Supporting Information for

Dynamics, bonding and magnetic resonance properties of $Sc_3C_2@C_{80}$ and its monoanion

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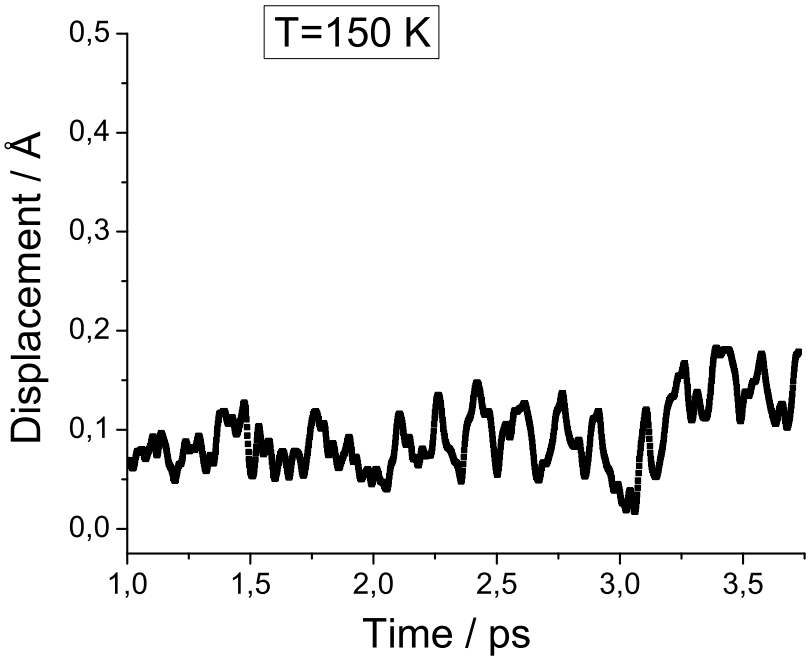
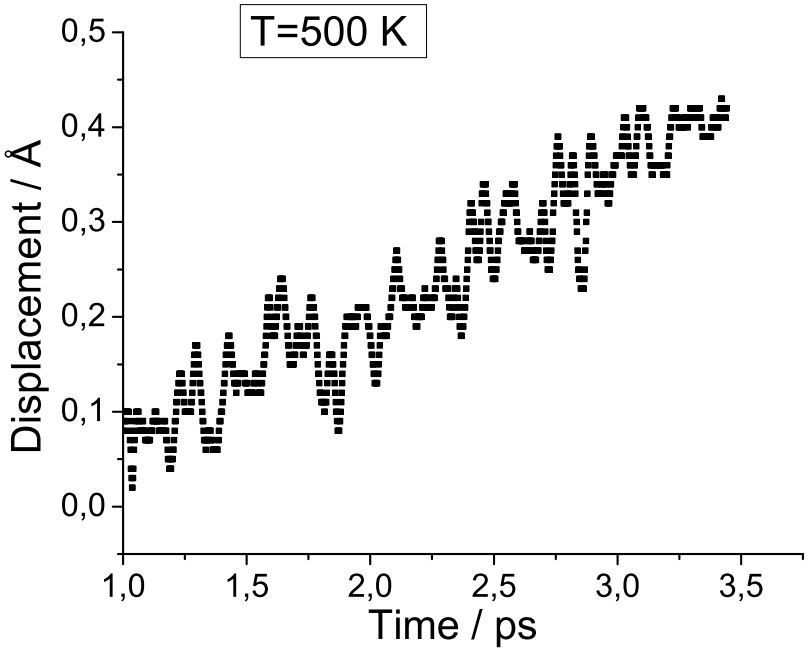
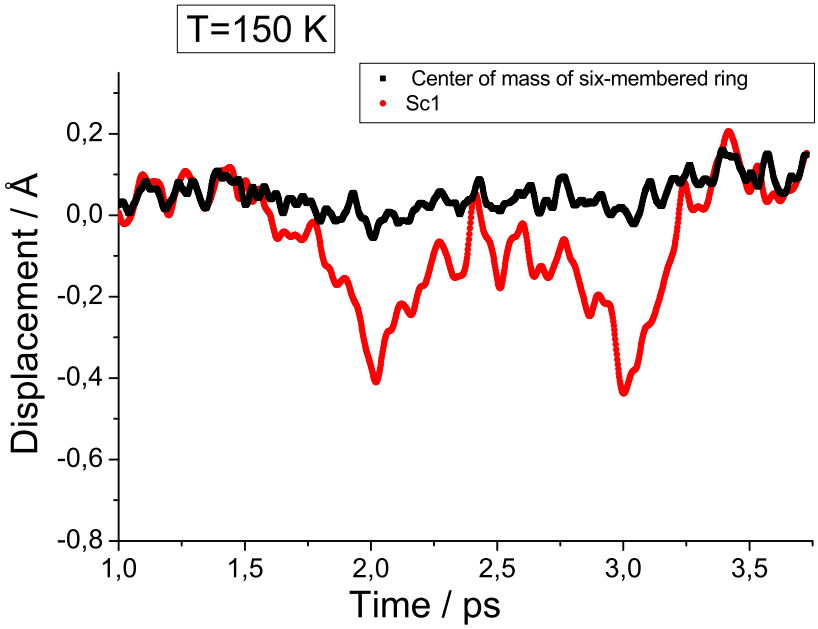


(a)

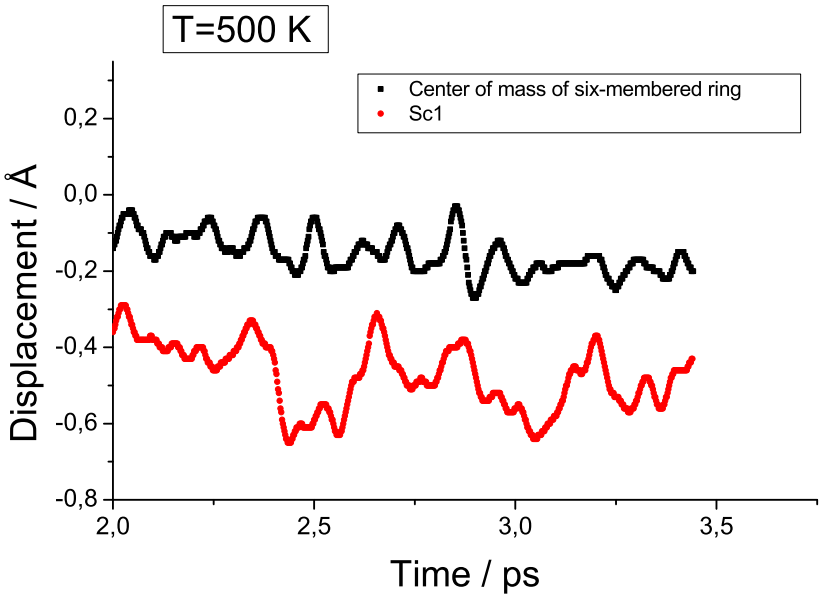


(b)

Figure S1: Total displacement from the original positions in the static 1a structure (in Å) of the center of mass of the six-membered ring closest to Sc1.



(a)



(b)

Figure S2: Displacement from the original positions in the static 1a structure (in Å) of the center of mass of the six-membered ring closest to Sc1, as well as of Sc1. The motion is directed towards the cage interior (negative direction on the y-axis). This plot illustrates the breathing-like dynamics of the cage, and it indicates a coupling between the Sc atoms and the cage. Although the amplitude of the motion of the scandium atom is larger than that of the cage, the phase is qualitatively the same throughout the trajectory.

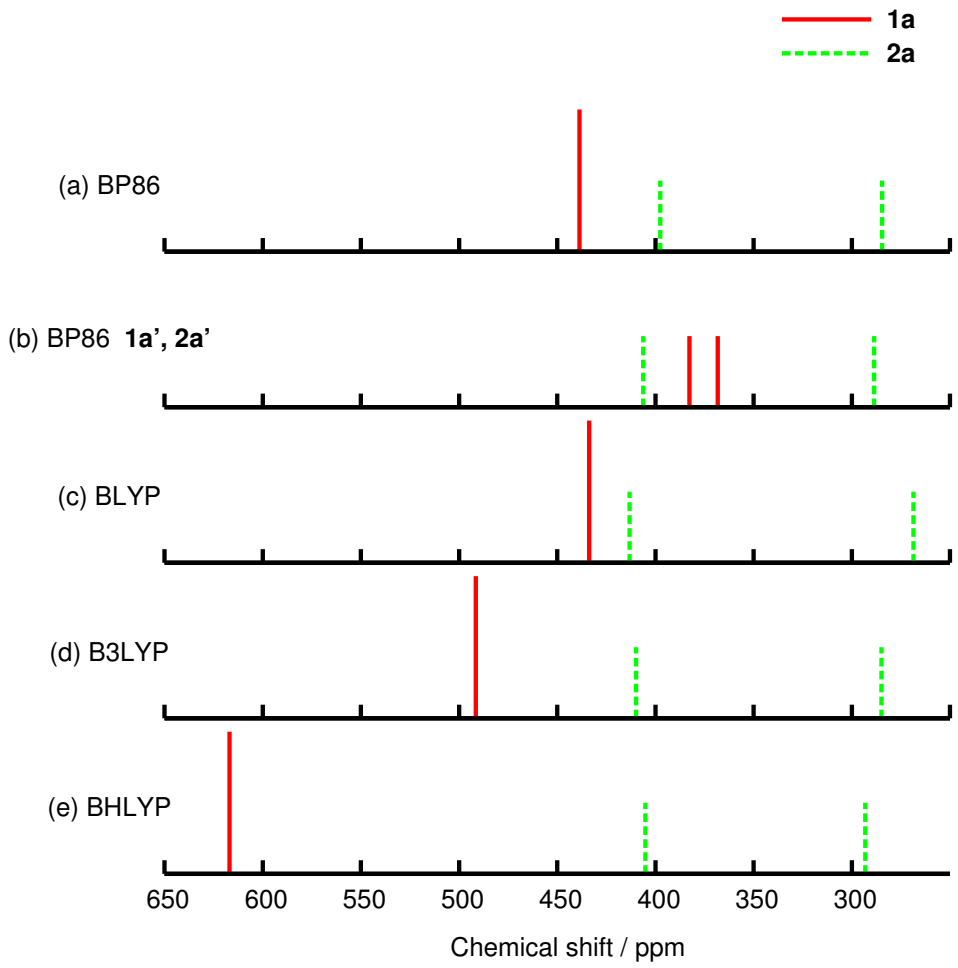


Figure S3: Calculated ^{13}C NMR spectrum of the endohedral carbon atoms in the $[Sc_3C_2@C_{80}]^-$ anion obtained with the indicated functionals. The def2-TZVP basis set is used. The x-scale is the chemical shift (in ppm) relative to TMS.

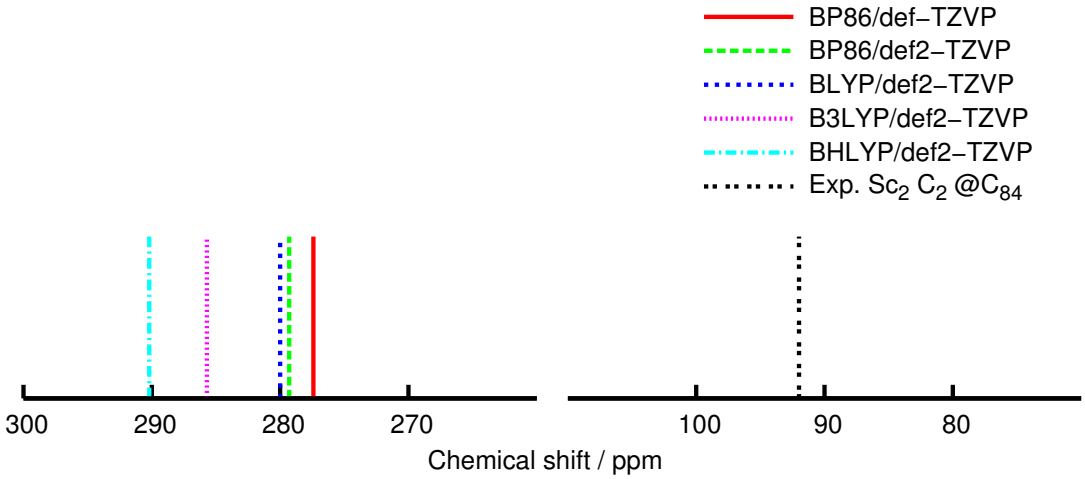


Figure S4: Calculated ^{13}C NMR spectrum of the endohedral carbon atoms in the $Sc_2C_2@C_{84}$ molecule obtained at the given computational levels. The x-scale is the chemical shift (in ppm) relative to TMS.

Table S1: Relative molecular energies in kJ mol^{-1} of the investigated structures and spin states of the Sc_3C_{82} molecule. The energies are given relative to **1a** and all structures are optimized at the BP86/def2-TZVP.

Molecule	Isomer	Singlet (anion)	Doublet	Quartet	Sextet
$Sc_3@C_{82}$[a]	C_{3v}		147.2	142.3	204.5
$Sc_3C_2@C_{80}$	**1a**	-301.1	**0.0**	127.2	290.4
	2a	-316.9	3.2	185.6	329.8
	$\mathbf{1a}_{TS}$		14.1		
	1a'	-303.3	0.1		
	2a'	-320.6	0.9		

[a] Structure (C_{3v}) optimized for the quartet state at the RI-BP86/def2-TZVP level.

Table S2: The energies in kJ mol^{-1} of the different isomers of the doublet $Sc_3C_2@C_{80}$ with different basis sets employed together with the BP86 DFT functional. The energies are given relative to **1a** and all structures are optimized at the BP86/def2-SVP level.

Single-point	**1a**	**2a**	**1a'**	**2a'**
def2-SVP	0.0	-4.2	-5.0	-0.1
ZPVE[a]	0.00	0.36	0.67	-2.62
def2-SVP/def2-TZVP[b]	0.0	-2.3	—	—
def2-TZVP	0.0	1.2	-10.5	-9.7

[a] Zero-point vibrational corrections have been calculated at the RI-BP86/def2-SVP level. The corrections are given relative to the ZPVE of **1a**.
[b] With the def2-TZVP basis set for the endohedral atoms and the def2-SVP basis set for the cage atoms.

Table S3: Calculated[a] ^{13}C NMR chemical shifts (in ppm with respect to TMS[b]) for cage carbon atoms in $[Sc_3C_2@C_{80}]^-$.

	Isomer **1a**		Isomer **2a**	
Level	Peak 1	Peak 2	Peak 1	Peak 2
BP86	149.4	138.2	151.1	141.4
BP86[c]	145.6	146.2	149.9	140.1
BLYP	150.3	139.1	151.0	141.4
B3LYP	153.3	144.2	154.6	146.3
BHLYP	156.4	150.4	157.7	151.2
Exp.[d]	145.6	138.9		

[a] Calculated with the specified functional and the def2-TZVP basis set. The shifts are averaged to correspond to the I_h cage.
[b] The ^{13}C shielding constants of TMS are 182.30 ppm (BP86); 178.48 ppm (BLYP); 181.84 (B3LYP); 186.00 (BHLYP). The basis set is def2-TZVP.
[c] Isomers **1a'** and **2a'** at the lower C_1 symmetry.
[d] Ref. 7. The isomers are experimentally indistinguishable.

Table S4: Calculated ^{45}Sc NMR chemical shielding constants for both the closed-shell anion and the open-shell neutral form of isomers **1a** and **2a**

Structure	Atom	NMR[a]	pNMR[b]
1a	Sc1	523.5	887
	Sc2	502.9	1688
	Sc3	502.9	1686
2a	Sc1	414.1	292
	Sc2	300.2	1143
	Sc3	300.2	1139
1a$_{TS}$	Sc1	420.0	929
	Sc2	413.2	1490
	Sc3	413.4	1473
1a'	Sc1	467.5	—
	Sc2	540.5	—
	Sc3	533.4	—
2a'	Sc1	422.9	—
	Sc2	310.2	—
	Sc3	291.9	—

[a] At the RI-BP86/def2-TZVP level.
[b] At the BP86 level with EPR-II basis on C and (15s11p6d)/[9s7p4d] basis on Sc. The value includes the contribution from SO-coupling. Note that no scalar relativistic effects are taken into account.

Table S5: Calculated[a] principal and isotropic g values for $Sc_3C_2@C_{80}$.

Structure	g_{iso}	g_{11}	g_{22}	g_{33}
1a	1.99923	1.99567	1.99976	2.00226
2a	1.99459	1.99283	1.99475	1.99619
1a$_{TS}$	1.99845	1.99668	1.99793	2.00075
Exp.[b] $Sc_3@C_{82}$	1.9987			
Exp.[c] $Sc_3C_2@C_{80}$	1.99835			

[a] At the BP86 level with EPR-II basis on C and (15s11p6d)/[9s7p4d] basis on Sc.
[b] Ref. 6 of the article.
[c] Ref. 4 of the article.

Cartesian coordinates for the neutral 1a isomer of $Sc_3C_2@C_{80}$ (in Å).

85

Energy =−5408.521373082 Hartree

C	4.1577582	-0.1385263	-0.0236560
C	4.0444752	0.5839164	-1.2890400
C	3.5121084	-0.0902163	-2.5000322
C	3.0751730	-1.4923077	-2.4290608
C	3.2941366	-2.2065454	-1.1939236
C	3.8246127	-1.5380683	-0.0187233
C	3.4412531	1.9147387	-1.2317009
C	3.1404234	2.6217834	-0.0028086
C	3.4295175	1.9448404	1.2209549
C	3.8889925	0.5732732	1.2005223
C	3.2688549	-2.1904100	1.1474666
C	2.9931575	-1.4591938	2.3382523
C	3.3411633	-0.0813519	2.3590227
C	2.4064774	-3.2541045	-0.7370202
C	2.4005937	-3.2420207	0.6977589
C	2.5855703	0.8561051	-3.1244582
C	2.5811759	2.0844704	-2.3681054
C	2.6078463	2.1285107	2.3776496
C	2.5417259	0.8719065	3.0966378
C	1.8835132	-1.8702817	-3.1380144
C	1.0692503	-0.9186612	-3.8661236
C	1.3784330	0.4677918	-3.8261685
C	0.2885575	1.3898548	-3.8700934
C	0.3232969	2.6307499	-3.1408830
C	1.4576705	2.9885595	-2.3538305
C	1.2431109	3.7511893	-1.1749167
C	2.0721475	3.5592708	-0.0120360
C	1.2452896	3.7470444	1.1553506
C	1.4773257	2.9949511	2.3384465
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C	1.4207952	0.4860729	3.9168123
C	1.0989938	-0.9318780	3.9539811
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C	0.9860775	-2.8871287	2.6542148
C	1.2256067	-3.5933949	1.4306318
C	1.0062532	-2.9325515	-2.6945566
C	1.2320745	-3.6195487	-1.4664550
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C	-4.1577582	0.1385263	-0.0236560
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C	-3.2688549	2.1904100	1.1474666
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C	-2.5417259	-0.8719065	3.0966378
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C	-2.0721475	-3.5592708	-0.0120360
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C	-1.3784330	-0.4677918	-3.8261685
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C	-1.0062532	2.9325515	-2.6945566
C	-1.2320745	3.6195487	-1.4664550
C	-0.9860775	2.8871287	2.6542148
C	-1.2256067	3.5933949	1.4306318
C	-0.0898123	4.0463774	0.7064847
C	-0.0911438	4.0634778	-0.7327061
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C	-0.0120664	-0.6552198	-0.0472278
Sc	0.0000000	0.0000000	2.1672489
Sc	1.9394220	-0.0555392	-0.9653948
Sc	-1.9394220	0.0555392	-0.9653948

Cartesian coordinates for the neutral 2a isomer of $Sc_3C_2@C_{80}$ (in Å).

85

Energy =−5408.520150710 Hartree

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C	-1.165967	0.487988	0.694535
C	0.743287	1.346453	1.807694
C	-1.219991	-1.979003	-0.799826
C	1.219991	-3.421437	-0.799826
C	3.092091	-2.700220	0.390926
C	-0.743287	1.346453	1.807694
C	3.131676	-0.321513	1.918152
C	2.377045	-3.867372	-0.062503
C	-2.358047	-0.340774	0.720221
C	-2.377045	-1.533068	-0.062503
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C	-3.092091	-2.700220	0.390926

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C	1.242734	-1.957949	7.094135
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C	2.347223	-5.060151	5.445068
C	-2.348864	-1.539056	6.244743
C	-3.121314	-5.082653	4.252799
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C	-3.037334	-2.700220	5.763206
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C	1.242734	-3.442491	7.094135
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C	-2.347223	-5.060151	5.445068
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C	0.000000	-2.700220	3.239197
C	0.000000	-2.700220	1.946083
Sc	0.000000	-0.611555	2.490479
Sc	0.000000	-4.788885	2.490479
Sc	0.000000	-2.700220	5.332461

Cartesian coordinates for the monoanionic 1a isomer of $Sc_3C_2@C_{80}$ (in Å).

85

Energy =–5408.636048460 Hartree

C	1.2461788	-3.7618038	1.1730790
C	2.0740194	-3.5661931	0.0111467
C	1.4594606	-2.9932865	2.3516391
C	2.5826938	-2.0908033	2.3671654
C	3.4422506	-1.9193046	1.2296136
C	3.1410838	-2.6221611	0.0013122
C	-0.0907222	-4.0717598	0.7310526
C	1.2465776	-3.7495444	-1.1556734
C	0.3234720	-2.6344787	3.1379713
C	2.5833678	-0.8591057	3.1202942
C	4.0339982	-0.5840804	1.2822885
C	-0.0888223	-4.0530271	-0.7082062
C	3.4370022	-1.9458558	-1.2242228
C	3.5012049	0.0885375	2.4891246
C	-1.2351376	-3.6327703	1.4655540
C	-1.0068488	-2.9380239	2.6930017
C	0.2884326	-1.3917713	3.8654968
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C	1.3779512	-0.4680537	3.8201503
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C	0.3352609	-2.6076526	-3.1207745
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C	-2.4039744	-3.2535230	-0.7022035
C	3.8218782	1.5447203	0.0152401
C	-0.9902215	-2.8958369	-2.6562301
C	1.8815722	1.8750428	3.1365521
C	3.2923571	2.2115261	1.1858828
C	-3.2923571	-2.2115261	1.1858828
C	-3.0650714	-1.4889689	2.4161478
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C	-3.5012049	-0.0885375	2.4891246
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C	1.0976382	0.9308694	-3.9344599

C	1.8688799	1.8606891	-3.1266419
C	1.2351376	3.6327703	1.4655540
C	-4.1542351	-0.1400831	0.0202542
C	-4.0339982	0.5840804	1.2822885
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C	-1.4191213	0.4847839	-3.8965912
C	-1.4594606	2.9932865	2.3516391
C	-0.2945091	1.4087028	-3.9330304
C	0.9902215	2.8958369	-2.6562301
C	1.2279024	3.6029474	-1.4331286
C	-3.3549853	-0.0813737	-2.3669297
C	-3.4422506	1.9193046	1.2296136
C	0.0907222	4.0717598	0.7310526
C	-3.8966846	0.5728785	-1.2054697
C	-2.5551265	0.8736456	-3.0983337
C	-0.3352609	2.6076526	-3.1207745
C	-1.2461788	3.7618038	1.1730790
C	0.0888223	4.0530271	-0.7082062
C	-3.1410838	2.6221611	0.0013122
C	-3.4370022	1.9458558	-1.2242228
C	-2.6161630	2.1297862	-2.3807696
C	-1.4791423	2.9944430	-2.3374907
C	-2.0740194	3.5661931	0.0111467
C	-1.2465776	3.7495444	-1.1556734
Sc	0.0000000	0.0000000	-2.1121601
Sc	1.9050383	0.0433133	0.9475671
Sc	-1.9050383	-0.0433133	0.9475671
C	-0.0027412	0.6709166	0.0743178
C	0.0027412	-0.6709166	0.0743178

Cartesian coordinates for the monoanionic 2a isomer of $Sc_3C_2@C_{80}$ (in Å).

85

Energy=–5408.642091246 Hartree

C	0.000000	0.000000	0.000000
C	1.165938	0.483255	0.699826
C	0.000000	-1.248315	-0.741416
C	1.222766	-1.979966	-0.798897
C	2.378879	-1.534839	-0.060045
C	2.356738	-0.343650	0.728640
C	-1.165938	0.483255	0.699826
C	0.739981	1.323600	1.823981
C	-1.222766	-1.979966	-0.798897
C	1.222766	-3.425586	-0.798897
C	3.091843	-2.702776	0.396951
C	-0.739981	1.323600	1.823981
C	3.129886	-0.322340	1.929071
C	2.378879	-3.870714	-0.060045
C	-2.356738	-0.343650	0.728640
C	-2.378879	-1.534839	-0.060045
C	-1.222766	-3.425586	-0.798897
C	1.470639	1.184978	3.087410
C	0.000000	-4.157238	-0.741416
C	2.671317	0.404053	3.094202
C	3.850074	-1.479543	2.376937
C	3.795143	-2.702776	1.636734
C	-1.470639	1.184978	3.087410
C	-3.091843	-2.702776	0.396951
C	-2.378879	-3.870714	-0.060045
C	-3.129886	-0.322340	1.929071

C	2.356738	-5.061903	0.728640
C	3.122543	-0.317617	4.267113
C	0.722683	1.177524	4.323745
C	3.837683	-1.480947	3.816563
C	0.000000	-5.405553	0.000000
C	-2.671317	0.404053	3.094202
C	3.850074	-3.926010	2.376937
C	-0.722683	1.177524	4.323745
C	1.165938	-5.888807	0.699826
C	3.129886	-5.083213	1.929071
C	-3.850074	-1.479543	2.376937
C	-3.795143	-2.702776	1.636734
C	-2.356738	-5.061903	0.728640
C	-1.165938	-5.888807	0.699826
C	1.163681	0.446354	5.490113
C	2.349590	-0.336797	5.463217
C	3.782795	-2.702776	4.548455
C	3.837683	-3.924605	3.816563
C	-3.122543	-0.317617	4.267113
C	-1.163681	0.446354	5.490113
C	0.739981	-6.729153	1.823981
C	-3.837683	-1.480947	3.816563
C	2.671317	-5.809606	3.094202
C	0.000000	-0.011022	6.222588
C	-3.850074	-3.926010	2.376937
C	-0.739981	-6.729153	1.823981
C	-3.129886	-5.083213	1.929071
C	-2.349590	-0.336797	5.463217
C	3.122543	-5.087936	4.267113
C	2.353003	-1.539542	6.259077
C	3.043414	-2.702776	5.779939
C	1.470639	-6.590531	3.087410
C	-3.782795	-2.702776	4.548455
C	-3.837683	-3.924605	3.816563
C	-2.671317	-5.809606	3.094202
C	0.000000	-1.194702	7.059327
C	-1.470639	-6.590531	3.087410
C	1.240979	-1.960649	7.098117
C	2.353003	-3.866011	6.259077
C	2.349590	-5.068756	5.463217
C	-2.353003	-1.539542	6.259077
C	-3.122543	-5.087936	4.267113
C	0.722683	-6.583077	4.323745
C	-3.043414	-2.702776	5.779939
C	-1.240979	-1.960649	7.098117
C	1.240979	-3.444904	7.098117
C	-0.722683	-6.583077	4.323745
C	1.163681	-5.851907	5.490113
C	-2.349590	-5.068756	5.463217
C	-2.353003	-3.866011	6.259077
C	-1.240979	-3.444904	7.098117
C	0.000000	-4.210851	7.059327
C	-1.163681	-5.851907	5.490113
C	0.000000	-5.394530	6.222588
C	0.000000	-2.702776	3.259977
C	0.000000	-2.702776	1.928201
Sc	0.000000	-4.715718	2.490892
Sc	0.000000	-2.702776	5.293784
Sc	0.000000	-0.689835	2.490892

Cartesian coordinates for the transition state bf $1a_{TS}$ of the neutral 1a isomer of $Sc_3C_2@C_{80}$ (in Å). The transition state has only one imaginary frequency.

85

Energy=–5408.515995012 Hartree

C	0.000000	0.000000	0.000000
C	0.778183	0.938491	-0.766665
C	0.877760	0.906283	-2.208417
C	0.005729	-0.025107	-2.905250
C	-0.729082	-0.997489	-2.150057
C	-0.715574	-0.996751	-0.706876
C	0.936409	2.295923	-0.327736
C	0.345340	2.767524	0.897682
C	-0.373720	1.818134	1.692071
C	-0.549969	0.467507	1.236906
C	-1.997154	-1.462092	-0.239115
C	-2.578035	-0.941895	0.953006
C	-1.812898	-0.002421	1.725746
C	-2.030651	-1.451347	-2.569290
C	-2.811043	-1.739093	-1.392467
C	1.137191	2.284075	-2.690887
C	1.118818	3.135210	-1.487776
C	-1.494824	2.184029	2.541080
C	-2.411805	1.029615	2.555329
C	-0.590417	0.438451	-4.118152
C	-0.410231	1.811124	-4.577256
C	0.423233	2.766362	-3.882116
C	-0.129475	4.102383	-3.827136
C	-0.025843	4.961256	-2.654780
C	0.551056	4.468849	-1.449015
C	0.018323	4.959100	-0.210989
C	-0.068252	4.120647	0.951886
C	-1.253781	4.487437	1.701687
C	-1.981812	3.553896	2.519809
C	-3.426311	3.729351	2.583291
C	-4.345293	2.573385	2.599306
C	-3.856244	1.202171	2.550425
C	-4.609018	0.269540	1.753495
C	-3.995528	-0.807893	1.006905
C	-4.808370	-1.093301	-0.138628
C	-4.219856	-1.520376	-1.369840
C	-1.891872	-0.012170	-4.533934
C	-2.647636	-0.933832	-3.743706
C	-4.072988	-0.799222	-3.751562
C	-4.851016	-1.097186	-2.584197
C	-6.013792	4.785260	-2.809386
C	-6.862292	3.852876	-2.085668
C	-6.716543	3.819553	-0.647930
C	-5.914367	4.757115	0.093486
C	-5.222484	5.754976	-0.634062
C	-5.255130	5.757198	-2.077135
C	-7.136933	2.475181	-2.560412
C	-6.463893	1.993351	-3.775778
C	-5.652366	2.949768	-4.496175
C	-5.457037	4.322212	-4.041389
C	-3.967321	6.211280	-2.536691
C	-3.387857	5.694082	-3.730228
C	-4.168570	4.772569	-4.496466

C	-3.926722	6.219570	-0.206456
C	-3.149959	6.498131	-1.384845
C	-6.859783	2.462079	-0.204890
C	-7.078811	1.623843	-1.359228
C	-4.448061	2.576292	-5.212898
C	-3.555709	3.701461	-5.230842
C	-5.322427	4.286427	1.310180
C	-5.485927	2.937087	1.774071
C	-6.231475	1.988583	1.000637
C	-5.818971	0.635226	1.041825
C	-5.941537	-0.201885	-0.118327
C	-6.511901	0.290122	-1.339047
C	-5.974177	-0.201813	-2.562559
C	-5.907981	0.657846	-3.737543
C	-4.708503	0.281001	-4.455819
C	-3.944361	1.241545	-5.181349
C	-2.527462	1.059466	-5.248370
C	-1.635250	2.184874	-5.257233
C	-2.137284	3.519398	-5.208799
C	-1.350671	4.479504	-4.507336
C	-1.963577	5.559478	-3.783157
C	-1.149151	5.856804	-2.640656
C	-1.741214	6.279515	-1.406874
C	-4.046959	4.757594	1.763039
C	-3.307588	5.699695	0.966472
C	-1.889436	5.567074	0.975638
C	-1.113567	5.852267	-0.194902
C	-2.939541	3.042769	-1.437989
C	-3.022713	1.725315	-1.426912
Sc	-2.972182	2.395076	0.782919
Sc	-0.994491	2.279319	-2.180132
Sc	-4.987272	2.482646	-2.129812

Cartesian coordinates of $Sc_3@C_{82}$, quartet state. The energies reported in Table S1 for doublet and sextet are calculated for the quartet structure.

85

Energy= See Table S1

C	2.745219	3.272188	-0.371030
C	3.094469	2.399416	-1.484370
C	2.217936	2.386733	-2.629091
C	3.774783	1.164437	-1.190544
C	4.018212	0.713283	0.172499
C	3.511829	1.450362	1.292378
C	2.946190	2.751875	0.982225
C	3.623476	0.000000	-2.027986
C	2.740942	0.000000	-3.167920
C	2.060444	1.223650	-3.472036
C	2.060444	-1.223650	-3.472036
C	3.774783	-1.164437	-1.190544
C	2.745219	-3.272188	-0.371030
C	3.094469	-2.399416	-1.484370
C	2.217936	-2.386733	-2.629091
C	2.184180	1.414176	3.400128
C	3.080222	0.737127	2.498603
C	3.080222	-0.737127	2.498603
C	3.511829	-1.450362	1.292378
C	4.018212	-0.713283	0.172499
C	2.946190	-2.751875	0.982225

C	0.708898	-1.227848	-3.982393
C	0.000000	0.000000	-4.210499
C	0.708898	1.227848	-3.982393
C	-1.417797	0.000000	-3.982393
C	0.029490	-2.396222	-3.472036
C	-1.811738	-3.138022	-2.027986
C	-1.370471	-2.373725	-3.167920
C	-2.089934	-1.172572	-3.472036
C	1.461189	-4.013523	-0.371030
C	0.530720	-3.879597	-1.484370
C	0.958003	-3.114155	-2.629091
C	-0.878960	-3.851276	-1.190544
C	-2.089934	1.172572	-3.472036
C	-1.370471	2.373725	-3.167920
C	0.029490	2.396222	-3.472036
C	-1.811738	3.138022	-2.027986
C	-3.175939	0.727422	-2.629091
C	-4.206407	0.741335	-0.371030
C	-3.625189	1.480181	-1.484370
C	-2.895823	2.686839	-1.190544
C	-2.895823	-2.686839	-1.190544
C	-3.625189	-1.480181	-1.484370
C	-3.175939	-0.727422	-2.629091
C	-4.206407	-0.741335	-0.371030
C	-0.878960	3.851276	-1.190544
C	0.530720	3.879597	-1.484370
C	0.958003	3.114155	-2.629091
C	1.461189	4.013523	-0.371030
C	-1.391385	3.836515	0.172499
C	-0.499864	3.766514	1.292378
C	0.910098	3.927413	0.982225
C	1.523796	2.639292	3.003035
C	1.884563	3.264159	1.806488
C	-2.316802	1.184468	3.400128
C	-2.178481	2.298987	2.498603
C	-0.901741	3.036114	2.498603
C	0.132622	2.598643	3.400128
C	-2.626827	3.123233	0.172499
C	-3.856288	1.175538	0.982225
C	-3.011965	2.316152	1.292378
C	-1.231146	-0.726311	4.232933
C	-1.231146	0.726311	4.232933
C	-0.013431	1.429359	4.232933
C	-0.013431	-1.429359	4.232933
C	-3.769126	0.000000	1.806488
C	-2.316802	-1.184468	3.400128
C	-3.047592	0.000000	3.003035
C	-2.626827	-3.123233	0.172499
C	0.132622	-2.598643	3.400128
C	-0.901741	-3.036114	2.498603
C	-2.178481	-2.298987	2.498603
C	-3.011965	-2.316152	1.292378
C	-3.856288	-1.175538	0.982225
C	1.523796	-2.639292	3.003035
C	1.884563	-3.264159	1.806488
C	0.910098	-3.927413	0.982225
C	-0.499864	-3.766514	1.292378
C	-1.391385	-3.836515	0.172499
C	1.244577	0.703048	4.232933
C	1.244577	-0.703048	4.232933
C	2.184180	-1.414176	3.400128
Sc	-2.094745	0.000000	-0.291519
Sc	1.047373	-1.814102	-0.291519
Sc	1.047373	1.814102	-0.291519

Cartesian coordinates of the distorted C_1-symmetric structure of the neutral doublet 1a isomer $Sc_3C_2@C_{80}$

85

Energy= See Table S1

C	4.1589651	-0.1553099	-0.2113666
C	3.9917104	0.5996067	-1.4532020
C	3.3937566	-0.0452785	-2.6492991
C	2.9563460	-1.4463476	-2.5925259
C	3.2321698	-2.1932067	-1.3880694
C	3.8194486	-1.5550122	-0.2225949
C	3.3931826	1.9301442	-1.3381659
C	3.1478218	2.6096288	-0.0814711
C	3.4866009	1.9016809	1.1113372
C	3.9357011	0.5278464	1.0380061
C	3.3109484	-2.2327231	0.9512537
C	3.0881018	-1.5306279	2.1711356
C	3.4354307	-0.1521393	2.2048615
C	2.3598891	-3.2472692	-0.9170310
C	2.4174693	-3.2694860	0.5165876
C	2.4436040	0.9168604	-3.2085695
C	2.4809977	2.1278747	-2.4285909
C	2.7193644	2.0614979	2.3077257
C	2.6764975	0.7876533	2.9981026
C	1.7344491	-1.8041671	-3.2586288
C	0.8934409	-0.8344208	-3.9283326
C	1.2081456	0.5494040	-3.8693660
C	0.1213012	1.4751939	-3.8449182
C	0.1934227	2.6983539	-3.0893454
C	1.3628678	3.0352189	-2.3458404
C	1.2037295	3.7724398	-1.1416663
C	2.0833727	3.5506476	-0.0216105
C	1.3088066	3.7117015	1.1860781
C	1.5913662	2.9309120	2.3391191
C	0.4851468	2.5211418	3.1690550
C	0.4778181	1.3203534	3.9906256
C	1.5923562	0.3866532	3.8594426
C	1.2636239	-1.0265111	3.8559291
C	1.9935114	-1.9425909	2.9979586
C	1.0954365	-2.9672888	2.5477712
C	1.2750596	-3.6375233	1.2943552
C	0.8745791	-2.8751970	-2.8028966
C	1.1521864	-3.5916922	-1.6023327
C	0.0435872	-4.0501168	-0.8293474
C	0.1059314	-4.0677403	0.6084522
C	-4.1475764	0.1435879	0.1628248
C	-3.8375188	-0.5982664	1.3588468
C	-3.2389419	0.0285596	2.5072677
C	-2.8820935	1.4035248	2.4998901
C	-3.2046339	2.1655887	1.3409218
C	-3.8097089	1.5405393	0.1853407
C	-3.3792733	-1.9684871	1.3264088
C	-3.1478757	-2.6169685	0.0751717
C	-3.5001874	-1.8819375	-1.1235899
C	-4.0958236	-0.5475530	-1.1229620
C	-3.3329847	2.2362313	-0.9959652
C	-3.1755657	1.5527075	-2.2576588
C	-3.6227492	0.1531015	-2.3440497
C	-2.3562252	3.2284349	0.8777043
C	-2.4251876	3.2747750	-0.5543745

C	-2.4065125	-0.9421384	3.1845525
C	-2.5051185	-2.1800806	2.4402620
C	-2.6938775	-2.0275887	-2.3022341
C	-2.7294366	-0.7825144	-3.0320597
C	-1.7121272	1.7742297	3.2492496
C	-0.9228332	0.8422852	4.0408850
C	-1.2479104	-0.5772812	3.9599079
C	-0.1285518	-1.5006004	3.9042772
C	-0.2068904	-2.6875176	3.0759355
C	-1.3818845	-3.0513078	2.3327379
C	-1.2072740	-3.7770523	1.1225003
C	-2.0839494	-3.5577946	-0.0022922
C	-1.3078010	-3.7245111	-1.2056184
C	-1.5718476	-2.9334402	-2.3559015
C	-0.4720555	-2.5593824	-3.1831091
C	-0.4648720	-1.3014815	-3.8837000
C	-1.5493988	-0.3787306	-3.7719593
C	-1.2367653	1.0081987	-3.7929690
C	-2.0147458	1.9458773	-3.0093618
C	-1.1142132	2.9944948	-2.5792704
C	-1.2831132	3.6546501	-1.3263927
C	-0.8547189	2.8142489	2.7562096
C	-1.1479423	3.5577743	1.5642614
C	-0.0437641	4.0261459	0.8029519
C	-0.1086207	4.0777682	-0.6339613
C	0.0053998	0.6854948	-0.0995069
C	-0.0124734	-0.6205249	0.0001677
Sc	0.0642604	0.0569876	2.1645436
Sc	1.9142574	-0.0402272	-1.0162930
Sc	-1.9647585	0.0678744	-0.9115234

Cartesian coordinates of the distorted C_1-symmetric structure of the neutral doublet 2a isomer $Sc_3C_2@C_{80}$

85

Energy= See Table S1

C	0.2672624	3.0871446	2.7058242
C	1.3687224	2.2821267	3.1858092
C	0.3361823	3.8354815	1.4581688
C	1.5631729	3.7789966	0.7238341
C	2.6560200	2.9391277	1.1706794
C	2.5661805	2.1562408	2.3659053
C	-0.9602558	2.5066181	3.2074778
C	0.8471664	1.2129233	4.0455024
C	-0.8801346	4.0077705	0.7239475
C	1.5631727	3.7789967	-0.7238340
C	3.3334507	2.4247210	0.0000000
C	-0.6357588	1.3537745	4.0694039
C	3.2380703	0.8910885	2.3902094
C	2.6560202	2.9391276	-1.1706792
C	-2.1524291	2.5874737	2.3713793
C	-2.1024761	3.3727947	1.1723159
C	-0.8801346	4.0077705	-0.7239475
C	1.4710951	-0.1128549	3.8994038
C	0.3361824	3.8354815	-1.4581688
C	2.6715725	-0.2297165	3.1173431
C	3.9211823	0.3804865	1.2299943
C	3.9312761	1.1240818	-0.0000000
C	-1.4800436	0.1530010	3.9212075

C	-2.8570709	2.9817416	0.0000000
C	-2.1024760	3.3727947	-1.1723159
C	-3.0319882	1.4557638	2.3886081
C	2.5661792	2.1562410	-2.3659070
C	3.0195989	-1.4429396	2.3939012
C	0.6126628	-1.2787783	3.8903933
C	3.7778870	-1.0574445	1.2274632
C	0.2672625	3.0871445	-2.7058242
C	-2.6716792	0.2501432	3.1180181
C	3.9211824	0.3804865	-1.2299944
C	-0.8337336	-1.1475831	3.8884686
C	1.3687227	2.2821268	-3.1858092
C	3.2380722	0.8910883	-2.3902088
C	-3.7943156	1.0736124	1.2294711
C	-3.6754858	1.8088354	-0.0000000
C	-2.1524291	2.5874738	-2.3713790
C	-0.9602558	2.5066181	-3.2074778
C	0.9500159	-2.4815864	3.1576084
C	2.1384681	-2.5654179	2.3729308
C	3.6548477	-1.7824566	-0.0000000
C	3.7778870	-1.0574445	-1.2274632
C	-3.2316080	-0.8795534	2.3935570
C	-1.3724170	-2.2697098	3.1452815
C	0.8471664	1.2129233	-4.0455024
C	-3.9084075	-0.3674725	1.2277531
C	2.6715724	-0.2297166	-3.1173438
C	-0.2754290	-3.1055532	2.6875010
C	-3.7943156	1.0736124	-1.2294710
C	-0.6357588	1.3537745	-4.0694038
C	-3.0319883	1.4557638	-2.3886082
C	-2.5614624	-2.1420537	2.3647875
C	3.0195989	-1.4429397	-2.3939013
C	2.0652761	-3.3710067	1.1658314
C	2.7914124	-2.9399741	0.0000000
C	1.4710952	-0.1128549	-3.8994039
C	-3.9212918	-1.1076739	-0.0000000
C	-3.9084075	-0.3674725	-1.2277531
C	-2.6716791	0.2501432	-3.1180181
C	-0.3483943	-3.9544278	1.5091977C
C	-1.4800436	0.1530010	-3.9212075C
C	0.8970586	-4.1503810	0.7479075C
C	2.0652762	-3.3710066	-1.1658314C
C	2.1384681	-2.5654179	-2.3729308C
C	-2.6409974	-2.9392777	1.1661679C
C	-3.2316080	-0.8795534	-2.3935570C
C	0.6126628	-1.2787782	-3.8903933C
C	-3.2951359	-2.4062534	-0.0000000C
C	-1.5814896	-3.8461769	0.7384288C
C	0.8970585	-4.1503810	-0.7479075C
C	-0.8337336	-1.1475831	-3.8884686C
C	0.9500159	-2.4815863	-3.1576083C
C	-2.5614623	-2.1420537	-2.3647875C
C	-2.6409974	-2.9392777	-1.1661679C
C	-1.5814896	-3.8461769	-0.7384288C
C	-0.3483943	-3.9544278	-1.5091977C
C	-1.3724170	-2.2697098	-3.1452815C
C	-0.2754289	-3.1055532	-2.6875011C
C	0.1844728	-0.1625080	-0.0000000C
C	0.0242648	1.1309134	0.0000000C
Sc	-0.0190192	0.6117929	2.0974719Sc
Sc	-0.0190195	0.6117930	-2.0974719Sc
Sc	0.0044587	-2.2544655	0.0000000Sc

Cartesian coordinates of the distorted C_1-symmetric structure of the anionic 1a isomer $Sc_3C_2@C_{80}$

85

Energy= See Table S1

C	3.9653195	-0.2399362	-1.3215777
C	3.4751487	0.5436859	-2.4605078
C	2.5340949	-0.0765606	-3.4189149
C	2.1036181	-1.4631692	-3.2583575
C	2.6953240	-2.2424609	-2.1986429
C	3.6004936	-1.6403129	-1.2421766
C	2.9552378	1.8903426	-2.1862374
C	3.0542381	2.5507065	-0.9013097
C	3.6811752	1.8137702	0.1519231
C	4.0692980	0.4297530	-0.0477875
C	3.4109470	-2.3248019	0.0228066
C	3.5403051	-1.6426593	1.2686911
C	3.8862677	-0.2564228	1.2084439
C	1.9612699	-3.2903831	-1.5274278
C	2.4053151	-3.3367252	-0.1627328
C	1.4994941	0.9067728	-3.7125041
C	1.7780517	2.1150657	-2.9823367
C	3.2708133	1.9727161	1.5114033
C	3.3917486	0.6914719	2.1784857
C	0.7533810	-1.8042369	-3.6077760
C	-0.2121469	-0.8122256	-4.0218199
C	0.1323483	0.5666696	-4.0341268
C	-0.8887276	1.5109346	-3.7153544
C	-0.5940537	2.7267726	-3.0028516
C	0.7401716	3.0390414	-2.6002769
C	0.9239588	3.7725165	-1.3927687
C	2.0646612	3.5162686	-0.5521210
C	1.6421309	3.6650563	0.8215377
C	2.2064187	2.8633301	1.8508039
C	1.3592468	2.4700310	2.9544877
C	1.5518419	1.2596434	3.7476125
C	2.5627868	0.3009642	3.2955656
C	2.2067244	-1.1015811	3.3384523
C	2.6945002	-2.0455152	2.3475625
C	1.6875095	-3.0530367	2.1556322
C	1.5049281	-3.6963466	0.8896756
C	0.0301380	-2.8687301	-2.9528934
C	0.6075717	-3.6021681	-1.8715779
C	-0.2636250	-4.0494800	-0.8337513
C	0.1807753	-4.0879610	0.5342695
C	-3.9321211	0.1958837	1.2675644
C	-3.3618701	-0.5669737	2.3465071
C	-2.4745569	0.0351976	3.3043677
C	-2.0928075	1.4041414	3.1958295
C	-2.6925473	2.1903623	2.1682107
C	-3.5851174	1.5894421	1.2097520
C	-2.9513203	-1.9404570	2.1753994
C	-3.0698883	-2.5753124	0.8996105
C	-3.7118086	-1.8254622	-0.1582195
C	-4.2318604	-0.4751827	0.0114029
C	-3.4335726	2.2902644	-0.0474748
C	-3.6384944	1.6200409	-1.3099263
C	-4.1239983	0.2278100	-1.2873883
C	-1.9803800	3.2512643	1.5033490
C	-2.4281544	3.3193336	0.1407491

C	-1.5072095	-0.9564984	3.7155407
C	-1.8121708	-2.1801143	3.0126533
C	-3.2694168	-1.9751379	-1.5169080
C	-3.4877292	-0.7213220	-2.2091774
C	-0.7568937	1.7500313	3.6025619
C	0.2002630	0.7980119	4.1402055
C	-0.1652428	-0.6107680	4.1016586
C	0.8747590	-1.5466756	3.7385050
C	0.5680187	-2.7474332	3.0005677
C	-0.7716607	-3.0697064	2.6011088
C	-0.9434481	-3.7829996	1.3811944
C	-2.0847089	-3.5391370	0.5350736
C	-1.6627659	-3.7017169	-0.8328742
C	-2.2117057	-2.8931307	-1.8678126
C	-1.3638736	-2.5276098	-2.9573463
C	-1.5194909	-1.2571177	-3.6190982
C	-2.5228843	-0.3189457	-3.2171517
C	-2.1949825	1.0678260	-3.3069169
C	-2.7197596	2.0160398	-2.3480053
C	-1.7169854	3.0443593	-2.1648023
C	-1.5330539	3.6981673	-0.9069682
C	-0.0395368	2.7832402	2.9062486
C	-0.6273780	3.5502760	1.8424488
C	0.2426379	4.0115907	0.8161949
C	-0.2026920	4.0871033	-0.5504011
C	-0.0780650	0.7655651	-0.2704702
C	-0.0209704	-0.5286864	0.0800328
Sc	0.6677613	0.2021624	1.9949798
Sc	1.6416820	0.0006416	-1.3472386
Sc	-2.0778707	0.0840456	-0.4867191

Cartesian coordinates of the distorted C_1-symmetric structure of the anionic 2a isomer $Sc_3C_2@C_{80}$

85

Energy= See Table S1

C	0.2789823	3.1076729	2.6976296
C	1.3738622	2.3014361	3.1758389
C	0.3498105	3.8483445	1.4519628
C	1.5698290	3.7863619	0.7207749
C	2.6553998	2.9466320	1.1663495
C	2.5638124	2.1685422	2.3564787
C	-0.9465557	2.5331628	3.1960747
C	0.8510136	1.2366161	4.0327848
C	-0.8592255	4.0230499	0.7204929
C	1.5700262	3.7860336	-0.7215001
C	3.3271708	2.4310172	0.0001241
C	-0.6281002	1.3825285	4.0564845
C	3.2275175	0.9070567	2.3802108
C	2.6556904	2.9461221	-1.1664596
C	-2.1323012	2.6153449	2.3611265
C	-2.0789236	3.3956600	1.1671256
C	-0.8589802	4.0227805	-0.7221227
C	1.4674958	-0.0876175	3.8875139
C	0.3502582	3.8477981	-1.4531135
C	2.6600006	-0.2071992	3.1056072
C	3.9043508	0.3954950	1.2243612
C	3.9176858	1.1353254	0.0004058
C	-1.4731581	0.1879469	3.9084969
C	-2.8308424	3.0082610	-0.0009822
C	-2.0785297	3.3952638	-1.1689476
C	-3.0107985	1.4917675	2.3779088
C	2.5644459	2.1676724	-2.3563454
C	3.0012768	-1.4168800	2.3835891
C	0.6080996	-1.2461790	3.8797543
C	3.7578401	-1.0359779	1.2222675
C	0.2798099	3.1067459	-2.6985689
C	-2.6571442	0.2898603	3.1059458
C	3.9047146	0.3951191	-1.2233026
C	-0.8334880	-1.1102756	3.8782516
C	1.3747913	2.3003246	-3.1761198
C	3.2281973	0.9062445	-2.3794934
C	-3.7695993	1.1130842	1.2226622
C	-3.6490911	1.8442624	-0.0009336
C	-2.1315412	2.6145633	-2.3627373
C	-0.9455432	2.5321333	-3.1972315
C	0.9395908	-2.4438859	3.1459173
C	2.1216380	-2.5313755	2.3642320
C	3.6333255	-1.7570333	0.0008240
C	3.7581474	-1.0363281	-1.2207700
C	-3.2158461	-0.8336610	2.3819059
C	-1.3729322	-2.2237461	3.1330776
C	0.8522338	1.2352097	-4.0328037
C	-3.8881059	-0.3214359	1.2211058
C	2.6609001	-0.2082234	-3.1046886
C	-0.2835115	-3.0620103	2.6793657
C	-3.7691449	1.1126790	-1.2242885
C	-0.6268381	1.3811802	-4.0571816
C	-3.0099734	1.4909202	-2.3793964
C	-2.5552357	-2.0930101	2.3554885
C	3.0019955	-1.4176262	-2.3822483
C	2.0475514	-3.3335267	1.1626716

C	2.7727225	-2.9088581	0.0008693
C	1.4686628	-0.0889281	-3.8868822
C	-3.9020630	-1.0573631	-0.0004802
C	-3.8876202	-0.3218051	-1.2223427
C	-2.6561198	0.2888214	-3.1069759
C	-0.3599777	-3.9068554	1.5055150
C	-1.4719445	0.1866695	-3.9090640
C	0.8798311	-4.1042219	0.7466397
C	2.0479419	-3.3338157	-1.1610178
C	2.1223419	-2.5320660	-2.3627903
C	-2.6363191	-2.8858142	1.1615583
C	-3.2149744	-0.8343946	-2.3826842
C	0.6093043	-1.2473851	-3.8790865
C	-3.2845381	-2.3524216	-0.0001780
C	-1.5884206	-3.7987988	0.7373628
C	0.8800504	-4.1043323	-0.7451007
C	-0.8322795	-1.1115100	-3.8781575
C	0.9405681	-2.4447659	-3.1448156
C	-2.5544069	-2.0937058	-2.3557125
C	-2.6359110	-2.8860883	-1.1615171
C	-1.5881843	-3.7989298	-0.7367023
C	-0.3594811	-3.9071067	-1.5043837
C	-1.3719382	-2.2247063	-3.1328570
C	-0.2826313	-3.0627498	-2.6785148
C	0.1936513	-0.1192590	0.0000416
C	0.0305798	1.1639587	-0.0001965
Sc	-0.0153712	0.6302588	2.0882052
Sc	-0.0152473	0.6295871	-2.0883535
Sc	-0.0150413	-2.2050586	0.0006553

Cartesian coordinates of the neutral closed-shell $Sc_2C_2@C_{84}$

88

Energy= -4800.124353642 Hartree

C	-1.1580717	-2.1957429	-3.3977383
C	0.1732505	-1.8192257	-3.8200476
C	-3.3031967	-2.3198927	-1.5121989
C	-2.3234511	-3.3003403	-1.5142301
C	-1.2452847	-3.2551755	-2.4686106
C	-3.8209458	-1.8272301	-0.2693216
C	-1.8289028	-3.8153109	-0.2697981
C	-2.2176466	-3.2515004	0.9764263
C	-3.2574036	-2.2150133	0.9776579
C	-2.3307877	-1.3184779	3.0920578
C	-3.3056517	-1.2271416	2.0540351
C	-3.8387158	0.0679175	1.8271817
C	-0.0699862	-3.8301117	-1.8260604
C	1.2270489	-3.2975187	-2.0518348
C	1.3197848	-2.3246991	-3.0892345
C	2.3307877	-1.3184779	-3.0920578
C	3.3056517	-1.2271416	-2.0540351
C	3.8387158	0.0679175	-1.8271817
C	-0.4660691	-4.2339172	-0.5131978
C	2.2176466	-3.2515004	-0.9764263
C	3.2574036	-2.2150133	-0.9776579
C	0.4660691	-4.2339172	0.5131978
C	1.8289028	-3.8153109	0.2697981
C	0.0699862	-3.8301117	1.8260604
C	-1.3197848	-2.3246991	3.0892345

C	-1.2270489	-3.2975187	2.0518348	
C	1.8242554	-0.1746950	-3.8209781	
C	3.2581970	1.2405279	-2.4663051	
C	2.2005618	1.1549141	-3.3982467	
C	3.3031967	2.3198927	-1.5121989	
C	2.3234511	3.3003403	-1.5142301	
C	4.2413755	-0.4649909	0.5133508	
C	4.2413755	0.4649909	-0.5133508	
C	3.8209458	1.8272301	-0.2693216	
C	3.8209458	-1.8272301	0.2693216	
C	0.5106146	-0.5105202	-4.3447688	
C	1.2452847	3.2551755	-2.4686106	
C	1.1580717	2.1957429	-3.3977383	
C	-0.1732505	1.8192257	-3.8200476	
C	-0.5106146	0.5105202	-4.3447688	
C	0.4660691	4.2339172	-0.5131978	
C	0.0699862	3.8301117	-1.8260604	
C	-1.2270489	3.2975187	-2.0518348	
C	-1.3197848	2.3246991	-3.0892345	
C	-0.4660691	4.2339172	0.5131978	
C	1.8289028	3.8153109	-0.2697981	
C	2.2176466	3.2515004	0.9764263	
C	3.2574036	2.2150133	0.9776579	
C	-3.2581970	-1.2405279	-2.4663051	
C	-2.2005618	-1.1549141	-3.3982467	
C	-1.8242554	0.1746950	-3.8209781	
C	-2.3307877	1.3184779	-3.0920578	
C	-3.3056517	1.2271416	-2.0540351	
C	-3.8387158	-0.0679175	-1.8271817	
C	-4.2413755	0.4649909	0.5133508	
C	-4.2413755	-0.4649909	-0.5133508	
C	-1.8289028	3.8153109	0.2697981	
C	-2.2176466	3.2515004	-0.9764263	
C	-3.2574036	2.2150133	-0.9776579	
C	-3.8209458	1.8272301	0.2693216	
C	-1.2452847	3.2551755	2.4686106	
C	-2.3234511	3.3003403	1.5142301	
C	-3.3031967	2.3198927	1.5121989	
C	0.1732505	1.8192257	3.8200476	
C	-1.1580717	2.1957429	3.3977383	
C	3.8387158	-0.0679175	1.8271817	
C	3.3056517	1.2271416	2.0540351	
C	2.3307877	1.3184779	3.0920578	
C	1.3197848	2.3246991	3.0892345	
C	1.2270489	3.2975187	2.0518348	
C	-0.0699862	3.8301117	1.8260604	
C	2.3234511	-3.3003403	1.5142301	
C	3.3031967	-2.3198927	1.5121989	
C	2.2005618	-1.1549141	3.3982467	
C	3.2581970	-1.2405279	2.4663051	
C	1.8242554	0.1746950	3.8209781	
C	-0.5106146	-0.5105202	4.3447688	
C	-0.1732505	-1.8192257	3.8200476	
C	1.1580717	-2.1957429	3.3977383	
C	1.2452847	-3.2551755	2.4686106	
C	0.5106146	0.5105202	4.3447688	
C	-3.2581970	1.2405279	2.4663051	
C	-2.2005618	1.1549141	3.3982467	
C	-1.8242554	-0.1746950	3.8209781	
C	0.6376532	0.0000000	0.0000000	
C	-0.6376532	0.0000000	0.0000000	
Sc	0.0000000	0.0000000	2.2188643	S24
Sc	0.0000000	0.0000000	-2.2188643	

Cartesian coordinates of the anionic doublet $Sc_2C_2@C_{84}$

88
Energy= -4800.236380102 Hartree

C	-1.1585393	-2.1943040	-3.4040934
C	0.1724453	-1.8195939	-3.8274004
C	-3.3010629	-2.3171563	-1.5130880
C	-2.3205848	-3.2981233	-1.5148697
C	-1.2466437	-3.2605818	-2.4759816
C	-3.8252477	-1.8280773	-0.2694361
C	-1.8296442	-3.8196939	-0.2698066
C	-2.2197321	-3.2509727	0.9824704
C	-3.2569381	-2.2171726	0.9835486
C	-2.3300288	-1.3183665	3.0988384
C	-3.3045120	-1.2282277	2.0567557
C	-3.8352436	0.0705421	1.8302892
C	-0.0723998	-3.8267871	-1.8290930
C	1.2281436	-3.2963985	-2.0545258
C	1.3196800	-2.3238700	-3.0960850
C	2.3300288	-1.3183665	-3.0988384
C	3.3045120	-1.2282277	-2.0567557
C	3.8352436	0.0705421	-1.8302892
C	-0.4694161	-4.2292834	-0.5123119
C	2.2197321	-3.2509727	-0.9824704
C	3.2569381	-2.2171726	-0.9835486
C	0.4694161	-4.2292834	0.5123119
C	1.8296442	-3.8196939	0.2698066
C	0.0723998	-3.8267871	1.8290930
C	-1.3196800	-2.3238700	3.0960850
C	-1.2281436	-3.2963985	2.0545258
C	1.8244408	-0.1735744	-3.8283560
C	3.2638773	1.2424108	-2.4741300
C	2.1992102	1.1557858	-3.4047607
C	3.3010629	2.3171563	-1.5130880
C	2.3205848	3.2981233	-1.5148697
C	4.2366809	-0.4684087	0.5125470
C	4.2366809	0.4684087	-0.5125470
C	3.8252477	1.8280773	-0.2694361
C	3.8252477	-1.8280773	0.2694361
C	0.5112961	-0.5109509	-4.3535173
C	1.2466437	3.2605818	-2.4759816
C	1.1585393	2.1943040	-3.4040934
C	-0.1724453	1.8195939	-3.8274004
C	-0.5112961	0.5109509	-4.3535173
C	0.4694161	4.2292834	-0.5123119
C	0.0723998	3.8267871	-1.8290930
C	-1.2281436	3.2963985	-2.0545258
C	-1.3196800	2.3238700	-3.0960850
C	-0.4694161	4.2292834	0.5123119
C	1.8296442	3.8196939	-0.2698066
C	2.2197321	3.2509727	0.9824704
C	3.2569381	2.2171726	0.9835486
C	-3.2638773	-1.2424108	-2.4741300
C	-2.1992102	-1.1557858	-3.4047607
C	-1.8244408	0.1735744	-3.8283560
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C	-4.2366809	0.4684087	0.5125470

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C	-1.8296442	3.8196939	0.2698066
C	-2.2197321	3.2509727	-0.9824704
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C	-3.8252477	1.8280773	0.2694361
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