

Supplementary Material:
SCCS⁻ radical: Renner-Teller Effect and Spin-orbit Coupling in the X ²Π_u Electronic State

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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

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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	0.0000000
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

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

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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

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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

54 Table S5.. The low-energy vibronic levels (in cm^{-1}) in the $X^2\Pi_{u1/2}$ component of the ground
55 state of SCCS^- . ΔE is relative energy (in cm^{-1}) in respect to the lowest vibronic level $1^2\Pi_{3/2u}$
56 of the lower $X^2\Pi_{u3/2}$ spin-orbit component (see Table III of the main text).

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$\Omega = \pm 1/2$									
$(\Lambda=1 \text{ and } \Sigma = -1/2, \text{ or } \Lambda = -1 \text{ and } \Sigma = -1/2)$									
v_4v_5	$v_4l_4v_5l_5\Lambda$	$^{2S+1}K_{ p ,u/g}$	E	ΔE	v_4v_5	$v_4l_4v_5l_5\Lambda$	$^{2S+1}K_{ p ,u/g}$	E	ΔE
00	00001	$^2\Pi_{1/2u}$	702.8	248.8	11	11111	$^2\Phi_{5/2g}$	1269.1	815.1
01	00111	$^2\Delta_{3/2g}$	876.3	422.3		111-11	$^2\Pi_{1/2g}$	1269.2	815.2
	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
02	00221	$^2\Phi_{5/2u}$	1049.7	595.7	04	00441	$^2H_{9/2u}$	1396.5	942.5
	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		00401	$^2\Pi_{1/2u}$	1396.8	942.8
10	11001	$^2\Delta_{3/2u}$	1095.7	641.7		004-21	$^2\Pi_{3/2u}$	1396.8	942.8
	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	12	11221	$^2\Gamma_{7/2u}$	1442.6	988.6
03	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
	003-11	$^2\Sigma_{1/2g}^-$	1223.3	769.3		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

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