**Supplementary Material:**

**SCCS− radical: Renner-Teller Effect and Spin-orbit Coupling in the *X* 2Πu Electronic State**

STANKA V. JEROSIMIĆ[[1]](#footnote-1)\*, MARKO Lj. MITIĆ, and MILAN Z. MILOVANOVIĆ

*Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, PAC 105305, 11158 Belgrade, Serbia*

Table S1. *Ab initio* calculated energies of two components of the ground electronic state of SCCS−  in respect to *trans*-bending angle (see main text for further details). Calculations were done with the use of SA-CAS-MRCISD(Q)-F12/cc-pVTZ-F12 method.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| roT | A' Bu | A'' Au | A' | A'' | Vavg | deltaV |
| 0 | -871.5910538 | -871.5910538 | 0 | 0 | 0.0000000 | 0.0000000 |
| 1 | -871.5910338 | -871.5910428 | 2.001E-05 | 1.103E-05 | 0.0000155 | 0.0000090 |
| 2 | -871.5909736 | -871.5910096 | 8.02E-05 | 4.422E-05 | 0.0000622 | 0.0000360 |
| 3 | -871.5908731 | -871.590954 | 0.0001807 | 9.981E-05 | 0.0001403 | 0.0000809 |
| 4 | -871.5907319 | -871.5908756 | 0.00032186 | 0.00017824 | 0.0002501 | 0.0001436 |
| 5 | -871.5905497 | -871.5907737 | 0.00050407 | 0.00028007 | 0.0003921 | 0.0002240 |
| 6 | -871.590326 | -871.5906479 | 0.00072779 | 0.00040591 | 0.0005669 | 0.0003219 |
| 7 | -871.5900603 | -871.5904973 | 0.00099352 | 0.00055645 | 0.0007750 | 0.0004371 |
| 8 | -871.589752 | -871.5903213 | 0.00130182 | 0.00073246 | 0.0010171 | 0.0005694 |
| 9 | -871.5894005 | -871.590119 | 0.00165331 | 0.00093479 | 0.0012941 | 0.0007185 |
| 10 | -871.5890051 | -871.5898895 | 0.00204865 | 0.00116432 | 0.0016065 | 0.0008843 |
| 11 | -871.5885653 | -871.5896318 | 0.00248853 | 0.00142203 | 0.0019553 | 0.0010665 |
| 12 | -871.5880801 | -871.5893448 | 0.00297369 | 0.00170895 | 0.0023413 | 0.0012647 |
| 13 | -871.5875489 | -871.5890276 | 0.00350493 | 0.0020262 | 0.0027656 | 0.0014787 |
| 14 | -871.5869707 | -871.5886788 | 0.00408309 | 0.00237495 | 0.0032290 | 0.0017081 |
| 15 | -871.5863448 | -871.5882973 | 0.00470904 | 0.00275647 | 0.0037328 | 0.0019526 |
| 16 | -871.5856701 | -871.5878817 | 0.00538372 | 0.00317208 | 0.0042779 | 0.0022116 |
| 17 | -871.5849457 | -871.5874306 | 0.00610813 | 0.00362323 | 0.0048657 | 0.0024849 |
| 18 | -871.5841705 | -871.5869424 | 0.00688327 | 0.00411138 | 0.0054973 | 0.0027719 |
| 19 | -871.5833435 | -871.5864157 | 0.00771029 | 0.00463812 | 0.0061742 | 0.0030722 |
| 20 | -871.5824635 | -871.5858487 | 0.00859031 | 0.00520509 | 0.0068977 | 0.0033852 |
| 21 | -871.5815293 | -871.5852398 | 0.00952452 | 0.00581404 | 0.0076693 | 0.0037105 |
| 22 | -871.5805396 | -871.584587 | 0.01051417 | 0.00646675 | 0.0084905 | 0.0040474 |
| 23 | -871.5794932 | -871.5838887 | 0.01156056 | 0.0071651 | 0.0093628 | 0.0043955 |
| 24 | -871.5783888 | -871.5831428 | 0.01266504 | 0.00791104 | 0.0102880 | 0.0047540 |
| 25 | -871.5772248 | -871.5823472 | 0.01382901 | 0.00870659 | 0.0112678 | 0.0051224 |

Table S2. *Ab initio* calculated energies of two components of the ground electronic state of SCCS−  in respect to *cis*-bending angle (see main text for further details). Calculations were done with the use of SA-CAS-MRCISD(Q)-F12/cc-pVTZ-F12 method.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| roC | A' A1 | A'' B1 | A' | A'' | Vavg | deltaV |
| 0 | -871.5910538 | -871.5910537 | 0 | 0 | 0.0000000 | 0.00000000 |
| 1 | -871.5910244 | -871.591025 | 2.937E-05 | 2.876E-05 | 0.0000291 | 0.00000061 |
| 2 | -871.5909361 | -871.5909386 | 0.00011769 | 0.00011519 | 0.0001164 | 0.00000250 |
| 3 | -871.5907889 | -871.5907945 | 0.00026487 | 0.00025924 | 0.0002621 | 0.00000563 |
| 4 | -871.5905829 | -871.5905928 | 0.00047088 | 0.00046092 | 0.0004659 | 0.00000996 |
| 5 | -871.5903181 | -871.5903336 | 0.00073567 | 0.0007202 | 0.0007279 | 0.00001547 |
| 6 | -871.5899946 | -871.5900167 | 0.00105919 | 0.00103705 | 0.0010481 | 0.00002214 |
| 7 | -871.5896125 | -871.5896424 | 0.00144131 | 0.00141138 | 0.0014263 | 0.00002993 |
| 8 | -871.5891718 | -871.5892107 | 0.001882 | 0.00184311 | 0.0018626 | 0.00003889 |
| 9 | -871.5886726 | -871.5887217 | 0.00238115 | 0.00233208 | 0.0023566 | 0.00004907 |
| 10 | -871.5881151 | -871.5881756 | 0.00293867 | 0.00287812 | 0.0029084 | 0.00006055 |
| 11 | -871.5874993 | -871.5875727 | 0.00355449 | 0.00348103 | 0.0035178 | 0.00007346 |
| 12 | -871.5868252 | -871.5869132 | 0.00422856 | 0.00414057 | 0.0041846 | 0.00008799 |
| 13 | -871.5860929 | -871.5861973 | 0.00496087 | 0.00485646 | 0.0049087 | 0.00010441 |
| 14 | -871.5853024 | -871.5854253 | 0.00575141 | 0.00562843 | 0.0056899 | 0.00012298 |
| 15 | -871.5844536 | -871.5845977 | 0.00660021 | 0.0064561 | 0.0065282 | 0.00014411 |
| 16 | -871.5835464 | -871.5837145 | 0.00750735 | 0.00733922 | 0.0074233 | 0.00016813 |
| 17 | -871.5825809 | -871.5827764 | 0.00847291 | 0.00827738 | 0.0083751 | 0.00019553 |
| 18 | -871.5815568 | -871.5817836 | 0.00949699 | 0.00927017 | 0.0093836 | 0.00022682 |
| 19 | -871.580474 | -871.5807366 | 0.01057972 | 0.01031718 | 0.0104485 | 0.00026254 |
| 20 | -871.5793325 | -871.5796358 | 0.01172126 | 0.01141795 | 0.0115696 | 0.00030331 |
| 21 | -871.578132 | -871.5784818 | 0.01292178 | 0.01257201 | 0.0127469 | 0.00034977 |
| 22 | -871.5768723 | -871.5772749 | 0.0141815 | 0.01377887 | 0.0139802 | 0.00040263 |
| 23 | -871.5755531 | -871.5760157 | 0.01550063 | 0.01503803 | 0.0152693 | 0.00046260 |
| 24 | -871.5741743 | -871.5747048 | 0.01687944 | 0.01634895 | 0.0166142 | 0.00053049 |
| 25 | -871.5727355 | -871.5733426 | 0.01831825 | 0.01771113 | 0.0180147 | 0.00060712 |

Table S3. *Ab initio* calculated energies of orbitals in the ground electronic state of SCCS−  in respect to *cis*-bending angle (see main text for further details). Calculations were done with the use of the SA-CAS /cc-pVTZ-F12 method.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| c2v | 8.1 | 8.3 | 9.1 | 10.1 | 9.3 | 2.4 | 2.2 | 3.2 | 3.4 |
| Angle | 15.1 | 16.1 | 17.1 | 18.1 | 19.1 | 3.2 | 4.2 | 5.2 | 6.2 |
| 0 | -0.374089 | -0.206212 | -0.304039 | -0.040461 | 0.43251 | -0.206212 | -0.30404 | -0.040461 | 0.432509 |
| 1 | -0.374082 | -0.206305 | -0.304207 | -0.040456 | 0.43238 | -0.206209 | -0.30404 | -0.04046 | 0.432518 |
| 2 | -0.374063 | -0.206581 | -0.304709 | -0.040442 | 0.43197 | -0.2062 | -0.30405 | -0.040456 | 0.432545 |
| 3 | -0.374031 | -0.207034 | -0.305528 | -0.040418 | 0.43131 | -0.206184 | -0.30406 | -0.04045 | 0.432589 |
| 4 | -0.373986 | -0.207656 | -0.306638 | -0.040384 | 0.43038 | -0.206162 | -0.30407 | -0.040441 | 0.432649 |
| 5 | -0.373929 | -0.208434 | -0.308003 | -0.040339 | 0.42919 | -0.206133 | -0.30409 | -0.040429 | 0.432722 |
| 6 | -0.37386 | -0.209352 | -0.309584 | -0.040284 | 0.42776 | -0.206097 | -0.30412 | -0.040413 | 0.432806 |
| 7 | -0.373778 | -0.210393 | -0.311337 | -0.040217 | 0.42609 | -0.206054 | -0.30414 | -0.040394 | 0.432899 |
| 8 | -0.373685 | -0.211539 | -0.313216 | -0.040139 | 0.42419 | -0.206003 | -0.30417 | -0.04037 | 0.432998 |
| 9 | -0.373581 | -0.212772 | -0.315178 | -0.040049 | 0.42207 | -0.205944 | -0.30421 | -0.040342 | 0.4331 |
| 10 | -0.373465 | -0.214072 | -0.317182 | -0.039948 | 0.41975 | -0.205877 | -0.30424 | -0.040309 | 0.433202 |
| 11 | -0.373338 | -0.215424 | -0.319192 | -0.039834 | 0.41723 | -0.2058 | -0.30428 | -0.040271 | 0.433302 |
| 12 | -0.373201 | -0.216811 | -0.321179 | -0.039708 | 0.41452 | -0.205715 | -0.30432 | -0.040228 | 0.433399 |
| 13 | -0.373052 | -0.21822 | -0.323117 | -0.039571 | 0.41165 | -0.205619 | -0.30436 | -0.040178 | 0.43349 |
| 14 | -0.372893 | -0.219639 | -0.324988 | -0.039421 | 0.40862 | -0.205515 | -0.3044 | -0.040123 | 0.433573 |
| 15 | -0.372723 | -0.221057 | -0.326776 | -0.039261 | 0.40544 | -0.205399 | -0.30444 | -0.040061 | 0.433648 |
| 16 | -0.372542 | -0.222465 | -0.328471 | -0.039089 | 0.40212 | -0.205274 | -0.30449 | -0.039993 | 0.433713 |
| 17 | -0.372351 | -0.223856 | -0.330066 | -0.038907 | 0.39869 | -0.205137 | -0.30453 | -0.039918 | 0.433768 |
| 18 | -0.372149 | -0.225223 | -0.331557 | -0.038716 | 0.39514 | -0.20499 | -0.30458 | -0.039837 | 0.433813 |
| 19 | -0.371936 | -0.22656 | -0.332942 | -0.038515 | 0.39148 | -0.20483 | -0.30463 | -0.039749 | 0.433846 |
| 20 | -0.371712 | -0.227862 | -0.334221 | -0.038306 | 0.38774 | -0.204659 | -0.30468 | -0.039655 | 0.433868 |
| 21 | -0.371478 | -0.229126 | -0.335396 | -0.038089 | 0.38391 | -0.204476 | -0.30473 | -0.039553 | 0.433879 |
| 22 | -0.371232 | -0.230346 | -0.336468 | -0.037866 | 0.38001 | -0.204279 | -0.30479 | -0.039445 | 0.433879 |
| 23 | -0.370975 | -0.23152 | -0.33744 | -0.037637 | 0.37604 | -0.20407 | -0.30485 | -0.03933 | 0.433867 |
| 24 | -0.370707 | -0.232643 | -0.338316 | -0.037404 | 0.37201 | -0.203846 | -0.3049 | -0.039208 | 0.433844 |
| 25 | -0.370427 | -0.233713 | -0.339101 | -0.037167 | 0.36792 | -0.203608 | -0.30496 | -0.039079 | 0.43381 |

Table S4. *Ab initio* calculated energies of orbitals in the ground electronic state of SCCS−  in respect to *trans*-bending angle (see main text for further details). Calculations were done with the use of the SA-CAS /cc-pVTZ-F12 method.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| C2h | 8.1 | 9.1 | 8.3 | 9.3 | 10.1 | 2.4 | 2.2 | 3.2 | 3.4 |
| Angle | 15.1 | 16.1 | 17.1 | 18.1 | 19.1 | 3.2 | 4.2 | 5.2 | 6.2 |
| 0 | -0.374088 | -0.206212 | -0.304038 | -0.040461 | 0.432508 | -0.206212 | -0.304038 | -0.040461 | 0.432508 |
| 1 | -0.374041 | -0.20625 | -0.304061 | -0.040463 | 0.432429 | -0.206208 | -0.304039 | -0.040457 | 0.43251 |
| 2 | -0.373898 | -0.206363 | -0.304131 | -0.040468 | 0.432188 | -0.206197 | -0.304043 | -0.040445 | 0.432509 |
| 3 | -0.373661 | -0.20655 | -0.304246 | -0.040476 | 0.431785 | -0.206178 | -0.30405 | -0.040424 | 0.432506 |
| 4 | -0.37333 | -0.206809 | -0.304405 | -0.040487 | 0.431224 | -0.206151 | -0.304059 | -0.040395 | 0.432504 |
| 5 | -0.372909 | -0.207137 | -0.304607 | -0.040502 | 0.430506 | -0.206117 | -0.30407 | -0.040358 | 0.432501 |
| 6 | -0.372398 | -0.207532 | -0.304851 | -0.040519 | 0.429633 | -0.206076 | -0.304084 | -0.040312 | 0.432497 |
| 7 | -0.371802 | -0.207989 | -0.305133 | -0.040539 | 0.428608 | -0.206027 | -0.304101 | -0.040259 | 0.432491 |
| 8 | -0.371123 | -0.208503 | -0.305451 | -0.040562 | 0.427433 | -0.20597 | -0.30412 | -0.040196 | 0.432485 |
| 9 | -0.370364 | -0.209069 | -0.305802 | -0.040588 | 0.426112 | -0.205905 | -0.304141 | -0.040126 | 0.432476 |
| 10 | -0.36953 | -0.209682 | -0.306183 | -0.040616 | 0.424649 | -0.205833 | -0.304166 | -0.040046 | 0.432465 |
| 11 | -0.368625 | -0.210336 | -0.306591 | -0.040647 | 0.423047 | -0.205754 | -0.304192 | -0.039959 | 0.432452 |
| 12 | -0.367654 | -0.211025 | -0.30702 | -0.040679 | 0.421312 | -0.205667 | -0.304221 | -0.039862 | 0.432436 |
| 13 | -0.366621 | -0.211742 | -0.307468 | -0.040713 | 0.419447 | -0.205572 | -0.304253 | -0.039757 | 0.432417 |
| 14 | -0.36553 | -0.212482 | -0.30793 | -0.040748 | 0.417458 | -0.205469 | -0.304287 | -0.039643 | 0.432395 |
| 15 | -0.364388 | -0.213237 | -0.308403 | -0.040785 | 0.415349 | -0.205358 | -0.304323 | -0.03952 | 0.432369 |
| 16 | -0.363197 | -0.214002 | -0.308883 | -0.040822 | 0.413126 | -0.20524 | -0.304362 | -0.039388 | 0.43234 |
| 17 | -0.361963 | -0.214771 | -0.309366 | -0.04086 | 0.410793 | -0.205114 | -0.304404 | -0.039247 | 0.432306 |
| 18 | -0.36069 | -0.215539 | -0.309849 | -0.040897 | 0.408355 | -0.20498 | -0.304448 | -0.039097 | 0.432268 |
| 19 | -0.359382 | -0.2163 | -0.310329 | -0.040934 | 0.405818 | -0.204839 | -0.304494 | -0.038937 | 0.432225 |
| 20 | -0.358043 | -0.21705 | -0.310803 | -0.040971 | 0.403187 | -0.204689 | -0.304543 | -0.038768 | 0.432177 |
| 21 | -0.356677 | -0.217784 | -0.311269 | -0.041006 | 0.400466 | -0.204532 | -0.304595 | -0.038589 | 0.432124 |
| 22 | -0.355286 | -0.218499 | -0.311725 | -0.041039 | 0.39766 | -0.204367 | -0.30465 | -0.038401 | 0.432066 |
| 23 | -0.353874 | -0.21919 | -0.31217 | -0.041069 | 0.394773 | -0.204193 | -0.304708 | -0.038203 | 0.432002 |
| 24 | -0.352443 | -0.219855 | -0.312601 | -0.041097 | 0.39181 | -0.204012 | -0.304769 | -0.037996 | 0.431932 |
| 25 | -0.350996 | -0.220492 | -0.31302 | -0.041122 | 0.388776 | -0.203824 | -0.304833 | -0.037778 | 0.431856 |

Table S5.. The low-energy vibronic levels (in cm−1) in the *X* 2Πu1/2 component of the ground state of SCCS−. ΔE is relative energy (in cm−1) in respect to the lowest vibronic level 12Π3/2u of the lower *X* 2Πu3/2 spin-orbit component (see Table III of the main text).

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| (Λ=1and, or and) | | | | | | | | | | |
| *v*4*v*5 | *v*4*l*4*v*5*l*5Λ |  | *E* | *ΔE* |  | *v*4*v*5 | *v*4*l*4*v*5*l*5Λ |  | *E* | *ΔE* |
| 00 | 00001 | 2Π1/2u | 702.8 | 248.8 |  | 11 | 11111 | 2Φ5/2g | 1269.1 | 815.1 |
| 01 | 00111 | 2Δ3/2g | 876.3 | 422.3 |  | 111-11 | 2Π1/2g | 1269.2 | 815.2 |
| 001-11 |  | 876.3 | 422.3 |  | 1-1111 | 2Π1/2g | 1327.5 | 873.5 |
| 0011-1 |  | 876.3 | 422.3 |  | 1-11-11 | 2Π3/2g | 1327.6 | 873.6 |
| 02 | 00221 | 2Φ5/2u | 1049.7 | 595.7 |  | 04 | 00441 | 2H9/2u | 1396.5 | 942.5 |
| 00201 | 2Π1/2u | 1049.8 | 595.8 |  | 00421 | 2Φ5/2u | 1396.7 | 942.7 |
| 002-21 | 2Π3/2u | 1049.8 | 595.8 |  | 00401 | 2Π1/2u | 1396.8 | 942.8 |
| 10 | 11001 | 2Δ3/2u | 1095.7 | 641.7 |  | 004-21 | 2Π3/2u | 1396.8 | 942.8 |
| 1-1001 |  | 1154.1 | 700.1 |  | 004-41 | 2Φ7/2u | 1396.9 | 942.9 |
| 1100-1 |  | 1154.1 | 700.1 |  | 12 | 11221 | 2Γ7/2u | 1442.6 | 988.6 |
| 03 | 00331 | 2Γ7/2g | 1223.1 | 769.1 |  | 11201 | 2Δ3/2u | 1442.6 | 988.6 |
| 00311 | 2Δ3/2g | 1223.2 | 769.2 |  | 112-21 |  | 1442.7 | 988.7 |
| 003-11 |  | 1223.3 | 769.3 |  | 1-122-1 |  | 1442.7 | 988.7 |
| 0031-1 |  | 1223.3 | 769.3 |  | 1-1221 | 2Δ3/2u | 1500.9 | 1046.9 |
| 003-31 | 2Δ5/2g | 1223.3 | 769.3 |  | 1-1201 |  | 1501.0 | 1047.0 |
|  |  |  |  |  |  | 1120-1 |  | 1501.0 | 1047.0 |
|  |  |  |  |  |  | 1-12-21 | 2Δ5/2u | 1501.1 | 1047.1 |

1. \*Corresponding author. E-mail: stanka@ffh.bg.ac.rs [↑](#footnote-ref-1)