**SuppleMentary material for**

**Spin state relaxation of iron complexes: the case for OPBE and S12g functionals**

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**Table S1**. Selected bond lenghts (Å) for compound **1** at the low (ground state), intermediate and high spin state. p. S3

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p. S12

**References**

p. S12

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**Table S1**. Selected bond lenghts (Å) for compound **1** at the low (ground state), intermediate and high spin state.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  | Fe-NNCO | Fe-Npyr | Fe-S |
| X-Ray[[1]](#footnote-1),[1](#_ENREF_1) | | 1.954 | 2.000 | 2.230 |
| **OPBE** | doublet | 1.947 | 1.980 | 2.195 |
| quartet | 2.150 | 2.051 | 2.262 |
| sextet | 2.160 | 2.243 | 2.342 |
| **OPBE**  **cosmo** | doublet | 1.945 | 1.981 | 2.203 |
| quartet | 2.140 | 2.022 | 2.279 |
| sextet | 2.133 | 2.208 | 2.378 |
| **S12g** | doublet | 1.989 | 1.984 | 2.238 |
| quartet | 2.233 | 2.069 | 2.291 |
| sextet | 2.257 | 2.230 | 2.357 |
| **S12g**  **cosmo** | doublet | 1.986 | 1.984 | 2.249 |
| quartet | 2.240 | 2.054 | 2.303 |
| sextet | 2.259 | 2.196 | 2.378 |

**Table S2**. Selected bond lenghts (Å) for compound **2** at the low, intermediate (ground state) and high spin state.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | Fe-Cl | Fe-S1 | Fe-S2 | Fe-N1 | Fe-N2 |
| X-Ray[[2]](#footnote-2),[2](#_ENREF_2) | | 2.336 | 2.195 | 2.187 | 1.979 | 2.031 |
| **OPBE** | doublet | 2.277 | 2.203 | 2.203 | 1.947 | 1.947 |
| quartet | 2.418 | 2.232 | 2.232 | 1.988 | 1.988 |
| sextet | 2.286 | 2.365 | 2.365 | 2.140 | 2.140 |
| **OPBE**  **cosmo** | doublet | 2.184 | 2.157 | 2.157 | 1.908 | 1.908 |
| quartet | 2.264 | 2.213 | 2.213 | 1.971 | 1.971 |
| sextet | 2.213 | 2.342 | 2.342 | 2.154 | 2.154 |
| **S12g** | doublet | 2.217 | 2.165 | 2.165 | 1.911 | 1.911 |
| quartet | 2.402 | 2.208 | 2.208 | 1.957 | 1.957 |
| sextet | 2.274 | 2.345 | 2.345 | 2.134 | 2.134 |
| **S12g**  **cosmo** | doublet | 2.226 | 2.194 | 2.194 | 1.937 | 1.937 |
| quartet | 2.287 | 2.239 | 2.239 | 2.002 | 2.002 |
| sextet | 2.232 | 2.368 | 2.368 | 2.161 | 2.161 |

**Table S3**. Selected bond lenghts (Å) for compound **3** at the low, intermediate and high spin state (ground state).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | Fe-N(CH2)3 | Fe-Nimidazole | Fe-S1 | Fe-S2 | Fe-S3 |
| X-Ray[[3]](#footnote-3),[3](#_ENREF_3) | | 2.211 | 2.148 | 2.297 | 2.304 | 2.307 |
| **OPBE** | doublet | 2.100 | 2.079 | 2.211 | 2.206 | 2.209 |
| quartet | 2.086 | 2.069 | 2.317 | 2.283 | 2.391 |
| sextet | 2.519 | 2.256 | 2.329 | 2.333 | 2.338 |
| **OPBE**  **cosmo** | doublet | 2.040 | 2.020 | 2.181 | 2.157 | 2.162 |
| quartet | 2.025 | 2.046 | 2.241 | 2.272 | 2.342 |
| sextet | 2.426 | 2.314 | 2.298 | 2.317 | 2.304 |
| **S12g** | doublet | 2.045 | 2.030 | 2.179 | 2.156 | 2.167 |
| quartet | 2.028 | 2.031 | 2.276 | 2.369 | 2.246 |
| sextet | 2.430 | 2.244 | 2.324 | 2.310 | 2.319 |
| **S12g**  **cosmo** | doublet | 2.095 | 2.063 | 2.210 | 2.208 | 2.205 |
| quartet | 2.078 | 2.073 | 2.287 | 2.292 | 2.382 |
| sextet | 2.481 | 2.303 | 2.312 | 2.336 | 2.334 |

**Table S4**. Selected bond lenghts (Å) for compound *trans***-4** at the low (ground state), intermediate and high spin state.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Fe-Sb | Fe-Snb | Fe-Sb | Fe-Snb | Fe-CO | Fe-Nax |
| X-Ray[[4]](#footnote-4),[4](#_ENREF_4) | | 2.241 | 2.304 | 2.241 | 2.304 | 1.749 | 2.074 |
| **OPBE** | singlet | 2.187 | 2.262 | 2.185 | 2.272 | 1.713 | 2.087 |
| triplet | 2.492 | 2.235 | 2.464 | 2.267 | 1.744 | 2.168 |
| quintet | 2.484 | 2.395 | 2.463 | 2.430 | 1.955 | 2.350 |
| **OPBE**  **cosmo** | singlet | 2.196 | 2.267 | 2.194 | 2.274 | 1.700 | 2.082 |
| triplet | 2.521 | 2.265 | 2.447 | 2.290 | 1.727 | 2.138 |
| quintet | 2.474 | 2.425 | 2.457 | 2.458 | 1.956 | 2.292 |
| **S12g** | singlet | 2.251 | 2.320 | 2.247 | 2.329 | 1.732 | 2.119 |
| triplet | 2.590 | 2.340 | 2.587 | 2.313 | 1.757 | 2.193 |
| quintet | 2.564 | 2.439 | 2.545 | 2.482 | 1.962 | 2.382 |
| **S12g**  **cosmo** | singlet | 2.262 | 2.328 | 2.259 | 2.336 | 1.719 | 2.115 |
| triplet | 2.563 | 2.421 | 2.559 | 2.380 | 1.736 | 2.148 |
| quintet | 2.546 | 2.476 | 2.537 | 2.521 | 1.964 | 2.314 |

**Table S5**. Selected bond lenghts (Å) for compound *trans***-5**  at the low (ground state), intermediate and high spin state.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Fe-Snb | Fe-Sb | Fe-Sb | Fe-Snb | Fe-PMe3 | Fe-Nax |
| X-Ray[[5]](#footnote-5),[5](#_ENREF_5) | | 2.308 | 2.230 | 2.230 | 2.308 | 2.216 | 2.066 |
| **OPBE** | singlet | 2.252 | 2.171 | 2.163 | 2.262 | 2.201 | 2.082 |
| triplet | 2.221 | 2.219 | 2.219 | 2.230 | 2.466 | 2.461 |
| quintet | 2.396 | 2.430 | 2.544 | 2.402 | 2.578 | 2.366 |
| **OPBE**  **cosmo** | singlet | 2.252 | 2.176 | 2.167 | 2.260 | 2.209 | 2.077 |
| triplet | 2.232 | 2.216 | 2.212 | 2.244 | 2.545 | 2.398 |
| quintet | 2.389 | 2.441 | 2.528 | 2.406 | 2.673 | 2.319 |
| **S12g** | singlet | 2.310 | 2.231 | 2.220 | 2.326 | 2.243 | 2.109 |
| triplet | 2.287 | 2.486 | 2.613 | 2.287 | 2.305 | 2.227 |
| quintet | 2.474 | 2.531 | 2.562 | 2.468 | 2.492 | 2.394 |
| **S12g**  **cosmo** | singlet | 2.311 | 2.237 | 2.226 | 2.329 | 2.256 | 2.108 |
| triplet | 2.310 | 2.512 | 2.627 | 2.305 | 2.319 | 2.193 |
| quintet | 2.485 | 2.499 | 2.586 | 2.490 | 2.564 | 2.347 |

**Table S6**. Selected bond lenghts (Å) for compound *mezo***-6** at the low, intermediate and high spin state (ground state).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Fe-Snb | Fe-Sb | Fe-Sb | Fe-Snb | Fe-Nax | Fe-NH3 |
| X-Ray[[6]](#footnote-6),[6](#_ENREF_6) | | 2.587 | 2.395 | 2.395 | 2.587 | 2.189 | 2.395 |
| **OPBE** | singlet | 2.255 | 2.174 | 2.174 | 2.255 | 2.017 | 2.025 |
| triplet | 2.235 | 2.249 | 2.249 | 2.235 | 2.334 | 2.503 |
| quintet | 2.322 | 2.565 | 2.565 | 2.322 | 2.326 | 2.296 |
| **OPBE**  **cosmo** | singlet | 2.254 | 2.174 | 2.174 | 2.254 | 2.032 | 2.028 |
| triplet | 2.242 | 2.252 | 2.252 | 2.242 | 2.402 | 2.414 |
| quintet | 2.354 | 2.536 | 2.536 | 2.354 | 2.349 | 2.271 |
| **S12g** | singlet | 2.305 | 2.231 | 2.231 | 2.305 | 2.057 | 2.065 |
| triplet | 2.278 | 2.308 | 2.308 | 2.278 | 2.351 | 2.411 |
| quintet | 2.353 | 2.674 | 2.674 | 2.353 | 2.312 | 2.260 |
| **S12g**  **cosmo** | singlet | 2.305 | 2.233 | 2.233 | 2.305 | 2.069 | 2.069 |
| triplet | 2.285 | 2.311 | 2.311 | 2.285 | 2.354 | 2.414 |
| quintet | 2.388 | 2.625 | 2.625 | 2.388 | 2.310 | 2.247 |

**Table S7**. Selected bond lenghts (Å) for compound *mezo***-7** at the low, intermediate and high spin state (ground state).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Fe-N2H4 | Fe-Snb | Fe-Sb | Fe-Snb | Fe-Sb | Fe-Nax |
| X-Ray[[7]](#footnote-7),[6](#_ENREF_6) | | 2.193 | 2.602 | 2.392 | 2.602 | 2.392 | 2.254 |
| **OPBE** | singlet | 2.048 | 2.256 | 2.175 | 2.256 | 2.175 | 2.036 |
| triplet | 2.467 | 2.237 | 2.250 | 2.237 | 2.250 | 2.384 |
| quintet | 2.263 | 2.323 | 2.578 | 2.323 | 2.578 | 2.341 |
| **OPBE**  **cosmo** | singlet | 2.053 | 2.254 | 2.179 | 2.254 | 2.179 | 2.043 |
| triplet | 2.528 | 2.237 | 2.251 | 2.237 | 2.251 | 2.386 |
| quintet | 2.270 | 2.349 | 2.548 | 2.349 | 2.548 | 2.331 |
| **S12g** | singlet | 2.093 | 2.314 | 2.229 | 2.314 | 2.229 | 2.072 |
| triplet | 2.425 | 2.286 | 2.303 | 2.286 | 2.303 | 2.377 |
| quintet | 2.237 | 2.361 | 2.682 | 2.361 | 2.682 | 2.353 |
| **S12g**  **cosmo** | singlet | 2.098 | 2.312 | 2.234 | 2.312 | 2.234 | 2.076 |
| triplet | 2.469 | 2.286 | 2.307 | 2.286 | 2.307 | 2.355 |
| quintet | 2.251 | 2.384 | 2.634 | 2.384 | 2.634 | 2.296 |

**Table S8**. Selected bond lenghts (Å) for compound **8** at the low, intermediate and high spin state (ground state).

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | Fe-Cl | Fe-N |
| X-Ray[[8]](#footnote-8),[7](#_ENREF_7) | | 2.203 | 2.015 |
| **OPBE** | doublet | 2.223 | 1.994 |
| quartet | 2.387 | 2.011 |
| sextet | 2.289 | 2.090 |
| **OPBE**  **cosmo** | doublet | 2.134 | 1.987 |
| quartet | 2.240 | 2.019 |
| sextet | 2.197 | 2.107 |
| **S12g** | doublet | 2.185 | 1.985 |
| quartet | 2.386 | 2.005 |
| sextet | 2.277 | 2.093 |
| **S12g**  **cosmo** | doublet | 2.168 | 1.995 |
| quartet | 2.251 | 2.026 |
| sextet | 2.207 | 2.107 |

**Table S9**. Selected bond lenghts (Å) for compound **9** at the low, intermediate (ground state) and high spin state.

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | Fe-Cl | Fe-N |
| X-Ray[[9]](#footnote-9),[8](#_ENREF_8) | | 2.326 | 1.931 |
| **OPBE** | doublet | 2.197 | 1.915 |
| quartet | 2.366 | 1.936 |
| sextet | 2.256 | 2.029 |
| **OPBE**  **cosmo** | doublet | 2.130 | 1.904 |
| quartet | 2.242 | 1.936 |
| sextet | 2.188 | 2.041 |
| **S12g** | doublet | 2.161 | 1.904 |
| quartet | 2.364 | 1.927 |
| sextet | 2.244 | 2.031 |
| **S12g**  **cosmo** | doublet | 2.163 | 1.916 |
| quartet | 2.254 | 1.947 |
| sextet | 2.198 | 2.044 |

**Table S10.** OPBE/TZP ligand binding energya (kcal/mol) for *trans/Meso*-(Fe(NH)S4)L

|  |  |  |  |
| --- | --- | --- | --- |
| *ligand L* | *singlet* | *triplet* | *quintet* |
| *trans* |  |  |  |
| CO (**4**) | -32.0 (-29.8) | -8.6 (-6.9) | 2.7 (3.8) |
| PMe3 (**5**) | -15.3 (-11.6) | 1.0 (3.9) | 4.7 (7.1) |
| NH3 (**6**) | -3.1 (-1.6) | 4.6 (5.5) | 5.3 (6.3) |
| N2H4 (**7**) | -3.5 (-1.8) | -1.9 (-1.5) | 5.2 (6.1) |
| *Meso* |  |  |  |
| CO (**4**) | -29.2 (-27.0) | 4.2 (5.8) | 9.6 (11.1) |
| PMe3 (**5**) | -12.2 (-8.5) | 7.5 (10.3) | 5.4 (7.8) |
| NH3 (**6**) | -0.6 (0.9) | 9.7 (10.7) | 6.0 (6.9) |
| N2H4 (**7**) | -1.0 (0.8) | 9.3 (10.3) | 6.6 (7.7) |

a) with respect to energy of infinitely separated *trans*-Fe(NH)S4 (triplet ground state) and ligand (in parentheses corrected for BSSE)

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**Coordinates of optimized structures**

**Iron (III) Complexes**

Fe-(PyPepS)2 **(1)** OPBE Doublet

Fe 0.00000000 0.00000000 -0.09321563

N 1.55604623 -1.17038397 -0.11840764

N 0.54602890 1.24265053 1.34774936

N -1.55604623 1.17038397 -0.11840764

N -0.54602890 -1.24265053 1.34774936

C 1.61524423 -2.16130011 0.80964119

C 3.59311775 -1.87153324 -1.38402923

C 2.51883872 -1.00388787 -1.11691696

C 0.38413453 -2.17222921 1.64429712

C 0.18766160 -3.11636133 2.65037896

C -1.00568496 -3.11357045 3.35843240

C -1.97212401 -2.16101542 3.03329214

C -1.70109265 -1.24260343 2.02916561

C 2.36531647 0.15779748 -1.91906658

C 3.28071373 0.41779390 -2.94843487

C -2.51883872 1.00388787 -1.11691696

C -3.59311775 1.87153324 -1.38402923

C -1.61524423 2.16130011 0.80964119

C -3.28071373 -0.41779390 -2.94843487

C -2.36531647 -0.15779748 -1.91906658

C -0.38413453 2.17222921 1.64429712

C -0.18766160 3.11636133 2.65037896

C 1.00568496 3.11357045 3.35843240

C 1.97212401 2.16101542 3.03329214

C 1.70109265 1.24260343 2.02916561

H 0.98593130 -3.83188253 2.83122846

H -1.18887395 -3.84619042 4.14525865

H -2.93249711 -2.12448684 3.54558176

H -2.42581095 -0.48779929 1.73790910

H -0.98593130 3.83188253 2.83122846

H 1.18887395 3.84619042 4.14525865

H 2.93249711 2.12448684 3.54558176

H 2.42581095 0.48779929 1.73790910

C -4.48608795 1.59738291 -2.41597196

C -4.33568202 0.45068915 -3.19810651

C 4.48608795 -1.59738291 -2.41597196

C 4.33568202 -0.45068915 -3.19810651

H -5.03543532 0.23743072 -4.00753286

H -5.30619045 2.29021881 -2.60924442

H -3.71025907 2.75531216 -0.76919723

H 5.03543532 -0.23743072 -4.00753286

H 5.30619045 -2.29021881 -2.60924442

H 3.71025907 -2.75531216 -0.76919723

O -2.51261189 3.00008415 1.01838309

O 2.51261189 -3.00008415 1.01838309

H 3.14431353 1.31176108 -3.55619282

H -3.14431353 -1.31176108 -3.55619282

S -1.05149266 -1.23617869 -1.57172998

S 1.05149266 1.23617869 -1.57172998

Fe-(PyPepS)2 **(1)** OPBE Quartet

Fe 0.00000000 0.00000000 -0.16881019

N 1.73325128 -1.27046938 -0.09454863

N 0.49503420 1.35444769 1.28907789

N -1.73325128 1.27046938 -0.09454863

N -0.49503420 -1.35444769 1.28907789

C 1.74597165 -2.22307362 0.86101478

C 3.89221296 -1.90849680 -1.17387072

C 2.75107980 -1.09745276 -1.01966899

C 0.45270849 -2.25097872 1.62413811

C 0.23606385 -3.20720466 2.61426473

C -0.99314769 -3.25897989 3.25747808

C -1.97701625 -2.34360062 2.88637349

C -1.68513002 -1.40775806 1.90534343

C 2.58540340 0.00457421 -1.90772314

C 3.52757703 0.23177858 -2.92066365

C -2.75107980 1.09745276 -1.01966899

C -3.89221296 1.90849680 -1.17387072

C -1.74597165 2.22307362 0.86101478

C -3.52757703 -0.23177858 -2.92066365

C -2.58540340 -0.00457421 -1.90772314

C -0.45270849 2.25097872 1.62413811

C -0.23606385 3.20720466 2.61426473

C 0.99314769 3.25897989 3.25747808

C 1.97701625 2.34360062 2.88637349

C 1.68513002 1.40775806 1.90534343

H 1.05127146 -3.89123240 2.83474272

H -1.18718270 -4.00397732 4.02989483

H -2.96408581 -2.34591894 3.34630525

H -2.41879935 -0.67426918 1.58345232

H -1.05127146 3.89123240 2.83474272

H 1.18718270 4.00397732 4.02989483

H 2.96408581 2.34591894 3.34630525

H 2.41879935 0.67426918 1.58345232

C -4.82295531 1.65593902 -2.17741674

C -4.64409975 0.58542032 -3.05512864

C 4.82295531 -1.65593902 -2.17741674

C 4.64409975 -0.58542032 -3.05512864

H -5.36715114 0.39022324 -3.84816319

H -5.69207549 2.30800869 -2.27663165

H -4.02463110 2.73942573 -0.49122836

H 5.36715114 -0.39022324 -3.84816319

H 5.69207549 -2.30800869 -2.27663165

H 4.02463110 -2.73942573 -0.49122836

O -2.63207313 3.04010636 1.17522382

O 2.63207313 -3.04010636 1.17522382

H 3.37086489 1.06691500 -3.60240428

H -3.37086489 -1.06691500 -3.60240428

S -1.24455398 -1.09319711 -1.70886997

S 1.24455398 1.09319711 -1.70886997

Fe-(PyPepS)2 **(1)** OPBE Sextet

Fe 0.00000000 0.00000000 -0.41723245

N 1.70195998 -1.30400122 -0.15192785

N 0.61178764 1.41313186 1.21304888

N -1.70195998 1.30400122 -0.15192785

N -0.61178764 -1.41313186 1.21304888

C 1.62574046 -2.29615353 0.76566391

C 4.04573469 -1.83031350 -0.82463119

C 2.86289389 -1.06409660 -0.88635019

C 0.29982760 -2.35618604 1.47734858

C 0.05432957 -3.37687688 2.39946269

C -1.16498212 -3.40971285 3.05889056

C -2.10860253 -2.42299044 2.78088148

C -1.78751100 -1.44641975 1.84705297

C 2.84417266 0.05668229 -1.77186905

C 3.98789033 0.35779632 -2.52970061

C -2.86289389 1.06409660 -0.88635019

C -4.04573469 1.83031350 -0.82463119

C -1.62574046 2.29615353 0.76566391

C -3.98789033 -0.35779632 -2.52970061

C -2.84417266 -0.05668229 -1.77186905

C -0.29982760 2.35618604 1.47734858

C -0.05432957 3.37687688 2.39946269

C 1.16498212 3.40971285 3.05889056

C 2.10860253 2.42299044 2.78088148

C 1.78751100 1.44641975 1.84705297

H 0.83779289 -4.11049170 2.56615352

H -1.38259410 -4.19739795 3.78168477

H -3.08074400 -2.40548155 3.27128326

H -2.49396051 -0.66259818 1.58581139

H -0.83779289 4.11049170 2.56615352

H 1.38259410 4.19739795 3.78168477

H 3.08074400 2.40548155 3.27128326

H 2.49396051 0.66259818 1.58581139

C -5.16190657 1.51271085 -1.59087191

C -5.14003091 0.41143055 -2.44673462

C 5.16190657 -1.51271085 -1.59087191

C 5.14003091 -0.41143055 -2.44673462

H -6.01151122 0.15645020 -3.05134661

H -6.05363744 2.13708285 -1.51710302

H -4.06204235 2.68538509 -0.16144351

H 6.01151122 -0.15645020 -3.05134661

H 6.05363744 -2.13708285 -1.51710302

H 4.06204235 -2.68538509 -0.16144351

O -2.47897210 3.13695003 1.10785797

O 2.47897210 -3.13695003 1.10785797

H 3.94573501 1.21613875 -3.19892092

H -3.94573501 -1.21613875 -3.19892092

S -1.42007731 -1.02454378 -1.97285375

S 1.42007731 1.02454378 -1.97285375

Fe(tsalen)Cl **(2)** OPBE Doublet

Fe -0.52016324 -0.12634477 0.00000000

Cl -2.64978998 0.35805032 0.00000000

S -0.44762363 -1.76868076 1.39692316

C -0.04892508 2.57299155 0.75761354

N -0.10383146 1.21121846 1.29534759

S -0.44762363 -1.76868076 -1.39692316

H -0.41922692 -3.34780652 -3.66625269

H -0.41922692 -3.34780652 3.66625269

C 0.02103638 1.16343904 2.59552974

C -0.27544258 -2.32285740 4.00356562

H 0.23031593 1.32189165 5.18737746

H -0.15410806 -2.86142384 6.06985196

H 0.22233964 2.11491561 3.10132000

C -0.06306205 0.04301100 3.47136465

H 0.16265903 -0.50420855 6.84441134

N -0.10383146 1.21121846 -1.29534759

C -0.12648289 -2.04657607 5.34717999

C -0.25970961 -1.29469194 3.03570043

C 0.08726397 0.29353356 4.85576324

C 0.05163817 -0.72407217 5.78414440

C -0.04892508 2.57299155 -0.75761354

C 0.02103638 1.16343904 -2.59552974

H 0.22233964 2.11491561 -3.10132000

C -0.06306205 0.04301100 -3.47136465

C -0.12648289 -2.04657607 -5.34717999

C -0.25970961 -1.29469194 -3.03570043

C 0.08726397 0.29353356 -4.85576324

C 0.05163817 -0.72407217 -5.78414440

C -0.27544258 -2.32285740 -4.00356562

H -0.15410806 -2.86142384 -6.06985196

H 0.23031593 1.32189165 -5.18737746

H 0.16265903 -0.50420855 -6.84441134

H -0.92676452 3.11624174 -1.12616327

H 0.84322119 3.08256648 -1.14220369

H 0.84322119 3.08256648 1.14220369

H -0.92676452 3.11624174 1.12616327

Fe(tsalen)Cl **(2)** OPBE Quartet

Fe -1.11714344 -0.02547195 0.00000000

Cl -3.24556419 0.74684055 0.00000000

S -1.05421263 -1.69950724 1.44583342

C -0.48368071 2.60345681 0.76657251

N -0.34540193 1.25136661 1.28859370

S -1.05421263 -1.69950724 -1.44583342

H -0.39354330 -3.37091569 -3.52764847

H -0.39354330 -3.37091569 3.52764847

C 0.24637328 1.11435785 2.43293156

C 0.03125691 -2.40027656 3.77676871

H 1.56148617 1.03456798 4.66024230

H 0.89374016 -3.09622031 5.60357801

H 0.67674626 2.01891810 2.88146854

C 0.39979235 -0.07053456 3.21609325

H 1.89942141 -0.88119865 6.18703191

N -0.34540193 1.25136661 -1.28859370

C 0.75756221 -2.24184618 4.94084171

C -0.16717503 -1.32970336 2.87605083

C 1.13696325 0.06104959 4.41500781

C 1.32460897 -1.00270304 5.27106842

C -0.48368071 2.60345681 -0.76657251

C 0.24637328 1.11435785 -2.43293156

H 0.67674626 2.01891810 -2.88146854

C 0.39979235 -0.07053456 -3.21609325

C 0.75756221 -2.24184618 -4.94084171

C -0.16717503 -1.32970336 -2.87605083

C 1.13696325 0.06104959 -4.41500781

C 1.32460897 -1.00270304 -5.27106842

C 0.03125691 -2.40027656 -3.77676871

H 0.89374016 -3.09622031 -5.60357801

H 1.56148617 1.03456798 -4.66024230

H 1.89942141 -0.88119865 -6.18703191

H -1.44346641 2.99311754 -1.12468634

H 0.31309989 3.25049189 -1.15612634

H 0.31309989 3.25049189 1.15612634

H -1.44346641 2.99311754 1.12468634

Fe(tsalen)Cl **(2)** OPBE Sextet

Fe -1.62537639 -0.02616676 0.00000000

Cl -3.69422871 0.76012131 0.00000000

S -1.49638255 -1.56292977 1.76303920

C -0.70243253 2.69162779 0.77264694

N -0.53990896 1.34030437 1.26246875

S -1.49638255 -1.56292977 -1.76303920

H -0.14078390 -3.38366675 -3.33522057

H -0.14078390 -3.38366675 3.33522057

C 0.34687780 1.12345388 2.17424432

C 0.40650814 -2.44776175 3.42644703

H 2.34052398 0.87080032 3.76301751

H 1.84928610 -3.26614495 4.77686873

H 0.94336957 1.98248795 2.51745334

C 0.67360559 -0.11718101 2.82122330

H 3.11777635 -1.11985230 5.00618558

N -0.53990896 1.34030437 -1.26246875

C 1.52536559 -2.37706314 4.23630042

C -0.05587794 -1.33496074 2.68921792

C 1.80206655 -0.07252639 3.66909649

C 2.23913256 -1.17989804 4.36681881

C -0.70243253 2.69162779 -0.77264694

C 0.34687780 1.12345388 -2.17424432

H 0.94336957 1.98248795 -2.51745334

C 0.67360559 -0.11718101 -2.82122330

C 1.52536559 -2.37706314 -4.23630042

C -0.05587794 -1.33496074 -2.68921792

C 1.80206655 -0.07252639 -3.66909649

C 2.23913256 -1.17989804 -4.36681881

C 0.40650814 -2.44776175 -3.42644703

H 1.84928610 -3.26614495 -4.77686873

H 2.34052398 0.87080032 -3.76301751

H 3.11777635 -1.11985230 -5.00618558

H -1.66553512 3.06678695 -1.13838515

H 0.08409579 3.35432863 -1.16008406

H 0.08409579 3.35432863 1.16008406

H -1.66553512 3.06678695 1.13838515

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** OPBE Doublet

Fe -0.00650094 -0.63931967 -0.94322405

H 3.02417548 -0.48244561 2.90736489

H 4.27944794 1.47723110 3.74829475

S -1.90717491 -0.86050094 0.06319593

N 0.04845517 1.39790902 -0.85839747

N -0.00773498 -2.64874592 -1.14481306

C 1.46293643 1.87859140 -0.82714426

C -0.63469202 1.95964072 0.35045451

C -0.61882199 1.99118868 -2.05846775

H 1.99661275 1.31680414 -1.60227251

C 2.18149299 1.75323619 0.47894298

H 1.47148476 2.93728352 -1.12223730

C 0.15553313 1.97399307 -3.33893275

H -0.86897572 3.03559512 -1.82498628

H -1.56370342 1.44799511 -2.18108976

H -0.22512523 1.42013287 1.21041464

C -2.12461966 1.88001013 0.37557826

H -0.33668691 3.01401686 0.44409137

C 1.45840615 1.99130510 -5.82434070

C 0.33054263 3.16202562 -4.05279286

C 0.64622491 0.77220825 -3.88360590

C 1.29758124 0.80147016 -5.12798472

C 0.97031581 3.18206927 -5.28791372

H -0.05344531 4.09352998 -3.63553448

S 0.44373788 -0.76043088 -3.07362921

H 1.67343732 -0.13273088 -5.54248555

H 1.08887374 4.12148906 -5.82625897

H 1.96307720 1.98986150 -6.79024052

C 3.69429327 1.56118877 2.83272920

C 2.24105612 0.53155908 1.17597949

C 2.87402673 2.85638237 0.98370717

C 3.63661930 2.77183837 2.14362665

C 2.99386579 0.45954705 2.36188846

S 1.45335991 -0.92222153 0.61898657

H 2.82401524 3.80292753 0.44431838

H 4.17487193 3.64514117 2.50945376

H -4.67104916 -0.38158813 0.41871361

C -4.90512489 1.74292412 0.66370733

C -2.77235061 0.63315052 0.31278291

C -2.88407263 3.03551310 0.56959951

C -4.26598250 2.98137827 0.71577890

C -4.16938225 0.58395556 0.46129704

H -5.98681717 1.67909581 0.78117304

H -2.37636357 3.99929727 0.62366714

H -4.83728649 3.89503930 0.87313717

C 1.08052173 -3.40637480 -1.17907517

C -1.06007009 -3.48499202 -1.42814144

H 2.08698140 -3.05333897 -1.00655704

C 1.70592404 -5.78624259 -1.54294697

C -0.59225094 -4.75520792 -1.61880612

H -2.07500665 -3.11740116 -1.47521546

N 0.77065194 -4.68939044 -1.45867285

H -1.10422358 -5.67931174 -1.85204734

H 2.72150514 -5.39945423 -1.43947483

H 1.61976129 -6.28708345 -2.51260396

H 1.52265461 -6.51270770 -0.74386446

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** OPBE Quartet

Fe 0.03264918 -0.65279517 -0.92299413

H 3.22983175 -0.45603119 2.92822241

H 4.35978181 1.57675135 3.76912898

S -2.06013518 -0.88556966 0.10282655

N 0.06656468 1.36959380 -0.81943944

N 0.06721080 -2.68797224 -1.13340929

C 1.49956079 1.82051367 -0.78590177

C -0.63544027 1.85786512 0.41807649

C -0.59954777 2.01030997 -2.00221991

H 2.02042149 1.23577652 -1.55431741

C 2.22079075 1.72802143 0.51980922

H 1.51610816 2.86765914 -1.11445416

C 0.14603863 1.98990807 -3.29613237

H -0.80287460 3.05528740 -1.73211144

H -1.56553967 1.50573047 -2.11576282

H -0.28610603 1.22351654 1.23933206

C -2.13038981 1.85958653 0.36753794

H -0.28755492 2.88275180 0.60401085

C 1.33260272 1.99679108 -5.83311711

C 0.40643670 3.18841675 -3.96533626

C 0.49917554 0.77083451 -3.90502223

C 1.09736597 0.79690495 -5.17691403

C 0.99123154 3.20572085 -5.22690541

H 0.12556159 4.13083169 -3.49369275

S 0.19783609 -0.77187963 -3.15483252

H 1.36913871 -0.14681917 -5.64702187

H 1.17510529 4.15223796 -5.73308514

H 1.78881595 1.98881691 -6.82293045

C 3.76217612 1.62716448 2.85917801

C 2.35931348 0.50836153 1.21296368

C 2.85069265 2.87129776 1.02058712

C 3.62310464 2.83441093 2.17547360

C 3.13221442 0.48414797 2.38820232

S 1.59718553 -0.96899974 0.69323701

H 2.74280929 3.81267022 0.48068821

H 4.10902165 3.73883517 2.53859556

H -4.81885313 -0.21823005 0.15971310

C -4.92984382 1.91193380 0.44198154

C -2.85487157 0.65627134 0.23270199

C -2.82456612 3.05966157 0.53854474

C -4.21375535 3.10004574 0.58291731

C -4.25972815 0.70958912 0.26603381

H -6.01937109 1.92152779 0.47056452

H -2.25988107 3.98553655 0.65392443

H -4.73092715 4.04788209 0.72463363

C 1.16132445 -3.43514511 -1.17144232

C -0.98303247 -3.52045536 -1.42955011

H 2.16444025 -3.07636982 -0.98959638

C 1.79565028 -5.80752927 -1.56350657

C -0.50647660 -4.78517735 -1.63031308

H -1.99863315 -3.15327726 -1.47151175

N 0.85619979 -4.71407550 -1.46690579

H -1.01380254 -5.71047869 -1.86845766

H 2.80905805 -5.42070970 -1.44166139

H 1.71920904 -6.28857150 -2.54376297

H 1.60434529 -6.54885685 -0.78050257

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** OPBE Sextet

Fe 0.04042544 -0.45777272 -0.98754529

H 3.58379523 -1.03817009 1.77738731

H 3.97424496 0.34339370 3.79597679

S -1.38622478 -0.61481242 0.81470383

N 0.06471573 1.95927030 -0.78182393

N 0.03239253 -2.76791981 -1.11722917

C 1.42913365 2.44282082 -0.46711481

C -0.85026031 2.39270509 0.29945770

C -0.37665725 2.56943071 -2.05770150

H 2.04751007 2.21085016 -1.34110766

C 2.07576073 1.83756376 0.74157577

H 1.40011039 3.54077630 -0.35349516

C 0.38768213 2.15528496 -3.27894046

H -0.33696737 3.66854191 -1.95953224

H -1.42527383 2.28135562 -2.18989844

H -0.43113605 1.99853948 1.23204529

C -2.27275596 1.93340147 0.18880145

H -0.83071514 3.49506597 0.35982942

C 1.69735613 1.45432354 -5.65937128

C 1.21583447 3.06368491 -3.94222233

C 0.21157406 0.86608588 -3.82840001

C 0.87533378 0.53490083 -5.01912820

C 1.87263340 2.72768858 -5.12180763

H 1.34294073 4.06380504 -3.52613608

S -0.87736477 -0.29582278 -3.08787201

H 0.73232681 -0.45920467 -5.43848264

H 2.51362104 3.45559252 -5.61760332

H 2.20205364 1.17447927 -6.58386457

C 3.44204082 0.76623596 2.94412842

C 2.54137268 0.50596595 0.70320724

C 2.31026774 2.60266357 1.88604063

C 2.98401357 2.08088740 2.98560216

C 3.22204596 -0.01226739 1.81413814

S 2.34468120 -0.46525740 -0.74703264

H 1.96162037 3.63570541 1.91272175

H 3.15291531 2.69841132 3.86694581

H -4.21554238 -0.83328589 0.61769696

C -4.96279304 1.13833435 0.17651977

C -2.60982546 0.58394392 0.43011633

C -3.29618052 2.85241989 -0.05527680

C -4.63359770 2.46968821 -0.06667527

C -3.96144840 0.20683739 0.42136638

H -6.00575483 0.82205410 0.17689707

H -3.03755467 3.89718988 -0.23133036

H -5.41203225 3.20675539 -0.25967151

C 1.07128706 -3.56961646 -0.96987130

C -1.03889559 -3.58294220 -1.37128558

H 2.08006453 -3.24236161 -0.75302081

C 1.59734798 -6.00694601 -1.01378454

C -0.63210857 -4.88922100 -1.37666678

H -2.03319530 -3.18679853 -1.53018798

N 0.71859148 -4.86590651 -1.11872674

H -1.17267107 -5.81327719 -1.53619150

H 2.61115687 -5.65851825 -0.80581841

H 1.60732985 -6.57310534 -1.95116700

H 1.27883779 -6.66555684 -0.19874733

FePCl **(8)** OPBE Doublet

Fe 0.00000000 0.00000000 -0.13493173

N 0.00000000 -1.97671357 0.06669009

N 1.97671357 0.00000000 0.06669009

N 0.00000000 1.97671357 0.06669009

N -1.97671357 0.00000000 0.06669009

C 2.40688545 -2.40688545 0.05850742

C 2.40688545 2.40688545 0.05850742

C -2.40688545 2.40688545 0.05850742

C -2.40688545 -2.40688545 0.05850742

H 3.17557679 -3.17557679 0.05605892

H 3.17557679 3.17557679 0.05605892

H -3.17557679 3.17557679 0.05605892

H -3.17557679 -3.17557679 0.05605892

C 1.08818157 -2.81652950 0.06370342

C -1.08818157 -2.81652950 0.06370342

C 0.67917148 -4.18988310 0.07848492

H 1.35542931 -5.03776688 0.09050624

C -0.67917148 -4.18988310 0.07848492

H -1.35542931 -5.03776688 0.09050624

C 2.81652950 1.08818157 0.06370342

C 2.81652950 -1.08818157 0.06370342

C 4.18988310 0.67917148 0.07848492

H 5.03776688 1.35542931 0.09050624

C 4.18988310 -0.67917148 0.07848492

H 5.03776688 -1.35542931 0.09050624

C -1.08818157 2.81652950 0.06370342

C 1.08818157 2.81652950 0.06370342

C -0.67917148 4.18988310 0.07848492

H -1.35542931 5.03776688 0.09050624

C 0.67917148 4.18988310 0.07848492

H 1.35542931 5.03776688 0.09050624

C -2.81652950 -1.08818157 0.06370342

C -2.81652950 1.08818157 0.06370342

C -4.18988310 -0.67917148 0.07848492

H -5.03776688 -1.35542931 0.09050624

C -4.18988310 0.67917148 0.07848492

H -5.03776688 1.35542931 0.09050624

Cl 0.00000000 0.00000000 -2.26849555

FePCl **(8)** OPBE Quartet

Fe 0.00000000 0.00000000 -0.23389793

N 0.00000000 -1.99459182 0.07806529

N 1.99459182 0.00000000 0.07806529

N 0.00000000 1.99459182 0.07806529

N -1.99459182 0.00000000 0.07806529

C 2.41098711 -2.41098711 0.10004043

C 2.41098711 2.41098711 0.10004043

C -2.41098711 2.41098711 0.10004043

C -2.41098711 -2.41098711 0.10004043

H 3.17939216 -3.17939216 0.11633962

H 3.17939216 3.17939216 0.11633962

H -3.17939216 3.17939216 0.11633962

H -3.17939216 -3.17939216 0.11633962

C 1.09028294 -2.82325111 0.09960439

C -1.09028294 -2.82325111 0.09960439

C 0.67974723 -4.19654598 0.13884129

H 1.35471545 -5.04505523 0.16740469

C -0.67974723 -4.19654598 0.13884129

H -1.35471545 -5.04505523 0.16740469

C 2.82325111 1.09028294 0.09960439

C 2.82325111 -1.09028294 0.09960439

C 4.19654598 0.67974723 0.13884129

H 5.04505523 1.35471545 0.16740469

C 4.19654598 -0.67974723 0.13884129

H 5.04505523 -1.35471545 0.16740469

C -1.09028294 2.82325111 0.09960439

C 1.09028294 2.82325111 0.09960439

C -0.67974723 4.19654598 0.13884129

H -1.35471545 5.04505523 0.16740469

C 0.67974723 4.19654598 0.13884129

H 1.35471545 5.04505523 0.16740469

C -2.82325111 -1.09028294 0.09960439

C -2.82325111 1.09028294 0.09960439

C -4.19654598 -0.67974723 0.13884129

H -5.04505523 -1.35471545 0.16740469

C -4.19654598 0.67974723 0.13884129

H -5.04505523 1.35471545 0.16740469

Cl 0.00000000 0.00000000 -2.47435661

FePCl **(8)** OPBE Sextet

Fe 0.00000000 0.00000000 -0.44777338

N 0.00000000 -2.03501620 0.09917734

N 2.03501620 0.00000000 0.09917734

N 0.00000000 2.03501620 0.09917734

N -2.03501620 0.00000000 0.09917734

C 2.41730760 -2.41730760 0.15789802

C 2.41730760 2.41730760 0.15789802

C -2.41730760 2.41730760 0.15789802

C -2.41730760 -2.41730760 0.15789802

H 3.18571900 -3.18571900 0.20153874

H 3.18571900 3.18571900 0.20153874

H -3.18571900 3.18571900 0.20153874

H -3.18571900 -3.18571900 0.20153874

C 1.09533023 -2.85188330 0.14865012

C -1.09533023 -2.85188330 0.14865012

C 0.68084051 -4.22669585 0.22218142

H 1.34941257 -5.07923321 0.27814456

C -0.68084051 -4.22669585 0.22218142

H -1.34941257 -5.07923321 0.27814456

C 2.85188330 1.09533023 0.14865012

C 2.85188330 -1.09533023 0.14865012

C 4.22669585 0.68084051 0.22218142

H 5.07923321 1.34941257 0.27814456

C 4.22669585 -0.68084051 0.22218142

H 5.07923321 -1.34941257 0.27814456

C -1.09533023 2.85188330 0.14865012

C 1.09533023 2.85188330 0.14865012

C -0.68084051 4.22669585 0.22218142

H -1.34941257 5.07923321 0.27814456

C 0.68084051 4.22669585 0.22218142

H 1.34941257 5.07923321 0.27814456

C -2.85188330 -1.09533023 0.14865012

C -2.85188330 1.09533023 0.14865012

C -4.22669585 -0.68084051 0.22218142

H -5.07923321 -1.34941257 0.27814456

C -4.22669585 0.68084051 0.22218142

H -5.07923321 1.34941257 0.27814456

Cl 0.00000000 0.00000000 -2.64427701

FePzCl **(9)** OPBE Doublet

Fe 0.00000000 0.00000000 -0.14948728

N 0.00000000 -1.89314378 0.05725539

N 1.89314378 0.00000000 0.05725539

N 0.00000000 1.89314378 0.05725539

N -1.89314378 0.00000000 0.05725539

N 2.37166606 -2.37166606 0.06327425

N 2.37166606 2.37166606 0.06327425

N -2.37166606 2.37166606 0.06327425

N -2.37166606 -2.37166606 0.06327425

C 1.09764538 -2.72094474 0.06550262

C -1.09764538 -2.72094474 0.06550262

C 0.67778133 -4.10076436 0.09410306

H 1.36722679 -4.93679774 0.11755725

C -0.67778133 -4.10076436 0.09410306

H -1.36722679 -4.93679774 0.11755725

C 2.72094474 1.09764538 0.06550262

C 2.72094474 -1.09764538 0.06550262

C 4.10076436 0.67778133 0.09410306

H 4.93679774 1.36722679 0.11755725

C 4.10076436 -0.67778133 0.09410306

H 4.93679774 -1.36722679 0.11755725

C -1.09764538 2.72094474 0.06550262

C 1.09764538 2.72094474 0.06550262

C -0.67778133 4.10076436 0.09410306

H -1.36722679 4.93679774 0.11755725

C 0.67778133 4.10076436 0.09410306

H 1.36722679 4.93679774 0.11755725

C -2.72094474 -1.09764538 0.06550262

C -2.72094474 1.09764538 0.06550262

C -4.10076436 -0.67778133 0.09410306

H -4.93679774 -1.36722679 0.11755725

C -4.10076436 0.67778133 0.09410306

H -4.93679774 1.36722679 0.11755725

Cl 0.00000000 0.00000000 -2.27929341

FePzCl **(9)** OPBE Quartet

Fe 0.00000000 0.00000000 -0.27136156

N 0.00000000 -1.90600755 0.06954024

N 1.90600755 0.00000000 0.06954024

N 0.00000000 1.90600755 0.06954024

N -1.90600755 0.00000000 0.06954024

N 2.37321444 -2.37321444 0.11458222

N 2.37321444 2.37321444 0.11458222

N -2.37321444 2.37321444 0.11458222

N -2.37321444 -2.37321444 0.11458222

C 1.09704635 -2.72350914 0.10767117

C -1.09704635 -2.72350914 0.10767117

C 0.67781943 -4.10541266 0.16375337

H 1.36707333 -4.94096607 0.20457463

C -0.67781943 -4.10541266 0.16375337

H -1.36707333 -4.94096607 0.20457463

C 2.72350914 1.09704635 0.10767117

C 2.72350914 -1.09704635 0.10767117

C 4.10541266 0.67781943 0.16375337

H 4.94096607 1.36707333 0.20457463

C 4.10541266 -0.67781943 0.16375337

H 4.94096607 -1.36707333 0.20457463

C -1.09704635 2.72350914 0.10767117

C 1.09704635 2.72350914 0.10767117

C -0.67781943 4.10541266 0.16375337

H -1.36707333 4.94096607 0.20457463

C 0.67781943 4.10541266 0.16375337

H 1.36707333 4.94096607 0.20457463

C -2.72350914 -1.09704635 0.10767117

C -2.72350914 1.09704635 0.10767117

C -4.10541266 -0.67781943 0.16375337

H -4.94096607 -1.36707333 0.20457463

C -4.10541266 0.67781943 0.16375337

H -4.94096607 1.36707333 0.20457463

Cl 0.00000000 0.00000000 -2.51324797

FePzCl **(9)** OPBE Sextet

Fe 0.00000000 0.00000000 -0.57295979

N 0.00000000 -1.93528110 0.07618671

N 1.93528110 0.00000000 0.07618671

N 0.00000000 1.93528110 0.07618671

N -1.93528110 0.00000000 0.07618671

N 2.37445959 -2.37445959 0.19467902

N 2.37445959 2.37445959 0.19467902

N -2.37445959 2.37445959 0.19467902

N -2.37445959 -2.37445959 0.19467902

C 1.09956841 -2.74209120 0.17111793

C -1.09956841 -2.74209120 0.17111793

C 0.67844227 -4.12301997 0.29956142

H 1.36282615 -4.95816856 0.39698242

C -0.67844227 -4.12301997 0.29956142

H -1.36282615 -4.95816856 0.39698242

C 2.74209120 1.09956841 0.17111793

C 2.74209120 -1.09956841 0.17111793

C 4.12301997 0.67844227 0.29956142

H 4.95816856 1.36282615 0.39698242

C 4.12301997 -0.67844227 0.29956142

H 4.95816856 -1.36282615 0.39698242

C -1.09956841 2.74209120 0.17111793

C 1.09956841 2.74209120 0.17111793

C -0.67844227 4.12301997 0.29956142

H -1.36282615 4.95816856 0.39698242

C 0.67844227 4.12301997 0.29956142

H 1.36282615 4.95816856 0.39698242

C -2.74209120 -1.09956841 0.17111793

C -2.74209120 1.09956841 0.17111793

C -4.12301997 -0.67844227 0.29956142

H -4.95816856 -1.36282615 0.39698242

C -4.12301997 0.67844227 0.29956142

H -4.95816856 1.36282615 0.39698242

Cl 0.00000000 0.00000000 -2.76114211

Fe-(PyPepS)2 **(1)** OPBE-Cosmo Doublet

Fe 0.00000000 0.00000000 -0.06274772

N 1.55574142 -1.16677551 -0.11796895

N 0.51908743 1.24408195 1.38931465

N -1.55574142 1.16677551 -0.11796895

N -0.51908743 -1.24408195 1.38931465

C 1.62708669 -2.15290313 0.80829179

C 3.52509572 -1.90932126 -1.47881228

C 2.49049229 -1.01273571 -1.14923381

C 0.41795054 -2.17148784 1.67270547

C 0.24254575 -3.11162255 2.68501784

C -0.93695277 -3.10329383 3.41873480

C -1.90718602 -2.15074356 3.11280632

C -1.65820390 -1.23684069 2.09806132

C 2.34146380 0.15757364 -1.93846040

C 3.22477123 0.41338850 -2.99551524

C -2.49049229 1.01273571 -1.14923381

C -3.52509572 1.90932126 -1.47881228

C -1.62708669 2.15290313 0.80829179

C -3.22477123 -0.41338850 -2.99551524

C -2.34146380 -0.15757364 -1.93846040

C -0.41795054 2.17148784 1.67270547

C -0.24254575 3.11162255 2.68501784

C 0.93695277 3.10329383 3.41873480

C 1.90718602 2.15074356 3.11280632

C 1.65820390 1.23684069 2.09806132

H 1.03196654 -3.83427017 2.87097443

H -1.10204125 -3.83025901 4.21195773

H -2.85238549 -2.10782411 3.64933648

H -2.39148851 -0.48339865 1.82903554

H -1.03196654 3.83427017 2.87097443

H 1.10204125 3.83025901 4.21195773

H 2.85238549 2.10782411 3.64933648

H 2.39148851 0.48339865 1.82903554

C -4.38624702 1.64584814 -2.54153990

C -4.24521070 0.48179101 -3.29894600

C 4.38624702 -1.64584814 -2.54153990

C 4.24521070 -0.48179101 -3.29894600

H -4.92104149 0.27485731 -4.12780797

H -5.17308914 2.36163022 -2.77731323

H -3.64679008 2.81378836 -0.89696284

H 4.92104149 -0.27485731 -4.12780797

H 5.17308914 -2.36163022 -2.77731323

H 3.64679008 -2.81378836 -0.89696284

O -2.53787429 2.99187079 0.98236570

O 2.53787429 -2.99187079 0.98236570

H 3.09560859 1.31907325 -3.58668772

H -3.09560859 -1.31907325 -3.58668772

S -1.04710472 -1.25646576 -1.53804203

S 1.04710472 1.25646576 -1.53804203

Fe-(PyPepS)2 **(1)** OPBE-Cosmo Quartet

Fe 0.00000000 0.00000000 0.07181994

N 1.68651488 -1.29956301 -0.14358484

N 0.34497065 1.37163166 1.51655585

N -1.68651488 1.29956301 -0.14358484

N -0.34497065 -1.37163166 1.51655585

C 1.76465319 -2.30720328 0.74444338

C 3.52666208 -2.05670029 -1.66055397

C 2.54898648 -1.14182797 -1.22115376

C 0.60040345 -2.31686076 1.68993654

C 0.47989815 -3.28909643 2.67943767

C -0.64877660 -3.30194167 3.49035629

C -1.62944788 -2.33375369 3.28898900

C -1.43556844 -1.38216864 2.29773153

C 2.36698655 0.05064650 -1.97609125

C 3.14014256 0.28677438 -3.11966022

C -2.54898648 1.14182797 -1.22115376

C -3.52666208 2.05670029 -1.66055397

C -1.76465319 2.30720328 0.74444338

C -3.14014256 -0.28677438 -3.11966022

C -2.36698655 -0.05064650 -1.97609125

C -0.60040345 2.31686076 1.68993654

C -0.47989815 3.28909643 2.67943767

C 0.64877660 3.30194167 3.49035629

C 1.62944788 2.33375369 3.28898900

C 1.43556844 1.38216864 2.29773153

H 1.27205109 -4.02423316 2.78575361

H -0.76488973 -4.05760784 4.26525541

H -2.53589993 -2.30410124 3.88911728

H -2.17265626 -0.60618894 2.11150824

H -1.27205109 4.02423316 2.78575361

H 0.76488973 4.05760784 4.26525541

H 2.53589993 2.30410124 3.88911728

H 2.17265626 0.60618894 2.11150824

C -4.28679081 1.80588351 -2.80028746

C -4.09975311 0.63293303 -3.53232428

C 4.28679081 -1.80588351 -2.80028746

C 4.09975311 -0.63293303 -3.53232428

H -4.69213211 0.43529644 -4.42482722

H -5.02842002 2.53838177 -3.11793034

H -3.67885240 2.97088997 -1.10003144

H 4.69213211 -0.43529644 -4.42482722

H 5.02842002 -2.53838177 -3.11793034

H 3.67885240 -2.97088997 -1.10003144

O -2.64153058 3.19135474 0.85919811

O 2.64153058 -3.19135474 0.85919811

H 2.98023948 1.20163188 -3.68847179

H -2.98023948 -1.20163188 -3.68847179

S -1.19566806 -1.22598250 -1.43211768

S 1.19566806 1.22598250 -1.43211768

Fe-(PyPepS)2 **(1)** OPBE-Cosmo Sextet

Fe 0.00000000 0.00000000 -0.09170218

N 1.65546858 -1.34097431 -0.20419786

N 0.37508242 1.44853752 1.53246344

N -1.65546858 1.34097431 -0.20419786

N -0.37508242 -1.44853752 1.53246344

C 1.75216196 -2.31338513 0.73153039

C 3.58106098 -2.13612874 -1.58146314

C 2.62246962 -1.17549635 -1.20011420

C 0.57301376 -2.38640788 1.65989250

C 0.47998969 -3.40010829 2.61150454

C -0.63290340 -3.44138676 3.44254301

C -1.61535324 -2.46522619 3.30458650

C -1.44489943 -1.48572757 2.33439558

C 2.59311775 0.05100157 -1.92421283

C 3.53182685 0.28565094 -2.94054748

C -2.62246962 1.17549635 -1.20011420

C -3.58106098 2.13612874 -1.58146314

C -1.75216196 2.31338513 0.73153039

C -3.53182685 -0.28565094 -2.94054748

C -2.59311775 -0.05100157 -1.92421283

C -0.57301376 2.38640788 1.65989250

C -0.47998969 3.40010829 2.61150454

C 0.63290340 3.44138676 3.44254301

C 1.61535324 2.46522619 3.30458650

C 1.44489943 1.48572757 2.33439558

H 1.27384817 -4.13726437 2.68045316

H -0.73313698 -4.22639739 4.19029375

H -2.50296023 -2.45626140 3.93298978

H -2.18955024 -0.70679559 2.19094992

H -1.27384817 4.13726437 2.68045316

H 0.73313698 4.22639739 4.19029375

H 2.50296023 2.45626140 3.93298978

H 2.18955024 0.70679559 2.19094992

C -4.49219148 1.89093235 -2.60519092

C -4.48079724 0.67147089 -3.28249706

C 4.49219148 -1.89093235 -2.60519092

C 4.48079724 -0.67147089 -3.28249706

H -5.19656556 0.46874838 -4.07808065

H -5.21391887 2.66254950 -2.87135914

H -3.60529147 3.08709677 -1.06542960

H 5.19656556 -0.46874838 -4.07808065

H 5.21391887 -2.66254950 -2.87135914

H 3.60529147 -3.08709677 -1.06542960

O -2.68579785 3.12014283 0.91743936

O 2.68579785 -3.12014283 0.91743936

H 3.49712976 1.23401647 -3.47467465

H -3.49712976 -1.23401647 -3.47467465

S -1.37552852 -1.25031884 -1.57469179

S 1.37552852 1.25031884 -1.57469179

Fe(tsalen)Cl **(2)** OPBE-Cosmo Doublet

Fe -0.40285417 -0.13988060 0.00000000

Cl -2.58929603 0.22858605 0.00000000

S -0.26826852 -1.77962044 1.40729186

C 0.15451764 2.56671445 0.75619746

N -0.04998661 1.21637794 1.29951909

S -0.26826852 -1.77962044 -1.40729186

H -0.38207550 -3.34182841 -3.71456234

H -0.38207550 -3.34182841 3.71456234

C -0.03667675 1.18136016 2.60322027

C -0.32868522 -2.30387264 4.03765733

H -0.12860859 1.38585700 5.18736687

H -0.39606377 -2.79948100 6.11866644

H 0.12840803 2.13367918 3.11548925

C -0.18656991 0.06385741 3.48313302

H -0.28411685 -0.41851464 6.87113215

N -0.04998661 1.21637794 -1.29951909

C -0.33685624 -1.99599043 5.38610838

C -0.26827329 -1.28823544 3.06071252

C -0.19238927 0.34674445 4.86889425

C -0.27430855 -0.66009729 5.81023548

C 0.15451764 2.56671445 -0.75619746

C -0.03667675 1.18136016 -2.60322027

H 0.12840803 2.13367918 -3.11548925

C -0.18656991 0.06385741 -3.48313302

C -0.33685624 -1.99599043 -5.38610838

C -0.26827329 -1.28823544 -3.06071252

C -0.19238927 0.34674445 -4.86889425

C -0.27430855 -0.66009729 -5.81023548

C -0.32868522 -2.30387264 -4.03765733

H -0.39606377 -2.79948100 -6.11866644

H -0.12860859 1.38585700 -5.18736687

H -0.28411685 -0.41851464 -6.87113215

H -0.63979964 3.21707699 -1.13595464

H 1.10487024 2.95498661 -1.13500212

H 1.10487024 2.95498661 1.13500212

H -0.63979964 3.21707699 1.13595464

Fe(tsalen)Cl **(2)** OPBE-Cosmo Quartet

Fe -1.03795895 -0.03426370 0.00000000

Cl -3.33243022 0.67473168 0.00000000

S -1.03946340 -1.69767205 1.45240634

C -0.43864296 2.61425467 0.76356308

N -0.33424846 1.25534867 1.29340392

S -1.03946340 -1.69767205 -1.45240634

H -0.40873968 -3.36599805 -3.57364191

H -0.40873968 -3.36599805 3.57364191

C 0.24790790 1.12074661 2.44155080

C 0.00914154 -2.39080270 3.81576114

H 1.52232600 1.05917313 4.68207616

H 0.84881089 -3.06566562 5.66571770

H 0.68052194 2.02183016 2.88572842

C 0.38619938 -0.06513907 3.23736882

H 1.83980377 -0.84310054 6.23762549

N -0.33424846 1.25534867 -1.29340392

C 0.72064575 -2.21868039 4.99328318

C -0.17031199 -1.32753744 2.90975413

C 1.10424686 0.08269929 4.44393899

C 1.27828585 -0.97621296 5.31538067

C -0.43864296 2.61425467 -0.76356308

C 0.24790790 1.12074661 -2.44155080

H 0.68052194 2.02183016 -2.88572842

C 0.38619938 -0.06513907 -3.23736882

C 0.72064575 -2.21868039 -4.99328318

C -0.17031199 -1.32753744 -2.90975413

C 1.10424686 0.08269929 -4.44393899

C 1.27828585 -0.97621296 -5.31538067

C 0.00914154 -2.39080270 -3.81576114

H 0.84881089 -3.06566562 -5.66571770

H 1.52232600 1.05917313 -4.68207616

H 1.83980377 -0.84310054 -6.23762549

H -1.37800772 3.03805421 -1.13371727

H 0.37819769 3.22940735 -1.15173999

H 0.37819769 3.22940735 1.15173999

H -1.37800772 3.03805421 1.13371727

Fe(tsalen)Cl **(2)** OPBE-Cosmo Sextet

Fe -1.58997707 -0.00685073 0.00000000

Cl -3.75284673 0.69445306 0.00000000

S -1.50889283 -1.54641203 1.76646139

C -0.66910441 2.70755550 0.77008096

N -0.52975881 1.34822033 1.26320271

S -1.50889283 -1.54641203 -1.76646139

H -0.15154790 -3.38732019 -3.34963430

H -0.15154790 -3.38732019 3.34963430

C 0.35065084 1.13000774 2.17952233

C 0.39674376 -2.45139297 3.43416296

H 2.34190408 0.86508785 3.75973079

H 1.84520614 -3.27340579 4.78185888

H 0.94857403 1.98241016 2.52276151

C 0.66962354 -0.11894476 2.82896093

H 3.11942209 -1.13105763 5.00127958

N -0.52975881 1.34822033 -1.26320271

C 1.52264668 -2.38413507 4.24235632

C -0.05733000 -1.33467763 2.70480325

C 1.80162681 -0.07607188 3.67014109

C 2.23749423 -1.18939043 4.36682198

C -0.66910441 2.70755550 -0.77008096

C 0.35065084 1.13000774 -2.17952233

H 0.94857403 1.98241016 -2.52276151

C 0.66962354 -0.11894476 -2.82896093

C 1.52264668 -2.38413507 -4.24235632

C -0.05733000 -1.33467763 -2.70480325

C 1.80162681 -0.07607188 -3.67014109

C 2.23749423 -1.18939043 -4.36682198

C 0.39674376 -2.45139297 -3.43416296

H 1.84520614 -3.27340579 -4.78185888

H 2.34190408 0.86508785 -3.75973079

H 3.11942209 -1.13105763 -5.00127958

H -1.61981526 3.10390026 -1.14368909

H 0.13175032 3.34699318 -1.15561516

H 0.13175032 3.34699318 1.15561516

H -1.61981526 3.10390026 1.14368909

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** OPBE-Cosmo Doublet

Fe 0.00728201 -0.63799355 -0.94384160

H 3.02346003 -0.46134731 2.92281052

H 4.23134097 1.51500218 3.79045747

S -1.87950000 -0.86497567 0.09843332

N 0.05524452 1.40449516 -0.86522967

N -0.00800751 -2.65693176 -1.15068270

C 1.46615912 1.90032630 -0.82305901

C -0.63566835 1.97988281 0.33364467

C -0.60387168 1.99987936 -2.07072296

H 2.01475083 1.34647563 -1.59328919

C 2.17425173 1.77730317 0.48984827

H 1.46525688 2.95894697 -1.11102510

C 0.17096129 1.97105931 -3.35175260

H -0.84142040 3.04623846 -1.84307567

H -1.55301669 1.46514575 -2.19708626

H -0.21816285 1.46312482 1.20353269

C -2.12511921 1.88009268 0.37229260

H -0.35450748 3.03832568 0.40512805

C 1.47078360 1.97295852 -5.84325297

C 0.35321364 3.15806473 -4.06782467

C 0.65385194 0.76718160 -3.89805826

C 1.30428856 0.78360461 -5.14362243

C 0.99101669 3.16811592 -5.30575123

H -0.01888104 4.09290555 -3.65001489

S 0.44242287 -0.76237561 -3.07504264

H 1.67686427 -0.15131400 -5.55952241

H 1.11679948 4.10555924 -5.84513525

H 1.97408038 1.96634434 -6.80919195

C 3.65734505 1.59463965 2.86808618

C 2.24520487 0.55493442 1.18410712

C 2.84297937 2.88978880 1.00948339

C 3.59058352 2.80743929 2.18109611

C 2.98011936 0.48250329 2.38127963

S 1.50005875 -0.91220527 0.58672369

H 2.78329188 3.83853746 0.47707499

H 4.11004137 3.68668581 2.55886040

H -4.65087534 -0.41098921 0.49491990

C -4.90350932 1.71607895 0.70338346

C -2.76209727 0.62694433 0.34507278

C -2.89533352 3.03269841 0.55263515

C -4.27592785 2.96278139 0.71914765

C -4.15659891 0.55920541 0.51289129

H -5.98221967 1.64255665 0.83696949

H -2.39895997 4.00238873 0.57540035

H -4.85579605 3.87291493 0.86341301

C 1.06164492 -3.45015205 -1.16326177

C -1.07612903 -3.46235911 -1.47885885

H 2.07734350 -3.14233282 -0.96353705

C 1.63166301 -5.84081399 -1.54660676

C -0.63418242 -4.74199913 -1.67363047

H -2.08251303 -3.07704028 -1.55661245

N 0.72209040 -4.71471369 -1.47061532

H -1.16255003 -5.64917933 -1.93454819

H 2.65175376 -5.48168785 -1.40894025

H 1.54729787 -6.32045601 -2.52474593

H 1.39605690 -6.56677585 -0.76378057

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** OPBE-Cosmo Quartet

Fe -0.04536901 -0.67976363 -0.93901656

H 3.28933667 -0.42701111 2.89862870

H 4.30170831 1.64797913 3.77765191

S -2.06259903 -0.86082533 0.03225124

N 0.03834365 1.34400120 -0.83186928

N -0.06108399 -2.70208010 -1.12142290

C 1.46676926 1.81486841 -0.80235759

C -0.65040064 1.89696867 0.38248244

C -0.62833078 1.93164566 -2.04733544

H 1.99936658 1.22352289 -1.55501751

C 2.18319906 1.74018509 0.50960510

H 1.46711693 2.85976117 -1.13245677

C 0.15853410 1.95211635 -3.31984268

H -0.89744122 2.96352065 -1.79600271

H -1.56252865 1.37489245 -2.18800981

H -0.27336820 1.32236632 1.23515738

C -2.14463209 1.88204005 0.37626302

H -0.31403495 2.93373803 0.50019262

C 1.45019014 2.06837712 -5.80938933

C 0.31712481 3.16741847 -3.99448070

C 0.66865038 0.77583100 -3.90234883

C 1.31631676 0.85339304 -5.14817918

C 0.94895504 3.23618346 -5.23255279

H -0.07540088 4.07783670 -3.54299832

S 0.51574144 -0.79099404 -3.14182428

H 1.71324045 -0.05597743 -5.59640342

H 1.05211761 4.19381383 -5.74009304

H 1.95000493 2.10227886 -6.77667295

C 3.70945631 1.68230845 2.86397183

C 2.37831518 0.51961502 1.18804790

C 2.75407653 2.90716698 1.02963552

C 3.51869109 2.89048678 2.19226122

C 3.14097813 0.51347762 2.37080033

S 1.72846964 -0.99206975 0.59926783

H 2.60257891 3.84852938 0.50249560

H 3.95754625 3.81211617 2.57095633

H -4.81940453 -0.23023814 0.26878765

C -4.94195087 1.89672790 0.57283278

C -2.86216469 0.67706377 0.26291589

C -2.84505268 3.07542735 0.57700535

C -4.23268508 3.09345642 0.68278735

C -4.26420393 0.70197108 0.35915842

H -6.02840150 1.89189545 0.65184741

H -2.28833229 4.00768262 0.66525253

H -4.75542965 4.03426372 0.84686828

C 1.04190926 -3.40757180 -1.37831940

C -1.09711408 -3.60805642 -1.09191756

H 2.03906123 -3.00498063 -1.47327391

C 1.70797990 -5.76972855 -1.76466695

C -0.59998222 -4.85759949 -1.32586312

H -2.12115355 -3.31295861 -0.91647414

N 0.75460464 -4.71016965 -1.50037678

H -1.08891025 -5.82067668 -1.38366833

H 2.69783822 -5.33171690 -1.89286808

H 1.42550667 -6.30056742 -2.67693889

H 1.72680485 -6.46996817 -0.92585751

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** OPBE-Cosmo Sextet

Fe 0.08393757 -0.49107067 -0.93448945

H 3.62946111 -0.92030062 1.87366106

H 3.99448652 0.53910832 3.83992655

S -1.30788009 -0.58061486 0.91802516

N 0.05594779 1.93499588 -0.80457485

N -0.01148315 -2.73008628 -1.05534454

C 1.41063520 2.45658049 -0.49333343

C -0.87114852 2.40121479 0.25717803

C -0.38758900 2.52622815 -2.09258698

H 2.03922633 2.22142576 -1.35839482

C 2.06456493 1.89327554 0.73294118

H 1.35859326 3.55248011 -0.40597843

C 0.39998974 2.13178896 -3.30537974

H -0.38009585 3.62277496 -1.99958990

H -1.42674494 2.21170160 -2.23541986

H -0.44399135 2.06630857 1.20835032

C -2.28057931 1.89662947 0.17193815

H -0.87906078 3.50168227 0.26185119

C 1.75031090 1.47952455 -5.68204864

C 1.18661912 3.07621212 -3.97260875

C 0.28990076 0.83404843 -3.84899347

C 0.97280453 0.52334413 -5.03588671

C 1.86052741 2.76432246 -5.15085682

H 1.26373454 4.08247759 -3.56165605

S -0.73879388 -0.38466212 -3.10496232

H 0.88320582 -0.47817038 -5.45291331

H 2.46514734 3.51984681 -5.65027314

H 2.26866383 1.21853963 -6.60391192

C 3.45312073 0.92193419 2.97571290

C 2.55658811 0.57014880 0.74511596

C 2.28461270 2.70176630 1.85250508

C 2.96932255 2.22968728 2.96986443

C 3.24762745 0.09901594 1.87224974

S 2.37747325 -0.47331465 -0.66239074

H 1.91727902 3.72765048 1.84351648

H 3.12656069 2.88113410 3.82819098

H -4.14317475 -0.91022879 0.73759265

C -4.94885981 1.01431213 0.20063067

C -2.58055825 0.55289762 0.48317746

C -3.33276360 2.77082129 -0.11853623

C -4.65847432 2.34274229 -0.10883112

C -3.91805163 0.12623841 0.49270159

H -5.98082529 0.66583727 0.21625992

H -3.10760927 3.81193889 -0.34827219

H -5.45932482 3.04405667 -0.33829984

C 0.98841102 -3.60285885 -1.08368092

C -1.15789644 -3.46711747 -1.23344126

H 2.03725409 -3.36538050 -0.97283257

C 1.35099904 -6.05261665 -1.34933954

C -0.83304829 -4.78954888 -1.36695162

H -2.13948584 -3.01244415 -1.24966954

N 0.53571735 -4.85699146 -1.26853629

H -1.44382520 -5.67014163 -1.51650928

H 2.39859748 -5.77366351 -1.23159866

H 1.21318911 -6.53402772 -2.32091902

H 1.07233483 -6.75036226 -0.55546836

FePCl **(8)** OPBE-Cosmo Doublet

Fe 0.00000000 0.00000000 -0.13710453

N 0.00000000 -1.97443387 0.07188450

N 1.97443387 0.00000000 0.07188450

N 0.00000000 1.97443387 0.07188450

N -1.97443387 0.00000000 0.07188450

C 2.41039760 -2.41039760 0.06536344

C 2.41039760 2.41039760 0.06536344

C -2.41039760 2.41039760 0.06536344

C -2.41039760 -2.41039760 0.06536344

H 3.17858728 -3.17858728 0.06594236

H 3.17858728 3.17858728 0.06594236

H -3.17858728 3.17858728 0.06594236

H -3.17858728 -3.17858728 0.06594236

C 1.09015646 -2.81863986 0.06962491

C -1.09015646 -2.81863986 0.06962491

C 0.68003986 -4.19132405 0.08558648

H 1.35855463 -5.03690167 0.10010711

C -0.68003986 -4.19132405 0.08558648

H -1.35855463 -5.03690167 0.10010711

C 2.81863986 1.09015646 0.06962491

C 2.81863986 -1.09015646 0.06962491

C 4.19132405 0.68003986 0.08558648

H 5.03690167 1.35855463 0.10010711

C 4.19132405 -0.68003986 0.08558648

H 5.03690167 -1.35855463 0.10010711

C -1.09015646 2.81863986 0.06962491

C 1.09015646 2.81863986 0.06962491

C -0.68003986 4.19132405 0.08558648

H -1.35855463 5.03690167 0.10010711

C 0.68003986 4.19132405 0.08558648

H 1.35855463 5.03690167 0.10010711

C -2.81863986 -1.09015646 0.06962491

C -2.81863986 1.09015646 0.06962491

C -4.19132405 -0.68003986 0.08558648

H -5.03690167 -1.35855463 0.10010711

C -4.19132405 0.68003986 0.08558648

H -5.03690167 1.35855463 0.10010711

Cl 0.00000000 0.00000000 -2.32185514

FePCl **(8)** OPBE-Cosmo Quartet

Fe 0.00000000 0.00000000 -0.19280308

N 0.00000000 -1.98660706 0.08048151

N 1.98660706 0.00000000 0.08048151

N 0.00000000 1.98660706 0.08048151

N -1.98660706 0.00000000 0.08048151

C 2.41496970 -2.41496970 0.10559732

C 2.41496970 2.41496970 0.10559732

C -2.41496970 2.41496970 0.10559732

C -2.41496970 -2.41496970 0.10559732

H 3.18269740 -3.18269740 0.12590661

H 3.18269740 3.18269740 0.12590661

H -3.18269740 3.18269740 0.12590661

H -3.18269740 -3.18269740 0.12590661

C 1.09334952 -2.82235098 0.10409287

C -1.09334952 -2.82235098 0.10409287

C 0.68089025 -4.19247819 0.14350070

H 1.35793761 -5.03864372 0.17387124

C -0.68089025 -4.19247819 0.14350070

H -1.35793761 -5.03864372 0.17387124

C 2.82235098 1.09334952 0.10409287

C 2.82235098 -1.09334952 0.10409287

C 4.19247819 0.68089025 0.14350070

H 5.03864372 1.35793761 0.17387124

C 4.19247819 -0.68089025 0.14350070

H 5.03864372 -1.35793761 0.17387124

C -1.09334952 2.82235098 0.10409287

C 1.09334952 2.82235098 0.10409287

C -0.68089025 4.19247819 0.14350070

H -1.35793761 5.03864372 0.17387124

C 0.68089025 4.19247819 0.14350070

H 1.35793761 5.03864372 0.17387124

C -2.82235098 -1.09334952 0.10409287

C -2.82235098 1.09334952 0.10409287

C -4.19247819 -0.68089025 0.14350070

H -5.03864372 -1.35793761 0.17387124

C -4.19247819 0.68089025 0.14350070

H -5.03864372 1.35793761 0.17387124

Cl 0.00000000 0.00000000 -2.57929564

FePCl **(8)** OPBE-Cosmo Sextet

Fe 0.00000000 0.00000000 -0.41034150

N 0.00000000 -2.02861051 0.10602701

N 2.02861051 0.00000000 0.10602701

N 0.00000000 2.02861051 0.10602701

N -2.02861051 0.00000000 0.10602701

C 2.42110339 -2.42110339 0.15834782

C 2.42110339 2.42110339 0.15834782

C -2.42110339 2.42110339 0.15834782

C -2.42110339 -2.42110339 0.15834782

H 3.18906975 -3.18906975 0.19838432

H 3.18906975 3.18906975 0.19838432

H -3.18906975 3.18906975 0.19838432

H -3.18906975 -3.18906975 0.19838432

C 1.09816715 -2.85245058 0.14951691

C -1.09816715 -2.85245058 0.14951691

C 0.68184806 -4.22535862 0.21265252

H 1.35279242 -5.07594014 0.26087486

C -0.68184806 -4.22535862 0.21265252

H -1.35279242 -5.07594014 0.26087486

C 2.85245058 1.09816715 0.14951691

C 2.85245058 -1.09816715 0.14951691

C 4.22535862 0.68184806 0.21265252

H 5.07594014 1.35279242 0.26087486

C 4.22535862 -0.68184806 0.21265252

H 5.07594014 -1.35279242 0.26087486

C -1.09816715 2.85245058 0.14951691

C 1.09816715 2.85245058 0.14951691

C -0.68184806 4.22535862 0.21265252

H -1.35279242 5.07594014 0.26087486

C 0.68184806 4.22535862 0.21265252

H 1.35279242 5.07594014 0.26087486

C -2.85245058 -1.09816715 0.14951691

C -2.85245058 1.09816715 0.14951691

C -4.22535862 -0.68184806 0.21265252

H -5.07594014 -1.35279242 0.26087486

C -4.22535862 0.68184806 0.21265252

H -5.07594014 1.35279242 0.26087486

Cl 0.00000000 0.00000000 -2.68761610

FePzCl **(9)** OPBE-Cosmo Doublet

Fe 0.00000000 0.00000000 -0.13760196

N 0.00000000 -1.89381901 0.05643040

N 1.89381901 0.00000000 0.05643040

N 0.00000000 1.89381901 0.05643040

N -1.89381901 0.00000000 0.05643040

N 2.37101623 -2.37101623 0.06232755

N 2.37101623 2.37101623 0.06232755

N -2.37101623 2.37101623 0.06232755

N -2.37101623 -2.37101623 0.06232755

C 1.09616368 -2.72399280 0.06581060

C -1.09616368 -2.72399280 0.06581060

C 0.67800359 -4.10427916 0.09461425

H 1.36162862 -4.94498305 0.12068310

C -0.67800359 -4.10427916 0.09461425

H -1.36162862 -4.94498305 0.12068310

C 2.72399280 1.09616368 0.06581060

C 2.72399280 -1.09616368 0.06581060

C 4.10427916 0.67800359 0.09461425

H 4.94498305 1.36162862 0.12068310

C 4.10427916 -0.67800359 0.09461425

H 4.94498305 -1.36162862 0.12068310

C -1.09616368 2.72399280 0.06581060

C 1.09616368 2.72399280 0.06581060

C -0.67800359 4.10427916 0.09461425

H -1.36162862 4.94498305 0.12068310

C 0.67800359 4.10427916 0.09461425

H 1.36162862 4.94498305 0.12068310

C -2.72399280 -1.09616368 0.06581060

C -2.72399280 1.09616368 0.06581060

C -4.10427916 -0.67800359 0.09461425

H -4.94498305 -1.36162862 0.12068310

C -4.10427916 0.67800359 0.09461425

H -4.94498305 1.36162862 0.12068310

Cl 0.00000000 0.00000000 -2.29843587

FePzCl **(9)** OPBE-Cosmo Quartet

Fe 0.00000000 0.00000000 -0.23085781

N 0.00000000 -1.90360032 0.06756906

N 1.90360032 0.00000000 0.06756906

N 0.00000000 1.90360032 0.06756906

N -1.90360032 0.00000000 0.06756906

N 2.37310966 -2.37310966 0.11639201

N 2.37310966 2.37310966 0.11639201

N -2.37310966 2.37310966 0.11639201

N -2.37310966 -2.37310966 0.11639201

C 1.09686220 -2.72608993 0.10995933

C -1.09686220 -2.72608993 0.10995933

C 0.67838883 -4.10578308 0.16709460

H 1.36170112 -4.94583291 0.21093799

C -0.67838883 -4.10578308 0.16709460

H -1.36170112 -4.94583291 0.21093799

C 2.72608993 1.09686220 0.10995933

C 2.72608993 -1.09686220 0.10995933

C 4.10578308 0.67838883 0.16709460

H 4.94583291 1.36170112 0.21093799

C 4.10578308 -0.67838883 0.16709460

H 4.94583291 -1.36170112 0.21093799

C -1.09686220 2.72608993 0.10995933

C 1.09686220 2.72608993 0.10995933

C -0.67838883 4.10578308 0.16709460

H -1.36170112 4.94583291 0.21093799

C 0.67838883 4.10578308 0.16709460

H 1.36170112 4.94583291 0.21093799

C -2.72608993 -1.09686220 0.10995933

C -2.72608993 1.09686220 0.10995933

C -4.10578308 -0.67838883 0.16709460

H -4.94583291 -1.36170112 0.21093799

C -4.10578308 0.67838883 0.16709460

H -4.94583291 1.36170112 0.21093799

Cl 0.00000000 0.00000000 -2.59470051

FePzCl **(9)** OPBE-Cosmo Sextet

Fe 0.00000000 0.00000000 -0.54245060

N 0.00000000 -1.93372162 0.07726835

N 1.93372162 0.00000000 0.07726835

N 0.00000000 1.93372162 0.07726835

N -1.93372162 0.00000000 0.07726835

N 2.37413044 -2.37413044 0.19281420

N 2.37413044 2.37413044 0.19281420

N -2.37413044 2.37413044 0.19281420

N -2.37413044 -2.37413044 0.19281420

C 1.09932605 -2.74554355 0.17042841

C -1.09932605 -2.74554355 0.17042841

C 0.67884762 -4.12547959 0.29309646

H 1.35766138 -4.96543205 0.38686349

C -0.67884762 -4.12547959 0.29309646

H -1.35766138 -4.96543205 0.38686349

C 2.74554355 1.09932605 0.17042841

C 2.74554355 -1.09932605 0.17042841

C 4.12547959 0.67884762 0.29309646

H 4.96543205 1.35766138 0.38686349

C 4.12547959 -0.67884762 0.29309646

H 4.96543205 -1.35766138 0.38686349

C -1.09932605 2.74554355 0.17042841

C 1.09932605 2.74554355 0.17042841

C -0.67884762 4.12547959 0.29309646

H -1.35766138 4.96543205 0.38686349

C 0.67884762 4.12547959 0.29309646

H 1.35766138 4.96543205 0.38686349

C -2.74554355 -1.09932605 0.17042841

C -2.74554355 1.09932605 0.17042841

C -4.12547959 -0.67884762 0.29309646

H -4.96543205 -1.35766138 0.38686349

C -4.12547959 0.67884762 0.29309646

H -4.96543205 1.35766138 0.38686349

Cl 0.00000000 0.00000000 -2.78671565

Fe-(PyPepS)2 **(1)** S12g Doublet

Fe 0.00000000 0.00000000 -0.11641476

N 1.59978908 -1.18087226 -0.09342942

N 0.53622430 1.25727381 1.32101215

N -1.59978908 1.18087226 -0.09342942

N -0.53622430 -1.25727381 1.32101215

C 1.66300459 -2.15414405 0.85785929

C 3.66586851 -1.87188038 -1.30992536

C 2.57732286 -1.01051105 -1.08109166

C 0.39947008 -2.17417023 1.64867976

C 0.17414429 -3.12219339 2.64263392

C -1.04768840 -3.13775702 3.30030969

C -2.01375280 -2.19591148 2.94306795

C -1.71688542 -1.26980473 1.95484637

C 2.42432185 0.13107932 -1.91295088

C 3.34596763 0.36701776 -2.94053584

C -2.57732286 1.01051105 -1.08109166

C -3.66586851 1.87188038 -1.30992536

C -1.66300459 2.15414405 0.85785929

C -3.34596763 -0.36701776 -2.94053584

C -2.42432185 -0.13107932 -1.91295088

C -0.39947008 2.17417023 1.64867976

C -0.17414429 3.12219339 2.64263392

C 1.04768840 3.13775702 3.30030969

C 2.01375280 2.19591148 2.94306795

C 1.71688542 1.26980473 1.95484637

H 0.97596107 -3.82790364 2.85030688

H -1.25361931 -3.87799821 4.07482145

H -2.99379859 -2.17602394 3.41810825

H -2.43418941 -0.51816189 1.63348338

H -0.97596107 3.82790364 2.85030688

H 1.25361931 3.87799821 4.07482145

H 2.99379859 2.17602394 3.41810825

H 2.43418941 0.51816189 1.63348338

C -4.56616041 1.61897863 -2.34015091

C -4.41077280 0.49754568 -3.15672168

C 4.56616041 -1.61897863 -2.34015091

C 4.41077280 -0.49754568 -3.15672168

H -5.11491457 0.30085685 -3.96697036

H -5.39646438 2.30744300 -2.50565956

H -3.78391790 2.73584585 -0.66636486

H 5.11491457 -0.30085685 -3.96697036

H 5.39646438 -2.30744300 -2.50565956

H 3.78391790 -2.73584585 -0.66636486

O -2.57686565 2.97388194 1.11836743

O 2.57686565 -2.97388194 1.11836743

H 3.20666596 1.24285426 -3.57437747

H -3.20666596 -1.24285426 -3.57437747

S -1.09906887 -1.23844145 -1.62274214

S 1.09906887 1.23844145 -1.62274214

Fe-(PyPepS)2 **(1)** S12g Quartet

Fe 0.00000000 0.00000000 -0.34860451

N 1.78840478 -1.30734721 -0.06639269

N 0.56705046 1.37424633 1.08968549

N -1.78840478 1.30734721 -0.06639269

N -0.56705046 -1.37424633 1.08968549

C 1.70645587 -2.27555425 0.87315093

C 4.15490343 -1.76429917 -0.71536721

C 2.93224310 -1.06900260 -0.81543304

C 0.33218414 -2.30201999 1.48526718

C 0.00055669 -3.28576790 2.41180786

C -1.28549060 -3.33393573 2.93079951

C -2.21038713 -2.38290367 2.50613582

C -1.81030002 -1.42111608 1.59175670

C 2.84018214 -0.01419835 -1.76593539

C 3.93594206 0.29109141 -2.58239450

C -2.93224310 1.06900260 -0.81543304

C -4.15490343 1.76429917 -0.71536721

C -1.70645587 2.27555425 0.87315093

C -3.93594206 -0.29109141 -2.58239450

C -2.84018214 0.01419835 -1.76593539

C -0.33218414 2.30201999 1.48526718

C -0.00055669 3.28576790 2.41180786

C 1.28549060 3.33393573 2.93079951

C 2.21038713 2.38290367 2.50613582

C 1.81030002 1.42111608 1.59175670

H 0.78032689 -3.99349220 2.68399388

H -1.56708328 -4.10373834 3.65086422

H -3.23627448 -2.37742457 2.87184440

H -2.49514111 -0.65797105 1.23303802

H -0.78032689 3.99349220 2.68399388

H 1.56708328 4.10373834 3.65086422

H 3.23627448 2.37742457 2.87184440

H 2.49514111 0.65797105 1.23303802

C -5.23406253 1.43863767 -1.52945137

C -5.12908329 0.41072939 -2.46714604

C 5.23406253 -1.43863767 -1.52945137

C 5.12908329 -0.41072939 -2.46714604

H -5.97245900 0.15656979 -3.11104257

H -6.16568807 1.99903638 -1.43295272

H -4.22487230 2.56680335 0.00978766

H 5.97245900 -0.15656979 -3.11104257

H 6.16568807 -1.99903638 -1.43295272

H 4.22487230 -2.56680335 0.00978766

O -2.55723688 3.10865915 1.26777057

O 2.55723688 -3.10865915 1.26777057

H 3.83752303 1.09485132 -3.31194101

H -3.83752303 -1.09485132 -3.31194101

S -1.36368501 -0.92218449 -1.94120577

S 1.36368501 0.92218449 -1.94120577

Fe-(PyPepS)2 **(1)** S12g Sextet

Fe 0.00000000 0.00000000 -0.53115849

N 1.77622630 -1.32320718 -0.09571017

N 0.62990931 1.45731445 1.03526861

N -1.77622630 1.32320718 -0.09571017

N -0.62990931 -1.45731445 1.03526861

C 1.65520029 -2.32012843 0.81394181

C 4.20890015 -1.71229110 -0.48309914

C 2.98762573 -1.04799797 -0.72841407

C 0.26714455 -2.38506854 1.40176566

C -0.05758560 -3.39657867 2.30659261

C -1.33807283 -3.44222603 2.83636095

C -2.26374248 -2.47660191 2.44909581

C -1.86513813 -1.50355608 1.54335920

C 2.99079021 0.00750056 -1.68914912

C 4.18269635 0.34624967 -2.34517704

C -2.98762573 1.04799797 -0.72841407

C -4.20890015 1.71229110 -0.48309914

C -1.65520029 2.32012843 0.81394181

C -4.18269635 -0.34624967 -2.34517704

C -2.99079021 -0.00750056 -1.68914912

C -0.26714455 2.38506854 1.40176566

C 0.05758560 3.39657867 2.30659261

C 1.33807283 3.44222603 2.83636095

C 2.26374248 2.47660191 2.44909581

C 1.86513813 1.50355608 1.54335920

H 0.71669914 -4.11619359 2.56054424

H -1.61720324 -4.22544435 3.54344970

H -3.28241980 -2.47173930 2.83456492

H -2.55157733 -0.73294859 1.20017559

H -0.71669914 4.11619359 2.56054424

H 1.61720324 4.22544435 3.54344970

H 3.28241980 2.47173930 2.83456492

H 2.55157733 0.73294859 1.20017559

C -5.37534862 1.35650143 -1.14829875

C -5.36894452 0.32464601 -2.08603788

C 5.37534862 -1.35650143 -1.14829875

C 5.36894452 -0.32464601 -2.08603788

H -6.28190492 0.04469643 -2.61385091

H -6.29761567 1.89957910 -0.93362107

H -4.21121847 2.52096231 0.23687826

H 6.28190492 -0.04469643 -2.61385091

H 6.29761567 -1.89957910 -0.93362107

H 4.21121847 -2.52096231 0.23687826

O -2.49322654 3.16050477 1.22158557

O 2.49322654 -3.16050477 1.22158557

H 4.15372337 1.15272268 -3.07722179

H -4.15372337 -1.15272268 -3.07722179

S -1.52091045 -0.85797624 -2.11393505

S 1.52091045 0.85797624 -2.11393505

Fe(tsalen)Cl **(2)** S12g Doublet

Fe -0.46860656 -0.16375919 0.00000000

Cl -2.62446568 0.39025605 0.00000000

S -0.36349079 -1.81878379 1.43602407

C -0.01230972 2.56807179 0.75986307

N -0.06781459 1.20255159 1.31365024

S -0.36349079 -1.81878379 -1.43602407

H -0.40399667 -3.33942489 -3.74535040

H -0.40399667 -3.33942489 3.74535040

C -0.00062443 1.16952352 2.61574378

C -0.29478348 -2.30514901 4.06837925

H 0.08010474 1.36967000 5.20312947

H -0.26903530 -2.80301802 6.14854749

H 0.16014385 2.12856309 3.12412701

C -0.10464163 0.05449891 3.50089380

H -0.03484209 -0.42730957 6.89118902

N -0.06781459 1.20255159 -1.31365024

C -0.21927835 -2.00113827 5.41216507

C -0.25288693 -1.29650913 3.08330892

C -0.02714626 0.33193278 4.88545485

C -0.08848214 -0.66864562 5.83080831

C -0.01230972 2.56807179 -0.75986307

C -0.00062443 1.16952352 -2.61574378

H 0.16014385 2.12856309 -3.12412701

C -0.10464163 0.05449891 -3.50089380

C -0.21927835 -2.00113827 -5.41216507

C -0.25288693 -1.29650913 -3.08330892

C -0.02714626 0.33193278 -4.88545485

C -0.08848214 -0.66864562 -5.83080831

C -0.29478348 -2.30514901 -4.06837925

H -0.26903530 -2.80301802 -6.14854749

H 0.08010474 1.36967000 -5.20312947

H -0.03484209 -0.42730957 -6.89118902

H -0.89289400 3.10948308 -1.12394178

H 0.88108700 3.07558187 -1.14348483

H 0.88108700 3.07558187 1.14348483

H -0.89289400 3.10948308 1.12394178

Fe(tsalen)Cl **(2)** S12g Quartet

Fe -0.92820494 -0.11054407 0.00000000

Cl -3.07640792 0.67546354 0.00000000

S -0.78828889 -1.80094893 1.46203842

C -0.31989294 2.58003807 0.76661855

N -0.22666090 1.22176020 1.31907748

S -0.78828889 -1.80094893 -1.46203842

H -0.39127789 -3.35369838 -3.69342118

H -0.39127789 -3.35369838 3.69342118

C 0.18315142 1.13495290 2.54512878

C -0.07580887 -2.35010579 3.97481965

H 1.05592346 1.20322788 4.97628336

H 0.47105454 -2.93211451 5.95678212

H 0.51709560 2.06467129 3.02603977

C 0.24311197 -0.01582875 3.39227329

H 1.20813124 -0.63617213 6.62103610

N -0.22666090 1.22176020 -1.31907748

C 0.41098233 -2.10966459 5.24386025

C -0.17719871 -1.32141115 3.01415074

C 0.74074708 0.19677826 4.69852140

C 0.82542866 -0.82425548 5.61955281

C -0.31989294 2.58003807 -0.76661855

C 0.18315142 1.13495290 -2.54512878

H 0.51709560 2.06467129 -3.02603977

C 0.24311197 -0.01582875 -3.39227329

C 0.41098233 -2.10966459 -5.24386025

C -0.17719871 -1.32141115 -3.01415074

C 0.74074708 0.19677826 -4.69852140

C 0.82542866 -0.82425548 -5.61955281

C -0.07580887 -2.35010579 -3.97481965

H 0.47105454 -2.93211451 -5.95678212

H 1.05592346 1.20322788 -4.97628336

H 1.20813124 -0.63617213 -6.62103610

H -1.26684716 3.00339998 -1.12057463

H 0.50003969 3.19944269 -1.15174211

H 0.50003969 3.19944269 1.15174211

H -1.26684716 3.00339998 1.12057463

Fe(tsalen)Cl **(2)** S12g Sextet

Fe -1.04365819 -0.21442315 0.00000000

Cl -3.12626541 0.58900709 0.00000000

S -0.66614155 -1.90081367 1.61864366

C -0.16454396 2.55731150 0.76991744

N -0.13683994 1.21198365 1.34603800

S -0.66614155 -1.90081367 -1.61864366

H -0.41092942 -3.28809416 -3.97119796

H -0.41092942 -3.28809416 3.97119796

C 0.23039372 1.14482576 2.58457471

C -0.10667737 -2.26909881 4.20366976

H 0.97472809 1.34068008 5.02333463

H 0.33277682 -2.71933022 6.24633839

H 0.56841415 2.07934061 3.05898423

C 0.24151279 0.02359496 3.48210430

H 1.04312266 -0.38267241 6.79207042

N -0.13683994 1.21198365 -1.34603800

C 0.31315281 -1.94572918 5.47861227

C -0.15614751 -1.30927341 3.17044589

C 0.67230911 0.31771590 4.79649116

C 0.71113855 -0.63935195 5.78765231

C -0.16454396 2.55731150 -0.76991744

C 0.23039372 1.14482576 -2.58457471

H 0.56841415 2.07934061 -3.05898423

C 0.24151279 0.02359496 -3.48210430

C 0.31315281 -1.94572918 -5.47861227

C -0.15614751 -1.30927341 -3.17044589

C 0.67230911 0.31771590 -4.79649116

C 0.71113855 -0.63935195 -5.78765231

C -0.10667737 -2.26909881 -4.20366976

H 0.33277682 -2.71933022 -6.24633839

H 0.97472809 1.34068008 -5.02333463

H 1.04312266 -0.38267241 -6.79207042

H -1.08628024 3.03994178 -1.11764669

H 0.68237935 3.14644347 -1.14526181

H 0.68237935 3.14644347 1.14526181

H -1.08628024 3.03994178 1.11764669

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** S12g Doublet

Fe 0.08476255 -0.66531392 -0.99431400

H 3.08220188 -0.42577866 2.90603560

H 4.16884196 1.59131378 3.84929140

S -1.84577501 -0.91638524 0.04179124

N 0.09203715 1.42417367 -0.84756044

N 0.05659498 -2.71786811 -1.20445134

C 1.51737978 1.92107005 -0.83644984

C -0.58569020 1.91838447 0.41343825

C -0.62864352 2.04925636 -2.01635423

H 2.04801015 1.34858440 -1.60623128

C 2.22367953 1.80637247 0.47941024

H 1.51875670 2.97614894 -1.14416059

C 0.10790295 2.05601977 -3.31935108

H -0.87503797 3.08687028 -1.74889588

H -1.57195806 1.50034133 -2.11648198

H -0.18081404 1.32025543 1.23516532

C -2.07655291 1.83257150 0.41261538

H -0.28475927 2.96385509 0.57188503

C 1.34672699 2.13511907 -5.83643240

C 0.32884291 3.26712657 -3.97610661

C 0.52851578 0.86268539 -3.93659136

C 1.14265772 0.92155742 -5.19638194

C 0.93981138 3.31937595 -5.22453417

H 0.00364497 4.19242792 -3.49816324

S 0.32901013 -0.71793107 -3.18981748

H 1.45963543 -0.00901771 -5.66584259

H 1.09645632 4.27821178 -5.71713839

H 1.82500427 2.15654281 -6.81570453

C 3.62778415 1.65739214 2.90535402

C 2.32942343 0.57817430 1.15992689

C 2.81783498 2.93779417 1.03929618

C 3.52496925 2.87507555 2.23517220

C 3.02437762 0.52549417 2.37819664

S 1.64555391 -0.92054034 0.54623528

H 2.72759227 3.89161076 0.51750466

H 3.98517935 3.77277343 2.64602647

H -4.61888710 -0.42901934 0.26164746

C -4.86763745 1.68802462 0.56144859

C -2.72163003 0.58962146 0.28558214

C -2.84475158 2.98205350 0.59493863

C -4.23171615 2.92347040 0.67574453

C -4.12203782 0.53541731 0.36215885

H -5.95421932 1.62210872 0.62147846

H -2.33873060 3.94434327 0.68753248

H -4.81201616 3.83303825 0.82518471

C 0.99693924 -3.60562803 -0.90674839

C -0.97933563 -3.43539859 -1.75674623

H 1.95403356 -3.37552800 -0.45893796

C 1.35609449 -6.08220772 -1.01864398

C -0.65369742 -4.76192371 -1.77932622

H -1.88319366 -2.94620650 -2.09196625

N 0.60673452 -4.85647340 -1.23827212

H -1.19975330 -5.62953838 -2.12752696

H 2.34647246 -5.83324570 -0.63154235

H 1.47136411 -6.62867954 -1.96049852

H 0.84073935 -6.71979433 -0.29171372

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** S12g Quartet

Fe 0.02936563 -0.68367954 -0.89171605

H 3.27057310 -0.41938461 2.89938913

H 4.28507786 1.64407381 3.81698830

S -2.07663969 -0.89369253 0.20073598

N 0.06715577 1.39249818 -0.80298044

N 0.09942870 -2.74346494 -1.11024033

C 1.51263147 1.85996754 -0.79683193

C -0.62813234 1.87548778 0.46315868

C -0.63307273 2.02913281 -1.99066638

H 2.02609374 1.26429970 -1.56147188

C 2.22988784 1.77396618 0.51192766

H 1.52039714 2.90393212 -1.13619912

C 0.11995654 1.99027479 -3.27986599

H -0.84147438 3.07465687 -1.72546762

H -1.59117936 1.50827951 -2.09037237

H -0.27852609 1.22736366 1.27283321

C -2.12282681 1.87832629 0.39532980

H -0.27181930 2.89550868 0.65866904

C 1.40871587 1.96266656 -5.76603701

C 0.48478139 3.17955726 -3.91218147

C 0.42363443 0.76307306 -3.89866734

C 1.07180936 0.76956395 -5.14381611

C 1.12165362 3.17936941 -5.14834693

H 0.25054955 4.12856575 -3.42724397

S 0.01649287 -0.78507043 -3.17647586

H 1.30602321 -0.18336309 -5.61674976

H 1.39073549 4.11984226 -5.62726663

H 1.90625785 1.94237790 -6.73587709

C 3.71020404 1.68808601 2.89190710

C 2.40767234 0.54930292 1.18545970

C 2.78849475 2.93210552 1.05596632

C 3.53097382 2.90217790 2.23074193

C 3.14704461 0.52940744 2.37897241

S 1.73572095 -0.96793028 0.61196862

H 2.64630482 3.87978100 0.53443515

H 3.96353759 3.81897219 2.62895786

H -4.81813927 -0.18341601 0.12970928

C -4.92141985 1.95699272 0.33344041

C -2.85463079 0.67864654 0.26847755

C -2.81101653 3.08873034 0.48591754

C -4.19984963 3.14251221 0.46259564

C -4.25684731 0.74382107 0.23428529

H -6.01110481 1.97711839 0.30660636

H -2.23912780 4.01276695 0.58428418

H -4.71388235 4.09957001 0.54008147

C 1.19168705 -3.48476765 -1.24474925

C -0.96783926 -3.57587028 -1.34812455

H 2.20522447 -3.12465512 -1.12959604

C 1.79566880 -5.86155456 -1.75245195

C -0.50298509 -4.83141685 -1.61738687

H -1.98497614 -3.20940815 -1.30548927

N 0.86959433 -4.75876611 -1.55113176

H -1.02174072 -5.75495022 -1.84134791

H 2.81939764 -5.48746699 -1.68598517

H 1.64330332 -6.30455212 -2.74206103

H 1.64631434 -6.62858217 -0.98496185

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** S12g Sextet

Fe 0.05491801 -0.49864319 -0.96864784

H 3.54099750 -1.03353450 1.76730119

H 3.86383054 0.32642987 3.81732486

S -1.45755047 -0.62161869 0.80477488

N 0.05398878 1.97448626 -0.77456468

N 0.09822165 -2.80113362 -0.98375532

C 1.43458470 2.46712488 -0.50062179

C -0.83691446 2.40817347 0.34000114

C -0.43758302 2.55825608 -2.05580704

H 2.03353715 2.22204543 -1.38404881

C 2.08194522 1.86091900 0.71064218

H 1.40788401 3.56711292 -0.39654373

C 0.33930951 2.15036202 -3.27490072

H -0.43417300 3.66025923 -1.97119001

H -1.47722634 2.23129333 -2.16478422

H -0.41128132 1.98466234 1.25650862

C -2.26923904 1.97925838 0.21835811

H -0.79261967 3.50960458 0.42073666

C 1.73574953 1.46088746 -5.61165219

C 1.16511019 3.07053140 -3.92178127

C 0.21916987 0.85282682 -3.81736613

C 0.92192943 0.52713674 -4.98456922

C 1.86188898 2.74198113 -5.08000051

H 1.25913122 4.07443515 -3.50479542

S -0.84517227 -0.36614197 -3.09412583

H 0.81693325 -0.47652094 -5.39395079

H 2.49914910 3.48096975 -5.56421410

H 2.27207279 1.18552479 -6.51990609

C 3.36511380 0.76021656 2.95046162

C 2.54899759 0.53070604 0.67995361

C 2.27212676 2.61043560 1.87134326

C 2.90567893 2.07434994 2.98788239

C 3.18607514 -0.00469116 1.80546863

S 2.38378105 -0.44762204 -0.78754645

H 1.91389282 3.64078127 1.89743064

H 3.04103612 2.68012295 3.88321007

H -4.27998082 -0.75319227 0.52716743

C -4.97342263 1.24293999 0.10762566

C -2.64436062 0.63516722 0.41996671

C -3.26346573 2.92246549 -0.04472183

C -4.60755424 2.57015886 -0.10163643

C -4.00018364 0.28655054 0.36321615

H -6.02248636 0.94880264 0.07105951

H -2.97228224 3.96210670 -0.20278707

H -5.36420150 3.32664896 -0.30641850

C 1.13761678 -3.59916730 -1.16822916

C -1.00185900 -3.61847381 -0.92919027

H 2.16749943 -3.27158701 -1.24272355

C 1.61439596 -6.05169800 -1.42320263

C -0.61433986 -4.92092242 -1.08215160

H -1.99272911 -3.21281870 -0.76720488

N 0.75401355 -4.89508111 -1.23412919

H -1.17597472 -5.84703341 -1.09041311

H 2.64776165 -5.71558155 -1.53428858

H 1.32153498 -6.59912022 -2.32549270

H 1.55019935 -6.72110722 -0.55843969

FePCl **(8)** S12g Doublet

Fe 0.00000000 0.00000000 -0.13928210

N 0.00000000 -1.98364314 0.07530139

N 1.98364314 0.00000000 0.07530139

N 0.00000000 1.98364314 0.07530139

N -1.98364314 0.00000000 0.07530139

C 2.40954192 -2.40954192 0.06338750

C 2.40954192 2.40954192 0.06338750

C -2.40954192 2.40954192 0.06338750

C -2.40954192 -2.40954192 0.06338750

H 3.17901644 -3.17901644 0.05811530

H 3.17901644 3.17901644 0.05811530

H -3.17901644 3.17901644 0.05811530

H -3.17901644 -3.17901644 0.05811530

C 1.09115767 -2.82227002 0.06979477

C -1.09115767 -2.82227002 0.06979477

C 0.67893970 -4.19325555 0.08134354

H 1.35575317 -5.04171771 0.09164927

C -0.67893970 -4.19325555 0.08134354

H -1.35575317 -5.04171771 0.09164927

C 2.82227002 1.09115767 0.06979477

C 2.82227002 -1.09115767 0.06979477

C 4.19325555 0.67893970 0.08134354

H 5.04171771 1.35575317 0.09164927

C 4.19325555 -0.67893970 0.08134354

H 5.04171771 -1.35575317 0.09164927

C -1.09115767 2.82227002 0.06979477

C 1.09115767 2.82227002 0.06979477

C -0.67893970 4.19325555 0.08134354

H -1.35575317 5.04171771 0.09164927

C 0.67893970 4.19325555 0.08134354

H 1.35575317 5.04171771 0.09164927

C -2.82227002 -1.09115767 0.06979477

C -2.82227002 1.09115767 0.06979477

C -4.19325555 -0.67893970 0.08134354

H -5.04171771 -1.35575317 0.09164927

C -4.19325555 0.67893970 0.08134354

H -5.04171771 1.35575317 0.09164927

Cl 0.00000000 0.00000000 -2.30709691

FePCl **(8)** S12g Quartet

Fe 0.00000000 0.00000000 -0.25900898

N 0.00000000 -1.99846857 0.07495425

N 1.99846857 0.00000000 0.07495425

N 0.00000000 1.99846857 0.07495425

N -1.99846857 0.00000000 0.07495425

C 2.41284928 -2.41284928 0.10809662

C 2.41284928 2.41284928 0.10809662

C -2.41284928 2.41284928 0.10809662

C -2.41284928 -2.41284928 0.10809662

H 3.18189146 -3.18189146 0.13330187

H 3.18189146 3.18189146 0.13330187

H -3.18189146 3.18189146 0.13330187

H -3.18189146 -3.18189146 0.13330187

C 1.09243298 -2.82677384 0.10535072

C -1.09243298 -2.82677384 0.10535072

C 0.67942072 -4.19745246 0.15559399

H 1.35551345 -5.04567755 0.19367041

C -0.67942072 -4.19745246 0.15559399

H -1.35551345 -5.04567755 0.19367041

C 2.82677384 1.09243298 0.10535072

C 2.82677384 -1.09243298 0.10535072

C 4.19745246 0.67942072 0.15559399

H 5.04567755 1.35551345 0.19367041

C 4.19745246 -0.67942072 0.15559399

H 5.04567755 -1.35551345 0.19367041

C -1.09243298 2.82677384 0.10535072

C 1.09243298 2.82677384 0.10535072

C -0.67942072 4.19745246 0.15559399

H -1.35551345 5.04567755 0.19367041

C 0.67942072 4.19745246 0.15559399

H 1.35551345 5.04567755 0.19367041

C -2.82677384 -1.09243298 0.10535072

C -2.82677384 1.09243298 0.10535072

C -4.19745246 -0.67942072 0.15559399

H -5.04567755 -1.35551345 0.19367041

C -4.19745246 0.67942072 0.15559399

H -5.04567755 1.35551345 0.19367041

Cl 0.00000000 0.00000000 -2.51004327

FePCl **(8)** S12g Sextet

Fe 0.00000000 0.00000000 -0.42801443

N 0.00000000 -2.03608355 0.11353657

N 2.03608355 0.00000000 0.11353657

N 0.00000000 2.03608355 0.11353657

N -2.03608355 0.00000000 0.11353657

C 2.41911421 -2.41911421 0.15519128

C 2.41911421 2.41911421 0.15519128

C -2.41911421 2.41911421 0.15519128

C -2.41911421 -2.41911421 0.15519128

H 3.18856439 -3.18856439 0.18498978

H 3.18856439 3.18856439 0.18498978

H -3.18856439 3.18856439 0.18498978

H -3.18856439 -3.18856439 0.18498978

C 1.09716012 -2.85391693 0.14954337

C -1.09716012 -2.85391693 0.14954337

C 0.68040605 -4.22742241 0.20294371

H 1.35049368 -5.08054980 0.24378614

C -0.68040605 -4.22742241 0.20294371

H -1.35049368 -5.08054980 0.24378614

C 2.85391693 1.09716012 0.14954337

C 2.85391693 -1.09716012 0.14954337

C 4.22742241 0.68040605 0.20294371

H 5.08054980 1.35049368 0.24378614

C 4.22742241 -0.68040605 0.20294371

H 5.08054980 -1.35049368 0.24378614

C -1.09716012 2.85391693 0.14954337

C 1.09716012 2.85391693 0.14954337

C -0.68040605 4.22742241 0.20294371

H -1.35049368 5.08054980 0.24378614

C 0.68040605 4.22742241 0.20294371

H 1.35049368 5.08054980 0.24378614

C -2.85391693 -1.09716012 0.14954337

C -2.85391693 1.09716012 0.14954337

C -4.22742241 -0.68040605 0.20294371

H -5.08054980 -1.35049368 0.24378614

C -4.22742241 0.68040605 0.20294371

H -5.08054980 1.35049368 0.24378614

Cl 0.00000000 0.00000000 -2.63497831

FePzCl **(9)** S12g Doublet

Fe 0.00000000 0.00000000 -0.15575962

N 0.00000000 -1.90271395 0.06543330

N 1.90271395 0.00000000 0.06543330

N 0.00000000 1.90271395 0.06543330

N -1.90271395 0.00000000 0.06543330

N 2.37588149 -2.37588149 0.06830514

N 2.37588149 2.37588149 0.06830514

N -2.37588149 2.37588149 0.06830514

N -2.37588149 -2.37588149 0.06830514

C 1.10072784 -2.72914064 0.07178924

C -1.10072784 -2.72914064 0.07178924

C 0.67773582 -4.10642762 0.09802321

H 1.36666216 -4.94366117 0.12061431

C -0.67773582 -4.10642762 0.09802321

H -1.36666216 -4.94366117 0.12061431

C 2.72914064 1.10072784 0.07178924

C 2.72914064 -1.10072784 0.07178924

C 4.10642762 0.67773582 0.09802321

H 4.94366117 1.36666216 0.12061431

C 4.10642762 -0.67773582 0.09802321

H 4.94366117 -1.36666216 0.12061431

C -1.10072784 2.72914064 0.07178924

C 1.10072784 2.72914064 0.07178924

C -0.67773582 4.10642762 0.09802321

H -1.36666216 4.94366117 0.12061431

C 0.67773582 4.10642762 0.09802321

H 1.36666216 4.94366117 0.12061431

C -2.72914064 -1.10072784 0.07178924

C -2.72914064 1.10072784 0.07178924

C -4.10642762 -0.67773582 0.09802321

H -4.94366117 -1.36666216 0.12061431

C -4.10642762 0.67773582 0.09802321

H -4.94366117 1.36666216 0.12061431

Cl 0.00000000 0.00000000 -2.31914469

FePzCl **(9)** S12g Quartet

Fe 0.00000000 0.00000000 -0.28678973

N 0.00000000 -1.91341497 0.07113677

N 1.91341497 0.00000000 0.07113677

N 0.00000000 1.91341497 0.07113677

N -1.91341497 0.00000000 0.07113677

N 2.37688957 -2.37688957 0.12046455

N 2.37688957 2.37688957 0.12046455

N -2.37688957 2.37688957 0.12046455

N -2.37688957 -2.37688957 0.12046455

C 1.09934033 -2.73006564 0.11281794

C -1.09934033 -2.73006564 0.11281794

C 0.67763687 -4.10959527 0.17234403

H 1.36698337 -4.94561860 0.21685472

C -0.67763687 -4.10959527 0.17234403

H -1.36698337 -4.94561860 0.21685472

C 2.73006564 1.09934033 0.11281794

C 2.73006564 -1.09934033 0.11281794

C 4.10959527 0.67763687 0.17234403

H 4.94561860 1.36698337 0.21685472

C 4.10959527 -0.67763687 0.17234403

H 4.94561860 -1.36698337 0.21685472

C -1.09934033 2.73006564 0.11281794

C 1.09934033 2.73006564 0.11281794

C -0.67763687 4.10959527 0.17234403

H -1.36698337 4.94561860 0.21685472

C 0.67763687 4.10959527 0.17234403

H 1.36698337 4.94561860 0.21685472

C -2.73006564 -1.09934033 0.11281794

C -2.73006564 1.09934033 0.11281794

C -4.10959527 -0.67763687 0.17234403

H -4.94561860 -1.36698337 0.21685472

C -4.10959527 0.67763687 0.17234403

H -4.94561860 1.36698337 0.21685472

Cl 0.00000000 0.00000000 -2.54109380

FePzCl **(9)** S12g Sextet

Fe 0.00000000 0.00000000 -0.54624110

N 0.00000000 -1.93959390 0.09822482

N 1.93959390 0.00000000 0.09822482

N 0.00000000 1.93959390 0.09822482

N -1.93959390 0.00000000 0.09822482

N 2.37862369 -2.37862369 0.19080809

N 2.37862369 2.37862369 0.19080809

N -2.37862369 2.37862369 0.19080809

N -2.37862369 -2.37862369 0.19080809

C 1.10182588 -2.74792855 0.17250067

C -1.10182588 -2.74792855 0.17250067

C 0.67819250 -4.12919388 0.27041222

H 1.36285949 -4.96718416 0.34460128

C -0.67819250 -4.12919388 0.27041222

H -1.36285949 -4.96718416 0.34460128

C 2.74792855 1.10182588 0.17250067

C 2.74792855 -1.10182588 0.17250067

C 4.12919388 0.67819250 0.27041222

H 4.96718416 1.36285949 0.34460128

C 4.12919388 -0.67819250 0.27041222

H 4.96718416 -1.36285949 0.34460128

C -1.10182588 2.74792855 0.17250067

C 1.10182588 2.74792855 0.17250067

C -0.67819250 4.12919388 0.27041222

H -1.36285949 4.96718416 0.34460128

C 0.67819250 4.12919388 0.27041222

H 1.36285949 4.96718416 0.34460128

C -2.74792855 -1.10182588 0.17250067

C -2.74792855 1.10182588 0.17250067

C -4.12919388 -0.67819250 0.27041222

H -4.96718416 -1.36285949 0.34460128

C -4.12919388 0.67819250 0.27041222

H -4.96718416 1.36285949 0.34460128

Cl 0.00000000 0.00000000 -2.74467517

Fe-(PyPepS)2 **(1)** S12g-Cosmo Doublet

Fe 0.00000000 0.00000000 -0.09967318

N 1.60179519 -1.17432792 -0.10451304

N 0.50103243 1.24906680 1.35853294

N -1.60179519 1.17432792 -0.10451304

N -0.50103243 -1.24906680 1.35853294

C 1.69344128 -2.12000101 0.86499789

C 3.59158684 -1.92928817 -1.42285549

C 2.54858907 -1.02947042 -1.13096714

C 0.45520250 -2.14250374 1.69334391

C 0.27046037 -3.05401155 2.72782352

C -0.93122125 -3.05321937 3.42509392

C -1.91587617 -2.13443484 3.06467553

C -1.66096832 -1.24609441 2.03021709

C 2.40152701 0.11644440 -1.95442727

C 3.28462805 0.33700283 -3.01710514

C -2.54858907 1.02947042 -1.13096714

C -3.59158684 1.92928817 -1.42285549

C -1.69344128 2.12000101 0.86499789

C -3.28462805 -0.33700283 -3.01710514

C -2.40152701 -0.11644440 -1.95442727

C -0.45520250 2.14250374 1.69334391

C -0.27046037 3.05401155 2.72782352

C 0.93122125 3.05321937 3.42509392

C 1.91587617 2.13443484 3.06467553

C 1.66096832 1.24609441 2.03021709

H 1.07341329 -3.74991244 2.95761821

H -1.10230955 -3.76045471 4.23501928

H -2.87637627 -2.10115277 3.57424464

H -2.39775344 -0.51324743 1.71195719

H -1.07341329 3.74991244 2.95761821

H 1.10230955 3.76045471 4.23501928

H 2.87637627 2.10115277 3.57424464

H 2.39775344 0.51324743 1.71195719

C -4.45484374 1.69919767 -2.49084789

C -4.30937927 0.56292182 -3.28804760

C 4.45484374 -1.69919767 -2.49084789

C 4.30937927 -0.56292182 -3.28804760

H -4.98562175 0.38128544 -4.12265590

H -5.24749728 2.41735576 -2.69922572

H -3.71452583 2.81166424 -0.80714718

H 4.98562175 -0.38128544 -4.12265590

H 5.24749728 -2.41735576 -2.69922572

H 3.71452583 -2.81166424 -0.80714718

O -2.63694209 2.91879565 1.10664245

O 2.63694209 -2.91879565 1.10664245

H 3.15357995 1.22272065 -3.63801209

H -3.15357995 -1.22272065 -3.63801209

S -1.10495014 -1.25690868 -1.60239633

S 1.10495014 1.25690868 -1.60239633

Fe-(PyPepS)2 **(1)** S12g-Cosmo Quartet

Fe 0.00000000 0.00000000 -0.20797830

N 1.80740013 -1.31794716 -0.09547416

N 0.44191698 1.36199958 1.26394832

N -1.80740013 1.31794716 -0.09547416

N -0.44191698 -1.36199958 1.26394832

C 1.80082669 -2.26262856 0.86457455

C 4.00334177 -1.93393435 -1.12939337

C 2.85150335 -1.13001727 -0.99656935

C 0.49351070 -2.27409001 1.60869725

C 0.24568271 -3.22081351 2.59738662

C -0.99066161 -3.24388405 3.23086364

C -1.95102942 -2.30696356 2.85841176

C -1.63380089 -1.37932484 1.87757485

C 2.70935206 -0.02990910 -1.88849654

C 3.67320608 0.21375956 -2.87358169

C -2.85150335 1.13001727 -0.99656935

C -4.00334177 1.93393435 -1.12939337

C -1.80082669 2.26262856 0.86457455

C -3.67320608 -0.21375956 -2.87358169

C -2.70935206 0.02990910 -1.88849654

C -0.49351070 2.27409001 1.60869725

C -0.24568271 3.22081351 2.59738662

C 0.99066161 3.24388405 3.23086364

C 1.95102942 2.30696356 2.85841176

C 1.63380089 1.37932484 1.87757485

H 1.03373505 -3.92835789 2.84162732

H -1.20443864 -3.98347593 4.00083136

H -2.93658818 -2.28535196 3.31796887

H -2.34630895 -0.62433761 1.55508524

H -1.03373505 3.92835789 2.84162732

H 1.20443864 3.98347593 4.00083136

H 2.93658818 2.28535196 3.31796887

H 2.34630895 0.62433761 1.55508524

C -4.95815481 1.67140793 -2.10841679

C -4.79748707 0.59803908 -2.98579954

C 4.95815481 -1.67140793 -2.10841679

C 4.79748707 -0.59803908 -2.98579954

H -5.53974812 0.39301518 -3.75631707

H -5.83288797 2.31678615 -2.18769812

H -4.13344159 2.77121552 -0.45430555

H 5.53974812 -0.39301518 -3.75631707

H 5.83288797 -2.31678615 -2.18769812

H 4.13344159 -2.77121552 -0.45430555

O -2.69264646 3.09110529 1.19232842

O 2.69264646 -3.09110529 1.19232842

H 3.53587771 1.05407874 -3.55327017

H -3.53587771 -1.05407874 -3.55327017

S -1.34074517 -1.07875798 -1.73814617

S 1.34074517 1.07875798 -1.73814617

Fe-(PyPepS)2 **(1)** S12g-Cosmo Sextet

Fe 0.00000000 0.00000000 -0.46419111

N 1.78290028 -1.33484961 -0.08813976

N 0.62424394 1.47414864 1.03960098

N -1.78290028 1.33484961 -0.08813976

N -0.62424394 -1.47414864 1.03960098

C 1.64604711 -2.34852197 0.79778497

C 4.23196857 -1.69741911 -0.46057894

C 3.00018364 -1.05533766 -0.71680551

C 0.26210149 -2.42328836 1.38618456

C -0.07669419 -3.45299320 2.26083836

C -1.36071844 -3.49827014 2.78849157

C -2.27192091 -2.50970618 2.42923737

C -1.86060943 -1.51761103 1.55050892

C 2.99905385 -0.01499530 -1.69071073

C 4.18105537 0.32582660 -2.36234725

C -3.00018364 1.05533766 -0.71680551

C -4.23196857 1.69741911 -0.46057894

C -1.64604711 2.34852197 0.79778497

C -4.18105537 -0.32582660 -2.36234725

C -2.99905385 0.01499530 -1.69071073

C -0.26210149 2.42328836 1.38618456

C 0.07669419 3.45299320 2.26083836

C 1.36071844 3.49827014 2.78849157

C 2.27192091 2.50970618 2.42923737

C 1.86060943 1.51761103 1.55050892

H 0.67306901 -4.19927653 2.50766409

H -1.64912110 -4.29658058 3.47082013

H -3.28817777 -2.50150499 2.81696343

H -2.53820767 -0.72825479 1.23636337

H -0.67306901 4.19927653 2.50766409

H 1.64912110 4.29658058 3.47082013

H 3.28817777 2.50150499 2.81696343

H 2.53820767 0.72825479 1.23636337

C -5.39403228 1.34201149 -1.13613456

C -5.37532163 0.33047013 -2.09617798

C 5.39403228 -1.34201149 -1.13613456

C 5.37532163 -0.33047013 -2.09617798

H -6.28219809 0.05250655 -2.63185140

H -6.32198586 1.86715430 -0.90991710

H -4.26069020 2.48830414 0.27698778

H 6.28219809 -0.05250655 -2.63185140

H 6.32198586 -1.86715430 -0.90991710

H 4.26069020 -2.48830414 0.27698778

O -2.48859307 3.20497100 1.17461738

O 2.48859307 -3.20497100 1.17461738

H 4.14833581 1.11989993 -3.10718222

H -4.14833581 -1.11989993 -3.10718222

S -1.51124608 -0.82310663 -2.10607729

S 1.51124608 0.82310663 -2.10607729

Fe(tsalen)Cl **(2)** S12g-Cosmo Doublet

Fe -0.35514673 -0.17294412 0.00000000

Cl -2.59571124 0.23074668 0.00000000

S -0.17725639 -1.82082536 1.45125643

C 0.22652226 2.56565715 0.75910212

N -0.00860389 1.21606784 1.31954951

S -0.17725639 -1.82082536 -1.45125643

H -0.37556080 -3.32725169 -3.78466616

H -0.37556080 -3.32725169 3.78466616

C -0.05173025 1.19295285 2.61977928

C -0.35496786 -2.28306697 4.09294683

H -0.27501024 1.42465046 5.18941902

H -0.52184973 -2.74945523 6.17570646

H 0.08124352 2.15008367 3.13439675

C -0.22679796 0.07801237 3.50588394

H -0.48531851 -0.35613682 6.89278714

N -0.00860389 1.21606784 -1.31954951

C -0.43748829 -1.95589944 5.43439898

C -0.26438648 -1.28333897 3.10533275

C -0.30619571 0.37960001 4.88440337

C -0.41776480 -0.61384931 5.83761458

C 0.22652226 2.56565715 -0.75910212

C -0.05173025 1.19295285 -2.61977928

H 0.08124352 2.15008367 -3.13439675

C -0.22679796 0.07801237 -3.50588394

C -0.43748829 -1.95589944 -5.43439898

C -0.26438648 -1.28333897 -3.10533275

C -0.30619571 0.37960001 -4.88440337

C -0.41776480 -0.61384931 -5.83761458

C -0.35496786 -2.28306697 -4.09294683

H -0.52184973 -2.74945523 -6.17570646

H -0.27501024 1.42465046 -5.18941902

H -0.48531851 -0.35613682 -6.89278714

H -0.55412743 3.23369792 -1.13614461

H 1.18732452 2.92849811 -1.13609487

H 1.18732452 2.92849811 1.13609487

H -0.55412743 3.23369792 1.13614461

Fe(tsalen)Cl **(2)** S12g-Cosmo Quartet

Fe -0.77025188 -0.13551277 0.00000000

Cl -3.09154133 0.54075988 0.00000000

S -0.67064326 -1.81541399 1.46642159

C -0.21245726 2.58783709 0.76284869

N -0.17824701 1.22228461 1.32629070

S -0.67064326 -1.81541399 -1.46642159

H -0.45131887 -3.33507029 -3.77206062

H -0.45131887 -3.33507029 3.77206062

C 0.17088774 1.14618363 2.57133152

C -0.16646329 -2.32182127 4.05089100

H 0.86062901 1.26684875 5.05229861

H 0.22503898 -2.85204576 6.08739842

H 0.48246995 2.07787109 3.05502969

C 0.17985412 0.00452288 3.44358126

H 0.89716764 -0.53779120 6.74834450

N -0.17824701 1.22228461 -1.32629070

C 0.21695050 -2.04709202 5.35355446

C -0.19451974 -1.31209393 3.07268463

C 0.57436951 0.25286153 4.77694652

C 0.59386546 -0.75197675 5.72561051

C -0.21245726 2.58783709 -0.76284869

C 0.17088774 1.14618363 -2.57133152

H 0.48246995 2.07787109 -3.05502969

C 0.17985412 0.00452288 -3.44358126

C 0.21695050 -2.04709202 -5.35355446

C -0.19451974 -1.31209393 -3.07268463

C 0.57436951 0.25286153 -4.77694652

C 0.59386546 -0.75197675 -5.72561051

C -0.16646329 -2.32182127 -4.05089100

H 0.22503898 -2.85204576 -6.08739842

H 0.86062901 1.26684875 -5.05229861

H 0.89716764 -0.53779120 -6.74834450

H -1.12916053 3.06141368 -1.12930976

H 0.63788137 3.15892676 -1.14635985

H 0.63788137 3.15892676 1.14635985

H -1.12916053 3.06141368 1.12930976

Fe(tsalen)Cl **(2)** S12g-Cosmo Sextet

Fe -0.16851914 -0.35347876 0.00000000

Cl -2.45050977 -0.22299212 0.00000000

S 0.45348691 -1.85594526 1.71758817

C 0.91983653 2.44136188 0.76813464

N 0.35611036 1.22056373 1.35167692

S 0.45348691 -1.85594526 -1.71758817

H -0.62010630 -3.17563871 -3.92482933

H -0.62010630 -3.17563871 3.92482933

C -0.01033271 1.28377818 2.58840860

C -0.74077036 -2.11271953 4.12618392

H -1.12737667 1.65521616 4.87224129

H -1.65303595 -2.44368285 6.03613172

H 0.02300969 2.25973872 3.08907060

C -0.45812621 0.20013272 3.43391901

H -1.92199452 -0.00630938 6.52496873

N 0.35611036 1.22056373 -1.35167692

C -1.31985802 -1.69787843 5.31558387

C -0.30404038 -1.18860248 3.16093605

C -1.03045363 0.59056922 4.66361898

C -1.47158107 -0.33532322 5.59055601

C 0.91983653 2.44136188 -0.76813464

C -0.01033271 1.28377818 -2.58840860

H 0.02300969 2.25973872 -3.08907060

C -0.45812621 0.20013272 -3.43391901

C -1.31985802 -1.69787843 -5.31558387

C -0.30404038 -1.18860248 -3.16093605

C -1.03045363 0.59056922 -4.66361898

C -1.47158107 -0.33532322 -5.59055601

C -0.74077036 -2.11271953 -4.12618392

H -1.65303595 -2.44368285 -6.03613172

H -1.12737667 1.65521616 -4.87224129

H -1.92199452 -0.00630938 -6.52496873

H 0.37815800 3.31574209 -1.14562429

H 1.95255080 2.51993518 -1.12452917

H 1.95255080 2.51993518 1.12452917

H 0.37815800 3.31574209 1.14562429

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** S12g-Cosmo Doublet

Fe 0.08403493 -0.66830271 -1.00116261

H 3.07681697 -0.42909448 2.90898629

H 4.15817957 1.58572037 3.85880971

S -1.85267071 -0.91517342 0.03289577

N 0.09160217 1.42621153 -0.85388782

N 0.06079241 -2.73672005 -1.20738351

C 1.51505828 1.93438203 -0.83494592

C -0.58931983 1.93086300 0.40160849

C -0.62296069 2.05645105 -2.02543386

H 2.05400255 1.37192853 -1.60597093

C 2.21930217 1.81351477 0.48251281

H 1.50825411 2.99077487 -1.13011199

C 0.11570196 2.06257998 -3.32862967

H -0.86321457 3.09328708 -1.75883118

H -1.56740661 1.51080104 -2.13274254

H -0.18057327 1.34534743 1.23026513

C -2.08101705 1.83733198 0.41201476

H -0.29709387 2.97857945 0.54577436

C 1.34758426 2.14927245 -5.85350789

C 0.32575940 3.27659197 -3.98609007

C 0.54591407 0.87497394 -3.94956996

C 1.15653593 0.93252197 -5.21133490

C 0.93232617 3.33025689 -5.23815678

H -0.00111233 4.19902200 -3.50647186

S 0.35251513 -0.70930918 -3.19493251

H 1.48178467 0.00691952 -5.68488609

H 1.08064080 4.28982352 -5.73072713

H 1.82166251 2.17407340 -6.83392940

C 3.61821081 1.65515160 2.91527768

C 2.32484287 0.58588812 1.16237910

C 2.81238022 2.94466977 1.04695549

C 3.51702630 2.87462258 2.24567055

C 3.01435871 0.52315362 2.38334289

S 1.65386094 -0.91797224 0.52810514

H 2.72125167 3.89993102 0.53039012

H 3.97688503 3.77027148 2.66009624

H -4.62957754 -0.42875528 0.30634494

C -4.87386322 1.68946504 0.60254185

C -2.72993864 0.59578373 0.29981490

C -2.84817800 2.98845496 0.60095591

C -4.23512458 2.92598452 0.70240660

C -4.12895734 0.53477912 0.39613891

H -5.95868187 1.62235002 0.67931595

H -2.34264122 3.95096116 0.67896669

H -4.81385293 3.83542166 0.85578015

C 0.99435739 -3.63410729 -0.89206372

C -0.97428464 -3.45569201 -1.76803622

H 1.95104476 -3.41876073 -0.43760365

C 1.34633434 -6.11517175 -0.99273281

C -0.65146376 -4.78424070 -1.77637288

H -1.87625879 -2.97515250 -2.12132024

N 0.59980759 -4.88042078 -1.21939742

H -1.19695025 -5.65220146 -2.12417568

H 2.32923187 -5.86665901 -0.59083592

H 1.46394716 -6.65194058 -1.93760260

H 0.80934961 -6.74637491 -0.27910554

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** S12g-Cosmo Quartet

Fe 0.08832921 -0.70721100 -0.95396793

H 3.30966554 -0.39316388 2.85553357

H 4.27092607 1.68021449 3.80357101

S -2.08464562 -0.93363589 0.01709348

N 0.07856007 1.37467178 -0.82559906

N 0.10865438 -2.76515168 -1.16579124

C 1.50617127 1.89849482 -0.81868377

C -0.61298411 1.82346913 0.45750231

C -0.65075308 2.01293257 -1.99578617

H 2.04105570 1.33854750 -1.59468834

C 2.22963542 1.81169705 0.48764001

H 1.46975541 2.94827611 -1.13001303

C 0.09914242 2.03592744 -3.28970551

H -0.89237117 3.04226964 -1.70627965

H -1.58828265 1.45843737 -2.10696208

H -0.24904140 1.16248282 1.25033524

C -2.10898248 1.82360565 0.42503199

H -0.26347841 2.83981806 0.66976377

C 1.38768372 2.14255824 -5.77847532

C 0.40862115 3.26054308 -3.88574536

C 0.45838656 0.84567869 -3.94901326

C 1.10583281 0.91488978 -5.19228769

C 1.04417413 3.32509530 -5.12236697

H 0.13688810 4.18142050 -3.37006319

S 0.11268882 -0.74600921 -3.27086786

H 1.38421655 -0.00888753 -5.69779061

H 1.27019738 4.29092527 -5.57101244

H 1.88481823 2.17392470 -6.74738246

C 3.69988138 1.72429443 2.87691868

C 2.43240820 0.58622679 1.14794632

C 2.76003348 2.97607168 1.04853667

C 3.49809233 2.94252184 2.22790078

C 3.16320886 0.55829999 2.34581946

S 1.81295543 -0.94214611 0.52403206

H 2.59516725 3.92678147 0.54210029

H 3.90852750 3.86244674 2.64075428

H -4.82365753 -0.22213326 0.16310407

C -4.91204177 1.90135132 0.49870934

C -2.85014601 0.63693097 0.25938999

C -2.79126817 3.02801148 0.61408691

C -4.18100563 3.07871989 0.65901777

C -4.25274460 0.69580723 0.29593073

H -6.00102187 1.92015722 0.52713568

H -2.21467452 3.94488991 0.73544736

H -4.68903007 4.02921590 0.81322742

C 1.08488321 -3.63681033 -0.90049934

C -0.91683504 -3.50118061 -1.72556975

H 2.04652739 -3.39962885 -0.46844358

C 1.52476021 -6.09322995 -1.10264557

C -0.54588655 -4.81338091 -1.77866104

H -1.84323019 -3.04353014 -2.04282632

N 0.72516757 -4.87964501 -1.25756751

H -1.06934075 -5.69117589 -2.13497884

H 2.50070488 -5.82512706 -0.69705767

H 1.65164580 -6.57320641 -2.07626345

H 1.01923719 -6.78051160 -0.41929359

Fe(N(CH2-o-C6H4S)3)(1MIm)  **(3)** S12g-Cosmo Sextet

Fe 0.08578122 -0.58299563 -0.94121847

H 3.56734576 -0.90254566 1.95414416

H 3.89717665 0.59749826 3.89810430

S -1.46400908 -0.63248799 0.80845160

N 0.05750305 1.93169487 -0.79278107

N 0.07240044 -2.83823423 -1.00650783

C 1.43983520 2.44252501 -0.54552724

C -0.81920289 2.39559440 0.32498257

C -0.45643496 2.51484714 -2.06918623

H 2.04042492 2.15103990 -1.41304772

C 2.08824931 1.90904555 0.69969933

H 1.41373300 3.54323062 -0.50353808

C 0.32510745 2.15179450 -3.29902485

H -0.48870048 3.61194217 -1.97259127

H -1.48599851 2.15818961 -2.17842641

H -0.39026187 1.98719868 1.24598540

C -2.25670336 1.97645374 0.22561737

H -0.76528820 3.49428279 0.38598453

C 1.71641181 1.56238948 -5.67063958

C 1.08125253 3.12601881 -3.95527343

C 0.27491393 0.85548487 -3.85142557

C 0.97514296 0.57455261 -5.03280584

C 1.77305441 2.84638780 -5.13083222

H 1.12168273 4.12978709 -3.53241847

S -0.70655905 -0.43591770 -3.12610401

H 0.92668250 -0.42963001 -5.45141891

H 2.35185737 3.62648555 -5.62279720

H 2.24870432 1.32569802 -6.59125930

C 3.38965704 0.96870499 3.00847056

C 2.55886834 0.58151023 0.76354826

C 2.28145034 2.73775459 1.80750597

C 2.92340902 2.28163873 2.95638999

C 3.20597750 0.12416985 1.91931424

S 2.39615639 -0.51903451 -0.62150915

H 1.92079064 3.76551735 1.76373084

H 3.06143802 2.94893388 3.80569248

H -4.29694413 -0.73924051 0.56765902

C -4.97511017 1.26557131 0.16388672

C -2.64694036 0.63855554 0.43583991

C -3.24707711 2.93082226 -0.01982245

C -4.59674527 2.58992575 -0.05094442

C -4.00612101 0.29694093 0.40082848

H -6.02698172 0.98238899 0.14678054

H -2.94876243 3.96633694 -0.18389544

H -5.34875747 3.35449585 -0.24003586

C 1.08323059 -3.67174767 -1.24246743

C -1.05601183 -3.62531766 -0.94518253

H 2.12222355 -3.38979145 -1.34962900

C 1.47430051 -6.13184348 -1.56204710

C -0.70937904 -4.93344911 -1.14295618

H -2.03387900 -3.20161390 -0.75473746

N 0.65340690 -4.94592181 -1.33001981

H -1.29963128 -5.84103942 -1.16045290

H 2.50849331 -5.82192554 -1.71672508

H 1.11504473 -6.65921783 -2.44965938

H 1.41777221 -6.79665256 -0.69575325

FePCl **(8)** S12g-Cosmo Doublet

Fe 0.00000000 0.00000000 -0.13818829

N 0.00000000 -1.98192649 0.08216535

N 1.98192649 0.00000000 0.08216535

N 0.00000000 1.98192649 0.08216535

N -1.98192649 0.00000000 0.08216535

C 2.41316150 -2.41316150 0.06990431

C 2.41316150 2.41316150 0.06990431

C -2.41316150 2.41316150 0.06990431

C -2.41316150 -2.41316150 0.06990431

H 3.18204175 -3.18204175 0.06623130

H 3.18204175 3.18204175 0.06623130

H -3.18204175 3.18204175 0.06623130

H -3.18204175 -3.18204175 0.06623130

C 1.09323469 -2.82483282 0.07575278

C -1.09323469 -2.82483282 0.07575278

C 0.67981390 -4.19525055 0.08627071

H 1.35828105 -5.04178492 0.09730194

C -0.67981390 -4.19525055 0.08627071

H -1.35828105 -5.04178492 0.09730194

C 2.82483282 1.09323469 0.07575278

C 2.82483282 -1.09323469 0.07575278

C 4.19525055 0.67981390 0.08627071

H 5.04178492 1.35828105 0.09730194

C 4.19525055 -0.67981390 0.08627071

H 5.04178492 -1.35828105 0.09730194

C -1.09323469 2.82483282 0.07575278

C 1.09323469 2.82483282 0.07575278

C -0.67981390 4.19525055 0.08627071

H -1.35828105 5.04178492 0.09730194

C 0.67981390 4.19525055 0.08627071

H 1.35828105 5.04178492 0.09730194

C -2.82483282 -1.09323469 0.07575278

C -2.82483282 1.09323469 0.07575278

C -4.19525055 -0.67981390 0.08627071

H -5.04178492 -1.35828105 0.09730194

C -4.19525055 0.67981390 0.08627071

H -5.04178492 1.35828105 0.09730194

Cl 0.00000000 0.00000000 -2.36090948

FePCl **(8)** S12g-Cosmo Quartet

Fe 0.00000000 0.00000000 -0.19605276

N 0.00000000 -1.99142946 0.08397990

N 1.99142946 0.00000000 0.08397990

N 0.00000000 1.99142946 0.08397990

N -1.99142946 0.00000000 0.08397990

C 2.41716314 -2.41716314 0.10709807

C 2.41716314 2.41716314 0.10709807

C -2.41716314 2.41716314 0.10709807

C -2.41716314 -2.41716314 0.10709807

H 3.18561264 -3.18561264 0.12591138

H 3.18561264 3.18561264 0.12591138

H -3.18561264 3.18561264 0.12591138

H -3.18561264 -3.18561264 0.12591138

C 1.09580437 -2.82704002 0.10599844

C -1.09580437 -2.82704002 0.10599844

C 0.68060767 -4.19503941 0.14232010

H 1.35807943 -5.04181932 0.17076074

C -0.68060767 -4.19503941 0.14232010

H -1.35807943 -5.04181932 0.17076074

C 2.82704002 1.09580437 0.10599844

C 2.82704002 -1.09580437 0.10599844

C 4.19503941 0.68060767 0.14232010

H 5.04181932 1.35807943 0.17076074

C 4.19503941 -0.68060767 0.14232010

H 5.04181932 -1.35807943 0.17076074

C -1.09580437 2.82704002 0.10599844

C 1.09580437 2.82704002 0.10599844

C -0.68060767 4.19503941 0.14232010

H -1.35807943 5.04181932 0.17076074

C 0.68060767 4.19503941 0.14232010

H 1.35807943 5.04181932 0.17076074

C -2.82704002 -1.09580437 0.10599844

C -2.82704002 1.09580437 0.10599844

C -4.19503941 -0.68060767 0.14232010

H -5.04181932 -1.35807943 0.17076074

C -4.19503941 0.68060767 0.14232010

H -5.04181932 1.35807943 0.17076074

Cl 0.00000000 0.00000000 -2.58303533

FePCl **(8)** S12g-Cosmo Sextet

Fe 0.00000000 0.00000000 -0.35186159

N 0.00000000 -2.03266189 0.13347438

N 2.03266189 0.00000000 0.13347438

N 0.00000000 2.03266189 0.13347438

N -2.03266189 0.00000000 0.13347438

C 2.42377309 -2.42377309 0.14569943

C 2.42377309 2.42377309 0.14569943

C -2.42377309 2.42377309 0.14569943

C -2.42377309 -2.42377309 0.14569943

H 3.19287454 -3.19287454 0.15455627

H 3.19287454 3.19287454 0.15455627

H -3.19287454 3.19287454 0.15455627

H -3.19287454 -3.19287454 0.15455627

C 1.10069873 -2.85681365 0.14546289

C -1.10069873 -2.85681365 0.14546289

C 0.68154907 -4.22880409 0.16461752

H 1.35300938 -5.08104881 0.17914819

C -0.68154907 -4.22880409 0.16461752

H -1.35300938 -5.08104881 0.17914819

C 2.85681365 1.10069873 0.14546289

C 2.85681365 -1.10069873 0.14546289

C 4.22880409 0.68154907 0.16461752

H 5.08104881 1.35300938 0.17914819

C 4.22880409 -0.68154907 0.16461752

H 5.08104881 -1.35300938 0.17914819

C -1.10069873 2.85681365 0.14546289

C 1.10069873 2.85681365 0.14546289

C -0.68154907 4.22880409 0.16461752

H -1.35300938 5.08104881 0.17914819

C 0.68154907 4.22880409 0.16461752

H 1.35300938 5.08104881 0.17914819

C -2.85681365 -1.10069873 0.14546289

C -2.85681365 1.10069873 0.14546289

C -4.22880409 -0.68154907 0.16461752

H -5.08104881 -1.35300938 0.17914819

C -4.22880409 0.68154907 0.16461752

H -5.08104881 1.35300938 0.17914819

Cl 0.00000000 0.00000000 -2.64086382

FePzCl **(9)** S12g-Cosmo Doublet

Fe 0.00000000 0.00000000 -0.14167715

N 0.00000000 -1.90339976 0.06549362

N 1.90339976 0.00000000 0.06549362

N 0.00000000 1.90339976 0.06549362

N -1.90339976 0.00000000 0.06549362

N 2.37537507 -2.37537507 0.06729600

N 2.37537507 2.37537507 0.06729600

N -2.37537507 2.37537507 0.06729600

N -2.37537507 -2.37537507 0.06729600

C 1.09929165 -2.73196962 0.07199404

C -1.09929165 -2.73196962 0.07199404

C 0.67791839 -4.10988315 0.09724690

H 1.36094016 -4.95180415 0.12130595

C -0.67791839 -4.10988315 0.09724690

H -1.36094016 -4.95180415 0.12130595

C 2.73196962 1.09929165 0.07199404

C 2.73196962 -1.09929165 0.07199404

C 4.10988315 0.67791839 0.09724690

H 4.95180415 1.36094016 0.12130595

C 4.10988315 -0.67791839 0.09724690

H 4.95180415 -1.36094016 0.12130595

C -1.09929165 2.73196962 0.07199404

C 1.09929165 2.73196962 0.07199404

C -0.67791839 4.10988315 0.09724690

H -1.36094016 4.95180415 0.12130595

C 0.67791839 4.10988315 0.09724690

H 1.36094016 4.95180415 0.12130595

C -2.73196962 -1.09929165 0.07199404

C -2.73196962 1.09929165 0.07199404

C -4.10988315 -0.67791839 0.09724690

H -4.95180415 -1.36094016 0.12130595

C -4.10988315 0.67791839 0.09724690

H -4.95180415 1.36094016 0.12130595

Cl 0.00000000 0.00000000 -2.33873854

FePzCl **(9)** S12g-Cosmo Quartet

Fe 0.00000000 0.00000000 -0.23491977

N 0.00000000 -1.91145543 0.07157440

N 1.91145543 0.00000000 0.07157440

N 0.00000000 1.91145543 0.07157440

N -1.91145543 0.00000000 0.07157440

N 2.37712876 -2.37712876 0.11822402

N 2.37712876 2.37712876 0.11822402

N -2.37712876 2.37712876 0.11822402

N -2.37712876 -2.37712876 0.11822402

C 1.09933663 -2.73292373 0.11232845

C -1.09933663 -2.73292373 0.11232845

C 0.67819938 -4.11069014 0.16634316

H 1.36127513 -4.95175652 0.20823813

C -0.67819938 -4.11069014 0.16634316

H -1.36127513 -4.95175652 0.20823813

C 2.73292373 1.09933663 0.11232845

C 2.73292373 -1.09933663 0.11232845

C 4.11069014 0.67819938 0.16634316

H 4.95175652 1.36127513 0.20823813

C 4.11069014 -0.67819938 0.16634316

H 4.95175652 -1.36127513 0.20823813

C -1.09933663 2.73292373 0.11232845

C 1.09933663 2.73292373 0.11232845

C -0.67819938 4.11069014 0.16634316

H -1.36127513 4.95175652 0.20823813

C 0.67819938 4.11069014 0.16634316

H 1.36127513 4.95175652 0.20823813

C -2.73292373 -1.09933663 0.11232845

C -2.73292373 1.09933663 0.11232845

C -4.11069014 -0.67819938 0.16634316

H -4.95175652 -1.36127513 0.20823813

C -4.11069014 0.67819938 0.16634316

H -4.95175652 1.36127513 0.20823813

Cl 0.00000000 0.00000000 -2.60137132

FePzCl **(9)** S12g-Cosmo Sextet

Fe 0.00000000 0.00000000 -0.47753114

N 0.00000000 -1.93986431 0.11677831

N 1.93986431 0.00000000 0.11677831

N 0.00000000 1.93986431 0.11677831

N -1.93986431 0.00000000 0.11677831

N 2.37949524 -2.37949524 0.17893599

N 2.37949524 2.37949524 0.17893599

N -2.37949524 2.37949524 0.17893599

N -2.37949524 -2.37949524 0.17893599

C 1.10242173 -2.75328276 0.16771426

C -1.10242173 -2.75328276 0.16771426

C 0.67865606 -4.13514607 0.23248291

H 1.35700891 -4.97992092 0.28170327

C -0.67865606 -4.13514607 0.23248291

H -1.35700891 -4.97992092 0.28170327

C 2.75328276 1.10242173 0.16771426

C 2.75328276 -1.10242173 0.16771426

C 4.13514607 0.67865606 0.23248291

H 4.97992092 1.35700891 0.28170327

C 4.13514607 -0.67865606 0.23248291

H 4.97992092 -1.35700891 0.28170327

C -1.10242173 2.75328276 0.16771426

C 1.10242173 2.75328276 0.16771426

C -0.67865606 4.13514607 0.23248291

H -1.35700891 4.97992092 0.28170327

C 0.67865606 4.13514607 0.23248291

H 1.35700891 4.97992092 0.28170327

C -2.75328276 -1.10242173 0.16771426

C -2.75328276 1.10242173 0.16771426

C -4.13514607 -0.67865606 0.23248291

H -4.97992092 -1.35700891 0.28170327

C -4.13514607 0.67865606 0.23248291

H -4.97992092 1.35700891 0.28170327

Cl 0.00000000 0.00000000 -2.73351270

**Iron(II) Complexes**

Meso-(Fe(NH)S4)CO **(4m)** OPBE Singlet

Fe -0.09006756 -0.16819211 0.00000000

S 0.98157935 -1.43951928 1.52194658

S -0.94842427 1.03481246 1.62509698

S -0.94842427 1.03481246 -1.62509698

S 0.98157935 -1.43951928 -1.52194658

C -0.55270923 0.16873081 3.12972729

C -1.12585582 0.56814586 4.33736110

C -0.80578560 -0.10794845 5.50792922

C 0.08120913 -1.18772722 5.44876350

C 0.62986010 -1.59851111 4.24405075

C 0.32295211 -0.92583581 3.04477476

C -0.55270923 0.16873081 -3.12972729

C -1.12585582 0.56814586 -4.33736110

C -0.80578560 -0.10794845 -5.50792922

C 0.08120913 -1.18772722 -5.44876350

C 0.62986010 -1.59851111 -4.24405075

C 0.32295211 -0.92583581 -3.04477476

N 1.52950693 1.18390021 0.00000000

C 0.24670243 2.41699168 1.71966519

C 1.60781405 1.95004409 1.25503328

C 0.24670243 2.41699168 -1.71966519

C 1.60781405 1.95004409 -1.25503328

H -1.82605522 1.40282507 4.35485676

H -1.24990819 0.19493673 6.45445110

H 0.33176821 -1.73170979 6.35951247

H 1.30095263 -2.45503794 4.21144020

H -1.82605522 1.40282507 -4.35485676

H -1.24990819 0.19493673 -6.45445110

H 0.33176821 -1.73170979 -6.35951247

H 1.30095263 -2.45503794 -4.21144020

H 2.28990447 0.50598658 0.00000000

H 0.27795670 2.77287344 2.75417972

H -0.16891126 3.22065264 1.10207089

H 2.01767506 1.27056992 2.00866052

H 2.29699757 2.80409807 1.15642533

H -0.16891126 3.22065264 -1.10207089

H 0.27795670 2.77287344 -2.75417972

H 2.29699757 2.80409807 -1.15642533

H 2.01767506 1.27056992 -2.00866052

C -1.35922563 -1.31318456 0.00000000

O -2.21216675 -2.10296414 0.00000000

Meso-(Fe(NH)S4)CO **(4m)** OPBE Triplet

Fe -0.20887896 -0.28105503 0.00000000

S 0.89724595 -1.51226845 1.47727079

S -0.94984935 1.02447445 1.73682641

S -0.94984935 1.02447445 -1.73682641

S 0.89724595 -1.51226845 -1.47727079

C -0.42586968 0.16510542 3.20710200

C -0.85926796 0.58750316 4.46399692

C -0.45991588 -0.10408229 5.60190845

C 0.35670886 -1.22998626 5.46473777

C 0.76820926 -1.66245848 4.21346959

C 0.38176858 -0.97168743 3.04922514

C -0.42586968 0.16510542 -3.20710200

C -0.85926796 0.58750316 -4.46399692

C -0.45991588 -0.10408229 -5.60190845

C 0.35670886 -1.22998626 -5.46473777

C 0.76820926 -1.66245848 -4.21346959

C 0.38176858 -0.97168743 -3.04922514

N 1.53148658 1.46251203 0.00000000

C 0.13011410 2.49637250 1.76215389

C 1.53180039 2.19610569 1.25486447

C 0.13011410 2.49637250 -1.76215389

C 1.53180039 2.19610569 -1.25486447

H -1.51505193 1.45335515 4.54877270

H -0.79559841 0.22144004 6.58498802

H 0.66518162 -1.78666167 6.34952319

H 1.39202404 -2.54935161 4.11665926

H -1.51505193 1.45335515 -4.54877270

H -0.79559841 0.22144004 -6.58498802

H 0.66518162 -1.78666167 -6.34952319

H 1.39202404 -2.54935161 -4.11665926

H 2.27033656 0.76993967 0.00000000

H 0.15431973 2.88165587 2.78684107

H -0.38786470 3.23918443 1.14500463

H 2.03950680 1.57349638 1.99817858

H 2.09734640 3.14261540 1.18094211

H -0.38786470 3.23918443 -1.14500463

H 0.15431973 2.88165587 -2.78684107

H 2.09734640 3.14261540 -1.18094211

H 2.03950680 1.57349638 -1.99817858

C -1.87851944 -1.23698886 0.00000000

O -2.67862115 -2.07116535 0.00000000

Meso-(Fe(NH)S4)CO **(4m)** OPBE Quintet

Fe -0.16641143 -0.44251707 0.00000000

S 0.73944636 -1.65968983 1.77926536

S -1.03949938 1.11487169 1.84761866

S -1.03949938 1.11487169 -1.84761866

S 0.73944636 -1.65968983 -1.77926536

C -0.47352738 0.31809003 3.33104960

C -0.83561533 0.87788865 4.55905779

C -0.39913617 0.31325388 5.75108458

C 0.39169171 -0.83603708 5.70383805

C 0.73371325 -1.40900480 4.48876189

C 0.31413073 -0.85272627 3.26261587

C -0.47352738 0.31809003 -3.33104960

C -0.83561533 0.87788865 -4.55905779

C -0.39913617 0.31325388 -5.75108458

C 0.39169171 -0.83603708 -5.70383805

C 0.73371325 -1.40900480 -4.48876189

C 0.31413073 -0.85272627 -3.26261587

N 1.52514863 1.25064587 0.00000000

C 0.17577628 2.46052974 1.72067856

C 1.54884942 2.01018403 1.24654157

C 0.17577628 2.46052974 -1.72067856

C 1.54884942 2.01018403 -1.24654157

H -1.46990993 1.76324664 4.57336569

H -0.68594442 0.75536083 6.70372163

H 0.73754820 -1.29802575 6.62848586

H 1.33792625 -2.31386033 4.46297878

H -1.46990993 1.76324664 -4.57336569

H -0.68594442 0.75536083 -6.70372163

H 0.73754820 -1.29802575 -6.62848586

H 1.33792625 -2.31386033 -4.46297878

H 2.31196111 0.60928357 0.00000000

H 0.26000595 2.93183564 2.70562453

H -0.28003478 3.19883255 1.05294736

H 1.97649184 1.35765874 2.01471590

H 2.20233940 2.89853769 1.17104385

H -0.28003478 3.19883255 -1.05294736

H 0.26000595 2.93183564 -2.70562453

H 2.20233940 2.89853769 -1.17104385

H 1.97649184 1.35765874 -2.01471590

C -1.57471296 -1.86902123 0.00000000

O -2.16540759 -2.85827524 0.00000000

trans-(Fe(NH)S4)CO **(4t)** OPBE Singlet

Fe 8.37201747 10.16261463 1.98792154

S 9.75461897 9.01403912 3.23442448

S 6.73551830 8.66677131 2.43368034

S 7.05582718 11.14915607 0.54938547

S 10.00054616 11.66333273 1.48058555

C 9.16733859 12.87633505 0.54919285

C 9.79383736 14.07984921 0.17398819

H 10.83037335 14.24778943 0.46103880

C 9.09983939 15.05099107 -0.53312438

H 9.60725846 15.97814453 -0.79968313

C 7.75974616 14.86840110 -0.88660208

H 7.21654624 15.64435487 -1.42306081

C 7.12221617 13.68470780 -0.53489236

H 6.07773617 13.51796352 -0.79504278

C 7.82876622 12.70187801 0.15762709

C 7.46294599 7.55810264 3.55346915

C 6.73284067 6.49261695 4.11879290

H 5.69306294 6.35402173 3.82760042

C 7.31830756 5.63641716 5.03775259

H 6.72611483 4.82375331 5.45849136

C 8.64578414 5.81039106 5.44528098

H 9.09294103 5.14672553 6.18304932

C 9.38486060 6.85384657 4.90348127

H 10.41613816 7.01984577 5.21380192

C 8.80338477 7.69466265 3.95339326

C 7.84882574 11.14432998 3.29011192

O 7.49294452 11.81540716 4.17045330

N 9.05383589 9.03059284 0.37288898

H 9.76003246 9.69598137 0.03711808

C 10.65341224 8.10240695 1.92771228

H 11.08852083 7.19800864 2.36324844

H 11.46765780 8.77224639 1.62181026

C 9.71782951 7.79329282 0.78492650

H 8.94697596 7.08719257 1.11146749

H 10.27233001 7.33650861 -0.05162283

C 7.45562376 10.22110936 -0.99770973

H 8.17993248 10.83210217 -1.54536637

H 6.54206380 10.13386972 -1.59568213

C 8.01534565 8.86525829 -0.64239313

H 7.23802872 8.22405739 -0.21062472

H 8.40624042 8.37700814 -1.55024856

trans-(Fe(NH)S4)CO **(4t)** OPBE Triplet

Fe 8.32848153 10.21496984 2.04748256

S 9.94128254 8.84064467 3.35914362

S 6.74266696 8.85430591 2.84064252

S 6.95898404 11.18986938 0.24549961

S 9.94556676 11.68757328 1.45278734

C 9.09614256 12.92260154 0.55603829

C 9.71288382 14.16747726 0.33588626

H 10.69390753 14.34761449 0.77136315

C 9.08537539 15.16170130 -0.40086447

H 9.58744235 16.11849451 -0.54381112

C 7.81570136 14.95278053 -0.94059774

H 7.31684068 15.73722971 -1.50740690

C 7.18405159 13.73227554 -0.73543890

H 6.18916185 13.55211397 -1.13933449

C 7.81767731 12.71776232 -0.01286906

C 7.52554872 7.54943736 3.69374610

C 6.74989923 6.48455070 4.19265758

H 5.68019811 6.47735707 3.99088970

C 7.32585733 5.46077953 4.92936492

H 6.69810230 4.64946561 5.29757756

C 8.69159925 5.47234628 5.21898257

H 9.13957689 4.68296941 5.82015068

C 9.47440427 6.51790845 4.74424443

H 10.53791666 6.55604096 4.97656541

C 8.90633409 7.53573749 3.97522130

C 7.72998417 11.39455620 3.18350228

O 7.33360396 12.18499090 3.93873294

N 9.02722251 8.94647535 0.43408886

H 9.73979672 9.60225456 0.10013727

C 10.69304709 7.99382031 1.93648286

H 11.16902297 7.06886028 2.27637341

H 11.48403425 8.67205620 1.59031998

C 9.68589684 7.71017601 0.84291744

H 8.92329792 7.01398566 1.20812965

H 10.19935117 7.22909251 -0.00758417

C 7.58074772 10.14783312 -1.12616327

H 8.41147980 10.68782517 -1.59250548

H 6.78470110 10.03258996 -1.87041879

C 8.02164815 8.79084750 -0.61523099

H 7.17280340 8.23985704 -0.19295284

H 8.41302394 8.20683849 -1.46551723

trans-(Fe(NH)S4)CO **(4t)** OPBE Quintet

Fe 8.39595903 10.17332571 1.99573643

S 9.94659919 8.67040094 3.22259472

S 6.69871032 8.57475268 2.54185158

S 7.06673299 11.15961738 0.17134865

S 10.05303472 11.83781888 1.37295831

C 9.08130125 13.02818616 0.55470158

C 9.57806586 14.33720769 0.39879062

H 10.55975739 14.56689072 0.80797534

C 8.84406844 15.32370785 -0.24367184

H 9.26361657 16.32531444 -0.33747379

C 7.57431557 15.04838646 -0.75311553

H 6.99155278 15.82383010 -1.24747715

C 7.05661936 13.76638313 -0.61731807

H 6.06579158 13.52912069 -1.00075144

C 7.79596887 12.76481729 0.01783010

C 7.45182162 7.54235803 3.72210206

C 6.65050016 6.63015224 4.43900494

H 5.58150497 6.61698048 4.23648298

C 7.18989847 5.76383087 5.37726954

H 6.53342022 5.07200200 5.90477088

C 8.55691306 5.78204991 5.65948188

H 8.98260916 5.11372392 6.40595677

C 9.37077549 6.67924454 4.98040988

H 10.43665119 6.72634608 5.19850023

C 8.83699440 7.53873475 4.01545623

C 7.82467198 11.35593261 3.44377388

O 7.46506958 12.09321622 4.25344258

N 9.17555460 8.86121749 0.20925044

H 9.97258867 9.43224102 -0.07204801

C 10.59222930 7.69859285 1.82162388

H 10.90353263 6.71822479 2.19596810

H 11.49963810 8.24027297 1.52011509

C 9.62808899 7.55486302 0.66003008

H 8.74923512 6.98235462 0.97653893

H 10.12872930 6.98228530 -0.14310170

C 7.80589624 10.26289372 -1.24743112

H 8.67701512 10.84212743 -1.57075312

H 7.07557713 10.24942193 -2.06427917

C 8.19531830 8.84819285 -0.86510373

H 7.31855892 8.28942137 -0.51387926

H 8.56785168 8.33680390 -1.77151133

Meso-(Fe(NH)S4)PMe3 **(5m)** OPBE Singlet

Fe 0.16199121 0.04998079 0.00000000

S 1.41384995 1.13727970 -1.51894085

S -0.82467035 -1.01654526 -1.61667565

S -0.82467035 -1.01654526 1.61667565

S 1.41384995 1.13727970 1.51894085

C -0.25290122 -0.28958643 -3.14665567

C -0.82300979 -0.65071127 -4.36751362

C -0.34082243 -0.09519105 -5.54721375

C 0.70555626 0.83213863 -5.48533388

C 1.25603395 1.20719036 -4.26979469

C 0.77913518 0.65966283 -3.06133589

C -0.25290122 -0.28958643 3.14665567

C -0.82300979 -0.65071127 4.36751362

C -0.34082243 -0.09519105 5.54721375

C 0.70555626 0.83213863 5.48533388

C 1.25603395 1.20719036 4.26979469

C 0.77913518 0.65966283 3.06133589

N 1.58193093 -1.50546218 0.00000000

C 0.14368485 -2.57158235 -1.70014913

C 1.55670876 -2.28623939 -1.24821218

C 0.14368485 -2.57158235 1.70014913

C 1.55670876 -2.28623939 1.24821218

H -1.64258893 -1.36903023 -4.39111863

H -0.77921879 -0.37360919 -6.50410909

H 1.08962728 1.27711637 -6.40357600

H 2.06082100 1.94001883 -4.23502827

H -1.64258893 -1.36903023 4.39111863

H -0.77921879 -0.37360919 6.50410909

H 1.08962728 1.27711637 6.40357600

H 2.06082100 1.94001883 4.23502827

H 2.42987821 -0.94188258 0.00000000

H 0.11895957 -2.94169685 -2.72962590

H -0.37564070 -3.29886557 -1.06712243

H 2.04811122 -1.67395803 -2.01065446

H 2.12970665 -3.22169724 -1.14209468

H -0.37564070 -3.29886557 1.06712243

H 0.11895957 -2.94169685 2.72962590

H 2.12970665 -3.22169724 1.14209468

H 2.04811122 -1.67395803 2.01065446

P -1.23739474 1.73769108 0.00000000

C -2.43583039 1.84462934 -1.39577855

H -1.90153494 1.92974538 -2.34767846

H -3.06545342 0.94821207 -1.42253005

H -3.07676141 2.72512577 -1.26595391

C -2.43583039 1.84462934 1.39577855

H -3.06545342 0.94821207 1.42253005

H -1.90153494 1.92974538 2.34767846

H -3.07676141 2.72512577 1.26595391

C -0.54732697 3.45257039 0.00000000

H -0.88895481 3.98740084 -0.89233995

H -0.88895481 3.98740084 0.89233995

H 0.54409476 3.42295975 0.00000000

Meso-(Fe(NH)S4)PMe3 **(5m)** OPBE Triplet

Fe 0.23547647 0.11812400 0.00000000

S 1.37256301 1.19296343 -1.68507658

S -0.86588638 -1.13921648 -1.73665919

S -0.86588638 -1.13921648 1.73665919

S 1.37256301 1.19296343 1.68507658

C -0.29097129 -0.38700214 -3.24400312

C -0.84555963 -0.79312081 -4.46012070

C -0.42076153 -0.22455689 -5.65489815

C 0.55884187 0.77176427 -5.61854949

C 1.09415704 1.19461764 -4.41170680

C 0.68750655 0.63028185 -3.18454793

C -0.29097129 -0.38700214 3.24400312

C -0.84555963 -0.79312081 4.46012070

C -0.42076153 -0.22455689 5.65489815

C 0.55884187 0.77176427 5.61854949

C 1.09415704 1.19461764 4.41170680

C 0.68750655 0.63028185 3.18454793

N 1.64283606 -1.46558920 0.00000000

C 0.22075423 -2.59759564 -1.69990730

C 1.62170760 -2.24220232 -1.24845401

C 0.22075423 -2.59759564 1.69990730

C 1.62170760 -2.24220232 1.24845401

H -1.61541568 -1.56458344 -4.46308091

H -0.85178963 -0.54848322 -6.60092101

H 0.90154552 1.23197226 -6.54574053

H 1.84702386 1.98127401 -4.39432333

H -1.61541568 -1.56458344 4.46308091

H -0.85178963 -0.54848322 6.60092101

H 0.90154552 1.23197226 6.54574053

H 1.84702386 1.98127401 4.39432333

H 2.48893121 -0.89982940 0.00000000

H 0.24618278 -3.03628464 -2.70323477

H -0.27100807 -3.32057030 -1.04092604

H 2.08205741 -1.61165852 -2.01538637

H 2.22956927 -3.15794037 -1.15229404

H -0.27100807 -3.32057030 1.04092604

H 0.24618278 -3.03628464 2.70323477

H 2.22956927 -3.15794037 1.15229404

H 2.08205741 -1.61165852 2.01538637

P -1.12311150 1.89786404 0.00000000

C -2.30792084 1.99723506 -1.40270283

H -1.76601688 2.04247125 -2.35266913

H -2.96058531 1.11749905 -1.40495977

H -2.92536803 2.89793495 -1.29663772

C -2.30792084 1.99723506 1.40270283

H -2.96058531 1.11749905 1.40495977

H -1.76601688 2.04247125 2.35266913

H -2.92536803 2.89793495 1.29663772

C -0.37750288 3.58367829 0.00000000

H -0.70065396 4.12784607 -0.89387086

H -0.70065396 4.12784607 0.89387086

H 0.71237259 3.51526731 0.00000000

Meso-(Fe(NH)S4)PMe3 **(5m)** OPBE Quintet

Fe 0.26968196 0.23835519 0.00000000

S 1.52738705 1.18421931 -1.69078746

S -0.86828091 -1.05591499 -1.90453855

S -0.86828091 -1.05591499 1.90453855

S 1.52738705 1.18421931 1.69078746

C -0.10501946 -0.35934416 -3.35186584

C -0.57236870 -0.75781145 -4.60812522

C -0.02877878 -0.22302069 -5.76918720

C 0.98093851 0.73572677 -5.66218545

C 1.43313370 1.14779656 -4.41780292

C 0.90750829 0.61814094 -3.22096221

C -0.10501946 -0.35934416 3.35186584

C -0.57236870 -0.75781145 4.60812522

C -0.02877878 -0.22302069 5.76918720

C 0.98093851 0.73572677 5.66218545

C 1.43313370 1.14779656 4.41780292

C 0.90750829 0.61814094 3.22096221

N 1.51599651 -1.79509888 0.00000000

C -0.01871647 -2.65352227 -1.76849608

C 1.40555192 -2.54009471 -1.24915253

C -0.01871647 -2.65352227 1.76849608

C 1.40555192 -2.54009471 1.24915253

H -1.37424897 -1.49307996 -4.66829162

H -0.39536843 -0.54175103 -6.74377029

H 1.41535229 1.17284570 -6.56161320

H 2.21591862 1.90090840 -4.34385199

H -1.37424897 -1.49307996 4.66829162

H -0.39536843 -0.54175103 6.74377029

H 1.41535229 1.17284570 6.56161320

H 2.21591862 1.90090840 4.34385199

H 2.39361475 -1.28526676 0.00000000

H -0.02270752 -3.13272667 -2.75367489

H -0.65603321 -3.25881055 -1.11443670

H 1.99672334 -2.00476737 -1.99900145

H 1.83359123 -3.55464127 -1.15721274

H -0.65603321 -3.25881055 1.11443670

H -0.02270752 -3.13272667 2.75367489

H 1.83359123 -3.55464127 1.15721274

H 1.99672334 -2.00476737 1.99900145

P -1.68227882 1.98396806 0.00000000

C -2.85855782 1.99905384 -1.41390393

H -2.30271533 2.10531316 -2.35176741

H -3.40752206 1.05117515 -1.44548575

H -3.57423671 2.82561389 -1.32289550

C -2.85855782 1.99905384 1.41390393

H -3.40752206 1.05117515 1.44548575

H -2.30271533 2.10531316 2.35176741

H -3.57423671 2.82561389 1.32289550

C -1.03354878 3.71232075 0.00000000

H -1.37908618 4.24627012 -0.89123768

H -1.37908618 4.24627012 0.89123768

H 0.05995578 3.69254275 0.00000000

trans-(Fe(NH)S4)PMe3 **(5t)** OPBE Singlet

Fe 3.12704066 2.99670483 8.08948338

S 3.31689781 5.05137520 8.99125804

S 4.86667752 3.39449160 6.85235429

S 1.24014858 2.72791083 9.11252271

S 2.84680373 0.97113921 7.12200291

P 4.30337099 2.20630505 9.77292480

C 4.68639795 0.40817399 9.83617207

C 5.99123950 2.89198118 10.02879735

C 3.59940120 2.46555269 11.45291651

C 5.43052117 5.03816270 7.25286791

C 6.57783724 5.56315627 6.65704820

C 6.99505487 6.85047307 6.97128476

C 6.25705846 7.59700246 7.89804981

C 5.13478888 7.06448557 8.51134296

C 4.69108804 5.76078493 8.20603150

C 0.78115240 1.01687018 8.91847870

C -0.25688433 0.46275280 9.66689567

C -0.62990032 -0.86029880 9.45603177

C 0.04471707 -1.61028108 8.48666583

C 1.08630246 -1.06150575 7.75304625

C 1.49448069 0.27072920 7.96269040

N 1.98295944 3.73375772 6.51447673

C 4.04176481 3.75282186 5.25863223

C 2.75619218 4.49273601 5.53099764

C 0.03288995 3.47527580 7.92076051

C 0.76886279 4.39876365 6.98123911

H 1.73951939 2.82354851 6.10555290

H 5.28437565 0.18641962 10.72863902

H 5.24410473 0.11938292 8.93965426

H 3.76103257 -0.17504919 9.86314264

H 6.43443656 2.45479663 10.93164411

H 5.93910760 3.97927638 10.13960230

H 6.63189587 2.65305342 9.17286320

H 4.30604809 2.11341751 12.21390091

H 2.65902148 1.91513903 11.56272450

H 3.40532862 3.53290743 11.60162379

H 7.14317106 4.95951267 5.94686111

H 7.88533844 7.26826327 6.50418371

H 6.57446850 8.60817181 8.15379588

H 4.57939778 7.65126324 9.24161761

H -0.76947717 1.07065099 10.41219579

H -1.43379041 -1.30401128 10.04114517

H -0.23908387 -2.64853848 8.31267288

H 1.61311535 -1.66496519 7.01524510

H 3.85908012 2.77239347 4.80016629

H 4.72117865 4.32326117 4.61812879

H 2.97389253 5.47936741 5.95337264

H 2.18706681 4.63647219 4.59750146

H -0.73470758 4.00992950 8.49058915

H -0.43775817 2.64155651 7.39038362

H 0.10918567 4.67874498 6.14293345

H 1.07873735 5.31225006 7.50091604

trans-(Fe(NH)S4)PMe3 **(5t)** OPBE Triplet

Fe 3.16635535 2.96932149 8.10950481

S 3.35584737 4.99647253 8.99779073

S 4.82269813 3.45567719 6.71546249

S 1.16096408 2.77546005 9.03845589

S 2.90996156 0.94803004 7.20221877

P 4.45306729 2.07159716 10.01175731

C 4.80112146 0.26562581 10.09520380

C 6.14948837 2.74224519 10.27092663

C 3.72529459 2.35942990 11.67951497

C 5.39609713 5.08651310 7.16158431

C 6.49744940 5.66167373 6.53016631

C 6.92328151 6.93300196 6.90034749

C 6.24788676 7.60964292 7.91852897

C 5.16387616 7.02781359 8.56050405

C 4.71631763 5.74599813 8.19491719

C 0.71187516 1.06020133 8.85139702

C -0.38195008 0.52595509 9.53070715

C -0.71715053 -0.81400479 9.36116087

C 0.05401471 -1.60711554 8.50877063

C 1.14873215 -1.07634017 7.83928468

C 1.50950985 0.27268239 8.00510237

N 1.80177127 3.83341555 6.25240223

C 3.95750973 3.86678970 5.15239302

C 2.65325768 4.61022024 5.38262111

C -0.02595456 3.51577532 7.81863565

C 0.65374346 4.46968557 6.85222306

H 1.55150853 2.94624407 5.82354905

H 5.38862885 0.01669290 10.98792264

H 5.35147744 -0.03809706 9.19837695

H 3.85805828 -0.29009867 10.11345618

H 6.60395637 2.33145970 11.18158987

H 6.10491312 3.83333512 10.34986135

H 6.78005915 2.48552701 9.41209577

H 4.38846533 1.99606399 12.47491389

H 2.76187978 1.84276981 11.75349766

H 3.55130164 3.43250981 11.81473140

H 7.02277159 5.11104099 5.75013206

H 7.78109317 7.38738371 6.40706381

H 6.57716889 8.60405217 8.22009491

H 4.64792041 7.56018019 9.35820383

H -0.96683753 1.16216637 10.19433563

H -1.56657368 -1.23742967 9.89498800

H -0.19634116 -2.65942207 8.37297210

H 1.75027386 -1.70738457 7.18656835

H 3.78172975 2.89369624 4.67615096

H 4.63856932 4.43975848 4.51507364

H 2.85999453 5.57104631 5.86803010

H 2.19372016 4.83316896 4.40028027

H -0.80931098 4.03543479 8.38163632

H -0.48336479 2.67381040 7.28914248

H -0.10520255 4.80262750 6.11803090

H 1.00662266 5.35921189 7.38771551

trans-(Fe(NH)S4)PMe3 **(5t)** OPBE Quintet

Fe 3.19569558 2.92923367 8.05375704

S 3.43904462 5.10296998 9.03126331

S 5.00222733 3.61543051 6.58048313

S 0.84563741 2.75802790 9.01205682

S 2.67576518 0.81491550 7.04013284

P 4.50791281 1.96966440 10.05500961

C 4.78640715 0.15725613 10.17920063

C 6.21928949 2.61194323 10.23348469

C 3.78925042 2.35736081 11.69989729

C 5.49242062 5.22291065 7.15179612

C 6.59489474 5.83760559 6.55298867

C 7.00972314 7.09849368 6.96198712

C 6.31706610 7.73208395 7.99576609

C 5.23669625 7.11544587 8.60757913

C 4.78751102 5.83767068 8.21232342

C 0.57630895 1.01127466 8.87982971

C -0.43363430 0.45197029 9.66984848

C -0.70164088 -0.91016423 9.62299566

C 0.05906465 -1.71645573 8.77420117

C 1.07080445 -1.17099517 7.99828392

C 1.37447546 0.20653047 8.02686954

N 1.91227459 3.84883895 6.29178625

C 4.03013614 4.04449324 5.10192591

C 2.70450109 4.70391160 5.42616922

C -0.10855172 3.39750156 7.58100437

C 0.66599073 4.41746107 6.76996139

H 1.73247286 2.95188034 5.83890630

H 5.37198200 -0.09858202 11.07121938

H 5.31451176 -0.18750867 9.28337975

H 3.82067085 -0.35762433 10.21568476

H 6.69211730 2.22726523 11.14563440

H 6.19405832 3.70576371 10.26740443

H 6.81624588 2.30698737 9.36650927

H 4.43831542 2.00327615 12.51044708

H 2.80752079 1.87989688 11.79225407

H 3.65750380 3.44148783 11.78167370

H 7.12720948 5.31721162 5.75738814

H 7.86601977 7.57542050 6.48785277

H 6.62853348 8.72105961 8.33283930

H 4.70913881 7.61740066 9.41667474

H -1.01087354 1.10475858 10.32300561

H -1.49065897 -1.33602597 10.24074501

H -0.13519473 -2.78809681 8.72182903

H 1.66618548 -1.81226591 7.35080910

H 3.88605652 3.08763653 4.58314382

H 4.63751996 4.68779550 4.45689166

H 2.88353763 5.65095260 5.94823803

H 2.18626670 4.94233928 4.47813019

H -1.03305824 3.84413245 7.96395460

H -0.37478979 2.52621810 6.97387932

H 0.01287224 4.76159668 5.94623245

H 0.90816341 5.29346109 7.38491563

Meso-(Fe(NH)S4)NH3  **(6m)** OPBE Singlet

Fe -0.27645225 -0.40703467 0.00000000

S 0.52208469 -1.86582341 1.52247946

S -0.94168256 0.88836689 1.61439014

S -0.94168256 0.88836689 -1.61439014

S 0.52208469 -1.86582341 -1.52247946

C -0.68261907 -0.00697085 3.13943134

C -1.15456474 0.49757690 4.35184786

C -0.93411162 -0.20943301 5.52819353

C -0.24732263 -1.42732704 5.47003431

C 0.20635161 -1.93535519 4.26249575

C -0.00817738 -1.23754026 3.05658282

C -0.68261907 -0.00697085 -3.13943134

C -1.15456474 0.49757690 -4.35184786

C -0.93411162 -0.20943301 -5.52819353

C -0.24732263 -1.42732704 -5.47003431

C 0.20635161 -1.93535519 -4.26249575

C -0.00817738 -1.23754026 -3.05658282

N 1.47733535 0.58919653 0.00000000

C 0.46412073 2.06027965 1.71698014

C 1.70902237 1.34389272 1.25103746

C 0.46412073 2.06027965 -1.71698014

C 1.70902237 1.34389272 -1.25103746

N -2.00957018 -1.45493421 0.00000000

H -1.69372545 1.44481370 4.37017379

H -1.29900367 0.17801523 6.47799473

H -0.07248670 -1.99359379 6.38517439

H 0.73072869 -2.88929719 4.23212785

H -1.69372545 1.44481370 -4.37017379

H -1.29900367 0.17801523 -6.47799473

H -0.07248670 -1.99359379 -6.38517439

H 0.73072869 -2.88929719 -4.23212785

H 2.12825141 -0.19591306 0.00000000

H 0.56285779 2.40329499 2.75117294

H 0.19912781 2.92263377 1.09598694

H 1.98869943 0.60528828 2.00904365

H 2.54868591 2.04738201 1.13291504

H 0.19912781 2.92263377 -1.09598694

H 0.56285779 2.40329499 -2.75117294

H 2.54868591 2.04738201 -1.13291504

H 1.98869943 0.60528828 -2.00904365

H -2.00032863 -2.06337004 0.81709254

H -2.00032863 -2.06337004 -0.81709254

H -2.87819717 -0.92707568 0.00000000

Meso-(Fe(NH)S4)NH3  **(6m)** OPBE Triplet

Fe -0.47398829 -0.52806121 0.00000000

S 0.25544232 -2.01060049 1.50575904

S -1.09894504 0.80443091 1.70064074

S -1.09894504 0.80443091 -1.70064074

S 0.25544232 -2.01060049 -1.50575904

C -0.76441135 -0.10048547 3.19874417

C -1.16061906 0.40133014 4.43910442

C -0.91630057 -0.33322344 5.59347178

C -0.28741468 -1.57797269 5.48704101

C 0.08581350 -2.08461969 4.25113643

C -0.15377150 -1.35835990 3.06857609

C -0.76441135 -0.10048547 -3.19874417

C -1.16061906 0.40133014 -4.43910442

C -0.91630057 -0.33322344 -5.59347178

C -0.28741468 -1.57797269 -5.48704101

C 0.08581350 -2.08461969 -4.25113643

C -0.15377150 -1.35835990 -3.06857609

N 1.42372969 0.83133428 0.00000000

C 0.20000307 2.09203822 1.74804020

C 1.53787322 1.56625776 1.25320338

C 0.20000307 2.09203822 -1.74804020

C 1.53787322 1.56625776 -1.25320338

N -2.80398959 -1.44143543 0.00000000

H -1.66394441 1.36622717 4.49749066

H -1.22234600 0.05373795 6.56405323

H -0.09679022 -2.16669984 6.38447535

H 0.56130413 -3.06161688 4.18028330

H -1.66394441 1.36622717 -4.49749066

H -1.22234600 0.05373795 -6.56405323

H -0.09679022 -2.16669984 -6.38447535

H 0.56130413 -3.06161688 -4.18028330

H 2.07864580 0.05775493 0.00000000

H 0.27760056 2.45967988 2.77624482

H -0.18195548 2.91382244 1.13230437

H 1.93011369 0.87073576 2.00193733

H 2.25141794 2.40599802 1.17813483

H -0.18195548 2.91382244 -1.13230437

H 0.27760056 2.45967988 -2.77624482

H 2.25141794 2.40599802 -1.17813483

H 1.93011369 0.87073576 -2.00193733

H -2.83593020 -2.04889916 0.81350418

H -2.83593020 -2.04889916 -0.81350418

H -3.65844045 -0.89068416 0.00000000

Meso-(Fe(NH)S4)NH3  **(6m)** OPBE Quintet

Fe -0.33841255 -0.65557547 0.00000000

S 0.44274197 -2.00038155 1.72431560

S -1.00132454 0.96017677 1.87871364

S -1.00132454 0.96017677 -1.87871364

S 0.44274197 -2.00038155 -1.72431560

C -0.58594262 0.04170075 3.34148444

C -0.92583846 0.58873403 4.58298877

C -0.65206173 -0.09822906 5.75835759

C -0.04790483 -1.35488638 5.67779353

C 0.27400533 -1.90796921 4.44765275

C 0.01707972 -1.23299675 3.23569609

C -0.58594262 0.04170075 -3.34148444

C -0.92583846 0.58873403 -4.58298877

C -0.65206173 -0.09822906 -5.75835759

C -0.04790483 -1.35488638 -5.67779353

C 0.27400533 -1.90796921 -4.44765275

C 0.01707972 -1.23299675 -3.23569609

N 1.50725926 0.75956779 0.00000000

C 0.38348364 2.12869433 1.75942175

C 1.66937324 1.49700275 1.25053739

C 0.38348364 2.12869433 -1.75942175

C 1.66937324 1.49700275 -1.25053739

N -2.47910598 -1.48482638 0.00000000

H -1.41293395 1.56278265 4.61869448

H -0.91579150 0.33544334 6.72173853

H 0.16782592 -1.91400183 6.58855943

H 0.73745877 -2.89170230 4.39693217

H -1.41293395 1.56278265 -4.61869448

H -0.91579150 0.33544334 -6.72173853

H 0.16782592 -1.91400183 -6.58855943

H 0.73745877 -2.89170230 -4.39693217

H 2.16166101 -0.01781105 0.00000000

H 0.54728199 2.56694940 2.74978861

H 0.02405957 2.93299030 1.10812838

H 2.01544564 0.78089258 2.00281365

H 2.44217205 2.28143552 1.16163243

H 0.02405957 2.93299030 -1.10812838

H 0.54728199 2.56694940 -2.74978861

H 2.44217205 2.28143552 -1.16163243

H 2.01544564 0.78089258 -2.00281365

H -2.55819575 -2.08347560 0.81704438

H -2.55819575 -2.08347560 -0.81704438

H -3.27455675 -0.85268182 0.00000000

trans-(Fe(NH)S4)NH3  **(6t)** OPBE Singlet

Fe 3.09965309 3.03411131 8.05270451

S 3.31550607 5.07231845 8.99307100

S 4.85960983 3.42619408 6.83612919

S 1.23667823 2.73153570 9.11371759

S 2.92338044 0.94506876 7.19486268

C 5.44800783 5.05295268 7.26750178

C 6.60253924 5.57268517 6.67944245

C 7.04648667 6.84149081 7.02871425

C 6.33041037 7.57185172 7.98511746

C 5.19927971 7.04495576 8.58713490

C 4.72476700 5.76133051 8.24523559

C 0.80178714 1.00947228 8.93921928

C -0.25255302 0.45909778 9.66792916

C -0.59414910 -0.87661069 9.48776282

C 0.13391518 -1.64718801 8.57556708

C 1.19188920 -1.10186028 7.86318020

C 1.56406221 0.24564884 8.03698953

N 1.98152537 3.71245357 6.52531005

C 4.03375042 3.78767188 5.24643205

C 2.73757255 4.49907661 5.53994233

C 0.01777824 3.46741646 7.93254952

C 0.75592494 4.37813897 6.98234509

H 1.73237708 2.81598551 6.09105027

H 7.15083248 4.97958384 5.94741886

H 7.94186780 7.25584612 6.56831523

H 6.67013052 8.56788872 8.26994500

H 4.65791974 7.62238021 9.33504915

H -0.80405784 1.08062069 10.37293031

H -1.41398172 -1.31461175 10.05467782

H -0.12394284 -2.69595805 8.42621315

H 1.75604189 -1.71776227 7.16430163

H 3.86993672 2.81057996 4.77387888

H 4.69935591 4.38223745 4.61373450

H 2.94182544 5.48224931 5.97752217

H 2.15208873 4.64463581 4.61713976

H -0.74537314 4.01109316 8.49943065

H -0.45645718 2.62758465 7.41502423

H 0.10263393 4.64371080 6.13448249

H 1.06345153 5.29906984 7.48986312

N 4.19813245 2.27294805 9.58757095

H 3.79398761 2.49761289 10.49237514

H 4.25379555 1.25984667 9.49884485

H 5.14593282 2.63839838 9.60959795

trans-(Fe(NH)S4)NH3  **(6t)** OPBE Triplet

Fe 3.13066234 3.00591463 8.05773698

S 3.36307540 4.99867867 9.03673236

S 4.86161065 3.45481251 6.77945430

S 1.21282769 2.75550531 9.08236384

S 2.94655047 0.90802371 7.24937587

C 5.44056654 5.08165366 7.23972580

C 6.55921550 5.64688852 6.63011466

C 6.98124758 6.91832682 7.00368364

C 6.28546311 7.60140363 8.00371328

C 5.18718166 7.02583764 8.62703275

C 4.74152128 5.74383538 8.25901325

C 0.76625130 1.03480876 8.92778640

C -0.31548066 0.50960139 9.63267166

C -0.65697726 -0.83019761 9.47756822

C 0.09835024 -1.62986857 8.61720381

C 1.18376686 -1.10707955 7.92637085

C 1.55252985 0.24191179 8.07597878

N 1.86614833 3.79591435 6.31792919

C 4.01584359 3.86555566 5.20493344

C 2.70191818 4.58882824 5.43593836

C 0.01329717 3.46892938 7.85482238

C 0.68887871 4.42174635 6.88679897

H 1.62543301 2.90929427 5.87841150

H 7.09730039 5.09144926 5.86231076

H 7.84881992 7.36930278 6.52465916

H 6.60974981 8.59732103 8.30567504

H 4.65593533 7.56439932 9.41030186

H -0.88829280 1.15273432 10.30004831

H -1.49986983 -1.24748139 10.02619538

H -0.15843143 -2.68170096 8.49015153

H 1.77086362 -1.74414228 7.26653815

H 3.85678878 2.89331629 4.72101937

H 4.69520240 4.45335781 4.57957558

H 2.89240981 5.55406765 5.91885176

H 2.22652915 4.79394317 4.45898085

H -0.78025016 3.98080253 8.41043309

H -0.42618242 2.61318997 7.33225561

H -0.05616423 4.72267305 6.12697135

H 1.01642514 5.32619546 7.41251646

N 4.49232748 1.99593805 9.95087917

H 4.11691538 2.20525887 10.87102421

H 4.49688264 0.98597681 9.84479713

H 5.46011223 2.30373029 9.95945026

trans-(Fe(NH)S4)NH3  **(6t)** OPBE Quintet

Fe 3.23494889 2.95734304 8.20696073

S 3.53821191 5.11288253 9.11111404

S 5.06838137 3.55676222 6.65357891

S 0.92454833 2.66661147 9.17371412

S 2.89221825 0.77610776 7.29915134

C 5.51605262 5.20640191 7.13680611

C 6.57201841 5.82988119 6.46587498

C 6.97340729 7.11221630 6.81529178

C 6.31964690 7.75803956 7.86688974

C 5.28706175 7.13393268 8.54925586

C 4.84831084 5.83608526 8.21256419

C 0.59212870 0.94602710 8.88558557

C -0.52469035 0.38254594 9.51203671

C -0.84278621 -0.95641485 9.32727659

C -0.02229106 -1.73663431 8.50983374

C 1.09583771 -1.18778067 7.90140003

C 1.45233490 0.16666332 8.07403511

N 1.93862656 3.76165435 6.45116861

C 4.02814220 3.86154608 5.19220302

C 2.72107492 4.55552024 5.51684109

C -0.05553133 3.46275388 7.83870840

C 0.74655215 4.41071671 6.96946651

H 1.70009515 2.86236419 6.03154534

H 7.07848813 5.29755428 5.66123769

H 7.79052734 7.59618488 6.28271774

H 6.62376612 8.76290059 8.16093237

H 4.78909220 7.64565555 9.37098028

H -1.14637890 1.01170117 10.14758282

H -1.71581013 -1.38593162 9.81606809

H -0.25421463 -2.79017859 8.35110756

H 1.73427365 -1.80794889 7.27436521

H 3.86053377 2.86494922 4.76357210

H 4.60731770 4.44721883 4.47080320

H 2.92714342 5.52669384 5.98122059

H 2.17582921 4.74859056 4.57435631

H -0.88584536 4.00216541 8.30795633

H -0.47526785 2.63875399 7.25280547

H 0.07979887 4.77362647 6.16529384

H 1.07179507 5.28176521 7.55146623

N 4.42661743 2.04094933 9.95795163

H 3.98530001 2.22227562 10.85455833

H 4.50854888 1.03413141 9.84620421

H 5.36226524 2.43202984 10.01593040

Meso-(Fe(NH)S4)N2H4 **(7m)** OPBE Singlet

Fe -0.10851679 0.39757510 0.00000000

N -1.62178592 1.77743547 0.00000000

H -2.23163730 1.62858532 0.80117594

H -2.23163730 1.62858532 -0.80117594

N -1.37149990 3.20601507 0.00000000

H -0.72777059 3.31416091 0.79155867

H -0.72777059 3.31416091 -0.79155867

S 1.00057046 1.62331789 1.53575969

S -1.02856711 -0.73689466 1.61147860

S 1.00057046 1.62331789 -1.53575969

S -1.02856711 -0.73689466 -1.61147860

N 1.39705492 -0.97305959 0.00000000

H 2.19988984 -0.34459705 0.00000000

C -0.58449056 0.07133521 3.14267573

C -1.15628192 -0.32702942 4.35146844

H -1.89387933 -1.12953413 4.36334106

C -0.78363530 0.30390755 5.53266614

H -1.22607246 0.00025453 6.47996591

C 0.16038198 1.33518246 5.48415117

H 0.45863633 1.83894280 6.40383688

C 0.71361616 1.74213511 4.27947863

H 1.43920442 2.55389354 4.25655415

C 0.34695242 1.12085351 3.06906823

C -0.58449056 0.07133521 -3.14267573

C -1.15628192 -0.32702942 -4.35146844

H -1.89387933 -1.12953413 -4.36334106

C -0.78363530 0.30390755 -5.53266614

H -1.22607246 0.00025453 -6.47996591

C 0.16038198 1.33518246 -5.48415117

H 0.45863633 1.83894280 -6.40383688

C 0.71361616 1.74213511 -4.27947863

H 1.43920442 2.55389354 -4.25655415

C 0.34695242 1.12085351 -3.06906823

C 0.08705124 -2.18710703 1.71317589

H -0.35917906 -2.97020416 1.09118783

H 0.10399285 -2.54293798 2.74757665

C 1.45979630 -1.76026049 1.24989655

H 2.12305383 -2.63195618 1.13125395

H 1.89499166 -1.10284402 2.00897327

C 0.08705124 -2.18710703 -1.71317589

H 0.10399285 -2.54293798 -2.74757665

H -0.35917906 -2.97020416 -1.09118783

C 1.45979630 -1.76026049 -1.24989655

H 1.89499166 -1.10284402 -2.00897327

H 2.12305383 -2.63195618 -1.13125395

Meso-(Fe(NH)S4)N2H4 **(7m)** OPBE Triplet

Fe -0.14068600 0.47052536 0.00000000

N -2.21293194 1.80878446 0.00000000

H -2.82307331 1.64338429 0.79967520

H -2.82307331 1.64338429 -0.79967520

N -1.97765021 3.24665482 0.00000000

H -1.33439822 3.36751679 0.78653572

H -1.33439822 3.36751679 -0.78653572

S 0.93522659 1.73148383 1.50171560

S -1.02962811 -0.68750708 1.71167144

S 0.93522659 1.73148383 -1.50171560

S -1.02962811 -0.68750708 -1.71167144

N 1.40933766 -1.34029273 0.00000000

H 2.23236333 -0.74977008 0.00000000

C -0.44521005 0.08247069 3.21075120

C -0.89153878 -0.34879554 4.46070120

H -1.60101836 -1.17311293 4.52985303

C -0.43046611 0.27748203 5.61285925

H -0.77184206 -0.05693153 6.59113864

C 0.46339999 1.34642960 5.49681756

H 0.82687173 1.84837221 6.39354439

C 0.88744771 1.78812485 4.25231226

H 1.57570940 2.62821648 4.17365694

C 0.43491279 1.16678450 3.07275977

C -0.44521005 0.08247069 -3.21075120

C -0.89153878 -0.34879554 -4.46070120

H -1.60101836 -1.17311293 -4.52985303

C -0.43046611 0.27748203 -5.61285925

H -0.77184206 -0.05693153 -6.59113864

C 0.46339999 1.34642960 -5.49681756

H 0.82687173 1.84837221 -6.39354439

C 0.88744771 1.78812485 -4.25231226

H 1.57570940 2.62821648 -4.17365694

C 0.43491279 1.16678450 -3.07275977

C -0.09719346 -2.26121090 1.74033062

H -0.67143544 -2.95429286 1.11618828

H -0.11494206 -2.64807174 2.76423673

C 1.33123110 -2.07917657 1.25139889

H 1.81568652 -3.06965191 1.18023248

H 1.87905285 -1.50351957 2.00440065

C -0.09719346 -2.26121090 -1.74033062

H -0.11494206 -2.64807174 -2.76423673

H -0.67143544 -2.95429286 -1.11618828

C 1.33123110 -2.07917657 -1.25139889

H 1.87905285 -1.50351957 -2.00440065

H 1.81568652 -3.06965191 -1.18023248

Meso-(Fe(NH)S4)N2H4 **(7m)** OPBE Quintet

Fe -0.13679602 0.63619858 0.00000000

N -2.03844791 1.86336327 0.00000000

H -2.64134643 1.68832731 0.80264335

H -2.64134643 1.68832731 -0.80264335

N -1.80577503 3.30034250 0.00000000

H -1.16604948 3.42385776 0.79046910

H -1.16604948 3.42385776 -0.79046910

S 0.95058067 1.76898292 1.71189157

S -1.11774406 -0.79035585 1.91029282

S 0.95058067 1.76898292 -1.71189157

S -1.11774406 -0.79035585 -1.91029282

N 1.35765768 -1.16517951 0.00000000

H 2.16434341 -0.54767041 0.00000000

C -0.46781333 0.00628133 3.36075602

C -0.88239936 -0.45795317 4.61334873

H -1.57284284 -1.29912009 4.66640616

C -0.42470231 0.14292760 5.77874891

H -0.74781106 -0.22742980 6.75034585

C 0.44009502 1.23473615 5.67875981

H 0.80400704 1.72590577 6.58146846

C 0.83858348 1.70906735 4.43840009

H 1.50890765 2.56432839 4.37167719

C 0.39936213 1.11556332 3.23690103

C -0.46781333 0.00628133 -3.36075602

C -0.88239936 -0.45795317 -4.61334873

H -1.57284284 -1.29912009 -4.66640616

C -0.42470231 0.14292760 -5.77874891

H -0.74781106 -0.22742980 -6.75034585

C 0.44009502 1.23473615 -5.67875981

H 0.80400704 1.72590577 -6.58146846

C 0.83858348 1.70906735 -4.43840009

H 1.50890765 2.56432839 -4.37167719

C 0.39936213 1.11556332 -3.23690103

C -0.04045454 -2.24488472 1.76348900

H -0.58015871 -2.93400473 1.10491416

H 0.02375688 -2.72362926 2.74662783

C 1.35274374 -1.91798918 1.25196669

H 1.92913259 -2.85626119 1.16331892

H 1.85275115 -1.29766644 2.00284275

C -0.04045454 -2.24488472 -1.76348900

H 0.02375688 -2.72362926 -2.74662783

H -0.58015871 -2.93400473 -1.10491416

C 1.35274374 -1.91798918 -1.25196669

H 1.85275115 -1.29766644 -2.00284275

H 1.92913259 -2.85626119 -1.16331892

trans-(Fe(NH)S4)N2H4 **(7t)** OPBE Singlet

Fe 3.08413602 3.02136555 8.06214503

S 3.27537116 5.06593604 8.99073309

S 4.86837724 3.42018527 6.88543157

S 1.19814249 2.74114397 9.09736760

S 2.88470658 0.93981086 7.18222328

C 5.44128411 5.05397769 7.31334229

C 6.60246145 5.57835583 6.74335330

C 7.02737967 6.85425192 7.09128099

C 6.28462013 7.58867374 8.02329442

C 5.14551213 7.05705222 8.60680759

C 4.69348733 5.76613015 8.26712501

C 0.77033390 1.01514506 8.93883033

C -0.28199432 0.46934741 9.67310768

C -0.62764973 -0.86612927 9.49752667

C 0.09351144 -1.64122842 8.58463401

C 1.15094358 -1.10083949 7.86681142

C 1.52593446 0.24567424 8.03615819

N 2.00498274 3.70667707 6.51067195

C 4.08140177 3.76885116 5.27339045

C 2.78006443 4.48502113 5.53431294

C 0.01099683 3.43465086 7.85812392

C 0.76055206 4.36033110 6.93226164

H 1.77213417 2.80312862 6.08048842

H 7.17194031 4.98400141 6.02875658

H 7.92882358 7.27221040 6.64620959

H 6.60923068 8.59066398 8.30464474

H 4.58189338 7.63673468 9.33639961

H -0.82729507 1.09406020 10.37978527

H -1.44552121 -1.30060232 10.07005677

H -0.16788042 -2.68967619 8.43935474

H 1.71141743 -1.72051399 7.16834508

H 3.92543207 2.78858047 4.80501673

H 4.76201790 4.35716873 4.65090074

H 2.97582614 5.47291039 5.96448324

H 2.21356589 4.62099428 4.59833703

H -0.78986054 3.95927771 8.39010792

H -0.41919464 2.58200396 7.32308868

H 0.12877793 4.61628778 6.06545661

H 1.03893105 5.28572187 7.44761414

N 4.16820165 2.12261408 9.55909168

H 3.78511966 1.18196713 9.62461229

H 5.10979107 2.00716930 9.18659641

N 4.19329259 2.67932866 10.87923493

H 5.12071964 2.52982973 11.27477111

H 4.09734112 3.68903642 10.72716156

trans-(Fe(NH)S4)N2H4 **(7t)** OPBE Triplet

Fe 3.08770850 3.02145286 8.07762770

S 3.30278254 5.12803076 8.98753369

S 4.92080653 3.46151613 6.81474461

S 1.09481322 2.71732147 9.10230112

S 2.85975905 0.88016041 7.17084226

C 5.46899395 5.09404805 7.26801455

C 6.61991424 5.63371730 6.68580157

C 7.05578696 6.90342942 7.05265423

C 6.34193638 7.62008464 8.01734330

C 5.20924729 7.07537234 8.61324292

C 4.73741487 5.80037585 8.24778676

C 0.70053807 0.99316568 8.90805074

C -0.36054433 0.43597696 9.62849646

C -0.68056586 -0.90908524 9.47181818

C 0.08080431 -1.69660523 8.60321712

C 1.14813153 -1.14851519 7.89906213

C 1.48880050 0.21142272 8.03199092

N 1.97662943 3.73647187 6.47950870

C 4.06485228 3.82897311 5.24408779

C 2.75072790 4.52332616 5.51400576

C -0.02860944 3.41804581 7.81121129

C 0.72038328 4.36282987 6.90048402

H 1.76434627 2.82655529 6.05725013

H 7.17450417 5.05305481 5.94905878

H 7.94914717 7.32656484 6.59594569

H 6.67528841 8.61541413 8.31141926

H 4.66289136 7.63899585 9.36746337

H -0.93186103 1.06342031 10.31159073

H -1.50890976 -1.34184057 10.03080716

H -0.16247329 -2.75098508 8.47081698

H 1.73565057 -1.77047361 7.22610689

H 3.92020803 2.85372114 4.76182634

H 4.71957789 4.43751901 4.61332756

H 2.93091169 5.51224307 5.94898681

H 2.18899090 4.65780121 4.57423195

H -0.85276702 3.93249394 8.31726350

H -0.43491596 2.56420826 7.26053093

H 0.09114814 4.61469972 6.03034252

H 0.97569331 5.29123696 7.42294971

N 4.17312671 2.15957606 9.58163622

H 3.80957347 1.21092847 9.65438592

H 5.13134446 2.05293890 9.25064908

N 4.14894278 2.72977512 10.90109418

H 5.07360011 2.59988698 11.31030854

H 4.04922620 3.73561460 10.72426431

trans-(Fe(NH)S4)N2H4 **(7t)** OPBE Quintet

Fe 3.18390922 2.95616456 8.22802675

S 3.48144971 5.12268977 9.10862955

S 5.05962719 3.53849766 6.70215209

S 0.85958864 2.66909913 9.13320401

S 2.89905099 0.76626665 7.34776421

C 5.49651592 5.19499443 7.17044961

C 6.56264456 5.81300837 6.51055130

C 6.95482576 7.10024526 6.85231672

C 6.28183401 7.75747070 7.88412028

C 5.23839490 7.13892229 8.55549327

C 4.81041063 5.83648161 8.22610055

C 0.53568190 0.94698544 8.83726005

C -0.60740923 0.38835048 9.41857131

C -0.92527912 -0.94832373 9.21714687

C -0.07814149 -1.73170556 8.43115726

C 1.06812840 -1.18870514 7.87116972

C 1.42333651 0.16297918 8.06188520

N 1.93616430 3.73702062 6.42973852

C 4.05217954 3.82069995 5.21374371

C 2.73761330 4.51740360 5.49988149

C -0.09211388 3.45450030 7.77115734

C 0.72957508 4.39136046 6.90802109

H 1.70847679 2.83150680 6.01777721

H 7.08478746 5.27274063 5.72145912

H 7.78034174 7.57964121 6.32864080

H 6.57892576 8.76623070 8.17163180

H 4.72433043 7.65917020 9.36183928

H -1.24961080 1.01890645 10.03178032

H -1.81930027 -1.37386532 9.67013424

H -0.31011903 -2.78327389 8.26027270

H 1.72855484 -1.81135785 7.26997145

H 3.89484880 2.81765189 4.79671817

H 4.64618577 4.39627334 4.49634658

H 2.93183405 5.49646354 5.95245610

H 2.21243028 4.69460496 4.54310733

H -0.92892727 4.00205482 8.21897412

H -0.50464353 2.62741161 7.18460722

H 0.08355550 4.74084023 6.08149915

H 1.03770388 5.27189447 7.48458352

N 4.37897719 1.97166627 9.97167796

H 3.89751850 1.10373039 10.19139499

H 5.24535676 1.70254366 9.50631842

N 4.60523962 2.68877606 11.18290858

H 5.54728360 2.50194156 11.52152699

H 4.56976834 3.67597050 10.92015091

Meso-(Fe(NH)S4)CO **(4m)** OPBE-Cosmo Singlet

Fe -0.07297936 -0.17890901 0.00000000

S 0.98678592 -1.45466010 1.53312650

S -0.94179792 1.03409754 1.62274055

S -0.94179792 1.03409754 -1.62274055

S 0.98678592 -1.45466010 -1.53312650

C -0.54568811 0.16532026 3.12909228

C -1.10876022 0.58310147 4.33651018

C -0.80332863 -0.09539372 5.51201023

C 0.05985524 -1.19484942 5.46279940

C 0.60581111 -1.62038519 4.25864545

C 0.31347243 -0.94313673 3.05884241

C -0.54568811 0.16532026 -3.12909228

C -1.10876022 0.58310147 -4.33651018

C -0.80332863 -0.09539372 -5.51201023

C 0.05985524 -1.19484942 -5.46279940

C 0.60581111 -1.62038519 -4.25864545

C 0.31347243 -0.94313673 -3.05884241

N 1.52598102 1.19750959 0.00000000

C 0.22602748 2.43169858 1.70709141

C 1.59087615 1.98085967 1.25071678

C 0.22602748 2.43169858 -1.70709141

C 1.59087615 1.98085967 -1.25071678

H -1.78328023 1.43790847 4.35342480

H -1.23758630 0.22700487 6.45647150

H 0.30023506 -1.73703014 6.37671391

H 1.26689849 -2.48522168 4.23659834

H -1.78328023 1.43790847 -4.35342480

H -1.23758630 0.22700487 -6.45647150

H 0.30023506 -1.73703014 -6.37671391

H 1.26689849 -2.48522168 -4.23659834

H 2.33800245 0.58431117 0.00000000

H 0.24248489 2.80369484 2.73528439

H -0.20866147 3.21347329 1.07791606

H 2.02774424 1.32731413 2.01040787

H 2.25597363 2.84748425 1.13281609

H -0.20866147 3.21347329 -1.07791606

H 0.24248489 2.80369484 -2.73528439

H 2.25597363 2.84748425 -1.13281609

H 2.02774424 1.32731413 -2.01040787

C -1.34964911 -1.29536399 0.00000000

O -2.21274038 -2.08690573 0.00000000

Meso-(Fe(NH)S4)CO **(4m)** OPBE-Cosmo Triplet

Fe 0.12338032 -0.23377622 0.00000000

S 1.18028487 -1.40632293 1.81559021

S -0.90472852 1.14005311 1.70221663

S -0.90472852 1.14005311 -1.70221663

S 1.18028487 -1.40632293 -1.81559021

C -0.63712200 0.19944108 3.17666425

C -1.37203701 0.56155443 4.31222888

C -1.24342101 -0.15539607 5.49550731

C -0.38727255 -1.25959743 5.52985356

C 0.32909374 -1.63735325 4.40225411

C 0.23303696 -0.91896021 3.19151614

C -0.63712200 0.19944108 -3.17666425

C -1.37203701 0.56155443 -4.31222888

C -1.24342101 -0.15539607 -5.49550731

C -0.38727255 -1.25959743 -5.52985356

C 0.32909374 -1.63735325 -4.40225411

C 0.23303696 -0.91896021 -3.19151614

N 1.64135119 1.19053345 0.00000000

C 0.36040992 2.45006050 1.74200017

C 1.70704378 1.96919660 1.25827131

C 0.36040992 2.45006050 -1.74200017

C 1.70704378 1.96919660 -1.25827131

H -2.04199710 1.41801087 4.26070872

H -1.81073765 0.13859840 6.37662447

H -0.28273570 -1.83960427 6.44612132

H 0.98116130 -2.50769690 4.44445229

H -2.04199710 1.41801087 -4.26070872

H -1.81073765 0.13859840 -6.37662447

H -0.28273570 -1.83960427 -6.44612132

H 0.98116130 -2.50769690 -4.44445229

H 2.47643840 0.60823474 0.00000000

H 0.42655867 2.83490888 2.76389965

H -0.05960600 3.24806243 1.12186529

H 2.13960173 1.30333340 2.00879176

H 2.38449438 2.82649867 1.13873599

H -0.05960600 3.24806243 -1.12186529

H 0.42655867 2.83490888 -2.76389965

H 2.38449438 2.82649867 -1.13873599

H 2.13960173 1.30333340 -2.00879176

C -1.10726106 -1.42304176 0.00000000

O -1.94728231 -2.23723811 0.00000000

Meso-(Fe(NH)S4)CO **(4m)** OPBE-Cosmo Quintet

Fe 0.06763785 -0.27923625 0.00000000

S 0.86282509 -1.62284268 1.71015428

S -0.99828600 1.07999732 1.84382869

S -0.99828600 1.07999732 -1.84382869

S 0.86282509 -1.62284268 -1.71015428

C -0.46248504 0.23912620 3.31731110

C -0.89022642 0.72830876 4.55589331

C -0.55729773 0.06781406 5.73399004

C 0.19448534 -1.10655937 5.66501337

C 0.61036680 -1.60464640 4.43648341

C 0.30099496 -0.94554502 3.23086312

C -0.46248504 0.23912620 -3.31731110

C -0.89022642 0.72830876 -4.55589331

C -0.55729773 0.06781406 -5.73399004

C 0.19448534 -1.10655937 -5.66501337

C 0.61036680 -1.60464640 -4.43648341

C 0.30099496 -0.94554502 -3.23086312

N 1.52489727 1.41793255 0.00000000

C 0.10630271 2.51889270 1.74986639

C 1.49904167 2.18733087 1.25411039

C 0.10630271 2.51889270 -1.74986639

C 1.49904167 2.18733087 -1.25411039

H -1.49453784 1.63344475 4.59248856

H -0.89353272 0.45908349 6.69255758

H 0.45186075 -1.64513004 6.57637777

H 1.18918087 -2.52595192 4.39580132

H -1.49453784 1.63344475 -4.59248856

H -0.89353272 0.45908349 -6.69255758

H 0.45186075 -1.64513004 -6.57637777

H 1.18918087 -2.52595192 -4.39580132

H 2.40385274 0.90703415 0.00000000

H 0.15681850 2.98140631 2.74004698

H -0.42129706 3.21951491 1.09600228

H 2.00837953 1.58021640 2.00829328

H 2.06823318 3.12396402 1.15191303

H -0.42129706 3.21951491 -1.09600228

H 0.15681850 2.98140631 -2.74004698

H 2.06823318 3.12396402 -1.15191303

H 2.00837953 1.58021640 -2.00829328

C -1.75659435 -1.60193701 0.00000000

O -2.40094756 -2.54733492 0.00000000

trans-(Fe(NH)S4)CO **(4t)** OPBE-Cosmo Singlet

Fe 8.38152837 10.14917194 1.96545532

S 9.77430966 8.98290286 3.19916804

S 6.73732121 8.65898129 2.43061958

S 7.07157708 11.13393852 0.50700790

S 9.99694670 11.68005209 1.49642700

C 9.15274812 12.90731520 0.58260245

C 9.76337262 14.13079152 0.24663047

H 10.79042787 14.31866108 0.55533236

C 9.06403578 15.10024106 -0.46275492

H 9.55752267 16.04120817 -0.70372583

C 7.73878757 14.88937293 -0.85602358

H 7.19332595 15.65767744 -1.40078827

C 7.11813092 13.68446385 -0.54031378

H 6.08882772 13.49608733 -0.84076369

C 7.82725754 12.70678295 0.15880662

C 7.45394574 7.57345937 3.59069941

C 6.71061364 6.53885381 4.19411652

H 5.66458368 6.40554719 3.92288090

C 7.29705898 5.69374452 5.12708512

H 6.69860184 4.90222342 5.57695563

C 8.63640342 5.85192248 5.50100335

H 9.08796941 5.19419167 6.24122230

C 9.38768324 6.86695006 4.91803735

H 10.43116732 7.00916697 5.19552149

C 8.80337418 7.70028516 3.96188867

C 7.85706344 11.11553585 3.26192952

O 7.49575445 11.78364330 4.15379851

N 9.05534828 9.01371632 0.35509328

H 9.78436297 9.63256001 -0.00945163

C 10.64179363 8.04371484 1.89545258

H 11.06184024 7.13648596 2.33722509

H 11.46835155 8.69562100 1.58895312

C 9.69687251 7.75734687 0.75873487

H 8.91568147 7.05769941 1.07055891

H 10.24378090 7.30805105 -0.08240242

C 7.49777538 10.22753939 -1.04053075

H 8.24803547 10.82965367 -1.56076649

H 6.59670135 10.16459058 -1.65687831

C 8.02902012 8.86486723 -0.68123686

H 7.23742652 8.22351763 -0.28242137

H 8.43959234 8.38582053 -1.58136789

trans-(Fe(NH)S4)CO **(4t)** OPBE-Cosmo Triplet

Fe 8.31802975 10.20153138 2.00255382

S 9.94841162 8.81377199 3.33304512

S 6.73218396 8.82886148 2.85864407

S 6.98851371 11.19068167 0.20246269

S 9.95656095 11.70970189 1.46747942

C 9.09686065 12.95382935 0.58722058

C 9.69575277 14.21465341 0.40322936

H 10.66674645 14.40829471 0.85550392

C 9.06539048 15.21083699 -0.33195765

H 9.55480852 16.17669766 -0.45175862

C 7.81172883 14.98564297 -0.90433640

H 7.31324651 15.76708536 -1.47500220

C 7.19695081 13.74990826 -0.73185954

H 6.21810255 13.55953357 -1.16816195

C 7.83193917 12.73411443 -0.00969241

C 7.52382836 7.54212413 3.74005704

C 6.75064960 6.49389015 4.27695605

H 5.67802848 6.47841595 4.09165352

C 7.33661127 5.48480947 5.03025785

H 6.71313887 4.68405157 5.42619515

C 8.70894885 5.49756052 5.29008917

H 9.16762329 4.71708917 5.89432810

C 9.48853701 6.52760192 4.77381326

H 10.55855616 6.55486248 4.97317021

C 8.91032144 7.53437486 3.99498871

C 7.71566411 11.36757716 3.12439107

O 7.30838549 12.16514040 3.87960902

N 9.01512869 8.94138837 0.42276711

H 9.75792845 9.54417312 0.06224659

C 10.66707613 7.94239010 1.90817347

H 11.12532510 7.01259287 2.25490046

H 11.46886539 8.60130203 1.55413272

C 9.64198254 7.68247835 0.83101043

H 8.86305903 7.00409745 1.19215538

H 10.13706860 7.19985705 -0.02487239

C 7.62567487 10.16018677 -1.17031359

H 8.47932033 10.68676787 -1.60778389

H 6.84124845 10.07075687 -1.92755617

C 8.02621442 8.79867403 -0.65156642

H 7.16105249 8.25523440 -0.25830888

H 8.43749998 8.21627531 -1.48888570

trans-(Fe(NH)S4)CO **(4t)** OPBE-Cosmo Quintet

Fe 8.45703085 10.13760201 1.94495923

S 9.94572552 8.60704149 3.19406783

S 6.67137938 8.63772266 2.61107220

S 7.12394340 11.13380993 0.13792105

S 10.05531177 11.92714294 1.41207932

C 9.04696029 13.09166097 0.58660991

C 9.48676268 14.42460449 0.46127852

H 10.44452534 14.70233311 0.89728141

C 8.72525598 15.38283918 -0.19698623

H 9.09943615 16.40331517 -0.27066464

C 7.48736170 15.04962050 -0.74925783

H 6.88506644 15.79917837 -1.25931591

C 7.02610699 13.74189493 -0.63920537

H 6.06188678 13.46382445 -1.06043734

C 7.79107293 12.76965186 0.01322096

C 7.41894384 7.57609414 3.78007872

C 6.60348329 6.70187586 4.52769769

H 5.52719974 6.72850724 4.36822219

C 7.14065852 5.81037889 5.44697806

H 6.47590818 5.14701605 5.99893427

C 8.51838736 5.76669531 5.67009506

H 8.94507462 5.07560358 6.39459004

C 9.34495006 6.63003476 4.95984341

H 10.41973180 6.62117686 5.13254940

C 8.81290096 7.51846092 4.01892022

C 7.88689634 11.31623056 3.39868004

O 7.51748564 12.05954097 4.20525253

N 9.20065718 8.84235073 0.20656011

H 10.03416532 9.34132413 -0.10453420

C 10.56919474 7.60609637 1.80671008

H 10.84324876 6.61804836 2.18639635

H 11.49467971 8.11853786 1.51556417

C 9.60577305 7.50844677 0.64499616

H 8.70741318 6.95591534 0.93828153

H 10.09494980 6.94369822 -0.16486729

C 7.88471349 10.26508504 -1.28431689

H 8.77093668 10.83513594 -1.57893791

H 7.16783971 10.27063611 -2.11067055

C 8.24493661 8.84685033 -0.89926053

H 7.35343117 8.29182118 -0.58646280

H 8.64770135 8.34368373 -1.79213019

Meso-(Fe(NH)S4)PMe3 **(5m)** OPBE-Cosmo Singlet

Fe 0.18277200 0.06165762 0.00000000

S 1.42724184 1.14557720 -1.52741192

S -0.81702692 -1.00155684 -1.61732125

S -0.81702692 -1.00155684 1.61732125

S 1.42724184 1.14557720 1.52741192

C -0.23534946 -0.28302198 -3.15030964

C -0.79991703 -0.65807583 -4.37028386

C -0.32446503 -0.10265721 -5.55530170

C 0.71124491 0.83788073 -5.50245911

C 1.26178187 1.22280638 -4.28685431

C 0.79138828 0.67281924 -3.07663229

C -0.23534946 -0.28302198 3.15030964

C -0.79991703 -0.65807583 4.37028386

C -0.32446503 -0.10265721 5.55530170

C 0.71124491 0.83788073 5.50245911

C 1.26178187 1.22280638 4.28685431

C 0.79138828 0.67281924 3.07663229

N 1.57058537 -1.52844805 0.00000000

C 0.10587831 -2.57702123 -1.69021277

C 1.52322295 -2.32277009 -1.24356865

C 0.10587831 -2.57702123 1.69021277

C 1.52322295 -2.32277009 1.24356865

H -1.60678851 -1.38997136 -4.39287497

H -0.75943920 -0.39474665 -6.50956756

H 1.08908012 1.28232400 -6.42305449

H 2.06159518 1.96206911 -4.26248464

H -1.60678851 -1.38997136 4.39287497

H -0.75943920 -0.39474665 6.50956756

H 1.08908012 1.28232400 6.42305449

H 2.06159518 1.96206911 4.26248464

H 2.46119439 -1.03757476 0.00000000

H 0.06384153 -2.96065780 -2.71336587

H -0.43503715 -3.27779849 -1.04826467

H 2.04031697 -1.73993638 -2.01098943

H 2.06491260 -3.27179339 -1.12218386

H -0.43503715 -3.27779849 1.04826467

H 0.06384153 -2.96065780 2.71336587

H 2.06491260 -3.27179339 1.12218386

H 2.04031697 -1.73993638 2.01098943

P -1.25959214 1.72591530 0.00000000

C -2.46370427 1.81940610 -1.39152396

H -1.93646381 1.90982503 -2.34679526

H -3.08565106 0.91766796 -1.41326521

H -3.11058218 2.69436047 -1.25715263

C -2.46370427 1.81940610 1.39152396

H -3.08565106 0.91766796 1.41326521

H -1.93646381 1.90982503 2.34679526

H -3.11058218 2.69436047 1.25715263

C -0.59931916 3.45476753 0.00000000

H -0.95338796 3.98609853 -0.88971312

H -0.95338796 3.98609853 0.88971312

H 0.49297041 3.44600912 0.00000000

Meso-(Fe(NH)S4)PMe3 **(5m)** OPBE-Cosmo Triplet

Fe 0.24733374 0.10851891 0.00000000

S 1.40388978 1.20243676 -1.68783835

S -0.86026440 -1.10544916 -1.74297280

S -0.86026440 -1.10544916 1.74297280

S 1.40388978 1.20243676 1.68783835

C -0.26311063 -0.36417555 -3.24978332

C -0.81242149 -0.77478323 -4.46802396

C -0.38495846 -0.20985053 -5.66582089

C 0.59437876 0.78781422 -5.63314896

C 1.13059672 1.21137298 -4.42421549

C 0.72048488 0.64891895 -3.19660312

C -0.26311063 -0.36417555 3.24978332

C -0.81242149 -0.77478323 4.46802396

C -0.38495846 -0.20985053 5.66582089

C 0.59437876 0.78781422 5.63314896

C 1.13059672 1.21137298 4.42421549

C 0.72048488 0.64891895 3.19660312

N 1.61660474 -1.49948723 0.00000000

C 0.16623733 -2.60469138 -1.69584692

C 1.57260418 -2.29052573 -1.24484397

C 0.16623733 -2.60469138 1.69584692

C 1.57260418 -2.29052573 1.24484397

H -1.57834735 -1.54971462 -4.47431693

H -0.81311471 -0.53960945 -6.61090923

H 0.93816776 1.24594466 -6.56038392

H 1.88589034 1.99644976 -4.41517714

H -1.57834735 -1.54971462 4.47431693

H -0.81311471 -0.53960945 6.61090923

H 0.93816776 1.24594466 6.56038392

H 1.88589034 1.99644976 4.41517714

H 2.50891347 -1.01119369 0.00000000

H 0.17177517 -3.05603195 -2.69271631

H -0.35796354 -3.29454907 -1.02912698

H 2.06772200 -1.69216861 -2.01463864

H 2.14374572 -3.22379066 -1.12918593

H -0.35796354 -3.29454907 1.02912698

H 0.17177517 -3.05603195 2.69271631

H 2.14374572 -3.22379066 1.12918593

H 2.06772200 -1.69216861 2.01463864

P -1.17751939 1.86958904 0.00000000

C -2.36366914 1.94145025 -1.40030725

H -1.82676802 1.99981850 -2.35221933

H -2.99960207 1.04981834 -1.39847576

H -2.99520990 2.83082628 -1.28828942

C -2.36366914 1.94145025 1.40030725

H -2.99960207 1.04981834 1.39847576

H -1.82676802 1.99981850 2.35221933

H -2.99520990 2.83082628 1.28828942

C -0.47154191 3.57337573 0.00000000

H -0.81240191 4.11146486 -0.89098420

H -0.81240191 4.11146486 0.89098420

H 0.62015128 3.53355409 0.00000000

Meso-(Fe(NH)S4)PMe3 **(5m)** OPBE-Cosmo Quintet

Fe 0.27937119 0.21836870 0.00000000

S 1.53049385 1.23783925 -1.69335026

S -0.85970189 -0.99166758 -1.90794222

S -0.85970189 -0.99166758 1.90794222

S 1.53049385 1.23783925 1.69335026

C -0.05484023 -0.34061711 -3.35704860

C -0.48752518 -0.77704493 -4.61400385

C 0.08312845 -0.27224000 -5.77780909

C 1.08499963 0.69560138 -5.67805971

C 1.50789163 1.14331549 -4.43257808

C 0.95460401 0.64037803 -3.23730214

C -0.05484023 -0.34061711 3.35704860

C -0.48752518 -0.77704493 4.61400385

C 0.08312845 -0.27224000 5.77780909

C 1.08499963 0.69560138 5.67805971

C 1.50789163 1.14331549 4.43257808

C 0.95460401 0.64037803 3.23730214

N 1.46537753 -1.83263130 0.00000000

C -0.11255124 -2.63625627 -1.75964929

C 1.31152189 -2.59282829 -1.24380413

C -0.11255124 -2.63625627 1.75964929

C 1.31152189 -2.59282829 1.24380413

H -1.28024275 -1.52124383 -4.67689869

H -0.25795380 -0.62330095 -6.75025907

H 1.53764515 1.10972491 -6.57857915

H 2.28716228 1.90143440 -4.36863336

H -1.28024275 -1.52124383 4.67689869

H -0.25795380 -0.62330095 6.75025907

H 1.53764515 1.10972491 6.57857915

H 2.28716228 1.90143440 4.36863336

H 2.40575090 -1.45076853 0.00000000

H -0.15193049 -3.12812759 -2.73633322

H -0.78744115 -3.18461884 -1.09557153

H 1.94326533 -2.11372973 -1.99766951

H 1.67466554 -3.62645909 -1.12791590

H -0.78744115 -3.18461884 1.09557153

H -0.15193049 -3.12812759 2.73633322

H 1.67466554 -3.62645909 1.12791590

H 1.94326533 -2.11372973 1.99766951

P -1.76372343 1.95962167 0.00000000

C -2.94509946 1.93841912 -1.40842959

H -2.40468884 2.06619691 -2.35236062

H -3.46795569 0.97588064 -1.43220023

H -3.68069500 2.74482387 -1.30440869

C -2.94509946 1.93841912 1.40842959

H -3.46795569 0.97588064 1.43220023

H -2.40468884 2.06619691 2.35236062

H -3.68069500 2.74482387 1.30440869

C -1.17637743 3.71159842 0.00000000

H -1.54587491 4.23222734 -0.88957818

H -1.54587491 4.23222734 0.88957818

H -0.08249344 3.73969350 0.00000000

trans-(Fe(NH)S4)PMe3 **(5t)** OPBE-Cosmo Singlet

Fe 3.11637033 3.00174313 8.07393616

S 3.32314898 5.05144611 8.98312617

S 4.84969040 3.40914240 6.82362314

S 1.22115111 2.73105309 9.08927648

S 2.84811344 0.96472346 7.13304525

P 4.29565135 2.21006750 9.76626775

C 4.70148426 0.41618626 9.83959955

C 5.98020563 2.89895679 10.04020800

C 3.58183305 2.45339643 11.44506934

C 5.43850169 5.03887921 7.25250384

C 6.58796675 5.55956051 6.65571679

C 7.02810940 6.83590746 6.99326731

C 6.31033867 7.57682282 7.94148097

C 5.17993193 7.04980249 8.55054282

C 4.71604775 5.75866028 8.22050344

C 0.77864252 1.01113813 8.92113729

C -0.26310269 0.46149283 9.66885892

C -0.61956284 -0.87209469 9.48229378

C 0.07413667 -1.63792000 8.53760814

C 1.11793298 -1.09133441 7.80098653

C 1.50682057 0.25111524 7.98710187

N 1.97284898 3.74615211 6.50738841

C 4.02516081 3.79922118 5.23974272

C 2.73862614 4.52621123 5.52934873

C 0.01242244 3.46229931 7.89436144

C 0.74561233 4.39840487 6.96849706

H 1.71335104 2.86372470 6.05791531

H 5.27614059 0.20702366 10.74993258

H 5.29516028 0.13529528 8.96352439

H 3.78575044 -0.18266828 9.84090026

H 6.41146127 2.45997040 10.94777449

H 5.92574482 3.98590221 10.15388797

H 6.63004534 2.66067833 9.19086264

H 4.29092368 2.10398969 12.20484352

H 2.64703562 1.89190497 11.54925588

H 3.37361344 3.51667122 11.60461840

H 7.13436449 4.96692327 5.92257134

H 7.91971539 7.24931660 6.52493804

H 6.64529041 8.57733189 8.21460152

H 4.63998910 7.63641876 9.29293987

H -0.79538463 1.07830395 10.39214897

H -1.42687247 -1.31017884 10.06670178

H -0.19633005 -2.68232010 8.38287248

H 1.65422819 -1.70805451 7.08067258

H 3.84836058 2.82923081 4.76020918

H 4.70586955 4.37921426 4.61089652

H 2.94296370 5.51130220 5.95974446

H 2.16436617 4.67034482 4.60239847

H -0.76754461 3.97874297 8.46158654

H -0.43765128 2.62712320 7.34998358

H 0.09174399 4.66542612 6.12508219

H 1.03101032 5.31855415 7.48661767

trans-(Fe(NH)S4)PMe3 **(5t)** OPBE-Cosmo Triplet

Fe 3.13494339 2.98880368 8.06544762

S 3.35987812 5.00564529 8.99368961

S 4.80514532 3.47533612 6.69335240

S 1.14923540 2.77757676 9.01589759

S 2.88861879 0.93852495 7.18769868

P 4.46995440 2.05137942 10.01908165

C 4.85149331 0.24986215 10.09924354

C 6.15757261 2.73981256 10.29750720

C 3.73502245 2.30782929 11.69061976

C 5.40623352 5.08959820 7.16775610

C 6.51313315 5.65721065 6.53699693

C 6.96093088 6.91770980 6.92487803

C 6.30215495 7.59143763 7.95717214

C 5.20866149 7.01762693 8.59536519

C 4.74000043 5.74827465 8.21067820

C 0.70951662 1.05536359 8.85914312

C -0.37973706 0.52779557 9.55288549

C -0.70905571 -0.81834563 9.40760094

C 0.06093635 -1.62369096 8.56377648

C 1.14988046 -1.09753108 7.87691765

C 1.50361640 0.25694783 8.01902079

N 1.80482462 3.84484049 6.26261588

C 3.94440836 3.91506866 5.13753372

C 2.64083842 4.64631806 5.39008938

C -0.04373756 3.50583790 7.79762890

C 0.63636157 4.47067567 6.84628198

H 1.53191257 2.99180412 5.78059415

H 5.41922218 0.00719734 11.00616021

H 5.43710837 -0.03658308 9.21862169

H 3.92003499 -0.32569272 10.08879705

H 6.61061872 2.32015119 11.20447414

H 6.09750676 3.82893818 10.39483930

H 6.79601861 2.50393762 9.43802757

H 4.40476929 1.94320236 12.47965108

H 2.77947492 1.77522880 11.75895400

H 3.54487054 3.37589631 11.84528239

H 7.02065382 5.11613062 5.73940564

H 7.82068410 7.36674421 6.43051324

H 6.64766377 8.57606186 8.27092662

H 4.70585632 7.55223671 9.40017076

H -0.96926751 1.17096236 10.20505147

H -1.55499952 -1.23533412 9.95146921

H -0.18505963 -2.67874550 8.44619648

H 1.74545094 -1.74038036 7.22989845

H 3.77091443 2.95137762 4.64355099

H 4.62855146 4.49713929 4.51338556

H 2.83616833 5.60618791 5.88040015

H 2.16590502 4.86483704 4.41824637

H -0.83646466 4.00703384 8.36178265

H -0.48147245 2.66222512 7.25554714

H -0.11220092 4.78357711 6.09774118

H 0.96169551 5.36944036 7.38096162

trans-(Fe(NH)S4)PMe3 **(5t)** OPBE-Cosmo Quintet

Fe 3.17041044 2.97332049 8.05871966

S 3.47471805 5.13120899 9.03813785

S 4.99127918 3.62310252 6.56930744

S 0.84325612 2.73114887 9.01623520

S 2.73248822 0.80225758 7.11748956

P 4.54237865 1.94468511 10.10858299

C 4.85980510 0.13718444 10.20244422

C 6.23810280 2.61542786 10.32502601

C 3.79009234 2.27634642 11.75091157

C 5.48780038 5.24117150 7.11712707

C 6.57345354 5.85324119 6.48346324

C 7.00458589 7.11560992 6.87722509

C 6.34671855 7.75589693 7.93023331

C 5.27969878 7.14300013 8.57422297

C 4.81660783 5.86607903 8.19227712

C 0.55031365 0.98850045 8.84973911

C -0.50872031 0.43409309 9.57784520

C -0.78951552 -0.92613797 9.50418108

C 0.00737938 -1.73697405 8.69188871

C 1.06762621 -1.19488805 7.97703745

C 1.38039801 0.18021343 8.03369117

N 1.89941559 3.83684409 6.32250075

C 3.99959255 4.01891176 5.09581815

C 2.68206768 4.68362400 5.43001157

C -0.12794924 3.43018037 7.62309937

C 0.66095032 4.43098737 6.80660110

H 1.67412896 2.97091379 5.83384843

H 5.41400502 -0.11664972 11.11434944

H 5.44054432 -0.17452160 9.32708609

H 3.90778295 -0.40358391 10.19152941

H 6.70360363 2.20962670 11.23115103

H 6.19265653 3.70692102 10.39555105

H 6.85068580 2.34634811 9.45688533

H 4.43418889 1.90442742 12.55680036

H 2.81419477 1.78213350 11.81529180

H 3.64227144 3.35497476 11.87151847

H 7.07811295 5.33440036 5.66946057

H 7.84571365 7.58891557 6.37365579

H 6.67141483 8.74380153 8.25607526

H 4.78102330 7.65476692 9.39605006

H -1.11721806 1.08449744 10.20423760

H -1.61677620 -1.34654443 10.07336148

H -0.19379582 -2.80575969 8.62143458

H 1.68574757 -1.84337783 7.35786515

H 3.85079638 3.05111007 4.60226723

H 4.60113744 4.64464374 4.43042062

H 2.85972836 5.64193172 5.92934111

H 2.14764840 4.89462231 4.48913813

H -1.02092420 3.90238322 8.04313063

H -0.44133806 2.57976449 7.01041689

H 0.01299977 4.77087845 5.98194027

H 0.91479083 5.30960417 7.40968642

Meso-(Fe(NH)S4)NH3  **(6m)** OPBE-Cosmo Singlet

Fe -0.24378984 -0.41994660 0.00000000

S 0.53677041 -1.87324460 1.53538133

S -0.92492616 0.87791299 1.60608205

S -0.92492616 0.87791299 -1.60608205

S 0.53677041 -1.87324460 -1.53538133

C -0.67764692 -0.01536149 3.13688282

C -1.15709050 0.49838178 4.34344928

C -0.96626601 -0.21203127 5.52560744

C -0.30143524 -1.44329337 5.48196673

C 0.16579388 -1.95927559 4.27955431

C -0.01824762 -1.25586514 3.07148392

C -0.67764692 -0.01536149 -3.13688282

C -1.15709050 0.49838178 -4.34344928

C -0.96626601 -0.21203127 -5.52560744

C -0.30143524 -1.44329337 -5.48196673

C 0.16579388 -1.95927559 -4.27955431

C -0.01824762 -1.25586514 -3.07148392

N 1.50015717 0.62389786 0.00000000

C 0.44783636 2.08008940 1.70820162

C 1.71040194 1.39637229 1.24718081

C 0.44783636 2.08008940 -1.70820162

C 1.71040194 1.39637229 -1.24718081

N -2.01541706 -1.40756385 0.00000000

H -1.67521853 1.45691281 4.35650938

H -1.33738966 0.18534274 6.46877275

H -0.15226440 -2.01171970 6.39974952

H 0.67531166 -2.92199241 4.26425579

H -1.67521853 1.45691281 -4.35650938

H -1.33738966 0.18534274 -6.46877275

H -0.15226440 -2.01171970 -6.39974952

H 0.67531166 -2.92199241 -4.26425579

H 2.20993521 -0.10589948 0.00000000

H 0.53255075 2.43975583 2.73722382

H 0.15560563 2.92553843 1.07855425

H 2.02649697 0.67836660 2.00930877

H 2.52119409 2.12709516 1.11705878

H 0.15560563 2.92553843 -1.07855425

H 0.53255075 2.43975583 -2.73722382

H 2.52119409 2.12709516 -1.11705878

H 2.02649697 0.67836660 -2.00930877

H -2.08320202 -2.01484502 0.81336607

H -2.08320202 -2.01484502 -0.81336607

H -2.84389590 -0.81793763 0.00000000

Meso-(Fe(NH)S4)NH3  **(6m)** OPBE-Cosmo Triplet

Fe -0.49286458 -0.57306403 0.00000000

S 0.22390971 -2.05458253 1.52297688

S -1.09909109 0.77756194 1.69731644

S -1.09909109 0.77756194 -1.69731644

S 0.22390971 -2.05458253 -1.52297688

C -0.73369738 -0.10685570 3.20395075

C -1.07982057 0.43224044 4.44498094

C -0.83135968 -0.28927104 5.60901107

C -0.25076016 -1.55824813 5.51763168

C 0.08008463 -2.10025476 4.28112438

C -0.15911937 -1.38301162 3.09381309

C -0.73369738 -0.10685570 -3.20395075

C -1.07982057 0.43224044 -4.44498094

C -0.83135968 -0.28927104 -5.60901107

C -0.25076016 -1.55824813 -5.51763168

C 0.08008463 -2.10025476 -4.28112438

C -0.15911937 -1.38301162 -3.09381309

N 1.41998153 0.87901262 0.00000000

C 0.14205075 2.11232688 1.73090385

C 1.49805158 1.63349714 1.24834553

C 0.14205075 2.11232688 -1.73090385

C 1.49805158 1.63349714 -1.24834553

N -2.78787349 -1.32145507 0.00000000

H -1.54282156 1.41656886 4.49925071

H -1.09703206 0.13052792 6.57769384

H -0.05956948 -2.13492275 6.42204534

H 0.52536929 -3.09252189 4.22430503

H -1.54282156 1.41656886 -4.49925071

H -1.09703206 0.13052792 -6.57769384

H -0.05956948 -2.13492275 -6.42204534

H 0.52536929 -3.09252189 -4.22430503

H 2.16577801 0.19291686 0.00000000

H 0.19589030 2.50365081 2.75093639

H -0.27741535 2.90186727 1.10019231

H 1.92654015 0.96799484 2.00416464

H 2.16887370 2.50403552 1.16420265

H -0.27741535 2.90186727 -1.10019231

H 0.19589030 2.50365081 -2.75093639

H 2.16887370 2.50403552 -1.16420265

H 1.92654015 0.96799484 -2.00416464

H -2.98055804 -1.90143598 0.81203995

H -2.98055804 -1.90143598 -0.81203995

H -3.49846011 -0.59365750 0.00000000

Meso-(Fe(NH)S4)NH3  **(6m)** OPBE-Cosmo Quintet

Fe -0.37904649 -0.62655327 0.00000000

S 0.38634331 -2.04916640 1.71212388

S -1.01025070 0.92330582 1.90563818

S -1.01025070 0.92330582 -1.90563818

S 0.38634331 -2.04916640 -1.71212388

C -0.53946181 0.00943576 3.35889808

C -0.81050057 0.57278992 4.61104469

C -0.50694545 -0.11433351 5.78141861

C 0.05898792 -1.38787052 5.69152515

C 0.31798208 -1.95768012 4.45112521

C 0.03168608 -1.27885049 3.24867681

C -0.53946181 0.00943576 -3.35889808

C -0.81050057 0.57278992 -4.61104469

C -0.50694545 -0.11433351 -5.78141861

C 0.05898792 -1.38787052 -5.69152515

C 0.31798208 -1.95768012 -4.45112521

C 0.03168608 -1.27885049 -3.24867681

N 1.46656288 0.82602822 0.00000000

C 0.30897548 2.16021213 1.76858762

C 1.61194957 1.58685757 1.24639181

C 0.30897548 2.16021213 -1.76858762

C 1.61194957 1.58685757 -1.24639181

N -2.56028494 -1.25695578 0.00000000

H -1.26510669 1.56108294 4.66330624

H -0.71773792 0.33580742 6.75002305

H 0.29537404 -1.94592550 6.59704320

H 0.75547196 -2.95338902 4.39662578

H -1.26510669 1.56108294 -4.66330624

H -0.71773792 0.33580742 -6.75002305

H 0.29537404 -1.94592550 -6.59704320

H 0.75547196 -2.95338902 -4.39662578

H 2.19809487 0.12154249 0.00000000

H 0.45880990 2.62130808 2.74947798

H -0.10662816 2.93017561 1.11140452

H 2.02112953 0.90436074 1.99727898

H 2.33500943 2.40946255 1.12920181

H -0.10662816 2.93017561 -1.11140452

H 0.45880990 2.62130808 -2.74947798

H 2.33500943 2.40946255 -1.12920181

H 2.02112953 0.90436074 -1.99727898

H -2.78014592 -1.82594568 0.81280567

H -2.78014592 -1.82594568 -0.81280567

H -3.22346680 -0.48647529 0.00000000

trans-(Fe(NH)S4)NH3  **(6t)** OPBE-Cosmo Singlet

Fe 3.09295952 3.03425101 8.03928722

S 3.32040996 5.06688221 8.98791734

S 4.84982799 3.43765077 6.81828533

S 1.21923814 2.73710476 9.08743018

S 2.90870794 0.94291131 7.18938199

C 5.45734993 5.05362685 7.27610356

C 6.61133628 5.57453147 6.68700810

C 7.06816018 6.83752516 7.05128366

C 6.36489420 7.56348596 8.02138145

C 5.22874747 7.03727528 8.62122185

C 4.74487415 5.76096114 8.26266140

C 0.80015728 1.00651100 8.94466610

C -0.25183175 0.46055460 9.68100460

C -0.57860452 -0.88496640 9.53012823

C 0.15949032 -1.67030353 8.63765175

C 1.21310656 -1.12730312 7.91190314

C 1.56759023 0.22931261 8.05717023

N 1.97836142 3.73112453 6.51041636

C 4.03106114 3.83588998 5.23490392

C 2.73216118 4.53615288 5.53531890

C 0.00302107 3.44573871 7.88974914

C 0.73619933 4.37654244 6.95772512

H 1.72124267 2.85833609 6.04096364

H 7.14639322 4.99312548 5.93674165

H 7.96218662 7.25119889 6.58784769

H 6.71282666 8.55345647 8.31573735

H 4.69606125 7.61595547 9.37506395

H -0.81674698 1.09052900 10.36709137

H -1.39647124 -1.31739364 10.10385744

H -0.08600189 -2.72462517 8.51168057

H 1.78008612 -1.75650915 7.22670010

H 3.87227780 2.86960069 4.74129479

H 4.70196369 4.43780582 4.61652591

H 2.92074355 5.51890859 5.97888057

H 2.14875279 4.68034045 4.61428061

H -0.78301352 3.96359210 8.44692198

H -0.43837043 2.60093846 7.35295226

H 0.08997072 4.62718936 6.10356108

H 1.01061900 5.30498869 7.46683703

N 4.18513691 2.25837609 9.57710699

H 3.79844329 2.48870631 10.48813008

H 4.23069114 1.24369036 9.51849109

H 5.14496231 2.59151593 9.59664898

trans-(Fe(NH)S4)NH3  **(6t)** OPBE-Cosmo Triplet

Fe 3.10842790 3.01849317 8.02252923

S 3.35831757 5.01440264 9.02743736

S 4.83342932 3.48227470 6.74130327

S 1.18537873 2.76138817 9.03490299

S 2.92351168 0.89766771 7.22331654

C 5.44500793 5.08735555 7.24202137

C 6.57297834 5.64232278 6.63745964

C 7.02462794 6.89784713 7.03616930

C 6.34954542 7.57719218 8.05373746

C 5.23744662 7.01334906 8.66896687

C 4.76346044 5.74877737 8.27438903

C 0.76412613 1.02925504 8.92617982

C -0.30803831 0.50876212 9.65095315

C -0.63014638 -0.84191941 9.53677681

C 0.13075017 -1.65709157 8.69471716

C 1.20473445 -1.13740299 7.97925576

C 1.55274840 0.22184169 8.08890393

N 1.85681258 3.81562250 6.30080713

C 3.99500829 3.93592724 5.17604301

C 2.67783638 4.64082308 5.42666241

C -0.01793540 3.43990189 7.79508038

C 0.65278141 4.41616512 6.85104034

H 1.60661388 2.95958304 5.80933112

H 7.09073012 5.09754433 5.84907762

H 7.89808738 7.33971278 6.55980870

H 6.69656504 8.55908162 8.37416434

H 4.72233173 7.55380731 9.46196385

H -0.89136838 1.16098948 10.29950855

H -1.46452555 -1.25402731 10.10166347

H -0.11089703 -2.71537145 8.59995157

H 1.79202436 -1.78869424 7.33321078

H 3.84241474 2.97660985 4.66689671

H 4.67896777 4.53767374 4.57108176

H 2.84968828 5.60319594 5.92039696

H 2.19324231 4.84598299 4.45793149

H -0.83447442 3.91911475 8.34372977

H -0.41603227 2.57694080 7.25306371

H -0.08039102 4.69559293 6.07619203

H 0.94030034 5.32943773 7.38219089

N 4.42334288 2.03909139 9.88238035

H 4.07218826 2.30787904 10.79764532

H 4.41059870 1.02326634 9.85687136

H 5.40323573 2.31026404 9.87315944

trans-(Fe(NH)S4)NH3  **(6t)** OPBE-Cosmo Quintet

Fe 3.21978426 2.95580419 8.17323468

S 3.55027397 5.13046815 9.12783234

S 5.06017806 3.58841231 6.65116375

S 0.91426165 2.66675488 9.11677571

S 2.84349267 0.73881505 7.24773648

C 5.53404729 5.22468181 7.16563834

C 6.59592981 5.84380384 6.49816749

C 7.01484663 7.11956287 6.85934419

C 6.37143483 7.76724196 7.91658530

C 5.32926099 7.14845648 8.59475346

C 4.87670173 5.85831335 8.24514669

C 0.59458885 0.93270718 8.89815671

C -0.50227441 0.38292747 9.57157074

C -0.80993012 -0.96786519 9.45055637

C -0.00111445 -1.77481128 8.64664247

C 1.09637906 -1.23782549 7.98621974

C 1.43804870 0.12789526 8.09261400

N 1.95488553 3.77722116 6.43026294

C 4.04604691 3.94022045 5.18130885

C 2.72996933 4.60742671 5.51398142

C -0.06820513 3.41184173 7.75394373

C 0.72734249 4.39182455 6.91939047

H 1.71558682 2.90784644 5.95354832

H 7.09054438 5.31895791 5.68193222

H 7.83506131 7.59798144 6.32693367

H 6.68619846 8.76628944 8.21714845

H 4.83987258 7.66713750 9.41781670

H -1.12039471 1.03006468 10.19181622

H -1.66741581 -1.38394085 9.97647230

H -0.22316251 -2.83621172 8.53835851

H 1.72148662 -1.88289520 7.37032304

H 3.89620084 2.95942905 4.71427659

H 4.63592184 4.55166360 4.49263229

H 2.90950012 5.57611371 5.99242274

H 2.18588675 4.79863432 4.57451400

H -0.93463339 3.90933026 8.19953426

H -0.42569717 2.57446266 7.14767383

H 0.07673864 4.73020853 6.09628648

H 0.99856752 5.27377146 7.50974219

N 4.36286109 2.01149004 9.88033773

H 3.99115959 2.27068370 10.79011883

H 4.35284959 0.99654712 9.83386168

H 5.33938415 2.29414424 9.88866063

Meso-(Fe(NH)S4)N2H4 **(7m)** OPBE-Cosmo Singlet

Fe -0.09804120 0.41059551 0.00000000

N -1.65164792 1.75218736 0.00000000

H -2.26033775 1.58448845 0.79791356

H -2.26033775 1.58448845 -0.79791356

N -1.43459158 3.18594496 0.00000000

H -0.79685521 3.31567647 0.79195185

H -0.79685521 3.31567647 -0.79195185

S 0.99121566 1.64450085 1.53962215

S -1.02843852 -0.72122890 1.61241048

S 0.99121566 1.64450085 -1.53962215

S -1.02843852 -0.72122890 -1.61241048

N 1.38558977 -0.99452884 0.00000000

H 2.23347407 -0.43134402 0.00000000

C -0.56461678 0.07423034 3.14795797

C -1.11296929 -0.34790017 4.36040306

H -1.83088819 -1.16748143 4.37526130

C -0.73821549 0.27733439 5.54669939

H -1.16182294 -0.04946114 6.49478764

C 0.18530200 1.32832644 5.50244271

H 0.48420618 1.82713844 6.42413930

C 0.72040497 1.75666579 4.29404953

H 1.43344750 2.58013121 4.27791915

C 0.35307129 1.13702463 3.08207858

C -0.56461678 0.07423034 -3.14795797

C -1.11296929 -0.34790017 -4.36040306

H -1.83088819 -1.16748143 -4.37526130

C -0.73821549 0.27733439 -5.54669939

H -1.16182294 -0.04946114 -6.49478764

C 0.18530200 1.32832644 -5.50244271

H 0.48420618 1.82713844 -6.42413930

C 0.72040497 1.75666579 -4.29404953

H 1.43344750 2.58013121 -4.27791915

C 0.35307129 1.13702463 -3.08207858

C 0.04541770 -2.19561250 1.69969351

H -0.42338784 -2.95222642 1.06453529

H 0.04729839 -2.57172576 2.72618677

C 1.42648723 -1.79664831 1.24488948

H 2.06163487 -2.68396848 1.11314763

H 1.88742919 -1.16610980 2.01037771

C 0.04541770 -2.19561250 -1.69969351

H 0.04729839 -2.57172576 -2.72618677

H -0.42338784 -2.95222642 -1.06453529

C 1.42648723 -1.79664831 -1.24488948

H 1.88742919 -1.16610980 -2.01037771

H 2.06163487 -2.68396848 -1.11314763

Meso-(Fe(NH)S4)N2H4 **(7m)** OPBE-Cosmo Triplet

Fe -0.08373595 0.48291128 0.00000000

N -2.26494636 1.76140034 0.00000000

H -2.85459428 1.53015094 0.79833108

H -2.85459428 1.53015094 -0.79833108

N -2.17820892 3.21487402 0.00000000

H -1.56124539 3.41316150 0.78983250

H -1.56124539 3.41316150 -0.78983250

S 0.94223925 1.76865748 1.51668285

S -1.01495138 -0.65704658 1.70321730

S 0.94223925 1.76865748 -1.51668285

S -1.01495138 -0.65704658 -1.70321730

N 1.38538286 -1.39735973 0.00000000

H 2.28782216 -0.93590288 0.00000000

C -0.41310698 0.08837313 3.20994686

C -0.83978630 -0.37469612 4.45634184

H -1.52293825 -1.22072724 4.51847730

C -0.38773611 0.24473389 5.61819653

H -0.71323145 -0.11868123 6.59132968

C 0.47459473 1.34125212 5.51923985

H 0.82771365 1.83831466 6.42220833

C 0.88533206 1.81163249 4.27769054

H 1.55419622 2.66887952 4.21533971

C 0.44701666 1.19113406 3.09261503

C -0.41310698 0.08837313 -3.20994686

C -0.83978630 -0.37469612 -4.45634184

H -1.52293825 -1.22072724 -4.51847730

C -0.38773611 0.24473389 -5.61819653

H -0.71323145 -0.11868123 -6.59132968

C 0.47459473 1.34125212 -5.51923985

H 0.82771365 1.83831466 -6.42220833

C 0.88533206 1.81163249 -4.27769054

H 1.55419622 2.66887952 -4.21533971

C 0.44701666 1.19113406 -3.09261503

C -0.16799631 -2.27042070 1.72741658

H -0.77835623 -2.92112668 1.09442216

H -0.21452158 -2.66777248 2.74551338

C 1.26501197 -2.15246074 1.24562080

H 1.69129017 -3.16470855 1.15600569

H 1.84928239 -1.62331577 2.00500444

C -0.16799631 -2.27042070 -1.72741658

H -0.21452158 -2.66777248 -2.74551338

H -0.77835623 -2.92112668 -1.09442216

C 1.26501197 -2.15246074 -1.24562080

H 1.84928239 -1.62331577 -2.00500444

H 1.69129017 -3.16470855 -1.15600569

Meso-(Fe(NH)S4)N2H4 **(7m)** OPBE-Cosmo Quintet

Fe -0.11255706 0.60438551 0.00000000

N -2.06835119 1.75691345 0.00000000

H -2.65160083 1.51727712 0.79980273

H -2.65160083 1.51727712 -0.79980273

N -1.98377861 3.20705067 0.00000000

H -1.37154064 3.40949166 0.79337534

H -1.37154064 3.40949166 -0.79337534

S 0.94472903 1.81407358 1.71310498

S -1.10968839 -0.74561392 1.91711286

S 0.94472903 1.81407358 -1.71310498

S -1.10968839 -0.74561392 -1.91711286

N 1.32061421 -1.23358943 0.00000000

H 2.20188960 -0.72855166 0.00000000

C -0.42941517 0.03062772 3.36777450

C -0.81670835 -0.45225022 4.62295912

H -1.48686900 -1.30877440 4.68087069

C -0.35493506 0.14657628 5.79036541

H -0.65793242 -0.24203350 6.76106222

C 0.48460571 1.25858458 5.69437001

H 0.84661269 1.75015003 6.59695165

C 0.86247636 1.74985263 4.45121782

H 1.51570281 2.61921042 4.39174200

C 0.42218502 1.15278406 3.25192543

C -0.42941517 0.03062772 -3.36777450

C -0.81670835 -0.45225022 -4.62295912

H -1.48686900 -1.30877440 -4.68087069

C -0.35493506 0.14657628 -5.79036541

H -0.65793242 -0.24203350 -6.76106222

C 0.48460571 1.25858458 -5.69437001

H 0.84661269 1.75015003 -6.59695165

C 0.86247636 1.74985263 -4.45121782

H 1.51570281 2.61921042 -4.39174200

C 0.42218502 1.15278406 -3.25192543

C -0.12135463 -2.25967046 1.76654606

H -0.70968543 -2.90333097 1.10580159

H -0.08317079 -2.75065910 2.74358083

C 1.27963314 -2.00729789 1.24701465

H 1.79082524 -2.97584942 1.13076605

H 1.83585029 -1.43938699 1.99897552

C -0.12135463 -2.25967046 -1.76654606

H -0.08317079 -2.75065910 -2.74358083

H -0.70968543 -2.90333097 -1.10580159

C 1.27963314 -2.00729789 -1.24701465

H 1.83585029 -1.43938699 -1.99897552

H 1.79082524 -2.97584942 -1.13076605

trans-(Fe(NH)S4)N2H4 **(7t)** OPBE-Cosmo Singlet

Fe 3.07816796 3.02465650 8.05427722

S 3.28102171 5.06616835 8.98225673

S 4.85425138 3.43152025 6.85620194

S 1.18673343 2.73860762 9.07738746

S 2.89349727 0.93149325 7.20156418

C 5.44705426 5.05342047 7.31106947

C 6.61017368 5.57476484 6.74071059

C 7.05422112 6.84155802 7.10746059

C 6.32823651 7.57220945 8.05668657

C 5.18195074 7.04574953 8.63700880

C 4.71362464 5.76511148 8.27732755

C 0.76560835 1.00798952 8.93639717

C -0.30085526 0.46894153 9.65680797

C -0.63469625 -0.87404418 9.49958411

C 0.11090391 -1.66423281 8.61813410

C 1.17890425 -1.12819108 7.90822430

C 1.53875325 0.22591529 8.05883873

N 1.99041926 3.71480841 6.50598291

C 4.06010344 3.80964861 5.25696797

C 2.75576937 4.51039624 5.53141093

C -0.00869332 3.43083391 7.84736680

C 0.73702061 4.35936746 6.92412078

H 1.74335910 2.83586881 6.04226330

H 7.16330255 4.99046848 6.00606546

H 7.95671440 7.25525979 6.66085616

H 6.66676389 8.56522855 8.35157059

H 4.63109363 7.62659882 9.37588682

H -0.87183963 1.10263182 10.33428079

H -1.46478750 -1.30076001 10.05990979

H -0.14062145 -2.71651500 8.48745590

H 1.75128723 -1.76068648 7.23068533

H 3.91132261 2.83769236 4.77192939

H 4.73952311 4.40641079 4.64294350

H 2.93558274 5.49949996 5.96380801

H 2.18389387 4.64041033 4.60129090

H -0.80879609 3.94752045 8.38529082

H -0.43386290 2.58003384 7.30700275

H 0.10786484 4.59880112 6.05439681

H 0.99587083 5.29350078 7.43041058

N 4.19023025 2.15094147 9.55580126

H 3.86817244 1.18776373 9.60665413

H 5.15031600 2.09208426 9.22053308

N 4.16707451 2.68030287 10.89002009

H 5.07342972 2.49051504 11.31796785

H 4.12482605 3.69468644 10.75394639

trans-(Fe(NH)S4)N2H4 **(7t)** OPBE-Cosmo Triplet

Fe 3.03429282 3.04004392 7.99349169

S 3.29523012 5.02071679 9.00868067

S 4.79076546 3.47504931 6.75292242

S 1.10670648 2.76598514 8.98875609

S 2.94610225 0.90100047 7.28650771

C 5.41564759 5.06992286 7.26408541

C 6.56558467 5.60664776 6.68512687

C 7.03015097 6.85216220 7.09970655

C 6.34500878 7.53950047 8.10498722

C 5.21069089 6.99275613 8.69481188

C 4.72484532 5.73824568 8.28495511

C 0.70477890 1.02869041 8.87923809

C -0.39574044 0.50361428 9.55696122

C -0.70376235 -0.84921730 9.43205581

C 0.09869685 -1.66320727 8.62832394

C 1.20283682 -1.13987002 7.96349528

C 1.53610842 0.22145803 8.08538702

N 1.82992879 3.79876238 6.27004871

C 3.98205879 3.92862089 5.17139313

C 2.65756889 4.62520971 5.40014269

C -0.07919455 3.42691588 7.72215606

C 0.60806117 4.39850330 6.78636113

H 1.59191439 2.94085229 5.77537593

H 7.09075764 5.05568058 5.90605731

H 7.92167599 7.28029887 6.64480833

H 6.70291464 8.51336230 8.43753543

H 4.68923328 7.53823944 9.48007811

H -1.01336226 1.15342278 10.17530695

H -1.56219368 -1.26397531 9.95757961

H -0.13466979 -2.72236823 8.52358653

H 1.82316009 -1.78905673 7.34692864

H 3.84502835 2.96973584 4.65713074

H 4.67458883 4.53568456 4.58197011

H 2.81446359 5.59173608 5.88993275

H 2.18154749 4.81808000 4.42521405

H -0.90734266 3.90690028 8.25206092

H -0.46263744 2.55766075 7.18020394

H -0.10451039 4.66662153 5.98946676

H 0.87811831 5.31790432 7.31565268

N 4.44991022 2.00289937 9.97521656

H 4.06416276 1.08608021 10.17798088

H 5.34361810 1.83822682 9.51657070

N 4.63135452 2.68590157 11.21651187

H 5.57420497 2.52242072 11.56949955

H 4.58882824 3.67770673 10.98316111

trans-(Fe(NH)S4)N2H4 **(7t)** OPBE-Cosmo Quintet

Fe 3.15799170 2.97539221 8.19682117

S 3.48776544 5.15980944 9.09859265

S 5.02889257 3.56026484 6.68037645

S 0.85553938 2.64591852 9.10708859

S 2.90858094 0.73249138 7.36257271

C 5.51383590 5.19696191 7.17732627

C 6.59765916 5.79223234 6.52358335

C 7.03266615 7.06277474 6.88392130

C 6.38395728 7.72921951 7.92597132

C 5.31805513 7.13491695 8.58914524

C 4.84911148 5.85184257 8.23860024

C 0.54052704 0.91607091 8.83766064

C -0.60876339 0.36336908 9.41437123

C -0.91926661 -0.98038288 9.23611417

C -0.06080194 -1.77806148 8.47612727

C 1.09047291 -1.23947335 7.91623763

C 1.43466937 0.11900403 8.08304224

N 1.91726315 3.74414388 6.43455457

C 4.02114859 3.89159541 5.20121121

C 2.70272887 4.56267048 5.51477783

C -0.12019626 3.41840036 7.75395961

C 0.69058372 4.37537772 6.90750779

H 1.67601177 2.87308955 5.96229933

H 7.09727869 5.25218579 5.72050025

H 7.87104431 7.52230327 6.36335430

H 6.71373155 8.72310117 8.22715043

H 4.82432852 7.66715020 9.40080471

H -1.26645768 1.00162934 10.00220143

H -1.81892402 -1.39858372 9.68413309

H -0.28640713 -2.83322134 8.32343529

H 1.75428873 -1.87647258 7.33334254

H 3.87444161 2.90384322 4.74838206

H 4.61492356 4.49308209 4.50714286

H 2.87751506 5.53655136 5.98409032

H 2.16608864 4.74204675 4.56907723

H -0.96719207 3.94063745 8.20834718

H -0.50871396 2.58950876 7.15535589

H 0.04887587 4.70683848 6.07507546

H 0.96796150 5.26354405 7.48491743

N 4.35315598 2.02688274 9.96147965

H 3.90112696 1.14536976 10.18780823

H 5.24274263 1.77365291 9.53211476

N 4.55840849 2.74354749 11.18288371

H 5.48375534 2.51789467 11.54625068

H 4.59179958 3.72695620 10.90735488

Meso-(Fe(NH)S4)CO **(4m)** S12g Singlet

Fe -0.01846934 -0.11944695 0.00000000

S 1.08558067 -1.38149023 1.57117117

S -0.90664520 1.10110620 1.67267054

S -0.90664520 1.10110620 -1.67267054

S 1.08558067 -1.38149023 -1.57117117

C -0.57106374 0.15244327 3.16331417

C -1.26850137 0.44890159 4.33298904

C -1.06043787 -0.31799266 5.47182451

C -0.15653486 -1.38303384 5.41775847

C 0.51624998 -1.68989526 4.24616005

C 0.31124777 -0.93587166 3.07628039

C -0.57106374 0.15244327 -3.16331417

C -1.26850137 0.44890159 -4.33298904

C -1.06043787 -0.31799266 -5.47182451

C -0.15653486 -1.38303384 -5.41775847

C 0.51624998 -1.68989526 -4.24616005

C 0.31124777 -0.93587166 -3.07628039

N 1.60571322 1.27761697 0.00000000

C 0.31471706 2.48999962 1.75781358

C 1.67781679 2.04371799 1.26954173

C 0.31471706 2.48999962 -1.75781358

C 1.67781679 2.04371799 -1.26954173

H -1.98398605 1.27086361 4.34120663

H -1.61050227 -0.10275670 6.38638250

H 0.00608818 -2.00010267 6.30170938

H 1.19212310 -2.54282580 4.20854295

H -1.98398605 1.27086361 -4.34120663

H -1.61050227 -0.10275670 -6.38638250

H 0.00608818 -2.00010267 -6.30170938

H 1.19212310 -2.54282580 -4.20854295

H 2.38134048 0.61562999 0.00000000

H 0.35111175 2.84453621 2.79300810

H -0.12521762 3.28115559 1.13883442

H 2.10740976 1.36472484 2.01269656

H 2.34492092 2.91424367 1.16674640

H -0.12521762 3.28115559 -1.13883442

H 0.35111175 2.84453621 -2.79300810

H 2.34492092 2.91424367 -1.16674640

H 2.10740976 1.36472484 -2.01269656

C -1.28497148 -1.29526451 0.00000000

O -2.12416087 -2.10255668 0.00000000

Meso-(Fe(NH)S4)CO **(4m)** S12g Triplet

Fe -0.19404506 -0.25825596 0.00000000

S 0.96407310 -1.47473179 1.51570705

S -0.93668977 1.08263527 1.81947754

S -0.93668977 1.08263527 -1.81947754

S 0.96407310 -1.47473179 -1.51570705

C -0.41992755 0.15724661 3.27425353

C -0.91892476 0.50985857 4.52732303

C -0.58143191 -0.24454445 5.64409446

C 0.24986162 -1.35707611 5.48942072

C 0.72484159 -1.72022823 4.23946384

C 0.39061430 -0.97395919 3.09535723

C -0.41992755 0.15724661 -3.27425353

C -0.91892476 0.50985857 -4.52732303

C -0.58143191 -0.24454445 -5.64409446

C 0.24986162 -1.35707611 -5.48942072

C 0.72484159 -1.72022823 -4.23946384

C 0.39061430 -0.97395919 -3.09535723

N 1.54796093 1.47903189 0.00000000

C 0.18630849 2.54793765 1.79176347

C 1.57546809 2.21780407 1.26403670

C 0.18630849 2.54793765 -1.79176347

C 1.57546809 2.21780407 -1.26403670

H -1.58870758 1.36443697 4.61976659

H -0.97732317 0.01945573 6.62349571

H 0.51354429 -1.96261681 6.35687664

H 1.35325651 -2.60224764 4.12469535

H -1.58870758 1.36443697 -4.61976659

H -0.97732317 0.01945573 -6.62349571

H 0.51354429 -1.96261681 -6.35687664

H 1.35325651 -2.60224764 -4.12469535

H 2.27924737 0.77546163 0.00000000

H 0.22640849 2.95795106 2.80680216

H -0.34323706 3.26808491 1.15561516

H 2.07667462 1.58217806 2.00140656

H 2.15370854 3.15527861 1.17911063

H -0.34323706 3.26808491 -1.15561516

H 0.22640849 2.95795106 -2.80680216

H 2.15370854 3.15527861 -1.17911063

H 2.07667462 1.58217806 -2.00140656

C -1.89829108 -1.18737532 0.00000000

O -2.69552254 -2.02604029 0.00000000

Meso-(Fe(NH)S4)CO **(4m)** S12g Quintet

Fe 0.24668973 -0.50054717 0.00000000

S 1.27906427 -1.32221762 1.96091286

S -0.85760476 1.22797486 1.76188189

S -0.85760476 1.22797486 -1.76188189

S 1.27906427 -1.32221762 -1.96091286

C -0.63508731 0.27107581 3.25795540

C -1.46719790 0.57010329 4.34040546

C -1.45534644 -0.22072512 5.48259486

C -0.60443842 -1.32485821 5.53338212

C 0.21496185 -1.63516828 4.45808283

C 0.21978530 -0.85547535 3.28720991

C -0.63508731 0.27107581 -3.25795540

C -1.46719790 0.57010329 -4.34040546

C -1.45534644 -0.22072512 -5.48259486

C -0.60443842 -1.32485821 -5.53338212

C 0.21496185 -1.63516828 -4.45808283

C 0.21978530 -0.85547535 -3.28720991

N 1.81062176 1.39059737 0.00000000

C 0.42293063 2.55334214 1.75896877

C 1.80548239 2.13897307 1.26576764

C 0.42293063 2.55334214 -1.75896877

C 1.80548239 2.13897307 -1.26576764

H -2.14177453 1.42206331 4.26831723

H -2.11402183 0.01350619 6.31776356

H -0.59141220 -1.96321425 6.41709330

H 0.86076447 -2.51029727 4.49826273

H -2.14177453 1.42206331 -4.26831723

H -2.11402183 0.01350619 -6.31776356

H -0.59141220 -1.96321425 -6.41709330

H 0.86076447 -2.51029727 -4.49826273

H 2.63100207 0.79102262 0.00000000

H 0.48696531 2.96328041 2.77279618

H -0.02904813 3.32467248 1.12314643

H 2.24756341 1.47742848 2.01737184

H 2.42937549 3.04967177 1.20260980

H -0.02904813 3.32467248 -1.12314643

H 0.48696531 2.96328041 -2.77279618

H 2.42937549 3.04967177 -1.20260980

H 2.24756341 1.47742848 -2.01737184

C -1.32106137 -1.67085070 0.00000000

O -2.15198342 -2.47016341 0.00000000

trans-(Fe(NH)S4)CO **(4t)** S12g Singlet

Fe 8.44921384 10.04794616 1.81050375

S 9.84663178 8.82822752 3.08531238

S 6.77325817 8.52715001 2.32002895

S 7.14199205 11.07143845 0.29662237

S 10.06432525 11.65273755 1.31906637

C 9.10019182 12.96061446 0.64718960

C 9.58209502 14.27879605 0.58436673

H 10.59015863 14.48886883 0.93777458

C 8.77449063 15.30899143 0.12153878

H 9.16487368 16.32684270 0.11059699

C 7.46440123 15.06795913 -0.29847449

H 6.82926735 15.88590841 -0.63474811

C 6.97066457 13.76935817 -0.26176229

H 5.94839202 13.55138688 -0.56872266

C 7.78846091 12.74009995 0.19539394

C 7.43481810 7.63069888 3.67217683

C 6.62560184 6.80132573 4.47136413

H 5.56881741 6.70559386 4.22767271

C 7.15047952 6.13867728 5.57030969

H 6.49352555 5.51878635 6.18085747

C 8.49634554 6.27397044 5.92303437

H 8.89479326 5.77117638 6.80268783

C 9.31621679 7.08301366 5.14739071

H 10.36417190 7.22803733 5.40920538

C 8.78794549 7.73208130 4.03352234

C 7.90818091 11.04891297 3.11666878

O 7.54260886 11.73649731 3.98237577

N 9.15884265 8.87504225 0.19526270

H 9.97408624 9.43678824 -0.07615019

C 10.55673209 7.69858915 1.79422256

H 10.79501214 6.74557479 2.27511926

H 11.49210738 8.18755739 1.48937677

C 9.59957004 7.53997938 0.63466715

H 8.70806883 6.98823431 0.95265505

H 10.08603369 6.98872803 -0.18702288

C 7.83116445 10.29964508 -1.25312242

H 8.70218121 10.89743386 -1.54286971

H 7.06730133 10.35575480 -2.03505271

C 8.20696761 8.87080830 -0.92738048

H 7.32825874 8.29398605 -0.61239566

H 8.63578322 8.38378266 -1.81822921

trans-(Fe(NH)S4)CO **(4t)** S12g Triplet

Fe 8.46577498 10.10164177 1.82999388

S 10.05125880 8.53168823 3.14462257

S 6.78941660 8.65701381 2.58921348

S 7.08696026 11.15924589 -0.08706077

S 10.02558947 11.70221403 1.23529973

C 9.00674441 13.02955885 0.66876997

C 9.42386044 14.36025600 0.82055441

H 10.37195080 14.55637809 1.31793023

C 8.63323629 15.41630011 0.38538074

H 8.97471490 16.44012315 0.53906545

C 7.40252823 15.17927104 -0.22434258

H 6.77599296 16.00736305 -0.55336753

C 6.97244948 13.86963778 -0.39939812

H 6.01087621 13.66053287 -0.86544928

C 7.76546445 12.80596770 0.03187340

C 7.50111501 7.63428882 3.82484500

C 6.64879409 6.87655621 4.65101133

H 5.57548928 6.92669734 4.47556103

C 7.14752407 6.10494435 5.68846598

H 6.45473739 5.54387782 6.31617550

C 8.51795873 6.06033735 5.95133054

H 8.90787399 5.47658499 6.78373429

C 9.37970271 6.79584187 5.14830724

H 10.45147503 6.79619694 5.34303283

C 8.88395306 7.56043790 4.09098940

C 7.81343701 11.22410609 3.01430156

O 7.39719572 11.98685265 3.78871013

N 9.15727047 8.79365796 0.21062842

H 10.04020905 9.25373260 -0.02738334

C 10.47482868 7.41042356 1.74339297

H 10.62544575 6.40429833 2.14556979

H 11.44294999 7.78339350 1.38050491

C 9.43593362 7.41395635 0.64153322

H 8.49488237 6.98452478 1.00352909

H 9.79954242 6.80176495 -0.20162447

C 8.08106788 10.31718307 -1.39588809

H 9.03068280 10.85510815 -1.48875446

H 7.53433782 10.37479989 -2.34277140

C 8.29292346 8.87280700 -0.98078770

H 7.33592069 8.39619240 -0.72951370

H 8.73058321 8.31330684 -1.82409991

trans-(Fe(NH)S4)CO **(4t)** S12g Quintet

Fe 8.45819980 10.04029849 1.82207421

S 10.01318926 8.37398759 2.99582428

S 6.73182094 8.42505796 2.42353020

S 7.21770991 11.11658362 -0.12263736

S 10.08171031 11.84442248 1.30475795

C 8.99196290 13.09170966 0.71395007

C 9.30717738 14.44992932 0.89617543

H 10.23287032 14.70147055 1.41025684

C 8.45338588 15.45618685 0.46515103

H 8.72363776 16.49766694 0.64134113

C 7.25295205 15.14974401 -0.17486345

H 6.57888396 15.93939394 -0.50398947

C 6.91871206 13.81670789 -0.37973865

H 5.98275520 13.54910507 -0.86740512

C 7.77408422 12.80379966 0.05416076

C 7.44012152 7.66010314 3.83731135

C 6.59563136 7.10557672 4.81694650

H 5.51964626 7.17866721 4.67132327

C 7.10447920 6.49673554 5.95479083

H 6.41632176 6.09020464 6.69624224

C 8.48039879 6.41535707 6.16553197

H 8.88082351 5.94958320 7.06485282

C 9.34006046 6.95631698 5.21842958

H 10.41793419 6.92921887 5.37089401

C 8.83223339 7.56405112 4.06859938

C 7.86825978 11.19716462 3.29270488

O 7.50031225 11.94007762 4.09438831

N 9.28066031 8.72504325 0.01398668

H 10.20502925 9.13787189 -0.12641621

C 10.34790022 7.19399694 1.60847129

H 10.33515129 6.18076486 2.02098348

H 11.38223484 7.43156102 1.32291878

C 9.41321551 7.32198852 0.41808495

H 8.41330017 6.96378262 0.68847283

H 9.80239521 6.68836438 -0.40022681

C 8.29119993 10.42109338 -1.46035034

H 9.23947656 10.96868123 -1.43306967

H 7.79492957 10.59072167 -2.42134681

C 8.49271010 8.93695281 -1.20391952

H 7.52299649 8.43912931 -1.06434055

H 8.96537122 8.47892873 -2.09063643

Meso-(Fe(NH)S4)PMe3 **(5m)** S12g Singlet

Fe 0.27073819 -0.02348753 0.00000000

S 1.50383601 1.06377645 -1.60816807

S -0.75504703 -1.13645418 -1.63004055

S -0.75504703 -1.13645418 1.63004055

S 1.50383601 1.06377645 1.60816807

C -0.31350312 -0.30199299 -3.16382006

C -1.03878870 -0.55358026 -4.32565570

C -0.74980924 0.15154525 -5.48741990

C 0.26984600 1.10852262 -5.46397152

C 0.98029609 1.36576997 -4.30219039

C 0.69304810 0.67502220 -3.11006941

C -0.31350312 -0.30199299 3.16382006

C -1.03878870 -0.55358026 4.32565570

C -0.74980924 0.15154525 5.48741990

C 0.26984600 1.10852262 5.46397152

C 0.98029609 1.36576997 4.30219039

C 0.69304810 0.67502220 3.11006941

N 1.71135446 -1.59782689 0.00000000

C 0.28377500 -2.67449039 -1.73415618

C 1.69209982 -2.37868348 -1.26307730

C 0.28377500 -2.67449039 1.73415618

C 1.69209982 -2.37868348 1.26307730

H -1.84164266 -1.29103373 -4.31015927

H -1.32033375 -0.02991915 -6.39698986

H 0.50036302 1.67558896 -6.36629017

H 1.75575666 2.13046443 -4.29069931

H -1.84164266 -1.29103373 4.31015927

H -1.32033375 -0.02991915 6.39698986

H 0.50036302 1.67558896 6.36629017

H 1.75575666 2.13046443 4.29069931

H 2.56484381 -1.04087366 0.00000000

H 0.26640370 -3.02664938 -2.77039953

H -0.23300997 -3.41202324 -1.10875016

H 2.18841357 -1.75823163 -2.01567318

H 2.26128339 -3.31580241 -1.15402710

H -0.23300997 -3.41202324 1.10875016

H 0.26640370 -3.02664938 2.77039953

H 2.26128339 -3.31580241 1.15402710

H 2.18841357 -1.75823163 2.01567318

P -1.08663479 1.74957429 0.00000000

C -2.28142335 1.91933593 -1.40816341

H -1.73534630 1.98808241 -2.35516579

H -2.94499151 1.04728517 -1.44191434

H -2.88241736 2.82670611 -1.26836801

C -2.28142335 1.91933593 1.40816341

H -2.94499151 1.04728517 1.44191434

H -1.73534630 1.98808241 2.35516579

H -2.88241736 2.82670611 1.26836801

C -0.31307872 3.44385061 0.00000000

H -0.63393053 3.98850523 -0.89457414

H -0.63393053 3.98850523 0.89457414

H 0.77513725 3.36049302 0.00000000

Meso-(Fe(NH)S4)PMe3 **(5m)** S12g Triplet

Fe 0.39505569 0.09839786 0.00000000

S 1.47925097 1.09665476 -1.81750953

S -0.79566562 -1.29709652 -1.77147852

S -0.79566562 -1.29709652 1.77147852

S 1.47925097 1.09665476 1.81750953

C -0.37709912 -0.41873902 -3.27694916

C -1.12820272 -0.68933539 -4.42247185

C -0.93243783 0.04342058 -5.58581300

C 0.02547777 1.05976264 -5.58960191

C 0.76080660 1.34210198 -4.44945301

C 0.57800708 0.62207802 -3.25305469

C -0.37709912 -0.41873902 3.27694916

C -1.12820272 -0.68933539 4.42247185

C -0.93243783 0.04342058 5.58581300

C 0.02547777 1.05976264 5.58960191

C 0.76080660 1.34210198 4.44945301

C 0.57800708 0.62207802 3.25305469

N 1.79955878 -1.56547934 0.00000000

C 0.38284122 -2.71458297 -1.73292372

C 1.77714601 -2.33776009 -1.26469658

C 0.38284122 -2.71458297 1.73292372

C 1.77714601 -2.33776009 1.26469658

H -1.88094042 -1.47670986 -4.38832351

H -1.52628689 -0.16698770 -6.47437515

H 0.18856067 1.65052342 -6.49174487

H 1.48773474 2.15310369 -4.45537715

H -1.88094042 -1.47670986 4.38832351

H -1.52628689 -0.16698770 6.47437515

H 0.18856067 1.65052342 6.49174487

H 1.48773474 2.15310369 4.45537715

H 2.65678306 -1.01412269 0.00000000

H 0.42233689 -3.14878984 -2.73781968

H -0.10151101 -3.44482535 -1.07361650

H 2.23325711 -1.69281156 -2.02241172

H 2.38666136 -3.25305575 -1.17354845

H -0.10151101 -3.44482535 1.07361650

H 0.42233689 -3.14878984 2.73781968

H 2.38666136 -3.25305575 1.17354845

H 2.23325711 -1.69281156 2.02241172

P -0.92139602 1.94067236 0.00000000

C -2.10266410 2.09152545 -1.41516654

H -1.55100740 2.13610652 -2.35991357

H -2.76819868 1.22030073 -1.43012850

H -2.69961573 3.00467530 -1.29299963

C -2.10266410 2.09152545 1.41516654

H -2.76819868 1.22030073 1.43012850

H -1.55100740 2.13610652 2.35991357

H -2.69961573 3.00467530 1.29299963

C -0.07368264 3.59059146 0.00000000

H -0.36313095 4.14970426 -0.89660883

H -0.36313095 4.14970426 0.89660883

H 1.00876636 3.44222550 0.00000000

Meso-(Fe(NH)S4)PMe3 **(5m)** S12g Quintet

Fe 0.49377423 0.19116264 0.00000000

S 1.65743288 1.00799164 -1.86098462

S -0.75893172 -1.30267669 -1.83000870

S -0.75893172 -1.30267669 1.83000870

S 1.65743288 1.00799164 1.86098462

C -0.30566918 -0.39977066 -3.31028627

C -1.07625286 -0.62048202 -4.45482945

C -0.87965557 0.13919055 -5.59996902

C 0.09813804 1.13457825 -5.58826997

C 0.85761905 1.36392631 -4.45167820

C 0.67721829 0.61545801 -3.27312162

C -0.30566918 -0.39977066 3.31028627

C -1.07625286 -0.62048202 4.45482945

C -0.87965557 0.13919055 5.59996902

C 0.09813804 1.13457825 5.58826997

C 0.85761905 1.36392631 4.45167820

C 0.67721829 0.61545801 3.27312162

N 1.79332984 -1.80333446 0.00000000

C 0.31728621 -2.79631493 -1.77619455

C 1.73072023 -2.54760215 -1.26590046

C 0.31728621 -2.79631493 1.77619455

C 1.73072023 -2.54760215 1.26590046

H -1.84750700 -1.38964591 -4.43125990

H -1.48903651 -0.03472779 -6.48590540

H 0.26204381 1.74815292 -6.47482707

H 1.60849034 2.15251736 -4.44704737

H -1.84750700 -1.38964591 4.43125990

H -1.48903651 -0.03472779 6.48590540

H 0.26204381 1.74815292 6.47482707

H 1.60849034 2.15251736 4.44704737

H 2.64917667 -1.25406859 0.00000000

H 0.34256501 -3.23300417 -2.78063805

H -0.24177844 -3.48562121 -1.13118569

H 2.25627261 -1.93949335 -2.00936433

H 2.24922662 -3.52067074 -1.19010799

H -0.24177844 -3.48562121 1.13118569

H 0.34256501 -3.23300417 2.78063805

H 2.24922662 -3.52067074 1.19010799

H 2.25627261 -1.93949335 2.00936433

P -1.28125295 2.01628385 0.00000000

C -2.44537463 2.15417527 -1.43164671

H -1.86674947 2.18472097 -2.36240387

H -3.09866194 1.27389950 -1.45628203

H -3.05778829 3.06155233 -1.34714610

C -2.44537463 2.15417527 1.43164671

H -3.09866194 1.27389950 1.45628203

H -1.86674947 2.18472097 2.36240387

H -3.05778829 3.06155233 1.34714610

C -0.44813111 3.67796180 0.00000000

H -0.73719630 4.24096141 -0.89410423

H -0.73719630 4.24096141 0.89410423

H 0.63655895 3.53495588 0.00000000

trans-(Fe(NH)S4)PMe3 **(5t)** S12g Singlet

Fe 3.02032624 3.05654843 7.94187362

S 3.25723466 5.15219246 8.88443567

S 4.79695419 3.50051861 6.66765714

S 1.07722866 2.75103429 8.97044550

S 2.71448190 0.95321544 6.99680698

P 4.19986180 2.24795924 9.66928438

C 4.53674768 0.43113235 9.78903190

C 5.91667737 2.89087943 9.93344807

C 3.47261562 2.56524228 11.34147390

C 5.50912040 5.02616784 7.30220575

C 6.77973583 5.41532796 6.88626767

C 7.36327651 6.55639075 7.42083248

C 6.65532626 7.29427021 8.37524121

C 5.39701473 6.89628923 8.79682509

C 4.79166241 5.73492509 8.27966387

C 0.81412279 0.97492494 8.99148241

C -0.03807589 0.40561542 9.93278184

C -0.20287121 -0.97486991 9.96408373

C 0.48586621 -1.75996944 9.03541576

C 1.33680598 -1.18660748 8.10022992

C 1.54094668 0.20454500 8.06648799

N 1.87859617 3.82787559 6.34538132

C 3.95559940 4.12407356 5.13421208

C 2.63705163 4.76447964 5.50044771

C -0.10451198 3.25790566 7.61519081

C 0.57326512 4.33324304 6.79692562

H 1.72251481 2.95521045 5.82631506

H 5.15436632 0.23472239 10.67428246

H 5.05740517 0.09674789 8.88578719

H 3.59479789 -0.12081593 9.87016006

H 6.33815170 2.43501123 10.83798133

H 5.89809319 3.97943619 10.04366194

H 6.54749316 2.63156141 9.07510511

H 4.14035688 2.17723047 12.12050219

H 2.49893372 2.06778762 11.42205966

H 3.33682186 3.64447652 11.46807268

H 7.31395455 4.81002698 6.15338682

H 8.36085765 6.86155086 7.10880470

H 7.10541479 8.18725047 8.80976453

H 4.86895986 7.46732916 9.55927901

H -0.55660186 1.04597810 10.64631333

H -0.85063073 -1.43412379 10.70924415

H 0.37087599 -2.84409381 9.05667122

H 1.88790810 -1.81580029 7.40285050

H 3.81614585 3.23196539 4.50843035

H 4.63312038 4.81643479 4.62629505

H 2.80670321 5.67661188 6.08306763

H 2.07310267 5.02739659 4.59000619

H -1.03210942 3.61258936 8.07550411

H -0.30765201 2.35947382 7.02202280

H -0.06719334 4.61602108 5.94508149

H 0.75927516 5.22983546 7.40109787

trans-(Fe(NH)S4)PMe3 **(5t)** S12g Triplet

Fe 3.07742658 3.02635093 7.93724703

S 3.43410528 5.06189207 8.91606618

S 4.90643990 3.66267916 6.37808500

S 0.69408793 2.71714313 8.96313121

S 2.67965992 0.94364739 7.07993332

P 4.18676943 2.20141016 9.78195415

C 4.47443229 0.38002917 9.93079425

C 5.91361237 2.80968195 10.05221979

C 3.40505504 2.55964728 11.41797494

C 5.60367591 5.11648252 7.16864565

C 6.84219620 5.58680256 6.73690898

C 7.44042791 6.67172599 7.36630076

C 6.78199436 7.28222508 8.43383701

C 5.55164508 6.81202093 8.86880642

C 4.93587591 5.70831065 8.25437184

C 0.64702820 0.93227908 8.99523692

C -0.19923788 0.30380436 9.91007061

C -0.20846620 -1.08126311 10.02392468

C 0.62386452 -1.83679804 9.19824572

C 1.46870341 -1.21476236 8.28815187

C 1.51983675 0.18407378 8.17651082

N 1.86400781 3.90315106 6.28822753

C 3.89743330 4.42889183 5.03525911

C 2.56840464 4.95089449 5.53989364

C -0.18982699 3.13500795 7.39513298

C 0.51495191 4.29409451 6.71598426

H 1.77854621 3.06736798 5.70426509

H 5.08132187 0.17937680 10.82274473

H 4.99130564 0.01865032 9.03559886

H 3.51641351 -0.14277043 10.01395710

H 6.32707443 2.36123704 10.96469335

H 5.91929256 3.90034642 10.13877837

H 6.53171892 2.52037122 9.19406945

H 4.03887444 2.18201476 12.23049856

H 2.42636553 2.06761934 11.46254119

H 3.27130443 3.64164701 11.51987648

H 7.34023931 5.08382593 5.90822482

H 8.41540736 7.02794642 7.03638468

H 7.24148849 8.12990353 8.94313148

H 5.05565730 7.28181285 9.71722784

H -0.84735354 0.91523639 10.53668950

H -0.86183077 -1.56592068 10.74846359

H 0.62624317 -2.92435307 9.27691532

H 2.13725695 -1.81047677 7.66823448

H 3.75674624 3.62160072 4.30334506

H 4.48694416 5.22202269 4.56580321

H 2.72529511 5.79630912 6.21940115

H 1.96825943 5.30298893 4.68251431

H -1.22599573 3.39690729 7.63349929

H -0.18097809 2.23719101 6.76742769

H -0.09426128 4.63106082 5.85977282

H 0.61796314 5.14385210 7.40435125

trans-(Fe(NH)S4)PMe3 **(5t)** S12g Quintet

Fe 3.03007845 3.00690419 7.88908502

S 3.30587346 5.26703398 8.85598128

S 4.84691275 3.80709533 6.31905528

S 0.65394243 2.72028592 8.80242167

S 2.56889942 0.78374537 6.92160084

P 4.31505469 2.13757181 9.83945455

C 4.48700343 0.31351900 10.08972523

C 6.08016139 2.67760248 9.96881828

C 3.65267771 2.66938277 11.48073695

C 5.58313907 5.15646504 7.23221148

C 6.88414514 5.52783052 6.89030159

C 7.55890858 6.49340596 7.62541875

C 6.91437916 7.08274272 8.71320450

C 5.62420375 6.71135237 9.05988174

C 4.91471941 5.73192307 8.33775747

C 0.67450149 0.94340185 8.97871230

C -0.09495821 0.39195735 10.00550720

C -0.06226088 -0.97386553 10.25555562

C 0.73842875 -1.78828942 9.45383410

C 1.50579450 -1.24398723 8.43413600

C 1.51679874 0.13879896 8.17171594

N 1.74849106 3.93422170 6.09257483

C 3.82939063 4.63186358 5.01087038

C 2.44483858 5.05578219 5.46433454

C -0.23237972 3.01513872 7.20234524

C 0.37724464 4.22281857 6.50932678

H 1.73562464 3.12702213 5.46631472

H 5.12039737 0.10121256 10.96076580

H 4.92499603 -0.13170110 9.18919361

H 3.49477069 -0.12704487 10.23849600

H 6.53437592 2.29675414 10.89317769

H 6.12920924 3.77198495 9.95513111

H 6.63675055 2.29424267 9.10506448

H 4.29653666 2.31794187 12.29748023

H 2.64399814 2.25806705 11.60760296

H 3.59133760 3.76317256 11.49067119

H 7.36855241 5.03889455 6.04596384

H 8.57654183 6.77480019 7.35849328

H 7.43096834 7.83709970 9.30741922

H 5.13814069 7.16784024 9.92029537

H -0.71567254 1.05048669 10.61127439

H -0.65860236 -1.39719516 11.06258902

H 0.77195054 -2.86323257 9.63344056

H 2.14504061 -1.88541250 7.83019288

H 3.77006033 3.87353724 4.21740297

H 4.40337861 5.48121582 4.62781697

H 2.52537671 5.85361849 6.21212073

H 1.89576268 5.45383566 4.59011679

H -1.29163911 3.18086486 7.42377735

H -0.11974117 2.10755317 6.59939487

H -0.26814734 4.51005545 5.65934112

H 0.41078442 5.08232889 7.19394561

Meso-(Fe(NH)S4)NH3  **(6m)** S12g Singlet

Fe -0.20404493 -0.38551145 0.00000000

S 0.61696035 -1.84862515 1.58102234

S -0.89776455 0.93579810 1.65837270

S -0.89776455 0.93579810 -1.65837270

S 0.61696035 -1.84862515 -1.58102234

C -0.70111487 -0.01739300 3.17711829

C -1.28222452 0.43474610 4.36112486

C -1.16756663 -0.32297328 5.52036277

C -0.47160594 -1.53540091 5.47190177

C 0.09030886 -1.98985251 4.28923031

C -0.02449614 -1.24633942 3.09860743

C -0.70111487 -0.01739300 -3.17711829

C -1.28222452 0.43474610 -4.36112486

C -1.16756663 -0.32297328 -5.52036277

C -0.47160594 -1.53540091 -5.47190177

C 0.09030886 -1.98985251 -4.28923031

C -0.02449614 -1.24633942 -3.09860743

N 1.56543225 0.66323160 0.00000000

C 0.53318365 2.11366940 1.75269749

C 1.78749830 1.42202045 1.26437855

C 0.53318365 2.11366940 -1.75269749

C 1.78749830 1.42202045 -1.26437855

N -1.94508094 -1.49508395 0.00000000

H -1.83158512 1.37643342 4.36632879

H -1.62655486 0.01737236 6.44733949

H -0.38016676 -2.14259476 6.37300173

H 0.61484046 -2.94401518 4.26178559

H -1.83158512 1.37643342 -4.36632879

H -1.62655486 0.01737236 -6.44733949

H -0.38016676 -2.14259476 -6.37300173

H 0.61484046 -2.94401518 -4.26178559

H 2.23370479 -0.10802783 0.00000000

H 0.63266950 2.45199623 2.78874928

H 0.24151544 2.96925693 1.13236523

H 2.09325956 0.68475853 2.01327918

H 2.60336738 2.15139339 1.14045370

H 0.24151544 2.96925693 -1.13236523

H 0.63266950 2.45199623 -2.78874928

H 2.60336738 2.15139339 -1.14045370

H 2.09325956 0.68475853 -2.01327918

H -1.92195377 -2.10527665 0.81891290

H -1.92195377 -2.10527665 -0.81891290

H -2.83063525 -0.99194275 0.00000000

Meso-(Fe(NH)S4)NH3  **(6m)** S12g Triplet

Fe -0.25956620 -0.45049177 0.00000000

S 0.51084126 -1.91953596 1.56172589

S -0.89009571 0.92768793 1.74082540

S -0.89009571 0.92768793 -1.74082540

S 0.51084126 -1.91953596 -1.56172589

C -0.61528603 -0.02681024 3.24069523

C -1.11042607 0.43478896 4.46007783

C -0.95868502 -0.33730605 5.60505970

C -0.31452179 -1.57494950 5.50981891

C 0.15794142 -2.03955760 4.29216301

C 0.00198071 -1.28136831 3.11722653

C -0.61528603 -0.02681024 -3.24069523

C -1.11042607 0.43478896 -4.46007783

C -0.95868502 -0.33730605 -5.60505970

C -0.31452179 -1.57494950 -5.50981891

C 0.15794142 -2.03955760 -4.29216301

C 0.00198071 -1.28136831 -3.11722653

N 1.66526735 0.89914993 0.00000000

C 0.46587760 2.19138596 1.76531149

C 1.79048657 1.63092587 1.26455212

C 0.46587760 2.19138596 -1.76531149

C 1.79048657 1.63092587 -1.26455212

N -2.45155860 -1.45546075 0.00000000

H -1.62611565 1.39428944 4.50396144

H -1.35156685 0.01227003 6.55879586

H -0.19555639 -2.19350055 6.39989981

H 0.63902704 -3.01450635 4.22562532

H -1.62611565 1.39428944 -4.50396144

H -1.35156685 0.01227003 -6.55879586

H -0.19555639 -2.19350055 -6.39989981

H 0.63902704 -3.01450635 -4.22562532

H 2.31121656 0.11574853 0.00000000

H 0.55152758 2.56606938 2.79076968

H 0.08718407 3.00541932 1.13576043

H 2.15914001 0.91818550 2.01000622

H 2.52087923 2.45657202 1.19387520

H 0.08718407 3.00541932 -1.13576043

H 0.55152758 2.56606938 -2.79076968

H 2.52087923 2.45657202 -1.19387520

H 2.15914001 0.91818550 -2.01000622

H -2.43151495 -2.06470251 0.81620775

H -2.43151495 -2.06470251 -0.81620775

H -3.34493203 -0.96689732 0.00000000

Meso-(Fe(NH)S4)NH3  **(6m)** S12g Quintet

Fe -0.06456650 -0.70262515 0.00000000

S 0.73244746 -1.89103554 1.86834071

S -0.90063586 1.03641534 1.85069477

S -0.90063586 1.03641534 -1.85069477

S 0.73244746 -1.89103554 -1.86834071

C -0.69037099 0.05846191 3.33759658

C -1.32977004 0.51146251 4.49617354

C -1.32713632 -0.25642395 5.65282800

C -0.68054523 -1.49357685 5.63740566

C -0.05460421 -1.95063042 4.48786811

C -0.04530022 -1.19975066 3.29493113

C -0.69037099 0.05846191 -3.33759658

C -1.32977004 0.51146251 -4.49617354

C -1.32713632 -0.25642395 -5.65282800

C -0.68054523 -1.49357685 -5.63740566

C -0.05460421 -1.95063042 -4.48786811

C -0.04530022 -1.19975066 -3.29493113

N 1.68573858 0.80744510 0.00000000

C 0.54037041 2.17878625 1.77400746

C 1.82921811 1.54566695 1.26693077

C 0.54037041 2.17878625 -1.77400746

C 1.82921811 1.54566695 -1.26693077

N -2.11842406 -1.64543009 0.00000000

H -1.84588137 1.47076720 4.47408251

H -1.83442362 0.09803432 6.54922516

H -0.67554873 -2.11621898 6.53273652

H 0.43455612 -2.92344871 4.48337698

H -1.84588137 1.47076720 -4.47408251

H -1.83442362 0.09803432 -6.54922516

H -0.67554873 -2.11621898 -6.53273652

H 0.43455612 -2.92344871 -4.48337698

H 2.37862686 0.06106176 0.00000000

H 0.68947668 2.59996900 2.77413394

H 0.18950525 2.98955882 1.12367561

H 2.16306280 0.81619082 2.01257855

H 2.59892229 2.33386005 1.18780501

H 0.18950525 2.98955882 -1.12367561

H 0.68947668 2.59996900 -2.77413394

H 2.59892229 2.33386005 -1.18780501

H 2.16306280 0.81619082 -2.01257855

H -2.16926794 -2.24709033 0.82094812

H -2.16926794 -2.24709033 -0.82094812

H -2.94153651 -1.04613421 0.00000000

trans-(Fe(NH)S4)NH3  **(6t)** S12g Singlet

Fe 2.95542953 3.10951960 7.85186798

S 3.22108022 5.17307009 8.86574619

S 4.76089658 3.56051832 6.61220466

S 1.01998703 2.77953313 8.90635949

S 2.75590801 0.93469847 7.03374408

C 5.51792538 5.02164020 7.33836285

C 6.80643282 5.38862356 6.95527821

C 7.42509659 6.47369622 7.56178889

C 6.73595223 7.17544134 8.55602404

C 5.45801669 6.80167922 8.94061207

C 4.81272578 5.69960992 8.34747370

C 0.83770293 0.99495695 9.02362040

C -0.01162338 0.44197095 9.97877581

C -0.11577446 -0.94001353 10.09121804

C 0.63600649 -1.74661248 9.23245332

C 1.48392466 -1.19142352 8.28413700

C 1.62227329 0.20399465 8.16284217

N 1.85784501 3.83184231 6.28670985

C 3.93568858 4.25050195 5.09883023

C 2.59253883 4.82827301 5.47904355

C -0.14073575 3.18698585 7.50744345

C 0.51557210 4.28621347 6.70360733

H 1.73594956 2.97836619 5.72712449

H 7.32476088 4.80985870 6.19025301

H 8.43662366 6.75958105 7.27733284

H 7.21471053 8.02195613 9.04923787

H 4.94120949 7.34965761 9.72732771

H -0.57922260 1.09899213 10.63751999

H -0.76357737 -1.38320900 10.84605710

H 0.56995088 -2.83185659 9.31687879

H 2.07590890 -1.83532481 7.63520853

H 3.83689066 3.39489748 4.41690491

H 4.60221061 4.99228727 4.65004506

H 2.72494532 5.72071086 6.10029605

H 2.02158303 5.10220902 4.57633172

H -1.10431513 3.49751130 7.92357044

H -0.26753085 2.26958195 6.92160190

H -0.10750183 4.54131077 5.83064955

H 0.65009954 5.19103037 7.30928879

N 4.06162165 2.30262537 9.40116085

H 4.29698223 3.03792139 10.07020864

H 3.56190158 1.56441411 9.89663321

H 4.92857803 1.87972014 9.07401924

trans-(Fe(NH)S4)NH3  **(6t)** S12g Triplet

Fe 2.99219677 3.08254320 7.88012393

S 3.26307837 5.11872147 8.89626596

S 4.74433915 3.61197763 6.54182514

S 0.98240222 2.78004379 8.86575466

S 2.80863947 0.90640919 7.11012870

C 5.51910650 5.05422058 7.29531745

C 6.79290652 5.44579481 6.89470382

C 7.42126852 6.50844253 7.53457383

C 6.76044308 7.15937393 8.57681965

C 5.49220101 6.76023935 8.97693162

C 4.84445896 5.68418917 8.34905435

C 0.79388705 0.99754145 9.00741329

C -0.09110316 0.45812039 9.93629928

C -0.18306675 -0.92327830 10.07815847

C 0.61151352 -1.74199911 9.27427526

C 1.49438650 -1.19830759 8.34905805

C 1.62066724 0.19338994 8.20566478

N 1.73509335 3.91179041 6.08998027

C 3.88786260 4.37252916 5.06922064

C 2.52072471 4.93718986 5.41403942

C -0.14954073 3.14899516 7.42158073

C 0.42787473 4.29624932 6.60889677

H 1.64479084 3.07963378 5.50572625

H 7.29411781 4.90588162 6.09111271

H 8.42327516 6.81331953 7.23555535

H 7.24913933 7.98478514 9.09545198

H 4.99316464 7.26704828 9.80187186

H -0.69384927 1.12346658 10.55398566

H -0.85951773 -1.35552509 10.81432287

H 0.55386548 -2.82557367 9.38312173

H 2.12305118 -1.84931891 7.74299294

H 3.80878447 3.54407149 4.35247017

H 4.55561338 5.13302354 4.65362653

H 2.63162333 5.78195572 6.10453582

H 2.04217861 5.30847332 4.48890741

H -1.13956892 3.39487049 7.81939925

H -0.21019291 2.22730228 6.83206881

H -0.29048285 4.56750928 5.81432390

H 0.56953548 5.18093419 7.24447781

N 4.24860379 2.15110604 9.70257069

H 4.46725030 2.88587447 10.37215930

H 3.73639990 1.41919200 10.19097483

H 5.12547801 1.73718519 9.39509383

trans-(Fe(NH)S4)NH3  **(6t)** S12g Quintet

Fe 3.01361257 3.05275846 7.86739616

S 3.37705786 5.20676281 8.92964646

S 4.87020025 3.83476601 6.32406500

S 0.58057623 2.71602392 8.77575431

S 2.63904133 0.77384817 7.02322404

C 5.62218018 5.16846413 7.25296793

C 6.91525759 5.55271032 6.89412913

C 7.60139939 6.49883373 7.64367537

C 6.97475722 7.05584570 8.75908787

C 5.69308834 6.66923727 9.12103770

C 4.97458364 5.70420635 8.38852780

C 0.66835192 0.94639964 9.01616376

C -0.11827059 0.40602659 10.03725254

C -0.04033918 -0.94481793 10.34964915

C 0.82438407 -1.75746061 9.61470768

C 1.60829666 -1.22467279 8.60171426

C 1.57230150 0.14537346 8.27280361

N 1.76504372 3.92259515 6.09467989

C 3.84103412 4.67126612 5.03548877

C 2.45102730 5.06971278 5.49490723

C -0.22877708 2.94019082 7.12727298

C 0.36382735 4.16413651 6.44855924

H 1.80335563 3.11878549 5.46399163

H 7.38437904 5.08928599 6.02675788

H 8.61393561 6.78967007 7.36725963

H 7.50105257 7.79419031 9.36510642

H 5.22180943 7.10126921 10.00238611

H -0.78868101 1.06285780 10.58960405

H -0.64977674 -1.35843927 11.15200569

H 0.89498584 -2.82171438 9.84231211

H 2.29051197 -1.86586469 8.04581991

H 3.79221857 3.93181553 4.22407272

H 4.40521379 5.53681753 4.67538788

H 2.51946051 5.85037940 6.26234124

H 1.89771005 5.47749359 4.62873879

H -1.30463147 3.06170526 7.28916365

H -0.04307450 2.02934130 6.54762916

H -0.24686701 4.41713933 5.56387278

H 0.33189468 5.03160196 7.12268290

N 4.05035124 2.09129049 9.62875946

H 4.26405470 2.81489646 10.31326716

H 3.46201673 1.38543366 10.07101934

H 4.91930737 1.62582619 9.37480888

Meso-(Fe(NH)S4)N2H4 **(7m)** S12g Singlet

Fe 0.00943735 0.35435508 0.00000000

N -1.47067671 1.83438076 0.00000000

H -2.08773125 1.72542211 0.80555965

H -2.08773125 1.72542211 -0.80555965

N -1.13111161 3.26907395 0.00000000

H -0.48159945 3.33311074 0.79395003

H -0.48159945 3.33311074 -0.79395003

S 1.13220700 1.55016654 1.63288012

S -0.96178759 -0.81969450 1.62706340

S 1.13220700 1.55016654 -1.63288012

S -0.96178759 -0.81969450 -1.62706340

N 1.52159732 -1.06228523 0.00000000

H 2.33675571 -0.44874866 0.00000000

C -0.63766864 0.07340376 3.15672062

C -1.36901964 -0.22573908 4.30485745

H -2.10820406 -1.02677214 4.27908228

C -1.16232089 0.50828745 5.46626127

H -1.73875632 0.29018440 6.36404117

C -0.21841738 1.53951103 5.45695516

H -0.05299287 2.12896209 6.35917327

C 0.49754515 1.84250416 4.30890724

H 1.21515818 2.66180813 4.31092288

C 0.29383360 1.12407990 3.11639308

C -0.63766864 0.07340376 -3.15672062

C -1.36901964 -0.22573908 -4.30485745

H -2.10820406 -1.02677214 -4.27908228

C -1.16232089 0.50828745 -5.46626127

H -1.73875632 0.29018440 -6.36404117

C -0.21841738 1.53951103 -5.45695516

H -0.05299287 2.12896209 -6.35917327

C 0.49754515 1.84250416 -4.30890724

H 1.21515818 2.66180813 -4.31092288

C 0.29383360 1.12407990 -3.11639308

C 0.20361259 -2.26230206 1.74637118

H -0.25074958 -3.04786833 1.13148521

H 0.22003719 -2.60076700 2.78697760

C 1.57727682 -1.84746096 1.26578087

H 2.22380071 -2.73117321 1.14664984

H 2.02510894 -1.18652123 2.01433066

C 0.20361259 -2.26230206 -1.74637118

H 0.22003719 -2.60076700 -2.78697760

H -0.25074958 -3.04786833 -1.13148521

C 1.57727682 -1.84746096 -1.26578087

H 2.02510894 -1.18652123 -2.01433066

H 2.22380071 -2.73117321 -1.14664984

Meso-(Fe(NH)S4)N2H4 **(7m)** S12g Triplet

Fe -0.02111576 0.40850684 0.00000000

N -1.90665050 1.93302945 0.00000000

H -2.53027054 1.85085722 0.80446690

H -2.53027054 1.85085722 -0.80446690

N -1.48170529 3.35125517 0.00000000

H -0.82349452 3.37465857 0.78795604

H -0.82349452 3.37465857 -0.78795604

S 1.09153656 1.62022273 1.58680730

S -0.96178388 -0.79635037 1.72287888

S 1.09153656 1.62022273 -1.58680730

S -0.96178388 -0.79635037 -1.72287888

N 1.54225746 -1.38187653 0.00000000

H 2.35846891 -0.77853033 0.00000000

C -0.50145577 0.06399393 3.23247975

C -1.12876788 -0.26137599 4.43461647

H -1.85447680 -1.07451875 4.46136903

C -0.84207552 0.46653007 5.58215480

H -1.33673083 0.22638679 6.52226040

C 0.07276558 1.52092579 5.50688674

H 0.29862001 2.10636728 6.39857580

C 0.68098868 1.85211825 4.30548928

H 1.37481413 2.69015562 4.25444590

C 0.39563937 1.13752100 3.12850806

C -0.50145577 0.06399393 -3.23247975

C -1.12876788 -0.26137599 -4.43461647

H -1.85447680 -1.07451875 -4.46136903

C -0.84207552 0.46653007 -5.58215480

H -1.33673083 0.22638679 -6.52226040

C 0.07276558 1.52092579 -5.50688674

H 0.29862001 2.10636728 -6.39857580

C 0.68098868 1.85211825 -4.30548928

H 1.37481413 2.69015562 -4.25444590

C 0.39563937 1.13752100 -3.12850806

C 0.05653042 -2.34673070 1.75762519

H -0.50078583 -3.05033694 1.12800586

H 0.04331739 -2.72589731 2.78493074

C 1.47981348 -2.11887333 1.26514003

H 1.99125218 -3.09608379 1.20100428

H 2.00373600 -1.51356600 2.01244414

C 0.05653042 -2.34673070 -1.75762519

H 0.04331739 -2.72589731 -2.78493074

H -0.50078583 -3.05033694 -1.12800586

C 1.47981348 -2.11887333 -1.26514003

H 2.00373600 -1.51356600 -2.01244414

H 1.99125218 -3.09608379 -1.20100428

Meso-(Fe(NH)S4)N2H4 **(7m)** S12g Quintet

Fe 0.16192665 0.64171420 0.00000000

N -1.54406566 2.08935053 0.00000000

H -2.16388250 2.01601397 0.80852251

H -2.16388250 2.01601397 -0.80852251

N -1.07411869 3.49176496 0.00000000

H -0.42253533 3.49919937 0.79488879

H -0.42253533 3.49919937 -0.79488879

S 1.19560932 1.58430271 1.90146985

S -0.97445821 -0.96727727 1.82036603

S 1.19560932 1.58430271 -1.90146985

S -0.97445821 -0.96727727 -1.82036603

N 1.63664363 -1.19242208 0.00000000

H 2.44675631 -0.57642008 0.00000000

C -0.64123741 -0.03211735 3.31127266

C -1.40001302 -0.34354504 4.44409721

H -2.08429424 -1.19043449 4.40477405

C -1.29949581 0.42335132 5.59684740

H -1.89933092 0.17921381 6.47268814

C -0.43315910 1.51751260 5.60485756

H -0.34848015 2.13871430 6.49704299

C 0.31411750 1.83488824 4.48085069

H 0.97722633 2.69843831 4.49367106

C 0.23026513 1.08134513 3.29427337

C -0.64123741 -0.03211735 -3.31127266

C -1.40001302 -0.34354504 -4.44409721

H -2.08429424 -1.19043449 -4.40477405

C -1.29949581 0.42335132 -5.59684740

H -1.89933092 0.17921381 -6.47268814

C -0.43315910 1.51751260 -5.60485756

H -0.34848015 2.13871430 -6.49704299

C 0.31411750 1.83488824 -4.48085069

H 0.97722633 2.69843831 -4.49367106

C 0.23026513 1.08134513 -3.29427337

C 0.25787813 -2.33645620 1.76608620

H -0.22125483 -3.08089640 1.11839918

H 0.32174030 -2.76791452 2.77092130

C 1.64156762 -1.94139310 1.26703925

H 2.25776119 -2.85550923 1.19333333

H 2.09678494 -1.28302358 2.01398140

C 0.25787813 -2.33645620 -1.76608620

H 0.32174030 -2.76791452 -2.77092130

H -0.22125483 -3.08089640 -1.11839918

C 1.64156762 -1.94139310 -1.26703925

H 2.09678494 -1.28302358 -2.01398140

H 2.25776119 -2.85550923 -1.19333333

trans-(Fe(NH)S4)N2H4 **(7t)** S12g Singlet

Fe 2.95296304 3.11688416 7.89080749

S 3.21656316 5.22519246 8.82874559

S 4.74366233 3.55181864 6.62007353

S 1.02182380 2.75081574 8.95558091

S 2.78264893 0.94989274 7.05838257

C 5.52901217 5.00241678 7.33637208

C 6.82720779 5.33963551 6.95877819

C 7.46553261 6.41464903 7.56377013

C 6.78634631 7.13668864 8.54973477

C 5.49704193 6.79382411 8.92753822

C 4.83213283 5.70437463 8.33483324

C 0.83993765 0.96131344 9.02535187

C -0.01987801 0.38433773 9.95469348

C -0.13730245 -1.00003387 10.01730785

C 0.61212896 -1.78513235 9.13814917

C 1.47451430 -1.20490220 8.21778823

C 1.62424024 0.19142458 8.14977255

N 1.84159556 3.82093967 6.32387291

C 3.90569905 4.24814817 5.11447112

C 2.56058340 4.81706715 5.50156692

C -0.14156126 3.16028727 7.55903452

C 0.49981426 4.26602854 6.75192756

H 1.72197293 2.96220406 5.77205481

H 7.33725369 4.74591769 6.19974910

H 8.48486187 6.67666215 7.28412535

H 7.28136675 7.97404972 9.04242260

H 4.98696851 7.35826997 9.70691100

H -0.58270670 1.02286099 10.63481484

H -0.79450937 -1.46253638 10.75221493

H 0.53368161 -2.87188303 9.18302552

H 2.06726161 -1.83043151 7.55159112

H 3.80869662 3.39444133 4.43015286

H 4.56724205 4.99442408 4.66588809

H 2.68942007 5.71609062 6.11342547

H 1.97962457 5.07724191 4.60119300

H -1.10602490 3.46394241 7.97879009

H -0.26939250 2.24640028 6.96790755

H -0.13108726 4.51833813 5.88372603

H 0.63199956 5.17171275 7.35643743

N 4.05146039 2.31134303 9.46194797

H 3.90417502 1.30305241 9.40069147

H 5.04637871 2.47692259 9.29252552

N 3.67505185 2.72760232 10.80184170

H 4.46692062 2.55777241 11.42587026

H 3.57721227 3.74568378 10.72008963

trans-(Fe(NH)S4)N2H4 **(7t)** S12g Triplet

Fe 3.07194960 3.03377317 8.07569461

S 3.23798319 5.16508163 8.90977480

S 4.88313758 3.45309269 6.86412425

S 1.12606326 2.73738628 9.08722804

S 2.84533526 0.92933791 7.13888366

C 5.46567018 5.09189377 7.29125866

C 6.65091027 5.59035175 6.75119730

C 7.10974293 6.84714031 7.12495995

C 6.37123851 7.59467937 8.04504043

C 5.19686349 7.09434652 8.58856579

C 4.70968492 5.82505086 8.22450613

C 0.73206751 0.99570361 8.92923793

C -0.29623131 0.42984010 9.68287947

C -0.59706646 -0.92028792 9.54717250

C 0.14312975 -1.69648458 8.65207394

C 1.17474280 -1.13790518 7.91071461

C 1.50397254 0.22499770 8.03264551

N 1.99002766 3.72582270 6.49829449

C 4.07661271 3.80792403 5.25565243

C 2.76732766 4.51458626 5.52066969

C -0.03247296 3.43185892 7.80969732

C 0.72703821 4.37160998 6.90108887

H 1.76619151 2.82087616 6.06760613

H 7.22135488 4.98175505 6.04896480

H 8.03840561 7.23754770 6.71060358

H 6.72474637 8.58036460 8.34934434

H 4.63527360 7.68169728 9.31342273

H -0.85274374 1.05266531 10.38267722

H -1.39485990 -1.36651611 10.13956261

H -0.08376453 -2.75714311 8.53778594

H 1.75239215 -1.75683513 7.22556395

H 3.92527808 2.82800048 4.78571393

H 4.75112109 4.40294944 4.63223242

H 2.95416004 5.50366881 5.95491995

H 2.20004541 4.65066366 4.58491286

H -0.85048203 3.94683358 8.32376179

H -0.44182490 2.57655926 7.26180942

H 0.11204005 4.62454295 6.02150738

H 0.98675999 5.29932914 7.42294548

N 4.07106270 2.15774616 9.46197073

H 3.67892437 1.21519099 9.49325780

H 5.02231596 2.02158356 9.10089668

N 4.14112048 2.58427202 10.85061755

H 5.06739498 2.34460553 11.20864882

H 4.09170538 3.60974715 10.81967021

trans-(Fe(NH)S4)N2H4 **(7t)** S12g Quintet

Fe 2.87052569 3.22546286 7.95415107

S 3.32960441 5.49621535 8.74161285

S 4.66934838 3.92398000 6.12755715

S 0.54906690 2.58430271 8.75284093

S 2.91751292 0.90888838 7.22605186

C 5.61696355 4.99828814 7.19738421

C 6.98763951 5.08145628 6.93950820

C 7.82687812 5.77946912 7.79826603

C 7.27753181 6.39869064 8.92081290

C 5.91699805 6.31502930 9.18197616

C 5.04122875 5.60583124 8.33806493

C 0.72818335 0.81591353 8.96865053

C -0.12045397 0.17394850 9.87129991

C 0.02779768 -1.18347528 10.12800379

C 1.02853800 -1.89162663 9.46158972

C 1.87311495 -1.25396857 8.56421782

C 1.76549670 0.12510650 8.30142152

N 1.62296492 3.95156496 6.08788367

C 3.60188939 4.98997582 5.04861766

C 2.17337700 5.19348628 5.53262539

C -0.24718451 2.72291275 7.08743758

C 0.19590883 4.01048514 6.41508031

H 1.77053870 3.17882435 5.43448048

H 7.38942210 4.58009947 6.06012356

H 8.89558755 5.83435115 7.59545409

H 7.92165799 6.94861428 9.60773789

H 5.50271894 6.79300971 10.06822740

H -0.89154407 0.75219477 10.37838560

H -0.62572564 -1.68084739 10.84341227

H 1.15830867 -2.95748856 9.65282220

H 2.65865000 -1.81461017 8.05997699

H 3.61592529 4.45489719 4.08960984

H 4.11527811 5.94574984 4.90935514

H 2.15326667 5.94209216 6.33115598

H 1.57169823 5.56451520 4.68275191

H -1.33276148 2.70491491 7.22696045

H 0.06294722 1.84269837 6.51289608

H -0.42861981 4.18288421 5.52046014

H 0.04026616 4.86648808 7.08572781

N 3.91109189 2.48103642 9.89140706

H 3.56081836 1.53701701 10.04678408

H 4.89726873 2.39230133 9.63607586

N 3.72354460 3.23986760 11.10848510

H 4.56601118 3.16784445 11.68060508

H 3.66173034 4.21381144 10.79204186

Meso-(Fe(NH)S4)CO **(4m)** S12g-Cosmo Singlet

Fe -0.00200241 -0.13068879 0.00000000

S 1.09399141 -1.39061325 1.58727562

S -0.89931133 1.10259371 1.67167939

S -0.89931133 1.10259371 -1.67167939

S 1.09399141 -1.39061325 -1.58727562

C -0.56791461 0.15001222 3.16552401

C -1.25951382 0.46166905 4.33596407

C -1.06554866 -0.30682385 5.47904249

C -0.18181684 -1.38906117 5.43353960

C 0.49135642 -1.70862549 4.26232430

C 0.30028533 -0.95014569 3.09363105

C -0.56791461 0.15001222 -3.16552401

C -1.25951382 0.46166905 -4.33596407

C -1.06554866 -0.30682385 -5.47904249

C -0.18181684 -1.38906117 -5.43353960

C 0.49135642 -1.70862549 -4.26232430

C 0.30028533 -0.95014569 -3.09363105

N 1.60247624 1.28477092 0.00000000

C 0.30207766 2.50394344 1.74652464

C 1.66544833 2.06550580 1.26723928

C 0.30207766 2.50394344 -1.74652464

C 1.66544833 2.06550580 -1.26723928

H -1.95521839 1.29964345 4.34614809

H -1.61013714 -0.07489604 6.39245904

H -0.02989799 -2.00431333 6.31991837

H 1.15873254 -2.56889042 4.23475839

H -1.95521839 1.29964345 -4.34614809

H -1.61013714 -0.07489604 -6.39245904

H -0.02989799 -2.00431333 -6.31991837

H 1.15873254 -2.56889042 -4.23475839

H 2.42252370 0.68026688 0.00000000

H 0.32536516 2.87281173 2.77595484

H -0.15363868 3.27348040 1.11516009

H 2.11391494 1.40605464 2.01535091

H 2.31583575 2.94285469 1.14903378

H -0.15363868 3.27348040 -1.11516009

H 0.32536516 2.87281173 -2.77595484

H 2.31583575 2.94285469 -1.14903378

H 2.11391494 1.40605464 -2.01535091

C -1.27318882 -1.28187738 0.00000000

O -2.11982902 -2.09514661 0.00000000

Meso-(Fe(NH)S4)CO **(4m)** S12g-Cosmo Triplet

Fe 0.18304506 -0.21401780 0.00000000

S 1.26772718 -1.33857025 1.88139340

S -0.87986724 1.21301343 1.78542128

S -0.87986724 1.21301343 -1.78542128

S 1.26772718 -1.33857025 -1.88139340

C -0.64348536 0.18988256 3.23774136

C -1.47091537 0.45238834 4.33545236

C -1.43692896 -0.36496931 5.45904541

C -0.57229990 -1.46217389 5.47670088

C 0.23412336 -1.74229175 4.38313917

C 0.22312917 -0.93028302 3.23152353

C -0.64348536 0.18988256 -3.23774136

C -1.47091537 0.45238834 -4.33545236

C -1.43692896 -0.36496931 -5.45904541

C -0.57229990 -1.46217389 -5.47670088

C 0.23412336 -1.74229175 -4.38313917

C 0.22312917 -0.93028302 -3.23152353

N 1.70349459 1.29473162 0.00000000

C 0.40823643 2.53703448 1.77709044

C 1.75710024 2.07573692 1.27333117

C 0.40823643 2.53703448 -1.77709044

C 1.75710024 2.07573692 -1.27333117

H -2.15096581 1.30160034 4.29763894

H -2.08528804 -0.15465893 6.30785577

H -0.53946234 -2.11830340 6.34607930

H 0.88649360 -2.61369798 4.40118041

H -2.15096581 1.30160034 -4.29763894

H -2.08528804 -0.15465893 -6.30785577

H -0.53946234 -2.11830340 -6.34607930

H 0.88649360 -2.61369798 -4.40118041

H 2.55415390 0.73297875 0.00000000

H 0.48332139 2.94573130 2.78909060

H -0.04798685 3.30197078 1.13876404

H 2.20762535 1.41283446 2.01610552

H 2.41103844 2.95056428 1.15052712

H -0.04798685 3.30197078 -1.13876404

H 0.48332139 2.94573130 -2.78909060

H 2.41103844 2.95056428 -1.15052712

H 2.20762535 1.41283446 -2.01610552

C -1.05831163 -1.41754414 0.00000000

O -1.89245056 -2.24151968 0.00000000

Meso-(Fe(NH)S4)CO **(4m)** S12g-Cosmo Quintet

Fe 0.29752409 -0.39034866 0.00000000

S 1.29730290 -1.32068830 1.97925944

S -0.83913171 1.22782351 1.77289142

S -0.83913171 1.22782351 -1.77289142

S 1.29730290 -1.32068830 -1.97925944

C -0.64808232 0.24198429 3.25872377

C -1.50792391 0.52112105 4.32614095

C -1.53617933 -0.29971594 5.44915562

C -0.69695078 -1.41362135 5.50013179

C 0.15379690 -1.70334324 4.44078403

C 0.19835415 -0.89139643 3.29228207

C -0.64808232 0.24198429 -3.25872377

C -1.50792391 0.52112105 -4.32614095

C -1.53617933 -0.29971594 -5.44915562

C -0.69695078 -1.41362135 -5.50013179

C 0.15379690 -1.70334324 -4.44078403

C 0.19835415 -0.89139643 -3.29228207

N 1.81879226 1.40408769 0.00000000

C 0.42827638 2.56978526 1.76444734

C 1.80774304 2.17017442 1.26637778

C 0.42827638 2.56978526 -1.76444734

C 1.80774304 2.17017442 -1.26637778

H -2.17203077 1.38130767 4.26167023

H -2.21610224 -0.07882254 6.27028154

H -0.71520422 -2.07353554 6.36700774

H 0.79160101 -2.58450168 4.48443798

H -2.17203077 1.38130767 -4.26167023

H -2.21610224 -0.07882254 -6.27028154

H -0.71520422 -2.07353554 -6.36700774

H 0.79160101 -2.58450168 -4.48443798

H 2.68734410 0.87475698 0.00000000

H 0.48635146 2.98764108 2.77403710

H -0.04593470 3.32156198 1.12361211

H 2.27927277 1.53094682 2.01789096

H 2.40950964 3.08900710 1.17900744

H -0.04593470 3.32156198 -1.12361211

H 0.48635146 2.98764108 -2.77403710

H 2.40950964 3.08900710 -1.17900744

H 2.27927277 1.53094682 -2.01789096

C -1.23403393 -1.62392538 0.00000000

O -2.05757926 -2.43412115 0.00000000

trans-(Fe(NH)S4)CO **(4t)** S12g-Cosmo Singlet

Fe 8.45641912 10.04167805 1.80023031

S 9.86065657 8.79310285 3.05946366

S 6.76814526 8.52979325 2.33065483

S 7.16256382 11.06557094 0.25698011

S 10.06003997 11.67884662 1.34649786

C 9.08533199 12.98949484 0.67783531

C 9.54993215 14.31516587 0.64293977

H 10.54485047 14.54262107 1.02258635

C 8.73938554 15.33773423 0.16154247

H 9.11396948 16.36090637 0.16702898

C 7.44812479 15.07454792 -0.30254386

H 6.81163251 15.88251321 -0.65889129

C 6.97365283 13.76604552 -0.29002141

H 5.96803508 13.53606667 -0.63866138

C 7.79180954 12.74483556 0.18741924

C 7.42714821 7.64612704 3.70312947

C 6.61090976 6.84551468 4.52350555

H 5.54854728 6.76240421 4.29921483

C 7.14112843 6.18317897 5.62349412

H 6.48312669 5.58257549 6.25086444

C 8.49667099 6.29415379 5.94641501

H 8.90253459 5.78843073 6.82064969

C 9.32180702 7.07745306 5.14624239

H 10.37861579 7.19151775 5.38426103

C 8.78864824 7.72961428 4.03540409

C 7.91521367 11.02532595 3.10197882

O 7.54407204 11.70731107 3.98289331

N 9.15653438 8.86370780 0.18920785

H 9.99068336 9.38027317 -0.10475487

C 10.54526587 7.65203002 1.76656140

H 10.77693121 6.69924955 2.24888795

H 11.48147462 8.13472698 1.46174208

C 9.58091919 7.51477678 0.61585595

H 8.68682977 6.96240252 0.92017468

H 10.06322350 6.97724806 -0.21283297

C 7.86575042 10.29613716 -1.28608434

H 8.74741898 10.88190992 -1.56410560

H 7.10730871 10.36420894 -2.06984559

C 8.21683730 8.86767292 -0.94951173

H 7.32724854 8.29987897 -0.65526590

H 8.66051485 8.37978526 -1.82818674

trans-(Fe(NH)S4)CO **(4t)** S12g-Cosmo Triplet

Fe 8.50242632 10.02618639 1.74018456

S 10.03319111 8.43533247 3.04169548

S 6.77418952 8.48286317 2.44225778

S 7.15011016 11.14970007 -0.11857645

S 10.07324083 11.73413506 1.20954097

C 8.99501202 13.05485723 0.74511702

C 9.35277235 14.39191033 0.98417549

H 10.29582019 14.60498196 1.48437076

C 8.51165888 15.43754552 0.61904266

H 8.80963276 16.46350590 0.83312078

C 7.28761369 15.18248791 -0.00004710

H 6.62360578 16.00011703 -0.27599610

C 6.91548620 13.86723585 -0.25811520

H 5.96174528 13.64910475 -0.73519706

C 7.75834490 12.81360585 0.10174068

C 7.46075943 7.68970902 3.85450538

C 6.60164916 7.10687320 4.80613806

H 5.52592760 7.16485674 4.64888933

C 7.10020716 6.48309547 5.94207523

H 6.40505452 6.05273043 6.66249661

C 8.47502341 6.42380115 6.17714211

H 8.86613408 5.95189729 7.07683340

C 9.34422932 6.99253917 5.25278482

H 10.41911372 6.97161126 5.42460762

C 8.85007566 7.61041287 4.10060879

C 7.88904321 11.06645572 2.98702565

O 7.47676704 11.79510581 3.80859926

N 9.19451661 8.79094117 0.12442121

H 10.10894653 9.19424143 -0.09584141

C 10.39545580 7.27953051 1.64484217

H 10.45740287 6.26498289 2.04671207

H 11.39897060 7.58979189 1.32902601

C 9.40708129 7.37663983 0.50586752

H 8.43725973 6.96079647 0.79291337

H 9.79649330 6.80599201 -0.34982532

C 8.17357653 10.38422454 -1.45726894

H 9.12107474 10.92848387 -1.51070579

H 7.62968127 10.48850685 -2.39956958

C 8.37326474 8.92784091 -1.10115488

H 7.41060136 8.43471121 -0.91792091

H 8.85442286 8.41408759 -1.94475179

trans-(Fe(NH)S4)CO **(4t)** S12g-Cosmo Quintet

Fe 8.52230698 9.98467878 1.74805872

S 9.98977846 8.28288497 2.94595567

S 6.69825946 8.47389044 2.47047827

S 7.30392399 11.09657755 -0.17993931

S 10.08863512 11.91703671 1.34038480

C 8.95078603 13.13848311 0.77036354

C 9.18799555 14.50315662 1.01383058

H 10.08322693 14.79121108 1.56224607

C 8.29257844 15.47968602 0.59158312

H 8.50083508 16.52646477 0.81139541

C 7.13037926 15.13015175 -0.09631926

H 6.42491084 15.89328831 -0.42089065

C 6.87521369 13.78752588 -0.35838265

H 5.97049469 13.49286305 -0.88697568

C 7.77076099 12.80416056 0.06566296

C 7.40986898 7.71725111 3.89638817

C 6.56845705 7.23769376 4.91704885

H 5.49190150 7.35513300 4.80713291

C 7.08459219 6.63764115 6.05904245

H 6.40270656 6.28707869 6.83319225

C 8.46189822 6.49483844 6.22501678

H 8.86955891 6.03454260 7.12348566

C 9.31690472 6.96421178 5.23341588

H 10.39553729 6.88026733 5.35342587

C 8.80341334 7.56392782 4.08069638

C 7.94461794 11.13888580 3.22853103

O 7.56880155 11.88709110 4.02968633

N 9.31162671 8.70424817 -0.00991043

H 10.27319733 9.02553708 -0.14160360

C 10.25206464 7.07033880 1.56839934

H 10.15630313 6.06322983 1.98202015

H 11.30293498 7.23676505 1.30279364

C 9.34884692 7.28094817 0.36981605

H 8.32404596 6.97307497 0.60125331

H 9.72378117 6.65326035 -0.45394412

C 8.42772449 10.44729876 -1.50147324

H 9.38020279 10.98027550 -1.42053240

H 7.96439170 10.65116588 -2.47022638

C 8.59129370 8.95784843 -1.26999523

H 7.61037424 8.47063811 -1.20421956

H 9.11645026 8.51904831 -2.13105764

Meso-(Fe(NH)S4)PMe3 **(5m)** S12g-Cosmo Singlet

Fe 0.30019961 -0.02420721 0.00000000

S 1.52494278 1.05712681 -1.62107470

S -0.73999458 -1.13376067 -1.63134180

S -0.73999458 -1.13376067 1.63134180

S 1.52494278 1.05712681 1.62107470

C -0.30510243 -0.29304672 -3.16768888

C -1.03803621 -0.54336978 -4.32593299

C -0.76954225 0.17609378 -5.48649913

C 0.23780061 1.14675938 -5.46879339

C 0.96072024 1.39976167 -4.31091864

C 0.69377995 0.69177331 -3.12434132

C -0.30510243 -0.29304672 3.16768888

C -1.03803621 -0.54336978 4.32593299

C -0.76954225 0.17609378 5.48649913

C 0.23780061 1.14675938 5.46879339

C 0.96072024 1.39976167 4.31091864

C 0.69377995 0.69177331 3.12434132

N 1.71083798 -1.62633843 0.00000000

C 0.26366944 -2.68967460 -1.72822357

C 1.67440836 -2.41841517 -1.26058011

C 0.26366944 -2.68967460 1.72822357

C 1.67440836 -2.41841517 1.26058011

H -1.82951233 -1.29239795 -4.31285913

H -1.34750965 -0.00640675 -6.39087733

H 0.45017109 1.72548825 -6.36757819

H 1.72821722 2.17304679 -4.30702760

H -1.82951233 -1.29239795 4.31285913

H -1.34750965 -0.00640675 6.39087733

H 0.45017109 1.72548825 6.36757819

H 1.72821722 2.17304679 4.30702760

H 2.60149409 -1.13274941 0.00000000

H 0.23332642 -3.05366070 -2.75928522

H -0.27231091 -3.40330187 -1.09401469

H 2.19324866 -1.82191176 -2.01628597

H 2.21753314 -3.36634890 -1.13912600

H -0.27231091 -3.40330187 1.09401469

H 0.23332642 -3.05366070 2.75928522

H 2.21753314 -3.36634890 1.13912600

H 2.19324866 -1.82191176 2.01628597

P -1.09628592 1.73419534 0.00000000

C -2.29602705 1.90177466 -1.40473858

H -1.75242496 1.97722158 -2.35264373

H -2.95561633 1.02687903 -1.43899857

H -2.89929864 2.80615181 -1.25835810

C -2.29602705 1.90177466 1.40473858

H -2.95561633 1.02687903 1.43899857

H -1.75242496 1.97722158 2.35264373

H -2.89929864 2.80615181 1.25835810

C -0.34247081 3.44023421 0.00000000

H -0.67162171 3.98432579 -0.89205208

H -0.67162171 3.98432579 0.89205208

H 0.74721785 3.36915671 0.00000000

Meso-(Fe(NH)S4)PMe3 **(5m)** S12g-Cosmo Triplet

Fe 0.39918962 0.04494937 0.00000000

S 1.51262882 1.09178051 -1.80469868

S -0.77842397 -1.26430076 -1.75638903

S -0.77842397 -1.26430076 1.75638903

S 1.51262882 1.09178051 1.80469868

C -0.35963785 -0.38485897 -3.26607404

C -1.11663861 -0.64624343 -4.41079820

C -0.92435306 0.09307699 -5.57299685

C 0.03556442 1.10856601 -5.57868233

C 0.78022105 1.38024296 -4.43956216

C 0.60126707 0.65007414 -3.24840375

C -0.35963785 -0.38485897 3.26607404

C -1.11663861 -0.64624343 4.41079820

C -0.92435306 0.09307699 5.57299685

C 0.03556442 1.10856601 5.57868233

C 0.78022105 1.38024296 4.43956216

C 0.60126707 0.65007414 3.24840375

N 1.77804191 -1.58749364 0.00000000

C 0.35021479 -2.72358481 -1.72746473

C 1.74709932 -2.37661863 -1.26182209

C 0.35021479 -2.72358481 1.72746473

C 1.74709932 -2.37661863 1.26182209

H -1.86997746 -1.43290245 -4.38234169

H -1.52278056 -0.11220674 -6.45927879

H 0.19467108 1.70461592 -6.47735866

H 1.50955324 2.18950209 -4.45198724

H -1.86997746 -1.43290245 4.38234169

H -1.52278056 -0.11220674 6.45927879

H 0.19467108 1.70461592 6.47735866

H 1.50955324 2.18950209 4.45198724

H 2.66998762 -1.09502119 0.00000000

H 0.36909954 -3.16107681 -2.73033182

H -0.15903787 -3.42930670 -1.06269534

H 2.23407363 -1.75953446 -2.02206564

H 2.32951233 -3.30293388 -1.14780926

H -0.15903787 -3.42930670 1.06269534

H 0.36909954 -3.16107681 2.73033182

H 2.32951233 -3.30293388 1.14780926

H 2.23407363 -1.75953446 2.02206564

P -0.96386884 1.89588386 0.00000000

C -2.14601800 2.04592995 -1.41337105

H -1.59502966 2.09397766 -2.35839377

H -2.81468373 1.17737757 -1.42778795

H -2.73718519 2.96139759 -1.28570703

C -2.14601800 2.04592995 1.41337105

H -2.81468373 1.17737757 1.42778795

H -1.59502966 2.09397766 2.35839377

H -2.73718519 2.96139759 1.28570703

C -0.13652826 3.55842224 0.00000000

H -0.43883875 4.11552259 -0.89377296

H -0.43883875 4.11552259 0.89377296

H 0.94870103 3.42990308 0.00000000

Meso-(Fe(NH)S4)PMe3 **(5m)** S12g-Cosmo Quintet

Fe 0.50078953 0.13479838 0.00000000

S 1.64741397 1.05140058 -1.86156989

S -0.75417654 -1.25610433 -1.84078592

S -0.75417654 -1.25610433 1.84078592

S 1.64741397 1.05140058 1.86156989

C -0.27621412 -0.37951058 -3.33255775

C -1.02191641 -0.62308610 -4.48975674

C -0.80766207 0.12101702 -5.64434424

C 0.16185839 1.12510703 -5.63203240

C 0.89976854 1.37575501 -4.48303195

C 0.70003641 0.64030606 -3.29964769

C -0.27621412 -0.37951058 3.33255775

C -1.02191641 -0.62308610 4.48975674

C -0.80766207 0.12101702 5.64434424

C 0.16185839 1.12510703 5.63203240

C 0.89976854 1.37575501 4.48303195

C 0.70003641 0.64030606 3.29964769

N 1.76407321 -1.82459469 0.00000000

C 0.25847927 -2.79424320 -1.76690802

C 1.67535718 -2.58411962 -1.26437378

C 0.25847927 -2.79424320 1.76690802

C 1.67535718 -2.58411962 1.26437378

H -1.78671247 -1.39846889 -4.47418993

H -1.39867897 -0.07190037 -6.53828601

H 0.33724254 1.72711177 -6.52349762

H 1.64381451 2.17125553 -4.48331506

H -1.78671247 -1.39846889 4.47418993

H -1.39867897 -0.07190037 6.53828601

H 0.33724254 1.72711177 6.52349762

H 1.64381451 2.17125553 4.48331506

H 2.67443112 -1.37038598 0.00000000

H 0.26074203 -3.24928748 -2.76218617

H -0.33018332 -3.44161642 -1.10745685

H 2.22855537 -2.00746829 -2.01233513

H 2.15892146 -3.56981120 -1.17205140

H -0.33018332 -3.44161642 1.10745685

H 0.26074203 -3.24928748 2.76218617

H 2.15892146 -3.56981120 1.17205140

H 2.22855537 -2.00746829 2.01233513

P -1.32465766 1.99399226 0.00000000

C -2.49122414 2.12460009 -1.42936067

H -1.91389335 2.15824941 -2.36089836

H -3.14343457 1.24361839 -1.44892699

H -3.10237359 3.03174377 -1.34167494

C -2.49122414 2.12460009 1.42936067

H -3.14343457 1.24361839 1.44892699

H -1.91389335 2.15824941 2.36089836

H -3.10237359 3.03174377 1.34167494

C -0.51232348 3.66728618 0.00000000

H -0.81311947 4.22734568 -0.89213199

H -0.81311947 4.22734568 0.89213199

H 0.57503046 3.54280411 0.00000000

trans-(Fe(NH)S4)PMe3 **(5t)** S12g-Cosmo Singlet

Fe 3.00354339 3.06541796 7.91063894

S 3.25638269 5.15142145 8.87231116

S 4.77364287 3.53327627 6.62559179

S 1.04741534 2.75708543 8.92747154

S 2.70528427 0.94137193 7.00190454

P 4.19095733 2.25159257 9.64772464

C 4.57530724 0.44155925 9.76644026

C 5.89593309 2.91508559 9.94685954

C 3.44373419 2.53037849 11.31953527

C 5.51477836 5.02803107 7.30593751

C 6.79404795 5.40491005 6.90334422

C 7.40666428 6.51014330 7.48477190

C 6.72057222 7.22601534 8.47217326

C 5.44871799 6.84393773 8.87533806

C 4.81652210 5.72149616 8.30739593

C 0.81184468 0.97616480 8.99792302

C -0.02943337 0.41882474 9.95703932

C -0.15855156 -0.96553734 10.03943222

C 0.55525140 -1.76901890 9.14517136

C 1.39434077 -1.20696281 8.18928092

C 1.55798355 0.18745839 8.10478349

N 1.86230333 3.84335456 6.31790220

C 3.93209335 4.18785900 5.10553437

C 2.60703669 4.80335988 5.48091208

C -0.12973468 3.23836685 7.56137296

C 0.53998093 4.32684211 6.75822477

H 1.70258017 2.99944544 5.75918893

H 5.16457097 0.26052560 10.67374482

H 5.14616037 0.12891128 8.88583852

H 3.64962012 -0.14086804 9.80700911

H 6.31218444 2.44107877 10.84430129

H 5.85856206 3.99984074 10.08581249

H 6.53868554 2.68764309 9.08805567

H 4.11131722 2.13982346 12.09733639

H 2.47580973 2.01908373 11.38429069

H 3.29055431 3.60486443 11.46670793

H 7.31354496 4.82247270 6.14250799

H 8.41090564 6.80273440 7.18277839

H 7.19406362 8.08651417 8.94465393

H 4.93870860 7.39990934 9.66123877

H -0.56944287 1.06817761 10.64553068

H -0.79752885 -1.41210949 10.79943606

H 0.47088520 -2.85379681 9.20820536

H 1.96314652 -1.85161183 7.52042734

H 3.80559935 3.30614334 4.46513200

H 4.60723568 4.89240612 4.61304710

H 2.75502376 5.71666213 6.06537035

H 2.03900143 5.05609176 4.57358212

H -1.06660172 3.57259890 8.01495247

H -0.30571522 2.34018690 6.96064724

H -0.09172864 4.59455183 5.89891500

H 0.69480867 5.22658261 7.36380569

trans-(Fe(NH)S4)PMe3 **(5t)** S12g-Cosmo Triplet

Fe 3.04561033 3.04142877 7.90121694

S 3.43937588 5.08606753 8.90229382

S 4.89609925 3.71055329 6.33936510

S 0.64702185 2.70044759 8.91732933

S 2.64195922 0.93387296 7.06088241

P 4.15875002 2.21363310 9.75900956

C 4.48040036 0.39618601 9.90140427

C 5.87716106 2.83108664 10.06625886

C 3.35594686 2.54279616 11.39153089

C 5.62695388 5.11895113 7.17907150

C 6.88791130 5.55923560 6.77619775

C 7.51828629 6.60360870 7.44547097

C 6.86919536 7.20836781 8.52355796

C 5.61551043 6.76986297 8.92969726

C 4.96934108 5.70580923 8.27551459

C 0.64837760 0.91713720 9.00686295

C -0.15841715 0.29507029 9.96326139

C -0.11893894 -1.08567433 10.12906903

C 0.71968317 -1.84780810 9.31397414

C 1.52690497 -1.23272475 8.36338447

C 1.52960324 0.16246906 8.20190444

N 1.85848055 3.91172479 6.27524470

C 3.87311496 4.50941832 5.02514177

C 2.54169971 4.99585075 5.54873249

C -0.20687814 3.08591988 7.32205678

C 0.48319545 4.26606240 6.67195089

H 1.78324266 3.11175378 5.64313771

H 5.04869968 0.20653206 10.82037507

H 5.05553294 0.05634044 9.03343241

H 3.53484793 -0.15339155 9.93224949

H 6.27458587 2.35896369 10.97344224

H 5.87355048 3.91863955 10.18457707

H 6.51062327 2.56630910 9.21121426

H 3.99167447 2.16273577 12.20101862

H 2.38289944 2.03897497 11.42541305

H 3.20894301 3.62155521 11.50973110

H 7.37863429 5.07064678 5.93508692

H 8.50874734 6.93370788 7.13612612

H 7.35164308 8.02323674 9.06307268

H 5.13127038 7.23547968 9.78724963

H -0.81572250 0.90384585 10.58240036

H -0.74135404 -1.56201217 10.88517759

H 0.75870418 -2.93043596 9.43262943

H 2.20175254 -1.83466493 7.75631815

H 3.74048144 3.71870845 4.27603316

H 4.45476542 5.31878434 4.57585282

H 2.67673939 5.83243341 6.24174831

H 1.93103922 5.34277459 4.70091857

H -1.25478668 3.31430484 7.53487494

H -0.14713403 2.19126848 6.69379744

H -0.10495596 4.58126260 5.79728599

H 0.53495004 5.11807640 7.36097036

trans-(Fe(NH)S4)PMe3 **(5t)** S12g-Cosmo Quintet

Fe 3.03093413 3.01680616 7.81395243

S 3.35951140 5.22653657 8.90182497

S 4.83113904 3.85488533 6.29680920

S 0.63909213 2.72827279 8.75471951

S 2.54596752 0.74122651 6.92660527

P 4.30461349 2.08043548 9.83236675

C 4.64148720 0.26964968 10.02080942

C 5.99263970 2.76765681 10.14954448

C 3.45772934 2.44758977 11.43425137

C 5.59196998 5.18705201 7.22306994

C 6.88163208 5.57633067 6.85614479

C 7.57187342 6.52700924 7.60036856

C 6.95478925 7.08642473 8.72037961

C 5.67387497 6.69814569 9.09024382

C 4.95416851 5.73360374 8.35884042

C 0.67358390 0.95671966 8.99375787

C -0.08172508 0.43891390 10.04976494

C -0.03523050 -0.91667470 10.35595536

C 0.76598883 -1.75847346 9.58251413

C 1.52165447 -1.24761686 8.53469608

C 1.51470320 0.12350574 8.21651662

N 1.75106074 3.95200417 6.08322268

C 3.81262047 4.69058480 4.99555441

C 2.43218912 5.09639495 5.46608717

C -0.24365861 3.01063912 7.15047000

C 0.36486824 4.22789232 6.48007545

H 1.72975236 3.18514273 5.40840685

H 5.17838832 0.08011638 10.95907349

H 5.24504084 -0.07722284 9.17420837

H 3.69390644 -0.27967229 10.01862233

H 6.38945385 2.37557192 11.09469580

H 5.93627121 3.86058298 10.19281742

H 6.65902785 2.48169101 9.32679716

H 4.06501527 2.10634347 12.28228437

H 2.48591808 1.93886681 11.45015738

H 3.29355739 3.52911376 11.50189557

H 7.34743189 5.11876751 5.98433903

H 8.58027094 6.82080633 7.31357460

H 7.48314892 7.82656008 9.32105876

H 5.21318861 7.13249332 9.97611934

H -0.70431216 1.11267507 10.63613937

H -0.62110169 -1.31042755 11.18491999

H 0.81172615 -2.82414436 9.80588566

H 2.16080322 -1.91309429 7.95674192

H 3.75300284 3.93434923 4.20306226

H 4.38381175 5.54295811 4.61772079

H 2.50188071 5.88968192 6.21838778

H 1.87306838 5.48882539 4.60041458

H -1.30346622 3.16588332 7.36939803

H -0.11679947 2.11057001 6.54057840

H -0.26085422 4.50538863 5.61711172

H 0.37116069 5.08424028 7.16764339

Meso-(Fe(NH)S4)NH3  **(6m)** S12g-Cosmo Singlet

Fe -0.16539594 -0.38986975 0.00000000

S 0.64228095 -1.84604224 1.59452535

S -0.87607728 0.93140329 1.65338045

S -0.87607728 0.93140329 -1.65338045

S 0.64228095 -1.84604224 -1.59452535

C -0.69888175 -0.02741509 3.17553340

C -1.29987840 0.42235224 4.35153352

C -1.22456219 -0.34785043 5.50886586

C -0.54571668 -1.57079069 5.47089951

C 0.04147638 -2.02246147 4.29630012

C -0.03499661 -1.26442829 3.11172838

C -0.69888175 -0.02741509 -3.17553340

C -1.29987840 0.42235224 -4.35153352

C -1.22456219 -0.34785043 -5.50886586

C -0.54571668 -1.57079069 -5.47089951

C 0.04147638 -2.02246147 -4.29630012

C -0.03499661 -1.26442829 -3.11172838

N 1.59218268 0.70246798 0.00000000

C 0.52647792 2.13697172 1.74812434

C 1.79444058 1.47449155 1.26266825

C 0.52647792 2.13697172 -1.74812434

C 1.79444058 1.47449155 -1.26266825

N -1.94614564 -1.44241124 0.00000000

H -1.83396853 1.37224921 4.35599078

H -1.70115510 -0.00687772 6.42637825

H -0.48673988 -2.18702342 6.36791527

H 0.55335959 -2.98412046 4.27925638

H -1.83396853 1.37224921 -4.35599078

H -1.70115510 -0.00687772 -6.42637825

H -0.48673988 -2.18702342 -6.36791527

H 0.55335959 -2.98412046 -4.27925638

H 2.31419794 -0.01668972 0.00000000

H 0.61468753 2.48866609 2.77994219

H 0.20808414 2.97634209 1.12119800

H 2.12917218 0.75245671 2.01313631

H 2.58525576 2.22596293 1.13083538

H 0.20808414 2.97634209 -1.12119800

H 0.61468753 2.48866609 -2.77994219

H 2.58525576 2.22596293 -1.13083538

H 2.12917218 0.75245671 -2.01313631

H -1.99483630 -2.05408880 0.81508748

H -1.99483630 -2.05408880 -0.81508748

H -2.79590799 -0.88011278 0.00000000

Meso-(Fe(NH)S4)NH3  **(6m)** S12g-Cosmo Triplet

Fe -0.36405913 -0.53365620 0.00000000

S 0.39167530 -1.98653192 1.59362152

S -1.04016720 0.84719796 1.72591689

S -1.04016720 0.84719796 -1.72591689

S 0.39167530 -1.98653192 -1.59362152

C -0.79803739 -0.10519303 3.23694283

C -1.33079082 0.35813182 4.44103010

C -1.23501450 -0.42323438 5.58866526

C -0.60922748 -1.67174660 5.51611400

C -0.09140796 -2.13664310 4.31378414

C -0.18812145 -1.36562603 3.14153958

C -0.79803739 -0.10519303 -3.23694283

C -1.33079082 0.35813182 -4.44103010

C -1.23501450 -0.42323438 -5.58866526

C -0.60922748 -1.67174660 -5.51611400

C -0.09140796 -2.13664310 -4.31378414

C -0.18812145 -1.36562603 -3.14153958

N 1.51437881 0.88565009 0.00000000

C 0.27307716 2.15079330 1.75997315

C 1.61271317 1.63409881 1.26397267

C 0.27307716 2.15079330 -1.75997315

C 1.61271317 1.63409881 -1.26397267

N -2.58211245 -1.48623717 0.00000000

H -1.83073685 1.32563346 4.47422009

H -1.65869603 -0.07014932 6.52745481

H -0.53815474 -2.29699862 6.40589644

H 0.37799131 -3.11868706 4.26693660

H -1.83073685 1.32563346 -4.47422009

H -1.65869603 -0.07014932 -6.52745481

H -0.53815474 -2.29699862 -6.40589644

H 0.37799131 -3.11868706 -4.26693660

H 2.24815874 0.18370441 0.00000000

H 0.33834800 2.53353980 2.78305798

H -0.13718285 2.94408397 1.12612305

H 2.01672307 0.94236625 2.01048619

H 2.30649101 2.48615515 1.18328848

H -0.13718285 2.94408397 -1.12612305

H 0.33834800 2.53353980 -2.78305798

H 2.30649101 2.48615515 -1.18328848

H 2.01672307 0.94236625 -2.01048619

H -2.66343958 -2.09180274 0.81498588

H -2.66343958 -2.09180274 -0.81498588

H -3.40577260 -0.88655657 0.00000000

Meso-(Fe(NH)S4)NH3  **(6m)** S12g-Cosmo Quintet

Fe -0.10332450 -0.65537544 0.00000000

S 0.69711271 -1.92513783 1.85765662

S -0.90521589 1.00466470 1.86908209

S -0.90521589 1.00466470 -1.86908209

S 0.69711271 -1.92513783 -1.85765662

C -0.66145092 0.03408854 3.36060150

C -1.25828137 0.50088055 4.53688103

C -1.23088057 -0.26124899 5.69978508

C -0.60488505 -1.50896057 5.67654890

C -0.01760414 -1.98074060 4.50977551

C -0.03337944 -1.23144044 3.31663851

C -0.66145092 0.03408854 -3.36060150

C -1.25828137 0.50088055 -4.53688103

C -1.23088057 -0.26124899 -5.69978508

C -0.60488505 -1.50896057 -5.67654890

C -0.01760414 -1.98074060 -4.50977551

C -0.03337944 -1.23144044 -3.31663851

N 1.66166313 0.83552590 0.00000000

C 0.49724722 2.19498860 1.77205321

C 1.79476338 1.59180803 1.26472622

C 0.49724722 2.19498860 -1.77205321

C 1.79476338 1.59180803 -1.26472622

N -2.17611073 -1.52401037 0.00000000

H -1.75979376 1.46768686 4.52946197

H -1.70580974 0.10705838 6.60774952

H -0.58361477 -2.12668822 6.57419439

H 0.45624075 -2.96144839 4.50345185

H -1.75979376 1.46768686 -4.52946197

H -1.70580974 0.10705838 -6.60774952

H -0.58361477 -2.12668822 -6.57419439

H 0.45624075 -2.96144839 -4.50345185

H 2.41164858 0.14712239 0.00000000

H 0.63557892 2.63888311 2.76263280

H 0.10891314 2.97579651 1.10881419

H 2.16633471 0.88424883 2.01272143

H 2.53636772 2.40005854 1.16669084

H 0.10891314 2.97579651 -1.10881419

H 0.63557892 2.63888311 -2.76263280

H 2.53636772 2.40005854 -1.16669084

H 2.16633471 0.88424883 -2.01272143

H -2.31479274 -2.11811290 0.81612202

H -2.31479274 -2.11811290 -0.81612202

H -2.93545680 -0.84467749 0.00000000

trans-(Fe(NH)S4)NH3  **(6t)** S12g-Cosmo Singlet

Fe 2.94750828 3.11441343 7.83391194

S 3.22287942 5.17734796 8.84929354

S 4.74250343 3.58416725 6.57626823

S 1.00200823 2.77269881 8.87541902

S 2.75276417 0.92310896 7.04139916

C 5.52558151 5.01789839 7.33941485

C 6.82020307 5.37581112 6.96589562

C 7.45751769 6.43825193 7.59881701

C 6.78217745 7.12961301 8.61051024

C 5.49521415 6.76754094 8.98499999

C 4.83441729 5.68992915 8.36329186

C 0.83042251 0.98696055 9.02162964

C -0.02007910 0.44240435 9.98087029

C -0.09996793 -0.94051202 10.12893091

C 0.67502749 -1.75799138 9.30142576

C 1.52253608 -1.21017862 8.34423196

C 1.63228903 0.18413304 8.19021069

N 1.84214485 3.84819653 6.26805529

C 3.91229154 4.30859767 5.08106680

C 2.56451519 4.86415335 5.46940776

C -0.15834518 3.17524659 7.47446671

C 0.49083994 4.28556999 6.68378488

H 1.71447290 3.02342722 5.67301823

H 7.32997063 4.81379525 6.18346155

H 8.47290035 6.71423056 7.31924791

H 7.27422021 7.95599207 9.12327453

H 4.99032243 7.31008309 9.78362741

H -0.60890680 1.10243655 10.61699003

H -0.74810476 -1.37424791 10.88863365

H 0.63029879 -2.84098701 9.41579842

H 2.13115871 -1.86460049 7.72112945

H 3.82257271 3.46407523 4.38687304

H 4.57582054 5.05949595 4.64492632

H 2.67810732 5.75732517 6.09117939

H 1.99167446 5.13006862 4.56914073

H -1.12444768 3.47142127 7.89134143

H -0.27114831 2.26299581 6.87913648

H -0.12846995 4.53315933 5.80977457

H 0.60463581 5.18966456 7.29247842

N 4.06094907 2.33693828 9.40997483

H 3.66160652 2.56755319 10.31824566

H 4.13079888 1.32035544 9.36062111

H 5.01552238 2.69259619 9.43810642

trans-(Fe(NH)S4)NH3  **(6t)** S12g-Cosmo Triplet

Fe 2.94694629 3.10945133 7.80723241

S 3.25408183 5.13393955 8.88330165

S 4.70496201 3.66545152 6.48875766

S 0.94647584 2.78323420 8.78989445

S 2.79196298 0.88349899 7.09200755

C 5.51980078 5.05449629 7.30345514

C 6.80830928 5.42231257 6.92296982

C 7.46886007 6.43883191 7.60829563

C 6.82633888 7.07190570 8.67388663

C 5.54151028 6.69880452 9.05305006

C 4.86334318 5.66971511 8.37851312

C 0.79550951 1.00286973 9.00298778

C -0.07442613 0.48438716 9.95892637

C -0.12881709 -0.89254633 10.16763917

C 0.68560945 -1.72978306 9.40279813

C 1.55243989 -1.20672680 8.44739982

C 1.63768452 0.17980967 8.23718205

N 1.71449777 3.92419326 6.05639762

C 3.84973062 4.47502921 5.03970049

C 2.46982315 4.99119505 5.39592303

C -0.18634024 3.10873006 7.33556562

C 0.37437650 4.27017358 6.53707260

H 1.63320609 3.12985535 5.42008844

H 7.29672665 4.90523602 6.09748136

H 8.48078138 6.72252700 7.32343529

H 7.33854594 7.85967758 9.22604552

H 5.05875669 7.19345560 9.89512612

H -0.69623639 1.15900136 10.54627449

H -0.79270328 -1.30531094 10.92560408

H 0.65906222 -2.80721651 9.56530475

H 2.19470390 -1.87419606 7.87396642

H 3.79554128 3.67092427 4.29578364

H 4.50940456 5.26014674 4.66064448

H 2.54564367 5.83168462 6.09427878

H 1.97861067 5.34930887 4.47649027

H -1.18393037 3.32564088 7.72742825

H -0.21019661 2.18796747 6.74312946

H -0.32154344 4.50308618 5.71580433

H 0.45814367 5.16517847 7.16552509

N 4.24741737 2.17749558 9.66753598

H 3.86088567 2.44721670 10.56982023

H 4.27303220 1.15979619 9.64459032

H 5.21457928 2.49646458 9.66858481

trans-(Fe(NH)S4)NH3  **(6t)** S12g-Cosmo Quintet

Fe 2.97674215 3.09303520 7.84967772

S 3.37805641 5.25122428 8.92665925

S 4.84414886 3.89604844 6.27701903

S 0.56113850 2.67845234 8.72596719

S 2.64212379 0.73002171 7.04799800

C 5.62757831 5.17965200 7.25784853

C 6.93572193 5.53116539 6.91479985

C 7.66103344 6.41915445 7.70142977

C 7.05979071 6.95787382 8.84020122

C 5.76122256 6.60749922 9.18662922

C 5.00499334 5.70500594 8.41273977

C 0.65552361 0.91440400 9.01259764

C -0.13460047 0.39411693 10.04183310

C -0.03777161 -0.94606361 10.40134607

C 0.85254582 -1.76868552 9.70827839

C 1.63913923 -1.25499147 8.68399603

C 1.57825791 0.10201426 8.30883370

N 1.75637792 3.92649889 6.08734497

C 3.79666948 4.76079656 5.01955260

C 2.40158469 5.10836547 5.49404678

C -0.23973105 2.88707200 7.06833111

C 0.33331764 4.12588917 6.40803009

H 1.80980312 3.15908234 5.41357903

H 7.38876381 5.08896213 6.02850469

H 8.68337636 6.68033094 7.43308346

H 7.61490506 7.64816702 9.47532134

H 5.31256439 7.02560481 10.08676131

H -0.82269599 1.05417558 10.56770352

H -0.64890466 -1.34170298 11.21108198

H 0.94329231 -2.82131009 9.97641991

H 2.33979742 -1.90761148 8.16486045

H 3.76268149 4.03938774 4.19404403

H 4.34468862 5.64449399 4.68242171

H 2.43786243 5.88958191 6.26069603

H 1.82990657 5.49027640 4.63281399

H -1.31684965 2.98578314 7.22616510

H -0.02925821 1.98500207 6.48538786

H -0.25379870 4.34997457 5.50459223

H 0.25034635 4.99364355 7.07479342

N 4.12695546 2.16753382 9.53557346

H 3.79604347 2.49791664 10.44061578

H 4.07722444 1.14966456 9.54325447

H 5.11510984 2.41407644 9.49384942

Meso-(Fe(NH)S4)N2H4 **(7m)** S12g-Cosmo Singlet

Fe 0.03078065 0.34727892 0.00000000

N -1.49325564 1.78909483 0.00000000

H -2.11060758 1.66188432 0.80209195

H -2.11060758 1.66188432 -0.80209195

N -1.18582218 3.23117586 0.00000000

H -0.53892364 3.31470014 0.79344307

H -0.53892364 3.31470014 -0.79344307

S 1.14041560 1.55241290 1.63153548

S -0.95554382 -0.81369998 1.63369346

S 1.14041560 1.55241290 -1.63153548

S -0.95554382 -0.81369998 -1.63369346

N 1.51485772 -1.10423999 0.00000000

H 2.37181847 -0.55304579 0.00000000

C -0.62278341 0.08641941 3.16323638

C -1.35106254 -0.20942031 4.31513671

H -2.08032118 -1.01914458 4.29972866

C -1.15354025 0.53737473 5.47296860

H -1.72859241 0.31853824 6.37114061

C -0.22178877 1.58052173 5.45992438

H -0.06509515 2.17969643 6.35672053

C 0.49498975 1.87958573 4.30860825

H 1.20400313 2.70687180 4.30983224

C 0.29972335 1.14534277 3.12379839

C -0.62278341 0.08641941 -3.16323638

C -1.35106254 -0.20942031 -4.31513671

H -2.08032118 -1.01914458 -4.29972866

C -1.15354025 0.53737473 -5.47296860

H -1.72859241 0.31853824 -6.37114061

C -0.22178877 1.58052173 -5.45992438

H -0.06509515 2.17969643 -6.35672053

C 0.49498975 1.87958573 -4.30860825

H 1.20400313 2.70687180 -4.30983224

C 0.29972335 1.14534277 -3.12379839

C 0.16871441 -2.28335061 1.74193561

H -0.31279138 -3.04246014 1.11705666

H 0.17409244 -2.63794382 2.77645755

C 1.54932832 -1.90114705 1.26317043

H 2.16476199 -2.80204592 1.13266897

H 2.02615671 -1.26605921 2.01507786

C 0.16871441 -2.28335061 -1.74193561

H 0.17409244 -2.63794382 -2.77645755

H -0.31279138 -3.04246014 -1.11705666

C 1.54932832 -1.90114705 -1.26317043

H 2.02615671 -1.26605921 -2.01507786

H 2.16476199 -2.80204592 -1.13266897

Meso-(Fe(NH)S4)N2H4 **(7m)** S12g-Cosmo Triplet

Fe 0.03017580 0.40304150 0.00000000

N -1.94982342 1.87872317 0.00000000

H -2.56912644 1.76238831 0.80315824

H -2.56912644 1.76238831 -0.80315824

N -1.58655012 3.31318510 0.00000000

H -0.93251826 3.37180630 0.78857782

H -0.93251826 3.37180630 -0.78857782

S 1.09350192 1.64479560 1.59774804

S -0.95177873 -0.77703117 1.72189884

S 1.09350192 1.64479560 -1.59774804

S -0.95177873 -0.77703117 -1.72189884

N 1.51987326 -1.42050912 0.00000000

H 2.40468037 -0.92231149 0.00000000

C -0.48363837 0.07477857 3.23921988

C -1.09700931 -0.26770759 4.44488092

H -1.80439705 -1.09588692 4.47565417

C -0.81743438 0.46075833 5.59665954

H -1.30157971 0.20353215 6.53731020

C 0.07546120 1.53461455 5.52652027

H 0.29411460 2.11932366 6.41982968

C 0.67460733 1.88145849 4.32232664

H 1.35543725 2.73083824 4.27787205

C 0.39817995 1.16164407 3.14660751

C -0.48363837 0.07477857 -3.23921988

C -1.09700931 -0.26770759 -4.44488092

H -1.80439705 -1.09588692 -4.47565417

C -0.81743438 0.46075833 -5.59665954

H -1.30157971 0.20353215 -6.53731020

C 0.07546120 1.53461455 -5.52652027

H 0.29411460 2.11932366 -6.41982968

C 0.67460733 1.88145849 -4.32232664

H 1.35543725 2.73083824 -4.27787205

C 0.39817995 1.16164407 -3.14660751

C 0.00620884 -2.36062690 1.75114594

H -0.57924324 -3.03009274 1.11228136

H -0.02597043 -2.75136132 2.77263160

C 1.43168005 -2.17259646 1.26296088

H 1.90628431 -3.16372746 1.18445426

H 1.98283085 -1.59626476 2.01348927

C 0.00620884 -2.36062690 -1.75114594

H -0.02597043 -2.75136132 -2.77263160

H -0.57924324 -3.03009274 -1.11228136

C 1.43168005 -2.17259646 -1.26296088

H 1.98283085 -1.59626476 -2.01348927

H 1.90628431 -3.16372746 -1.18445426

Meso-(Fe(NH)S4)N2H4 **(7m)** S12g-Cosmo Quintet

Fe 0.15248825 0.56899942 0.00000000

N -1.62944576 1.94395908 0.00000000

H -2.24378562 1.81688510 0.80549879

H -2.24378562 1.81688510 -0.80549879

N -1.27044398 3.37607570 0.00000000

H -0.62457838 3.44456129 0.79487450

H -0.62457838 3.44456129 -0.79487450

S 1.18465429 1.61775306 1.87531580

S -0.98897618 -0.91919252 1.84898447

S 1.18465429 1.61775306 -1.87531580

S -0.98897618 -0.91919252 -1.84898447

N 1.58276756 -1.22743509 0.00000000

H 2.44949375 -0.69347408 0.00000000

C -0.60482367 0.00630144 3.33929312

C -1.33034631 -0.30381124 4.49458971

H -2.01965736 -1.14691231 4.47723429

C -1.19098960 0.45843525 5.64900311

H -1.76678578 0.21345581 6.54012490

C -0.31870652 1.54835834 5.63970123

H -0.20399201 2.16495779 6.53101882

C 0.39816513 1.86534504 4.49348585

H 1.06500943 2.72656566 4.49604866

C 0.27134728 1.11482829 3.30889824

C -0.60482367 0.00630144 -3.33929312

C -1.33034631 -0.30381124 -4.49458971

H -2.01965736 -1.14691231 -4.47723429

C -1.19098960 0.45843525 -5.64900311

H -1.76678578 0.21345581 -6.54012490

C -0.31870652 1.54835834 -5.63970123

H -0.20399201 2.16495779 -6.53101882

C 0.39816513 1.86534504 -4.49348585

H 1.06500943 2.72656566 -4.49604866

C 0.27134728 1.11482829 -3.30889824

C 0.18021290 -2.34331010 1.76948193

H -0.34038056 -3.04646337 1.11017947

H 0.22937558 -2.79578205 2.76453731

C 1.56827234 -1.99096801 1.26747212

H 2.14865542 -2.92243216 1.17573554

H 2.05963194 -1.35925685 2.01419625

C 0.18021290 -2.34331010 -1.76948193

H 0.22937558 -2.79578205 -2.76453731

H -0.34038056 -3.04646337 -1.11017947

C 1.56827234 -1.99096801 -1.26747212

H 2.05963194 -1.35925685 -2.01419625

H 2.14865542 -2.92243216 -1.17573554

trans-(Fe(NH)S4)N2H4 **(7t)** S12g-Cosmo Singlet

Fe 2.93285483 3.12550234 7.85950136

S 3.20215895 5.22752666 8.80816324

S 4.71987634 3.58276016 6.58092764

S 0.98986785 2.75396223 8.90060733

S 2.77756671 0.93789312 7.06420352

C 5.53036634 4.99640427 7.34864212

C 6.84206814 5.31268610 6.99908085

C 7.50242790 6.34975127 7.65085365

C 6.83314039 7.05600921 8.65539876

C 5.52666950 6.73663699 9.00338837

C 4.84282062 5.68696999 8.36178265

C 0.83499513 0.96264485 9.02453905

C -0.02348700 0.39702899 9.96416099

C -0.10161949 -0.98882749 10.08364710

C 0.68192638 -1.78940069 9.24795398

C 1.53868181 -1.22099977 8.31152722

C 1.64640801 0.17606944 8.18803048

N 1.82032899 3.83765585 6.28872072

C 3.88253114 4.31435776 5.09209645

C 2.52931432 4.85678402 5.48103961

C -0.17111423 3.14376371 7.49625240

C 0.46514733 4.26216184 6.70668026

H 1.69958873 3.00755137 5.69958134

H 7.34696304 4.73760907 6.22312127

H 8.53179883 6.59232082 7.39225373

H 7.34471509 7.85960508 9.18486653

H 5.02646947 7.28965790 9.79760563

H -0.62088790 1.04237969 10.60719866

H -0.75714204 -1.43874086 10.82738085

H 0.63598268 -2.87459083 9.33833269

H 2.15404192 -1.86100155 7.68005418

H 3.80101826 3.47397720 4.39203569

H 4.54114144 5.07311592 4.66217274

H 2.63366807 5.75518094 6.09608645

H 1.95112679 5.10872267 4.58015820

H -1.14156074 3.42840181 7.91134856

H -0.27360316 2.23177435 6.89858692

H -0.15718575 4.50471764 5.83352986

H 0.57031760 5.16666017 7.31614164

N 4.06750981 2.33541372 9.42960254

H 3.95557824 1.32263038 9.39187644

H 5.05776290 2.51242404 9.25020352

N 3.73598079 2.74540755 10.78845563

H 4.56738810 2.60037964 11.36590496

H 3.62378833 3.76164165 10.71068986

trans-(Fe(NH)S4)N2H4 **(7t)** S12g-Cosmo Triplet

Fe 2.88201995 3.13285631 7.76862840

S 3.21231175 5.12274110 8.87760029

S 4.66227911 3.67073482 6.48364581

S 0.88587817 2.78131646 8.74514564

S 2.83069293 0.89950819 7.14294404

C 5.49355253 5.03370068 7.32323949

C 6.79427391 5.38034088 6.96539819

C 7.46818802 6.36612930 7.68199044

C 6.82704110 6.98992979 8.75374847

C 5.52916563 6.63796025 9.10922858

C 4.83812788 5.64093633 8.40222502

C 0.75655360 0.99978939 8.96960040

C -0.14114427 0.47367820 9.89524359

C -0.18389068 -0.90285100 10.10765269

C 0.66969709 -1.73277344 9.37810830

C 1.56593020 -1.20201130 8.45508771

C 1.63890956 0.18453839 8.24341152

N 1.68694775 3.92321428 6.02932703

C 3.82648862 4.50361007 5.03446693

C 2.43856306 5.00361060 5.38082878

C -0.22777853 3.08227332 7.27126529

C 0.33096227 4.25199687 6.48402629

H 1.62461278 3.13265417 5.38588031

H 7.28202187 4.86955201 6.13569272

H 8.48977052 6.63296587 7.41600691

H 7.35081333 7.75189793 9.33060988

H 5.04731958 7.12318932 9.95722507

H -0.79459139 1.14136230 10.45535390

H -0.87100617 -1.32192604 10.84098653

H 0.65002810 -2.80988356 9.54347143

H 2.23869705 -1.86233455 7.90905723

H 3.78913717 3.71270916 4.27571089

H 4.48673090 5.29994774 4.68094107

H 2.49789495 5.84048854 6.08465410

H 1.94977950 5.35914257 4.45974286

H -1.23571513 3.28428091 7.64405479

H -0.22611903 2.16070056 6.67953294

H -0.34853624 4.47449262 5.64695890

H 0.39003644 5.14805218 7.11366519

N 4.25140208 2.08241990 9.77558762

H 3.85488533 1.16782592 9.97920074

H 5.15768797 1.91531736 9.33882112

N 4.39865041 2.79650914 11.02412472

H 5.34492781 2.66860700 11.38642433

H 4.32155616 3.78351678 10.76531259

trans-(Fe(NH)S4)N2H4 **(7t)** S12g-Cosmo Quintet

Fe 2.89422913 3.15909345 7.84768960

S 3.31655279 5.35554416 8.83009393

S 4.75656526 3.94067608 6.20408888

S 0.50977655 2.63242503 8.69562523

S 2.76854371 0.78952875 7.13595625

C 5.62079267 5.10283557 7.26161945

C 6.97749201 5.30950627 6.99700965

C 7.75849042 6.07486326 7.85660200

C 7.16664695 6.63624465 8.98892701

C 5.81854780 6.43035713 9.25668805

C 5.00745719 5.65096477 8.41047119

C 0.67339287 0.87248046 8.99278577

C -0.14096647 0.31200873 9.98098195

C -0.00097104 -1.02503961 10.33842689

C 0.95879086 -1.80292541 9.68822522

C 1.77011113 -1.24924090 8.70504247

C 1.66520332 0.10585238 8.33524812

N 1.68548034 3.93908219 6.06541110

C 3.69374610 4.90509314 5.02866979

C 2.27737303 5.16514249 5.50306079

C -0.26362923 2.78794758 7.01820850

C 0.24778989 4.05653308 6.36390782

H 1.78993305 3.18772141 5.37966883

H 7.42116268 4.85315387 6.11345087

H 8.81705765 6.22259368 7.64898936

H 7.76496226 7.23059908 9.67931123

H 5.37555553 6.86004641 10.15409594

H -0.88307406 0.93680830 10.47530600

H -0.63120262 -1.45271167 11.11651906

H 1.08355656 -2.85188648 9.95676574

H 2.52421040 -1.86593878 8.21797873

H 3.69574797 4.26824314 4.13603614

H 4.21879206 5.83335629 4.78862388

H 2.26579833 5.92878706 6.28640505

H 1.69407894 5.53441560 4.64451992

H -1.34799861 2.82225679 7.15162466

H 0.01303416 1.89781059 6.44442266

H -0.33650487 4.24470587 5.45075479

H 0.10423363 4.91891314 7.02717646

N 4.02137772 2.24768354 9.66164253

H 3.62579603 1.32144502 9.81804298

H 4.96963372 2.08565529 9.31497534

N 4.05026128 2.93668237 10.93826571

H 4.95644503 2.76944807 11.37793104

H 4.02622234 3.93070056 10.68875864

1. CSD entry VACBOQ [↑](#footnote-ref-1)
2. CSD entry DABMUO [↑](#footnote-ref-2)
3. CSD entry ZAZNUJ [↑](#footnote-ref-3)
4. CSD entry VADPEV [↑](#footnote-ref-4)
5. CSD entry HEYNII [↑](#footnote-ref-5)
6. CSD entry YAJLEA [↑](#footnote-ref-6)
7. CSD entry YAJKUP [↑](#footnote-ref-7)
8. CSD entry QEFWUV [↑](#footnote-ref-8)
9. CSD entry NEGJIT [↑](#footnote-ref-9)