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Supplementary material

SUPPLEMENTARY MATERIAL TO

$SCCS^-$ radical: Renner–Teller effect and spin–orbit coupling in the X $^2\Pi_u$ electronic state

STANKA V. JEROSIMIĆ*, MARKO LJ. MITIĆ and MILAN Z. MILOVANOVIĆ

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

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TABLE S-I. *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). The calculations were realized using the 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

* Corresponding author. E-mail: stanka@ffh.bg.ac.rs

TABLE S-II. *Ab initio* calculated energies of two components of the ground electronic state of $SCCS^-$ in respect to the *cis*-bending angle (see main text for further details). The calculations were realized using the 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 S-III. *Ab initio* calculated energies of orbitals in the ground electronic state of $SCCS^-$ in respect to the *cis*-bending angle (see main text for further details). The calculations were realized using 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 S-IV. *Ab initio* calculated energies of orbitals in the ground electronic state of $SCCS^-$ in respect to the *trans*-bending angle (see main text for further details). The calculations were realize using 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 S-V. The low-energy vibronic levels in the $X\,^2\Pi_{u1/2}$ component of the ground state of $SCCS^-$. ΔE is the relative energy in respect to the lowest vibronic level 1 $^2\Pi_{3/2u}$ of the lower $X\,^2\Pi_{u3/2}$ spin–orbit component (see Table III of the main text)

$\Omega = \pm 1/2$ (Λ=1 and $\Sigma = -1/2$, or $\Lambda = -1$ and $\Sigma = -1/2$)									
v_4v_5	$v_4l_4v_5l_5\Lambda$	$^{2S+1}K_{\|P\|,u/g}$	E / cm^{-1}	ΔE / cm^{-1}	v_4v_5	$v_4l_4v_5l_5\Lambda$	$^{2S+1}K_{\|P\|,u/g}$	E / cm^{-1}	ΔE / cm^{-1}
00	00001	$^2\Pi_{1/2u}$	702.8	248.8		11111	$^2\Phi_{5/2g}$	1269.1	815.1
	00111	$^2\Delta_{3/2g}$	876.3	422.3	11	111–11	$^2\Pi_{1/2g}$	1269.2	815.2
01	001–11	$^2\Sigma_{1/2g}^-$	876.3	422.3		1–1111	$^2\Pi_{1/2g}$	1327.5	873.5
	0011–1	$^2\Sigma_{1/2g}^+$	876.3	422.3		1–11–11	$^2\Pi_{3/2g}$	1327.6	873.6
	00221	$^2\Phi_{5/2u}$	1049.7	595.7		00441	$^2H_{9/2u}$	1396.5	942.5
02	00201	$^2\Pi_{1/2u}$	1049.8	595.8		00421	$^2\Phi_{5/2u}$	1396.7	942.7
	002–21	$^2\Pi_{3/2u}$	1049.8	595.8	04	00401	$^2\Pi_{1/2u}$	1396.8	942.8
	11001	$^2\Delta_{3/2u}$	1095.7	641.7		004–21	$^2\Pi_{3/2u}$	1396.8	942.8
10	1–1001	$^2\Sigma_{1/2u}^-$	1154.1	700.1		004–41	$^2\Phi_{7/2u}$	1396.9	942.9
	1100–1	$^2\Sigma_{1/2u}^+$	1154.1	700.1		11221	$^2\Gamma_{7/2u}$	1442.6	988.6
	00331	$^2\Gamma_{7/2g}$	1223.1	769.1		11201	$^2\Delta_{3/2u}$	1442.6	988.6
	00311	$^2\Delta_{3/2g}$	1223.2	769.2		112–21	$^2\Sigma_{1/2u}^-$	1442.7	988.7
03	003–11	$^2\Sigma_{1/2g}^-$	1223.3	769.3	12	1–122–1	$^2\Sigma_{1/2u}^+$	1442.7	988.7
	0031–1	$^2\Sigma_{1/2g}^+$	1223.3	769.3		1–1221	$^2\Delta_{3/2u}$	1500.9	1046.9
	003–31	$^2\Delta_{5/2g}$	1223.3	769.3		1–1201	$^2\Sigma_{1/2u}^-$	1501.0	1047.0
						1120–1	$^2\Sigma_{1/2u}^+$	1501.0	1047.0
						1–12–21	$^2\Delta_{5/2u}$	1501.1	1047.1