



SUPPLEMENTARY MATERIAL TO  
**Spin state relaxation of iron complexes:  
The case for OPBE and S12g**

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TABLE S-I. Selected bond lengths (Å) for compound **1** at the low (ground state), intermediate and high spin state

Data		Fe–N <sub>NCO</sub>	Fe–N <sub>pyr</sub>	Fe–S
X-Ray <sup>a1</sup>		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

<sup>a</sup>CSD entry VACBOQ

TABLE S-II. Selected bond lengths (Å) for compound **2** at the low, intermediate (ground state) and high spin state

Data		Fe–Cl	Fe–S1	Fe–S2	Fe–N1	Fe–N2
X-Ray <sup>a2</sup>		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

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TABLE S-II. Continued

Data		Fe-Cl	Fe-S1	Fe-S2	Fe-N1	Fe-N2
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

<sup>a</sup>CSD entry DABMUOTABLE S-III. Selected bond lengths (Å) for compound **3** at the low, intermediate and high spin state (ground state)

Data		Fe-N <sub>(CH<sub>2</sub>)<sub>3</sub></sub>	Fe-N <sub>imidazole</sub>	Fe-S1	Fe-S2	Fe-S3
X-Ray <sup>a3</sup>		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

<sup>a</sup>CSD entry ZAZNUJTABLE S-IV. Selected bond lengths (Å) for compound *trans-4* at the low (ground state), intermediate and high spin state

Data		Fe-S <sub>b</sub>	Fe-S <sub>nb</sub>	Fe-S <sub>b</sub>	Fe-S <sub>nb</sub>	Fe-CO	Fe-N <sub>ax</sub>
X-Ray <sup>a4</sup>		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

<sup>a</sup>CSD entry VADPEV

TABLE S-V. Selected bond lengths (Å) for compound *trans-5* at the low (ground state), intermediate and high spin state

Data		Fe-S <sub>nb</sub>	Fe-S <sub>b</sub>	Fe-S <sub>b</sub>	Fe-S <sub>nb</sub>	Fe-PMe <sub>3</sub>	Fe-N <sub>ax</sub>
X-Ray <sup>a5</sup>		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

<sup>a</sup>CSD entry HEYNIITABLE S-VI. Selected bond lengths (Å) for compound *meso-6* at the low, intermediate and high spin state (ground state)

Data		Fe-S <sub>nb</sub>	Fe-S <sub>b</sub>	Fe-S <sub>b</sub>	Fe-S <sub>nb</sub>	Fe-N <sub>ax</sub>	Fe-NH <sub>3</sub>
X-Ray <sup>a6</sup>		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

<sup>a</sup>CSD entry YAJLEATABLE S-VII. Selected bond lengths (Å) for compound *meso-7* at the low, intermediate and high spin state (ground state)

Data		Fe-N <sub>2</sub> H <sub>4</sub>	Fe-S <sub>nb</sub>	Fe-S <sub>b</sub>	Fe-S <sub>nb</sub>	Fe-S <sub>b</sub>	Fe-N <sub>ax</sub>
X-Ray <sup>a6</sup>		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

TABLE S-VII. Continued

Data		Fe–N <sub>2</sub> H <sub>4</sub>	Fe–S <sub>nb</sub>	Fe–S <sub>b</sub>	Fe–S <sub>nb</sub>	Fe–S <sub>b</sub>	Fe–N <sub>ax</sub>
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

<sup>a</sup>CSD entry YAJKUPTABLE S-VIII. OPBE/TZP ligand binding energy (kcal mol<sup>-1</sup>) for *trans/meso*-(Fe(NH)S<sub>4</sub>)L with respect to energy of infinitely separated *trans*-Fe(NH)S<sub>4</sub> (triplet ground state) and ligand (in parentheses corrected for basis set superposition error)

ligand L	Singlet	Triplet	Quintet
<i>trans</i>			
CO (4)	-32.0 (-29.8)	-8.6 (-6.9)	2.7 (3.8)
PMe <sub>3</sub> (5)	-15.3 (-11.6)	1.0 (3.9)	4.7 (7.1)
NH <sub>3</sub> (6)	-3.1 (-1.6)	4.6 (5.5)	5.3 (6.3)
N <sub>2</sub> H <sub>4</sub> (7)	-3.5 (-1.8)	-1.9 (-1.5)	5.2 (6.1)
<i>meso</i>			
CO (4)	-29.2 (-27.0)	4.2 (5.8)	9.6 (11.1)
PMe <sub>3</sub> (5)	-12.2 (-8.5)	7.5 (10.3)	5.4 (7.8)
NH <sub>3</sub> (6)	-0.6 (0.9)	9.7 (10.7)	6.0 (6.9)
N <sub>2</sub> H <sub>4</sub> (7)	-1.0 (0.8)	9.3 (10.3)	6.6 (7.7)

TABLE S-IX. Selected bond lengths (Å) for compound **8** at the low, intermediate and high spin state (ground state)

Data		Fe–Cl	Fe–N
X-Ray <sup>a7</sup>		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

<sup>a</sup>CSD entry QEFWUV

TABLE S-X. Selected bond lengths (Å) for compound **9** at the low, intermediate (ground state) and high spin state

Data		Fe-Cl	Fe-N
X-Ray <sup>a8</sup>		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

<sup>a</sup>CSD entry NEGJIT

## COORDINATES OF THE OPTIMIZED STRUCTURES

*Iron (III) Complexes*TABLE S-XI. Fe-(PyPepS)<sub>2</sub> (1) OPBE Doublet

Fe	0.00000000	0.00000000	0.09321563	H	0.98593130	-3.83188253	2.83122846
N	1.55604623	-1.17038397	-0.11840764	H	-1.18887395	-3.84619042	4.14525865
N	0.54602890	1.24265053	1.34774936	H	-2.93249711	-2.12448684	3.54558176
N	-1.55604623	1.17038397	-0.11840764	H	-2.42581095	-0.48779929	1.73790910
N	-0.54602890	-1.24265053	1.34774936	H	-0.98593130	3.83188253	2.83122846
C	1.61524423	-2.16130011	0.80964119	H	1.18887395	3.84619042	4.14525865
C	3.59311775	-1.87153324	-1.38402923	H	2.93249711	2.12448684	3.54558176
C	2.51883872	-1.00388787	-1.11691696	H	2.42581095	0.48779929	1.73790910
C	0.38413453	-2.17222921	1.64429712	C	-4.48608795	1.59738291	-2.41597196
C	0.18766160	-3.11636133	2.65037896	C	-4.33568202	0.45068915	-3.19810651
C	-1.00568496	-3.11357045	3.35843240	C	4.48608795	-1.59738291	-2.41597196
C	-1.97212401	-2.16101542	3.03329214	C	4.33568202	-0.45068915	-3.19810651
C	-1.70109265	-1.24260343	2.02916561	H	-5.03543532	0.23743072	-4.00753286
C	2.36531647	0.15779748	-1.91906658	H	-5.30619045	2.29021881	-2.60924442
C	3.28071373	0.41779390	-2.94843487	H	-3.71025907	2.75531216	-0.76919723
C	-2.51883872	1.00388787	-1.11691696	H	5.03543532	-0.23743072	-4.00753286
C	-3.59311775	1.87153324	-1.38402923	H	5.30619045	-2.29021881	-2.60924442
C	-1.61524423	2.16130011	0.80964119	H	3.71025907	-2.75531216	-0.76919723
C	-3.28071373	-0.41779390	-2.94843487	O	-2.51261189	3.00008415	1.01838309
C	-2.36531647	-0.15779748	-1.91906658	O	2.51261189	-3.00008415	1.01838309
C	-0.38413453	2.17222921	1.64429712	H	3.14431353	1.31176108	-3.55619282
C	-0.18766160	3.11636133	2.65037896	H	-3.14431353	-1.31176108	-3.55619282
C	1.00568496	3.11357045	3.35843240	S	-1.05149266	-1.23617869	-1.57172998
C	1.97212401	2.16101542	3.03329214	S	1.05149266	1.23617869	-1.57172998
C	1.70109265	1.24260343	2.02916561				

TABLE S-XII. Fe-(PyPepS)<sub>2</sub> (1) OPBE Quartet

Fe	0.00000000	0.00000000	-0.16881019	H	1.05127146	-3.89123240	2.83474272
N	1.73325128	-1.27046938	-0.09454863	H	-1.18718270	-4.00397732	4.02989483
N	0.49503420	1.35444769	1.28907789	H	-2.96408581	-2.34591894	3.34630525
N	-1.73325128	1.27046938	-0.09454863	H	-2.41879935	-0.67426918	1.58345232
N	-0.49503420	-1.35444769	1.28907789	H	-1.05127146	3.89123240	2.83474272
C	1.74597165	-2.22307362	0.86101478	H	1.18718270	4.00397732	4.02989483
C	3.89221296	-1.90849680	-1.17387072	H	2.96408581	2.34591894	3.34630525
C	2.75107980	-1.09745276	-1.01966899	H	2.41879935	0.67426918	1.58345232

C	0.45270849	-2.25097872	1.62413811	C	-4.82295531	1.65593902	-2.17741674
C	0.23606385	-3.20720466	2.61426473	C	-4.64409975	0.58542032	-3.05512864
C	-0.99314769	-3.25897989	3.25747808	C	4.82295531	-1.65593902	-2.17741674
C	-1.97701625	-2.34360062	2.88637349	C	4.64409975	-0.58542032	-3.05512864
C	-1.68513002	-1.40775806	1.90534343	H	-5.36715114	0.39022324	-3.84816319
C	2.58540340	0.00457421	-1.90772314	H	-5.69207549	2.30800869	-2.27663165
C	3.52757703	0.23177858	-2.92066365	H	-4.02463110	2.73942573	-0.49122836
C	-2.75107980	1.09745276	-1.01966899	H	5.36715114	-0.39022324	-3.84816319
C	-3.89221296	1.90849680	-1.17387072	H	5.69207549	-2.30800869	-2.27663165
C	-1.74597165	2.22307362	0.86101478	H	4.02463110	-2.73942573	-0.49122836
C	-3.52757703	-0.23177858	-2.92066365	O	-2.63207313	3.04010636	1.17522382
C	-2.58540340	-0.00457421	-1.90772314	O	2.63207313	-3.04010636	1.17522382
C	-0.45270849	2.25097872	1.62413811	H	3.37086489	1.06691500	-3.60240428
C	-0.23606385	3.20720466	2.61426473	H	-3.37086489	-1.06691500	-3.60240428
C	0.99314769	3.25897989	3.25747808	S	-1.24455398	-1.09319711	-1.70886997
C	1.97701625	2.34360062	2.88637349	S	1.24455398	1.09319711	-1.70886997
C	1.68513002	1.40775806	1.90534343				

TABLE S-XIII. Fe-(PyPepS)<sub>2</sub> (1) OPBE Sextet

Fe	0.00000000	0.00000000	-0.41723245	H	0.83779289	-4.11049170	2.56615352
N	1.70195998	-1.30400122	-0.15192785	H	-1.38259410	-4.19739795	3.78168477
N	0.61178764	1.41313186	1.21304888	H	-3.08074400	-2.40548155	3.27128326
N	-1.70195998	1.30400122	-0.15192785	H	-2.49396051	-0.66259818	1.58581139
N	-0.61178764	-1.41313186	1.21304888	H	-0.83779289	4.11049170	2.56615352
C	1.62574046	-2.29615353	0.76566391	H	1.38259410	4.19739795	3.78168477
C	4.04573469	-1.83031350	-0.82463119	H	3.08074400	2.40548155	3.27128326
C	2.86289389	-1.06409660	-0.88635019	H	2.49396051	0.66259818	1.58581139
C	0.29982760	-2.35618604	1.47734858	C	-5.16190657	1.51271085	-1.59087191
C	0.05432957	-3.37687688	2.39946269	C	-5.14003091	0.41143055	-2.44673462
C	-1.16498212	-3.40971285	3.05889056	C	5.16190657	-1.51271085	-1.59087191
C	-2.10860253	-2.42299044	2.78088148	C	5.14003091	-0.41143055	-2.44673462
C	-1.78751100	-1.44641975	1.84705297	H	-6.01151122	0.15645020	-3.05134661
C	2.84417266	0.05668229	-1.77186905	H	-6.05363744	2.13708285	-1.51710302
C	3.98789033	0.35779632	-2.52970061	H	-4.06204235	2.68538509	-0.16144351
C	-2.86289389	1.06409660	-0.88635019	H	6.01151122	-0.15645020	-3.05134661
C	-4.04573469	1.83031350	-0.82463119	H	6.05363744	-2.13708285	-1.51710302
C	-1.62574046	2.29615353	0.76566391	H	4.06204235	-2.68538509	-0.16144351
C	-3.98789033	-0.35779632	-2.52970061	O	-2.47897210	3.13695003	1.10785797
C	-2.84417266	-0.05668229	-1.77186905	O	2.47897210	-3.13695003	1.10785797
C	-0.29982760	2.35618604	1.47734858	H	3.94573501	1.21613875	-3.19892092

C	-0.05432957	3.37687688	2.39946269	H	-3.94573501	-1.21613875	-3.19892092
C	1.16498212	3.40971285	3.05889056	S	-1.42007731	-1.02454378	-1.97285375
C	2.10860253	2.42299044	2.78088148	S	1.42007731	1.02454378	-1.97285375
C	1.78751100	1.44641975	1.84705297				

TABLE S-XIV. Fe(tsalen)Cl (2) OPBE Doublet

Fe	-0.52016324	-0.12634477	0.00000000	C	0.08726397	0.29353356	4.85576324
Cl	-2.64978998	0.35805032	0.00000000	C	0.05163817	-0.72407217	5.78414440
S	-0.44762363	-1.76868076	1.39692316	C	-0.04892508	2.57299155	-0.75761354
C	-0.04892508	2.57299155	0.75761354	C	0.02103638	1.16343904	-2.59552974
N	-0.10383146	1.21121846	1.29534759	H	0.22233964	2.11491561	-3.10132000
S	-0.44762363	-1.76868076	-1.39692316	C	-0.06306205	0.04301100	-3.47136465
H	-0.41922692	-3.34780652	-3.66625269	C	-0.12648289	-2.04657607	-5.34717999
H	-0.41922692	-3.34780652	3.66625269	C	-0.25970961	-1.29469194	-3.03570043
C	0.02103638	1.16343904	2.59552974	C	0.08726397	0.29353356	-4.85576324
C	-0.27544258	-2.32285740	4.00356562	C	0.05163817	-0.72407217	-5.78414440
H	0.23031593	1.32189165	5.18737746	C	-0.27544258	-2.32285740	-4.00356562
H	-0.15410806	-2.86142384	6.06985196	H	-0.15410806	-2.86142384	-6.06985196
H	0.22233964	2.11491561	3.10132000	H	0.23031593	1.32189165	-5.18737746
C	-0.06306205	0.04301100	3.47136465	H	0.16265903	-0.50420855	-6.84441134
H	0.16265903	-0.50420855	6.84441134	H	-0.92676452	3.11624174	-1.12616327
N	-0.10383146	1.21121846	-1.29534759	H	0.84322119	3.08256648	-1.14220369
C	-0.12648289	-2.04657607	5.34717999	H	0.84322119	3.08256648	1.14220369
C	-0.25970961	-1.29469194	3.03570043	H	-0.92676452	3.11624174	1.12616327

TABLE S-XV. Fe(tsalen)Cl (2) OPBE Quartet

Fe	-1.11714344	-0.02547195	0.00000000	C	1.13696325	0.06104959	4.41500781
Cl	-3.24556419	0.74684055	0.00000000	C	1.32460897	-1.00270304	5.27106842
S	-1.05421263	-1.69950724	1.44583342	C	-0.48368071	2.60345681	-0.76657251
C	-0.48368071	2.60345681	0.76657251	C	0.24637328	1.11435785	-2.43293156
N	-0.34540193	1.25136661	1.28859370	H	0.67674626	2.01891810	-2.88146854
S	-1.05421263	-1.69950724	-1.44583342	C	0.39979235	-0.07053456	-3.21609325
H	-0.39354330	-3.37091569	-3.52764847	C	0.75756221	-2.24184618	-4.94084171
H	-0.39354330	-3.37091569	3.52764847	C	-0.16717503	-1.32970336	-2.87605083
C	0.24637328	1.11435785	2.43293156	C	1.13696325	0.06104959	-4.41500781
C	0.03125691	-2.40027656	3.77676871	C	1.32460897	-1.00270304	-5.27106842
H	1.56148617	1.03456798	4.66024230	C	0.03125691	-2.40027656	-3.77676871
H	0.89374016	-3.09622031	5.60357801	H	0.89374016	-3.09622031	-5.60357801
H	0.67674626	2.01891810	2.88146854	H	1.56148617	1.03456798	-4.66024230
C	0.39979235	-0.07053456	3.21609325	H	1.89942141	-0.88119865	-6.18703191



H	1.89942141	-0.88119865	6.18703191	H	-1.44346641	2.99311754	-1.12468634
N	-0.34540193	1.25136661	-1.28859370	H	0.31309989	3.25049189	-1.15612634
C	0.75756221	-2.24184618	4.94084171	H	0.31309989	3.25049189	1.15612634
C	-0.16717503	-1.32970336	2.87605083	H	-1.44346641	2.99311754	1.12468634

TABLE S-XVI. Fe(tsalen)Cl (2) OPBE Sextet

Fe	-1.62537639	-0.02616676	0.00000000	C	1.80206655	-0.07252639	3.66909649
Cl	-3.69422871	0.76012131	0.00000000	C	2.23913256	-1.17989804	4.36681881
S	-1.49638255	-1.56292977	1.76303920	C	-0.70243253	2.69162779	-0.77264694
C	-0.70243253	2.69162779	0.77264694	C	0.34687780	1.12345388	-2.17424432
N	-0.53990896	1.34030437	1.26246875	H	0.94336957	1.98248795	-2.51745334
S	-1.49638255	-1.56292977	-1.76303920	C	0.67360559	-0.11718101	-2.82122330
H	-0.14078390	-3.38366675	-3.33522057	C	1.52536559	-2.37706314	-4.23630042
H	-0.14078390	-3.38366675	3.33522057	C	-0.05587794	-1.33496074	-2.68921792
C	0.34687780	1.12345388	2.17424432	C	1.80206655	-0.07252639	-3.66909649
C	0.40650814	-2.44776175	3.42644703	C	2.23913256	-1.17989804	-4.36681881
H	2.34052398	0.87080032	3.76301751	C	0.40650814	-2.44776175	-3.42644703
H	1.84928610	-3.26614495	4.77686873	H	1.84928610	-3.26614495	-4.77686873
H	0.94336957	1.98248795	2.51745334	H	2.34052398	0.87080032	-3.76301751
C	0.67360559	-0.11718101	2.82122330	H	3.11777635	-1.11985230	-5.00618558
H	3.11777635	-1.11985230	5.00618558	H	-1.66553512	3.06678695	-1.13838515
N	-0.53990896	1.34030437	-1.26246875	H	0.08409579	3.35432863	-1.16008406
C	1.52536559	-2.37706314	4.23630042	H	0.08409579	3.35432863	1.16008406
C	-0.05587794	-1.33496074	2.68921792	H	-1.66553512	3.06678695	1.13838515

TABLE S-XVII. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(1MIm) (3) OPBE Doublet

Fe	-0.00650094	-0.63931967	-0.94322405	C	3.69429327	1.56118877	2.83272920
H	3.02417548	-0.48244561	2.90736489	C	2.24105612	0.53155908	1.17597949
H	4.27944794	1.47723110	3.74829475	C	2.87402673	2.85638237	0.98370717
S	-1.90717491	-0.86050094	0.06319593	C	3.63661930	2.77183837	2.14362665
N	0.04845517	1.39790902	-0.85839747	C	2.99386579	0.45954705	2.36188846
N	-0.00773498	-2.64874592	-1.14481306	S	1.45335991	-0.92222153	0.61898657
C	1.46293643	1.87859140	-0.82714426	H	2.82401524	3.80292753	0.44431838
C	-0.63469202	1.95964072	0.35045451	H	4.17487193	3.64514117	2.50945376
C	-0.61882199	1.99118868	-2.05846775	H	-4.67104916	-0.38158813	0.41871361
H	1.99661275	1.31680414	-1.60227251	C	-4.90512489	1.74292412	0.66370733
C	2.18149299	1.75323619	0.47894298	C	-2.77235061	0.63315052	0.31278291
H	1.47148476	2.93728352	-1.12223730	C	-2.88407263	3.03551310	0.56959951
C	0.15553313	1.97399307	-3.33893275	C	-4.26598250	2.98137827	0.71577890
H	-0.86897572	3.03559512	-1.82498628	C	-4.16938225	0.58395556	0.46129704

H	-1.56370342	1.44799511	-2.18108976	H	-5.98681717	1.67909581	0.78117304
H	-0.22512523	1.42013287	1.21041464	H	-2.37636357	3.99929727	0.62366714
C	-2.12461966	1.88001013	0.37557826	H	-4.83728649	3.89503930	0.87313717
H	-0.33668691	3.01401686	0.44409137	C	1.08052173	-3.40637480	-1.17907517
C	1.45840615	1.99130510	-5.82434070	C	-1.06007009	-3.48499202	-1.42814144
C	0.33054263	3.16202562	-4.05279286	H	2.08698140	-3.05333897	-1.00655704
C	0.64622491	0.77220825	-3.88360590	C	1.70592404	-5.78624259	-1.54294697
C	1.29758124	0.80147016	-5.12798472	C	-0.59225094	-4.75520792	-1.61880612
C	0.97031581	3.18206927	-5.28791372	H	-2.07500665	-3.11740116	-1.47521546
H	-0.05344531	4.09352998	-3.63553448	N	0.77065194	-4.68939044	-1.45867285
S	0.44373788	-0.76043088	-3.07362921	H	-1.10422358	-5.67931174	-1.85204734
H	1.67343732	-0.13273088	-5.54248555	H	2.72150514	-5.39945423	-1.43947483
H	1.08887374	4.12148906	-5.82625897	H	1.61976129	-6.28708345	-2.51260396
H	1.96307720	1.98986150	-6.79024052	H	1.52265461	-6.51270770	-0.74386446

TABLE S-XVIII. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(IMIm) (3) OPBE Quartet

Fe	0.03264918	-0.65279517	-0.92299413	C	3.76217612	1.62716448	2.85917801
H	3.22983175	-0.45603119	2.92822241	C	2.35931348	0.50836153	1.21296368
H	4.35978181	1.57675135	3.76912898	C	2.85069265	2.87129776	1.02058712
S	-2.06013518	-0.88556966	0.10282655	C	3.62310464	2.83441093	2.17547360
N	0.06656468	1.36959380	-0.81943944	C	3.13221442	0.48414797	2.38820232
N	0.06721080	-2.68797224	-1.13340929	S	1.59718553	-0.96899974	0.69323701
C	1.49956079	1.82051367	-0.78590177	H	2.74280929	3.81267022	0.48068821
C	-0.63544027	1.85786512	0.41807649	H	4.10902165	3.73883517	2.53859556
C	-0.59954777	2.01030997	-2.00221991	H	-4.81885313	-0.21823005	0.15971310
H	2.02042149	1.23577652	-1.55431741	C	-4.92984382	1.91193380	0.44198154
C	2.22079075	1.72802143	0.51980922	C	-2.85487157	0.65627134	0.23270199
H	1.51610816	2.86765914	-1.11445416	C	-2.82456612	3.05966157	0.53854474
C	0.14603863	1.98990807	-3.29613237	C	-4.21375535	3.10004574	0.58291731
H	-0.80287460	3.05528740	-1.73211144	C	-4.25972815	0.70958912	0.26603381
H	-1.56553967	1.50573047	-2.11576282	H	-6.01937109	1.92152779	0.47056452
H	-0.28610603	1.22351654	1.23933206	H	-2.25988107	3.98553655	0.65392443
C	-2.13038981	1.85958653	0.36753794	H	-4.73092715	4.04788209	0.72463363
H	-0.28755492	2.88275180	0.60401085	C	1.16132445	-3.43514511	-1.17144232
C	1.33260272	1.99679108	-5.83311711	C	-0.98303247	-3.52045536	-1.42955011
C	0.40643670	3.18841675	-3.96533626	H	2.16444025	-3.07636982	-0.98959638
C	0.49917554	0.77083451	-3.90502223	C	1.79565028	-5.80752927	-1.56350657
C	1.09736597	0.79690495	-5.17691403	C	-0.50647660	-4.78517735	-1.63031308
C	0.99123154	3.20572085	-5.22690541	H	-1.99863315	-3.15327726	-1.47151175
H	0.12556159	4.13083169	-3.49369275	N	0.85619979	-4.71407550	-1.46690579

S	0.19783609	-0.77187963	-3.15483252	H	-1.01380254	-5.71047869	-1.86845766
H	1.36913871	-0.14681917	-5.64702187	H	2.80905805	-5.42070970	-1.44166139
H	1.17510529	4.15223796	-5.73308514	H	1.71920904	-6.28857150	-2.54376297
H	1.78881595	1.98881691	-6.82293045	H	1.60434529	-6.54885685	-0.78050257

TABLE S-XIX. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(IMIm) (3) OPBE Sextet

Fe	0.04042544	-0.45777272	-0.98754529	C	3.44204082	0.76623596	2.94412842
H	3.58379523	-1.03817009	1.77738731	C	2.54137268	0.50596595	0.70320724
H	3.97424496	0.34339370	3.79597679	C	2.31026774	2.60266357	1.88604063
S	-1.38622478	-0.61481242	0.81470383	C	2.98401357	2.08088740	2.98560216
N	0.06471573	1.95927030	-0.78182393	C	3.22204596	-0.01226739	1.81413814
N	0.03239253	-2.76791981	-1.11722917	S	2.34468120	-0.46525740	-0.74703264
C	1.42913365	2.44282082	-0.46711481	H	1.96162037	3.63570541	1.91272175
C	-0.85026031	2.39270509	0.29945770	H	3.15291531	2.69841132	3.86694581
C	-0.37665725	2.56943071	-2.05770150	H	-4.21554238	-0.83328589	0.61769696
H	2.04751007	2.21085016	-1.34110766	C	-4.96279304	1.13833435	0.17651977
C	2.07576073	1.83756376	0.74157577	C	-2.60982546	0.58394392	0.43011633
H	1.40011039	3.54077630	-0.35349516	C	-3.29618052	2.85241989	-0.05527680
C	0.38768213	2.15528496	-3.27894046	C	-4.63359770	2.46968821	-0.06667527
H	-0.33696737	3.66854191	-1.95953224	C	-3.96144840	0.20683739	0.42136638
H	-1.42527383	2.28135562	-2.18989844	H	-6.00575483	0.82205410	0.17689707
H	-0.43113605	1.99853948	1.23204529	H	-3.03755467	3.89718988	-0.23133036
C	-2.27275596	1.93340147	0.18880145	H	-5.41203225	3.20675539	-0.25967151
H	-0.83071514	3.49506597	0.35982942	C	1.07128706	-3.56961646	-0.96987130
C	1.69735613	1.45432354	-5.65937128	C	-1.03889559	-3.58294220	-1.37128558
C	1.21583447	3.06368491	-3.94222233	H	2.08006453	-3.24236161	-0.75302081
C	0.21157406	0.86608588	-3.82840001	C	1.59734798	-6.00694601	-1.01378454
C	0.87533378	0.53490083	-5.01912820	C	-0.63210857	-4.88922100	-1.37666678
C	1.87263340	2.72768858	-5.12180763	H	-2.03319530	-3.18679853	-1.53018798
H	1.34294073	4.06380504	-3.52613608	N	0.71859148	-4.86590651	-1.11872674
S	-0.87736477	-0.29582278	-3.08787201	H	-1.17267107	-5.81327719	-1.53619150
H	0.73232681	-0.45920467	-5.43848264	H	2.61115687	-5.65851825	-0.80581841
H	2.51362104	3.45559252	-5.61760332	H	1.60732985	-6.57310534	-1.95116700
H	2.20205364	1.17447927	-6.58386457	H	1.27883779	-6.66555684	-0.19874733

TABLE S-XX. FePCl (8) OPBE Doublet

Fe	0.00000000	0.00000000	-0.13493173	C	2.81652950	1.08818157	0.06370342
N	0.00000000	-1.97671357	0.06669009	C	2.81652950	-1.08818157	0.06370342
N	1.97671357	0.00000000	0.06669009	C	4.18988310	0.67917148	0.07848492
N	0.00000000	1.97671357	0.06669009	H	5.03776688	1.35542931	0.09050624

N	-1.97671357	0.00000000	0.06669009	C	4.18988310	-0.67917148	0.07848492
C	2.40688545	-2.40688545	0.05850742	H	5.03776688	-1.35542931	0.09050624
C	2.40688545	2.40688545	0.05850742	C	-1.08818157	2.81652950	0.06370342
C	-2.40688545	2.40688545	0.05850742	C	1.08818157	2.81652950	0.06370342
C	-2.40688545	-2.40688545	0.05850742	C	-0.67917148	4.18988310	0.07848492
H	3.17557679	-3.17557679	0.05605892	H	-1.35542931	5.03776688	0.09050624
H	3.17557679	3.17557679	0.05605892	C	0.67917148	4.18988310	0.07848492
H	-3.17557679	3.17557679	0.05605892	H	1.35542931	5.03776688	0.09050624
H	-3.17557679	-3.17557679	0.05605892	C	-2.81652950	-1.08818157	0.06370342
C	1.08818157	-2.81652950	0.06370342	C	-2.81652950	1.08818157	0.06370342
C	-1.08818157	-2.81652950	0.06370342	C	-4.18988310	-0.67917148	0.07848492
C	0.67917148	-4.18988310	0.07848492	H	-5.03776688	-1.35542931	0.09050624
H	1.35542931	-5.03776688	0.09050624	C	-4.18988310	0.67917148	0.07848492
C	-0.67917148	-4.18988310	0.07848492	H	-5.03776688	1.35542931	0.09050624
H	-1.35542931	-5.03776688	0.09050624	Cl	0.00000000	0.00000000	-2.26849555

TABLE S-XXI. FePCl (**8**) OPBE Quartet

Fe	0.00000000	0.00000000	-0.23389793	C	2.82325111	1.09028294	0.09960439
N	0.00000000	-1.99459182	0.07806529	C	2.82325111	-1.09028294	0.09960439
N	1.99459182	0.00000000	0.07806529	C	4.19654598	0.67974723	0.13884129
N	0.00000000	1.99459182	0.07806529	H	5.04505523	1.35471545	0.16740469
N	-1.99459182	0.00000000	0.07806529	C	4.19654598	-0.67974723	0.13884129
C	2.41098711	-2.41098711	0.10004043	H	5.04505523	-1.35471545	0.16740469
C	2.41098711	2.41098711	0.10004043	C	-1.09028294	2.82325111	0.09960439
C	-2.41098711	2.41098711	0.10004043	C	1.09028294	2.82325111	0.09960439
C	-2.41098711	-2.41098711	0.10004043	C	-0.67974723	4.19654598	0.13884129
H	3.17939216	-3.17939216	0.11633962	H	-1.35471545	5.04505523	0.16740469
H	3.17939216	3.17939216	0.11633962	C	0.67974723	4.19654598	0.13884129
H	-3.17939216	3.17939216	0.11633962	H	1.35471545	5.04505523	0.16740469
H	-3.17939216	-3.17939216	0.11633962	C	-2.82325111	-1.09028294	0.09960439
C	1.09028294	-2.82325111	0.09960439	C	-2.82325111	1.09028294	0.09960439
C	-1.09028294	-2.82325111	0.09960439	C	-4.19654598	-0.67974723	0.13884129
C	0.67974723	-4.19654598	0.13884129	H	-5.04505523	-1.35471545	0.16740469
H	1.35471545	-5.04505523	0.16740469	C	-4.19654598	0.67974723	0.13884129
C	-0.67974723	-4.19654598	0.13884129	H	-5.04505523	1.35471545	0.16740469
H	-1.35471545	-5.04505523	0.16740469	Cl	0.00000000	0.00000000	-2.47435661
Fe	0.00000000	0.00000000	-0.23389793	C	2.82325111	1.09028294	0.09960439
N	0.00000000	-1.99459182	0.07806529	C	2.82325111	-1.09028294	0.09960439
N	1.99459182	0.00000000	0.07806529	C	4.19654598	0.67974723	0.13884129
N	0.00000000	1.99459182	0.07806529	H	5.04505523	1.35471545	0.16740469

TABLE S-XXII. FePcI (8) OPBE Sextet

Fe	0.00000000	0.00000000	-0.44777338	C	2.85188330	1.09533023	0.14865012
N	0.00000000	-2.03501620	0.09917734	C	2.85188330	-1.09533023	0.14865012
N	2.03501620	0.00000000	0.09917734	C	4.22669585	0.68084051	0.22218142
N	0.00000000	2.03501620	0.09917734	H	5.07923321	1.34941257	0.27814456
N	-2.03501620	0.00000000	0.09917734	C	4.22669585	-0.68084051	0.22218142
C	2.41730760	-2.41730760	0.15789802	H	5.07923321	-1.34941257	0.27814456
C	2.41730760	2.41730760	0.15789802	C	-1.09533023	2.85188330	0.14865012
C	-2.41730760	2.41730760	0.15789802	C	1.09533023	2.85188330	0.14865012
C	-2.41730760	-2.41730760	0.15789802	C	-0.68084051	4.22669585	0.22218142
H	3.18571900	-3.18571900	0.20153874	H	-1.34941257	5.07923321	0.27814456
H	3.18571900	3.18571900	0.20153874	C	0.68084051	4.22669585	0.22218142
H	-3.18571900	3.18571900	0.20153874	H	1.34941257	5.07923321	0.27814456
H	-3.18571900	-3.18571900	0.20153874	C	-2.85188330	-1.09533023	0.14865012
C	1.09533023	-2.85188330	0.14865012	C	-2.85188330	1.09533023	0.14865012
C	-1.09533023	-2.85188330	0.14865012	C	-4.22669585	-0.68084051	0.22218142
C	0.68084051	-4.22669585	0.22218142	H	-5.07923321	-1.34941257	0.27814456
H	1.34941257	-5.07923321	0.27814456	C	-4.22669585	0.68084051	0.22218142
C	-0.68084051	-4.22669585	0.22218142	H	-5.07923321	1.34941257	0.27814456
H	-1.34941257	-5.07923321	0.27814456	Cl	0.00000000	0.00000000	-2.64427701
Fe	0.00000000	0.00000000	-0.44777338	C	2.85188330	1.09533023	0.14865012
N	0.00000000	-2.03501620	0.09917734	C	2.85188330	-1.09533023	0.14865012
N	2.03501620	0.00000000	0.09917734	C	4.22669585	0.68084051	0.22218142
N	0.00000000	2.03501620	0.09917734	H	5.07923321	1.34941257	0.27814456

TABLE S-XXIII. FePzCl (9) OPBE Doublet

Fe	0.00000000	0.00000000	-0.14948728	C	4.10076436	0.67778133	0.09410306
N	0.00000000	-1.89314378	0.05725539	H	4.93679774	1.36722679	0.11755725
N	1.89314378	0.00000000	0.05725539	C	4.10076436	-0.67778133	0.09410306
N	0.00000000	1.89314378	0.05725539	H	4.93679774	-1.36722679	0.11755725
N	-1.89314378	0.00000000	0.05725539	C	-1.09764538	2.72094474	0.06550262
N	2.37166606	-2.37166606	0.06327425	C	1.09764538	2.72094474	0.06550262
N	2.37166606	2.37166606	0.06327425	C	-0.67778133	4.10076436	0.09410306
N	-2.37166606	2.37166606	0.06327425	H	-1.36722679	4.93679774	0.11755725
N	-2.37166606	-2.37166606	0.06327425	C	0.67778133	4.10076436	0.09410306
C	1.09764538	-2.72094474	0.06550262	H	1.36722679	4.93679774	0.11755725
C	-1.09764538	-2.72094474	0.06550262	C	-2.72094474	-1.09764538	0.06550262
C	0.67778133	-4.10076436	0.09410306	C	-2.72094474	1.09764538	0.06550262
H	1.36722679	-4.93679774	0.11755725	C	-4.10076436	-0.67778133	0.09410306

C	-0.67778133	-4.10076436	0.09410306	H	-4.93679774	-1.36722679	0.11755725
H	-1.36722679	-4.93679774	0.11755725	C	-4.10076436	0.67778133	0.09410306
C	2.72094474	1.09764538	0.06550262	H	-4.93679774	1.36722679	0.11755725
C	2.72094474	-1.09764538	0.06550262	Cl	0.00000000	0.00000000	-2.27929341

TABLE S-XXIV. FePzCl (9) OPBE Quartet

Fe	0.00000000	0.00000000	-0.27136156	C	4.10541266	0.67781943	0.16375337
N	0.00000000	-1.90600755	0.06954024	H	4.94096607	1.36707333	0.20457463
N	1.90600755	0.00000000	0.06954024	C	4.10541266	-0.67781943	0.16375337
N	0.00000000	1.90600755	0.06954024	H	4.94096607	-1.36707333	0.20457463
N	-1.90600755	0.00000000	0.06954024	C	-1.09704635	2.72350914	0.10767117
N	2.37321444	-2.37321444	0.11458222	C	1.09704635	2.72350914	0.10767117
N	2.37321444	2.37321444	0.11458222	C	-0.67781943	4.10541266	0.16375337
N	-2.37321444	2.37321444	0.11458222	H	-1.36707333	4.94096607	0.20457463
N	-2.37321444	-2.37321444	0.11458222	C	0.67781943	4.10541266	0.16375337
C	1.09704635	-2.72350914	0.10767117	H	1.36707333	4.94096607	0.20457463
C	-1.09704635	-2.72350914	0.10767117	C	-2.72350914	-1.09704635	0.10767117
C	0.67781943	-4.10541266	0.16375337	C	-2.72350914	1.09704635	0.10767117
H	1.36707333	-4.94096607	0.20457463	C	-4.10541266	-0.67781943	0.16375337
C	-0.67781943	-4.10541266	0.16375337	H	-4.94096607	-1.36707333	0.20457463
H	-1.36707333	-4.94096607	0.20457463	C	-4.10541266	0.67781943	0.16375337
C	2.72350914	1.09704635	0.10767117	H	-4.94096607	1.36707333	0.20457463
C	2.72350914	-1.09704635	0.10767117	Cl	0.00000000	0.00000000	-2.51324797

TABLE S-XXV. FePzCl (9) OPBE Sextet

Fe	0.00000000	0.00000000	-0.57295979	C	4.12301997	0.67844227	0.29956142
N	0.00000000	-1.93528110	0.07618671	H	4.95816856	1.36282615	0.39698242
N	1.93528110	0.00000000	0.07618671	C	4.12301997	-0.67844227	0.29956142
N	0.00000000	1.93528110	0.07618671	H	4.95816856	-1.36282615	0.39698242
N	-1.93528110	0.00000000	0.07618671	C	-1.09956841	2.74209120	0.17111793
N	2.37445959	-2.37445959	0.19467902	C	1.09956841	2.74209120	0.17111793
N	2.37445959	2.37445959	0.19467902	C	-0.67844227	4.12301997	0.29956142
N	-2.37445959	2.37445959	0.19467902	H	-1.36282615	4.95816856	0.39698242
N	-2.37445959	-2.37445959	0.19467902	C	0.67844227	4.12301997	0.29956142
C	1.09956841	-2.74209120	0.17111793	H	1.36282615	4.95816856	0.39698242
C	-1.09956841	-2.74209120	0.17111793	C	-2.74209120	-1.09956841	0.17111793
C	0.67844227	-4.12301997	0.29956142	C	-2.74209120	1.09956841	0.17111793
H	1.36282615	-4.95816856	0.39698242	C	-4.12301997	-0.67844227	0.29956142
C	-0.67844227	-4.12301997	0.29956142	H	-4.95816856	-1.36282615	0.39698242
H	-1.36282615	-4.95816856	0.39698242	C	-4.12301997	0.67844227	0.29956142

C	2.74209120	1.09956841	0.17111793	H	-4.95816856	1.36282615	0.39698242
C	2.74209120	-1.09956841	0.17111793	Cl	0.00000000	0.00000000	-2.76114211

TABLE S-XXVI. Fe-(PyPepS)<sub>2</sub> (1) OPBE–Cosmo Doublet

Fe	0.00000000	0.00000000	-0.06274772	H	1.03196654	-3.83427017	2.87097443
N	1.55574142	-1.16677551	-0.11796895	H	-1.10204125	-3.83025901	4.21195773
N	0.51908743	1.24408195	1.38931465	H	-2.85238549	-2.10782411	3.64933648
N	-1.55574142	1.16677551	-0.11796895	H	-2.39148851	-0.48339865	1.82903554
N	-0.51908743	-1.24408195	1.38931465	H	-1.03196654	3.83427017	2.87097443
C	1.62708669	-2.15290313	0.80829179	H	1.10204125	3.83025901	4.21195773
C	3.52509572	-1.90932126	-1.47881228	H	2.85238549	2.10782411	3.64933648
C	2.49049229	-1.01273571	-1.14923381	H	2.39148851	0.48339865	1.82903554
C	0.41795054	-2.17148784	1.67270547	C	-4.38624702	1.64584814	-2.54153990
C	0.24254575	-3.11162255	2.68501784	C	-4.24521070	0.48179101	-3.29894600
C	-0.93695277	-3.10329383	3.41873480	C	4.38624702	-1.64584814	-2.54153990
C	-1.90718602	-2.15074356	3.11280632	C	4.24521070	-0.48179101	-3.29894600
C	-1.65820390	-1.23684069	2.09806132	H	-4.92104149	0.27485731	-4.12780797
C	2.34146380	0.15757364	-1.93846040	H	-5.17308914	2.36163022	-2.77731323
C	3.22477123	0.41338850	-2.99551524	H	-3.64679008	2.81378836	-0.89696284
C	-2.49049229	1.01273571	-1.14923381	H	4.92104149	-0.27485731	-4.12780797
C	-3.52509572	1.90932126	-1.47881228	H	5.17308914	-2.36163022	-2.77731323
C	-1.62708669	2.15290313	0.80829179	H	3.64679008	-2.81378836	-0.89696284
C	-3.22477123	-0.41338850	-2.99551524	O	-2.53787429	2.99187079	0.98236570
C	-2.34146380	-0.15757364	-1.93846040	O	2.53787429	-2.99187079	0.98236570
C	-0.41795054	2.17148784	1.67270547	H	3.09560859	1.31907325	-3.58668772
C	-0.24254575	3.11162255	2.68501784	H	-3.09560859	-1.31907325	-3.58668772
C	0.93695277	3.10329383	3.41873480	S	-1.04710472	-1.25646576	-1.53804203
C	1.90718602	2.15074356	3.11280632	S	1.04710472	1.25646576	-1.53804203

TABLE S-XXVII. Fe-(PyPepS)<sub>2</sub> (1) OPBE–Cosmo Quartet

Fe	0.00000000	0.00000000	0.07181994	H	1.27205109	-4.02423316	2.78575361
N	1.68651488	-1.29956301	-0.14358484	H	-0.76488973	-4.05760784	4.26525541
N	0.34497065	1.37163166	1.51655585	H	-2.53589993	-2.30410124	3.88911728
N	-1.68651488	1.29956301	-0.14358484	H	-2.17265626	-0.60618894	2.11150824
N	-0.34497065	-1.37163166	1.51655585	H	-1.27205109	4.02423316	2.78575361
C	1.76465319	-2.30720328	0.74444338	H	0.76488973	4.05760784	4.26525541
C	3.52666208	-2.05670029	-1.66055397	H	2.53589993	2.30410124	3.88911728
C	2.54898648	-1.14182797	-1.22115376	H	2.17265626	0.60618894	2.11150824
C	0.60040345	-2.31686076	1.68993654	C	-4.28679081	1.80588351	-2.80028746
C	0.47989815	-3.28909643	2.67943767	C	-4.09975311	0.63293303	-3.53232428

C	-0.64877660	-3.30194167	3.49035629	C	4.28679081	-1.80588351	-2.80028746
C	-1.62944788	-2.33375369	3.28898900	C	4.09975311	-0.63293303	-3.53232428
C	-1.43556844	-1.38216864	2.29773153	H	-4.69213211	0.43529644	-4.42482722
C	2.36698655	0.05064650	-1.97609125	H	-5.02842002	2.53838177	-3.11793034
C	3.14014256	0.28677438	-3.11966022	H	-3.67885240	2.97088997	-1.10003144
C	-2.54898648	1.14182797	-1.22115376	H	4.69213211	-0.43529644	-4.42482722
C	-3.52666208	2.05670029	-1.66055397	H	5.02842002	-2.53838177	-3.11793034
C	-1.76465319	2.30720328	0.74444338	H	3.67885240	-2.97088997	-1.10003144
C	-3.14014256	-0.28677438	-3.11966022	O	-2.64153058	3.19135474	0.85919811
C	-2.36698655	-0.05064650	-1.97609125	O	2.64153058	-3.19135474	0.85919811
C	-0.60040345	2.31686076	1.68993654	H	2.98023948	1.20163188	-3.68847179
C	-0.47989815	3.28909643	2.67943767	H	-2.98023948	-1.20163188	-3.68847179
C	0.64877660	3.30194167	3.49035629	S	-1.19566806	-1.22598250	-1.43211768
C	1.62944788	2.33375369	3.28898900	S	1.19566806	1.22598250	-1.43211768

TABLE S-XXVIII. Fe-(PyPepS)<sub>2</sub> (1) OPBE–Cosmo Sextet

Fe	0.00000000	0.00000000	-0.09170218	H	1.27384817	-4.13726437	2.68045316
N	1.65546858	-1.34097431	-0.20419786	H	-0.73313698	-4.22639739	4.19029375
N	0.37508242	1.44853752	1.53246344	H	-2.50296023	-2.45626140	3.93298978
N	-1.65546858	1.34097431	-0.20419786	H	-2.18955024	-0.70679559	2.19094992
N	-0.37508242	-1.44853752	1.53246344	H	-1.27384817	4.13726437	2.68045316
C	1.75216196	-2.31338513	0.73153039	H	0.73313698	4.22639739	4.19029375
C	3.58106098	-2.13612874	-1.58146314	H	2.50296023	2.45626140	3.93298978
C	2.62246962	-1.17549635	-1.20011420	H	2.18955024	0.70679559	2.19094992
C	0.57301376	-2.38640788	1.65989250	C	-4.49219148	1.89093235	-2.60519092
C	0.47998969	-3.40010829	2.61150454	C	-4.48079724	0.67147089	-3.28249706
C	-0.63290340	-3.44138676	3.44254301	C	4.49219148	-1.89093235	-2.60519092
C	-1.61535324	-2.46522619	3.30458650	C	4.48079724	-0.67147089	-3.28249706
C	-1.44489943	-1.48572757	2.33439558	H	-5.19656556	0.46874838	-4.07808065
C	2.59311775	0.05100157	-1.92421283	H	-5.21391887	2.66254950	-2.87135914
C	3.53182685	0.28565094	-2.94054748	H	-3.60529147	3.08709677	-1.06542960
C	-2.62246962	1.17549635	-1.20011420	H	5.19656556	-0.46874838	-4.07808065
C	-3.58106098	2.13612874	-1.58146314	H	5.21391887	-2.66254950	-2.87135914
C	-1.75216196	2.31338513	0.73153039	H	3.60529147	-3.08709677	-1.06542960
C	-3.53182685	-0.28565094	-2.94054748	O	-2.68579785	3.12014283	0.91743936
C	-2.59311775	-0.05100157	-1.92421283	O	2.68579785	-3.12014283	0.91743936
C	-0.57301376	2.38640788	1.65989250	H	3.49712976	1.23401647	-3.47467465
C	-0.47998969	3.40010829	2.61150454	H	-3.49712976	-1.23401647	-3.47467465
C	0.63290340	3.44138676	3.44254301	S	-1.37552852	-1.25031884	-1.57469179
C	1.61535324	2.46522619	3.30458650	S	1.37552852	1.25031884	-1.57469179



TABLE S-XXIX. Fe(tsalen)Cl (2) OPBE–Cosmo Doublet

Fe	-0.40285417	-0.13988060	0.00000000	C	-0.19238927	0.34674445	4.86889425
Cl	-2.58929603	0.22858605	0.00000000	C	-0.27430855	-0.66009729	5.81023548
S	-0.26826852	-1.77962044	1.40729186	C	0.15451764	2.56671445	-0.75619746
C	0.15451764	2.56671445	0.75619746	C	-0.03667675	1.18136016	-2.60322027
N	-0.04998661	1.21637794	1.29951909	H	0.12840803	2.13367918	-3.11548925
S	-0.26826852	-1.77962044	-1.40729186	C	-0.18656991	0.06385741	-3.48313302
H	-0.38207550	-3.34182841	-3.71456234	C	-0.33685624	-1.99599043	-5.38610838
H	-0.38207550	-3.34182841	3.71456234	C	-0.26827329	-1.28823544	-3.06071252
C	-0.03667675	1.18136016	2.60322027	C	-0.19238927	0.34674445	-4.86889425
C	-0.32868522	-2.30387264	4.03765733	C	-0.27430855	-0.66009729	-5.81023548
H	-0.12860859	1.38585700	5.18736687	C	-0.32868522	-2.30387264	-4.03765733
H	-0.39606377	-2.79948100	6.11866644	H	-0.39606377	-2.79948100	-6.11866644
H	0.12840803	2.13367918	3.11548925	H	-0.12860859	1.38585700	-5.18736687
C	-0.18656991	0.06385741	3.48313302	H	-0.28411685	-0.41851464	-6.87113215
H	-0.28411685	-0.41851464	6.87113215	H	-0.63979964	3.21707699	-1.13595464
N	-0.04998661	1.21637794	-1.29951909	H	1.10487024	2.95498661	-1.13500212
C	-0.33685624	-1.99599043	5.38610838	H	1.10487024	2.95498661	1.13500212
C	-0.26827329	-1.28823544	3.06071252	H	-0.63979964	3.21707699	1.13595464

TABLE S-XXX. Fe(tsalen)Cl (2) OPBE–Cosmo Quartet

Fe	-1.03795895	-0.03426370	0.00000000	C	1.10424686	0.08269929	4.44393899
Cl	-3.33243022	0.67473168	0.00000000	C	1.27828585	-0.97621296	5.31538067
S	-1.03946340	-1.69767205	1.45240634	C	-0.43864296	2.61425467	-0.76356308
C	-0.43864296	2.61425467	0.76356308	C	0.24790790	1.12074661	-2.44155080
N	-0.33424846	1.25534867	1.29340392	H	0.68052194	2.02183016	-2.88572842
S	-1.03946340	-1.69767205	-1.45240634	C	0.38619938	-0.06513907	-3.23736882
H	-0.40873968	-3.36599805	-3.57364191	C	0.72064575	-2.21868039	-4.99328318
H	-0.40873968	-3.36599805	3.57364191	C	-0.17031199	-1.32753744	-2.90975413
C	0.24790790	1.12074661	2.44155080	C	1.10424686	0.08269929	-4.44393899
C	0.00914154	-2.39080270	3.81576114	C	1.27828585	-0.97621296	-5.31538067
H	1.52232600	1.05917313	4.68207616	C	0.00914154	-2.39080270	-3.81576114
H	0.84881089	-3.06566562	5.66571770	H	0.84881089	-3.06566562	-5.66571770
H	0.68052194	2.02183016	2.88572842	H	1.52232600	1.05917313	-4.68207616
C	0.38619938	-0.06513907	3.23736882	H	1.83980377	-0.84310054	-6.23762549
H	1.83980377	-0.84310054	6.23762549	H	-1.37800772	3.03805421	-1.13371727
N	-0.33424846	1.25534867	-1.29340392	H	0.37819769	3.22940735	-1.15173999
C	0.72064575	-2.21868039	4.99328318	H	0.37819769	3.22940735	1.15173999
C	-0.17031199	-1.32753744	2.90975413	H	-1.37800772	3.03805421	1.13371727

TABLE S-XXXI. Fe(tsalen)Cl (2) OPBE–Cosmo Sextet

Fe	-1.58997707	-0.00685073	0.00000000	C	1.80162681	-0.07607188	3.67014109
Cl	-3.75284673	0.69445306	0.00000000	C	2.23749423	-1.18939043	4.36682198
S	-1.50889283	-1.54641203	1.76646139	C	-0.66910441	2.70755550	-0.77008096
C	-0.66910441	2.70755550	0.77008096	C	0.35065084	1.13000774	-2.17952233
N	-0.52975881	1.34822033	1.26320271	H	0.94857403	1.98241016	-2.52276151
S	-1.50889283	-1.54641203	-1.76646139	C	0.66962354	-0.11894476	-2.82896093
H	-0.15154790	-3.38732019	-3.34963430	C	1.52264668	-2.38413507	-4.24235632
H	-0.15154790	-3.38732019	3.34963430	C	-0.05733000	-1.33467763	-2.70480325
C	0.35065084	1.13000774	2.17952233	C	1.80162681	-0.07607188	-3.67014109
C	0.39674376	-2.45139297	3.43416296	C	2.23749423	-1.18939043	-4.36682198
H	2.34190408	0.86508785	3.75973079	C	0.39674376	-2.45139297	-3.43416296
H	1.84520614	-3.27340579	4.78185888	H	1.84520614	-3.27340579	-4.78185888
H	0.94857403	1.98241016	2.52276151	H	2.34190408	0.86508785	-3.75973079
C	0.66962354	-0.11894476	2.82896093	H	3.11942209	-1.13105763	-5.00127958
H	3.11942209	-1.13105763	5.00127958	H	-1.61981526	3.10390026	-1.14368909
N	-0.52975881	1.34822033	-1.26320271	H	0.13175032	3.34699318	-1.15561516
C	1.52264668	-2.38413507	4.24235632	H	0.13175032	3.34699318	1.15561516
C	-0.05733000	-1.33467763	2.70480325	H	-1.61981526	3.10390026	1.14368909

TABLE S-XXXII. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(1MIm) (3) OPBE–Cosmo Doublet

Fe	0.00728201	-0.63799355	-0.94384160	C	3.65734505	1.59463965	2.86808618
H	3.02346003	-0.46134731	2.92281052	C	2.24520487	0.55493442	1.18410712
H	4.23134097	1.51500218	3.79045747	C	2.84297937	2.88978880	1.00948339
S	-1.87950000	-0.86497567	0.09843332	C	3.59058352	2.80743929	2.18109611
N	0.05524452	1.40449516	-0.86522967	C	2.98011936	0.48250329	2.38127963
N	-0.00800751	-2.65693176	-1.15068270	S	1.50005875	-0.91220527	0.58672369
C	1.46615912	1.90032630	-0.82305901	H	2.78329188	3.83853746	0.47707499
C	-0.63566835	1.97988281	0.33364467	H	4.11004137	3.68668581	2.55886040
C	-0.60387168	1.99987936	-2.07072296	H	-4.65087534	-0.41098921	0.49491990
H	2.01475083	1.34647563	-1.59328919	C	-4.90350932	1.71607895	0.70338346
C	2.17425173	1.77730317	0.48984827	C	-2.76209727	0.62694433	0.34507278
H	1.46525688	2.95894697	-1.11102510	C	-2.89533352	3.03269841	0.55263515
C	0.17096129	1.97105931	-3.35175260	C	-4.27592785	2.96278139	0.71914765
H	-0.84142040	3.04623846	-1.84307567	C	-4.15659891	0.55920541	0.51289129
H	-1.55301669	1.46514575	-2.19708626	H	-5.98221967	1.64255665	0.83696949
H	-0.21816285	1.46312482	1.20353269	H	-2.39895997	4.00238873	0.57540035
C	-2.12511921	1.88009268	0.37229260	H	-4.85579605	3.87291493	0.86341301
H	-0.35450748	3.03832568	0.40512805	C	1.06164492	-3.45015205	-1.16326177
C	1.47078360	1.97295852	-5.84325297	C	-1.07612903	-3.46235911	-1.47885885

C	0.35321364	3.15806473	-4.06782467	H	2.07734350	-3.14233282	-0.96353705
C	0.65385194	0.76718160	-3.89805826	C	1.63166301	-5.84081399	-1.54660676
C	1.30428856	0.78360461	-5.14362243	C	-0.63418242	-4.74199913	-1.67363047
C	0.99101669	3.16811592	-5.30575123	H	-2.08251303	-3.07704028	-1.55661245
H	-0.01888104	4.09290555	-3.65001489	N	0.72209040	-4.71471369	-1.47061532
S	0.44242287	-0.76237561	-3.07504264	H	-1.16255003	-5.64917933	-1.93454819
H	1.67686427	-0.15131400	-5.55952241	H	2.65175376	-5.48168785	-1.40894025
H	1.11679948	4.10555924	-5.84513525	H	1.54729787	-6.32045601	-2.52474593
H	1.97408038	1.96634434	-6.80919195	H	1.39605690	-6.56677585	-0.76378057

TABLE S-XXXIII. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(1MIm) (3) OPBE-Cosmo Quartet

Fe	-0.04536901	-0.67976363	-0.93901656	C	3.70945631	1.68230845	2.86397183
H	3.28933667	-0.42701111	2.89862870	C	2.37831518	0.51961502	1.18804790
H	4.30170831	1.64797913	3.77765191	C	2.75407653	2.90716698	1.02963552
S	-2.06259903	-0.86082533	0.03225124	C	3.51869109	2.89048678	2.19226122
N	0.03834365	1.34400120	-0.83186928	C	3.14097813	0.51347762	2.37080033
N	-0.06108399	-2.70208010	-1.12142290	S	1.72846964	-0.99206975	0.59926783
C	1.46676926	1.81486841	-0.80235759	H	2.60257891	3.84852938	0.50249560
C	-0.65040064	1.89696867	0.38248244	H	3.95754625	3.81211617	2.57095633
C	-0.62833078	1.93164566	-2.04733544	H	-4.81940453	-0.23023814	0.26878765
H	1.99936658	1.22352289	-1.55501751	C	-4.94195087	1.89672790	0.57283278
C	2.18319906	1.74018509	0.50960510	C	-2.86216469	0.67706377	0.26291589
H	1.46711693	2.85976117	-1.13245677	C	-2.84505268	3.07542735	0.57700535
C	0.15853410	1.95211635	-3.31984268	C	-4.23268508	3.09345642	0.68278735
H	-0.89744122	2.96352065	-1.79600271	C	-4.26420393	0.70197108	0.35915842
H	-1.56252865	1.37489245	-2.18800981	H	-6.02840150	1.89189545	0.65184741
H	-0.27336820	1.32236632	1.23515738	H	-2.28833229	4.00768262	0.66525253
C	-2.14463209	1.88204005	0.37626302	H	-4.75542965	4.03426372	0.84686828
H	-0.31403495	2.93373803	0.50019262	C	1.04190926	-3.40757180	-1.37831940
C	1.45019014	2.06837712	-5.80938933	C	-1.09711408	-3.60805642	-1.09191756
C	0.31712481	3.16741847	-3.99448070	H	2.03906123	-3.00498063	-1.47327391
C	0.66865038	0.77583100	-3.90234883	C	1.70797990	-5.76972855	-1.76466695
C	1.31631676	0.85339304	-5.14817918	C	-0.59998222	-4.85759949	-1.32586312
C	0.94895504	3.23618346	-5.23255279	H	-2.12115355	-3.31295861	-0.91647414
H	-0.07540088	4.07783670	-3.54299832	N	0.75460464	-4.71016965	-1.50037678
S	0.51574144	-0.79099404	-3.14182428	H	-1.08891025	-5.82067668	-1.38366833
H	1.71324045	-0.05597743	-5.59640342	H	2.69783822	-5.33171690	-1.89286808
H	1.05211761	4.19381383	-5.74009304	H	1.42550667	-6.30056742	-2.67693889
H	1.95000493	2.10227886	-6.77667295	H	1.72680485	-6.46996817	-0.92585751

TABLE S-XXXIV. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(1MIm) (3) OPBE–Cosmo Sextet

Fe	0.08393757	-0.49107067	-0.93448945	C	3.45312073	0.92193419	2.97571290
H	3.62946111	-0.92030062	1.87366106	C	2.55658811	0.57014880	0.74511596
H	3.99448652	0.53910832	3.83992655	C	2.28461270	2.70176630	1.85250508
S	-1.30788009	-0.58061486	0.91802516	C	2.96932255	2.22968728	2.96986443
N	0.05594779	1.93499588	-0.80457485	C	3.24762745	0.09901594	1.87224974
N	-0.01148315	-2.73008628	-1.05534454	S	2.37747325	-0.47331465	-0.66239074
C	1.41063520	2.45658049	-0.49333343	H	1.91727902	3.72765048	1.84351648
C	-0.87114852	2.40121479	0.25717803	H	3.12656069	2.88113410	3.82819098
C	-0.38758900	2.52622815	-2.09258698	H	-4.14317475	-0.91022879	0.73759265
H	2.03922633	2.22142576	-1.35839482	C	-4.94885981	1.01431213	0.20063067
C	2.06456493	1.89327554	0.73294118	C	-2.58055825	0.55289762	0.48317746
H	1.35859326	3.55248011	-0.40597843	C	-3.33276360	2.77082129	-0.11853623
C	0.39998974	2.13178896	-3.30537974	C	-4.65847432	2.34274229	-0.10883112
H	-0.38009585	3.62277496	-1.99958990	C	-3.91805163	0.12623841	0.49270159
H	-1.42674494	2.21170160	-2.23541986	H	-5.98082529	0.66583727	0.21625992
H	-0.44399135	2.06630857	1.20835032	H	-3.10760927	3.81193889	-0.34827219
C	-2.28057931	1.89662947	0.17193815	H	-5.45932482	3.04405667	-0.33829984
H	-0.87906078	3.50168227	0.26185119	C	0.98841102	-3.60285885	-1.08368092
C	1.75031090	1.47952455	-5.68204864	C	-1.15789644	-3.46711747	-1.23344126
C	1.18661912	3.07621212	-3.97260875	H	2.03725409	-3.36538050	-0.97283257
C	0.28990076	0.83404843	-3.84899347	C	1.35099904	-6.05261665	-1.34933954
C	0.97280453	0.52334413	-5.03588671	C	-0.83304829	-4.78954888	-1.36695162
C	1.86052741	2.76432246	-5.15085682	H	-2.13948584	-3.01244415	-1.24966954
H	1.26373454	4.08247759	-3.56165605	N	0.53571735	-4.85699146	-1.26853629
S	-0.73879388	-0.38466212	-3.10496232	H	-1.44382520	-5.67014163	-1.51650928
H	0.88320582	-0.47817038	-5.45291331	H	2.39859748	-5.77366351	-1.23159866
H	2.46514734	3.51984681	-5.65027314	H	1.21318911	-6.53402772	-2.32091902
H	2.26866383	1.21853963	-6.60391192	H	1.07233483	-6.75036226	-0.55546836

TABLE S-XXXV. FePCl (8) OPBE–Cosmo Doublet

Fe	0.00000000	0.00000000	-0.13710453	C	2.81863986	1.09015646	0.06962491
N	0.00000000	-1.97443387	0.07188450	C	2.81863986	-1.09015646	0.06962491
N	1.97443387	0.00000000	0.07188450	C	4.19132405	0.68003986	0.08558648
N	0.00000000	1.97443387	0.07188450	H	5.03690167	1.35855463	0.10010711
N	-1.97443387	0.00000000	0.07188450	C	4.19132405	-0.68003986	0.08558648
C	2.41039760	-2.41039760	0.06536344	H	5.03690167	-1.35855463	0.10010711
C	2.41039760	2.41039760	0.06536344	C	-1.09015646	2.81863986	0.06962491
C	-2.41039760	2.41039760	0.06536344	C	1.09015646	2.81863986	0.06962491
C	-2.41039760	-2.41039760	0.06536344	C	-0.68003986	4.19132405	0.08558648

H	3.17858728	-3.17858728	0.06594236	H	-1.35855463	5.03690167	0.10010711
H	3.17858728	3.17858728	0.06594236	C	0.68003986	4.19132405	0.08558648
H	-3.17858728	3.17858728	0.06594236	H	1.35855463	5.03690167	0.10010711
H	-3.17858728	-3.17858728	0.06594236	C	-2.81863986	-1.09015646	0.06962491
C	1.09015646	-2.81863986	0.06962491	C	-2.81863986	1.09015646	0.06962491
C	-1.09015646	-2.81863986	0.06962491	C	-4.19132405	-0.68003986	0.08558648
C	0.68003986	-4.19132405	0.08558648	H	-5.03690167	-1.35855463	0.10010711
H	1.35855463	-5.03690167	0.10010711	C	-4.19132405	0.68003986	0.08558648
C	-0.68003986	-4.19132405	0.08558648	H	-5.03690167	1.35855463	0.10010711
H	-1.35855463	-5.03690167	0.10010711	Cl	0.00000000	0.00000000	-2.32185514

TABLE S-XXXVI. FePCl (**8**) OPBE–Cosmo Quartet

Fe	0.00000000	0.00000000	-0.19280308	C	2.82235098	1.09334952	0.10409287
N	0.00000000	-1.98660706	0.08048151	C	2.82235098	-1.09334952	0.10409287
N	1.98660706	0.00000000	0.08048151	C	4.19247819	0.68089025	0.14350070
N	0.00000000	1.98660706	0.08048151	H	5.03864372	1.35793761	0.17387124
N	-1.98660706	0.00000000	0.08048151	C	4.19247819	-0.68089025	0.14350070
C	2.41496970	-2.41496970	0.10559732	H	5.03864372	-1.35793761	0.17387124
C	2.41496970	2.41496970	0.10559732	C	-1.09334952	2.82235098	0.10409287
C	-2.41496970	2.41496970	0.10559732	C	1.09334952	2.82235098	0.10409287
C	-2.41496970	-2.41496970	0.10559732	C	-0.68089025	4.19247819	0.14350070
H	3.18269740	-3.18269740	0.12590661	H	-1.35793761	5.03864372	0.17387124
H	3.18269740	3.18269740	0.12590661	C	0.68089025	4.19247819	0.14350070
H	-3.18269740	3.18269740	0.12590661	H	1.35793761	5.03864372	0.17387124
H	-3.18269740	-3.18269740	0.12590661	C	-2.82235098	-1.09334952	0.10409287
C	1.09334952	-2.82235098	0.10409287	C	-2.82235098	1.09334952	0.10409287
C	-1.09334952	-2.82235098	0.10409287	C	-4.19247819	-0.68089025	0.14350070
C	0.68089025	-4.19247819	0.14350070	H	-5.03864372	-1.35793761	0.17387124
H	1.35793761	-5.03864372	0.17387124	C	-4.19247819	0.68089025	0.14350070
C	-0.68089025	-4.19247819	0.14350070	H	-5.03864372	1.35793761	0.17387124
H	-1.35793761	-5.03864372	0.17387124	Cl	0.00000000	0.00000000	-2.57929564

TABLE S-XXXVII. FePCl (**8**) OPBE–Cosmo Sextet

Fe	0.00000000	0.00000000	-0.41034150	C	2.85245058	1.09816715	0.14951691
N	0.00000000	-2.02861051	0.10602701	C	2.85245058	-1.09816715	0.14951691
N	2.02861051	0.00000000	0.10602701	C	4.22535862	0.68184806	0.21265252
N	0.00000000	2.02861051	0.10602701	H	5.07594014	1.35279242	0.26087486
N	-2.02861051	0.00000000	0.10602701	C	4.22535862	-0.68184806	0.21265252
C	2.42110339	-2.42110339	0.15834782	H	5.07594014	-1.35279242	0.26087486
C	2.42110339	2.42110339	0.15834782	C	-1.09816715	2.85245058	0.14951691

C	-2.42110339	2.42110339	0.15834782	C	1.09816715	2.85245058	0.14951691
C	-2.42110339	-2.42110339	0.15834782	C	-0.68184806	4.22535862	0.21265252
H	3.18906975	-3.18906975	0.19838432	H	-1.35279242	5.07594014	0.26087486
H	3.18906975	3.18906975	0.19838432	C	0.68184806	4.22535862	0.21265252
H	-3.18906975	3.18906975	0.19838432	H	1.35279242	5.07594014	0.26087486
H	-3.18906975	-3.18906975	0.19838432	C	-2.85245058	-1.09816715	0.14951691
C	1.09816715	-2.85245058	0.14951691	C	-2.85245058	1.09816715	0.14951691
C	-1.09816715	-2.85245058	0.14951691	C	-4.22535862	-0.68184806	0.21265252
C	0.68184806	-4.22535862	0.21265252	H	-5.07594014	-1.35279242	0.26087486
H	1.35279242	-5.07594014	0.26087486	C	-4.22535862	0.68184806	0.21265252
C	-0.68184806	-4.22535862	0.21265252	H	-5.07594014	1.35279242	0.26087486
H	-1.35279242	-5.07594014	0.26087486	Cl	0.00000000	0.00000000	-2.68761610

TABLE S-XXXVIII. FePzCl (9) OPBE–Cosmo Doublet

Fe	0.00000000	0.00000000	-0.13760196	C	4.10427916	0.67800359	0.09461425
N	0.00000000	-1.89381901	0.05643040	H	4.94498305	1.36162862	0.12068310
N	1.89381901	0.00000000	0.05643040	C	4.10427916	-0.67800359	0.09461425
N	0.00000000	1.89381901	0.05643040	H	4.94498305	-1.36162862	0.12068310
N	-1.89381901	0.00000000	0.05643040	C	-1.09616368	2.72399280	0.06581060
N	2.37101623	-2.37101623	0.06232755	C	1.09616368	2.72399280	0.06581060
N	2.37101623	2.37101623	0.06232755	C	-0.67800359	4.10427916	0.09461425
N	-2.37101623	2.37101623	0.06232755	H	-1.36162862	4.94498305	0.12068310
N	-2.37101623	-2.37101623	0.06232755	C	0.67800359	4.10427916	0.09461425
C	1.09616368	-2.72399280	0.06581060	H	1.36162862	4.94498305	0.12068310
C	-1.09616368	-2.72399280	0.06581060	C	-2.72399280	-1.09616368	0.06581060
C	0.67800359	-4.10427916	0.09461425	C	-2.72399280	1.09616368	0.06581060
H	1.36162862	-4.94498305	0.12068310	C	-4.10427916	-0.67800359	0.09461425
C	-0.67800359	-4.10427916	0.09461425	H	-4.94498305	-1.36162862	0.12068310
H	-1.36162862	-4.94498305	0.12068310	C	-4.10427916	0.67800359	0.09461425
C	2.72399280	1.09616368	0.06581060	H	-4.94498305	1.36162862	0.12068310
C	2.72399280	-1.09616368	0.06581060	Cl	0.00000000	0.00000000	-2.29843587

TABLE S-XXXIX. FePzCl (9) OPBE–Cosmo Quartet

Fe	0.00000000	0.00000000	-0.23085781	C	4.10578308	0.67838883	0.16709460
N	0.00000000	-1.90360032	0.06756906	H	4.94583291	1.36170112	0.21093799
N	1.90360032	0.00000000	0.06756906	C	4.10578308	-0.67838883	0.16709460
N	0.00000000	1.90360032	0.06756906	H	4.94583291	-1.36170112	0.21093799
N	-1.90360032	0.00000000	0.06756906	C	-1.09686220	2.72608993	0.10995933
N	2.37310966	-2.37310966	0.11639201	C	1.09686220	2.72608993	0.10995933
N	2.37310966	2.37310966	0.11639201	C	-0.67838883	4.10578308	0.16709460

N	-2.37310966	2.37310966	0.11639201	H	-1.36170112	4.94583291	0.21093799
N	-2.37310966	-2.37310966	0.11639201	C	0.67838883	4.10578308	0.16709460
C	1.09686220	-2.72608993	0.10995933	H	1.36170112	4.94583291	0.21093799
C	-1.09686220	-2.72608993	0.10995933	C	-2.72608993	-1.09686220	0.10995933
C	0.67838883	-4.10578308	0.16709460	C	-2.72608993	1.09686220	0.10995933
H	1.36170112	-4.94583291	0.21093799	C	-4.10578308	-0.67838883	0.16709460
C	-0.67838883	-4.10578308	0.16709460	H	-4.94583291	-1.36170112	0.21093799
H	-1.36170112	-4.94583291	0.21093799	C	-4.10578308	0.67838883	0.16709460
C	2.72608993	1.09686220	0.10995933	H	-4.94583291	1.36170112	0.21093799
C	2.72608993	-1.09686220	0.10995933	Cl	0.00000000	0.00000000	-2.59470051

TABLE S-XL. FePzCl (9) OPBE–Cosmo Sextet

Fe	0.00000000	0.00000000	-0.54245060	C	4.12547959	0.67884762	0.29309646
N	0.00000000	-1.93372162	0.07726835	H	4.96543205	1.35766138	0.38686349
N	1.93372162	0.00000000	0.07726835	C	4.12547959	-0.67884762	0.29309646
N	0.00000000	1.93372162	0.07726835	H	4.96543205	-1.35766138	0.38686349
N	-1.93372162	0.00000000	0.07726835	C	-1.09932605	2.74554355	0.17042841
N	2.37413044	-2.37413044	0.19281420	C	1.09932605	2.74554355	0.17042841
N	2.37413044	2.37413044	0.19281420	C	-0.67884762	4.12547959	0.29309646
N	-2.37413044	2.37413044	0.19281420	H	-1.35766138	4.96543205	0.38686349
N	-2.37413044	-2.37413044	0.19281420	C	0.67884762	4.12547959	0.29309646
C	1.09932605	-2.74554355	0.17042841	H	1.35766138	4.96543205	0.38686349
C	-1.09932605	-2.74554355	0.17042841	C	-2.74554355	-1.09932605	0.17042841
C	0.67884762	-4.12547959	0.29309646	C	-2.74554355	1.09932605	0.17042841
H	1.35766138	-4.96543205	0.38686349	C	-4.12547959	-0.67884762	0.29309646
C	-0.67884762	-4.12547959	0.29309646	H	-4.96543205	-1.35766138	0.38686349
H	-1.35766138	-4.96543205	0.38686349	C	-4.12547959	0.67884762	0.29309646
C	2.74554355	1.09932605	0.17042841	H	-4.96543205	1.35766138	0.38686349
C	2.74554355	-1.09932605	0.17042841	Cl	0.00000000	0.00000000	-2.78671565

TABLE S-XLI. Fe-(PyPepS)<sub>2</sub> (1) S12g Doublet

Fe	0.00000000	0.00000000	-0.11641476	H	0.97596107	-3.82790364	2.85030688
N	1.59978908	-1.18087226	-0.09342942	H	-1.25361931	-3.87799821	4.07482145
N	0.53622430	1.25727381	1.32101215	H	-2.99379859	-2.17602394	3.41810825
N	-1.59978908	1.18087226	-0.09342942	H	-2.43418941	-0.51816189	1.63348338
N	-0.53622430	-1.25727381	1.32101215	H	-0.97596107	3.82790364	2.85030688
C	1.66300459	-2.15414405	0.85785929	H	1.25361931	3.87799821	4.07482145
C	3.66586851	-1.87188038	-1.30992536	H	2.99379859	2.17602394	3.41810825
C	2.57732286	-1.01051105	-1.08109166	H	2.43418941	0.51816189	1.63348338
C	0.39947008	-2.17417023	1.64867976	C	-4.56616041	1.61897863	-2.34015091

C	0.17414429	-3.12219339	2.64263392	C	-4.41077280	0.49754568	-3.15672168
C	-1.04768840	-3.13775702	3.30030969	C	4.56616041	-1.61897863	-2.34015091
C	-2.01375280	-2.19591148	2.94306795	C	4.41077280	-0.49754568	-3.15672168
C	-1.71688542	-1.26980473	1.95484637	H	-5.11491457	0.30085685	-3.96697036
C	2.42432185	0.13107932	-1.91295088	H	-5.39646438	2.30744300	-2.50565956
C	3.34596763	0.36701776	-2.94053584	H	-3.78391790	2.73584585	-0.66636486
C	-2.57732286	1.01051105	-1.08109166	H	5.11491457	-0.30085685	-3.96697036
C	-3.66586851	1.87188038	-1.30992536	H	5.39646438	-2.30744300	-2.50565956
C	-1.66300459	2.15414405	0.85785929	H	3.78391790	-2.73584585	-0.66636486
C	-3.34596763	-0.36701776	-2.94053584	O	-2.57686565	2.97388194	1.11836743
C	-2.42432185	-0.13107932	-1.91295088	O	2.57686565	-2.97388194	1.11836743
C	-0.39947008	2.17417023	1.64867976	H	3.20666596	1.24285426	-3.57437747
C	-0.17414429	3.12219339	2.64263392	H	-3.20666596	-1.24285426	-3.57437747
C	1.04768840	3.13775702	3.30030969	S	-1.09906887	-1.23844145	-1.62274214
C	2.01375280	2.19591148	2.94306795	S	1.09906887	1.23844145	-1.62274214
C	1.71688542	1.26980473	1.95484637				

TABLE S-XLII. Fe-(PyPepS)<sub>2</sub> (I) S12g Quartet

Fe	0.00000000	0.00000000	-0.34860451	H	0.78032689	-3.99349220	2.68399388
N	1.78840478	-1.30734721	-0.06639269	H	-1.56708328	-4.10373834	3.65086422
N	0.56705046	1.37424633	1.08968549	H	-3.23627448	-2.37742457	2.87184440
N	-1.78840478	1.30734721	-0.06639269	H	-2.49514111	-0.65797105	1.23303802
N	-0.56705046	-1.37424633	1.08968549	H	-0.78032689	3.99349220	2.68399388
C	1.70645587	-2.27555425	0.87315093	H	1.56708328	4.10373834	3.65086422
C	4.15490343	-1.76429917	-0.71536721	H	3.23627448	2.37742457	2.87184440
C	2.93224310	-1.06900260	-0.81543304	H	2.49514111	0.65797105	1.23303802
C	0.33218414	-2.30201999	1.48526718	C	-5.23406253	1.43863767	-1.52945137
C	0.00055669	-3.28576790	2.41180786	C	-5.12908329	0.41072939	-2.46714604
C	-1.28549060	-3.33393573	2.93079951	C	5.23406253	-1.43863767	-1.52945137
C	-2.21038713	-2.38290367	2.50613582	C	5.12908329	-0.41072939	-2.46714604
C	-1.81030002	-1.42111608	1.59175670	H	-5.97245900	0.15656979	-3.11104257
C	2.84018214	-0.01419835	-1.76593539	H	-6.16568807	1.99903638	-1.43295272
C	3.93594206	0.29109141	-2.58239450	H	-4.22487230	2.56680335	0.00978766
C	-2.93224310	1.06900260	-0.81543304	H	5.97245900	-0.15656979	-3.11104257
C	-4.15490343	1.76429917	-0.71536721	H	6.16568807	-1.99903638	-1.43295272
C	-1.70645587	2.27555425	0.87315093	H	4.22487230	-2.56680335	0.00978766
C	-3.93594206	-0.29109141	-2.58239450	O	-2.55723688	3.10865915	1.26777057
C	-2.84018214	0.01419835	-1.76593539	O	2.55723688	-3.10865915	1.26777057
C	-0.33218414	2.30201999	1.48526718	H	3.83752303	1.09485132	-3.31194101
C	-0.00055669	3.28576790	2.41180786	H	-3.83752303	-1.09485132	-3.31194101



C	1.28549060	3.33393573	2.93079951	S	-1.36368501	-0.92218449	-1.94120577
C	2.21038713	2.38290367	2.50613582	S	1.36368501	0.92218449	-1.94120577
C	1.81030002	1.42111608	1.59175670				

TABLE S-XLIII. Fe-(PyPepS)<sub>2</sub> (1) S12g Sextet

Fe	0.00000000	0.00000000	-0.53115849	H	0.71669914	-4.11619359	2.56054424
N	1.77622630	-1.32320718	-0.09571017	H	-1.61720324	-4.22544435	3.54344970
N	0.62990931	1.45731445	1.03526861	H	-3.28241980	-2.47173930	2.83456492
N	-1.77622630	1.32320718	-0.09571017	H	-2.55157733	-0.73294859	1.20017559
N	-0.62990931	-1.45731445	1.03526861	H	-0.71669914	4.11619359	2.56054424
C	1.65520029	-2.32012843	0.81394181	H	1.61720324	4.22544435	3.54344970
C	4.20890015	-1.71229110	-0.48309914	H	3.28241980	2.47173930	2.83456492
C	2.98762573	-1.04799797	-0.72841407	H	2.55157733	0.73294859	1.20017559
C	0.26714455	-2.38506854	1.40176566	C	-5.37534862	1.35650143	-1.14829875
C	-0.05758560	-3.39657867	2.30659261	C	-5.36894452	0.32464601	-2.08603788
C	-1.33807283	-3.44222603	2.83636095	C	5.37534862	-1.35650143	-1.14829875
C	-2.26374248	-2.47660191	2.44909581	C	5.36894452	-0.32464601	-2.08603788
C	-1.86513813	-1.50355608	1.54335920	H	-6.28190492	0.04469643	-2.61385091
C	2.99079021	0.00750056	-1.68914912	H	-6.29761567	1.89957910	-0.93362107
C	4.18269635	0.34624967	-2.34517704	H	-4.21121847	2.52096231	0.23687826
C	-2.98762573	1.04799797	-0.72841407	H	6.28190492	-0.04469643	-2.61385091
C	-4.20890015	1.71229110	-0.48309914	H	6.29761567	-1.89957910	-0.93362107
C	-1.65520029	2.32012843	0.81394181	H	4.21121847	-2.52096231	0.23687826
C	-4.18269635	-0.34624967	-2.34517704	O	-2.49322654	3.16050477	1.22158557
C	-2.99079021	-0.00750056	-1.68914912	O	2.49322654	-3.16050477	1.22158557
C	-0.26714455	2.38506854	1.40176566	H	4.15372337	1.15272268	-3.07722179
C	0.05758560	3.39657867	2.30659261	H	-4.15372337	-1.15272268	-3.07722179
C	1.33807283	3.44222603	2.83636095	S	-1.52091045	-0.85797624	-2.11393505
C	2.26374248	2.47660191	2.44909581	S	1.52091045	0.85797624	-2.11393505
C	1.86513813	1.50355608	1.54335920				

TABLE S-XLIV. Fe(tsalen)Cl (2) S12g Doublet

Fe	-0.46860656	-0.16375919	0.00000000	C	-0.02714626	0.33193278	4.88545485
Cl	-2.62446568	0.39025605	0.00000000	C	-0.08848214	-0.66864562	5.83080831
S	-0.36349079	-1.81878379	1.43602407	C	-0.01230972	2.56807179	-0.75986307
C	-0.01230972	2.56807179	0.75986307	C	-0.00062443	1.16952352	-2.61574378
N	-0.06781459	1.20255159	1.31365024	H	0.16014385	2.12856309	-3.12412701
S	-0.36349079	-1.81878379	-1.43602407	C	-0.10464163	0.05449891	-3.50089380
H	-0.40399667	-3.33942489	-3.74535040	C	-0.21927835	-2.00113827	-5.41216507
H	-0.40399667	-3.33942489	3.74535040	C	-0.25288693	-1.29650913	-3.08330892

C	-0.00062443	1.16952352	2.61574378	C	-0.02714626	0.33193278	-4.88545485
C	-0.29478348	-2.30514901	4.06837925	C	-0.08848214	-0.66864562	-5.83080831
H	0.08010474	1.36967000	5.20312947	C	-0.29478348	-2.30514901	-4.06837925
H	-0.26903530	-2.80301802	6.14854749	H	-0.26903530	-2.80301802	-6.14854749
H	0.16014385	2.12856309	3.12412701	H	0.08010474	1.36967000	-5.20312947
C	-0.10464163	0.05449891	3.50089380	H	-0.03484209	-0.42730957	-6.89118902
H	-0.03484209	-0.42730957	6.89118902	H	-0.89289400	3.10948308	-1.12394178
N	-0.06781459	1.20255159	-1.31365024	H	0.88108700	3.07558187	-1.14348483
C	-0.21927835	-2.00113827	5.41216507	H	0.88108700	3.07558187	1.14348483
C	-0.25288693	-1.29650913	3.08330892	H	-0.89289400	3.10948308	1.12394178

TABLE S-XLV. Fe(tsalen)Cl (2) S12g Quartet

Fe	-0.92820494	-0.11054407	0.00000000	C	0.74074708	0.19677826	4.69852140
Cl	-3.07640792	0.67546354	0.00000000	C	0.82542866	-0.82425548	5.61955281
S	-0.78828889	-1.80094893	1.46203842	C	-0.31989294	2.58003807	-0.76661855
C	-0.31989294	2.58003807	0.76661855	C	0.18315142	1.13495290	-2.54512878
N	-0.22666090	1.22176020	1.31907748	H	0.51709560	2.06467129	-3.02603977
S	-0.78828889	-1.80094893	-1.46203842	C	0.24311197	-0.01582875	-3.39227329
H	-0.39127789	-3.35369838	-3.69342118	C	0.41098233	-2.10966459	-5.24386025
H	-0.39127789	-3.35369838	3.69342118	C	-0.17719871	-1.32141115	-3.01415074
C	0.18315142	1.13495290	2.54512878	C	0.74074708	0.19677826	-4.69852140
C	-0.07580887	-2.35010579	3.97481965	C	0.82542866	-0.82425548	-5.61955281
H	1.05592346	1.20322788	4.97628336	C	-0.07580887	-2.35010579	-3.97481965
H	0.47105454	-2.93211451	5.95678212	H	0.47105454	-2.93211451	-5.95678212
H	0.51709560	2.06467129	3.02603977	H	1.05592346	1.20322788	-4.97628336
C	0.24311197	-0.01582875	3.39227329	H	1.20813124	-0.63617213	-6.62103610
H	1.20813124	-0.63617213	6.62103610	H	-1.26684716	3.00339998	-1.12057463
N	-0.22666090	1.22176020	-1.31907748	H	0.50003969	3.19944269	-1.15174211
C	0.41098233	-2.10966459	5.24386025	H	0.50003969	3.19944269	1.15174211
C	-0.17719871	-1.32141115	3.01415074	H	-1.26684716	3.00339998	1.12057463

TABLE S-XLVI. Fe(tsalen)Cl (2) S12g Sextet

Fe	-1.04365819	-0.21442315	0.00000000	C	0.67230911	0.31771590	4.79649116
Cl	-3.12626541	0.58900709	0.00000000	C	0.71113855	-0.63935195	5.78765231
S	-0.66614155	-1.90081367	1.61864366	C	-0.16454396	2.55731150	-0.76991744
C	-0.16454396	2.55731150	0.76991744	C	0.23039372	1.14482576	-2.58457471
N	-0.13683994	1.21198365	1.34603800	H	0.56841415	2.07934061	-3.05898423
S	-0.66614155	-1.90081367	-1.61864366	C	0.24151279	0.02359496	-3.48210430
H	-0.41092942	-3.28809416	-3.97119796	C	0.31315281	-1.94572918	-5.47861227
H	-0.41092942	-3.28809416	3.97119796	C	-0.15614751	-1.30927341	-3.17044589

C	0.23039372	1.14482576	2.58457471	C	0.67230911	0.31771590	-4.79649116
C	-0.10667737	-2.26909881	4.20366976	C	0.71113855	-0.63935195	-5.78765231
H	0.97472809	1.34068008	5.02333463	C	-0.10667737	-2.26909881	-4.20366976
H	0.33277682	-2.71933022	6.24633839	H	0.33277682	-2.71933022	-6.24633839
H	0.56841415	2.07934061	3.05898423	H	0.97472809	1.34068008	-5.02333463
C	0.24151279	0.02359496	3.48210430	H	1.04312266	-0.38267241	-6.79207042
H	1.04312266	-0.38267241	6.79207042	H	-1.08628024	3.03994178	-1.11764669
N	-0.13683994	1.21198365	-1.34603800	H	0.68237935	3.14644347	-1.14526181
C	0.31315281	-1.94572918	5.47861227	H	0.68237935	3.14644347	1.14526181
C	-0.15614751	-1.30927341	3.17044589	H	-1.08628024	3.03994178	1.11764669

TABLE S-XLVII. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(1MIm) (3) S12g Doublet

Fe	0.08476255	-0.66531392	-0.99431400	C	3.62778415	1.65739214	2.90535402
H	3.08220188	-0.42577866	2.90603560	C	2.32942343	0.57817430	1.15992689
H	4.16884196	1.59131378	3.84929140	C	2.81783498	2.93779417	1.03929618
S	-1.84577501	-0.91638524	0.04179124	C	3.52496925	2.87507555	2.23517220
N	0.09203715	1.42417367	-0.84756044	C	3.02437762	0.52549417	2.37819664
N	0.05659498	-2.71786811	-1.20445134	S	1.64555391	-0.92054034	0.54623528
C	1.51737978	1.92107005	-0.83644984	H	2.72759227	3.89161076	0.51750466
C	-0.58569020	1.91838447	0.41343825	H	3.98517935	3.77277343	2.64602647
C	-0.62864352	2.04925636	-2.01635423	H	-4.61888710	-0.42901934	0.26164746
H	2.04801015	1.34858440	-1.60623128	C	-4.86763745	1.68802462	0.56144859
C	2.22367953	1.80637247	0.47941024	C	-2.72163003	0.58962146	0.28558214
H	1.51875670	2.97614894	-1.14416059	C	-2.84475158	2.98205350	0.59493863
C	0.10790295	2.05601977	-3.31935108	C	-4.23171615	2.92347040	0.67574453
H	-0.87503797	3.08687028	-1.74889588	C	-4.12203782	0.53541731	0.36215885
H	-1.57195806	1.50034133	-2.11648198	H	-5.95421932	1.62210872	0.62147846
H	-0.18081404	1.32025543	1.23516532	H	-2.33873060	3.94434327	0.68753248
C	-2.07655291	1.83257150	0.41261538	H	-4.81201616	3.83303825	0.82518471
H	-0.28475927	2.96385509	0.57188503	C	0.99693924	-3.60562803	-0.90674839
C	1.34672699	2.13511907	-5.83643240	C	-0.97933563	-3.43539859	-1.75674623
C	0.32884291	3.26712657	-3.97610661	H	1.95403356	-3.37552800	-0.45893796
C	0.52851578	0.86268539	-3.93659136	C	1.35609449	-6.08220772	-1.01864398
C	1.14265772	0.92155742	-5.19638194	C	-0.65369742	-4.76192371	-1.77932622
C	0.93981138	3.31937595	-5.22453417	H	-1.88319366	-2.94620650	-2.09196625
H	0.00364497	4.19242792	-3.49816324	N	0.60673452	-4.85647340	-1.23827212
S	0.32901013	-0.71793107	-3.18981748	H	-1.19975330	-5.62953838	-2.12752696
H	1.45963543	-0.00901771	-5.66584259	H	2.34647246	-5.83324570	-0.63154235
H	1.09645632	4.27821178	-5.71713839	H	1.47136411	-6.62867954	-1.96049852
H	1.82500427	2.15654281	-6.81570453	H	0.84073935	-6.71979433	-0.29171372

TABLE S-XLVIII. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(IMIm) (3) S12g Quartet

Fe	0.02936563	-0.68367954	-0.89171605	C	3.71020404	1.68808601	2.89190710
H	3.27057310	-0.41938461	2.89938913	C	2.40767234	0.54930292	1.18545970
H	4.28507786	1.64407381	3.81698830	C	2.78849475	2.93210552	1.05596632
S	-2.07663969	-0.89369253	0.20073598	C	3.53097382	2.90217790	2.23074193
N	0.06715577	1.39249818	-0.80298044	C	3.14704461	0.52940744	2.37897241
N	0.09942870	-2.74346494	-1.11024033	S	1.73572095	-0.96793028	0.61196862
C	1.51263147	1.85996754	-0.79683193	H	2.64630482	3.87978100	0.53443515
C	-0.62813234	1.87548778	0.46315868	H	3.96353759	3.81897219	2.62895786
C	-0.63307273	2.02913281	-1.99066638	H	-4.81813927	-0.18341601	0.12970928
H	2.02609374	1.26429970	-1.56147188	C	-4.92141985	1.95699272	0.33344041
C	2.22988784	1.77396618	0.51192766	C	-2.85463079	0.67864654	0.26847755
H	1.52039714	2.90393212	-1.13619912	C	-2.81101653	3.08873034	0.48591754
C	0.11995654	1.99027479	-3.27986599	C	-4.19984963	3.14251221	0.46259564
H	-0.84147438	3.07465687	-1.72546762	C	-4.25684731	0.74382107	0.23428529
H	-1.59117936	1.50827951	-2.09037237	H	-6.01110481	1.97711839	0.30660636
H	-0.27852609	1.22736366	1.27283321	H	-2.23912780	4.01276695	0.58428418
C	-2.12282681	1.87832629	0.39532980	H	-4.71388235	4.09957001	0.54008147
H	-0.27181930	2.89550868	0.65866904	C	1.19168705	-3.48476765	-1.24474925
C	1.40871587	1.96266656	-5.76603701	C	-0.96783926	-3.57587028	-1.34812455
C	0.48478139	3.17955726	-3.91218147	H	2.20522447	-3.12465512	-1.12959604
C	0.42363443	0.76307306	-3.89866734	C	1.79566880	-5.86155456	-1.75245195
C	1.07180936	0.76956395	-5.14381611	C	-0.50298509	-4.83141685	-1.61738687
C	1.12165362	3.17936941	-5.14834693	H	-1.98497614	-3.20940815	-1.30548927
H	0.25054955	4.12856575	-3.42724397	N	0.86959433	-4.75876611	-1.55113176
S	0.01649287	-0.78507043	-3.17647586	H	-1.02174072	-5.75495022	-1.84134791
H	1.30602321	-0.18336309	-5.61674976	H	2.81939764	-5.48746699	-1.68598517
H	1.39073549	4.11984226	-5.62726663	H	1.64330332	-6.30455212	-2.74206103
H	1.90625785	1.94237790	-6.73587709	H	1.64631434	-6.62858217	-0.98496185

TABLE S-XLIX. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(IMIm) (3) S12g Sextet

Fe	0.05491801	-0.49864319	-0.96864784	C	3.36511380	0.76021656	2.95046162
H	3.54099750	-1.03353450	1.76730119	C	2.54899759	0.53070604	0.67995361
H	3.86383054	0.32642987	3.81732486	C	2.27212676	2.61043560	1.87134326
S	-1.45755047	-0.62161869	0.80477488	C	2.90567893	2.07434994	2.98788239
N	0.05398878	1.97448626	-0.77456468	C	3.18607514	-0.00469116	1.80546863
N	0.09822165	-2.80113362	-0.98375532	S	2.38378105	-0.44762204	-0.78754645
C	1.43458470	2.46712488	-0.50062179	H	1.91389282	3.64078127	1.89743064
C	-0.83691446	2.40817347	0.34000114	H	3.04103612	2.68012295	3.88321007
C	-0.43758302	2.55825608	-2.05580704	H	-4.27998082	-0.75319227	0.52716743

H	2.03353715	2.22204543	-1.38404881	C	-4.97342263	1.24293999	0.10762566
C	2.08194522	1.86091900	0.71064218	C	-2.64436062	0.63516722	0.41996671
H	1.40788401	3.56711292	-0.39654373	C	-3.26346573	2.92246549	-0.04472183
C	0.33930951	2.15036202	-3.27490072	C	-4.60755424	2.57015886	-0.10163643
H	-0.43417300	3.66025923	-1.97119001	C	-4.00018364	0.28655054	0.36321615
H	-1.47722634	2.23129333	-2.16478422	H	-6.02248636	0.94880264	0.07105951
H	-0.41128132	1.98466234	1.25650862	H	-2.97228224	3.96210670	-0.20278707
C	-2.26923904	1.97925838	0.21835811	H	-5.36420150	3.32664896	-0.30641850
H	-0.79261967	3.50960458	0.42073666	C	1.13761678	-3.59916730	-1.16822916
C	1.73574953	1.46088746	-5.61165219	C	-1.00185900	-3.61847381	-0.92919027
C	1.16511019	3.07053140	-3.92178127	H	2.16749943	-3.27158701	-1.24272355
C	0.21916987	0.85282682	-3.81736613	C	1.61439596	-6.05169800	-1.42320263
C	0.92192943	0.52713674	-4.98456922	C	-0.61433986	-4.92092242	-1.08215160
C	1.86188898	2.74198113	-5.08000051	H	-1.99272911	-3.21281870	-0.76720488
H	1.25913122	4.07443515	-3.50479542	N	0.75401355	-4.89508111	-1.23412919
S	-0.84517227	-0.36614197	-3.09412583	H	-1.17597472	-5.84703341	-1.09041311
H	0.81693325	-0.47652094	-5.39395079	H	2.64776165	-5.71558155	-1.53428858
H	2.49914910	3.48096975	-5.56421410	H	1.32153498	-6.59912022	-2.32549270
H	2.27207279	1.18552479	-6.51990609	H	1.55019935	-6.72110722	-0.55843969

TABLE S-L. FePCI (8) S12g Doublet

Fe	0.00000000	0.00000000	-0.13928210	C	2.82227002	1.09115767	0.06979477
N	0.00000000	-1.98364314	0.07530139	C	2.82227002	-1.09115767	0.06979477
N	1.98364314	0.00000000	0.07530139	C	4.19325555	0.67893970	0.08134354
N	0.00000000	1.98364314	0.07530139	H	5.04171771	1.35575317	0.09164927
N	-1.98364314	0.00000000	0.07530139	C	4.19325555	-0.67893970	0.08134354
C	2.40954192	-2.40954192	0.06338750	H	5.04171771	-1.35575317	0.09164927
C	2.40954192	2.40954192	0.06338750	C	-1.09115767	2.82227002	0.06979477
C	-2.40954192	2.40954192	0.06338750	C	1.09115767	2.82227002	0.06979477
C	-2.40954192	-2.40954192	0.06338750	C	-0.67893970	4.19325555	0.08134354
H	3.17901644	-3.17901644	0.05811530	H	-1.35575317	5.04171771	0.09164927
H	3.17901644	3.17901644	0.05811530	C	0.67893970	4.19325555	0.08134354
H	-3.17901644	3.17901644	0.05811530	H	1.35575317	5.04171771	0.09164927
H	-3.17901644	-3.17901644	0.05811530	C	-2.82227002	-1.09115767	0.06979477
C	1.09115767	-2.82227002	0.06979477	C	-2.82227002	1.09115767	0.06979477
C	-1.09115767	-2.82227002	0.06979477	C	-4.19325555	-0.67893970	0.08134354
C	0.67893970	-4.19325555	0.08134354	H	-5.04171771	-1.35575317	0.09164927
H	1.35575317	-5.04171771	0.09164927	C	-4.19325555	0.67893970	0.08134354
C	-0.67893970	-4.19325555	0.08134354	H	-5.04171771	1.35575317	0.09164927
H	-1.35575317	-5.04171771	0.09164927	Cl	0.00000000	0.00000000	-2.30709691

TABLE S-LI. FePCI (8) S12g Quartet

Fe	0.00000000	0.00000000	-0.25900898	C	2.82677384	1.09243298	0.10535072
N	0.00000000	-1.99846857	0.07495425	C	2.82677384	-1.09243298	0.10535072
N	1.99846857	0.00000000	0.07495425	C	4.19745246	0.67942072	0.15559399
N	0.00000000	1.99846857	0.07495425	H	5.04567755	1.35551345	0.19367041
N	-1.99846857	0.00000000	0.07495425	C	4.19745246	-0.67942072	0.15559399
C	2.41284928	-2.41284928	0.10809662	H	5.04567755	-1.35551345	0.19367041
C	2.41284928	2.41284928	0.10809662	C	-1.09243298	2.82677384	0.10535072
C	-2.41284928	2.41284928	0.10809662	C	1.09243298	2.82677384	0.10535072
C	-2.41284928	-2.41284928	0.10809662	C	-0.67942072	4.19745246	0.15559399
H	3.18189146	-3.18189146	0.13330187	H	-1.35551345	5.04567755	0.19367041
H	3.18189146	3.18189146	0.13330187	C	0.67942072	4.19745246	0.15559399
H	-3.18189146	3.18189146	0.13330187	H	1.35551345	5.04567755	0.19367041
H	-3.18189146	-3.18189146	0.13330187	C	-2.82677384	-1.09243298	0.10535072
C	1.09243298	-2.82677384	0.10535072	C	-2.82677384	1.09243298	0.10535072
C	-1.09243298	-2.82677384	0.10535072	C	-4.19745246	-0.67942072	0.15559399
C	0.67942072	-4.19745246	0.15559399	H	-5.04567755	-1.35551345	0.19367041
H	1.35551345	-5.04567755	0.19367041	C	-4.19745246	0.67942072	0.15559399
C	-0.67942072	-4.19745246	0.15559399	H	-5.04567755	1.35551345	0.19367041
H	-1.35551345	-5.04567755	0.19367041	Cl	0.00000000	0.00000000	-2.51004327

TABLE S-LII. FePCI (8) S12g Sextet

Fe	0.00000000	0.00000000	-0.42801443	C	2.85391693	1.09716012	0.14954337
N	0.00000000	-2.03608355	0.11353657	C	2.85391693	-1.09716012	0.14954337
N	2.03608355	0.00000000	0.11353657	C	4.22742241	0.68040605	0.20294371
N	0.00000000	2.03608355	0.11353657	H	5.08054980	1.35049368	0.24378614
N	-2.03608355	0.00000000	0.11353657	C	4.22742241	-0.68040605	0.20294371
C	2.41911421	-2.41911421	0.15519128	H	5.08054980	-1.35049368	0.24378614
C	2.41911421	2.41911421	0.15519128	C	-1.09716012	2.85391693	0.14954337
C	-2.41911421	2.41911421	0.15519128	C	1.09716012	2.85391693	0.14954337
C	-2.41911421	-2.41911421	0.15519128	C	-0.68040605	4.22742241	0.20294371
H	3.18856439	-3.18856439	0.18498978	H	-1.35049368	5.08054980	0.24378614
H	3.18856439	3.18856439	0.18498978	C	0.68040605	4.22742241	0.20294371
H	-3.18856439	3.18856439	0.18498978	H	1.35049368	5.08054980	0.24378614
H	-3.18856439	-3.18856439	0.18498978	C	-2.85391693	-1.09716012	0.14954337
C	1.09716012	-2.85391693	0.14954337	C	-2.85391693	1.09716012	0.14954337
C	-1.09716012	-2.85391693	0.14954337	C	-4.22742241	-0.68040605	0.20294371
C	0.68040605	-4.22742241	0.20294371	H	-5.08054980	-1.35049368	0.24378614
H	1.35049368	-5.08054980	0.24378614	C	-4.22742241	0.68040605	0.20294371
C	-0.68040605	-4.22742241	0.20294371	H	-5.08054980	1.35049368	0.24378614

H	-1.35049368	-5.08054980	0.24378614	Cl	0.00000000	0.00000000	-2.63497831
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TABLE S-LIII. FePzCl (9) S12g Doublet

Fe	0.00000000	0.00000000	-0.15575962	C	4.10642762	0.67773582	0.09802321
N	0.00000000	-1.90271395	0.06543330	H	4.94366117	1.36666216	0.12061431
N	1.90271395	0.00000000	0.06543330	C	4.10642762	-0.67773582	0.09802321
N	0.00000000	1.90271395	0.06543330	H	4.94366117	-1.36666216	0.12061431
N	-1.90271395	0.00000000	0.06543330	C	-1.10072784	2.72914064	0.07178924
N	2.37588149	-2.37588149	0.06830514	C	1.10072784	2.72914064	0.07178924
N	2.37588149	2.37588149	0.06830514	C	-0.67773582	4.10642762	0.09802321
N	-2.37588149	2.37588149	0.06830514	H	-1.36666216	4.94366117	0.12061431
N	-2.37588149	-2.37588149	0.06830514	C	0.67773582	4.10642762	0.09802321
C	1.10072784	-2.72914064	0.07178924	H	1.36666216	4.94366117	0.12061431
C	-1.10072784	-2.72914064	0.07178924	C	-2.72914064	-1.10072784	0.07178924
C	0.67773582	-4.10642762	0.09802321	C	-2.72914064	1.10072784	0.07178924
H	1.36666216	-4.94366117	0.12061431	C	-4.10642762	-0.67773582	0.09802321
C	-0.67773582	-4.10642762	0.09802321	H	-4.94366117	-1.36666216	0.12061431
H	-1.36666216	-4.94366117	0.12061431	C	-4.10642762	0.67773582	0.09802321
C	2.72914064	1.10072784	0.07178924	H	-4.94366117	1.36666216	0.12061431
C	2.72914064	-1.10072784	0.07178924	Cl	0.00000000	0.00000000	-2.31914469

TABLE S-LIV. FePzCl (9) S12g Quartet

Fe	0.00000000	0.00000000	-0.28678973	C	4.10959527	0.67763687	0.17234403
N	0.00000000	-1.91341497	0.07113677	H	4.94561860	1.36698337	0.21685472
N	1.91341497	0.00000000	0.07113677	C	4.10959527	-0.67763687	0.17234403
N	0.00000000	1.91341497	0.07113677	H	4.94561860	-1.36698337	0.21685472
N	-1.91341497	0.00000000	0.07113677	C	-1.09934033	2.73006564	0.11281794
N	2.37688957	-2.37688957	0.12046455	C	1.09934033	2.73006564	0.11281794
N	2.37688957	2.37688957	0.12046455	C	-0.67763687	4.10959527	0.17234403
N	-2.37688957	2.37688957	0.12046455	H	-1.36698337	4.94561860	0.21685472
N	-2.37688957	-2.37688957	0.12046455	C	0.67763687	4.10959527	0.17234403
C	1.09934033	-2.73006564	0.11281794	H	1.36698337	4.94561860	0.21685472
C	-1.09934033	-2.73006564	0.11281794	C	-2.73006564	-1.09934033	0.11281794
C	0.67763687	-4.10959527	0.17234403	C	-2.73006564	1.09934033	0.11281794
H	1.36698337	-4.94561860	0.21685472	C	-4.10959527	-0.67763687	0.17234403
C	-0.67763687	-4.10959527	0.17234403	H	-4.94561860	-1.36698337	0.21685472
H	-1.36698337	-4.94561860	0.21685472	C	-4.10959527	0.67763687	0.17234403
C	2.73006564	1.09934033	0.11281794	H	-4.94561860	1.36698337	0.21685472
C	2.73006564	-1.09934033	0.11281794	Cl	0.00000000	0.00000000	-2.54109380

TABLE S-LV. FePzCl (9) S12g Sextet

Fe	0.00000000	0.00000000	-0.54624110	C	4.12919388	0.67819250	0.27041222
N	0.00000000	-1.93959390	0.09822482	H	4.96718416	1.36285949	0.34460128
N	1.93959390	0.00000000	0.09822482	C	4.12919388	-0.67819250	0.27041222
N	0.00000000	1.93959390	0.09822482	H	4.96718416	-1.36285949	0.34460128
N	-1.93959390	0.00000000	0.09822482	C	-1.10182588	2.74792855	0.17250067
N	2.37862369	-2.37862369	0.19080809	C	1.10182588	2.74792855	0.17250067
N	2.37862369	2.37862369	0.19080809	C	-0.67819250	4.12919388	0.27041222
N	-2.37862369	2.37862369	0.19080809	H	-1.36285949	4.96718416	0.34460128
N	-2.37862369	-2.37862369	0.19080809	C	0.67819250	4.12919388	0.27041222
C	1.10182588	-2.74792855	0.17250067	H	1.36285949	4.96718416	0.34460128
C	-1.10182588	-2.74792855	0.17250067	C	-2.74792855	-1.10182588	0.17250067
C	0.67819250	-4.12919388	0.27041222	C	-2.74792855	1.10182588	0.17250067
H	1.36285949	-4.96718416	0.34460128	C	-4.12919388	-0.67819250	0.27041222
C	-0.67819250	-4.12919388	0.27041222	H	-4.96718416	-1.36285949	0.34460128
H	-1.36285949	-4.96718416	0.34460128	C	-4.12919388	0.67819250	0.27041222
C	2.74792855	1.10182588	0.17250067	H	-4.96718416	1.36285949	0.34460128
C	2.74792855	-1.10182588	0.17250067	Cl	0.00000000	0.00000000	-2.74467517

TABLE S-LVI. Fe-(PyPepS)<sub>2</sub> (1) S12g-Cosmo Doublet

Fe	0.00000000	0.00000000	-0.09967318	H	1.07341329	-3.74991244	2.95761821
N	1.60179519	-1.17432792	-0.10451304	H	-1.10230955	-3.76045471	4.23501928
N	0.50103243	1.24906680	1.35853294	H	-2.87637627	-2.10115277	3.57424464
N	-1.60179519	1.17432792	-0.10451304	H	-2.39775344	-0.51324743	1.71195719
N	-0.50103243	-1.24906680	1.35853294	H	-1.07341329	3.74991244	2.95761821
C	1.69344128	-2.12000101	0.86499789	H	1.10230955	3.76045471	4.23501928
C	3.59158684	-1.92928817	-1.42285549	H	2.87637627	2.10115277	3.57424464
C	2.54858907	-1.02947042	-1.13096714	H	2.39775344	0.51324743	1.71195719
C	0.45520250	-2.14250374	1.69334391	C	-4.45484374	1.69919767	-2.49084789
C	0.27046037	-3.05401155	2.72782352	C	-4.30937927	0.56292182	-3.28804760
C	-0.93122125	-3.05321937	3.42509392	C	4.45484374	-1.69919767	-2.49084789
C	-1.91587617	-2.13443484	3.06467553	C	4.30937927	-0.56292182	-3.28804760
C	-1.66096832	-1.24609441	2.03021709	H	-4.98562175	0.38128544	-4.12265590
C	2.40152701	0.11644440	-1.95442727	H	-5.24749728	2.41735576	-2.69922572
C	3.28462805	0.33700283	-3.01710514	H	-3.71452583	2.81166424	-0.80714718
C	-2.54858907	1.02947042	-1.13096714	H	4.98562175	-0.38128544	-4.12265590
C	-3.59158684	1.92928817	-1.42285549	H	5.24749728	-2.41735576	-2.69922572
C	-1.69344128	2.12000101	0.86499789	H	3.71452583	-2.81166424	-0.80714718
C	-3.28462805	-0.33700283	-3.01710514	O	-2.63694209	2.91879565	1.10664245
C	-2.40152701	-0.11644440	-1.95442727	O	2.63694209	-2.91879565	1.10664245



C	-0.45520250	2.14250374	1.69334391	H	3.15357995	1.22272065	-3.63801209
C	-0.27046037	3.05401155	2.72782352	H	-3.15357995	-1.22272065	-3.63801209
C	0.93122125	3.05321937	3.42509392	S	-1.10495014	-1.25690868	-1.60239633
C	1.91587617	2.13443484	3.06467553	S	1.10495014	1.25690868	-1.60239633
C	1.66096832	1.24609441	2.03021709				

TABLE S-LVII. Fe-(PyPepS)<sub>2</sub> (1) S12g–Cosmo Quartet

Fe	0.00000000	0.00000000	-0.20797830	H	1.03373505	-3.92835789	2.84162732
N	1.80740013	-1.31794716	-0.09547416	H	-1.20443864	-3.98347593	4.00083136
N	0.44191698	1.36199958	1.26394832	H	-2.93658818	-2.28535196	3.31796887
N	-1.80740013	1.31794716	-0.09547416	H	-2.34630895	-0.62433761	1.55508524
N	-0.44191698	-1.36199958	1.26394832	H	-1.03373505	3.92835789	2.84162732
C	1.80082669	-2.26262856	0.86457455	H	1.20443864	3.98347593	4.00083136
C	4.00334177	-1.93393435	-1.12939337	H	2.93658818	2.28535196	3.31796887
C	2.85150335	-1.13001727	-0.99656935	H	2.34630895	0.62433761	1.55508524
C	0.49351070	-2.27409001	1.60869725	C	-4.95815481	1.67140793	-2.10841679
C	0.24568271	-3.22081351	2.59738662	C	-4.79748707	0.59803908	-2.98579954
C	-0.99066161	-3.24388405	3.23086364	C	4.95815481	-1.67140793	-2.10841679
C	-1.95102942	-2.30696356	2.85841176	C	4.79748707	-0.59803908	-2.98579954
C	-1.63380089	-1.37932484	1.87757485	H	-5.53974812	0.39301518	-3.75631707
C	2.70935206	-0.02990910	-1.88849654	H	-5.83288797	2.31678615	-2.18769812
C	3.67320608	0.21375956	-2.87358169	H	-4.13344159	2.77121552	-0.45430555
C	-2.85150335	1.13001727	-0.99656935	H	5.53974812	-0.39301518	-3.75631707
C	-4.00334177	1.93393435	-1.12939337	H	5.83288797	-2.31678615	-2.18769812
C	-1.80082669	2.26262856	0.86457455	H	4.13344159	-2.77121552	-0.45430555
C	-3.67320608	-0.21375956	-2.87358169	O	-2.69264646	3.09110529	1.19232842
C	-2.70935206	0.02990910	-1.88849654	O	2.69264646	-3.09110529	1.19232842
C	-0.49351070	2.27409001	1.60869725	H	3.53587771	1.05407874	-3.55327017
C	-0.24568271	3.22081351	2.59738662	H	-3.53587771	-1.05407874	-3.55327017
C	0.99066161	3.24388405	3.23086364	S	-1.34074517	-1.07875798	-1.73814617
C	1.95102942	2.30696356	2.85841176	S	1.34074517	1.07875798	-1.73814617
C	1.63380089	1.37932484	1.87757485				

TABLE S-LVIII. Fe-(PyPepS)<sub>2</sub> (1) S12g–Cosmo Sextet

Fe	0.00000000	0.00000000	-0.46419111	H	0.67306901	-4.19927653	2.50766409
N	1.78290028	-1.33484961	-0.08813976	H	-1.64912110	-4.29658058	3.47082013
N	0.62424394	1.47414864	1.03960098	H	-3.28817777	-2.50150499	2.81696343
N	-1.78290028	1.33484961	-0.08813976	H	-2.53820767	-0.72825479	1.23636337
N	-0.62424394	-1.47414864	1.03960098	H	-0.67306901	4.19927653	2.50766409
C	1.64604711	-2.34852197	0.79778497	H	1.64912110	4.29658058	3.47082013

C	4.23196857	-1.69741911	-0.46057894	H	3.28817777	2.50150499	2.81696343
C	3.00018364	-1.05533766	-0.71680551	H	2.53820767	0.72825479	1.23636337
C	0.26210149	-2.42328836	1.38618456	C	-5.39403228	1.34201149	-1.13613456
C	-0.07669419	-3.45299320	2.26083836	C	-5.37532163	0.33047013	-2.09617798
C	-1.36071844	-3.49827014	2.78849157	C	5.39403228	-1.34201149	-1.13613456
C	-2.27192091	-2.50970618	2.42923737	C	5.37532163	-0.33047013	-2.09617798
C	-1.86060943	-1.51761103	1.55050892	H	-6.28219809	0.05250655	-2.63185140
C	2.99905385	-0.01499530	-1.69071073	H	-6.32198586	1.86715430	-0.90991710
C	4.18105537	0.32582660	-2.36234725	H	-4.26069020	2.48830414	0.27698778
C	-3.00018364	1.05533766	-0.71680551	H	6.28219809	-0.05250655	-2.63185140
C	-4.23196857	1.69741911	-0.46057894	H	6.32198586	-1.86715430	-0.90991710
C	-1.64604711	2.34852197	0.79778497	H	4.26069020	-2.48830414	0.27698778
C	-4.18105537	-0.32582660	-2.36234725	O	-2.48859307	3.20497100	1.17461738
C	-2.99905385	0.01499530	-1.69071073	O	2.48859307	-3.20497100	1.17461738
C	-0.26210149	2.42328836	1.38618456	H	4.14833581	1.11989993	-3.10718222
C	0.07669419	3.45299320	2.26083836	H	-4.14833581	-1.11989993	-3.10718222
C	1.36071844	3.49827014	2.78849157	S	-1.51124608	-0.82310663	-2.10607729
C	2.27192091	2.50970618	2.42923737	S	1.51124608	0.82310663	-2.10607729
C	1.86060943	1.51761103	1.55050892				

TABLE S-LIX. Fe(tsalen)Cl (2) S12g–Cosmo Doublet

Fe	-0.35514673	-0.17294412	0.00000000	C	-0.30619571	0.37960001	4.88440337
Cl	-2.59571124	0.23074668	0.00000000	C	-0.41776480	-0.61384931	5.83761458
S	-0.17725639	-1.82082536	1.45125643	C	0.22652226	2.56565715	-0.75910212
C	0.22652226	2.56565715	0.75910212	C	-0.05173025	1.19295285	-2.61977928
N	-0.00860389	1.21606784	1.31954951	H	0.08124352	2.15008367	-3.13439675
S	-0.17725639	-1.82082536	-1.45125643	C	-0.22679796	0.07801237	-3.50588394
H	-0.37556080	-3.32725169	-3.78466616	C	-0.43748829	-1.95589944	-5.43439898
H	-0.37556080	-3.32725169	3.78466616	C	-0.26438648	-1.28333897	-3.10533275
C	-0.05173025	1.19295285	2.61977928	C	-0.30619571	0.37960001	-4.88440337
C	-0.35496786	-2.28306697	4.09294683	C	-0.41776480	-0.61384931	-5.83761458
H	-0.27501024	1.42465046	5.18941902	C	-0.35496786	-2.28306697	-4.09294683
H	-0.52184973	-2.74945523	6.17570646	H	-0.52184973	-2.74945523	-6.17570646
H	0.08124352	2.15008367	3.13439675	H	-0.27501024	1.42465046	-5.18941902
C	-0.22679796	0.07801237	3.50588394	H	-0.48531851	-0.35613682	-6.89278714
H	-0.48531851	-0.35613682	6.89278714	H	-0.55412743	3.23369792	-1.13614461
N	-0.00860389	1.21606784	-1.31954951	H	1.18732452	2.92849811	-1.13609487
C	-0.43748829	-1.95589944	5.43439898	H	1.18732452	2.92849811	1.13609487
C	-0.26438648	-1.28333897	3.10533275	H	-0.55412743	3.23369792	1.13614461

TABLE S-LX. Fe(tsalen)Cl (2) S12g–Cosmo Quartet

Fe	-0.77025188	-0.13551277	0.00000000	C	0.57436951	0.25286153	4.77694652
Cl	-3.09154133	0.54075988	0.00000000	C	0.59386546	-0.75197675	5.72561051
S	-0.67064326	-1.81541399	1.46642159	C	-0.21245726	2.58783709	-0.76284869
C	-0.21245726	2.58783709	0.76284869	C	0.17088774	1.14618363	-2.57133152
N	-0.17824701	1.22228461	1.32629070	H	0.48246995	2.07787109	-3.05502969
S	-0.67064326	-1.81541399	-1.46642159	C	0.17985412	0.00452288	-3.44358126
H	-0.45131887	-3.33507029	-3.77206062	C	0.21695050	-2.04709202	-5.35355446
H	-0.45131887	-3.33507029	3.77206062	C	-0.19451974	-1.31209393	-3.07268463
C	0.17088774	1.14618363	2.57133152	C	0.57436951	0.25286153	-4.77694652
C	-0.16646329	-2.32182127	4.05089100	C	0.59386546	-0.75197675	-5.72561051
H	0.86062901	1.26684875	5.05229861	C	-0.16646329	-2.32182127	-4.05089100
H	0.22503898	-2.85204576	6.08739842	H	0.22503898	-2.85204576	-6.08739842
H	0.48246995	2.07787109	3.05502969	H	0.86062901	1.26684875	-5.05229861
C	0.17985412	0.00452288	3.44358126	H	0.89716764	-0.53779120	-6.74834450
H	0.89716764	-0.53779120	6.74834450	H	-1.12916053	3.06141368	-1.12930976
N	-0.17824701	1.22228461	-1.32629070	H	0.63788137	3.15892676	-1.14635985
C	0.21695050	-2.04709202	5.35355446	H	0.63788137	3.15892676	1.14635985
C	-0.19451974	-1.31209393	3.07268463	H	-1.12916053	3.06141368	1.12930976

TABLE S-LXI. Fe(tsalen)Cl (2) S12g–Cosmo Sextet

Fe	-0.16851914	-0.35347876	0.00000000	C	-1.03045363	0.59056922	4.66361898
Cl	-2.45050977	-0.22299212	0.00000000	C	-1.47158107	-0.33532322	5.59055601
S	0.45348691	-1.85594526	1.71758817	C	0.91983653	2.44136188	-0.76813464
C	0.91983653	2.44136188	0.76813464	C	-0.01033271	1.28377818	-2.58840860
N	0.35611036	1.22056373	1.35167692	H	0.02300969	2.25973872	-3.08907060
S	0.45348691	-1.85594526	-1.71758817	C	-0.45812621	0.20013272	-3.43391901
H	-0.62010630	-3.17563871	-3.92482933	C	-1.31985802	-1.69787843	-5.31558387
H	-0.62010630	-3.17563871	3.92482933	C	-0.30404038	-1.18860248	-3.16093605
C	-0.01033271	1.28377818	2.58840860	C	-1.03045363	0.59056922	-4.66361898
C	-0.74077036	-2.11271953	4.12618392	C	-1.47158107	-0.33532322	-5.59055601
H	-1.12737667	1.65521616	4.87224129	C	-0.74077036	-2.11271953	-4.12618392
H	-1.65303595	-2.44368285	6.03613172	H	-1.65303595	-2.44368285	-6.03613172
H	0.02300969	2.25973872	3.08907060	H	-1.12737667	1.65521616	-4.87224129
C	-0.45812621	0.20013272	3.43391901	H	-1.92199452	-0.00630938	-6.52496873
H	-1.92199452	-0.00630938	6.52496873	H	0.37815800	3.31574209	-1.14562429
N	0.35611036	1.22056373	-1.35167692	H	1.95255080	2.51993518	-1.12452917
C	-1.31985802	-1.69787843	5.31558387	H	1.95255080	2.51993518	1.12452917
C	-0.30404038	-1.18860248	3.16093605	H	0.37815800	3.31574209	1.14562429

TABLE S-LXII. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(1MIm) (3) S12g–Cosmo Doublet

Fe	0.08403493	-0.66830271	-1.00116261	C	3.61821081	1.65515160	2.91527768
H	3.07681697	-0.42909448	2.90898629	C	2.32484287	0.58588812	1.16237910
H	4.15817957	1.58572037	3.85880971	C	2.81238022	2.94466977	1.04695549
S	-1.85267071	-0.91517342	0.03289577	C	3.51702630	2.87462258	2.24567055
N	0.09160217	1.42621153	-0.85388782	C	3.01435871	0.52315362	2.38334289
N	0.06079241	-2.73672005	-1.20738351	S	1.65386094	-0.91797224	0.52810514
C	1.51505828	1.93438203	-0.83494592	H	2.72125167	3.89993102	0.53039012
C	-0.58931983	1.93086300	0.40160849	H	3.97688503	3.77027148	2.66009624
C	-0.62296069	2.05645105	-2.02543386	H	-4.62957754	-0.42875528	0.30634494
H	2.05400255	1.37192853	-1.60597093	C	-4.87386322	1.68946504	0.60254185
C	2.21930217	1.81351477	0.48251281	C	-2.72993864	0.59578373	0.29981490
H	1.50825411	2.99077487	-1.13011199	C	-2.84817800	2.98845496	0.60095591
C	0.11570196	2.06257998	-3.32862967	C	-4.23512458	2.92598452	0.70240660
H	-0.86321457	3.09328708	-1.75883118	C	-4.12895734	0.53477912	0.39613891
H	-1.56740661	1.51080104	-2.13274254	H	-5.95868187	1.62235002	0.67931595
H	-0.18057327	1.34534743	1.23026513	H	-2.34264122	3.95096116	0.67896669
C	-2.08101705	1.83733198	0.41201476	H	-4.81385293	3.83542166	0.85578015
H	-0.29709387	2.97857945	0.54577436	C	0.99435739	-3.63410729	-0.89206372
C	1.34758426	2.14927245	-5.85350789	C	-0.97428464	-3.45569201	-1.76803622
C	0.32575940	3.27659197	-3.98609007	H	1.95104476	-3.41876073	-0.43760365
C	0.54591407	0.87497394	-3.94956996	C	1.34633434	-6.11517175	-0.99273281
C	1.15653593	0.93252197	-5.21133490	C	-0.65146376	-4.78424070	-1.77637288
C	0.93232617	3.33025689	-5.23815678	H	-1.87625879	-2.97515250	-2.12132024
H	-0.00111233	4.19902200	-3.50647186	N	0.59980759	-4.88042078	-1.21939742
S	0.35251513	-0.70930918	-3.19493251	H	-1.19695025	-5.65220146	-2.12417568
H	1.48178467	0.00691952	-5.68488609	H	2.32923187	-5.86665901	-0.59083592
H	1.08064080	4.28982352	-5.73072713	H	1.46394716	-6.65194058	-1.93760260
H	1.82166251	2.17407340	-6.83392940	H	0.80934961	-6.74637491	-0.27910554

TABLE S-LXIII. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(1MIm) (3) S12g–Cosmo Quartet

Fe	0.08832921	-0.70721100	-0.95396793	C	3.69988138	1.72429443	2.87691868
H	3.30966554	-0.39316388	2.85553357	C	2.43240820	0.58622679	1.14794632
H	4.27092607	1.68021449	3.80357101	C	2.76003348	2.97607168	1.04853667
S	-2.08464562	-0.93363589	0.01709348	C	3.49809233	2.94252184	2.22790078
N	0.07856007	1.37467178	-0.82559906	C	3.16320886	0.55829999	2.34581946
N	0.10865438	-2.76515168	-1.16579124	S	1.81295543	-0.94214611	0.52403206
C	1.50617127	1.89849482	-0.81868377	H	2.59516725	3.92678147	0.54210029
C	-0.61298411	1.82346913	0.45750231	H	3.90852750	3.86244674	2.64075428
C	-0.65075308	2.01293257	-1.99578617	H	-4.82365753	-0.22213326	0.16310407

H	2.04105570	1.33854750	-1.59468834	C	-4.91204177	1.90135132	0.49870934
C	2.22963542	1.81169705	0.48764001	C	-2.85014601	0.63693097	0.25938999
H	1.46975541	2.94827611	-1.13001303	C	-2.79126817	3.02801148	0.61408691
C	0.09914242	2.03592744	-3.28970551	C	-4.18100563	3.07871989	0.65901777
H	-0.89237117	3.04226964	-1.70627965	C	-4.25274460	0.69580723	0.29593073
H	-1.58828265	1.45843737	-2.10696208	H	-6.00102187	1.92015722	0.52713568
H	-0.24904140	1.16248282	1.25033524	H	-2.21467452	3.94488991	0.73544736
C	-2.10898248	1.82360565	0.42503199	H	-4.68903007	4.02921590	0.81322742
H	-0.26347841	2.83981806	0.66976377	C	1.08488321	-3.63681033	-0.90049934
C	1.38768372	2.14255824	-5.77847532	C	-0.91683504	-3.50118061	-1.72556975
C	0.40862115	3.26054308	-3.88574536	H	2.04652739	-3.39962885	-0.46844358
C	0.45838656	0.84567869	-3.94901326	C	1.52476021	-6.09322995	-1.10264557
C	1.10583281	0.91488978	-5.19228769	C	-0.54588655	-4.81338091	-1.77866104
C	1.04417413	3.32509530	-5.12236697	H	-1.84323019	-3.04353014	-2.04282632
H	0.13688810	4.18142050	-3.37006319	N	0.72516757	-4.87964501	-1.25756751
S	0.11268882	-0.74600921	-3.27086786	H	-1.06934075	-5.69117589	-2.13497884
H	1.38421655	-0.00888753	-5.69779061	H	2.50070488	-5.82512706	-0.69705767
H	1.27019738	4.29092527	-5.57101244	H	1.65164580	-6.57320641	-2.07626345
H	1.88481823	2.17392470	-6.74738246	H	1.01923719	-6.78051160	-0.41929359

TABLE S-LXIV. Fe(N(CH<sub>2</sub>-o-C<sub>6</sub>H<sub>4</sub>S)<sub>3</sub>)(1MIm) (3) S12g-Cosmo Sextet

Fe	0.08578122	-0.58299563	-0.94121847	C	3.38965704	0.96870499	3.00847056
H	3.56734576	-0.90254566	1.95414416	C	2.55886834	0.58151023	0.76354826
H	3.89717665	0.59749826	3.89810430	C	2.28145034	2.73775459	1.80750597
S	-1.46400908	-0.63248799	0.80845160	C	2.92340902	2.28163873	2.95638999
N	0.05750305	1.93169487	-0.79278107	C	3.20597750	0.12416985	1.91931424
N	0.07240044	-2.83823423	-1.00650783	S	2.39615639	-0.51903451	-0.62150915
C	1.43983520	2.44252501	-0.54552724	H	1.92079064	3.76551735	1.76373084
C	-0.81920289	2.39559440	0.32498257	H	3.06143802	2.94893388	3.80569248
C	-0.45643496	2.51484714	-2.06918623	H	-4.29694413	-0.73924051	0.56765902
H	2.04042492	2.15103990	-1.41304772	C	-4.97511017	1.26557131	0.16388672
C	2.08824931	1.90904555	0.69969933	C	-2.64694036	0.63855554	0.43583991
H	1.41373300	3.54323062	-0.50353808	C	-3.24707711	2.93082226	-0.01982245
C	0.32510745	2.15179450	-3.29902485	C	-4.59674527	2.58992575	-0.05094442
H	-0.48870048	3.61194217	-1.97259127	C	-4.00612101	0.29694093	0.40082848
H	-1.48599851	2.15818961	-2.17842641	H	-6.02698172	0.98238899	0.14678054
H	-0.39026187	1.98719868	1.24598540	H	-2.94876243	3.96633694	-0.18389544
C	-2.25670336	1.97645374	0.22561737	H	-5.34875747	3.35449585	-0.24003586
H	-0.76528820	3.49428279	0.38598453	C	1.08323059	-3.67174767	-1.24246743
C	1.71641181	1.56238948	-5.67063958	C	-1.05601183	-3.62531766	-0.94518253

C	1.08125253	3.12601881	-3.95527343	H	2.12222355	-3.38979145	-1.34962900
C	0.27491393	0.85548487	-3.85142557	C	1.47430051	-6.13184348	-1.56204710
C	0.97514296	0.57455261	-5.03280584	C	-0.70937904	-4.93344911	-1.14295618
C	1.77305441	2.84638780	-5.13083222	H	-2.03387900	-3.20161390	-0.75473746
H	1.12168273	4.12978709	-3.53241847	N	0.65340690	-4.94592181	-1.33001981
S	-0.70655905	-0.43591770	-3.12610401	H	-1.29963128	-5.84103942	-1.16045290
H	0.92668250	-0.42963001	-5.45141891	H	2.50849331	-5.82192554	-1.71672508
H	2.35185737	3.62648555	-5.62279720	H	1.11504473	-6.65921783	-2.44965938
H	2.24870432	1.32569802	-6.59125930	H	1.41777221	-6.79665256	-0.69575325

TABLE S-LXV. FePCl (**8**) S12g–Cosmo Doublet

Fe	0.00000000	0.00000000	-0.13818829	C	2.82483282	1.09323469	0.07575278
N	0.00000000	-1.98192649	0.08216535	C	2.82483282	-1.09323469	0.07575278
N	1.98192649	0.00000000	0.08216535	C	4.19525055	0.67981390	0.08627071
N	0.00000000	1.98192649	0.08216535	H	5.04178492	1.35828105	0.09730194
N	-1.98192649	0.00000000	0.08216535	C	4.19525055	-0.67981390	0.08627071
C	2.41316150	-2.41316150	0.06990431	H	5.04178492	-1.35828105	0.09730194
C	2.41316150	2.41316150	0.06990431	C	-1.09323469	2.82483282	0.07575278
C	-2.41316150	2.41316150	0.06990431	C	1.09323469	2.82483282	0.07575278
C	-2.41316150	-2.41316150	0.06990431	C	-0.67981390	4.19525055	0.08627071
H	3.18204175	-3.18204175	0.06623130	H	-1.35828105	5.04178492	0.09730194
H	3.18204175	3.18204175	0.06623130	C	0.67981390	4.19525055	0.08627071
H	-3.18204175	3.18204175	0.06623130	H	1.35828105	5.04178492	0.09730194
H	-3.18204175	-3.18204175	0.06623130	C	-2.82483282	-1.09323469	0.07575278
C	1.09323469	-2.82483282	0.07575278	C	-2.82483282	1.09323469	0.07575278
C	-1.09323469	-2.82483282	0.07575278	C	-4.19525055	-0.67981390	0.08627071
C	0.67981390	-4.19525055	0.08627071	H	-5.04178492	-1.35828105	0.09730194
H	1.35828105	-5.04178492	0.09730194	C	-4.19525055	0.67981390	0.08627071
C	-0.67981390	-4.19525055	0.08627071	H	-5.04178492	1.35828105	0.09730194
H	-1.35828105	-5.04178492	0.09730194	Cl	0.00000000	0.00000000	-2.36090948

TABLE S-LXVI. FePCl (**8**) S12g–Cosmo Quartet

Fe	0.00000000	0.00000000	-0.19605276	C	2.82704002	1.09580437	0.10599844
N	0.00000000	-1.99142946	0.08397990	C	2.82704002	-1.09580437	0.10599844
N	1.99142946	0.00000000	0.08397990	C	4.19503941	0.68060767	0.14232010
N	0.00000000	1.99142946	0.08397990	H	5.04181932	1.35807943	0.17076074
N	-1.99142946	0.00000000	0.08397990	C	4.19503941	-0.68060767	0.14232010
C	2.41716314	-2.41716314	0.10709807	H	5.04181932	-1.35807943	0.17076074
C	2.41716314	2.41716314	0.10709807	C	-1.09580437	2.82704002	0.10599844
C	-2.41716314	2.41716314	0.10709807	C	1.09580437	2.82704002	0.10599844

C	-2.41716314	-2.41716314	0.10709807	C	-0.68060767	4.19503941	0.14232010
H	3.18561264	-3.18561264	0.12591138	H	-1.35807943	5.04181932	0.17076074
H	3.18561264	3.18561264	0.12591138	C	0.68060767	4.19503941	0.14232010
H	-3.18561264	3.18561264	0.12591138	H	1.35807943	5.04181932	0.17076074
H	-3.18561264	-3.18561264	0.12591138	C	-2.82704002	-1.09580437	0.10599844
C	1.09580437	-2.82704002	0.10599844	C	-2.82704002	1.09580437	0.10599844
C	-1.09580437	-2.82704002	0.10599844	C	-4.19503941	-0.68060767	0.14232010
C	0.68060767	-4.19503941	0.14232010	H	-5.04181932	-1.35807943	0.17076074
H	1.35807943	-5.04181932	0.17076074	C	-4.19503941	0.68060767	0.14232010
C	-0.68060767	-4.19503941	0.14232010	H	-5.04181932	1.35807943	0.17076074
H	-1.35807943	-5.04181932	0.17076074	Cl	0.00000000	0.00000000	-2.58303533

TABLE S-LXVII. FePCl (**8**) S12g–Cosmo Sextet

Fe	0.00000000	0.00000000	-0.35186159	C	2.85681365	1.10069873	0.14546289
N	0.00000000	-2.03266189	0.13347438	C	2.85681365	-1.10069873	0.14546289
N	2.03266189	0.00000000	0.13347438	C	4.22880409	0.68154907	0.16461752
N	0.00000000	2.03266189	0.13347438	H	5.08104881	1.35300938	0.17914819
N	-2.03266189	0.00000000	0.13347438	C	4.22880409	-0.68154907	0.16461752
C	2.42377309	-2.42377309	0.14569943	H	5.08104881	-1.35300938	0.17914819
C	2.42377309	2.42377309	0.14569943	C	-1.10069873	2.85681365	0.14546289
C	-2.42377309	2.42377309	0.14569943	C	1.10069873	2.85681365	0.14546289
C	-2.42377309	-2.42377309	0.14569943	C	-0.68154907	4.22880409	0.16461752
H	3.19287454	-3.19287454	0.15455627	H	-1.35300938	5.08104881	0.17914819
H	3.19287454	3.19287454	0.15455627	C	0.68154907	4.22880409	0.16461752
H	-3.19287454	3.19287454	0.15455627	H	1.35300938	5.08104881	0.17914819
H	-3.19287454	-3.19287454	0.15455627	C	-2.85681365	-1.10069873	0.14546289
C	1.10069873	-2.85681365	0.14546289	C	-2.85681365	1.10069873	0.14546289
C	-1.10069873	-2.85681365	0.14546289	C	-4.22880409	-0.68154907	0.16461752
C	0.68154907	-4.22880409	0.16461752	H	-5.08104881	-1.35300938	0.17914819
H	1.35300938	-5.08104881	0.17914819	C	-4.22880409	0.68154907	0.16461752
C	-0.68154907	-4.22880409	0.16461752	H	-5.08104881	1.35300938	0.17914819
H	-1.35300938	-5.08104881	0.17914819	Cl	0.00000000	0.00000000	-2.64086382

TABLE S-LXVIII. FePzCl (**9**) S12g–Cosmo Doublet

Fe	0.00000000	0.00000000	-0.14167715	C	4.10988315	0.67791839	0.09724690
N	0.00000000	-1.90339976	0.06549362	H	4.95180415	1.36094016	0.12130595
N	1.90339976	0.00000000	0.06549362	C	4.10988315	-0.67791839	0.09724690
N	0.00000000	1.90339976	0.06549362	H	4.95180415	-1.36094016	0.12130595
N	-1.90339976	0.00000000	0.06549362	C	-1.09929165	2.73196962	0.07199404
N	2.37537507	-2.37537507	0.06729600	C	1.09929165	2.73196962	0.07199404

N	2.37537507	2.37537507	0.06729600	C	-0.67791839	4.10988315	0.09724690
N	-2.37537507	2.37537507	0.06729600	H	-1.36094016	4.95180415	0.12130595
N	-2.37537507	-2.37537507	0.06729600	C	0.67791839	4.10988315	0.09724690
C	1.09929165	-2.73196962	0.07199404	H	1.36094016	4.95180415	0.12130595
C	-1.09929165	-2.73196962	0.07199404	C	-2.73196962	-1.09929165	0.07199404
C	0.67791839	-4.10988315	0.09724690	C	-2.73196962	1.09929165	0.07199404
H	1.36094016	-4.95180415	0.12130595	C	-4.10988315	-0.67791839	0.09724690
C	-0.67791839	-4.10988315	0.09724690	H	-4.95180415	-1.36094016	0.12130595
H	-1.36094016	-4.95180415	0.12130595	C	-4.10988315	0.67791839	0.09724690
C	2.73196962	1.09929165	0.07199404	H	-4.95180415	1.36094016	0.12130595
C	2.73196962	-1.09929165	0.07199404	Cl	0.00000000	0.00000000	-2.33873854

TABLE S-LXIX. FePzCl (9) S12g–Cosmo Quartet

Fe	0.00000000	0.00000000	-0.23491977	C	4.11069014	0.67819938	0.16634316
N	0.00000000	-1.91145543	0.07157440	H	4.95175652	1.36127513	0.20823813
N	1.91145543	0.00000000	0.07157440	C	4.11069014	-0.67819938	0.16634316
N	0.00000000	1.91145543	0.07157440	H	4.95175652	-1.36127513	0.20823813
N	-1.91145543	0.00000000	0.07157440	C	-1.09933663	2.73292373	0.11232845
N	2.37712876	-2.37712876	0.11822402	C	1.09933663	2.73292373	0.11232845
N	2.37712876	2.37712876	0.11822402	C	-0.67819938	4.11069014	0.16634316
N	-2.37712876	2.37712876	0.11822402	H	-1.36127513	4.95175652	0.20823813
N	-2.37712876	-2.37712876	0.11822402	C	0.67819938	4.11069014	0.16634316
C	1.09933663	-2.73292373	0.11232845	H	1.36127513	4.95175652	0.20823813
C	-1.09933663	-2.73292373	0.11232845	C	-2.73292373	-1.09933663	0.11232845
C	0.67819938	-4.11069014	0.16634316	C	-2.73292373	1.09933663	0.11232845
H	1.36127513	-4.95175652	0.20823813	C	-4.11069014	-0.67819938	0.16634316
C	-0.67819938	-4.11069014	0.16634316	H	-4.95175652	-1.36127513	0.20823813
H	-1.36127513	-4.95175652	0.20823813	C	-4.11069014	0.67819938	0.16634316
C	2.73292373	1.09933663	0.11232845	H	-4.95175652	1.36127513	0.20823813
C	2.73292373	-1.09933663	0.11232845	Cl	0.00000000	0.00000000	-2.60137132

TABLE S-LXX. FePzCl (9) S12g–Cosmo Sextet

Fe	0.00000000	0.00000000	-0.47753114	C	4.13514607	0.67865606	0.23248291
N	0.00000000	-1.93986431	0.11677831	H	4.97992092	1.35700891	0.28170327
N	1.93986431	0.00000000	0.11677831	C	4.13514607	-0.67865606	0.23248291
N	0.00000000	1.93986431	0.11677831	H	4.97992092	-1.35700891	0.28170327
N	-1.93986431	0.00000000	0.11677831	C	-1.10242173	2.75328276	0.16771426
N	2.37949524	-2.37949524	0.17893599	C	1.10242173	2.75328276	0.16771426
N	2.37949524	2.37949524	0.17893599	C	-0.67865606	4.13514607	0.23248291
N	-2.37949524	2.37949524	0.17893599	H	-1.35700891	4.97992092	0.28170327



N	-2.37949524	-2.37949524	0.17893599	C	0.67865606	4.13514607	0.23248291
C	1.10242173	-2.75328276	0.16771426	H	1.35700891	4.97992092	0.28170327
C	-1.10242173	-2.75328276	0.16771426	C	-2.75328276	-1.10242173	0.16771426
C	0.67865606	-4.13514607	0.23248291	C	-2.75328276	1.10242173	0.16771426
H	1.35700891	-4.97992092	0.28170327	C	-4.13514607	-0.67865606	0.23248291
C	-0.67865606	-4.13514607	0.23248291	H	-4.97992092	-1.35700891	0.28170327
H	-1.35700891	-4.97992092	0.28170327	C	-4.13514607	0.67865606	0.23248291
C	2.75328276	1.10242173	0.16771426	H	-4.97992092	1.35700891	0.28170327
C	2.75328276	-1.10242173	0.16771426	Cl	0.00000000	0.00000000	-2.73351270

*Iron(II) complexes*TABLE S-LXXI. *Meso*-(Fe(NH)<sub>4</sub>S<sub>4</sub>)CO (**4m**) OPBE Singlet

Fe	-0.09006756	-0.16819211	0.00000000	C	1.60781405	1.95004409	-1.25503328
S	0.98157935	-1.43951928	1.52194658	H	-1.82605522	1.40282507	4.35485676
S	-0.94842427	1.03481246	1.62509698	H	-1.24990819	0.19493673	6.45445110
S	-0.94842427	1.03481246	-1.62509698	H	0.33176821	-1.73170979	6.35951247
S	0.98157935	-1.43951928	-1.52194658	H	1.30095263	-2.45503794	4.21144020
C	-0.55270923	0.16873081	3.12972729	H	-1.82605522	1.40282507	-4.35485676
C	-1.12585582	0.56814586	4.33736110	H	-1.24990819	0.19493673	-6.45445110
C	-0.80578560	-0.10794845	5.50792922	H	0.33176821	-1.73170979	-6.35951247
C	0.08120913	-1.18772722	5.44876350	H	1.30095263	-2.45503794	-4.21144020
C	0.62986010	-1.59851111	4.24405075	H	2.28990447	0.50598658	0.00000000
C	0.32295211	-0.92583581	3.04477476	H	0.27795670	2.77287344	2.75417972
C	-0.55270923	0.16873081	-3.12972729	H	-0.16891126	3.22065264	1.10207089
C	-1.12585582	0.56814586	-4.33736110	H	2.01767506	1.27056992	2.00866052
C	-0.80578560	-0.10794845	-5.50792922	H	2.29699757	2.80409807	1.15642533
C	0.08120913	-1.18772722	-5.44876350	H	-0.16891126	3.22065264	-1.10207089
C	0.62986010	-1.59851111	-4.24405075	H	0.27795670	2.77287344	-2.75417972
C	0.32295211	-0.92583581	-3.04477476	H	2.29699757	2.80409807	-1.15642533
N	1.52950693	1.18390021	0.00000000	H	2.01767506	1.27056992	-2.00866052
C	0.24670243	2.41699168	1.71966519	C	-1.35922563	-1.31318456	0.00000000
C	1.60781405	1.95004409	1.25503328	O	-2.21216675	-2.10296414	0.00000000
C	0.24670243	2.41699168	-1.71966519				

TABLE S-LXXII. *Meso*-(Fe(NH)<sub>4</sub>S<sub>4</sub>)CO (**4m**) OPBE Triplet

Fe	-0.20887896	-0.28105503	0.00000000	C	1.53180039	2.19610569	-1.25486447
S	0.89724595	-1.51226845	1.47727079	H	-1.51505193	1.45335515	4.54877270
S	-0.94984935	1.02447445	1.73682641	H	-0.79559841	0.22144004	6.58498802
S	-0.94984935	1.02447445	-1.73682641	H	0.66518162	-1.78666167	6.34952319

S	0.89724595	-1.51226845	-1.47727079	H	1.39202404	-2.54935161	4.11665926
C	-0.42586968	0.16510542	3.20710200	H	-1.51505193	1.45335515	-4.54877270
C	-0.85926796	0.58750316	4.46399692	H	-0.79559841	0.22144004	-6.58498802
C	-0.45991588	-0.10408229	5.60190845	H	0.66518162	-1.78666167	-6.34952319
C	0.35670886	-1.22998626	5.46473777	H	1.39202404	-2.54935161	-4.11665926
C	0.76820926	-1.66245848	4.21346959	H	2.27033656	0.76993967	0.00000000
C	0.38176858	-0.97168743	3.04922514	H	0.15431973	2.88165587	2.78684107
C	-0.42586968	0.16510542	-3.20710200	H	-0.38786470	3.23918443	1.14500463
C	-0.85926796	0.58750316	-4.46399692	H	2.03950680	1.57349638	1.99817858
C	-0.45991588	-0.10408229	-5.60190845	H	2.09734640	3.14261540	1.18094211
C	0.35670886	-1.22998626	-5.46473777	H	-0.38786470	3.23918443	-1.14500463
C	0.76820926	-1.66245848	-4.21346959	H	0.15431973	2.88165587	-2.78684107
C	0.38176858	-0.97168743	-3.04922514	H	2.09734640	3.14261540	-1.18094211
N	1.53148658	1.46251203	0.00000000	H	2.03950680	1.57349638	-1.99817858
C	0.13011410	2.49637250	1.76215389	C	-1.87851944	-1.23698886	0.00000000
C	1.53180039	2.19610569	1.25486447	O	-2.67862115	-2.07116535	0.00000000
C	0.13011410	2.49637250	-1.76215389				

TABLE S-LXXIII. *Meso*-(Fe(NH)S<sub>4</sub>)CO (**4m**) OPBE Quintet

Fe	-0.16641143	-0.44251707	0.00000000	C	1.54884942	2.01018403	-1.24654157
S	0.73944636	-1.65968983	1.77926536	H	-1.46990993	1.76324664	4.57336569
S	-1.03949938	1.11487169	1.84761866	H	-0.68594442	0.75536083	6.70372163
S	-1.03949938	1.11487169	-1.84761866	H	0.73754820	-1.29802575	6.62848586
S	0.73944636	-1.65968983	-1.77926536	H	1.33792625	-2.31386033	4.46297878
C	-0.47352738	0.31809003	3.33104960	H	-1.46990993	1.76324664	-4.57336569
C	-0.83561533	0.87788865	4.55905779	H	-0.68594442	0.75536083	-6.70372163
C	-0.39913617	0.31325388	5.75108458	H	0.73754820	-1.29802575	-6.62848586
C	0.39169171	-0.83603708	5.70383805	H	1.33792625	-2.31386033	-4.46297878
C	0.73371325	-1.40900480	4.48876189	H	2.31196111	0.60928357	0.00000000
C	0.31413073	-0.85272627	3.26261587	H	0.26000595	2.93183564	2.70562453
C	-0.47352738	0.31809003	-3.33104960	H	-0.28003478	3.19883255	1.05294736
C	-0.83561533	0.87788865	-4.55905779	H	1.97649184	1.35765874	2.01471590
C	-0.39913617	0.31325388	-5.75108458	H	2.20233940	2.89853769	1.17104385
C	0.39169171	-0.83603708	-5.70383805	H	-0.28003478	3.19883255	-1.05294736
C	0.73371325	-1.40900480	-4.48876189	H	0.26000595	2.93183564	-2.70562453
C	0.31413073	-0.85272627	-3.26261587	H	2.20233940	2.89853769	-1.17104385
N	1.52514863	1.25064587	0.00000000	H	1.97649184	1.35765874	-2.01471590
C	0.17577628	2.46052974	1.72067856	C	-1.57471296	-1.86902123	0.00000000
C	1.54884942	2.01018403	1.24654157	O	-2.16540759	-2.85827524	0.00000000
C	0.17577628	2.46052974	-1.72067856				

TABLE S-LXXIV. *trans*-(Fe(NH)S<sub>4</sub>)CO (**4t**) OPBE Singlet

Fe	8.37201747	10.16261463	1.98792154	H	9.09294103	5.14672553	6.18304932
S	9.75461897	9.01403912	3.23442448	C	9.38486060	6.85384657	4.90348127
S	6.73551830	8.66677131	2.43368034	H	10.41613816	7.01984577	5.21380192
S	7.05582718	11.14915607	0.54938547	C	8.80338477	7.69466265	3.95339326
S	10.00054616	11.66333273	1.48058555	C	7.84882574	11.14432998	3.29011192
C	9.16733859	12.87633505	0.54919285	O	7.49294452	11.81540716	4.17045330
C	9.79383736	14.07984921	0.17398819	N	9.05383589	9.03059284	0.37288898
H	10.83037335	14.24778943	0.46103880	H	9.76003246	9.69598137	0.03711808
C	9.09983939	15.05099107	-0.53312438	C	10.65341224	8.10240695	1.92771228
H	9.60725846	15.97814453	-0.79968313	H	11.08852083	7.19800864	2.36324844
C	7.75974616	14.86840110	-0.88660208	H	11.46765780	8.77224639	1.62181026
H	7.21654624	15.64435487	-1.42306081	C	9.71782951	7.79329282	0.78492650
C	7.12221617	13.68470780	-0.53489236	H	8.94697596	7.08719257	1.11146749
H	6.07773617	13.51796352	-0.79504278	H	10.27233001	7.33650861	-0.05162283
C	7.82876622	12.70187801	0.15762709	C	7.45562376	10.22110936	-0.99770973
C	7.46294599	7.55810264	3.55346915	H	8.17993248	10.83210217	-1.54536637
C	6.73284067	6.49261695	4.11879290	H	6.54206380	10.13386972	-1.59568213
H	5.69306294	6.35402173	3.82760042	C	8.01534565	8.86525829	-0.64239313
C	7.31830756	5.63641716	5.03775259	H	7.23802872	8.22405739	-0.21062472
H	6.72611483	4.82375331	5.45849136	H	8.40624042	8.37700814	-1.55024856
C	8.64578414	5.81039106	5.44528098				

TABLE S-LXV. *trans*-(Fe(NH)S<sub>4</sub>)CO (**4t**) OPBE Triplet

Fe	8.32848153	10.21496984	2.04748256	H	9.13957689	4.68296941	5.82015068
S	9.94128254	8.84064467	3.35914362	C	9.47440427	6.51790845	4.74424443
S	6.74266696	8.85430591	2.84064252	H	10.53791666	6.55604096	4.97656541
S	6.95898404	11.18986938	0.24549961	C	8.90633409	7.53573749	3.97522130
S	9.94556676	11.68757328	1.45278734	C	7.72998417	11.39455620	3.18350228
C	9.09614256	12.92260154	0.55603829	O	7.33360396	12.18499090	3.93873294
C	9.71288382	14.16747726	0.33588626	N	9.02722251	8.94647535	0.43408886
H	10.69390753	14.34761449	0.77136315	H	9.73979672	9.60225456	0.10013727
C	9.08537539	15.16170130	-0.40086447	C	10.69304709	7.99382031	1.93648286
H	9.58744235	16.11849451	-0.54381112	H	11.16902297	7.06886028	2.27637341
C	7.81570136	14.95278053	-0.94059774	H	11.48403425	8.67205620	1.59031998
H	7.31684068	15.73722971	-1.50740690	C	9.68589684	7.71017601	0.84291744
C	7.18405159	13.73227554	-0.73543890	H	8.92329792	7.01398566	1.20812965
H	6.18916185	13.55211397	-1.13933449	H	10.19935117	7.22909251	-0.00758417
C	7.81767731	12.71776232	-0.01286906	C	7.58074772	10.14783312	-1.12616327
C	7.52554872	7.54943736	3.69374610	H	8.41147980	10.68782517	-1.59250548

C	6.74989923	6.48455070	4.19265758	H	6.78470110	10.03258996	-1.87041879
H	5.68019811	6.47735707	3.99088970	C	8.02164815	8.79084750	-0.61523099
C	7.32585733	5.46077953	4.92936492	H	7.17280340	8.23985704	-0.19295284
H	6.69810230	4.64946561	5.29757756	H	8.41302394	8.20683849	-1.46551723
C	8.69159925	5.47234628	5.21898257				

TABLE S-LXXVI. *trans*-(Fe(NH)S<sub>4</sub>)CO (**4t**) OPBE Quintet

Fe	8.39595903	10.17332571	1.99573643	H	8.98260916	5.11372392	6.40595677
S	9.94659919	8.67040094	3.22259472	C	9.37077549	6.67924454	4.98040988
S	6.69871032	8.57475268	2.54185158	H	10.43665119	6.72634608	5.19850023
S	7.06673299	11.15961738	0.17134865	C	8.83699440	7.53873475	4.01545623
S	10.05303472	11.83781888	1.37295831	C	7.82467198	11.35593261	3.44377388
C	9.08130125	13.02818616	0.55470158	O	7.46506958	12.09321622	4.25344258
C	9.57806586	14.33720769	0.39879062	N	9.17555460	8.86121749	0.20925044
H	10.55975739	14.56689072	0.80797534	H	9.97258867	9.43224102	-0.07204801
C	8.84406844	15.32370785	-0.24367184	C	10.59222930	7.69859285	1.82162388
H	9.26361657	16.32531444	-0.33747379	H	10.90353263	6.71822479	2.19596810
C	7.57431557	15.04838646	-0.75311553	H	11.49963810	8.24027297	1.52011509
H	6.99155278	15.82383010	-1.24747715	C	9.62808899	7.55486302	0.66003008
C	7.05661936	13.76638313	-0.61731807	H	8.74923512	6.98235462	0.97653893
H	6.06579158	13.52912069	-1.00075144	H	10.12872930	6.98228530	-0.14310170
C	7.79596887	12.76481729	0.01783010	C	7.80589624	10.26289372	-1.24743112
C	7.45182162	7.54235803	3.72210206	H	8.67701512	10.84212743	-1.57075312
C	6.65050016	6.63015224	4.43900494	H	7.07557713	10.24942193	-2.06427917
H	5.58150497	6.61698048	4.23648298	C	8.19531830	8.84819285	-0.86510373
C	7.18989847	5.76383087	5.37726954	H	7.31855892	8.28942137	-0.51387926
H	6.53342022	5.07200200	5.90477088	H	8.56785168	8.33680390	-1.77151133
C	8.55691306	5.78204991	5.65948188				

TABLE S-LXXVII. *Meso*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5m**) OPBE Singlet

Fe	0.16199121	0.04998079	0.00000000	H	-1.64258893	-1.36903023	4.39111863
S	1.41384995	1.13727970	-1.51894085	H	-0.77921879	-0.37360919	6.50410909
S	-0.82467035	-1.01654526	-1.61667565	H	1.08962728	1.27711637	6.40357600
S	-0.82467035	-1.01654526	1.61667565	H	2.06082100	1.94001883	4.23502827
S	1.41384995	1.13727970	1.51894085	H	2.42987821	-0.94188258	0.00000000
C	-0.25290122	-0.28958643	-3.14665567	H	0.11895957	-2.94169685	-2.72962590
C	-0.82300979	-0.65071127	-4.36751362	H	-0.37564070	-3.29886557	-1.06712243
C	-0.34082243	-0.09519105	-5.54721375	H	2.04811122	-1.67395803	-2.01065446
C	0.70555626	0.83213863	-5.48533388	H	2.12970665	-3.22169724	-1.14209468
C	1.25603395	1.20719036	-4.26979469	H	-0.37564070	-3.29886557	1.06712243

C	0.77913518	0.65966283	-3.06133589	H	0.11895957	-2.94169685	2.72962590
C	-0.25290122	-0.28958643	3.14665567	H	2.12970665	-3.22169724	1.14209468
C	-0.82300979	-0.65071127	4.36751362	H	2.04811122	-1.67395803	2.01065446
C	-0.34082243	-0.09519105	5.54721375	P	-1.23739474	1.73769108	0.00000000
C	0.70555626	0.83213863	5.48533388	C	-2.43583039	1.84462934	-1.39577855
C	1.25603395	1.20719036	4.26979469	H	-1.90153494	1.92974538	-2.34767846
C	0.77913518	0.65966283	3.06133589	H	-3.06545342	0.94821207	-1.42253005
N	1.58193093	-1.50546218	0.00000000	H	-3.07676141	2.72512577	-1.26595391
C	0.14368485	-2.57158235	-1.70014913	C	-2.43583039	1.84462934	1.39577855
C	1.55670876	-2.28623939	-1.24821218	H	-3.06545342	0.94821207	1.42253005
C	0.14368485	-2.57158235	1.70014913	H	-1.90153494	1.92974538	2.34767846
C	1.55670876	-2.28623939	1.24821218	H	-3.07676141	2.72512577	1.26595391
H	-1.64258893	-1.36903023	-4.39111863	C	-0.54732697	3.45257039	0.00000000
H	-0.77921879	-0.37360919	-6.50410909	H	-0.88895481	3.98740084	-0.89233995
H	1.08962728	1.27711637	-6.40357600	H	-0.88895481	3.98740084	0.89233995
H	2.06082100	1.94001883	-4.23502827	H	0.54409476	3.42295975	0.00000000

TABLE S-LXXVIII. *Meso*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5m**) OPBE Triplet

Fe	0.23547647	0.11812400	0.00000000	H	-1.61541568	-1.56458344	4.46308091
S	1.37256301	1.19296343	-1.68507658	H	-0.85178963	-0.54848322	6.60092101
S	-0.86588638	-1.13921648	-1.73665919	H	0.90154552	1.23197226	6.54574053
S	-0.86588638	-1.13921648	1.73665919	H	1.84702386	1.98127401	4.39432333
S	1.37256301	1.19296343	1.68507658	H	2.48893121	-0.89982940	0.00000000
C	-0.29097129	-0.38700214	-3.24400312	H	0.24618278	-3.03628464	-2.70323477
C	-0.84555963	-0.79312081	-4.46012070	H	-0.27100807	-3.32057030	-1.04092604
C	-0.42076153	-0.22455689	-5.65489815	H	2.08205741	-1.61165852	-2.01538637
C	0.55884187	0.77176427	-5.61854949	H	2.22956927	-3.15794037	-1.15229404
C	1.09415704	1.19461764	-4.41170680	H	-0.27100807	-3.32057030	1.04092604
C	0.68750655	0.63028185	-3.18454793	H	0.24618278	-3.03628464	2.70323477
C	-0.29097129	-0.38700214	3.24400312	H	2.22956927	-3.15794037	1.15229404
C	-0.84555963	-0.79312081	4.46012070	H	2.08205741	-1.61165852	2.01538637
C	-0.42076153	-0.22455689	5.65489815	P	-1.12311150	1.89786404	0.00000000
C	0.55884187	0.77176427	5.61854949	C	-2.30792084	1.99723506	-1.40270283
C	1.09415704	1.19461764	4.41170680	H	-1.76601688	2.04247125	-2.35266913
C	0.68750655	0.63028185	3.18454793	H	-2.96058531	1.11749905	-1.40495977
N	1.64283606	-1.46558920	0.00000000	H	-2.92536803	2.89793495	-1.29663772
C	0.22075423	-2.59759564	-1.69990730	C	-2.30792084	1.99723506	1.40270283
C	1.62170760	-2.24220232	-1.24845401	H	-2.96058531	1.11749905	1.40495977
C	0.22075423	-2.59759564	1.69990730	H	-1.76601688	2.04247125	2.35266913
C	1.62170760	-2.24220232	1.24845401	H	-2.92536803	2.89793495	1.29663772

H	-1.61541568	-1.56458344	-4.46308091	C	-0.37750288	3.58367829	0.00000000
H	-0.85178963	-0.54848322	-6.60092101	H	-0.70065396	4.12784607	-0.89387086
H	0.90154552	1.23197226	-6.54574053	H	-0.70065396	4.12784607	0.89387086
H	1.84702386	1.98127401	-4.39432333	H	0.71237259	3.51526731	0.00000000

TABLE S-LXXIX. *Meso*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5m**) OPBE Quintet

Fe	0.26968196	0.23835519	0.00000000	H	-1.37424897	-1.49307996	4.66829162
S	1.52738705	1.18421931	-1.69078746	H	-0.39536843	-0.54175103	6.74377029
S	-0.86828091	-1.05591499	-1.90453855	H	1.41535229	1.17284570	6.56161320
S	-0.86828091	-1.05591499	1.90453855	H	2.21591862	1.90090840	4.34385199
S	1.52738705	1.18421931	1.69078746	H	2.39361475	-1.28526676	0.00000000
C	-0.10501946	-0.35934416	-3.35186584	H	-0.02270752	-3.13272667	-2.75367489
C	-0.57236870	-0.75781145	-4.60812522	H	-0.65603321	-3.25881055	-1.11443670
C	-0.02877878	-0.22302069	-5.76918720	H	1.99672334	-2.00476737	-1.99900145
C	0.98093851	0.73572677	-5.66218545	H	1.83359123	-3.55464127	-1.15721274
C	1.43313370	1.14779656	-4.41780292	H	-0.65603321	-3.25881055	1.11443670
C	0.90750829	0.61814094	-3.22096221	H	-0.02270752	-3.13272667	2.75367489
C	-0.10501946	-0.35934416	3.35186584	H	1.83359123	-3.55464127	1.15721274
C	-0.57236870	-0.75781145	4.60812522	H	1.99672334	-2.00476737	1.99900145
C	-0.02877878	-0.22302069	5.76918720	P	-1.68227882	1.98396806	0.00000000
C	0.98093851	0.73572677	5.66218545	C	-2.85855782	1.99905384	-1.41390393
C	1.43313370	1.14779656	4.41780292	H	-2.30271533	2.10531316	-2.35176741
C	0.90750829	0.61814094	3.22096221	H	-3.40752206	1.05117515	-1.44548575
N	1.51599651	-1.79509888	0.00000000	H	-3.57423671	2.82561389	-1.32289550
C	-0.01871647	-2.65352227	-1.76849608	C	-2.85855782	1.99905384	1.41390393
C	1.40555192	-2.54009471	-1.24915253	H	-3.40752206	1.05117515	1.44548575
C	-0.01871647	-2.65352227	1.76849608	H	-2.30271533	2.10531316	2.35176741
C	1.40555192	-2.54009471	1.24915253	H	-3.57423671	2.82561389	1.32289550
H	-1.37424897	-1.49307996	-4.66829162	C	-1.03354878	3.71232075	0.00000000
H	-0.39536843	-0.54175103	-6.74377029	H	-1.37908618	4.24627012	-0.89123768
H	1.41535229	1.17284570	-6.56161320	H	-1.37908618	4.24627012	0.89123768
H	2.21591862	1.90090840	-4.34385199	H	0.05995578	3.69254275	0.00000000

TABLE S-LXXX. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) OPBE Singlet

Fe	3.12704066	2.99670483	8.08948338	H	1.73951939	2.82354851	6.10555290
S	3.31689781	5.05137520	8.99125804	H	5.28437565	0.18641962	10.72863902
S	4.86667752	3.39449160	6.85235429	H	5.24410473	0.11938292	8.93965426
S	1.24014858	2.72791083	9.11252271	H	3.76103257	-0.17504919	9.86314264
S	2.84680373	0.97113921	7.12200291	H	6.43443656	2.45479663	10.93164411
P	4.30337099	2.20630505	9.77292480	H	5.93910760	3.97927638	10.13960230

C	4.68639795	0.40817399	9.83617207	H	6.63189587	2.65305342	9.17286320
C	5.99123950	2.89198118	10.02879735	H	4.30604809	2.11341751	12.21390091
C	3.59940120	2.46555269	11.45291651	H	2.65902148	1.91513903	11.56272450
C	5.43052117	5.03816270	7.25286791	H	3.40532862	3.53290743	11.60162379
C	6.57783724	5.56315627	6.65704820	H	7.14317106	4.95951267	5.94686111
C	6.99505487	6.85047307	6.97128476	H	7.88533844	7.26826327	6.50418371
C	6.25705846	7.59700246	7.89804981	H	6.57446850	8.60817181	8.15379588
C	5.13478888	7.06448557	8.51134296	H	4.57939778	7.65126324	9.24161761
C	4.69108804	5.76078493	8.20603150	H	-0.76947717	1.07065099	10.41219579
C	0.78115240	1.01687018	8.91847870	H	-1.43379041	-1.30401128	10.04114517
C	-0.25688433	0.46275280	9.66689567	H	-0.23908387	-2.64853848	8.31267288
C	-0.62990032	-0.86029880	9.45603177	H	1.61311535	-1.66496519	7.01524510
C	0.04471707	-1.61028108	8.48666583	H	3.85908012	2.77239347	4.80016629
C	1.08630246	-1.06150575	7.75304625	H	4.72117865	4.32326117	4.61812879
C	1.49448069	0.27072920	7.96269040	H	2.97389253	5.47936741	5.95337264
N	1.98295944	3.73375772	6.51447673	H	2.18706681	4.63647219	4.59750146
C	4.04176481	3.75282186	5.25863223	H	-0.73470758	4.00992950	8.49058915
C	2.75619218	4.49273601	5.53099764	H	-0.43775817	2.64155651	7.39038362
C	0.03288995	3.47527580	7.92076051	H	0.10918567	4.67874498	6.14293345
C	0.76886279	4.39876365	6.98123911	H	1.07873735	5.31225006	7.50091604

TABLE S-LXXXI. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) OPBE Triplet

Fe	3.16635535	2.96932149	8.10950481	H	1.55150853	2.94624407	5.82354905
S	3.35584737	4.99647253	8.99779073	H	5.38862885	0.01669290	10.98792264
S	4.82269813	3.45567719	6.71546249	H	5.35147744	-0.03809706	9.19837695
S	1.16096408	2.77546005	9.03845589	H	3.85805828	-0.29009867	10.11345618
S	2.90996156	0.94803004	7.20221877	H	6.60395637	2.33145970	11.18158987
P	4.45306729	2.07159716	10.01175731	H	6.10491312	3.83333512	10.34986135
C	4.80112146	0.26562581	10.09520380	H	6.78005915	2.48552701	9.41209577
C	6.14948837	2.74224519	10.27092663	H	4.38846533	1.99606399	12.47491389
C	3.72529459	2.35942990	11.67951497	H	2.76187978	1.84276981	11.75349766
C	5.39609713	5.08651310	7.16158431	H	3.55130164	3.43250981	11.81473140
C	6.49744940	5.66167373	6.53016631	H	7.02277159	5.11104099	5.75013206
C	6.92328151	6.93300196	6.90034749	H	7.78109317	7.38738371	6.40706381
C	6.24788676	7.60964292	7.91852897	H	6.57716889	8.60405217	8.22009491
C	5.16387616	7.02781359	8.56050405	H	4.64792041	7.56018019	9.35820383
C	4.71631763	5.74599813	8.19491719	H	-0.96683753	1.16216637	10.19433563
C	0.71187516	1.06020133	8.85139702	H	-1.56657368	-1.23742967	9.89498800
C	-0.38195008	0.52595509	9.53070715	H	-0.19634116	-2.65942207	8.37297210
C	-0.71715053	-0.81400479	9.36116087	H	1.75027386	-1.70738457	7.18656835

C	0.05401471	-1.60711554	8.50877063	H	3.78172975	2.89369624	4.67615096
C	1.14873215	-1.07634017	7.83928468	H	4.63856932	4.43975848	4.51507364
C	1.50950985	0.27268239	8.00510237	H	2.85999453	5.57104631	5.86803010
N	1.80177127	3.83341555	6.25240223	H	2.19372016	4.83316896	4.40028027
C	3.95750973	3.86678970	5.15239302	H	-0.80931098	4.03543479	8.38163632
C	2.65325768	4.61022024	5.38262111	H	-0.48336479	2.67381040	7.28914248
C	-0.02595456	3.51577532	7.81863565	H	-0.10520255	4.80262750	6.11803090
C	0.65374346	4.46968557	6.85222306	H	1.00662266	5.35921189	7.38771551

TABLE S-LXXXII. *trans*-(Fe(NH)<sub>4</sub>)PMe<sub>3</sub> (**5t**) OPBE Quintet

Fe	3.19569558	2.92923367	8.05375704	H	1.73247286	2.95188034	5.83890630
S	3.43904462	5.10296998	9.03126331	H	5.37198200	-0.09858202	11.07121938
S	5.00222733	3.61543051	6.58048313	H	5.31451176	-0.18750867	9.28337975
S	0.84563741	2.75802790	9.01205682	H	3.82067085	-0.35762433	10.21568476
S	2.67576518	0.81491550	7.04013284	H	6.69211730	2.22726523	11.14563440
P	4.50791281	1.96966440	10.05500961	H	6.19405832	3.70576371	10.26740443
C	4.78640715	0.15725613	10.17920063	H	6.81624588	2.30698737	9.36650927
C	6.21928949	2.61194323	10.23348469	H	4.43831542	2.00327615	12.51044708
C	3.78925042	2.35736081	11.69989729	H	2.80752079	1.87989688	11.79225407
C	5.49242062	5.22291065	7.15179612	H	3.65750380	3.44148783	11.78167370
C	6.59489474	5.83760559	6.55298867	H	7.12720948	5.31721162	5.75738814
C	7.00972314	7.09849368	6.96198712	H	7.86601977	7.57542050	6.48785277
C	6.31706610	7.73208395	7.99576609	H	6.62853348	8.72105961	8.33283930
C	5.23669625	7.11544587	8.60757913	H	4.70913881	7.61740066	9.41667474
C	4.78751102	5.83767068	8.21232342	H	-1.01087354	1.10475858	10.32300561
C	0.57630895	1.01127466	8.87982971	H	-1.49065897	-1.33602597	10.24074501
C	-0.43363430	0.45197029	9.66984848	H	-0.13519473	-2.78809681	8.72182903
C	-0.70164088	-0.91016423	9.62299566	H	1.66618548	-1.81226591	7.35080910
C	0.05906465	-1.71645573	8.77420117	H	3.88605652	3.08763653	4.58314382
C	1.07080445	-1.17099517	7.99828392	H	4.63751996	4.68779550	4.45689166
C	1.37447546	0.20653047	8.02686954	H	2.88353763	5.65095260	5.94823803
N	1.91227459	3.84883895	6.29178625	H	2.18626670	4.94233928	4.47813019
C	4.03013614	4.04449324	5.10192591	H	-1.03305824	3.84413245	7.96395460
C	2.70450109	4.70391160	5.42616922	H	-0.37478979	2.52621810	6.97387932
C	-0.10855172	3.39750156	7.58100437	H	0.01287224	4.76159668	5.94623245
C	0.66599073	4.41746107	6.76996139	H	0.90816341	5.29346109	7.38491563

TABLE S-LXXXIII. *Meso*-(Fe(NH)<sub>4</sub>)NH<sub>3</sub> (**6m**) OPBE Singlet

Fe	-0.27645225	-0.40703467	0.00000000	N	-2.00957018	-1.45493421	0.00000000
S	0.52208469	-1.86582341	1.52247946	H	-1.69372545	1.44481370	4.37017379



S	-0.94168256	0.88836689	1.61439014	H	-1.29900367	0.17801523	6.47799473
S	-0.94168256	0.88836689	-1.61439014	H	-0.07248670	-1.99359379	6.38517439
S	0.52208469	-1.86582341	-1.52247946	H	0.73072869	-2.88929719	4.23212785
C	-0.68261907	-0.00697085	3.13943134	H	-1.69372545	1.44481370	-4.37017379
C	-1.15456474	0.49757690	4.35184786	H	-1.29900367	0.17801523	-6.47799473
C	-0.93411162	-0.20943301	5.52819353	H	-0.07248670	-1.99359379	-6.38517439
C	-0.24732263	-1.42732704	5.47003431	H	0.73072869	-2.88929719	-4.23212785
C	0.20635161	-1.93535519	4.26249575	H	2.12825141	-0.19591306	0.00000000
C	-0.00817738	-1.23754026	3.05658282	H	0.56285779	2.40329499	2.75117294
C	-0.68261907	-0.00697085	-3.13943134	H	0.19912781	2.92263377	1.09598694
C	-1.15456474	0.49757690	-4.35184786	H	1.98869943	0.60528828	2.00904365
C	-0.93411162	-0.20943301	-5.52819353	H	2.54868591	2.04738201	1.13291504
C	-0.24732263	-1.42732704	-5.47003431	H	0.19912781	2.92263377	-1.09598694
C	0.20635161	-1.93535519	-4.26249575	H	0.56285779	2.40329499	-2.75117294
C	-0.00817738	-1.23754026	-3.05658282	H	2.54868591	2.04738201	-1.13291504
N	1.47733535	0.58919653	0.00000000	H	1.98869943	0.60528828	-2.00904365
C	0.46412073	2.06027965	1.71698014	H	-2.00032863	-2.06337004	0.81709254
C	1.70902237	1.34389272	1.25103746	H	-2.00032863	-2.06337004	-0.81709254
C	0.46412073	2.06027965	-1.71698014	H	-2.87819717	-0.92707568	0.00000000
C	1.70902237	1.34389272	-1.25103746	N			

TABLE S-LXXXIV. *Meso*-(Fe(NH)<sub>4</sub>)NH<sub>3</sub> (**6m**) OPBE Triplet

Fe	-0.47398829	-0.52806121	0.00000000	N	-2.80398959	-1.44143543	0.00000000
S	0.25544232	-2.01060049	1.50575904	H	-1.66394441	1.36622717	4.49749066
S	-1.09894504	0.80443091	1.70064074	H	-1.22234600	0.05373795	6.56405323
S	-1.09894504	0.80443091	-1.70064074	H	-0.09679022	-2.16669984	6.38447535
S	0.25544232	-2.01060049	-1.50575904	H	0.56130413	-3.06161688	4.18028330
C	-0.76441135	-0.10048547	3.19874417	H	-1.66394441	1.36622717	-4.49749066
C	-1.16061906	0.40133014	4.43910442	H	-1.22234600	0.05373795	-6.56405323
C	-0.91630057	-0.33322344	5.59347178	H	-0.09679022	-2.16669984	-6.38447535
C	-0.28741468	-1.57797269	5.48704101	H	0.56130413	-3.06161688	-4.18028330
C	0.08581350	-2.08461969	4.25113643	H	2.07864580	0.05775493	0.00000000
C	-0.15377150	-1.35835990	3.06857609	H	0.27760056	2.45967988	2.77624482
C	-0.76441135	-0.10048547	-3.19874417	H	-0.18195548	2.91382244	1.13230437
C	-1.16061906	0.40133014	-4.43910442	H	1.93011369	0.87073576	2.00193733
C	-0.91630057	-0.33322344	-5.59347178	H	2.25141794	2.40599802	1.17813483
C	-0.28741468	-1.57797269	-5.48704101	H	-0.18195548	2.91382244	-1.13230437
C	0.08581350	-2.08461969	-4.25113643	H	0.27760056	2.45967988	-2.77624482
C	-0.15377150	-1.35835990	-3.06857609	H	2.25141794	2.40599802	-1.17813483
N	1.42372969	0.83133428	0.00000000	H	1.93011369	0.87073576	-2.00193733

C	0.20000307	2.09203822	1.74804020	H	-2.83593020	-2.04889916	0.81350418
C	1.53787322	1.56625776	1.25320338	H	-2.83593020	-2.04889916	-0.81350418
C	0.20000307	2.09203822	-1.74804020	H	-3.65844045	-0.89068416	0.00000000
C	1.53787322	1.56625776	-1.25320338				

TABLE S-LXXXV. *Meso*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6m**) OPBE Quintet

Fe	-0.33841255	-0.65557547	0.00000000	N	-2.47910598	-1.48482638	0.00000000
S	0.44274197	-2.00038155	1.72431560	H	-1.41293395	1.56278265	4.61869448
S	-1.00132454	0.96017677	1.87871364	H	-0.91579150	0.33544334	6.72173853
S	-1.00132454	0.96017677	-1.87871364	H	0.16782592	-1.91400183	6.58855943
S	0.44274197	-2.00038155	-1.72431560	H	0.73745877	-2.89170230	4.39693217
C	-0.58594262	0.04170075	3.34148444	H	-1.41293395	1.56278265	-4.61869448
C	-0.92583846	0.58873403	4.58298877	H	-0.91579150	0.33544334	-6.72173853
C	-0.65206173	-0.09822906	5.75835759	H	0.16782592	-1.91400183	-6.58855943
C	-0.04790483	-1.35488638	5.67779353	H	0.73745877	-2.89170230	-4.39693217
C	0.27400533	-1.90796921	4.44765275	H	2.16166101	-0.01781105	0.00000000
C	0.01707972	-1.23299675	3.23569609	H	0.54728199	2.56694940	2.74978861
C	-0.58594262	0.04170075	-3.34148444	H	0.02405957	2.93299030	1.10812838
C	-0.92583846	0.58873403	-4.58298877	H	2.01544564	0.78089258	2.00281365
C	-0.65206173	-0.09822906	-5.75835759	H	2.44217205	2.28143552	1.16163243
C	-0.04790483	-1.35488638	-5.67779353	H	0.02405957	2.93299030	-1.10812838
C	0.27400533	-1.90796921	-4.44765275	H	0.54728199	2.56694940	-2.74978861
C	0.01707972	-1.23299675	-3.23569609	H	2.44217205	2.28143552	-1.16163243
N	1.50725926	0.75956779	0.00000000	H	2.01544564	0.78089258	-2.00281365
C	0.38348364	2.12869433	1.75942175	H	-2.55819575	-2.08347560	0.81704438
C	1.66937324	1.49700275	1.25053739	H	-2.55819575	-2.08347560	-0.81704438
C	0.38348364	2.12869433	-1.75942175	H	-3.27455675	-0.85268182	0.00000000
C	1.66937324	1.49700275	-1.25053739				

TABLE S-LXXXVI. *trans*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6t**) OPBE Singlet

Fe	3.09965309	3.03411131	8.05270451	H	1.73237708	2.81598551	6.09105027
S	3.31550607	5.07231845	8.99307100	H	7.15083248	4.97958384	5.94741886
S	4.85960983	3.42619408	6.83612919	H	7.94186780	7.25584612	6.56831523
S	1.23667823	2.73153570	9.11371759	H	6.67013052	8.56788872	8.26994500
S	2.92338044	0.94506876	7.19486268	H	4.65791974	7.62238021	9.33504915
C	5.44800783	5.05295268	7.26750178	H	-0.80405784	1.08062069	10.37293031
C	6.60253924	5.57268517	6.67944245	H	-1.41398172	-1.31461175	10.05467782
C	7.04648667	6.84149081	7.02871425	H	-0.12394284	-2.69595805	8.42621315
C	6.33041037	7.57185172	7.98511746	H	1.75604189	-1.71776227	7.16430163
C	5.19927971	7.04495576	8.58713490	H	3.86993672	2.81057996	4.77387888

C	4.72476700	5.76133051	8.24523559	H	4.69935591	4.38223745	4.61373450
C	0.80178714	1.00947228	8.93921928	H	2.94182544	5.48224931	5.97752217
C	-0.25255302	0.45909778	9.66792916	H	2.15208873	4.64463581	4.61713976
C	-0.59414910	-0.87661069	9.48776282	H	-0.74537314	4.01109316	8.49943065
C	0.13391518	-1.64718801	8.57556708	H	-0.45645718	2.62758465	7.41502423
C	1.19188920	-1.10186028	7.86318020	H	0.10263393	4.64371080	6.13448249
C	1.56406221	0.24564884	8.03698953	H	1.06345153	5.29906984	7.48986312
N	1.98152537	3.71245357	6.52531005	N	4.19813245	2.27294805	9.58757095
C	4.03375042	3.78767188	5.24643205	H	3.79398761	2.49761289	10.49237514
C	2.73757255	4.49907661	5.53994233	H	4.25379555	1.25984667	9.49884485
C	0.01777824	3.46741646	7.93254952	H	5.14593282	2.63839838	9.60959795
C	0.75592494	4.37813897	6.98234509				

TABLE S-LXXXVII. *trans*-(Fe(NH)<sub>4</sub>)NH<sub>3</sub> (**6t**) OPBE Triplet

Fe	3.13066234	3.00591463	8.05773698	H	1.62543301	2.90929427	5.87841150
S	3.36307540	4.99867867	9.03673236	H	7.09730039	5.09144926	5.86231076
S	4.86161065	3.45481251	6.77945430	H	7.84881992	7.36930278	6.52465916
S	1.21282769	2.75550531	9.08236384	H	6.60974981	8.59732103	8.30567504
S	2.94655047	0.90802371	7.24937587	H	4.65593533	7.56439932	9.41030186
C	5.44056654	5.08165366	7.23972580	H	-0.88829280	1.15273432	10.30004831
C	6.55921550	5.64688852	6.63011466	H	-1.49986983	-1.24748139	10.02619538
C	6.98124758	6.91832682	7.00368364	H	-0.15843143	-2.68170096	8.49015153
C	6.28546311	7.60140363	8.00371328	H	1.77086362	-1.74414228	7.26653815
C	5.18718166	7.02583764	8.62703275	H	3.85678878	2.89331629	4.72101937
C	4.74152128	5.74383538	8.25901325	H	4.69520240	4.45335781	4.57957558
C	0.76625130	1.03480876	8.92778640	H	2.89240981	5.55406765	5.91885176
C	-0.31548066	0.50960139	9.63267166	H	2.22652915	4.79394317	4.45898085
C	-0.65697726	-0.83019761	9.47756822	H	-0.78025016	3.98080253	8.41043309
C	0.09835024	-1.62986857	8.61720381	H	-0.42618242	2.61318997	7.33225561
C	1.18376686	-1.10707955	7.92637085	H	-0.05616423	4.72267305	6.12697135
C	1.55252985	0.24191179	8.07597878	H	1.01642514	5.32619546	7.41251646
N	1.86614833	3.79591435	6.31792919	N	4.49232748	1.99593805	9.95087917
C	4.01584359	3.86555566	5.20493344	H	4.11691538	2.20525887	10.87102421
C	2.70191818	4.58882824	5.43593836	H	4.49688264	0.98597681	9.84479713
C	0.01329717	3.46892938	7.85482238	H	5.46011223	2.30373029	9.95945026
C	0.68887871	4.42174635	6.88679897				

TABLE S-LXXXVIII. *trans*-(Fe(NH)<sub>4</sub>)NH<sub>3</sub> (**6t**) OPBE Quintet

Fe	3.23494889	2.95734304	8.20696073	H	1.70009515	2.86236419	6.03154534
S	3.53821191	5.11288253	9.11111404	H	7.07848813	5.29755428	5.66123769

S	5.06838137	3.55676222	6.65357891	H	7.79052734	7.59618488	6.28271774
S	0.92454833	2.66661147	9.17371412	H	6.62376612	8.76290059	8.16093237
S	2.89221825	0.77610776	7.29915134	H	4.78909220	7.64565555	9.37098028
C	5.51605262	5.20640191	7.13680611	H	-1.14637890	1.01170117	10.14758282
C	6.57201841	5.82988119	6.46587498	H	-1.71581013	-1.38593162	9.81606809
C	6.97340729	7.11221630	6.81529178	H	-0.25421463	-2.79017859	8.35110756
C	6.31964690	7.75803956	7.86688974	H	1.73427365	-1.80794889	7.27436521
C	5.28706175	7.13393268	8.54925586	H	3.86053377	2.86494922	4.76357210
C	4.84831084	5.83608526	8.21256419	H	4.60731770	4.44721883	4.47080320
C	0.59212870	0.94602710	8.88558557	H	2.92714342	5.52669384	5.98122059
C	-0.52469035	0.38254594	9.51203671	H	2.17582921	4.74859056	4.57435631
C	-0.84278621	-0.95641485	9.32727659	H	-0.88584536	4.00216541	8.30795633
C	-0.02229106	-1.73663431	8.50983374	H	-0.47526785	2.63875399	7.25280547
C	1.09583771	-1.18778067	7.90140003	H	0.07979887	4.77362647	6.16529384
C	1.45233490	0.16666332	8.07403511	H	1.07179507	5.28176521	7.55146623
N	1.93862656	3.76165435	6.45116861	N	4.42661743	2.04094933	9.95795163
C	4.02814220	3.86154608	5.19220302	H	3.98530001	2.22227562	10.85455833
C	2.72107492	4.55552024	5.51684109	H	4.50854888	1.03413141	9.84620421
C	-0.05553133	3.46275388	7.83870840	H	5.36226524	2.43202984	10.01593040
C	0.74655215	4.41071671	6.96946651				

TABLE S-LXXXIX. *Meso*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) OPBE Singlet

Fe	-0.10851679	0.39757510	0.00000000	C	-0.58449056	0.07133521	-3.14267573
N	-1.62178592	1.77743547	0.00000000	C	-1.15628192	-0.32702942	-4.35146844
H	-2.23163730	1.62858532	0.80117594	H	-1.89387933	-1.12953413	-4.36334106
H	-2.23163730	1.62858532	-0.80117594	C	-0.78363530	0.30390755	-5.53266614
N	-1.37149990	3.20601507	0.00000000	H	-1.22607246	0.00025453	-6.47996591
H	-0.72777059	3.31416091	0.79155867	C	0.16038198	1.33518246	-5.48415117
H	-0.72777059	3.31416091	-0.79155867	H	0.45863633	1.83894280	-6.40383688
S	1.00057046	1.62331789	1.53575969	C	0.71361616	1.74213511	-4.27947863
S	-1.02856711	-0.73689466	1.61147860	H	1.43920442	2.55389354	-4.25655415
S	1.00057046	1.62331789	-1.53575969	C	0.34695242	1.12085351	-3.06906823
S	-1.02856711	-0.73689466	-1.61147860	C	0.08705124	-2.18710703	1.71317589
N	1.39705492	-0.97305959	0.00000000	H	-0.35917906	-2.97020416	1.09118783
H	2.19988984	-0.34459705	0.00000000	H	0.10399285	-2.54293798	2.74757665
C	-0.58449056	0.07133521	3.14267573	C	1.45979630	-1.76026049	1.24989655
C	-1.15628192	-0.32702942	4.35146844	H	2.12305383	-2.63195618	1.13125395
H	-1.89387933	-1.12953413	4.36334106	H	1.89499166	-1.10284402	2.00897327
C	-0.78363530	0.30390755	5.53266614	C	0.08705124	-2.18710703	-1.71317589
H	-1.22607246	0.00025453	6.47996591	H	0.10399285	-2.54293798	-2.74757665

C	0.16038198	1.33518246	5.48415117	H	-0.35917906	-2.97020416	-1.09118783
H	0.45863633	1.83894280	6.40383688	C	1.45979630	-1.76026049	-1.24989655
C	0.71361616	1.74213511	4.27947863	H	1.89499166	-1.10284402	-2.00897327
H	1.43920442	2.55389354	4.25655415	H	2.12305383	-2.63195618	-1.13125395
C	0.34695242	1.12085351	3.06906823				

TABLE S-XC. *Meso*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) OPBE Triplet

Fe	-0.14068600	0.47052536	0.00000000	C	-0.44521005	0.08247069	-3.21075120
N	-2.21293194	1.80878446	0.00000000	C	-0.89153878	-0.34879554	-4.46070120
H	-2.82307331	1.64338429	0.79967520	H	-1.60101836	-1.17311293	-4.52985303
H	-2.82307331	1.64338429	-0.79967520	C	-0.43046611	0.27748203	-5.61285925
N	-1.97765021	3.24665482	0.00000000	H	-0.77184206	-0.05693153	-6.59113864
H	-1.33439822	3.36751679	0.78653572	C	0.46339999	1.34642960	-5.49681756
H	-1.33439822	3.36751679	-0.78653572	H	0.82687173	1.84837221	-6.39354439
S	0.93522659	1.73148383	1.50171560	C	0.88744771	1.78812485	-4.25231226
S	-1.02962811	-0.68750708	1.71167144	H	1.57570940	2.62821648	-4.17365694
S	0.93522659	1.73148383	-1.50171560	C	0.43491279	1.16678450	-3.07275977
S	-1.02962811	-0.68750708	-1.71167144	C	-0.09719346	-2.26121090	1.74033062
N	1.40933766	-1.34029273	0.00000000	H	-0.67143544	-2.95429286	1.11618828
H	2.23236333	-0.74977008	0.00000000	H	-0.11494206	-2.64807174	2.76423673
C	-0.44521005	0.08247069	3.21075120	C	1.33123110	-2.07917657	1.25139889
C	-0.89153878	-0.34879554	4.46070120	H	1.81568652	-3.06965191	1.18023248
H	-1.60101836	-1.17311293	4.52985303	H	1.87905285	-1.50351957	2.00440065
C	-0.43046611	0.27748203	5.61285925	C	-0.09719346	-2.26121090	-1.74033062
H	-0.77184206	-0.05693153	6.59113864	H	-0.11494206	-2.64807174	-2.76423673
C	0.46339999	1.34642960	5.49681756	H	-0.67143544	-2.95429286	-1.11618828
H	0.82687173	1.84837221	6.39354439	C	1.33123110	-2.07917657	-1.25139889
C	0.88744771	1.78812485	4.25231226	H	1.87905285	-1.50351957	-2.00440065
H	1.57570940	2.62821648	4.17365694	H	1.81568652	-3.06965191	-1.18023248
C	0.43491279	1.16678450	3.07275977				

TABLE S-XCI. *Meso*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) OPBE Quintet

Fe	-0.13679602	0.63619858	0.00000000	C	-0.46781333	0.00628133	-3.36075602
N	-2.03844791	1.86336327	0.00000000	C	-0.88239936	-0.45795317	-4.61334873
H	-2.64134643	1.68832731	0.80264335	H	-1.57284284	-1.29912009	-4.66640616
H	-2.64134643	1.68832731	-0.80264335	C	-0.42470231	0.14292760	-5.77874891
N	-1.80577503	3.30034250	0.00000000	H	-0.74781106	-0.22742980	-6.75034585
H	-1.16604948	3.42385776	0.79046910	C	0.44009502	1.23473615	-5.67875981
H	-1.16604948	3.42385776	-0.79046910	H	0.80400704	1.72590577	-6.58146846
S	0.95058067	1.76898292	1.71189157	C	0.83858348	1.70906735	-4.43840009

S	-1.11774406	-0.79035585	1.91029282	H	1.50890765	2.56432839	-4.37167719
S	0.95058067	1.76898292	-1.71189157	C	0.39936213	1.11556332	-3.23690103
S	-1.11774406	-0.79035585	-1.91029282	C	-0.04045454	-2.24488472	1.76348900
N	1.35765768	-1.16517951	0.00000000	H	-0.58015871	-2.93400473	1.10491416
H	2.16434341	-0.54767041	0.00000000	H	0.02375688	-2.72362926	2.74662783
C	-0.46781333	0.00628133	3.36075602	C	1.35274374	-1.91798918	1.25196669
C	-0.88239936	-0.45795317	4.61334873	H	1.92913259	-2.85626119	1.16331892
H	-1.57284284	-1.29912009	4.66640616	H	1.85275115	-1.29766644	2.00284275
C	-0.42470231	0.14292760	5.77874891	C	-0.04045454	-2.24488472	-1.76348900
H	-0.74781106	-0.22742980	6.75034585	H	0.02375688	-2.72362926	-2.74662783
C	0.44009502	1.23473615	5.67875981	H	-0.58015871	-2.93400473	-1.10491416
H	0.80400704	1.72590577	6.58146846	C	1.35274374	-1.91798918	-1.25196669
C	0.83858348	1.70906735	4.43840009	H	1.85275115	-1.29766644	-2.00284275
H	1.50890765	2.56432839	4.37167719	H	1.92913259	-2.85626119	-1.16331892
C	0.39936213	1.11556332	3.23690103				

TABLE S-XCII. *trans*-(Fe(NH)<sub>4</sub>)<sub>2</sub>N<sub>2</sub>H<sub>4</sub> (**7t**) OPBE Singlet

Fe	3.08413602	3.02136555	8.06214503	H	7.17194031	4.98400141	6.02875658
S	3.27537116	5.06593604	8.99073309	H	7.92882358	7.27221040	6.64620959
S	4.86837724	3.42018527	6.88543157	H	6.60923068	8.59066398	8.30464474
S	1.19814249	2.74114397	9.09736760	H	4.58189338	7.63673468	9.33639961
S	2.88470658	0.93981086	7.18222328	H	-0.82729507	1.09406020	10.37978527
C	5.44128411	5.05397769	7.31334229	H	-1.44552121	-1.30060232	10.07005677
C	6.60246145	5.57835583	6.74335330	H	-0.16788042	-2.68967619	8.43935474
C	7.02737967	6.85425192	7.09128099	H	1.71141743	-1.72051399	7.16834508
C	6.28462013	7.58867374	8.02329442	H	3.92543207	2.78858047	4.80501673
C	5.14551213	7.05705222	8.60680759	H	4.76201790	4.35716873	4.65090074
C	4.69348733	5.76613015	8.26712501	H	2.97582614	5.47291039	5.96448324
C	0.77033390	1.01514506	8.93883033	H	2.21356589	4.62099428	4.59833703
C	-0.28199432	0.46934741	9.67310768	H	-0.78986054	3.95927771	8.39010792
C	-0.62764973	-0.86612927	9.49752667	H	-0.41919464	2.58200396	7.32308868
C	0.09351144	-1.64122842	8.58463401	H	0.12877793	4.61628778	6.06545661
C	1.15094358	-1.10083949	7.86681142	H	1.03893105	5.28572187	7.44761414
C	1.52593446	0.24567424	8.03615819	N	4.16820165	2.12261408	9.55909168
N	2.00498274	3.70667707	6.51067195	H	3.78511966	1.18196713	9.62461229
C	4.08140177	3.76885116	5.27339045	H	5.10979107	2.00716930	9.18659641
C	2.78006443	4.48502113	5.53431294	N	4.19329259	2.67932866	10.87923493
C	0.01099683	3.43465086	7.85812392	H	5.12071964	2.52982973	11.27477111
C	0.76055206	4.36033110	6.93226164	H	4.09734112	3.68903642	10.72716156
H	1.77213417	2.80312862	6.08048842				

TABLE S-XCIII. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (7t) OPBE Triplet

Fe	3.08770850	3.02145286	8.07762770	H	7.17450417	5.05305481	5.94905878
S	3.30278254	5.12803076	8.98753369	H	7.94914717	7.32656484	6.59594569
S	4.92080653	3.46151613	6.81474461	H	6.67528841	8.61541413	8.31141926
S	1.09481322	2.71732147	9.10230112	H	4.66289136	7.63899585	9.36746337
S	2.85975905	0.88016041	7.17084226	H	-0.93186103	1.06342031	10.31159073
C	5.46899395	5.09404805	7.26801455	H	-1.50890976	-1.34184057	10.03080716
C	6.61991424	5.63371730	6.68580157	H	-0.16247329	-2.75098508	8.47081698
C	7.05578696	6.90342942	7.05265423	H	1.73565057	-1.77047361	7.22610689
C	6.34193638	7.62008464	8.01734330	H	3.92020803	2.85372114	4.76182634
C	5.20924729	7.07537234	8.61324292	H	4.71957789	4.43751901	4.61332756
C	4.73741487	5.80037585	8.24778676	H	2.93091169	5.51224307	5.94898681
C	0.70053807	0.99316568	8.90805074	H	2.18899090	4.65780121	4.57423195
C	-0.36054433	0.43597696	9.62849646	H	-0.85276702	3.93249394	8.31726350
C	-0.68056586	-0.90908524	9.47181818	H	-0.43491596	2.56420826	7.26053093
C	0.08080431	-1.69660523	8.60321712	H	0.09114814	4.61469972	6.03034252
C	1.14813153	-1.14851519	7.89906213	H	0.97569331	5.29123696	7.42294971
C	1.48880050	0.21142272	8.03199092	N	4.17312671	2.15957606	9.58163622
N	1.97662943	3.73647187	6.47950870	H	3.80957347	1.21092847	9.65438592
C	4.06485228	3.82897311	5.24408779	H	5.13134446	2.05293890	9.25064908
C	2.75072790	4.52332616	5.51400576	N	4.14894278	2.72977512	10.90109418
C	-0.02860944	3.41804581	7.81121129	H	5.07360011	2.59988698	11.31030854
C	0.72038328	4.36282987	6.90048402	H	4.04922620	3.73561460	10.72426431
H	1.76434627	2.82655529	6.05725013				

TABLE S-XCIV. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (7t) OPBE Quintet

Fe	3.18390922	2.95616456	8.22802675	H	7.08478746	5.27274063	5.72145912
S	3.48144971	5.12268977	9.10862955	H	7.78034174	7.57964121	6.32864080
S	5.05962719	3.53849766	6.70215209	H	6.57892576	8.76623070	8.17163180
S	0.85958864	2.66909913	9.13320401	H	4.72433043	7.65917020	9.36183928
S	2.89905099	0.76626665	7.34776421	H	-1.24961080	1.01890645	10.03178032
C	5.49651592	5.19499443	7.17044961	H	-1.81930027	-1.37386532	9.67013424
C	6.56264456	5.81300837	6.51055130	H	-0.31011903	-2.78327389	8.26027270
C	6.95482576	7.10024526	6.85231672	H	1.72855484	-1.81135785	7.26997145
C	6.28183401	7.75747070	7.88412028	H	3.89484880	2.81765189	4.79671817
C	5.23839490	7.13892229	8.55549327	H	4.64618577	4.39627334	4.49634658
C	4.81041063	5.83648161	8.22610055	H	2.93183405	5.49646354	5.95245610
C	0.53568190	0.94698544	8.83726005	H	2.21243028	4.69460496	4.54310733
C	-0.60740923	0.38835048	9.41857131	H	-0.92892727	4.00205482	8.21897412
C	-0.92527912	-0.94832373	9.21714687	H	-0.50464353	2.62741161	7.18460722

C	-0.07814149	-1.73170556	8.43115726	H	0.08355550	4.74084023	6.08149915
C	1.06812840	-1.18870514	7.87116972	H	1.03770388	5.27189447	7.48458352
C	1.42333651	0.16297918	8.06188520	N	4.37897719	1.97166627	9.97167796
N	1.93616430	3.73702062	6.42973852	H	3.89751850	1.10373039	10.19139499
C	4.05217954	3.82069995	5.21374371	H	5.24535676	1.70254366	9.50631842
C	2.73761330	4.51740360	5.49988149	N	4.60523962	2.68877606	11.18290858
C	-0.09211388	3.45450030	7.77115734	H	5.54728360	2.50194156	11.52152699
C	0.72957508	4.39136046	6.90802109	H	4.56976834	3.67597050	10.92015091
H	1.70847679	2.83150680	6.01777721				

TABLE S-XCV. *Meso*-(Fe(NH)S<sub>4</sub>)CO (4m) OPBE–Cosmo Singlet

Fe	-0.07297936	-0.17890901	0.00000000	C	1.59087615	1.98085967	-1.25071678
S	0.98678592	-1.45466010	1.53312650	H	-1.78328023	1.43790847	4.35342480
S	-0.94179792	1.03409754	1.62274055	H	-1.23758630	0.22700487	6.45647150
S	-0.94179792	1.03409754	-1.62274055	H	0.30023506	-1.73703014	6.37671391
S	0.98678592	-1.45466010	-1.53312650	H	1.26689849	-2.48522168	4.23659834
C	-0.54568811	0.16532026	3.12909228	H	-1.78328023	1.43790847	-4.35342480
C	-1.10876022	0.58310147	4.33651018	H	-1.23758630	0.22700487	-6.45647150
C	-0.80332863	-0.09539372	5.51201023	H	0.30023506	-1.73703014	-6.37671391
C	0.05985524	-1.19484942	5.46279940	H	1.26689849	-2.48522168	-4.23659834
C	0.60581111	-1.62038519	4.25864545	H	2.33800245	0.58431117	0.00000000
C	0.31347243	-0.94313673	3.05884241	H	0.24248489	2.80369484	2.73528439
C	-0.54568811	0.16532026	-3.12909228	H	-0.20866147	3.21347329	1.07791606
C	-1.10876022	0.58310147	-4.33651018	H	2.02774424	1.32731413	2.01040787
C	-0.80332863	-0.09539372	-5.51201023	H	2.25597363	2.84748425	1.13281609
C	0.05985524	-1.19484942	-5.46279940	H	-0.20866147	3.21347329	-1.07791606
C	0.60581111	-1.62038519	-4.25864545	H	0.24248489	2.80369484	-2.73528439
C	0.31347243	-0.94313673	-3.05884241	H	2.25597363	2.84748425	-1.13281609
N	1.52598102	1.19750959	0.00000000	H	2.02774424	1.32731413	-2.01040787
C	0.22602748	2.43169858	1.70709141	C	-1.34964911	-1.29536399	0.00000000
C	1.59087615	1.98085967	1.25071678	O	-2.21274038	-2.08690573	0.00000000
C	0.22602748	2.43169858	-1.70709141				

TABLE S-XCVI. *Meso*-(Fe(NH)S<sub>4</sub>)CO (4m) OPBE–Cosmo Triplet

Fe	0.12338032	-0.23377622	0.00000000	C	1.70704378	1.96919660	-1.25827131
S	1.18028487	-1.40632293	1.81559021	H	-2.04199710	1.41801087	4.26070872
S	-0.90472852	1.14005311	1.70221663	H	-1.81073765	0.13859840	6.37662447
S	-0.90472852	1.14005311	-1.70221663	H	-0.28273570	-1.83960427	6.44612132
S	1.18028487	-1.40632293	-1.81559021	H	0.98116130	-2.50769690	4.44445229
C	-0.63712200	0.19944108	3.17666425	H	-2.04199710	1.41801087	-4.26070872



C	-1.37203701	0.56155443	4.31222888	H	-1.81073765	0.13859840	-6.37662447
C	-1.24342101	-0.15539607	5.49550731	H	-0.28273570	-1.83960427	-6.44612132
C	-0.38727255	-1.25959743	5.52985356	H	0.98116130	-2.50769690	-4.44445229
C	0.32909374	-1.63735325	4.40225411	H	2.47643840	0.60823474	0.00000000
C	0.23303696	-0.91896021	3.19151614	H	0.42655867	2.83490888	2.76389965
C	-0.63712200	0.19944108	-3.17666425	H	-0.05960600	3.24806243	1.12186529
C	-1.37203701	0.56155443	-4.31222888	H	2.13960173	1.30333340	2.00879176
C	-1.24342101	-0.15539607	-5.49550731	H	2.38449438	2.82649867	1.13873599
C	-0.38727255	-1.25959743	-5.52985356	H	-0.05960600	3.24806243	-1.12186529
C	0.32909374	-1.63735325	-4.40225411	H	0.42655867	2.83490888	-2.76389965
C	0.23303696	-0.91896021	-3.19151614	H	2.38449438	2.82649867	-1.13873599
N	1.64135119	1.19053345	0.00000000	H	2.13960173	1.30333340	-2.00879176
C	0.36040992	2.45006050	1.74200017	C	-1.10726106	-1.42304176	0.00000000
C	1.70704378	1.96919660	1.25827131	O	-1.94728231	-2.23723811	0.00000000
C	0.36040992	2.45006050	-1.74200017				

TABLE S-XCVII. *Meso*-(Fe(NH)S<sub>4</sub>)CO (4m) OPBE–Cosmo Quintet

Fe	0.06763785	-0.27923625	0.00000000	C	1.49904167	2.18733087	-1.25411039
S	0.86282509	-1.62284268	1.71015428	H	-1.49453784	1.63344475	4.59248856
S	-0.99828600	1.07999732	1.84382869	H	-0.89353272	0.45908349	6.69255758
S	-0.99828600	1.07999732	-1.84382869	H	0.45186075	-1.64513004	6.57637777
S	0.86282509	-1.62284268	-1.71015428	H	1.18918087	-2.52595192	4.39580132
C	-0.46248504	0.23912620	3.31731110	H	-1.49453784	1.63344475	-4.59248856
C	-0.89022642	0.72830876	4.55589331	H	-0.89353272	0.45908349	-6.69255758
C	-0.55729773	0.06781406	5.73399004	H	0.45186075	-1.64513004	-6.57637777
C	0.19448534	-1.10655937	5.66501337	H	1.18918087	-2.52595192	-4.39580132
C	0.61036680	-1.60464640	4.43648341	H	2.40385274	0.90703415	0.00000000
C	0.30099496	-0.94554502	3.23086312	H	0.15681850	2.98140631	2.74004698
C	-0.46248504	0.23912620	-3.31731110	H	-0.42129706	3.21951491	1.09600228
C	-0.89022642	0.72830876	-4.55589331	H	2.00837953	1.58021640	2.00829328
C	-0.55729773	0.06781406	-5.73399004	H	2.06823318	3.12396402	1.15191303
C	0.19448534	-1.10655937	-5.66501337	H	-0.42129706	3.21951491	-1.09600228
C	0.61036680	-1.60464640	-4.43648341	H	0.15681850	2.98140631	-2.74004698
C	0.30099496	-0.94554502	-3.23086312	H	2.06823318	3.12396402	-1.15191303
N	1.52489727	1.41793255	0.00000000	H	2.00837953	1.58021640	-2.00829328
C	0.10630271	2.51889270	1.74986639	C	-1.75659435	-1.60193701	0.00000000
C	1.49904167	2.18733087	1.25411039	O	-2.40094756	-2.54733492	0.00000000
C	0.10630271	2.51889270	-1.74986639				

TABLE S-XCVIII. *trans*-(Fe(NH)S<sub>4</sub>)CO (4t) OPBE–Cosmo Singlet

Fe	8.38152837	10.14917194	1.96545532	H	9.08796941	5.19419167	6.24122230
S	9.77430966	8.98290286	3.19916804	C	9.38768324	6.86695006	4.91803735
S	6.73732121	8.65898129	2.43061958	H	10.43116732	7.00916697	5.19552149
S	7.07157708	11.13393852	0.50700790	C	8.80337418	7.70028516	3.96188867
S	9.99694670	11.68005209	1.49642700	C	7.85706344	11.11553585	3.26192952
C	9.15274812	12.90731520	0.58260245	O	7.49575445	11.78364330	4.15379851
C	9.76337262	14.13079152	0.24663047	N	9.05534828	9.01371632	0.35509328
H	10.79042787	14.31866108	0.55533236	H	9.78436297	9.63256001	-0.00945163
C	9.06403578	15.10024106	-0.46275492	C	10.64179363	8.04371484	1.89545258
H	9.55752267	16.04120817	-0.70372583	H	11.06184024	7.13648596	2.33722509
C	7.73878757	14.88937293	-0.85602358	H	11.46835155	8.69562100	1.58895312
H	7.19332595	15.65767744	-1.40078827	C	9.69687251	7.75734687	0.75873487
C	7.11813092	13.68446385	-0.54031378	H	8.91568147	7.05769941	1.07055891
H	6.08882772	13.49608733	-0.84076369	H	10.24378090	7.30805105	-0.08240242
C	7.82725754	12.70678295	0.15880662	C	7.49777538	10.22753939	-1.04053075
C	7.45394574	7.57345937	3.59069941	H	8.24803547	10.82965367	-1.56076649
C	6.71061364	6.53885381	4.19411652	H	6.59670135	10.16459058	-1.65687831
H	5.66458368	6.40554719	3.92288090	C	8.02902012	8.86486723	-0.68123686
C	7.29705898	5.69374452	5.12708512	H	7.23742652	8.22351763	-0.28242137
H	6.69860184	4.90222342	5.57695563	H	8.43959234	8.38582053	-1.58136789
C	8.63640342	5.85192248	5.50100335				

TABLE S-XCIX. *trans*-(Fe(NH)S<sub>4</sub>)CO (4t) OPBE–Cosmo Triplet

Fe	8.31802975	10.20153138	2.00255382	H	9.16762329	4.71708917	5.89432810
S	9.94841162	8.81377199	3.33304512	C	9.48853701	6.52760192	4.77381326
S	6.73218396	8.82886148	2.85864407	H	10.55855616	6.55486248	4.97317021
S	6.98851371	11.19068167	0.20246269	C	8.91032144	7.53437486	3.99498871
S	9.95656095	11.70970189	1.46747942	C	7.71566411	11.36757716	3.12439107
C	9.09686065	12.95382935	0.58722058	O	7.30838549	12.16514040	3.87960902
C	9.69575277	14.21465341	0.40322936	N	9.01512869	8.94138837	0.42276711
H	10.66674645	14.40829471	0.85550392	H	9.75792845	9.54417312	0.06224659
C	9.06539048	15.21083699	-0.33195765	C	10.66707613	7.94239010	1.90817347
H	9.55480852	16.17669766	-0.45175862	H	11.12532510	7.01259287	2.25490046
C	7.81172883	14.98564297	-0.90433640	H	11.46886539	8.60130203	1.55413272
H	7.31324651	15.76708536	-1.47500220	C	9.64198254	7.68247835	0.83101043
C	7.19695081	13.74990826	-0.73185954	H	8.86305903	7.00409745	1.19215538
H	6.21810255	13.55953357	-1.16816195	H	10.13706860	7.19985705	-0.02487239
C	7.83193917	12.73411443	-0.00969241	C	7.62567487	10.16018677	-1.17031359

C	7.52382836	7.54212413	3.74005704	H	8.47932033	10.68676787	-1.60778389
C	6.75064960	6.49389015	4.27695605	H	6.84124845	10.07075687	-1.92755617
H	5.67802848	6.47841595	4.09165352	C	8.02621442	8.79867403	-0.65156642
C	7.33661127	5.48480947	5.03025785	H	7.16105249	8.25523440	-0.25830888
H	6.71313887	4.68405157	5.42619515	H	8.43749998	8.21627531	-1.48888570
C	8.70894885	5.49756052	5.29008917				

TABLE S-C. *trans*-(Fe(NH)<sub>4</sub>)CO (**4t**) OPBE–Cosmo Quintet

Fe	8.45703085	10.13760201	1.94495923	H	8.94507462	5.07560358	6.39459004
S	9.94572552	8.60704149	3.19406783	C	9.34495006	6.63003476	4.95984341
S	6.67137938	8.63772266	2.61107220	H	10.41973180	6.62117686	5.13254940
S	7.12394340	11.13380993	0.13792105	C	8.81290096	7.51846092	4.01892022
S	10.05531177	11.92714294	1.41207932	C	7.88689634	11.31623056	3.39868004
C	9.04696029	13.09166097	0.58660991	O	7.51748564	12.05954097	4.20525253
C	9.48676268	14.42460449	0.46127852	N	9.20065718	8.84235073	0.20656011
H	10.44452534	14.70233311	0.89728141	H	10.03416532	9.34132413	-0.10453420
C	8.72525598	15.38283918	-0.19698623	C	10.56919474	7.60609637	1.80671008
H	9.09943615	16.40331517	-0.27066464	H	10.84324876	6.61804836	2.18639635
C	7.48736170	15.04962050	-0.74925783	H	11.49467971	8.11853786	1.51556417
H	6.88506644	15.79917837	-1.25931591	C	9.60577305	7.50844677	0.64499616
C	7.02610699	13.74189493	-0.63920537	H	8.70741318	6.95591534	0.93828153
H	6.06188678	13.46382445	-1.06043734	H	10.09494980	6.94369822	-0.16486729
C	7.79107293	12.76965186	0.01322096	C	7.88471349	10.26508504	-1.28431689
C	7.41894384	7.57609414	3.78007872	H	8.77093668	10.83513594	-1.57893791
C	6.60348329	6.70187586	4.52769769	H	7.16783971	10.27063611	-2.11067055
H	5.52719974	6.72850724	4.36822219	C	8.24493661	8.84685033	-0.89926053
C	7.14065852	5.81037889	5.44697806	H	7.35343117	8.29182118	-0.58646280
H	6.47590818	5.14701605	5.99893427	H	8.64770135	8.34368373	-1.79213019
C	8.51838736	5.76669531	5.67009506				

TABLE S-CI. *Meso*-(Fe(NH)<sub>4</sub>)PMe<sub>3</sub> (**5m**) OPBE–Cosmo Singlet

Fe	0.18277200	0.06165762	0.00000000	H	-1.60678851	-1.38997136	4.39287497
S	1.42724184	1.14557720	-1.52741192	H	-0.75943920	-0.39474665	6.50956756
S	-0.81702692	-1.00155684	-1.61732125	H	1.08908012	1.28232400	6.42305449
S	-0.81702692	-1.00155684	1.61732125	H	2.06159518	1.96206911	4.26248464
S	1.42724184	1.14557720	1.52741192	H	2.46119439	-1.03757476	0.00000000
C	-0.23534946	-0.28302198	-3.15030964	H	0.06384153	-2.96065780	-2.71336587
C	-0.79991703	-0.65807583	-4.37028386	H	-0.43503715	-3.27779849	-1.04826467
C	-0.32446503	-0.10265721	-5.55530170	H	2.04031697	-1.73993638	-2.01098943
C	0.71124491	0.83788073	-5.50245911	H	2.06491260	-3.27179339	-1.12218386

C	1.26178187	1.22280638	-4.28685431	H	-0.43503715	-3.27779849	1.04826467
C	0.79138828	0.67281924	-3.07663229	H	0.06384153	-2.96065780	2.71336587
C	-0.23534946	-0.28302198	3.15030964	H	2.06491260	-3.27179339	1.12218386
C	-0.79991703	-0.65807583	4.37028386	H	2.04031697	-1.73993638	2.01098943
C	-0.32446503	-0.10265721	5.55530170	P	-1.25959214	1.72591530	0.00000000
C	0.71124491	0.83788073	5.50245911	C	-2.46370427	1.81940610	-1.39152396
C	1.26178187	1.22280638	4.28685431	H	-1.93646381	1.90982503	-2.34679526
C	0.79138828	0.67281924	3.07663229	H	-3.08565106	0.91766796	-1.41326521
N	1.57058537	-1.52844805	0.00000000	H	-3.11058218	2.69436047	-1.25715263
C	0.10587831	-2.57702123	-1.69021277	C	-2.46370427	1.81940610	1.39152396
C	1.52322295	-2.32277009	-1.24356865	H	-3.08565106	0.91766796	1.41326521
C	0.10587831	-2.57702123	1.69021277	H	-1.93646381	1.90982503	2.34679526
C	1.52322295	-2.32277009	1.24356865	H	-3.11058218	2.69436047	1.25715263
H	-1.60678851	-1.38997136	-4.39287497	C	-0.59931916	3.45476753	0.00000000
H	-0.75943920	-0.39474665	-6.50956756	H	-0.95338796	3.98609853	-0.88971312
H	1.08908012	1.28232400	-6.42305449	H	-0.95338796	3.98609853	0.88971312
H	2.06159518	1.96206911	-4.26248464	H	0.49297041	3.44600912	0.00000000

TABLE S-CII. *Meso*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5m**) OPBE–Cosmo Triplet

Fe	0.24733374	0.10851891	0.00000000	H	-1.57834735	-1.54971462	4.47431693
S	1.40388978	1.20243676	-1.68783835	H	-0.81311471	-0.53960945	6.61090923
S	-0.86026440	-1.10544916	-1.74297280	H	0.93816776	1.24594466	6.56038392
S	-0.86026440	-1.10544916	1.74297280	H	1.88589034	1.99644976	4.41517714
S	1.40388978	1.20243676	1.68783835	H	2.50891347	-1.01119369	0.00000000
C	-0.26311063	-0.36417555	-3.24978332	H	0.17177517	-3.05603195	-2.69271631
C	-0.81242149	-0.77478323	-4.46802396	H	-0.35796354	-3.29454907	-1.02912698
C	-0.38495846	-0.20985053	-5.66582089	H	2.06772200	-1.69216861	-2.01463864
C	0.59437876	0.78781422	-5.63314896	H	2.14374572	-3.22379066	-1.12918593
C	1.13059672	1.21137298	-4.42421549	H	-0.35796354	-3.29454907	1.02912698
C	0.72048488	0.64891895	-3.19660312	H	0.17177517	-3.05603195	2.69271631
C	-0.26311063	-0.36417555	3.24978332	H	2.14374572	-3.22379066	1.12918593
C	-0.81242149	-0.77478323	4.46802396	H	2.06772200	-1.69216861	2.01463864
C	-0.38495846	-0.20985053	5.66582089	P	-1.17751939	1.86958904	0.00000000
C	0.59437876	0.78781422	5.63314896	C	-2.36366914	1.94145025	-1.40030725
C	1.13059672	1.21137298	4.42421549	H	-1.82676802	1.99981850	-2.35221933
C	0.72048488	0.64891895	3.19660312	H	-2.99960207	1.04981834	-1.39847576
N	1.61660474	-1.49948723	0.00000000	H	-2.99520990	2.83082628	-1.28828942
C	0.16623733	-2.60469138	-1.69584692	C	-2.36366914	1.94145025	1.40030725
C	1.57260418	-2.29052573	-1.24484397	H	-2.99960207	1.04981834	1.39847576
C	0.16623733	-2.60469138	1.69584692	H	-1.82676802	1.99981850	2.35221933

C	1.57260418	-2.29052573	1.24484397	H	-2.99520990	2.83082628	1.28828942
H	-1.57834735	-1.54971462	-4.47431693	C	-0.47154191	3.57337573	0.00000000
H	-0.81311471	-0.53960945	-6.61090923	H	-0.81240191	4.11146486	-0.89098420
H	0.93816776	1.24594466	-6.56038392	H	-0.81240191	4.11146486	0.89098420
H	1.88589034	1.99644976	-4.41517714	H	0.62015128	3.53355409	0.00000000

TABLE S-CIII. *Meso*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5m**) OPBE–Cosmo Quintet

Fe	0.27937119	0.21836870	0.00000000	H	-1.28024275	-1.52124383	4.67689869
S	1.53049385	1.23783925	-1.69335026	H	-0.25795380	-0.62330095	6.75025907
S	-0.85970189	-0.99166758	-1.90794222	H	1.53764515	1.10972491	6.57857915
S	-0.85970189	-0.99166758	1.90794222	H	2.28716228	1.90143440	4.36863336
S	1.53049385	1.23783925	1.69335026	H	2.40575090	-1.45076853	0.00000000
C	-0.05484023	-0.34061711	-3.35704860	H	-0.15193049	-3.12812759	-2.73633322
C	-0.48752518	-0.77704493	-4.61400385	H	-0.78744115	-3.18461884	-1.09557153
C	0.08312845	-0.27224000	-5.77780909	H	1.94326533	-2.11372973	-1.99766951
C	1.08499963	0.69560138	-5.67805971	H	1.67466554	-3.62645909	-1.12791590
C	1.50789163	1.14331549	-4.43257808	H	-0.78744115	-3.18461884	1.09557153
C	0.95460401	0.64037803	-3.23730214	H	-0.15193049	-3.12812759	2.73633322
C	-0.05484023	-0.34061711	3.35704860	H	1.67466554	-3.62645909	1.12791590
C	-0.48752518	-0.77704493	4.61400385	H	1.94326533	-2.11372973	1.99766951
C	0.08312845	-0.27224000	5.77780909	P	-1.76372343	1.95962167	0.00000000
C	1.08499963	0.69560138	5.67805971	C	-2.94509946	1.93841912	-1.40842959
C	1.50789163	1.14331549	4.43257808	H	-2.40468884	2.06619691	-2.35236062
C	0.95460401	0.64037803	3.23730214	H	-3.46795569	0.97588064	-1.43220023
N	1.46537753	-1.83263130	0.00000000	H	-3.68069500	2.74482387	-1.30440869
C	-0.11255124	-2.63625627	-1.75964929	C	-2.94509946	1.93841912	1.40842959
C	1.31152189	-2.59282829	-1.24380413	H	-3.46795569	0.97588064	1.43220023
C	-0.11255124	-2.63625627	1.75964929	H	-2.40468884	2.06619691	2.35236062
C	1.31152189	-2.59282829	1.24380413	H	-3.68069500	2.74482387	1.30440869
H	-1.28024275	-1.52124383	-4.67689869	C	-1.17637743	3.71159842	0.00000000
H	-0.25795380	-0.62330095	-6.75025907	H	-1.54587491	4.23222734	-0.88957818
H	1.53764515	1.10972491	-6.57857915	H	-1.54587491	4.23222734	0.88957818
H	2.28716228	1.90143440	-4.36863336	H	-0.08249344	3.73969350	0.00000000

TABLE S-CIV. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) OPBE–Cosmo Singlet

Fe	3.11637033	3.00174313	8.07393616	H	1.71335104	2.86372470	6.05791531
S	3.32314898	5.05144611	8.98312617	H	5.27614059	0.20702366	10.74993258
S	4.84969040	3.40914240	6.82362314	H	5.29516028	0.13529528	8.96352439
S	1.22115111	2.73105309	9.08927648	H	3.78575044	-0.18266828	9.84090026
S	2.84811344	0.96472346	7.13304525	H	6.41146127	2.45997040	10.94777449

P	4.29565135	2.21006750	9.76626775	H	5.92574482	3.98590221	10.15388797
C	4.70148426	0.41618626	9.83959955	H	6.63004534	2.66067833	9.19086264
C	5.98020563	2.89895679	10.04020800	H	4.29092368	2.10398969	12.20484352
C	3.58183305	2.45339643	11.44506934	H	2.64703562	1.89190497	11.54925588
C	5.43850169	5.03887921	7.25250384	H	3.37361344	3.51667122	11.60461840
C	6.58796675	5.55956051	6.65571679	H	7.13436449	4.96692327	5.92257134
C	7.02810940	6.83590746	6.99326731	H	7.91971539	7.24931660	6.52493804
C	6.31033867	7.57682282	7.94148097	H	6.64529041	8.57733189	8.21460152
C	5.17993193	7.04980249	8.55054282	H	4.63998910	7.63641876	9.29293987
C	4.71604775	5.75866028	8.22050344	H	-0.79538463	1.07830395	10.39214897
C	0.77864252	1.01113813	8.92113729	H	-1.42687247	-1.31017884	10.06670178
C	-0.26310269	0.46149283	9.66885892	H	-0.19633005	-2.68232010	8.38287248
C	-0.61956284	-0.87209469	9.48229378	H	1.65422819	-1.70805451	7.08067258
C	0.07413667	-1.63792000	8.53760814	H	3.84836058	2.82923081	4.76020918
C	1.11793298	-1.09133441	7.80098653	H	4.70586955	4.37921426	4.61089652
C	1.50682057	0.25111524	7.98710187	H	2.94296370	5.51130220	5.95974446
N	1.97284898	3.74615211	6.50738841	H	2.16436617	4.67034482	4.60239847
C	4.02516081	3.79922118	5.23974272	H	-0.76754461	3.97874297	8.46158654
C	2.73862614	4.52621123	5.52934873	H	-0.43765128	2.62712320	7.34998358
C	0.01242244	3.46229931	7.89436144	H	0.09174399	4.66542612	6.12508219
C	0.74561233	4.39840487	6.96849706	H	1.03101032	5.31855415	7.48661767

TABLE S-CV. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) OPBE–Cosmo Triplet

Fe	3.13494339	2.98880368	8.06544762	H	1.53191257	2.99180412	5.78059415
S	3.35987812	5.00564529	8.99368961	H	5.41922218	0.00719734	11.00616021
S	4.80514532	3.47533612	6.69335240	H	5.43710837	-0.03658308	9.21862169
S	1.14923540	2.77757676	9.01589759	H	3.92003499	-0.32569272	10.08879705
S	2.88861879	0.93852495	7.18769868	H	6.61061872	2.32015119	11.20447414
P	4.46995440	2.05137942	10.01908165	H	6.09750676	3.82893818	10.39483930
C	4.85149331	0.24986215	10.09924354	H	6.79601861	2.50393762	9.43802757
C	6.15757261	2.73981256	10.29750720	H	4.40476929	1.94320236	12.47965108
C	3.73502245	2.30782929	11.69061976	H	2.77947492	1.77522880	11.75895400
C	5.40623352	5.08959820	7.16775610	H	3.54487054	3.37589631	11.84528239
C	6.51313315	5.65721065	6.53699693	H	7.02065382	5.11613062	5.73940564
C	6.96093088	6.91770980	6.92487803	H	7.82068410	7.36674421	6.43051324
C	6.30215495	7.59143763	7.95717214	H	6.64766377	8.57606186	8.27092662
C	5.20866149	7.01762693	8.59536519	H	4.70585632	7.55223671	9.40017076
C	4.74000043	5.74827465	8.21067820	H	-0.96926751	1.17096236	10.20505147
C	0.70951662	1.05536359	8.85914312	H	-1.55499952	-1.23533412	9.95146921
C	-0.37973706	0.52779557	9.55288549	H	-0.18505963	-2.67874550	8.44619648

C	-0.70905571	-0.81834563	9.40760094	H	1.74545094	-1.74038036	7.22989845
C	0.06093635	-1.62369096	8.56377648	H	3.77091443	2.95137762	4.64355099
C	1.14988046	-1.09753108	7.87691765	H	4.62855146	4.49713929	4.51338556
C	1.50361640	0.25694783	8.01902079	H	2.83616833	5.60618791	5.88040015
N	1.80482462	3.84484049	6.26261588	H	2.16590502	4.86483704	4.41824637
C	3.94440836	3.91506866	5.13753372	H	-0.83646466	4.00703384	8.36178265
C	2.64083842	4.64631806	5.39008938	H	-0.48147245	2.66222512	7.25554714
C	-0.04373756	3.50583790	7.79762890	H	-0.11220092	4.78357711	6.09774118
C	0.63636157	4.47067567	6.84628198	H	0.96169551	5.36944036	7.38096162

TABLE S-CVI. *trans*-(Fe(NH)<sub>4</sub>)PMe<sub>3</sub> (**5t**) OPBE–Cosmo Quintet

Fe	3.17041044	2.97332049	8.05871966	H	1.67412896	2.97091379	5.83384843
S	3.47471805	5.13120899	9.03813785	H	5.41400502	-0.11664972	11.11434944
S	4.99127918	3.62310252	6.56930744	H	5.44054432	-0.17452160	9.32708609
S	0.84325612	2.73114887	9.01623520	H	3.90778295	-0.40358391	10.19152941
S	2.73248822	0.80225758	7.11748956	H	6.70360363	2.20962670	11.23115103
P	4.54237865	1.94468511	10.10858299	H	6.19265653	3.70692102	10.39555105
C	4.85980510	0.13718444	10.20244422	H	6.85068580	2.34634811	9.45688533
C	6.23810280	2.61542786	10.32502601	H	4.43418889	1.90442742	12.55680036
C	3.79009234	2.27634642	11.75091157	H	2.81419477	1.78213350	11.81529180
C	5.48780038	5.24117150	7.11712707	H	3.64227144	3.35497476	11.87151847
C	6.57345354	5.85324119	6.48346324	H	7.07811295	5.33440036	5.66946057
C	7.00458589	7.11560992	6.87722509	H	7.84571365	7.58891557	6.37365579
C	6.34671855	7.75589693	7.93023331	H	6.67141483	8.74380153	8.25607526
C	5.27969878	7.14300013	8.57422297	H	4.78102330	7.65476692	9.39605006
C	4.81660783	5.86607903	8.19227712	H	-1.11721806	1.08449744	10.20423760
C	0.55031365	0.98850045	8.84973911	H	-1.61677620	-1.34654443	10.07336148
C	-0.50872031	0.43409309	9.57784520	H	-0.19379582	-2.80575969	8.62143458
C	-0.78951552	-0.92613797	9.50418108	H	1.68574757	-1.84337783	7.35786515
C	0.00737938	-1.73697405	8.69188871	H	3.85079638	3.05111007	4.60226723
C	1.06762621	-1.19488805	7.97703745	H	4.60113744	4.64464374	4.43042062
C	1.38039801	0.18021343	8.03369117	H	2.85972836	5.64193172	5.92934111
N	1.89941559	3.83684409	6.32250075	H	2.14764840	4.89462231	4.48913813
C	3.99959255	4.01891176	5.09581815	H	-1.02092420	3.90238322	8.04313063
C	2.68206768	4.68362400	5.43001157	H	-0.44133806	2.57976449	7.01041689
C	-0.12794924	3.43018037	7.62309937	H	0.01299977	4.77087845	5.98194027
C	0.66095032	4.43098737	6.80660110	H	0.91479083	5.30960417	7.40968642

TABLE S-VII. *Meso*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6m**) OPBE–Cosmo Singlet

Fe	-0.24378984	-0.41994660	0.00000000	N	-2.01541706	-1.40756385	0.00000000
S	0.53677041	-1.87324460	1.53538133	H	-1.67521853	1.45691281	4.35650938
S	-0.92492616	0.87791299	1.60608205	H	-1.33738966	0.18534274	6.46877275
S	-0.92492616	0.87791299	-1.60608205	H	-0.15226440	-2.01171970	6.39974952
S	0.53677041	-1.87324460	-1.53538133	H	0.67531166	-2.92199241	4.26425579
C	-0.67764692	-0.01536149	3.13688282	H	-1.67521853	1.45691281	-4.35650938
C	-1.15709050	0.49838178	4.34344928	H	-1.33738966	0.18534274	-6.46877275
C	-0.96626601	-0.21203127	5.52560744	H	-0.15226440	-2.01171970	-6.39974952
C	-0.30143524	-1.44329337	5.48196673	H	0.67531166	-2.92199241	-4.26425579
C	0.16579388	-1.95927559	4.27955431	H	2.20993521	-0.10589948	0.00000000
C	-0.01824762	-1.25586514	3.07148392	H	0.53255075	2.43975583	2.73722382
C	-0.67764692	-0.01536149	-3.13688282	H	0.15560563	2.92553843	1.07855425
C	-1.15709050	0.49838178	-4.34344928	H	2.02649697	0.67836660	2.00930877
C	-0.96626601	-0.21203127	-5.52560744	H	2.52119409	2.12709516	1.11705878
C	-0.30143524	-1.44329337	-5.48196673	H	0.15560563	2.92553843	-1.07855425
C	0.16579388	-1.95927559	-4.27955431	H	0.53255075	2.43975583	-2.73722382
C	-0.01824762	-1.25586514	-3.07148392	H	2.52119409	2.12709516	-1.11705878
N	1.50015717	0.62389786	0.00000000	H	2.02649697	0.67836660	-2.00930877
C	0.44783636	2.08008940	1.70820162	H	-2.08320202	-2.01484502	0.81336607
C	1.71040194	1.39637229	1.24718081	H	-2.08320202	-2.01484502	-0.81336607
C	0.44783636	2.08008940	-1.70820162	H	-2.84389590	-0.81793763	0.00000000
C	1.71040194	1.39637229	-1.24718081				

TABLE S-CVIII. *Meso*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6m**) OPBE–Cosmo Triplet

Fe	-0.49286458	-0.57306403	0.00000000	N	-2.78787349	-1.32145507	0.00000000
S	0.22390971	-2.05458253	1.52297688	H	-1.54282156	1.41656886	4.49925071
S	-1.09909109	0.77756194	1.69731644	H	-1.09703206	0.13052792	6.57769384
S	-1.09909109	0.77756194	-1.69731644	H	-0.05956948	-2.13492275	6.42204534
S	0.22390971	-2.05458253	-1.52297688	H	0.52536929	-3.09252189	4.22430503
C	-0.73369738	-0.10685570	3.20395075	H	-1.54282156	1.41656886	-4.49925071
C	-1.07982057	0.43224044	4.44498094	H	-1.09703206	0.13052792	-6.57769384
C	-0.83135968	-0.28927104	5.60901107	H	-0.05956948	-2.13492275	-6.42204534
C	-0.25076016	-1.55824813	5.51763168	H	0.52536929	-3.09252189	-4.22430503
C	0.08008463	-2.10025476	4.28112438	H	2.16577801	0.19291686	0.00000000
C	-0.15911937	-1.38301162	3.09381309	H	0.19589030	2.50365081	2.75093639
C	-0.73369738	-0.10685570	-3.20395075	H	-0.27741535	2.90186727	1.10019231
C	-1.07982057	0.43224044	-4.44498094	H	1.92654015	0.96799484	2.00416464
C	-0.83135968	-0.28927104	-5.60901107	H	2.16887370	2.50403552	1.16420265



C	-0.25076016	-1.55824813	-5.51763168	H	-0.27741535	2.90186727	-1.10019231
C	0.08008463	-2.10025476	-4.28112438	H	0.19589030	2.50365081	-2.75093639
C	-0.15911937	-1.38301162	-3.09381309	H	2.16887370	2.50403552	-1.16420265
N	1.41998153	0.87901262	0.00000000	H	1.92654015	0.96799484	-2.00416464
C	0.14205075	2.11232688	1.73090385	H	-2.98055804	-1.90143598	0.81203995
C	1.49805158	1.63349714	1.24834553	H	-2.98055804	-1.90143598	-0.81203995
C	0.14205075	2.11232688	-1.73090385	H	-3.49846011	-0.59365750	0.00000000
C	1.49805158	1.63349714	-1.24834553				

TABLE S-CIX. *Meso*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6m**) OPBE–Cosmo Quintet

Fe	-0.37904649	-0.62655327	0.00000000	N	-2.56028494	-1.25695578	0.00000000
S	0.38634331	-2.04916640	1.71212388	H	-1.26510669	1.56108294	4.66330624
S	-1.01025070	0.92330582	1.90563818	H	-0.71773792	0.33580742	6.75002305
S	-1.01025070	0.92330582	-1.90563818	H	0.29537404	-1.94592550	6.59704320
S	0.38634331	-2.04916640	-1.71212388	H	0.75547196	-2.95338902	4.39662578
C	-0.53946181	0.00943576	3.35889808	H	-1.26510669	1.56108294	-4.66330624
C	-0.81050057	0.57278992	4.61104469	H	-0.71773792	0.33580742	-6.75002305
C	-0.50694545	-0.11433351	5.78141861	H	0.29537404	-1.94592550	-6.59704320
C	0.05898792	-1.38787052	5.69152515	H	0.75547196	-2.95338902	-4.39662578
C	0.31798208	-1.95768012	4.45112521	H	2.19809487	0.12154249	0.00000000
C	0.03168608	-1.27885049	3.24867681	H	0.45880990	2.62130808	2.74947798
C	-0.53946181	0.00943576	-3.35889808	H	-0.10662816	2.93017561	1.11140452
C	-0.81050057	0.57278992	-4.61104469	H	2.02112953	0.90436074	1.99727898
C	-0.50694545	-0.11433351	-5.78141861	H	2.33500943	2.40946255	1.12920181
C	0.05898792	-1.38787052	-5.69152515	H	-0.10662816	2.93017561	-1.11140452
C	0.31798208	-1.95768012	-4.45112521	H	0.45880990	2.62130808	-2.74947798
C	0.03168608	-1.27885049	-3.24867681	H	2.33500943	2.40946255	-1.12920181
N	1.46656288	0.82602822	0.00000000	H	2.02112953	0.90436074	-1.99727898
C	0.30897548	2.16021213	1.76858762	H	-2.78014592	-1.82594568	0.81280567
C	1.61194957	1.58685757	1.24639181	H	-2.78014592	-1.82594568	-0.81280567
C	0.30897548	2.16021213	-1.76858762				

TABLE S-CX. *trans*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6t**) OPBE–Cosmo Singlet

Fe	3.09295952	3.03425101	8.03928722	H	1.72124267	2.85833609	6.04096364
S	3.32040996	5.06688221	8.98791734	H	7.14639322	4.99312548	5.93674165
S	4.84982799	3.43765077	6.81828533	H	7.96218662	7.25119889	6.58784769
S	1.21923814	2.73710476	9.08743018	H	6.71282666	8.55345647	8.31573735
S	2.90870794	0.94291131	7.18938199	H	4.69606125	7.61595547	9.37506395
C	5.45734993	5.05362685	7.27610356	H	-0.81674698	1.09052900	10.36709137
C	6.61133628	5.57453147	6.68700810	H	-1.39647124	-1.31739364	10.10385744

C	7.06816018	6.83752516	7.05128366	H	-0.08600189	-2.72462517	8.51168057
C	6.36489420	7.56348596	8.02138145	H	1.78008612	-1.75650915	7.22670010
C	5.22874747	7.03727528	8.62122185	H	3.87227780	2.86960069	4.74129479
C	4.74487415	5.76096114	8.26266140	H	4.70196369	4.43780582	4.61652591
C	0.80015728	1.00651100	8.94466610	H	2.92074355	5.51890859	5.97888057
C	-0.25183175	0.46055460	9.68100460	H	2.14875279	4.68034045	4.61428061
C	-0.57860452	-0.88496640	9.53012823	H	-0.78301352	3.96359210	8.44692198
C	0.15949032	-1.67030353	8.63765175	H	-0.43837043	2.60093846	7.35295226
C	1.21310656	-1.12730312	7.91190314	H	0.08997072	4.62718936	6.10356108
C	1.56759023	0.22931261	8.05717023	H	1.01061900	5.30498869	7.46683703
N	1.97836142	3.73112453	6.51041636	N	4.18513691	2.25837609	9.57710699
C	4.03106114	3.83588998	5.23490392	H	3.79844329	2.48870631	10.48813008
C	2.73216118	4.53615288	5.53531890	H	4.23069114	1.24369036	9.51849109
C	0.00302107	3.44573871	7.88974914	H	5.14496231	2.59151593	9.59664898
C	0.73619933	4.37654244	6.95772512				

TABLE S-CXI. *trans*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6t**) OPBE–Cosmo Triplet

Fe	3.10842790	3.01849317	8.02252923	H	1.60661388	2.95958304	5.80933112
S	3.35831757	5.01440264	9.02743736	H	7.09073012	5.09754433	5.84907762
S	4.83342932	3.48227470	6.74130327	H	7.89808738	7.33971278	6.55980870
S	1.18537873	2.76138817	9.03490299	H	6.69656504	8.55908162	8.37416434
S	2.92351168	0.89766771	7.22331654	H	4.72233173	7.55380731	9.46196385
C	5.44500793	5.08735555	7.24202137	H	-0.89136838	1.16098948	10.29950855
C	6.57297834	5.64232278	6.63745964	H	-1.46452555	-1.25402731	10.10166347
C	7.02462794	6.89784713	7.03616930	H	-0.11089703	-2.71537145	8.59995157
C	6.34954542	7.57719218	8.05373746	H	1.79202436	-1.78869424	7.33321078
C	5.23744662	7.01334906	8.66896687	H	3.84241474	2.97660985	4.66689671
C	4.76346044	5.74877737	8.27438903	H	4.67896777	4.53767374	4.57108176
C	0.76412613	1.02925504	8.92617982	H	2.84968828	5.60319594	5.92039696
C	-0.30803831	0.50876212	9.65095315	H	2.19324231	4.84598299	4.45793149
C	-0.63014638	-0.84191941	9.53677681	H	-0.83447442	3.91911475	8.34372977
C	0.13075017	-1.65709157	8.69471716	H	-0.41603227	2.57694080	7.25306371
C	1.20473445	-1.13740299	7.97925576	H	-0.08039102	4.69559293	6.07619203
C	1.55274840	0.22184169	8.08890393	H	0.94030034	5.32943773	7.38219089
N	1.85681258	3.81562250	6.30080713	N	4.42334288	2.03909139	9.88238035
C	3.99500829	3.93592724	5.17604301	H	4.07218826	2.30787904	10.79764532
C	2.67783638	4.64082308	5.42666241	H	4.41059870	1.02326634	9.85687136
C	-0.01793540	3.43990189	7.79508038	H	5.40323573	2.31026404	9.87315944
C	0.65278141	4.41616512	6.85104034				

TABLE S-CXII. *trans*-(Fe(NH)<sub>4</sub>S<sub>4</sub>)NH<sub>3</sub> (**6t**) OPBE–Cosmo Quintet

Fe	3.21978426	2.95580419	8.17323468	H	1.71558682	2.90784644	5.95354832
S	3.55027397	5.13046815	9.12783234	H	7.09054438	5.31895791	5.68193222
S	5.06017806	3.58841231	6.65116375	H	7.83506131	7.59798144	6.32693367
S	0.91426165	2.66675488	9.11677571	H	6.68619846	8.76628944	8.21714845
S	2.84349267	0.73881505	7.24773648	H	4.83987258	7.66713750	9.41781670
C	5.53404729	5.22468181	7.16563834	H	-1.12039471	1.03006468	10.19181622
C	6.59592981	5.84380384	6.49816749	H	-1.66741581	-1.38394085	9.97647230
C	7.01484663	7.11956287	6.85934419	H	-0.22316251	-2.83621172	8.53835851
C	6.37143483	7.76724196	7.91658530	H	1.72148662	-1.88289520	7.37032304
C	5.32926099	7.14845648	8.59475346	H	3.89620084	2.95942905	4.71427659
C	4.87670173	5.85831335	8.24514669	H	4.63592184	4.55166360	4.49263229
C	0.59458885	0.93270718	8.89815671	H	2.90950012	5.57611371	5.99242274
C	-0.50227441	0.38292747	9.57157074	H	2.18588675	4.79863432	4.57451400
C	-0.80993012	-0.96786519	9.45055637	H	-0.93463339	3.90933026	8.19953426
C	-0.00111445	-1.77481128	8.64664247	H	-0.42569717	2.57446266	7.14767383
C	1.09637906	-1.23782549	7.98621974	H	0.07673864	4.73020853	6.09628648
C	1.43804870	0.12789526	8.09261400	H	0.99856752	5.27377146	7.50974219
N	1.95488553	3.77722116	6.43026294	N	4.36286109	2.01149004	9.88033773
C	4.04604691	3.94022045	5.18130885	H	3.99115959	2.27068370	10.79011883
C	2.72996933	4.60742671	5.51398142	H	4.35284959	0.99654712	9.83386168
C	-0.06820513	3.41184173	7.75394373	H	5.33938415	2.29414424	9.88866063
C	0.72734249	4.39182455	6.91939047				

TABLE S-CXIII. *Meso*-(Fe(NH)<sub>4</sub>S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) OPBE–Cosmo Singlet

Fe	-0.09804120	0.41059551	0.00000000	C	-0.56461678	0.07423034	-3.14795797
N	-1.65164792	1.75218736	0.00000000	C	-1.11296929	-0.34790017	-4.36040306
H	-2.26033775	1.58448845	0.79791356	H	-1.83088819	-1.16748143	-4.37526130
H	-2.26033775	1.58448845	-0.79791356	C	-0.73821549	0.27733439	-5.54669939
N	-1.43459158	3.18594496	0.00000000	H	-1.16182294	-0.04946114	-6.49478764
H	-0.79685521	3.31567647	0.79195185	C	0.18530200	1.32832644	-5.50244271
H	-0.79685521	3.31567647	-0.79195185	H	0.48420618	1.82713844	-6.42413930
S	0.99121566	1.64450085	1.53962215	C	0.72040497	1.75666579	-4.29404953
S	-1.02843852	-0.72122890	1.61241048	H	1.43344750	2.58013121	-4.27791915
S	0.99121566	1.64450085	-1.53962215	C	0.35307129	1.13702463	-3.08207858
S	-1.02843852	-0.72122890	-1.61241048	C	0.04541770	-2.19561250	1.69969351
N	1.38558977	-0.99452884	0.00000000	H	-0.42338784	-2.95222642	1.06453529
H	2.23347407	-0.43134402	0.00000000	H	0.04729839	-2.57172576	2.72618677
C	-0.56461678	0.07423034	3.14795797	C	1.42648723	-1.79664831	1.24488948

C	-1.11296929	-0.34790017	4.36040306	H	2.06163487	-2.68396848	1.11314763
H	-1.83088819	-1.16748143	4.37526130	H	1.88742919	-1.16610980	2.01037771
C	-0.73821549	0.27733439	5.54669939	C	0.04541770	-2.19561250	-1.69969351
H	-1.16182294	-0.04946114	6.49478764	H	0.04729839	-2.57172576	-2.72618677
C	0.18530200	1.32832644	5.50244271	H	-0.42338784	-2.95222642	-1.06453529
H	0.48420618	1.82713844	6.42413930	C	1.42648723	-1.79664831	-1.24488948
C	0.72040497	1.75666579	4.29404953	H	1.88742919	-1.16610980	-2.01037771
H	1.43344750	2.58013121	4.27791915	H	2.06163487	-2.68396848	-1.11314763
C	0.35307129	1.13702463	3.08207858				

TABLE S-CXIV. *Meso*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) OPBE–Cosmo Triplet

Fe	-0.08373595	0.48291128	0.00000000	C	-0.41310698	0.08837313	-3.20994686
N	-2.26494636	1.76140034	0.00000000	C	-0.83978630	-0.37469612	-4.45634184
H	-2.85459428	1.53015094	0.79833108	H	-1.52293825	-1.22072724	-4.51847730
H	-2.85459428	1.53015094	-0.79833108	C	-0.38773611	0.24473389	-5.61819653
N	-2.17820892	3.21487402	0.00000000	H	-0.71323145	-0.11868123	-6.59132968
H	-1.56124539	3.41316150	0.78983250	C	0.47459473	1.34125212	-5.51923985
H	-1.56124539	3.41316150	-0.78983250	H	0.82771365	1.83831466	-6.42220833
S	0.94223925	1.76865748	1.51668285	C	0.88533206	1.81163249	-4.27769054
S	-1.01495138	-0.65704658	1.70321730	H	1.55419622	2.66887952	-4.21533971
S	0.94223925	1.76865748	-1.51668285	C	0.44701666	1.19113406	-3.09261503
S	-1.01495138	-0.65704658	-1.70321730	C	-0.16799631	-2.27042070	1.72741658
N	1.38538286	-1.39735973	0.00000000	H	-0.77835623	-2.92112668	1.09442216
H	2.28782216	-0.93590288	0.00000000	H	-0.21452158	-2.66777248	2.74551338
C	-0.41310698	0.08837313	3.20994686	C	1.26501197	-2.15246074	1.24562080
C	-0.83978630	-0.37469612	4.45634184	H	1.69129017	-3.16470855	1.15600569
H	-1.52293825	-1.22072724	4.51847730	H	1.84928239	-1.62331577	2.00500444
C	-0.38773611	0.24473389	5.61819653	C	-0.16799631	-2.27042070	-1.72741658
H	-0.71323145	-0.11868123	6.59132968	H	-0.21452158	-2.66777248	-2.74551338
C	0.47459473	1.34125212	5.51923985	H	-0.77835623	-2.92112668	-1.09442216
H	0.82771365	1.83831466	6.42220833	C	1.26501197	-2.15246074	-1.24562080
C	0.88533206	1.81163249	4.27769054	H	1.84928239	-1.62331577	-2.00500444
H	1.55419622	2.66887952	4.21533971	H	1.69129017	-3.16470855	-1.15600569
C	0.44701666	1.19113406	3.09261503				

TABLE S-CXV. *Meso*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) OPBE–Cosmo Quintet

Fe	-0.11255706	0.60438551	0.00000000	C	-0.42941517	0.03062772	-3.36777450
N	-2.06835119	1.75691345	0.00000000	C	-0.81670835	-0.45225022	-4.62295912
H	-2.65160083	1.51727712	0.79980273	H	-1.48686900	-1.30877440	-4.68087069
H	-2.65160083	1.51727712	-0.79980273	C	-0.35493506	0.14657628	-5.79036541

N	-1.98377861	3.20705067	0.00000000	H	-0.65793242	-0.24203350	-6.76106222
H	-1.37154064	3.40949166	0.79337534	C	0.48460571	1.25858458	-5.69437001
H	-1.37154064	3.40949166	-0.79337534	H	0.84661269	1.75015003	-6.59695165
S	0.94472903	1.81407358	1.71310498	C	0.86247636	1.74985263	-4.45121782
S	-1.10968839	-0.74561392	1.91711286	H	1.51570281	2.61921042	-4.39174200
S	0.94472903	1.81407358	-1.71310498	C	0.42218502	1.15278406	-3.25192543
S	-1.10968839	-0.74561392	-1.91711286	C	-0.12135463	-2.25967046	1.76654606
N	1.32061421	-1.23358943	0.00000000	H	-0.70968543	-2.90333097	1.10580159
H	2.20188960	-0.72855166	0.00000000	H	-0.08317079	-2.75065910	2.74358083
C	-0.42941517	0.03062772	3.36777450	C	1.27963314	-2.00729789	1.24701465
C	-0.81670835	-0.45225022	4.62295912	H	1.79082524	-2.97584942	1.13076605
H	-1.48686900	-1.30877440	4.68087069	H	1.83585029	-1.43938699	1.99897552
C	-0.35493506	0.14657628	5.79036541	C	-0.12135463	-2.25967046	-1.76654606
H	-0.65793242	-0.24203350	6.76106222	H	-0.08317079	-2.75065910	-2.74358083
C	0.48460571	1.25858458	5.69437001	H	-0.70968543	-2.90333097	-1.10580159
H	0.84661269	1.75015003	6.59695165	C	1.27963314	-2.00729789	-1.24701465
C	0.86247636	1.74985263	4.45121782	H	1.83585029	-1.43938699	-1.99897552
H	1.51570281	2.61921042	4.39174200	H	1.79082524	-2.97584942	-1.13076605
C	0.42218502	1.15278406	3.25192543				

TABLE S-CXVI. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7t**) OPBE–Cosmo Singlet

Fe	3.07816796	3.02465650	8.05427722	H	7.16330255	4.99046848	6.00606546
S	3.28102171	5.06616835	8.98225673	H	7.95671440	7.25525979	6.66085616
S	4.85425138	3.43152025	6.85620194	H	6.66676389	8.56522855	8.35157059
S	1.18673343	2.73860762	9.07738746	H	4.63109363	7.62659882	9.37588682
S	2.89349727	0.93149325	7.20156418	H	-0.87183963	1.10263182	10.33428079
C	5.44705426	5.05342047	7.31106947	H	-1.46478750	-1.30076001	10.05990979
C	6.61017368	5.57476484	6.74071059	H	-0.14062145	-2.71651500	8.48745590
C	7.05422112	6.84155802	7.10746059	H	1.75128723	-1.76068648	7.23068533
C	6.32823651	7.57220945	8.05668657	H	3.91132261	2.83769236	4.77192939
C	5.18195074	7.04574953	8.63700880	H	4.73952311	4.40641079	4.64294350
C	4.71362464	5.76511148	8.27732755	H	2.93558274	5.49949996	5.96380801
C	0.76560835	1.00798952	8.93639717	H	2.18389387	4.64041033	4.60129090
C	-0.30085526	0.46894153	9.65680797	H	-0.80879609	3.94752045	8.38529082
C	-0.63469625	-0.87404418	9.49958411	H	-0.43386290	2.58003384	7.30700275
C	0.11090391	-1.66423281	8.61813410	H	0.10786484	4.59880112	6.05439681
C	1.17890425	-1.12819108	7.90822430	H	0.99587083	5.29350078	7.43041058
C	1.53875325	0.22591529	8.05883873	N	4.19023025	2.15094147	9.55580126
N	1.99041926	3.71480841	6.50598291	H	3.86817244	1.18776373	9.60665413
C	4.06010344	3.80964861	5.25696797	H	5.15031600	2.09208426	9.22053308

C	2.75576937	4.51039624	5.53141093	N	4.16707451	2.68030287	10.89002009
C	-0.00869332	3.43083391	7.84736680	H	5.07342972	2.49051504	11.31796785
C	0.73702061	4.35936746	6.92412078	H	7.16330255	4.99046848	6.00606546
H	1.74335910	2.83586881	6.04226330				

TABLE S-CXVII. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7t**) OPBE–Cosmo Triplet

Fe	3.03429282	3.04004392	7.99349169	H	7.09075764	5.05568058	5.90605731
S	3.29523012	5.02071679	9.00868067	H	7.92167599	7.28029887	6.64480833
S	4.79076546	3.47504931	6.75292242	H	6.70291464	8.51336230	8.43753543
S	1.10670648	2.76598514	8.98875609	H	4.68923328	7.53823944	9.48007811
S	2.94610225	0.90100047	7.28650771	H	-1.01336226	1.15342278	10.17530695
C	5.41564759	5.06992286	7.26408541	H	-1.56219368	-1.26397531	9.95757961
C	6.56558467	5.60664776	6.68512687	H	-0.13466979	-2.72236823	8.52358653
C	7.03015097	6.85216220	7.09970655	H	1.82316009	-1.78905673	7.34692864
C	6.34500878	7.53950047	8.10498722	H	3.84502835	2.96973584	4.65713074
C	5.21069089	6.99275613	8.69481188	H	4.67458883	4.53568456	4.58197011
C	4.72484532	5.73824568	8.28495511	H	2.81446359	5.59173608	5.88993275
C	0.70477890	1.02869041	8.87923809	H	2.18154749	4.81808000	4.42521405
C	-0.39574044	0.50361428	9.55696122	H	-0.90734266	3.90690028	8.25206092
C	-0.70376235	-0.84921730	9.43205581	H	-0.46263744	2.55766075	7.18020394
C	0.09869685	-1.66320727	8.62832394	H	-0.10451039	4.66662153	5.98946676
C	1.20283682	-1.13987002	7.96349528	H	0.87811831	5.31790432	7.31565268
C	1.53610842	0.22145803	8.08538702	N	4.44991022	2.00289937	9.97521656
N	1.82992879	3.79876238	6.27004871	H	4.06416276	1.08608021	10.17798088
C	3.98205879	3.92862089	5.17139313	H	5.34361810	1.83822682	9.51657070
C	2.65756889	4.62520971	5.40014269	N	4.63135452	2.68590157	11.21651187
C	-0.07919455	3.42691588	7.72215606	H	5.57420497	2.52242072	11.56949955
C	0.60806117	4.39850330	6.78636113	H	4.58882824	3.67770673	10.98316111
H	1.59191439	2.94085229	5.77537593				

TABLE S-CXVIII. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7t**) OPBE–Cosmo Quintet

Fe	3.15799170	2.97539221	8.19682117	H	7.09727869	5.25218579	5.72050025
S	3.48776544	5.15980944	9.09859265	H	7.87104431	7.52230327	6.36335430
S	5.02889257	3.56026484	6.68037645	H	6.71373155	8.72310117	8.22715043
S	0.85553938	2.64591852	9.10708859	H	4.82432852	7.66715020	9.40080471
S	2.90858094	0.73249138	7.36257271	H	-1.26645768	1.00162934	10.00220143
C	5.51383590	5.19696191	7.17732627	H	-1.81892402	-1.39858372	9.68413309
C	6.59765916	5.79223234	6.52358335	H	-0.28640713	-2.83322134	8.32343529
C	7.03266615	7.06277474	6.88392130	H	1.75428873	-1.87647258	7.33334254
C	6.38395728	7.72921951	7.92597132	H	3.87444161	2.90384322	4.74838206

C	5.31805513	7.13491695	8.58914524	H	4.61492356	4.49308209	4.50714286
C	4.84911148	5.85184257	8.23860024	H	2.87751506	5.53655136	5.98409032
C	0.54052704	0.91607091	8.83766064	H	2.16608864	4.74204675	4.56907723
C	-0.60876339	0.36336908	9.41437123	H	-0.96719207	3.94063745	8.20834718
C	-0.91926661	-0.98038288	9.23611417	H	-0.50871396	2.58950876	7.15535589
C	-0.06080194	-1.77806148	8.47612727	H	0.04887587	4.70683848	6.07507546
C	1.09047291	-1.23947335	7.91623763	H	0.96796150	5.26354405	7.48491743
C	1.43466937	0.11900403	8.08304224	N	4.35315598	2.02688274	9.96147965
N	1.91726315	3.74414388	6.43455457	H	3.90112696	1.14536976	10.18780823
C	4.02114859	3.89159541	5.20121121	H	5.24274263	1.77365291	9.53211476
C	2.70272887	4.56267048	5.51477783	N	4.55840849	2.74354749	11.18288371
C	-0.12019626	3.41840036	7.75395961	H	5.48375534	2.51789467	11.54625068
C	0.69058372	4.37537772	6.90750779	H	4.59179958	3.72695620	10.90735488
H	1.67601177	2.87308955	5.96229933				

TABLE S-CXIX. *Meso*-(Fe(NH)<sub>4</sub>S<sub>4</sub>)CO (4m) S12g Singlet

Fe	-0.01846934	-0.11944695	0.00000000	C	1.67781679	2.04371799	-1.26954173
S	1.08558067	-1.38149023	1.57117117	H	-1.98398605	1.27086361	4.34120663
S	-0.90664520	1.10110620	1.67267054	H	-1.61050227	-0.10275670	6.38638250
S	-0.90664520	1.10110620	-1.67267054	H	0.00608818	-2.00010267	6.30170938
S	1.08558067	-1.38149023	-1.57117117	H	1.19212310	-2.54282580	4.20854295
C	-0.57106374	0.15244327	3.16331417	H	-1.98398605	1.27086361	-4.34120663
C	-1.26850137	0.44890159	4.33298904	H	-1.61050227	-0.10275670	-6.38638250
C	-1.06043787	-0.31799266	5.47182451	H	0.00608818	-2.00010267	-6.30170938
C	-0.15653486	-1.38303384	5.41775847	H	1.19212310	-2.54282580	-4.20854295
C	0.51624998	-1.68989526	4.24616005	H	2.38134048	0.61562999	0.00000000
C	0.31124777	-0.93587166	3.07628039	H	0.35111175	2.84453621	2.79300810
C	-0.57106374	0.15244327	-3.16331417	H	-0.12521762	3.28115559	1.13883442
C	-1.26850137	0.44890159	-4.33298904	H	2.10740976	1.36472484	2.01269656
C	-1.06043787	-0.31799266	-5.47182451	H	2.34492092	2.91424367	1.16674640
C	-0.15653486	-1.38303384	-5.41775847	H	-0.12521762	3.28115559	-1.13883442
C	0.51624998	-1.68989526	-4.24616005	H	0.35111175	2.84453621	-2.79300810
C	0.31124777	-0.93587166	-3.07628039	H	2.34492092	2.91424367	-1.16674640
N	1.60571322	1.27761697	0.00000000	H	2.10740976	1.36472484	-2.01269656
C	0.31471706	2.48999962	1.75781358	C	-1.28497148	-1.29526451	0.00000000
C	1.67781679	2.04371799	1.26954173	O	-2.12416087	-2.10255668	0.00000000
C	0.31471706	2.48999962	-1.75781358				

TABLE S-CXX. *Meso*-(Fe(NH)<sub>4</sub>)CO (4m) S12g Triplet

Fe	-0.19404506	-0.25825596	0.00000000	C	1.57546809	2.21780407	-1.26403670
S	0.96407310	-1.47473179	1.51570705	H	-1.58870758	1.36443697	4.61976659
S	-0.93668977	1.08263527	1.81947754	H	-0.97732317	0.01945573	6.62349571
S	-0.93668977	1.08263527	-1.81947754	H	0.51354429	-1.96261681	6.35687664
S	0.96407310	-1.47473179	-1.51570705	H	1.35325651	-2.60224764	4.12469535
C	-0.41992755	0.15724661	3.27425353	H	-1.58870758	1.36443697	-4.61976659
C	-0.91892476	0.50985857	4.52732303	H	-0.97732317	0.01945573	-6.62349571
C	-0.58143191	-0.24454445	5.64409446	H	0.51354429	-1.96261681	-6.35687664
C	0.24986162	-1.35707611	5.48942072	H	1.35325651	-2.60224764	-4.12469535
C	0.72484159	-1.72022823	4.23946384	H	2.27924737	0.77546163	0.00000000
C	0.39061430	-0.97395919	3.09535723	H	0.22640849	2.95795106	2.80680216
C	-0.41992755	0.15724661	-3.27425353	H	-0.34323706	3.26808491	1.15561516
C	-0.91892476	0.50985857	-4.52732303	H	2.07667462	1.58217806	2.00140656
C	-0.58143191	-0.24454445	-5.64409446	H	2.15370854	3.15527861	1.17911063
C	0.24986162	-1.35707611	-5.48942072	H	-0.34323706	3.26808491	-1.15561516
C	0.72484159	-1.72022823	-4.23946384	H	0.22640849	2.95795106	-2.80680216
C	0.39061430	-0.97395919	-3.09535723	H	2.15370854	3.15527861	-1.17911063
N	1.54796093	1.47903189	0.00000000	H	2.07667462	1.58217806	-2.00140656
C	0.18630849	2.54793765	1.79176347	C	-1.89829108	-1.18737532	0.00000000
C	1.57546809	2.21780407	1.26403670	O	-2.69552254	-2.02604029	0.00000000
C	0.18630849	2.54793765	-1.79176347				

TABLE S-CXXI. *Meso*-(Fe(NH)<sub>4</sub>)CO (4m) S12g Quintet

Fe	0.24668973	-0.50054717	0.00000000	C	1.80548239	2.13897307	-1.26576764
S	1.27906427	-1.32221762	1.96091286	H	-2.14177453	1.42206331	4.26831723
S	-0.85760476	1.22797486	1.76188189	H	-2.11402183	0.01350619	6.31776356
S	-0.85760476	1.22797486	-1.76188189	H	-0.59141220	-1.96321425	6.41709330
S	1.27906427	-1.32221762	-1.96091286	H	0.86076447	-2.51029727	4.49826273
C	-0.63508731	0.27107581	3.25795540	H	-2.14177453	1.42206331	-4.26831723
C	-1.46719790	0.57010329	4.34040546	H	-2.11402183	0.01350619	-6.31776356
C	-1.45534644	-0.22072512	5.48259486	H	-0.59141220	-1.96321425	-6.41709330
C	-0.60443842	-1.32485821	5.53338212	H	0.86076447	-2.51029727	-4.49826273
C	0.21496185	-1.63516828	4.45808283	H	2.63100207	0.79102262	0.00000000
C	0.21978530	-0.85547535	3.28720991	H	0.48696531	2.96328041	2.77279618
C	-0.63508731	0.27107581	-3.25795540	H	-0.02904813	3.32467248	1.12314643
C	-1.46719790	0.57010329	-4.34040546	H	2.24756341	1.47742848	2.01737184
C	-1.45534644	-0.22072512	-5.48259486	H	2.42937549	3.04967177	1.20260980
C	-0.60443842	-1.32485821	-5.53338212	H	-0.02904813	3.32467248	-1.12314643



C	0.21496185	-1.63516828	-4.45808283	H	0.48696531	2.96328041	-2.77279618
C	0.21978530	-0.85547535	-3.28720991	H	2.42937549	3.04967177	-1.20260980
N	1.81062176	1.39059737	0.00000000	H	2.24756341	1.47742848	-2.01737184
C	0.42293063	2.55334214	1.75896877	C	-1.32106137	-1.67085070	0.00000000
C	1.80548239	2.13897307	1.26576764	O	-2.15198342	-2.47016341	0.00000000
C	0.42293063	2.55334214	-1.75896877				

TABLE S-CXXII. *trans*-(Fe(NH)S<sub>4</sub>)CO (**4t**) S12g Singlet

Fe	8.44921384	10.04794616	1.81050375	H	8.89479326	5.77117638	6.80268783
S	9.84663178	8.82822752	3.08531238	C	9.31621679	7.08301366	5.14739071
S	6.77325817	8.52715001	2.32002895	H	10.36417190	7.22803733	5.40920538
S	7.14199205	11.07143845	0.29662237	C	8.78794549	7.73208130	4.03352234
S	10.06432525	11.65273755	1.31906637	C	7.90818091	11.04891297	3.11666878
C	9.10019182	12.96061446	0.64718960	O	7.54260886	11.73649731	3.98237577
C	9.58209502	14.27879605	0.58436673	N	9.15884265	8.87504225	0.19526270
H	10.59015863	14.48886883	0.93777458	H	9.97408624	9.43678824	-0.07615019
C	8.77449063	15.30899143	0.12153878	C	10.55673209	7.69858915	1.79422256
H	9.16487368	16.32684270	0.11059699	H	10.79501214	6.74557479	2.27511926
C	7.46440123	15.06795913	-0.29847449	H	11.49210738	8.18755739	1.48937677
H	6.82926735	15.88590841	-0.63474811	C	9.59957004	7.53997938	0.63466715
C	6.97066457	13.76935817	-0.26176229	H	8.70806883	6.98823431	0.95265505
H	5.94839202	13.55138688	-0.56872266	H	10.08603369	6.98872803	-0.18702288
C	7.78846091	12.74009995	0.19539394	C	7.83116445	10.29964508	-1.25312242
C	7.43481810	7.63069888	3.67217683	H	8.70218121	10.89743386	-1.54286971
C	6.62560184	6.80132573	4.47136413	H	7.06730133	10.35575480	-2.03505271
H	5.56881741	6.70559386	4.22767271	C	8.20696761	8.87080830	-0.92738048
C	7.15047952	6.13867728	5.57030969	H	7.32825874	8.29398605	-0.61239566
H	6.49352555	5.51878635	6.18085747	H	8.63578322	8.38378266	-1.81822921
C	8.49634554	6.27397044	5.92303437				

TABLE S-CXXIII. *trans*-(Fe(NH)S<sub>4</sub>)CO (**4t**) S12g Triplet

Fe	8.46577498	10.10164177	1.82999388	H	8.90787399	5.47658499	6.78373429
S	10.05125880	8.53168823	3.14462257	C	9.37970271	6.79584187	5.14830724
S	6.78941660	8.65701381	2.58921348	H	10.45147503	6.79619694	5.34303283
S	7.08696026	11.15924589	-0.08706077	C	8.88395306	7.56043790	4.09098940
S	10.02558947	11.70221403	1.23529973	C	7.81343701	11.22410609	3.01430156
C	9.00674441	13.02955885	0.66876997	O	7.39719572	11.98685265	3.78871013
C	9.42386044	14.36025600	0.82055441	N	9.15727047	8.79365796	0.21062842
H	10.37195080	14.55637809	1.31793023	H	10.04020905	9.25373260	-0.02738334
C	8.63323629	15.41630011	0.38538074	C	10.47482868	7.41042356	1.74339297

H	8.97471490	16.44012315	0.53906545	H	10.62544575	6.40429833	2.14556979
C	7.40252823	15.17927104	-0.22434258	H	11.44294999	7.78339350	1.38050491
H	6.77599296	16.00736305	-0.55336753	C	9.43593362	7.41395635	0.64153322
C	6.97244948	13.86963778	-0.39939812	H	8.49488237	6.98452478	1.00352909
H	6.01087621	13.66053287	-0.86544928	H	9.79954242	6.80176495	-0.20162447
C	7.76546445	12.80596770	0.03187340	C	8.08106788	10.31718307	-1.39588809
C	7.50111501	7.63428882	3.82484500	H	9.03068280	10.85510815	-1.48875446
C	6.64879409	6.87655621	4.65101133	H	7.53433782	10.37479989	-2.34277140
H	5.57548928	6.92669734	4.47556103	C	8.29292346	8.87280700	-0.98078770
C	7.14752407	6.10494435	5.68846598	H	7.33592069	8.39619240	-0.72951370
H	6.45473739	5.54387782	6.31617550	H	8.73058321	8.31330684	-1.82409991
C	8.51795873	6.06033735	5.95133054				

TABLE S-CXXIV. *trans*-(Fe(NH)<sub>4</sub>S<sub>4</sub>)CO (**4t**) S12g Quintet

Fe	8.45819980	10.04029849	1.82207421	H	8.88082351	5.94958320	7.06485282
S	10.01318926	8.37398759	2.99582428	C	9.34006046	6.95631698	5.21842958
S	6.73182094	8.42505796	2.42353020	H	10.41793419	6.92921887	5.37089401
S	7.21770991	11.11658362	-0.12263736	C	8.83223339	7.56405112	4.06859938
S	10.08171031	11.84442248	1.30475795	C	7.86825978	11.19716462	3.29270488
C	8.99196290	13.09170966	0.71395007	O	7.50031225	11.94007762	4.09438831
C	9.30717738	14.44992932	0.89617543	N	9.28066031	8.72504325	0.01398668
H	10.23287032	14.70147055	1.41025684	H	10.20502925	9.13787189	-0.12641621
C	8.45338588	15.45618685	0.46515103	C	10.34790022	7.19399694	1.60847129
H	8.72363776	16.49766694	0.64134113	H	10.33515129	6.18076486	2.02098348
C	7.25295205	15.14974401	-0.17486345	H	11.38223484	7.43156102	1.32291878
H	6.57888396	15.93939394	-0.50398947	C	9.41321551	7.32198852	0.41808495
C	6.91871206	13.81670789	-0.37973865	H	8.41330017	6.96378262	0.68847283
H	5.98275520	13.54910507	-0.86740512	H	9.80239521	6.68836438	-0.40022681
C	7.77408422	12.80379966	0.05416076	C	8.29119993	10.42109338	-1.46035034
C	7.44012152	7.66010314	3.83731135	H	9.23947656	10.96868123	-1.43306967
C	6.59563136	7.10557672	4.81694650	H	7.79492957	10.59072167	-2.42134681
H	5.51964626	7.17866721	4.67132327	C	8.49271010	8.93695281	-1.20391952
C	7.10447920	6.49673554	5.95479083	H	7.52299649	8.43912931	-1.06434055
H	6.41632176	6.09020464	6.69624224	H	8.96537122	8.47892873	-2.09063643
C	8.48039879	6.41535707	6.16553197				

TABLE S-CXXV. *Meso*-(Fe(NH)<sub>4</sub>)PMe<sub>3</sub> (**5m**) S12g Singlet

Fe	0.27073819	-0.02348753	0.00000000	H	-1.84164266	-1.29103373	4.31015927
S	1.50383601	1.06377645	-1.60816807	H	-1.32033375	-0.02991915	6.39698986
S	-0.75504703	-1.13645418	-1.63004055	H	0.50036302	1.67558896	6.36629017

S	-0.75504703	-1.13645418	1.63004055	H	1.75575666	2.13046443	4.29069931
S	1.50383601	1.06377645	1.60816807	H	2.56484381	-1.04087366	0.00000000
C	-0.31350312	-0.30199299	-3.16382006	H	0.26640370	-3.02664938	-2.77039953
C	-1.03878870	-0.55358026	-4.32565570	H	-0.23300997	-3.41202324	-1.10875016
C	-0.74980924	0.15154525	-5.48741990	H	2.18841357	-1.75823163	-2.01567318
C	0.26984600	1.10852262	-5.46397152	H	2.26128339	-3.31580241	-1.15402710
C	0.98029609	1.36576997	-4.30219039	H	-0.23300997	-3.41202324	1.10875016
C	0.69304810	0.67502220	-3.11006941	H	0.26640370	-3.02664938	2.77039953
C	-0.31350312	-0.30199299	3.16382006	H	2.26128339	-3.31580241	1.15402710
C	-1.03878870	-0.55358026	4.32565570	H	2.18841357	-1.75823163	2.01567318
C	-0.74980924	0.15154525	5.48741990	P	-1.08663479	1.74957429	0.00000000
C	0.26984600	1.10852262	5.46397152	C	-2.28142335	1.91933593	-1.40816341
C	0.98029609	1.36576997	4.30219039	H	-1.73534630	1.98808241	-2.35516579
C	0.69304810	0.67502220	3.11006941	H	-2.94499151	1.04728517	-1.44191434
N	1.71135446	-1.59782689	0.00000000	H	-2.88241736	2.82670611	-1.26836801
C	0.28377500	-2.67449039	-1.73415618	C	-2.28142335	1.91933593	1.40816341
C	1.69209982	-2.37868348	-1.26307730	H	-2.94499151	1.04728517	1.44191434
C	0.28377500	-2.67449039	1.73415618	H	-1.73534630	1.98808241	2.35516579
C	1.69209982	-2.37868348	1.26307730	H	-2.88241736	2.82670611	1.26836801
H	-1.84164266	-1.29103373	-4.31015927	C	-0.31307872	3.44385061	0.00000000
H	-1.32033375	-0.02991915	-6.39698986	H	-0.63393053	3.98850523	-0.89457414
H	0.50036302	1.67558896	-6.36629017	H	-0.63393053	3.98850523	0.89457414
H	1.75575666	2.13046443	-4.29069931	H	0.77513725	3.36049302	0.00000000

TABLE S-CXXVI. *Meso*-(Fe(NH)<sub>4</sub>)PMe<sub>3</sub> (**5m**) S12g Triplet

Fe	0.39505569	0.09839786	0.00000000	H	-1.88094042	-1.47670986	4.38832351
S	1.47925097	1.09665476	-1.81750953	H	-1.52628689	-0.16698770	6.47437515
S	-0.79566562	-1.29709652	-1.77147852	H	0.18856067	1.65052342	6.49174487
S	-0.79566562	-1.29709652	1.77147852	H	1.48773474	2.15310369	4.45537715
S	1.47925097	1.09665476	1.81750953	H	2.65678306	-1.01412269	0.00000000
C	-0.37709912	-0.41873902	-3.27694916	H	0.42233689	-3.14878984	-2.73781968
C	-1.12820272	-0.68933539	-4.42247185	H	-0.10151101	-3.44482535	-1.07361650
C	-0.93243783	0.04342058	-5.58581300	H	2.23325711	-1.69281156	-2.02241172
C	0.02547777	1.05976264	-5.58960191	H	2.38666136	-3.25305575	-1.17354845
C	0.76080660	1.34210198	-4.44945301	H	-0.10151101	-3.44482535	1.07361650
C	0.57800708	0.62207802	-3.25305469	H	0.42233689	-3.14878984	2.73781968
C	-0.37709912	-0.41873902	3.27694916	H	2.38666136	-3.25305575	1.17354845
C	-1.12820272	-0.68933539	4.42247185	H	2.23325711	-1.69281156	2.02241172
C	-0.93243783	0.04342058	5.58581300	P	-0.92139602	1.94067236	0.00000000
C	0.02547777	1.05976264	5.58960191	C	-2.10266410	2.09152545	-1.41516654

C	0.76080660	1.34210198	4.44945301	H	-1.55100740	2.13610652	-2.35991357
C	0.57800708	0.62207802	3.25305469	H	-2.76819868	1.22030073	-1.43012850
N	1.79955878	-1.56547934	0.00000000	H	-2.69961573	3.00467530	-1.29299963
C	0.38284122	-2.71458297	-1.73292372	C	-2.10266410	2.09152545	1.41516654
C	1.77714601	-2.33776009	-1.26469658	H	-2.76819868	1.22030073	1.43012850
C	0.38284122	-2.71458297	1.73292372	H	-1.55100740	2.13610652	2.35991357
C	1.77714601	-2.33776009	1.26469658	H	-2.69961573	3.00467530	1.29299963
H	-1.88094042	-1.47670986	-4.38832351	C	-0.07368264	3.59059146	0.00000000
H	-1.52628689	-0.16698770	-6.47437515	H	-0.36313095	4.14970426	-0.89660883
H	0.18856067	1.65052342	-6.49174487	H	-0.36313095	4.14970426	0.89660883
H	1.48773474	2.15310369	-4.45537715	H	1.00876636	3.44222550	0.00000000

TABLE S-CXXVII. *Meso*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5m**) S12g Quintet

Fe	0.49377423	0.19116264	0.00000000	H	-1.84750700	-1.38964591	4.43125990
S	1.65743288	1.00799164	-1.86098462	H	-1.48903651	-0.03472779	6.48590540
S	-0.75893172	-1.30267669	-1.83000870	H	0.26204381	1.74815292	6.47482707
S	-0.75893172	-1.30267669	1.83000870	H	1.60849034	2.15251736	4.44704737
S	1.65743288	1.00799164	1.86098462	H	2.64917667	-1.25406859	0.00000000
C	-0.30566918	-0.39977066	-3.31028627	H	0.34256501	-3.23300417	-2.78063805
C	-1.07625286	-0.62048202	-4.45482945	H	-0.24177844	-3.48562121	-1.13118569
C	-0.87965557	0.13919055	-5.59996902	H	2.25627261	-1.93949335	-2.00936433
C	0.09813804	1.13457825	-5.58826997	H	2.24922662	-3.52067074	-1.19010799
C	0.85761905	1.36392631	-4.45167820	H	-0.24177844	-3.48562121	1.13118569
C	0.67721829	0.61545801	-3.27312162	H	0.34256501	-3.23300417	2.78063805
C	-0.30566918	-0.39977066	3.31028627	H	2.24922662	-3.52067074	1.19010799
C	-1.07625286	-0.62048202	4.45482945	H	2.25627261	-1.93949335	2.00936433
C	-0.87965557	0.13919055	5.59996902	P	-1.28125295	2.01628385	0.00000000
C	0.09813804	1.13457825	5.58826997	C	-2.44537463	2.15417527	-1.43164671
C	0.85761905	1.36392631	4.45167820	H	-1.86674947	2.18472097	-2.36240387
C	0.67721829	0.61545801	3.27312162	H	-3.09866194	1.27389950	-1.45628203
N	1.79332984	-1.80333446	0.00000000	H	-3.05778829	3.06155233	-1.34714610
C	0.31728621	-2.79631493	-1.77619455	C	-2.44537463	2.15417527	1.43164671
C	1.73072023	-2.54760215	-1.26590046	H	-3.09866194	1.27389950	1.45628203
C	0.31728621	-2.79631493	1.77619455	H	-1.86674947	2.18472097	2.36240387
C	1.73072023	-2.54760215	1.26590046	H	-3.05778829	3.06155233	1.34714610
H	-1.84750700	-1.38964591	-4.43125990	C	-0.44813111	3.67796180	0.00000000
H	-1.48903651	-0.03472779	-6.48590540	H	-0.73719630	4.24096141	-0.89410423
H	0.26204381	1.74815292	-6.47482707	H	-0.73719630	4.24096141	0.89410423
H	1.60849034	2.15251736	-4.44704737	H	0.63655895	3.53495588	0.00000000

TABLE S-CXXVIII. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) S12g Singlet

Fe	3.02032624	3.05654843	7.94187362	H	1.72251481	2.95521045	5.82631506
S	3.25723466	5.15219246	8.88443567	H	5.15436632	0.23472239	10.67428246
S	4.79695419	3.50051861	6.66765714	H	5.05740517	0.09674789	8.88578719
S	1.07722866	2.75103429	8.97044550	H	3.59479789	-0.12081593	9.87016006
S	2.71448190	0.95321544	6.99680698	H	6.33815170	2.43501123	10.83798133
P	4.19986180	2.24795924	9.66928438	H	5.89809319	3.97943619	10.04366194
C	4.53674768	0.43113235	9.78903190	H	6.54749316	2.63156141	9.07510511
C	5.91667737	2.89087943	9.93344807	H	4.14035688	2.17723047	12.12050219
C	3.47261562	2.56524228	11.34147390	H	2.49893372	2.06778762	11.42205966
C	5.50912040	5.02616784	7.30220575	H	3.33682186	3.64447652	11.46807268
C	6.77973583	5.41532796	6.88626767	H	7.31395455	4.81002698	6.15338682
C	7.36327651	6.55639075	7.42083248	H	8.36085765	6.86155086	7.10880470
C	6.65532626	7.29427021	8.37524121	H	7.10541479	8.18725047	8.80976453
C	5.39701473	6.89628923	8.79682509	H	4.86895986	7.46732916	9.55927901
C	4.79166241	5.73492509	8.27966387	H	-0.55660186	1.04597810	10.64631333
C	0.81412279	0.97492494	8.99148241	H	-0.85063073	-1.43412379	10.70924415
C	-0.03807589	0.40561542	9.93278184	H	0.37087599	-2.84409381	9.05667122
C	-0.20287121	-0.97486991	9.96408373	H	1.88790810	-1.81580029	7.40285050
C	0.48586621	-1.75996944	9.03541576	H	3.81614585	3.23196539	4.50843035
C	1.33680598	-1.18660748	8.10022992	H	4.63312038	4.81643479	4.62629505
C	1.54094668	0.20454500	8.06648799	H	2.80670321	5.67661188	6.08306763
N	1.87859617	3.82787559	6.34538132	H	2.07310267	5.02739659	4.59000619
C	3.95559940	4.12407356	5.13421208	H	-1.03210942	3.61258936	8.07550411
C	2.63705163	4.76447964	5.50044771	H	-0.30765201	2.35947382	7.02202280
C	-0.10451198	3.25790566	7.61519081	H	-0.06719334	4.61602108	5.94508149
C	0.57326512	4.33324304	6.79692562	H	0.75927516	5.22983546	7.40109787

TABLE S-CXXIX. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) S12g Triplet

Fe	3.07742658	3.02635093	7.93724703	H	1.77854621	3.06736798	5.70426509
S	3.43410528	5.06189207	8.91606618	H	5.08132187	0.17937680	10.82274473
S	4.90643990	3.66267916	6.37808500	H	4.99130564	0.01865032	9.03559886
S	0.69408793	2.71714313	8.96313121	H	3.51641351	-0.14277043	10.01395710
S	2.67965992	0.94364739	7.07993332	H	6.32707443	2.36123704	10.96469335
P	4.18676943	2.20141016	9.78195415	H	5.91929256	3.90034642	10.13877837
C	4.47443229	0.38002917	9.93079425	H	6.53171892	2.52037122	9.19406945
C	5.91361237	2.80968195	10.05221979	H	4.03887444	2.18201476	12.23049856
C	3.40505504	2.55964728	11.41797494	H	2.42636553	2.06761934	11.46254119
C	5.60367591	5.11648252	7.16864565	H	3.27130443	3.64164701	11.51987648
C	6.84219620	5.58680256	6.73690898	H	7.34023931	5.08382593	5.90822482

C	7.44042791	6.67172599	7.36630076	H	8.41540736	7.02794642	7.03638468
C	6.78199436	7.28222508	8.43383701	H	7.24148849	8.12990353	8.94313148
C	5.55164508	6.81202093	8.86880642	H	5.05565730	7.28181285	9.71722784
C	4.93587591	5.70831065	8.25437184	H	-0.84735354	0.91523639	10.53668950
C	0.64702820	0.93227908	8.99523692	H	-0.86183077	-1.56592068	10.74846359
C	-0.19923788	0.30380436	9.91007061	H	0.62624317	-2.92435307	9.27691532
C	-0.20846620	-1.08126311	10.02392468	H	2.13725695	-1.81047677	7.66823448
C	0.62386452	-1.83679804	9.19824572	H	3.75674624	3.62160072	4.30334506
C	1.46870341	-1.21476236	8.28815187	H	4.48694416	5.22202269	4.56580321
C	1.51983675	0.18407378	8.17651082	H	2.72529511	5.79630912	6.21940115
N	1.86400781	3.90315106	6.28822753	H	1.96825943	5.30298893	4.68251431
C	3.89743330	4.42889183	5.03525911	H	-1.22599573	3.39690729	7.63349929
C	2.56840464	4.95089449	5.53989364	H	-0.18097809	2.23719101	6.76742769
C	-0.18982699	3.13500795	7.39513298	H	-0.09426128	4.63106082	5.85977282
C	0.51495191	4.29409451	6.71598426	H	0.61796314	5.14385210	7.40435125

TABLE S-CXXX. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) S12g Quintet

Fe	3.03007845	3.00690419	7.88908502	H	1.73562464	3.12702213	5.46631472
S	3.30587346	5.26703398	8.85598128	H	5.12039737	0.10121256	10.96076580
S	4.84691275	3.80709533	6.31905528	H	4.92499603	-0.13170110	9.18919361
S	0.65394243	2.72028592	8.80242167	H	3.49477069	-0.12704487	10.23849600
S	2.56889942	0.78374537	6.92160084	H	6.53437592	2.29675414	10.89317769
P	4.31505469	2.13757181	9.83945455	H	6.12920924	3.77198495	9.95513111
C	4.48700343	0.31351900	10.08972523	H	6.63675055	2.29424267	9.10506448
C	6.08016139	2.67760248	9.96881828	H	4.29653666	2.31794187	12.29748023
C	3.65267771	2.66938277	11.48073695	H	2.64399814	2.25806705	11.60760296
C	5.58313907	5.15646504	7.23221148	H	3.59133760	3.76317256	11.49067119
C	6.88414514	5.52783052	6.89030159	H	7.36855241	5.03889455	6.04596384
C	7.55890858	6.49340596	7.62541875	H	8.57654183	6.77480019	7.35849328
C	6.91437916	7.08274272	8.71320450	H	7.43096834	7.83709970	9.30741922
C	5.62420375	6.71135237	9.05988174	H	5.13814069	7.16784024	9.92029537
C	4.91471941	5.73192307	8.33775747	H	-0.71567254	1.05048669	10.61127439
C	0.67450149	0.94340185	8.97871230	H	-0.65860236	-1.39719516	11.06258902
C	-0.09495821	0.39195735	10.00550720	H	0.77195054	-2.86323257	9.63344056
C	-0.06226088	-0.97386553	10.25555562	H	2.14504061	-1.88541250	7.83019288
C	0.73842875	-1.78828942	9.45383410	H	3.77006033	3.87353724	4.21740297
C	1.50579450	-1.24398723	8.43413600	H	4.40337861	5.48121582	4.62781697
C	1.51679874	0.13879896	8.17171594	H	2.52537671	5.85361849	6.21212073
N	1.74849106	3.93422170	6.09257483	H	1.89576268	5.45383566	4.59011679
C	3.82939063	4.63186358	5.01087038	H	-1.29163911	3.18086486	7.42377735

C	2.44483858	5.05578219	5.46433454	H	-0.11974117	2.10755317	6.59939487
C	-0.23237972	3.01513872	7.20234524	H	-0.26814734	4.51005545	5.65934112
C	0.37724464	4.22281857	6.50932678	H	0.41078442	5.08232889	7.19394561

TABLE S-CXXXI. *Meso*-(Fe(NH)<sub>4</sub>)NH<sub>3</sub> (**6m**) S12g Singlet

Fe	-0.20404493	-0.38551145	0.00000000	N	-1.94508094	-1.49508395	0.00000000
S	0.61696035	-1.84862515	1.58102234	H	-1.83158512	1.37643342	4.36632879
S	-0.89776455	0.93579810	1.65837270	H	-1.62655486	0.01737236	6.44733949
S	-0.89776455	0.93579810	-1.65837270	H	-0.38016676	-2.14259476	6.37300173
S	0.61696035	-1.84862515	-1.58102234	H	0.61484046	-2.94401518	4.26178559
C	-0.70111487	-0.01739300	3.17711829	H	-1.83158512	1.37643342	-4.36632879
C	-1.28222452	0.43474610	4.36112486	H	-1.62655486	0.01737236	-6.44733949
C	-1.16756663	-0.32297328	5.52036277	H	-0.38016676	-2.14259476	-6.37300173
C	-0.47160594	-1.53540091	5.47190177	H	0.61484046	-2.94401518	-4.26178559
C	0.09030886	-1.98985251	4.28923031	H	2.23370479	-0.10802783	0.00000000
C	-0.02449614	-1.24633942	3.09860743	H	0.63266950	2.45199623	2.78874928
C	-0.70111487	-0.01739300	-3.17711829	H	0.24151544	2.96925693	1.13236523
C	-1.28222452	0.43474610	-4.36112486	H	2.09325956	0.68475853	2.01327918
C	-1.16756663	-0.32297328	-5.52036277	H	2.60336738	2.15139339	1.14045370
C	-0.47160594	-1.53540091	-5.47190177	H	0.24151544	2.96925693	-1.13236523
C	0.09030886	-1.98985251	-4.28923031	H	0.63266950	2.45199623	-2.78874928
C	-0.02449614	-1.24633942	-3.09860743	H	2.60336738	2.15139339	-1.14045370
N	1.56543225	0.66323160	0.00000000	H	2.09325956	0.68475853	-2.01327918
C	0.53318365	2.11366940	1.75269749	H	-1.92195377	-2.10527665	0.81891290
C	1.78749830	1.42202045	1.26437855	H	-1.92195377	-2.10527665	-0.81891290
C	0.53318365	2.11366940	-1.75269749	H	-2.83063525	-0.99194275	0.00000000
C	1.78749830	1.42202045	-1.26437855				

TABLE S-CXXXII. *Meso*-(Fe(NH)<sub>4</sub>)NH<sub>3</sub> (**6m**) S12g Triplet

Fe	-0.25956620	-0.45049177	0.00000000	N	-2.45155860	-1.45546075	0.00000000
S	0.51084126	-1.91953596	1.56172589	H	-1.62611565	1.39428944	4.50396144
S	-0.89009571	0.92768793	1.74082540	H	-1.35156685	0.01227003	6.55879586
S	-0.89009571	0.92768793	-1.74082540	H	-0.19555639	-2.19350055	6.39989981
S	0.51084126	-1.91953596	-1.56172589	H	0.63902704	-3.01450635	4.22562532
C	-0.61528603	-0.02681024	3.24069523	H	-1.62611565	1.39428944	-4.50396144
C	-1.11042607	0.43478896	4.46007783	H	-1.35156685	0.01227003	-6.55879586
C	-0.95868502	-0.33730605	5.60505970	H	-0.19555639	-2.19350055	-6.39989981
C	-0.31452179	-1.57494950	5.50981891	H	0.63902704	-3.01450635	-4.22562532
C	0.15794142	-2.03955760	4.29216301	H	2.31121656	0.11574853	0.00000000
C	0.00198071	-1.28136831	3.11722653	H	0.55152758	2.56606938	2.79076968

C	-0.61528603	-0.02681024	-3.24069523	H	0.08718407	3.00541932	1.13576043
C	-1.11042607	0.43478896	-4.46007783	H	2.15914001	0.91818550	2.01000622
C	-0.95868502	-0.33730605	-5.60505970	H	2.52087923	2.45657202	1.19387520
C	-0.31452179	-1.57494950	-5.50981891	H	0.08718407	3.00541932	-1.13576043
C	0.15794142	-2.03955760	-4.29216301	H	0.55152758	2.56606938	-2.79076968
C	0.00198071	-1.28136831	-3.11722653	H	2.52087923	2.45657202	-1.19387520
N	1.66526735	0.89914993	0.00000000	H	2.15914001	0.91818550	-2.01000622
C	0.46587760	2.19138596	1.76531149	H	-2.43151495	-2.06470251	0.81620775
C	1.79048657	1.63092587	1.26455212	H	-2.43151495	-2.06470251	-0.81620775
C	0.46587760	2.19138596	-1.76531149	H	-3.34493203	-0.96689732	0.00000000
C	1.79048657	1.63092587	-1.26455212				

TABLE S-CXXXIII. *Meso*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6m**) S12g Quintet

Fe	-0.06456650	-0.70262515	0.00000000	N	-2.11842406	-1.64543009	0.00000000
S	0.73244746	-1.89103554	1.86834071	H	-1.84588137	1.47076720	4.47408251
S	-0.90063586	1.03641534	1.85069477	H	-1.83442362	0.09803432	6.54922516
S	-0.90063586	1.03641534	-1.85069477	H	-0.67554873	-2.11621898	6.53273652
S	0.73244746	-1.89103554	-1.86834071	H	0.43455612	-2.92344871	4.48337698
C	-0.69037099	0.05846191	3.33759658	H	-1.84588137	1.47076720	-4.47408251
C	-1.32977004	0.51146251	4.49617354	H	-1.83442362	0.09803432	-6.54922516
C	-1.32713632	-0.25642395	5.65282800	H	-0.67554873	-2.11621898	-6.53273652
C	-0.68054523	-1.49357685	5.63740566	H	0.43455612	-2.92344871	-4.48337698
C	-0.05460421	-1.95063042	4.48786811	H	2.37862686	0.06106176	0.00000000
C	-0.04530022	-1.19975066	3.29493113	H	0.68947668	2.59996900	2.77413394
C	-0.69037099	0.05846191	-3.33759658	H	0.18950525	2.98955882	1.12367561
C	-1.32977004	0.51146251	-4.49617354	H	2.16306280	0.81619082	2.01257855
C	-1.32713632	-0.25642395	-5.65282800	H	2.59892229	2.33386005	1.18780501
C	-0.68054523	-1.49357685	-5.63740566	H	0.18950525	2.98955882	-1.12367561
C	-0.05460421	-1.95063042	-4.48786811	H	0.68947668	2.59996900	-2.77413394
C	-0.04530022	-1.19975066	-3.29493113	H	2.59892229	2.33386005	-1.18780501
N	1.68573858	0.80744510	0.00000000	H	2.16306280	0.81619082	-2.01257855
C	0.54037041	2.17878625	1.77400746	H	-2.16926794	-2.24709033	0.82094812
C	1.82921811	1.54566695	1.26693077	H	-2.16926794	-2.24709033	-0.82094812
C	0.54037041	2.17878625	-1.77400746	H	-2.94153651	-1.04613421	0.00000000
C	1.82921811	1.54566695	-1.26693077				

TABLE S-CXXXIV. *trans*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6t**) S12g Singlet

Fe	2.95542953	3.10951960	7.85186798	H	1.73594956	2.97836619	5.72712449
S	3.22108022	5.17307009	8.86574619	H	7.32476088	4.80985870	6.19025301
S	4.76089658	3.56051832	6.61220466	H	8.43662366	6.75958105	7.27733284



S	1.01998703	2.77953313	8.90635949	H	7.21471053	8.02195613	9.04923787
S	2.75590801	0.93469847	7.03374408	H	4.94120949	7.34965761	9.72732771
C	5.51792538	5.02164020	7.33836285	H	-0.57922260	1.09899213	10.63751999
C	6.80643282	5.38862356	6.95527821	H	-0.76357737	-1.38320900	10.84605710
C	7.42509659	6.47369622	7.56178889	H	0.56995088	-2.83185659	9.31687879
C	6.73595223	7.17544134	8.55602404	H	2.07590890	-1.83532481	7.63520853
C	5.45801669	6.80167922	8.94061207	H	3.83689066	3.39489748	4.41690491
C	4.81272578	5.69960992	8.34747370	H	4.60221061	4.99228727	4.65004506
C	0.83770293	0.99495695	9.02362040	H	2.72494532	5.72071086	6.10029605
C	-0.01162338	0.44197095	9.97877581	H	2.02158303	5.10220902	4.57633172
C	-0.11577446	-0.94001353	10.09121804	H	-1.10431513	3.49751130	7.92357044
C	0.63600649	-1.74661248	9.23245332	H	-0.26753085	2.26958195	6.92160190
C	1.48392466	-1.19142352	8.28413700	H	-0.10750183	4.54131077	5.83064955
C	1.62227329	0.20399465	8.16284217	H	0.65009954	5.19103037	7.30928879
N	1.85784501	3.83184231	6.28670985	N	4.06162165	2.30262537	9.40116085
C	3.93568858	4.25050195	5.09883023	H	4.29698223	3.03792139	10.07020864
C	2.59253883	4.82827301	5.47904355	H	3.56190158	1.56441411	9.89663321
C	-0.14073575	3.18698585	7.50744345	H	4.92857803	1.87972014	9.07401924
C	0.51557210	4.28621347	6.70360733				

TABLE S-CXXXV. *trans*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6t**) S12g Triplet

Fe	2.99219677	3.08254320	7.88012393	H	1.64479084	3.07963378	5.50572625
S	3.26307837	5.11872147	8.89626596	H	7.29411781	4.90588162	6.09111271
S	4.74433915	3.61197763	6.54182514	H	8.42327516	6.81331953	7.23555535
S	0.98240222	2.78004379	8.86575466	H	7.24913933	7.98478514	9.09545198
S	2.80863947	0.90640919	7.11012870	H	4.99316464	7.26704828	9.80187186
C	5.51910650	5.05422058	7.29531745	H	-0.69384927	1.12346658	10.55398566
C	6.79290652	5.44579481	6.89470382	H	-0.85951773	-1.35552509	10.81432287
C	7.42126852	6.50844253	7.53457383	H	0.55386548	-2.82557367	9.38312173
C	6.76044308	7.15937393	8.57681965	H	2.12305118	-1.84931891	7.74299294
C	5.49220101	6.76023935	8.97693162	H	3.80878447	3.54407149	4.35247017
C	4.84445896	5.68418917	8.34905435	H	4.55561338	5.13302354	4.65362653
C	0.79388705	0.99754145	9.00741329	H	2.63162333	5.78195572	6.10453582
C	-0.09110316	0.45812039	9.93629928	H	2.04217861	5.30847332	4.48890741
C	-0.18306675	-0.92327830	10.07815847	H	-1.13956892	3.39487049	7.81939925
C	0.61151352	-1.74199911	9.27427526	H	-0.21019291	2.22730228	6.83206881
C	1.49438650	-1.19830759	8.34905805	H	-0.29048285	4.56750928	5.81432390
C	1.62066724	0.19338994	8.20566478	H	0.56953548	5.18093419	7.24447781
N	1.73509335	3.91179041	6.08998027	N	4.24860379	2.15110604	9.70257069
C	3.88786260	4.37252916	5.06922064	H	4.46725030	2.88587447	10.37215930

C	2.52072471	4.93718986	5.41403942	H	3.73639990	1.41919200	10.19097483
C	-0.14954073	3.14899516	7.42158073	H	5.12547801	1.73718519	9.39509383
C	0.42787473	4.29624932	6.60889677				

TABLE S-CXXXVI. *trans*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6t**) S12g Quintet

Fe	3.01361257	3.05275846	7.86739616	H	1.80335563	3.11878549	5.46399163
S	3.37705786	5.20676281	8.92964646	H	7.38437904	5.08928599	6.02675788
S	4.87020025	3.83476601	6.32406500	H	8.61393561	6.78967007	7.36725963
S	0.58057623	2.71602392	8.77575431	H	7.50105257	7.79419031	9.36510642
S	2.63904133	0.77384817	7.02322404	H	5.22180943	7.10126921	10.00238611
C	5.62218018	5.16846413	7.25296793	H	-0.78868101	1.06285780	10.58960405
C	6.91525759	5.55271032	6.89412913	H	-0.64977674	-1.35843927	11.15200569
C	7.60139939	6.49883373	7.64367537	H	0.89498584	-2.82171438	9.84231211
C	6.97475722	7.05584570	8.75908787	H	2.29051197	-1.86586469	8.04581991
C	5.69308834	6.66923727	9.12103770	H	3.79221857	3.93181553	4.22407272
C	4.97458364	5.70420635	8.38852780	H	4.40521379	5.53681753	4.67538788
C	0.66835192	0.94639964	9.01616376	H	2.51946051	5.85037940	6.26234124
C	-0.11827059	0.40602659	10.03725254	H	1.89771005	5.47749359	4.62873879
C	-0.04033918	-0.94481793	10.34964915	H	-1.30463147	3.06170526	7.28916365
C	0.82438407	-1.75746061	9.61470768	H	-0.04307450	2.02934130	6.54762916
C	1.60829666	-1.22467279	8.60171426	H	-0.24686701	4.41713933	5.56387278
C	1.57230150	0.14537346	8.27280361	H	0.33189468	5.03160196	7.12268290
N	1.76504372	3.92259515	6.09467989	N	4.05035124	2.09129049	9.62875946
C	3.84103412	4.67126612	5.03548877	H	4.26405470	2.81489646	10.31326716
C	2.45102730	5.06971278	5.49490723	H	3.46201673	1.38543366	10.07101934
C	-0.22877708	2.94019082	7.12727298	H	4.91930737	1.62582619	9.37480888
C	0.36382735	4.16413651	6.44855924				

TABLE S-CXXXVII. *Meso*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) S12g Singlet

Fe	0.00943735	0.35435508	0.00000000	C	-0.63766864	0.07340376	-3.15672062
N	-1.47067671	1.83438076	0.00000000	C	-1.36901964	-0.22573908	-4.30485745
H	-2.08773125	1.72542211	0.80555965	H	-2.10820406	-1.02677214	-4.27908228
H	-2.08773125	1.72542211	-0.80555965	C	-1.16232089	0.50828745	-5.46626127
N	-1.13111161	3.26907395	0.00000000	H	-1.73875632	0.29018440	-6.36404117
H	-0.48159945	3.33311074	0.79395003	C	-0.21841738	1.53951103	-5.45695516
H	-0.48159945	3.33311074	-0.79395003	H	-0.05299287	2.12896209	-6.35917327
S	1.13220700	1.55016654	1.63288012	C	0.49754515	1.84250416	-4.30890724
S	-0.96178759	-0.81969450	1.62706340	H	1.21515818	2.66180813	-4.31092288
S	1.13220700	1.55016654	-1.63288012	C	0.29383360	1.12407990	-3.11639308
S	-0.96178759	-0.81969450	-1.62706340	C	0.20361259	-2.26230206	1.74637118

N	1.52159732	-1.06228523	0.00000000	H	-0.25074958	-3.04786833	1.13148521
H	2.33675571	-0.44874866	0.00000000	H	0.22003719	-2.60076700	2.78697760
C	-0.63766864	0.07340376	3.15672062	C	1.57727682	-1.84746096	1.26578087
C	-1.36901964	-0.22573908	4.30485745	H	2.22380071	-2.73117321	1.14664984
H	-2.10820406	-1.02677214	4.27908228	H	2.02510894	-1.18652123	2.01433066
C	-1.16232089	0.50828745	5.46626127	C	0.20361259	-2.26230206	-1.74637118
H	-1.73875632	0.29018440	6.36404117	H	0.22003719	-2.60076700	-2.78697760
C	-0.21841738	1.53951103	5.45695516	H	-0.25074958	-3.04786833	-1.13148521
H	-0.05299287	2.12896209	6.35917327	C	1.57727682	-1.84746096	-1.26578087
C	0.49754515	1.84250416	4.30890724	H	2.02510894	-1.18652123	-2.01433066
H	1.21515818	2.66180813	4.31092288	H	2.22380071	-2.73117321	-1.14664984
C	0.29383360	1.12407990	3.11639308				

TABLE S-CXXVIII. *Meso*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) S12g Triplet

Fe	-0.02111576	0.40850684	0.00000000	C	-0.50145577	0.06399393	-3.23247975
N	-1.90665050	1.93302945	0.00000000	C	-1.12876788	-0.26137599	-4.43461647
H	-2.53027054	1.85085722	0.80446690	H	-1.85447680	-1.07451875	-4.46136903
H	-2.53027054	1.85085722	-0.80446690	C	-0.84207552	0.46653007	-5.58215480
N	-1.48170529	3.35125517	0.00000000	H	-1.33673083	0.22638679	-6.52226040
H	-0.82349452	3.37465857	0.78795604	C	0.07276558	1.52092579	-5.50688674
H	-0.82349452	3.37465857	-0.78795604	H	0.29862001	2.10636728	-6.39857580
S	1.09153656	1.62022273	1.58680730	C	0.68098868	1.85211825	-4.30548928
S	-0.96178388	-0.79635037	1.72287888	H	1.37481413	2.69015562	-4.25444590
S	1.09153656	1.62022273	-1.58680730	C	0.39563937	1.13752100	-3.12850806
S	-0.96178388	-0.79635037	-1.72287888	C	0.05653042	-2.34673070	1.75762519
N	1.54225746	-1.38187653	0.00000000	H	-0.50078583	-3.05033694	1.12800586
H	2.35846891	-0.77853033	0.00000000	H	0.04331739	-2.72589731	2.78493074
C	-0.50145577	0.06399393	3.23247975	C	1.47981348	-2.11887333	1.26514003
C	-1.12876788	-0.26137599	4.43461647	H	1.99125218	-3.09608379	1.20100428
H	-1.85447680	-1.07451875	4.46136903	H	2.00373600	-1.51356600	2.01244414
C	-0.84207552	0.46653007	5.58215480	C	0.05653042	-2.34673070	-1.75762519
H	-1.33673083	0.22638679	6.52226040	H	0.04331739	-2.72589731	-2.78493074
C	0.07276558	1.52092579	5.50688674	H	-0.50078583	-3.05033694	-1.12800586
H	0.29862001	2.10636728	6.39857580	C	1.47981348	-2.11887333	-1.26514003
C	0.68098868	1.85211825	4.30548928	H	2.00373600	-1.51356600	-2.01244414
H	1.37481413	2.69015562	4.25444590	H	1.99125218	-3.09608379	-1.20100428
C	0.39563937	1.13752100	3.12850806				

TABLE S-CXXXIX. *Meso*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) S12g Quintet

Fe	0.16192665	0.64171420	0.00000000	C	-0.64123741	-0.03211735	-3.31127266
N	-1.54406566	2.08935053	0.00000000	C	-1.40001302	-0.34354504	-4.44409721
H	-2.16388250	2.01601397	0.80852251	H	-2.08429424	-1.19043449	-4.40477405
H	-2.16388250	2.01601397	-0.80852251	C	-1.29949581	0.42335132	-5.59684740
N	-1.07411869	3.49176496	0.00000000	H	-1.89933092	0.17921381	-6.47268814
H	-0.42253533	3.49919937	0.79488879	C	-0.43315910	1.51751260	-5.60485756
H	-0.42253533	3.49919937	-0.79488879	H	-0.34848015	2.13871430	-6.49704299
S	1.19560932	1.58430271	1.90146985	C	0.31411750	1.83488824	-4.48085069
S	-0.97445821	-0.96727727	1.82036603	H	0.97722633	2.69843831	-4.49367106
S	1.19560932	1.58430271	-1.90146985	C	0.23026513	1.08134513	-3.29427337
S	-0.97445821	-0.96727727	-1.82036603	C	0.25787813	-2.33645620	1.76608620
N	1.63664363	-1.19242208	0.00000000	H	-0.22125483	-3.08089640	1.11839918
H	2.44675631	-0.57642008	0.00000000	H	0.32174030	-2.76791452	2.77092130
C	-0.64123741	-0.03211735	3.31127266	C	1.64156762	-1.94139310	1.26703925
C	-1.40001302	-0.34354504	4.44409721	H	2.25776119	-2.85550923	1.19333333
H	-2.08429424	-1.19043449	4.40477405	H	2.09678494	-1.28302358	2.01398140
C	-1.29949581	0.42335132	5.59684740	C	0.25787813	-2.33645620	-1.76608620
H	-1.89933092	0.17921381	6.47268814	H	0.32174030	-2.76791452	-2.77092130
C	-0.43315910	1.51751260	5.60485756	H	-0.22125483	-3.08089640	-1.11839918
H	-0.34848015	2.13871430	6.49704299	C	1.64156762	-1.94139310	-1.26703925
C	0.31411750	1.83488824	4.48085069	H	2.09678494	-1.28302358	-2.01398140
H	0.97722633	2.69843831	4.49367106	H	2.25776119	-2.85550923	-1.19333333
C	0.23026513	1.08134513	3.29427337				

TABLE S-CXL. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7t**) S12g Singlet

Fe	2.95296304	3.11688416	7.89080749	H	7.33725369	4.74591769	6.19974910
S	3.21656316	5.22519246	8.82874559	H	8.48486187	6.67666215	7.28412535
S	4.74366233	3.55181864	6.62007353	H	7.28136675	7.97404972	9.04242260
S	1.02182380	2.75081574	8.95558091	H	4.98696851	7.35826997	9.70691100
S	2.78264893	0.94989274	7.05838257	H	-0.58270670	1.02286099	10.63481484
C	5.52901217	5.00241678	7.33637208	H	-0.79450937	-1.46253638	10.75221493
C	6.82720779	5.33963551	6.95877819	H	0.53368161	-2.87188303	9.18302552
C	7.46553261	6.41464903	7.56377013	H	2.06726161	-1.83043151	7.55159112
C	6.78634631	7.13668864	8.54973477	H	3.80869662	3.39444133	4.43015286
C	5.49704193	6.79382411	8.92753822	H	4.56724205	4.99442408	4.66588809
C	4.83213283	5.70437463	8.33483324	H	2.68942007	5.71609062	6.11342547
C	0.83993765	0.96131344	9.02535187	H	1.97962457	5.07724191	4.60119300
C	-0.01987801	0.38433773	9.95469348	H	-1.10602490	3.46394241	7.97879009

C	-0.13730245	-1.00003387	10.01730785	H	-0.26939250	2.24640028	6.96790755
C	0.61212896	-1.78513235	9.13814917	H	-0.13108726	4.51833813	5.88372603
C	1.47451430	-1.20490220	8.21778823	H	0.63199956	5.17171275	7.35643743
C	1.62424024	0.19142458	8.14977255	N	4.05146039	2.31134303	9.46194797
N	1.84159556	3.82093967	6.32387291	H	3.90417502	1.30305241	9.40069147
C	3.90569905	4.24814817	5.11447112	H	5.04637871	2.47692259	9.29252552
C	2.56058340	4.81706715	5.50156692	N	3.67505185	2.72760232	10.80184170
C	-0.14156126	3.16028727	7.55903452	H	4.46692062	2.55777241	11.42587026
C	0.49981426	4.26602854	6.75192756	H	3.57721227	3.74568378	10.72008963
H	1.72197293	2.96220406	5.77205481				

TABLE S-CXLI. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7t**) S12g Triplet

Fe	3.07194960	3.03377317	8.07569461	H	7.22135488	4.98175505	6.04896480
S	3.23798319	5.16508163	8.90977480	H	8.03840561	7.23754770	6.71060358
S	4.88313758	3.45309269	6.86412425	H	6.72474637	8.58036460	8.34934434
S	1.12606326	2.73738628	9.08722804	H	4.63527360	7.68169728	9.31342273
S	2.84533526	0.92933791	7.13888366	H	-0.85274374	1.05266531	10.38267722
C	5.46567018	5.09189377	7.29125866	H	-1.39485990	-1.36651611	10.13956261
C	6.65091027	5.59035175	6.75119730	H	-0.08376453	-2.75714311	8.53778594
C	7.10974293	6.84714031	7.12495995	H	1.75239215	-1.75683513	7.22556395
C	6.37123851	7.59467937	8.04504043	H	3.92527808	2.82800048	4.78571393
C	5.19686349	7.09434652	8.58856579	H	4.75112109	4.40294944	4.63223242
C	4.70968492	5.82505086	8.22450613	H	2.95416004	5.50366881	5.95491995
C	0.73206751	0.99570361	8.92923793	H	2.20004541	4.65066366	4.58491286
C	-0.29623131	0.42984010	9.68287947	H	-0.85048203	3.94683358	8.32376179
C	-0.59706646	-0.92028792	9.54717250	H	-0.44182490	2.57655926	7.26180942
C	0.14312975	-1.69648458	8.65207394	H	0.11204005	4.62454295	6.02150738
C	1.17474280	-1.13790518	7.91071461	H	0.98675999	5.29932914	7.42294548
C	1.50397254	0.22499770	8.03264551	N	4.07106270	2.15774616	9.46197073
N	1.99002766	3.72582270	6.49829449	H	3.67892437	1.21519099	9.49325780
C	4.07661271	3.80792403	5.25565243	H	5.02231596	2.02158356	9.10089668
C	2.76732766	4.51458626	5.52066969	N	4.14112048	2.58427202	10.85061755
C	-0.03247296	3.43185892	7.80969732	H	5.06739498	2.34460553	11.20864882
C	0.72703821	4.37160998	6.90108887	H	4.09170538	3.60974715	10.81967021
H	1.76619151	2.82087616	6.06760613				

TABLE S-CXLII. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7t**) S12g Quintet

Fe	2.87052569	3.22546286	7.95415107	H	7.38942210	4.58009947	6.06012356
S	3.32960441	5.49621535	8.74161285	H	8.89558755	5.83435115	7.59545409
S	4.66934838	3.92398000	6.12755715	H	7.92165799	6.94861428	9.60773789

S	0.54906690	2.58430271	8.75284093	H	5.50271894	6.79300971	10.06822740
S	2.91751292	0.90888838	7.22605186	H	-0.89154407	0.75219477	10.37838560
C	5.61696355	4.99828814	7.19738421	H	-0.62572564	-1.68084739	10.84341227
C	6.98763951	5.08145628	6.93950820	H	1.15830867	-2.95748856	9.65282220
C	7.82687812	5.77946912	7.79826603	H	2.65865000	-1.81461017	8.05997699
C	7.27753181	6.39869064	8.92081290	H	3.61592529	4.45489719	4.08960984
C	5.91699805	6.31502930	9.18197616	H	4.11527811	5.94574984	4.90935514
C	5.04122875	5.60583124	8.33806493	H	2.15326667	5.94209216	6.33115598
C	0.72818335	0.81591353	8.96865053	H	1.57169823	5.56451520	4.68275191
C	-0.12045397	0.17394850	9.87129991	H	-1.33276148	2.70491491	7.22696045
C	0.02779768	-1.18347528	10.12800379	H	0.06294722	1.84269837	6.51289608
C	1.02853800	-1.89162663	9.46158972	H	-0.42861981	4.18288421	5.52046014
C	1.87311495	-1.25396857	8.56421782	H	0.04026616	4.86648808	7.08572781
C	1.76549670	0.12510650	8.30142152	N	3.91109189	2.48103642	9.89140706
N	1.62296492	3.95156496	6.08788367	H	3.56081836	1.53701701	10.04678408
C	3.60188939	4.98997582	5.04861766	H	4.89726873	2.39230133	9.63607586
C	2.17337700	5.19348628	5.53262539	N	3.72354460	3.23986760	11.10848510
C	-0.24718451	2.72291275	7.08743758	H	4.56601118	3.16784445	11.68060508
C	0.19590883	4.01048514	6.41508031	H	3.66173034	4.21381144	10.79204186
H	1.77053870	3.17882435	5.43448048				

TABLE S-CXLIII. *Meso*-(Fe(NH)<sub>4</sub>)CO (**4m**) S12g-Cosmo Singlet

Fe	-0.00200241	-0.13068879	0.00000000	C	1.66544833	2.06550580	-1.26723928
S	1.09399141	-1.39061325	1.58727562	H	-1.95521839	1.29964345	4.34614809
S	-0.89931133	1.10259371	1.67167939	H	-1.61013714	-0.07489604	6.39245904
S	-0.89931133	1.10259371	-1.67167939	H	-0.02989799	-2.00431333	6.31991837
S	1.09399141	-1.39061325	-1.58727562	H	1.15873254	-2.56889042	4.23475839
C	-0.56791461	0.15001222	3.16552401	H	-1.95521839	1.29964345	-4.34614809
C	-1.25951382	0.46166905	4.33596407	H	-1.61013714	-0.07489604	-6.39245904
C	-1.06554866	-0.30682385	5.47904249	H	-0.02989799	-2.00431333	-6.31991837
C	-0.18181684	-1.38906117	5.43353960	H	1.15873254	-2.56889042	-4.23475839
C	0.49135642	-1.70862549	4.26232430	H	2.42252370	0.68026688	0.00000000
C	0.30028533	-0.95014569	3.09363105	H	0.32536516	2.87281173	2.77595484
C	-0.56791461	0.15001222	-3.16552401	H	-0.15363868	3.27348040	1.11516009
C	-1.25951382	0.46166905	-4.33596407	H	2.11391494	1.40605464	2.01535091
C	-1.06554866	-0.30682385	-5.47904249	H	2.31583575	2.94285469	1.14903378
C	-0.18181684	-1.38906117	-5.43353960	H	-0.15363868	3.27348040	-1.11516009
C	0.49135642	-1.70862549	-4.26232430	H	0.32536516	2.87281173	-2.77595484
C	0.30028533	-0.95014569	-3.09363105	H	2.31583575	2.94285469	-1.14903378
N	1.60247624	1.28477092	0.00000000	H	2.11391494	1.40605464	-2.01535091

C	0.30207766	2.50394344	1.74652464	C	-1.27318882	-1.28187738	0.00000000
C	1.66544833	2.06550580	1.26723928	O	-2.11982902	-2.09514661	0.00000000
C	0.30207766	2.50394344	-1.74652464				

TABLE S-CXLIV. *Meso*-(Fe(NH)S<sub>4</sub>)CO (**4m**) S12g–Cosmo Triplet

Fe	0.18304506	-0.21401780	0.00000000	C	1.75710024	2.07573692	-1.27333117
S	1.26772718	-1.33857025	1.88139340	H	-2.15096581	1.30160034	4.29763894
S	-0.87986724	1.21301343	1.78542128	H	-2.08528804	-0.15465893	6.30785577
S	-0.87986724	1.21301343	-1.78542128	H	-0.53946234	-2.11830340	6.34607930
S	1.26772718	-1.33857025	-1.88139340	H	0.88649360	-2.61369798	4.40118041
C	-0.64348536	0.18988256	3.23774136	H	-2.15096581	1.30160034	-4.29763894
C	-1.47091537	0.45238834	4.33545236	H	-2.08528804	-0.15465893	-6.30785577
C	-1.43692896	-0.36496931	5.45904541	H	-0.53946234	-2.11830340	-6.34607930
C	-0.57229990	-1.46217389	5.47670088	H	0.88649360	-2.61369798	-4.40118041
C	0.23412336	-1.74229175	4.38313917	H	2.55415390	0.73297875	0.00000000
C	0.22312917	-0.93028302	3.23152353	H	0.48332139	2.94573130	2.78909060
C	-0.64348536	0.18988256	-3.23774136	H	-0.04798685	3.30197078	1.13876404
C	-1.47091537	0.45238834	-4.33545236	H	2.20762535	1.41283446	2.01610552
C	-1.43692896	-0.36496931	-5.45904541	H	2.41103844	2.95056428	1.15052712
C	-0.57229990	-1.46217389	-5.47670088	H	-0.04798685	3.30197078	-1.13876404
C	0.23412336	-1.74229175	-4.38313917	H	0.48332139	2.94573130	-2.78909060
C	0.22312917	-0.93028302	-3.23152353	H	2.41103844	2.95056428	-1.15052712
N	1.70349459	1.29473162	0.00000000	H	2.20762535	1.41283446	-2.01610552
C	0.40823643	2.53703448	1.77709044	C	-1.05831163	-1.41754414	0.00000000
C	1.75710024	2.07573692	1.27333117	O	-1.89245056	-2.24151968	0.00000000
C	0.40823643	2.53703448	-1.77709044				

TABLE S-CXLV. *Meso*-(Fe(NH)S<sub>4</sub>)CO (**4m**) S12g–Cosmo Quintet

Fe	0.29752409	-0.39034866	0.00000000	C	1.80774304	2.17017442	-1.26637778
S	1.29730290	-1.32068830	1.97925944	H	-2.17203077	1.38130767	4.26167023
S	-0.83913171	1.22782351	1.77289142	H	-2.21610224	-0.07882254	6.27028154
S	-0.83913171	1.22782351	-1.77289142	H	-0.71520422	-2.07353554	6.36700774
S	1.29730290	-1.32068830	-1.97925944	H	0.79160101	-2.58450168	4.48443798
C	-0.64808232	0.24198429	3.25872377	H	-2.17203077	1.38130767	-4.26167023
C	-1.50792391	0.52112105	4.32614095	H	-2.21610224	-0.07882254	-6.27028154
C	-1.53617933	-0.29971594	5.44915562	H	-0.71520422	-2.07353554	-6.36700774
C	-0.69695078	-1.41362135	5.50013179	H	0.79160101	-2.58450168	-4.48443798
C	0.15379690	-1.70334324	4.44078403	H	2.68734410	0.87475698	0.00000000
C	0.19835415	-0.89139643	3.29228207	H	0.48635146	2.98764108	2.77403710
C	-0.64808232	0.24198429	-3.25872377	H	-0.04593470	3.32156198	1.12361211

C	-1.50792391	0.52112105	-4.32614095	H	2.27927277	1.53094682	2.01789096
C	-1.53617933	-0.29971594	-5.44915562	H	2.40950964	3.08900710	1.17900744
C	-0.69695078	-1.41362135	-5.50013179	H	-0.04593470	3.32156198	-1.12361211
C	0.15379690	-1.70334324	-4.44078403	H	0.48635146	2.98764108	-2.77403710
C	0.19835415	-0.89139643	-3.29228207	H	2.40950964	3.08900710	-1.17900744
N	1.81879226	1.40408769	0.00000000	H	2.27927277	1.53094682	-2.01789096
C	0.42827638	2.56978526	1.76444734	C	-1.23403393	-1.62392538	0.00000000
C	1.80774304	2.17017442	1.26637778	O	-2.05757926	-2.43412115	0.00000000
C	0.42827638	2.56978526	-1.76444734				

TABLE S-CXLVI. *trans*-(Fe(NH)<sub>4</sub>)CO (**4t**) S12g–Cosmo Singlet

Fe	8.45641912	10.04167805	1.80023031	H	8.90253459	5.78843073	6.82064969
S	9.86065657	8.79310285	3.05946366	C	9.32180702	7.07745306	5.14624239
S	6.76814526	8.52979325	2.33065483	H	10.37861579	7.19151775	5.38426103
S	7.16256382	11.06557094	0.25698011	C	8.78864824	7.72961428	4.03540409
S	10.06003997	11.67884662	1.34649786	C	7.91521367	11.02532595	3.10197882
C	9.08533199	12.98949484	0.67783531	O	7.54407204	11.70731107	3.98289331
C	9.54993215	14.31516587	0.64293977	N	9.15653438	8.86370780	0.18920785
H	10.54485047	14.54262107	1.02258635	H	9.99068336	9.38027317	-0.10475487
C	8.73938554	15.33773423	0.16154247	C	10.54526587	7.65203002	1.76656140
H	9.11396948	16.36090637	0.16702898	H	10.77693121	6.69924955	2.24888795
C	7.44812479	15.07454792	-0.30254386	H	11.48147462	8.13472698	1.46174208
H	6.81163251	15.88251321	-0.65889129	C	9.58091919	7.51477678	0.61585595
C	6.97365283	13.76604552	-0.29002141	H	8.68682977	6.96240252	0.92017468
H	5.96803508	13.53606667	-0.63866138	H	10.06322350	6.97724806	-0.21283297
C	7.79180954	12.74483556	0.18741924	C	7.86575042	10.29613716	-1.28608434
C	7.42714821	7.64612704	3.70312947	H	8.74741898	10.88190992	-1.56410560
C	6.61090976	6.84551468	4.52350555	H	7.10730871	10.36420894	-2.06984559
H	5.54854728	6.76240421	4.29921483	C	8.21683730	8.86767292	-0.94951173
C	7.14112843	6.18317897	5.62349412	H	7.32724854	8.29987897	-0.65526590
H	6.48312669	5.58257549	6.25086444	H	8.66051485	8.37978526	-1.82818674
C	8.49667099	6.29415379	5.94641501	H			

TABLE S-CXLVII. *trans*-(Fe(NH)<sub>4</sub>)CO (**4t**) S12g–Cosmo Triplet

Fe	8.50242632	10.02618639	1.74018456	H	8.86613408	5.95189729	7.07683340
S	10.03319111	8.43533247	3.04169548	C	9.34422932	6.99253917	5.25278482
S	6.77418952	8.48286317	2.44225778	H	10.41911372	6.97161126	5.42460762
S	7.15011016	11.14970007	-0.11857645	C	8.85007566	7.61041287	4.10060879
S	10.07324083	11.73413506	1.20954097	C	7.88904321	11.06645572	2.98702565
C	8.99501202	13.05485723	0.74511702	O	7.47676704	11.79510581	3.80859926



C	9.35277235	14.39191033	0.98417549	N	9.19451661	8.79094117	0.12442121
H	10.29582019	14.60498196	1.48437076	H	10.10894653	9.19424143	-0.09584141
C	8.51165888	15.43754552	0.61904266	C	10.39545580	7.27953051	1.64484217
H	8.80963276	16.46350590	0.83312078	H	10.45740287	6.26498289	2.04671207
C	7.28761369	15.18248791	-0.00004710	H	11.39897060	7.58979189	1.32902601
H	6.62360578	16.00011703	-0.27599610	C	9.40708129	7.37663983	0.50586752
C	6.91548620	13.86723585	-0.25811520	H	8.43725973	6.96079647	0.79291337
H	5.96174528	13.64910475	-0.73519706	H	9.79649330	6.80599201	-0.34982532
C	7.75834490	12.81360585	0.10174068	C	8.17357653	10.38422454	-1.45726894
C	7.46075943	7.68970902	3.85450538	H	9.12107474	10.92848387	-1.51070579
C	6.60164916	7.10687320	4.80613806	H	7.62968127	10.48850685	-2.39956958
H	5.52592760	7.16485674	4.64888933	C	8.37326474	8.92784091	-1.10115488
C	7.10020716	6.48309547	5.94207523	H	7.41060136	8.43471121	-0.91792091
H	6.40505452	6.05273043	6.66249661	H	8.85442286	8.41408759	-1.94475179
C	8.47502341	6.42380115	6.17714211				

TABLE S-CXLVIII. *trans*-(Fe(NH)S<sub>4</sub>)CO (**4t**) S12g–Cosmo Quintet

Fe	8.52230698	9.98467878	1.74805872	H	8.86955891	6.03454260	7.12348566
S	9.98977846	8.28288497	2.94595567	C	9.31690472	6.96421178	5.23341588
S	6.69825946	8.47389044	2.47047827	H	10.39553729	6.88026733	5.35342587
S	7.30392399	11.09657755	-0.17993931	C	8.80341334	7.56392782	4.08069638
S	10.08863512	11.91703671	1.34038480	C	7.94461794	11.13888580	3.22853103
C	8.95078603	13.13848311	0.77036354	O	7.56880155	11.88709110	4.02968633
C	9.18799555	14.50315662	1.01383058	N	9.31162671	8.70424817	-0.00991043
H	10.08322693	14.79121108	1.56224607	H	10.27319733	9.02553708	-0.14160360
C	8.29257844	15.47968602	0.59158312	C	10.25206464	7.07033880	1.56839934
H	8.50083508	16.52646477	0.81139541	H	10.15630313	6.06322983	1.98202015
C	7.13037926	15.13015175	-0.09631926	H	11.30293498	7.23676505	1.30279364
H	6.42491084	15.89328831	-0.42089065	C	9.34884692	7.28094817	0.36981605
C	6.87521369	13.78752588	-0.35838265	H	8.32404596	6.97307497	0.60125331
H	5.97049469	13.49286305	-0.88697568	H	9.72378117	6.65326035	-0.45394412
C	7.77076099	12.80416056	0.06566296	C	8.42772449	10.44729876	-1.50147324
C	7.40986898	7.71725111	3.89638817	H	9.38020279	10.98027550	-1.42053240
C	6.56845705	7.23769376	4.91704885	H	7.96439170	10.65116588	-2.47022638
H	5.49190150	7.35513300	4.80713291	C	8.59129370	8.95784843	-1.26999523
C	7.08459219	6.63764115	6.05904245	H	7.61037424	8.47063811	-1.20421956
H	6.40270656	6.28707869	6.83319225	H	9.11645026	8.51904831	-2.13105764
C	8.46189822	6.49483844	6.22501678				

TABLE S-CXLIX. *Meso*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5m**) S12g–Cosmo Singlet

Fe	0.30019961	-0.02420721	0.00000000	H	-1.82951233	-1.29239795	4.31285913
S	1.52494278	1.05712681	-1.62107470	H	-1.34750965	-0.00640675	6.39087733
S	-0.73999458	-1.13376067	-1.63134180	H	0.45017109	1.72548825	6.36757819
S	-0.73999458	-1.13376067	1.63134180	H	1.72821722	2.17304679	4.30702760
S	1.52494278	1.05712681	1.62107470	H	2.60149409	-1.13274941	0.00000000
C	-0.30510243	-0.29304672	-3.16768888	H	0.23332642	-3.05366070	-2.75928522
C	-1.03803621	-0.54336978	-4.32593299	H	-0.27231091	-3.40330187	-1.09401469
C	-0.76954225	0.17609378	-5.48649913	H	2.19324866	-1.82191176	-2.01628597
C	0.23780061	1.14675938	-5.46879339	H	2.21753314	-3.36634890	-1.13912600
C	0.96072024	1.39976167	-4.31091864	H	-0.27231091	-3.40330187	1.09401469
C	0.69377995	0.69177331	-3.12434132	H	0.23332642	-3.05366070	2.75928522
C	-0.30510243	-0.29304672	3.16768888	H	2.21753314	-3.36634890	1.13912600
C	-1.03803621	-0.54336978	4.32593299	H	2.19324866	-1.82191176	2.01628597
C	-0.76954225	0.17609378	5.48649913	P	-1.09628592	1.73419534	0.00000000
C	0.23780061	1.14675938	5.46879339	C	-2.29602705	1.90177466	-1.40473858
C	0.96072024	1.39976167	4.31091864	H	-1.75242496	1.97722158	-2.35264373
C	0.69377995	0.69177331	3.12434132	H	-2.95561633	1.02687903	-1.43899857
N	1.71083798	-1.62633843	0.00000000	H	-2.89929864	2.80615181	-1.25835810
C	0.26366944	-2.68967460	-1.72822357	C	-2.29602705	1.90177466	1.40473858
C	1.67440836	-2.41841517	-1.26058011	H	-2.95561633	1.02687903	1.43899857
C	0.26366944	-2.68967460	1.72822357	H	-1.75242496	1.97722158	2.35264373
C	1.67440836	-2.41841517	1.26058011	H	-2.89929864	2.80615181	1.25835810
H	-1.82951233	-1.29239795	-4.31285913	C	-0.34247081	3.44023421	0.00000000
H	-1.34750965	-0.00640675	-6.39087733	H	-0.67162171	3.98432579	-0.89205208
H	0.45017109	1.72548825	-6.36757819	H	-0.67162171	3.98432579	0.89205208
H	1.72821722	2.17304679	-4.30702760	H	0.74721785	3.36915671	0.00000000

TABLE S-CL. *Meso*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5m**) S12g–Cosmo Triplet

Fe	0.39918962	0.04494937	0.00000000	H	-1.86997746	-1.43290245	4.38234169
S	1.51262882	1.09178051	-1.80469868	H	-1.52278056	-0.11220674	6.45927879
S	-0.77842397	-1.26430076	-1.75638903	H	0.19467108	1.70461592	6.47735866
S	-0.77842397	-1.26430076	1.75638903	H	1.50955324	2.18950209	4.45198724
S	1.51262882	1.09178051	1.80469868	H	2.66998762	-1.09502119	0.00000000
C	-0.35963785	-0.38485897	-3.26607404	H	0.36909954	-3.16107681	-2.73033182
C	-1.11663861	-0.64624343	-4.41079820	H	-0.15903787	-3.42930670	-1.06269534
C	-0.92435306	0.09307699	-5.57299685	H	2.23407363	-1.75953446	-2.02206564
C	0.03556442	1.10856601	-5.57868233	H	2.32951233	-3.30293388	-1.14780926
C	0.78022105	1.38024296	-4.43956216	H	-0.15903787	-3.42930670	1.06269534

C	0.60126707	0.65007414	-3.24840375	H	0.36909954	-3.16107681	2.73033182
C	-0.35963785	-0.38485897	3.26607404	H	2.32951233	-3.30293388	1.14780926
C	-1.11663861	-0.64624343	4.41079820	H	2.23407363	-1.75953446	2.02206564
C	-0.92435306	0.09307699	5.57299685	P	-0.96386884	1.89588386	0.00000000
C	0.03556442	1.10856601	5.57868233	C	-2.14601800	2.04592995	-1.41337105
C	0.78022105	1.38024296	4.43956216	H	-1.59502966	2.09397766	-2.35839377
C	0.60126707	0.65007414	3.24840375	H	-2.81468373	1.17737757	-1.42778795
N	1.77804191	-1.58749364	0.00000000	H	-2.73718519	2.96139759	-1.28570703
C	0.35021479	-2.72358481	-1.72746473	C	-2.14601800	2.04592995	1.41337105
C	1.74709932	-2.37661863	-1.26182209	H	-2.81468373	1.17737757	1.42778795
C	0.35021479	-2.72358481	1.72746473	H	-1.59502966	2.09397766	2.35839377
C	1.74709932	-2.37661863	1.26182209	H	-2.73718519	2.96139759	1.28570703
H	-1.86997746	-1.43290245	-4.38234169	C	-0.13652826	3.55842224	0.00000000
H	-1.52278056	-0.11220674	-6.45927879	H	-0.43883875	4.11552259	-0.89377296
H	0.19467108	1.70461592	-6.47735866	H	-0.43883875	4.11552259	0.89377296
H	1.50955324	2.18950209	-4.45198724	H	0.94870103	3.42990308	0.00000000

TABLE S-CLI. *Meso*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5m**) S12g–Cosmo Quintet

Fe	0.50078953	0.13479838	0.00000000	H	-1.78671247	-1.39846889	4.47418993
S	1.64741397	1.05140058	-1.86156989	H	-1.39867897	-0.07190037	6.53828601
S	-0.75417654	-1.25610433	-1.84078592	H	0.33724254	1.72711177	6.52349762
S	-0.75417654	-1.25610433	1.84078592	H	1.64381451	2.17125553	4.48331506
S	1.64741397	1.05140058	1.86156989	H	2.67443112	-1.37038598	0.00000000
C	-0.27621412	-0.37951058	-3.33255775	H	0.26074203	-3.24928748	-2.76218617
C	-1.02191641	-0.62308610	-4.48975674	H	-0.33018332	-3.44161642	-1.10745685
C	-0.80766207	0.12101702	-5.64434424	H	2.22855537	-2.00746829	-2.01233513
C	0.16185839	1.12510703	-5.63203240	H	2.15892146	-3.56981120	-1.17205140
C	0.89976854	1.37575501	-4.48303195	H	-0.33018332	-3.44161642	1.10745685
C	0.70003641	0.64030606	-3.29964769	H	0.26074203	-3.24928748	2.76218617
C	-0.27621412	-0.37951058	3.33255775	H	2.15892146	-3.56981120	1.17205140
C	-1.02191641	-0.62308610	4.48975674	H	2.22855537	-2.00746829	2.01233513
C	-0.80766207	0.12101702	5.64434424	P	-1.32465766	1.99399226	0.00000000
C	0.16185839	1.12510703	5.63203240	C	-2.49122414	2.12460009	-1.42936067
C	0.89976854	1.37575501	4.48303195	H	-1.91389335	2.15824941	-2.36089836
C	0.70003641	0.64030606	3.29964769	H	-3.14343457	1.24361839	-1.44892699
N	1.76407321	-1.82459469	0.00000000	H	-3.10237359	3.03174377	-1.34167494
C	0.25847927	-2.79424320	-1.76690802	C	-2.49122414	2.12460009	1.42936067
C	1.67535718	-2.58411962	-1.26437378	H	-3.14343457	1.24361839	1.44892699
C	0.25847927	-2.79424320	1.76690802	H	-1.91389335	2.15824941	2.36089836
C	1.67535718	-2.58411962	1.26437378	H	-3.10237359	3.03174377	1.34167494

H	-1.78671247	-1.39846889	-4.47418993	C	-0.51232348	3.66728618	0.00000000
H	-1.39867897	-0.07190037	-6.53828601	H	-0.81311947	4.22734568	-0.89213199
H	0.33724254	1.72711177	-6.52349762	H	-0.81311947	4.22734568	0.89213199
H	1.64381451	2.17125553	-4.48331506	H	0.57503046	3.54280411	0.00000000

TABLE S-CLII. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) S12g–Cosmo Singlet

Fe	3.00354339	3.06541796	7.91063894	H	1.70258017	2.99944544	5.75918893
S	3.25638269	5.15142145	8.87231116	H	5.16457097	0.26052560	10.67374482
S	4.77364287	3.53327627	6.62559179	H	5.14616037	0.12891128	8.88583852
S	1.04741534	2.75708543	8.92747154	H	3.64962012	-0.14086804	9.80700911
S	2.70528427	0.94137193	7.00190454	H	6.31218444	2.44107877	10.84430129
P	4.19095733	2.25159257	9.64772464	H	5.85856206	3.99984074	10.08581249
C	4.57530724	0.44155925	9.76644026	H	6.53868554	2.68764309	9.08805567
C	5.89593309	2.91508559	9.94685954	H	4.11131722	2.13982346	12.09733639
C	3.44373419	2.53037849	11.31953527	H	2.47580973	2.01908373	11.38429069
C	5.51477836	5.02803107	7.30593751	H	3.29055431	3.60486443	11.46670793
C	6.79404795	5.40491005	6.90334422	H	7.31354496	4.82247270	6.14250799
C	7.40666428	6.51014330	7.48477190	H	8.41090564	6.80273440	7.18277839
C	6.72057222	7.22601534	8.47217326	H	7.19406362	8.08651417	8.94465393
C	5.44871799	6.84393773	8.87533806	H	4.93870860	7.39990934	9.66123877
C	4.81652210	5.72149616	8.30739593	H	-0.56944287	1.06817761	10.64553068
C	0.81184468	0.97616480	8.99792302	H	-0.79752885	-1.41210949	10.79943606
C	-0.02943337	0.41882474	9.95703932	H	0.47088520	-2.85379681	9.20820536
C	-0.15855156	-0.96553734	10.03943222	H	1.96314652	-1.85161183	7.52042734
C	0.55525140	-1.76901890	9.14517136	H	3.80559935	3.30614334	4.46513200
C	1.39434077	-1.20696281	8.18928092	H	4.60723568	4.89240612	4.61304710
C	1.55798355	0.18745839	8.10478349	H	2.75502376	5.71666213	6.06537035
N	1.86230333	3.84335456	6.31790220	H	2.03900143	5.05609176	4.57358212
C	3.93209335	4.18785900	5.10553437	H	-1.06660172	3.57259890	8.01495247
C	2.60703669	4.80335988	5.48091208	H	-0.30571522	2.34018690	6.96064724
C	-0.12973468	3.23836685	7.56137296	H	-0.09172864	4.59455183	5.89891500
C	0.53998093	4.32684211	6.75822477	H	0.69480867	5.22658261	7.36380569

TABLE S-CLIII. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) S12g–Cosmo Triplet

Fe	3.04561033	3.04142877	7.90121694	H	1.78324266	3.11175378	5.64313771
S	3.43937588	5.08606753	8.90229382	H	5.04869968	0.20653206	10.82037507
S	4.89609925	3.71055329	6.33936510	H	5.05553294	0.05634044	9.03343241
S	0.64702185	2.70044759	8.91732933	H	3.53484793	-0.15339155	9.93224949
S	2.64195922	0.93387296	7.06088241	H	6.27458587	2.35896369	10.97344224
P	4.15875002	2.21363310	9.75900956	H	5.87355048	3.91863955	10.18457707

C	4.48040036	0.39618601	9.90140427	H	6.51062327	2.56630910	9.21121426
C	5.87716106	2.83108664	10.06625886	H	3.99167447	2.16273577	12.20101862
C	3.35594686	2.54279616	11.39153089	H	2.38289944	2.03897497	11.42541305
C	5.62695388	5.11895113	7.17907150	H	3.20894301	3.62155521	11.50973110
C	6.88791130	5.55923560	6.77619775	H	7.37863429	5.07064678	5.93508692
C	7.51828629	6.60360870	7.44547097	H	8.50874734	6.93370788	7.13612612
C	6.86919536	7.20836781	8.52355796	H	7.35164308	8.02323674	9.06307268
C	5.61551043	6.76986297	8.92969726	H	5.13127038	7.23547968	9.78724963
C	4.96934108	5.70580923	8.27551459	H	-0.81572250	0.90384585	10.58240036
C	0.64837760	0.91713720	9.00686295	H	-0.74135404	-1.56201217	10.88517759
C	-0.15841715	0.29507029	9.96326139	H	0.75870418	-2.93043596	9.43262943
C	-0.11893894	-1.08567433	10.12906903	H	2.20175254	-1.83466493	7.75631815
C	0.71968317	-1.84780810	9.31397414	H	3.74048144	3.71870845	4.27603316
C	1.52690497	-1.23272475	8.36338447	H	4.45476542	5.31878434	4.57585282
C	1.52960324	0.16246906	8.20190444	H	2.67673939	5.83243341	6.24174831
N	1.85848055	3.91172479	6.27524470	H	1.93103922	5.34277459	4.70091857
C	3.87311496	4.50941832	5.02514177	H	-1.25478668	3.31430484	7.53487494
C	2.54169971	4.99585075	5.54873249	H	-0.14713403	2.19126848	6.69379744
C	-0.20687814	3.08591988	7.32205678	H	-0.10495596	4.58126260	5.79728599
C	0.48319545	4.26606240	6.67195089	H	0.53495004	5.11807640	7.36097036

TABLE S-CLIV. *trans*-(Fe(NH)S<sub>4</sub>)PMe<sub>3</sub> (**5t**) S12g-Cosmo Quintet

Fe	3.03093413	3.01680616	7.81395243	H	1.72975236	3.18514273	5.40840685
S	3.35951140	5.22653657	8.90182497	H	5.17838832	0.08011638	10.95907349
S	4.83113904	3.85488533	6.29680920	H	5.24504084	-0.07722284	9.17420837
S	0.63909213	2.72827279	8.75471951	H	3.69390644	-0.27967229	10.01862233
S	2.54596752	0.74122651	6.92660527	H	6.38945385	2.37557192	11.09469580
P	4.30461349	2.08043548	9.83236675	H	5.93627121	3.86058298	10.19281742
C	4.64148720	0.26964968	10.02080942	H	6.65902785	2.48169101	9.32679716
C	5.99263970	2.76765681	10.14954448	H	4.06501527	2.10634347	12.28228437
C	3.45772934	2.44758977	11.43425137	H	2.48591808	1.93886681	11.45015738
C	5.59196998	5.18705201	7.22306994	H	3.29355739	3.52911376	11.50189557
C	6.88163208	5.57633067	6.85614479	H	7.34743189	5.11876751	5.98433903
C	7.57187342	6.52700924	7.60036856	H	8.58027094	6.82080633	7.31357460
C	6.95478925	7.08642473	8.72037961	H	7.48314892	7.82656008	9.32105876
C	5.67387497	6.69814569	9.09024382	H	5.21318861	7.13249332	9.97611934
C	4.95416851	5.73360374	8.35884042	H	-0.70431216	1.11267507	10.63613937
C	0.67358390	0.95671966	8.99375787	H	-0.62110169	-1.31042755	11.18491999
C	-0.08172508	0.43891390	10.04976494	H	0.81172615	-2.82414436	9.80588566
C	-0.03523050	-0.91667470	10.35595536	H	2.16080322	-1.91309429	7.95674192

C	0.76598883	-1.75847346	9.58251413	H	3.75300284	3.93434923	4.20306226
C	1.52165447	-1.24761686	8.53469608	H	4.38381175	5.54295811	4.61772079
C	1.51470320	0.12350574	8.21651662	H	2.50188071	5.88968192	6.21838778
N	1.75106074	3.95200417	6.08322268	H	1.87306838	5.48882539	4.60041458
C	3.81262047	4.69058480	4.99555441	H	-1.30346622	3.16588332	7.36939803
C	2.43218912	5.09639495	5.46608717	H	-0.11679947	2.11057001	6.54057840
C	-0.24365861	3.01063912	7.15047000	H	-0.26085422	4.50538863	5.61711172
C	0.36486824	4.22789232	6.48007545	H	0.37116069	5.08424028	7.16764339

TABLE S-CLV. *Meso*-(Fe(NH)<sub>4</sub>)NH<sub>3</sub> (**6m**) S12g–Cosmo Singlet

Fe	-0.16539594	-0.38986975	0.00000000	N	-1.94614564	-1.44241124	0.00000000
S	0.64228095	-1.84604224	1.59452535	H	-1.83396853	1.37224921	4.35599078
S	-0.87607728	0.93140329	1.65338045	H	-1.70115510	-0.00687772	6.42637825
S	-0.87607728	0.93140329	-1.65338045	H	-0.48673988	-2.18702342	6.36791527
S	0.64228095	-1.84604224	-1.59452535	H	0.55335959	-2.98412046	4.27925638
C	-0.69888175	-0.02741509	3.17553340	H	-1.83396853	1.37224921	-4.35599078
C	-1.29987840	0.42235224	4.35153352	H	-1.70115510	-0.00687772	-6.42637825
C	-1.22456219	-0.34785043	5.50886586	H	-0.48673988	-2.18702342	-6.36791527
C	-0.54571668	-1.57079069	5.47089951	H	0.55335959	-2.98412046	-4.27925638
C	0.04147638	-2.02246147	4.29630012	H	2.31419794	-0.01668972	0.00000000
C	-0.03499661	-1.26442829	3.11172838	H	0.61468753	2.48866609	2.77994219
C	-0.69888175	-0.02741509	-3.17553340	H	0.20808414	2.97634209	1.12119800
C	-1.29987840	0.42235224	-4.35153352	H	2.12917218	0.75245671	2.01313631
C	-1.22456219	-0.34785043	-5.50886586	H	2.58525576	2.22596293	1.13083538
C	-0.54571668	-1.57079069	-5.47089951	H	0.20808414	2.97634209	-1.12119800
C	0.04147638	-2.02246147	-4.29630012	H	0.61468753	2.48866609	-2.77994219
C	-0.03499661	-1.26442829	-3.11172838	H	2.58525576	2.22596293	-1.13083538
N	1.59218268	0.70246798	0.00000000	H	2.12917218	0.75245671	-2.01313631
C	0.52647792	2.13697172	1.74812434	H	-1.99483630	-2.05408880	0.81508748
C	1.79444058	1.47449155	1.26266825	H	-1.99483630	-2.05408880	-0.81508748
C	0.52647792	2.13697172	-1.74812434	H	-2.79590799	-0.88011278	0.00000000
C	1.79444058	1.47449155	-1.26266825				

TABLE S-CLVI. *Meso*-(Fe(NH)<sub>4</sub>)NH<sub>3</sub> (**6m**) S12g–Cosmo Triplet

Fe	-0.36405913	-0.53365620	0.00000000	N	-2.58211245	-1.48623717	0.00000000
S	0.39167530	-1.98653192	1.59362152	H	-1.83073685	1.32563346	4.47422009
S	-1.04016720	0.84719796	1.72591689	H	-1.65869603	-0.07014932	6.52745481
S	-1.04016720	0.84719796	-1.72591689	H	-0.53815474	-2.29699862	6.40589644
S	0.39167530	-1.98653192	-1.59362152	H	0.37799131	-3.11868706	4.26693660
C	-0.79803739	-0.10519303	3.23694283	H	-1.83073685	1.32563346	-4.47422009

C	-1.33079082	0.35813182	4.44103010	H	-1.65869603	-0.07014932	-6.52745481
C	-1.23501450	-0.42323438	5.58866526	H	-0.53815474	-2.29699862	-6.40589644
C	-0.60922748	-1.67174660	5.51611400	H	0.37799131	-3.11868706	-4.26693660
C	-0.09140796	-2.13664310	4.31378414	H	2.24815874	0.18370441	0.00000000
C	-0.18812145	-1.36562603	3.14153958	H	0.33834800	2.53353980	2.78305798
C	-0.79803739	-0.10519303	-3.23694283	H	-0.13718285	2.94408397	1.12612305
C	-1.33079082	0.35813182	-4.44103010	H	2.01672307	0.94236625	2.01048619
C	-1.23501450	-0.42323438	-5.58866526	H	2.30649101	2.48615515	1.18328848
C	-0.60922748	-1.67174660	-5.51611400	H	-0.13718285	2.94408397	-1.12612305
C	-0.09140796	-2.13664310	-4.31378414	H	0.33834800	2.53353980	-2.78305798
C	-0.18812145	-1.36562603	-3.14153958	H	2.30649101	2.48615515	-1.18328848
N	1.51437881	0.88565009	0.00000000	H	2.01672307	0.94236625	-2.01048619
C	0.27307716	2.15079330	1.75997315	H	-2.66343958	-2.09180274	0.81498588
C	1.61271317	1.63409881	1.26397267	H	-2.66343958	-2.09180274	-0.81498588
C	0.27307716	2.15079330	-1.75997315	H	-3.40577260	-0.88655657	0.00000000
C	1.61271317	1.63409881	-1.26397267				

TABLE S-CLVII. *Meso*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6m**) S12g–Cosmo Quintet

Fe	-0.10332450	-0.65537544	0.00000000	N	-2.17611073	-1.52401037	0.00000000
S	0.69711271	-1.92513783	1.85765662	H	-1.75979376	1.46768686	4.52946197
S	-0.90521589	1.00466470	1.86908209	H	-1.70580974	0.10705838	6.60774952
S	-0.90521589	1.00466470	-1.86908209	H	-0.58361477	-2.12668822	6.57419439
S	0.69711271	-1.92513783	-1.85765662	H	0.45624075	-2.96144839	4.50345185
C	-0.66145092	0.03408854	3.36060150	H	-1.75979376	1.46768686	-4.52946197
C	-1.25828137	0.50088055	4.53688103	H	-1.70580974	0.10705838	-6.60774952
C	-1.23088057	-0.26124899	5.69978508	H	-0.58361477	-2.12668822	-6.57419439
C	-0.60488505	-1.50896057	5.67654890	H	0.45624075	-2.96144839	-4.50345185
C	-0.01760414	-1.98074060	4.50977551	H	2.41164858	0.14712239	0.00000000
C	-0.03337944	-1.23144044	3.31663851	H	0.63557892	2.63888311	2.76263280
C	-0.66145092	0.03408854	-3.36060150	H	0.10891314	2.97579651	1.10881419
C	-1.25828137	0.50088055	-4.53688103	H	2.16633471	0.88424883	2.01272143
C	-1.23088057	-0.26124899	-5.69978508	H	2.53636772	2.40005854	1.16669084
C	-0.60488505	-1.50896057	-5.67654890	H	0.10891314	2.97579651	-1.10881419
C	-0.01760414	-1.98074060	-4.50977551	H	0.63557892	2.63888311	-2.76263280
C	-0.03337944	-1.23144044	-3.31663851	H	2.53636772	2.40005854	-1.16669084
N	1.66166313	0.83552590	0.00000000	H	2.16633471	0.88424883	-2.01272143
C	0.49724722	2.19498860	1.77205321	H	-2.31479274	-2.11811290	0.81612202
C	1.79476338	1.59180803	1.26472622	H	-2.31479274	-2.11811290	-0.81612202
C	0.49724722	2.19498860	-1.77205321	H	-2.93545680	-0.84467749	0.00000000
C	1.79476338	1.59180803	-1.26472622				

TABLE S-CLVIII. *trans*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6t**) S12g–Cosmo Singlet

Fe	2.94750828	3.11441343	7.83391194	H	1.71447290	3.02342722	5.67301823
S	3.22287942	5.17734796	8.84929354	H	7.32997063	4.81379525	6.18346155
S	4.74250343	3.58416725	6.57626823	H	8.47290035	6.71423056	7.31924791
S	1.00200823	2.77269881	8.87541902	H	7.27422021	7.95599207	9.12327453
S	2.75276417	0.92310896	7.04139916	H	4.99032243	7.31008309	9.78362741
C	5.52558151	5.01789839	7.33941485	H	-0.60890680	1.10243655	10.61699003
C	6.82020307	5.37581112	6.96589562	H	-0.74810476	-1.37424791	10.88863365
C	7.45751769	6.43825193	7.59881701	H	0.63029879	-2.84098701	9.41579842
C	6.78217745	7.12961301	8.61051024	H	2.13115871	-1.86460049	7.72112945
C	5.49521415	6.76754094	8.98499999	H	3.82257271	3.46407523	4.38687304
C	4.83441729	5.68992915	8.36329186	H	4.57582054	5.05949595	4.64492632
C	0.83042251	0.98696055	9.02162964	H	2.67810732	5.75732517	6.09117939
C	-0.02007910	0.44240435	9.98087029	H	1.99167446	5.13006862	4.56914073
C	-0.09996793	-0.94051202	10.12893091	H	-1.12444768	3.47142127	7.89134143
C	0.67502749	-1.75799138	9.30142576	H	-0.27114831	2.26299581	6.87913648
C	1.52253608	-1.21017862	8.34423196	H	-0.12846995	4.53315933	5.80977457
C	1.63228903	0.18413304	8.19021069	H	0.60463581	5.18966456	7.29247842
N	1.84214485	3.84819653	6.26805529	N	4.06094907	2.33693828	9.40997483
C	3.91229154	4.30859767	5.08106680	H	3.66160652	2.56755319	10.31824566
C	2.56451519	4.86415335	5.46940776	H	4.13079888	1.32035544	9.36062111
C	-0.15834518	3.17524659	7.47446671	H	5.01552238	2.69259619	9.43810642
C	0.49083994	4.28556999	6.68378488				

TABLE S-CLIX. *trans*-(Fe(NH)S<sub>4</sub>)NH<sub>3</sub> (**6t**) S12g–Cosmo Triplet

Fe	2.94694629	3.10945133	7.80723241	H	1.63320609	3.12985535	5.42008844
S	3.25408183	5.13393955	8.88330165	H	7.29672665	4.90523602	6.09748136
S	4.70496201	3.66545152	6.48875766	H	8.48078138	6.72252700	7.32343529
S	0.94647584	2.78323420	8.78989445	H	7.33854594	7.85967758	9.22604552
S	2.79196298	0.88349899	7.09200755	H	5.05875669	7.19345560	9.89512612
C	5.51980078	5.05449629	7.30345514	H	-0.69623639	1.15900136	10.54627449
C	6.80830928	5.42231257	6.92296982	H	-0.79270328	-1.30531094	10.92560408
C	7.46886007	6.43883191	7.60829563	H	0.65906222	-2.80721651	9.56530475
C	6.82633888	7.07190570	8.67388663	H	2.19470390	-1.87419606	7.87396642
C	5.54151028	6.69880452	9.05305006	H	3.79554128	3.67092427	4.29578364
C	4.86334318	5.66971511	8.37851312	H	4.50940456	5.26014674	4.66064448
C	0.79550951	1.00286973	9.00298778	H	2.54564367	5.83168462	6.09427878
C	-0.07442613	0.48438716	9.95892637	H	1.97861067	5.34930887	4.47649027
C	-0.12881709	-0.89254633	10.16763917	H	-1.18393037	3.32564088	7.72742825
C	0.68560945	-1.72978306	9.40279813	H	-0.21019661	2.18796747	6.74312946



C	1.55243989	-1.20672680	8.44739982	H	-0.32154344	4.50308618	5.71580433
C	1.63768452	0.17980967	8.23718205	H	0.45814367	5.16517847	7.16552509
N	1.71449777	3.92419326	6.05639762	N	4.24741737	2.17749558	9.66753598
C	3.84973062	4.47502921	5.03970049	H	3.86088567	2.44721670	10.56982023
C	2.46982315	4.99119505	5.39592303	H	4.27303220	1.15979619	9.64459032
C	-0.18634024	3.10873006	7.33556562	H	5.21457928	2.49646458	9.66858481
C	0.37437650	4.27017358	6.53707260				

TABLE S-CLX. *trans*-(Fe(NH)<sub>4</sub>)NH<sub>3</sub> (**6t**) S12g–Cosmo Quintet

Fe	2.97674215	3.09303520	7.84967772	H	1.80980312	3.15908234	5.41357903
S	3.37805641	5.25122428	8.92665925	H	7.38876381	5.08896213	6.02850469
S	4.84414886	3.89604844	6.27701903	H	8.68337636	6.68033094	7.43308346
S	0.56113850	2.67845234	8.72596719	H	7.61490506	7.64816702	9.47532134
S	2.64212379	0.73002171	7.04799800	H	5.31256439	7.02560481	10.08676131
C	5.62757831	5.17965200	7.25784853	H	-0.82269599	1.05417558	10.56770352
C	6.93572193	5.53116539	6.91479985	H	-0.64890466	-1.34170298	11.21108198
C	7.66103344	6.41915445	7.70142977	H	0.94329231	-2.82131009	9.97641991
C	7.05979071	6.95787382	8.84020122	H	2.33979742	-1.90761148	8.16486045
C	5.76122256	6.60749922	9.18662922	H	3.76268149	4.03938774	4.19404403
C	5.00499334	5.70500594	8.41273977	H	4.34468862	5.64449399	4.68242171
C	0.65552361	0.91440400	9.01259764	H	2.43786243	5.88958191	6.26069603
C	-0.13460047	0.39411693	10.04183310	H	1.82990657	5.49027640	4.63281399
C	-0.03777161	-0.94606361	10.40134607	H	-1.31684965	2.98578314	7.22616510
C	0.85254582	-1.76868552	9.70827839	H	-0.02925821	1.98500207	6.48538786
C	1.63913923	-1.25499147	8.68399603	H	-0.25379870	4.34997457	5.50459223
C	1.57825791	0.10201426	8.30883370	H	0.25034635	4.99364355	7.07479342
N	1.75637792	3.92649889	6.08734497	N	4.12695546	2.16753382	9.53557346
C	3.79666948	4.76079656	5.01955260	H	3.79604347	2.49791664	10.44061578
C	2.40158469	5.10836547	5.49404678	H	4.07722444	1.14966456	9.54325447
C	-0.23973105	2.88707200	7.06833111	H	5.11510984	2.41407644	9.49384942
C	0.33331764	4.12588917	6.40803009				

TABLE S-CLXI. *Meso*-(Fe(NH)<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) S12g–Cosmo Singlet

Fe	0.03078065	0.34727892	0.00000000	C	-0.62278341	0.08641941	-3.16323638
N	-1.49325564	1.78909483	0.00000000	C	-1.35106254	-0.20942031	-4.31513671
H	-2.11060758	1.66188432	0.80209195	H	-2.08032118	-1.01914458	-4.29972866
H	-2.11060758	1.66188432	-0.80209195	C	-1.15354025	0.53737473	-5.47296860
N	-1.18582218	3.23117586	0.00000000	H	-1.72859241	0.31853824	-6.37114061
H	-0.53892364	3.31470014	0.79344307	C	-0.22178877	1.58052173	-5.45992438
H	-0.53892364	3.31470014	-0.79344307	H	-0.06509515	2.17969643	-6.35672053

S	1.14041560	1.55241290	1.63153548	C	0.49498975	1.87958573	-4.30860825
S	-0.95554382	-0.81369998	1.63369346	H	1.20400313	2.70687180	-4.30983224
S	1.14041560	1.55241290	-1.63153548	C	0.29972335	1.14534277	-3.12379839
S	-0.95554382	-0.81369998	-1.63369346	C	0.16871441	-2.28335061	1.74193561
N	1.51485772	-1.10423999	0.00000000	H	-0.31279138	-3.04246014	1.11705666
H	2.37181847	-0.55304579	0.00000000	H	0.17409244	-2.63794382	2.77645755
C	-0.62278341	0.08641941	3.16323638	C	1.54932832	-1.90114705	1.26317043
C	-1.35106254	-0.20942031	4.31513671	H	2.16476199	-2.80204592	1.13266897
H	-2.08032118	-1.01914458	4.29972866	H	2.02615671	-1.26605921	2.01507786
C	-1.15354025	0.53737473	5.47296860	C	0.16871441	-2.28335061	-1.74193561
H	-1.72859241	0.31853824	6.37114061	H	0.17409244	-2.63794382	-2.77645755
C	-0.22178877	1.58052173	5.45992438	H	-0.31279138	-3.04246014	-1.11705666
H	-0.06509515	2.17969643	6.35672053	C	1.54932832	-1.90114705	-1.26317043
C	0.49498975	1.87958573	4.30860825	H	2.02615671	-1.26605921	-2.01507786
H	1.20400313	2.70687180	4.30983224	H	2.16476199	-2.80204592	-1.13266897
C	0.29972335	1.14534277	3.12379839				

TABLE S-CLXII. *Meso*-(Fe(NH)<sub>4</sub>)<sub>2</sub>N<sub>2</sub>H<sub>4</sub> (**7m**) S12g–Cosmo Triplet

Fe	0.03017580	0.40304150	0.00000000	C	-0.48363837	0.07477857	-3.23921988
N	-1.94982342	1.87872317	0.00000000	C	-1.09700931	-0.26770759	-4.44488092
H	-2.56912644	1.76238831	0.80315824	H	-1.80439705	-1.09588692	-4.47565417
H	-2.56912644	1.76238831	-0.80315824	C	-0.81743438	0.46075833	-5.59665954
N	-1.58655012	3.31318510	0.00000000	H	-1.30157971	0.20353215	-6.53731020
H	-0.93251826	3.37180630	0.78857782	C	0.07546120	1.53461455	-5.52652027
H	-0.93251826	3.37180630	-0.78857782	H	0.29411460	2.11932366	-6.41982968
S	1.09350192	1.64479560	1.59774804	C	0.67460733	1.88145849	-4.32232664
S	-0.95177873	-0.77703117	1.72189884	H	1.35543725	2.73083824	-4.27787205
S	1.09350192	1.64479560	-1.59774804	C	0.39817995	1.16164407	-3.14660751
S	-0.95177873	-0.77703117	-1.72189884	C	0.00620884	-2.36062690	1.75114594
N	1.51987326	-1.42050912	0.00000000	H	-0.57924324	-3.03009274	1.11228136
H	2.40468037	-0.92231149	0.00000000	H	-0.02597043	-2.75136132	2.77263160
C	-0.48363837	0.07477857	3.23921988	C	1.43168005	-2.17259646	1.26296088
C	-1.09700931	-0.26770759	4.44488092	H	1.90628431	-3.16372746	1.18445426
H	-1.80439705	-1.09588692	4.47565417	H	1.98283085	-1.59626476	2.01348927
C	-0.81743438	0.46075833	5.59665954	C	0.00620884	-2.36062690	-1.75114594
H	-1.30157971	0.20353215	6.53731020	H	-0.02597043	-2.75136132	-2.77263160
C	0.07546120	1.53461455	5.52652027	H	-0.57924324	-3.03009274	-1.11228136
H	0.29411460	2.11932366	6.41982968	C	1.43168005	-2.17259646	-1.26296088
C	0.67460733	1.88145849	4.32232664	H	1.98283085	-1.59626476	-2.01348927
H	1.35543725	2.73083824	4.27787205	H	1.90628431	-3.16372746	-1.18445426

C	0.39817995	1.16164407	3.14660751			
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TABLE S-CLXIII. *Meso*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7m**) S12g–Cosmo Quintet

Fe	0.15248825	0.56899942	0.00000000	C	-0.60482367	0.00630144	-3.33929312
N	-1.62944576	1.94395908	0.00000000	C	-1.33034631	-0.30381124	-4.49458971
H	-2.24378562	1.81688510	0.80549879	H	-2.01965736	-1.14691231	-4.47723429
H	-2.24378562	1.81688510	-0.80549879	C	-1.19098960	0.45843525	-5.64900311
N	-1.27044398	3.37607570	0.00000000	H	-1.76678578	0.21345581	-6.54012490
H	-0.62457838	3.44456129	0.79487450	C	-0.31870652	1.54835834	-5.63970123
H	-0.62457838	3.44456129	-0.79487450	H	-0.20399201	2.16495779	-6.53101882
S	1.18465429	1.61775306	1.87531580	C	0.39816513	1.86534504	-4.49348585
S	-0.98897618	-0.91919252	1.84898447	H	1.06500943	2.72656566	-4.49604866
S	1.18465429	1.61775306	-1.87531580	C	0.27134728	1.11482829	-3.30889824
S	-0.98897618	-0.91919252	-1.84898447	C	0.18021290	-2.34331010	1.76948193
N	1.58276756	-1.22743509	0.00000000	H	-0.34038056	-3.04646337	1.11017947
H	2.44949375	-0.69347408	0.00000000	H	0.22937558	-2.79578205	2.76453731
C	-0.60482367	0.00630144	3.33929312	C	1.56827234	-1.99096801	1.26747212
C	-1.33034631	-0.30381124	4.49458971	H	2.14865542	-2.92243216	1.17573554
H	-2.01965736	-1.14691231	4.47723429	H	2.05963194	-1.35925685	2.01419625
C	-1.19098960	0.45843525	5.64900311	C	0.18021290	-2.34331010	-1.76948193
H	-1.76678578	0.21345581	6.54012490	H	0.22937558	-2.79578205	-2.76453731
C	-0.31870652	1.54835834	5.63970123	H	-0.34038056	-3.04646337	-1.11017947
H	-0.20399201	2.16495779	6.53101882	C	1.56827234	-1.99096801	-1.26747212
C	0.39816513	1.86534504	4.49348585	H	2.05963194	-1.35925685	-2.01419625
H	1.06500943	2.72656566	4.49604866	H	2.14865542	-2.92243216	-1.17573554
C	0.27134728	1.11482829	3.30889824				

TABLE S-CLXIV. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7t**) S12g–Cosmo Singlet

Fe	2.93285483	3.12550234	7.85950136	H	7.34696304	4.73760907	6.22312127
S	3.20215895	5.22752666	8.80816324	H	8.53179883	6.59232082	7.39225373
S	4.71987634	3.58276016	6.58092764	H	7.34471509	7.85960508	9.18486653
S	0.98986785	2.75396223	8.90060733	H	5.02646947	7.28965790	9.79760563
S	2.77756671	0.93789312	7.06420352	H	-0.62088790	1.04237969	10.60719866
C	5.53036634	4.99640427	7.34864212	H	-0.75714204	-1.43874086	10.82738085
C	6.84206814	5.31268610	6.99908085	H	0.63598268	-2.87459083	9.33833269
C	7.50242790	6.34975127	7.65085365	H	2.15404192	-1.86100155	7.68005418
C	6.83314039	7.05600921	8.65539876	H	3.80101826	3.47397720	4.39203569
C	5.52666950	6.73663699	9.00338837	H	4.54114144	5.07311592	4.66217274
C	4.84282062	5.68696999	8.36178265	H	2.63366807	5.75518094	6.09608645
C	0.83499513	0.96264485	9.02453905	H	1.95112679	5.10872267	4.58015820

C	-0.02348700	0.39702899	9.96416099	H	-1.14156074	3.42840181	7.91134856
C	-0.10161949	-0.98882749	10.08364710	H	-0.27360316	2.23177435	6.89858692
C	0.68192638	-1.78940069	9.24795398	H	-0.15718575	4.50471764	5.83352986
C	1.53868181	-1.22099977	8.31152722	H	0.57031760	5.16666017	7.31614164
C	1.64640801	0.17606944	8.18803048	N	4.06750981	2.33541372	9.42960254
N	1.82032899	3.83765585	6.28872072	H	3.95557824	1.32263038	9.39187644
C	3.88253114	4.31435776	5.09209645	H	5.05776290	2.51242404	9.25020352
C	2.52931432	4.85678402	5.48103961	N	3.73598079	2.74540755	10.78845563
C	-0.17111423	3.14376371	7.49625240	H	4.56738810	2.60037964	11.36590496
C	0.46514733	4.26216184	6.70668026	H	3.62378833	3.76164165	10.71068986
H	1.69958873	3.00755137	5.69958134				

TABLE S-CLXV. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7t**) S12g–Cosmo Triplet

Fe	2.88201995	3.13285631	7.76862840	H	7.28202187	4.86955201	6.13569272
S	3.21231175	5.12274110	8.87760029	H	8.48977052	6.63296587	7.41600691
S	4.66227911	3.67073482	6.48364581	H	7.35081333	7.75189793	9.33060988
S	0.88587817	2.78131646	8.74514564	H	5.04731958	7.12318932	9.95722507
S	2.83069293	0.89950819	7.14294404	H	-0.79459139	1.14136230	10.45535390
C	5.49355253	5.03370068	7.32323949	H	-0.87100617	-1.32192604	10.84098653
C	6.79427391	5.38034088	6.96539819	H	0.65002810	-2.80988356	9.54347143
C	7.46818802	6.36612930	7.68199044	H	2.23869705	-1.86233455	7.90905723
C	6.82704110	6.98992979	8.75374847	H	3.78913717	3.71270916	4.27571089
C	5.52916563	6.63796025	9.10922858	H	4.48673090	5.29994774	4.68094107
C	4.83812788	5.64093633	8.40222502	H	2.49789495	5.84048854	6.08465410
C	0.75655360	0.99978939	8.96960040	H	1.94977950	5.35914257	4.45974286
C	-0.14114427	0.47367820	9.89524359	H	-1.23571513	3.28428091	7.64405479
C	-0.18389068	-0.90285100	10.10765269	H	-0.22611903	2.16070056	6.67953294
C	0.66969709	-1.73277344	9.37810830	H	-0.34853624	4.47449262	5.64695890
C	1.56593020	-1.20201130	8.45508771	H	0.39003644	5.14805218	7.11366519
C	1.63890956	0.18453839	8.24341152	N	4.25140208	2.08241990	9.77558762
N	1.68694775	3.92321428	6.02932703	H	3.85488533	1.16782592	9.97920074
C	3.82648862	4.50361007	5.03446693	H	5.15768797	1.91531736	9.33882112
C	2.43856306	5.00361060	5.38082878	N	4.39865041	2.79650914	11.02412472
C	-0.22777853	3.08227332	7.27126529	H	5.34492781	2.66860700	11.38642433
C	0.33096227	4.25199687	6.48402629	H	4.32155616	3.78351678	10.76531259
H	1.62461278	3.13265417	5.38588031				

TABLE S-CLXVI. *trans*-(Fe(NH)S<sub>4</sub>)N<sub>2</sub>H<sub>4</sub> (**7t**) S12g–Cosmo Quintet

Fe	2.89422913	3.15909345	7.84768960	H	7.42116268	4.85315387	6.11345087
S	3.31655279	5.35554416	8.83009393	H	8.81705765	6.22259368	7.64898936

S	4.75656526	3.94067608	6.20408888	H	7.76496226	7.23059908	9.67931123
S	0.50977655	2.63242503	8.69562523	H	5.37555553	6.86004641	10.15409594
S	2.76854371	0.78952875	7.13595625	H	-0.88307406	0.93680830	10.47530600
C	5.62079267	5.10283557	7.26161945	H	-0.63120262	-1.45271167	11.11651906
C	6.97749201	5.30950627	6.99700965	H	1.08355656	-2.85188648	9.95676574
C	7.75849042	6.07486326	7.85660200	H	2.52421040	-1.86593878	8.21797873
C	7.16664695	6.63624465	8.98892701	H	3.69574797	4.26824314	4.13603614
C	5.81854780	6.43035713	9.25668805	H	4.21879206	5.83335629	4.78862388
C	5.00745719	5.65096477	8.41047119	H	2.26579833	5.92878706	6.28640505
C	0.67339287	0.87248046	8.99278577	H	1.69407894	5.53441560	4.64451992
C	-0.14096647	0.31200873	9.98098195	H	-1.34799861	2.82225679	7.15162466
C	-0.00097104	-1.02503961	10.33842689	H	0.01303416	1.89781059	6.44442266
C	0.95879086	-1.80292541	9.68822522	H	-0.33650487	4.24470587	5.45075479
C	1.77011113	-1.24924090	8.70504247	H	0.10423363	4.91891314	7.02717646
C	1.66520332	0.10585238	8.33524812	N	4.02137772	2.24768354	9.66164253
N	1.68548034	3.93908219	6.06541110	H	3.62579603	1.32144502	9.81804298
C	3.69374610	4.90509314	5.02866979	H	4.96963372	2.08565529	9.31497534
C	2.27737303	5.16514249	5.50306079	N	4.05026128	2.93668237	10.93826571
C	-0.26362923	2.78794758	7.01820850	H	4.95644503	2.76944807	11.37793104
C	0.24778989	4.05653308	6.36390782	H	4.02622234	3.93070056	10.68875864
H	1.78993305	3.18772141	5.37966883				

## REFERENCES

1. J. C. Noveron, M. M. Olmstead, P. K. Mascharak, *Inorg. Chem.* **37** (1998) 1138
2. G. D. Fallon, B. M. Gatehouse, P. J. Minari, K. S. Murray, B. O. West, *J. Chem. Soc. Dalton Trans.* (1984) 2733
3. N. Govindaswamy, D. A. Quarless, S. A. Koch, *J. Am. Chem. Soc.* **117** (1995) 8468
4. D. Sellmann, H. Kunstmann, F. Knoch, M. Moll, *Inorg. Chem.* **27** (1988) 4183
5. D. Sellmann, T. Hofmann, F. Knoch, *Inorg. Chim. Acta* **224** (1994) 61
6. D. Sellmann, W. Soglowek, F. Knoch, G. Ritter, J. Dengler, *Inorg. Chem.* **31** (1992) 3711
7. W. Morris, B. Voloskiy, S. Demir, F. Gándara, P. L. McGrier, H. Furukawa, D. Cascio, J. F. Stoddart, O. M. Yaghi, *Inorg. Chem.* **51** (2012) 6443
8. T. Goslinski, C. Zhong, M. J. Fuchter, C. L. Stern, A. J. P. White, A. G. M. Barrett, B. M. Hoffman, *Inorg. Chem.* **45** (2006) 3686.