

Supplementary Information for:

A Computational Search for Molecular Switches that Exploit Baird's Rule on Excited State Aromaticity and Antiaromaticity

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Interference in 1-OFF

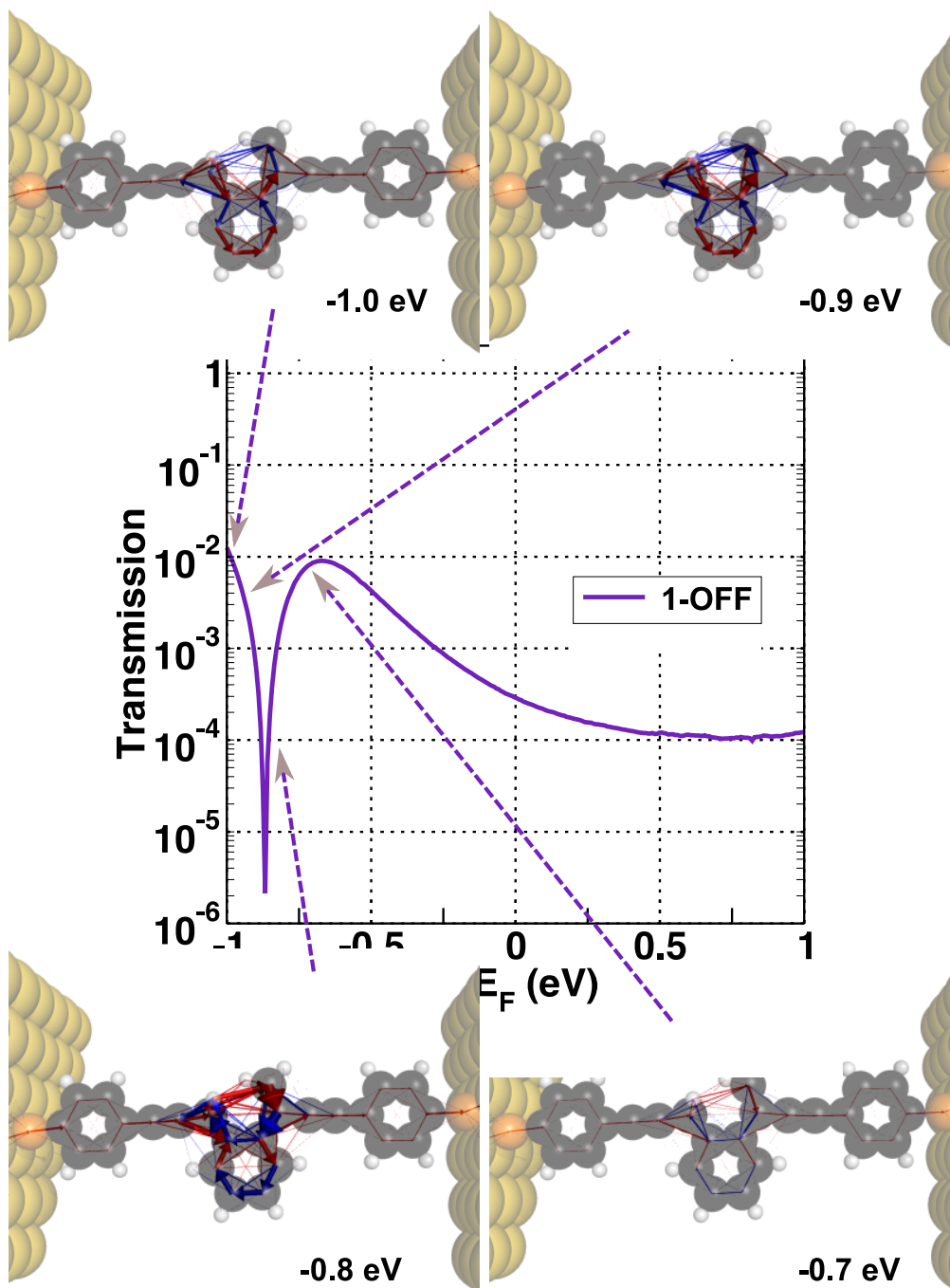


Figure S1. Transmission spectra ($V = 0$) for switch **1-OFF** together with local currents plotted at different energies. The energy at which the currents are plotted is given at each plot and marked in the transmission spectra with a dashed line. Note the two reversals of the ring currents in the central part going from -0.9 eV to -0.8 eV.

Full reference 41

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Energy and geometry tables

All energies and geometry data obtained at B3LYP/6-31G(d) level of computation.

Table S1: Switches of type **1-ON/OFF** (ΔG in kJ/mol and distances d in Å)

State/isomer	1	1B	1C
OFF	0.00	0.00	0.00
OFF@S---S(ON)	3.5	11.4	-
d(S---S(OFF))	17.191	15.075	7.811
TS	130.7	131.3	136.8
TS@S---S(OFF)	116.2	-	-
TS@S---S(ON)	145.1	-	-
ON	42.3	26.8	10.4
ON@S---S(OFF)	5.5	6.8	-
d(S---S(ON))	20.303	20.258	20.302

Table S2: Energy data of switch **2**

State/isomer	ΔG (kJ/mol)	d(S---S) (Å)
OFF	0.0	19.242
TS	166.8	19.667
ON	86.8	20.405

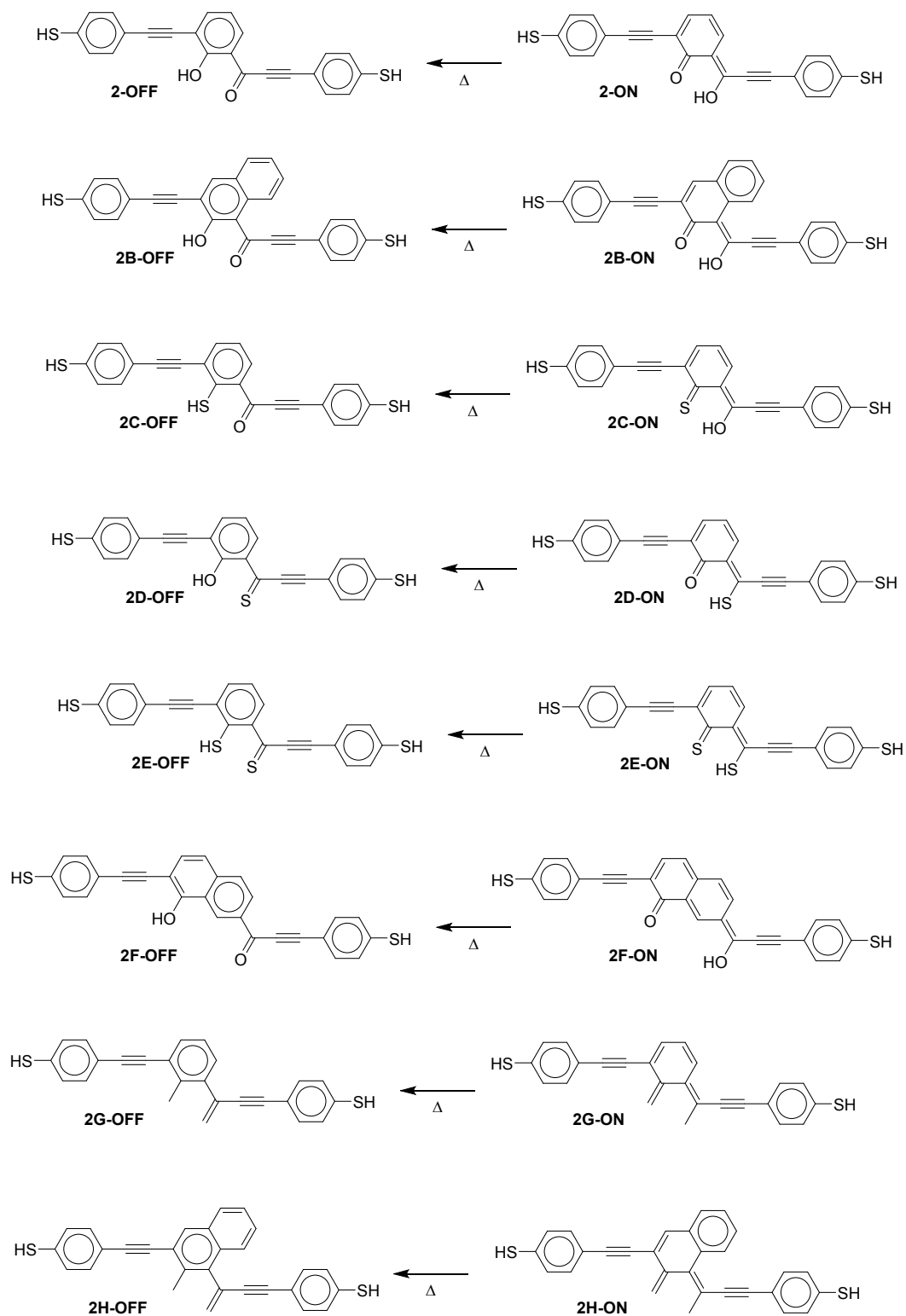
Table S3: Energy data for modified switches **2** (see Scheme S1 p. S6 for structures)

State/isomer	2	2B	2C	2D	2E	2F
ON	0.0	0.0	0.0	0.0	0.0	0.0
TS (OH rot.)	20.8	17.8	20.5	53.9	57.5	22.1
Intermediate	-	-	-84.4	-	-	3.0
TS (H-shift)	-	-	-90.6	-	-	199.6
OFF	-113.3	-82.8	-112.0	-52.3	-37.9	-83.9
State/isomer	2G	2H				
ON	0.0	0.0				
TS (OH rot.)	-	-				
Intermediate	-	-				
TS (H-shift)	80.0	68.5				
OFF	-86.8	-118.8				

Table S4: Energy and geometry data of switch **5**

	ΔG (kJ/mol)	ΔH (kJ/mol)	d SS (Å)	CCC (Arm-CO)	HCC (Ring)	HCC (Arm)	HCC (CO)	d CC (CO)	d CS
<i>cis</i> -OFF	0.0	0.0	16.024	114.4	109.3	108.6	104.7	1.563	1.785
<i>cis</i> -OFF@S---S(ON)	44.7	50.6	20.154	124.8	107.5	104.9	101.5	1.599	1.843
<i>trans</i> -OFF	-0.4	0.3	18.235	110.4	112.3	109.7	107.5	1.563	1.785
<i>trans</i> -OFF@S---S(ON)	53.4	53.6	20.154	123.5	107.6	104.5	101.2	1.595	1.855
<i>cis</i> -ON@S---S(OFF)	-	-	16.024						
<i>trans</i> -ON@S---S(OFF)	-3.3	13.1	18.235						

Scheme S1



Cartesian coordinates and absolute energies

1-OFF@ S---S(ON)

B3LYP/6-31G(d): -1759.740165 a.u.

C	0.659463	3.356020	0.370003
C	1.136936	4.433313	1.131119
C	2.480689	4.510453	1.480707
C	3.395218	3.515131	1.082632
C	2.906336	2.444482	0.310472
C	1.561593	2.364901	-0.040463
C	4.769044	3.580031	1.478887
C	5.925739	3.633711	1.844614
C	7.279227	3.709389	2.406692
C	8.315202	2.738445	1.833081
C	7.869087	1.716529	0.987993
C	8.736960	0.782771	0.426544
C	10.098249	0.866020	0.702985
C	10.563846	1.879737	1.533077
C	9.706178	2.827756	2.123318
C	10.355063	3.848543	3.011193
C	11.759836	4.092288	2.821708
C	12.958127	4.293642	2.740580
C	14.366683	4.519303	2.702745
C	15.014884	5.184834	3.764017
C	16.390678	5.379973	3.755901
C	17.169668	4.915856	2.684951
C	16.535702	4.261225	1.619145
C	15.157611	4.067189	1.628383
S	18.937433	5.186243	2.755310
S	-1.087315	3.311285	-0.022663
C	9.765725	4.520357	4.028336
H	8.348076	0.003444	-0.223344
H	6.808659	1.663544	0.764675
H	10.797401	0.151947	0.276456
H	11.625855	1.947202	1.742912
H	7.179646	3.528249	3.486823
H	8.738490	4.371779	4.326026
H	10.344142	5.221603	4.620137
H	14.425531	5.543149	4.602313
H	14.682085	3.555984	0.796894
H	16.863016	5.892033	4.589792
H	17.116905	3.896128	0.776728
H	2.834097	5.347432	2.075008
H	3.590198	1.664730	-0.010851
H	0.454706	5.214252	1.455894
H	1.217452	1.521648	-0.633178
H	19.234885	4.605336	1.575091
H	-1.060378	2.169501	-0.739935
H	7.654930	4.738388	2.319591

1-OFF

B3LYP/6-31G(d): -1759.744187 a.u.

C	-0.616437	-3.137888	2.427538
C	-1.355289	-2.836810	1.288058
C	-0.733790	-2.412446	0.101702
C	0.669223	-2.249502	0.081778
C	1.396969	-2.547557	1.240897
C	0.771021	-2.996225	2.401310
H	-1.120804	-3.475623	3.328811
H	-2.437262	-2.932697	1.301953
H	2.473268	-2.403503	1.229477
H	1.364575	-3.221052	3.283457
C	1.409269	-1.747707	-1.161139
H	1.646450	-2.598243	-1.817820
H	0.739538	-1.110621	-1.750913
C	-1.611652	-2.147225	-1.085809
C	-1.383532	-2.682702	-2.303694
H	-0.544082	-3.346887	-2.479889
H	-2.045681	-2.482948	-3.139855
C	2.649630	-1.020119	-0.886551
C	3.679338	-0.412552	-0.681396
C	-2.754874	-1.320285	-0.862605
C	-3.717287	-0.610379	-0.636674
C	-4.843920	0.221085	-0.382888
C	-5.830610	0.425310	-1.367039
C	-5.001662	0.863094	0.862158
C	-6.930591	1.238015	-1.118505
H	-5.726161	-0.061239	-2.331881
C	-6.100288	1.674853	1.111838
H	-4.249789	0.718159	1.631606
C	-7.076713	1.871037	0.123583
H	-7.676316	1.377538	-1.896314
H	-6.200343	2.160359	2.078743
C	4.885177	0.313163	-0.438311
C	6.132459	-0.198690	-0.841308
C	4.858089	1.562552	0.211222
C	7.307100	0.508062	-0.605945
H	6.174000	-1.160284	-1.343724
C	6.030086	2.270415	0.447917
H	3.904904	1.973437	0.529110
C	7.267243	1.750036	0.041417
H	8.255750	0.087612	-0.928624
H	5.983669	3.232608	0.950680
S	8.729990	2.716015	0.380873
H	9.618468	1.862719	-0.168087
S	-8.459464	2.926674	0.518616
H	-9.082348	2.832442	-0.673867

1-ON@S---S(OFF)

B3LYP/6-31G(d): -1759.721907 a.u.

C	-0.690717	-3.073882	2.422789
C	-0.219902	-3.924195	1.412321
C	0.355515	-3.395663	0.265328
C	0.483943	-2.000493	0.093614
C	-0.029919	-1.155449	1.100446
C	-0.607336	-1.684094	2.246222
C	1.192413	-1.483768	-1.017587
C	1.927983	-1.086523	-1.910721
C	2.909918	-0.751057	-2.848121
C	3.408254	0.520467	-3.084097
C	4.650048	0.733586	-3.849754
C	5.351479	1.974161	-3.599604
C	4.796710	2.988258	-2.881084
C	3.490664	2.840331	-2.301132
C	2.828549	1.657869	-2.402527
C	5.191283	-0.176639	-4.763751
C	6.572465	-0.155928	-5.032444
C	7.781809	-0.310948	-5.134251
C	9.175198	-0.552515	-5.054092
C	9.798904	-1.544739	-5.838302
C	11.135062	-1.871730	-5.643481
C	11.890147	-1.210870	-4.664146
C	11.293676	-0.188962	-3.909428
C	9.959103	0.134205	-4.100460
S	13.579856	-1.630067	-4.290591
S	-1.364739	-3.678614	3.955816
C	4.416246	-1.260835	-5.482830
H	5.326868	3.930381	-2.772087
H	6.311302	2.112242	-4.086584
H	1.862031	1.518256	-1.928004
H	3.044939	3.674432	-1.765826
H	3.401752	-1.602101	-3.305592
H	3.341027	-1.061079	-5.477558
H	4.759536	-1.320033	-6.521689
H	9.215720	-2.076611	-6.583680
H	9.496122	0.905981	-3.493713
H	11.585096	-2.656813	-6.244986
H	11.872933	0.340286	-3.157747
H	0.737443	-4.059976	-0.503550
H	0.051579	-0.079503	0.982094
H	-0.286404	-5.002566	1.527637
H	-0.981689	-1.015630	3.016730
H	-1.304994	-4.991788	3.654601
H	13.736675	-2.558816	-5.255860
H	4.581319	-2.254678	-5.043405

1-ON

B3LYP/6-31G(d): -1759.730975 a.u.

C	0.682669	3.305484	0.194953
H	1.186611	4.264681	0.278174
C	1.394476	2.150253	0.256322
H	2.474594	2.170046	0.360184
C	-0.738158	3.266297	-0.015603
H	-1.292679	4.196433	-0.104905
C	-1.391065	2.075757	-0.070563
H	-2.470007	2.051241	-0.176767
C	0.767352	0.854344	0.097038
C	1.566627	-0.255245	-0.141022
H	1.103838	-1.193137	-0.422670
C	-0.707647	0.807651	0.100019
C	-1.475561	-0.336153	0.337750
C	-0.940099	-1.678039	0.792758
H	-0.702375	-2.340104	-0.051480
H	-0.028604	-1.564366	1.389468
H	-1.696855	-2.190260	1.394006
C	2.967412	-0.263217	-0.126519
C	4.188964	-0.324579	-0.121730
C	-2.881422	-0.294081	0.228323
C	-4.099975	-0.350760	0.148367
C	-5.513271	-0.406274	0.048299
C	-6.219065	-1.576756	0.402248
C	-6.256300	0.703033	-0.407390
C	-7.602174	-1.634128	0.304766
H	-5.665959	-2.441323	0.755761
C	-7.640786	0.645820	-0.505535
H	-5.733713	1.612853	-0.686160
C	-8.329146	-0.523179	-0.150512
H	-8.122365	-2.546352	0.583833
H	-8.185784	1.516144	-0.860776
C	5.603862	-0.399726	-0.115720
C	6.267635	-1.594865	-0.469959
C	6.392100	0.713873	0.244292
C	7.653147	-1.671453	-0.463400
H	5.679444	-2.463034	-0.750369
C	7.779063	0.637312	0.250630
H	5.902337	1.642505	0.520605
C	8.425093	-0.556100	-0.102676
H	8.140257	-2.602709	-0.739368
H	8.359287	1.511830	0.532244
S	-10.103089	-0.673549	-0.250200
H	-10.346557	0.573549	-0.701995
S	10.199683	-0.731590	-0.119025
H	10.490315	0.518295	0.295756

1-TS

B3LYP/6-31G(d): -1759.693119 a.u.

C	0.572224	3.495191	-1.161512
H	1.079729	4.441161	-0.992384
C	1.307154	2.330808	-1.275343
H	2.389481	2.358545	-1.193022
C	-0.830601	3.458913	-1.289351
H	-1.409127	4.375703	-1.214059
C	-1.468089	2.253970	-1.489427
H	-2.551606	2.208788	-1.542211
C	0.696030	1.091081	-1.577017
C	1.523278	-0.112380	-1.746066
H	1.554791	-0.520455	-2.759103
C	-0.740789	1.040856	-1.619418
C	-1.412936	-0.234480	-1.518467
C	-0.713204	-1.430828	-1.854602
H	-0.353185	-1.531349	-2.880726
H	0.517065	-1.113629	-1.413841
H	-1.135754	-2.360900	-1.474106
C	2.769230	-0.204630	-1.071697
C	3.817014	-0.340115	-0.460547
C	-2.648649	-0.313209	-0.846115
C	-3.728739	-0.392240	-0.280345
C	-4.979429	-0.484466	0.382000
C	-5.682256	-1.707094	0.441493
C	-5.555868	0.643464	1.002686
C	-6.903376	-1.797311	1.094904
H	-5.255391	-2.586241	-0.030936
C	-6.780859	0.555039	1.651690
H	-5.028944	1.592054	0.970809
C	-7.467147	-0.666692	1.706358
H	-7.424298	-2.750234	1.129890
H	-7.201246	1.441157	2.119431
C	5.037586	-0.490666	0.249544
C	6.080075	-1.295181	-0.257337
C	5.242988	0.159707	1.483761
C	7.272272	-1.442446	0.438816
H	5.941794	-1.804445	-1.206010
C	6.436605	0.013945	2.180306
H	4.452379	0.781666	1.892072
C	7.464028	-0.789016	1.665542
H	8.059779	-2.068281	0.027745
H	6.565748	0.528056	3.128934
S	-9.040907	-0.859454	2.522022
H	-9.157749	0.413591	2.951504
S	9.023467	-1.024372	2.500411
H	8.749537	-0.257160	3.575174

1B-OFF@S---S(ON)

B3LYP/6-31G(d): -1913.377077 a.u.

C	0.826569	4.181535	-0.311515
C	0.263248	2.878134	-0.339601
C	0.954906	1.784351	0.275993
C	2.171467	2.083914	0.954606
C	2.687477	3.361446	0.977620
C	2.019718	4.423840	0.327373
C	0.386465	0.455001	0.236405
C	-0.890228	0.278139	-0.312781
C	-1.553510	1.388419	-0.904295
C	-0.994499	2.637452	-0.943767
C	-1.642686	-1.063273	-0.410530
C	-3.112657	-0.968648	-0.275611
C	-4.327612	-0.918683	-0.209664
C	-5.765164	-0.866423	-0.140928
C	-6.569213	-1.476144	-1.127299
C	-7.961131	-1.422625	-1.070531
C	-8.615134	-0.753919	-0.023224
C	-7.826621	-0.144240	0.964962
C	-6.433496	-0.200605	0.906657
S	-10.423046	-0.718878	-0.013678
C	1.208964	-0.673471	0.818576
C	0.738610	-1.449120	1.819354
C	2.568282	-0.874508	0.375615
C	3.761280	-1.001368	0.144977
C	5.180204	-1.103784	-0.042765
C	5.945399	-2.051720	0.672148
C	7.331969	-2.110638	0.550286
C	8.020527	-1.222756	-0.292830
C	7.269419	-0.286549	-1.021673
C	5.881081	-0.229194	-0.899954
S	9.822166	-1.331681	-0.375269
H	-1.521866	3.462369	-1.417032
H	-2.536031	1.223277	-1.335474
H	-1.256633	-1.778576	0.319341
H	1.336831	-2.251129	2.240195
H	-0.241641	-1.277066	2.252344
H	5.440589	-2.743348	1.339796
H	5.327613	0.513367	-1.466678
H	7.882028	-2.851593	1.124157
H	7.766127	0.413776	-1.687951
H	-6.091144	-1.998760	-1.950351
H	-5.850035	0.281270	1.685473
H	-8.540903	-1.906512	-1.852021
H	-8.295779	0.382215	1.791990
H	9.992509	-0.339643	-1.273000
H	-10.554131	-0.005556	1.123330
H	2.700189	1.297429	1.476885

H	3.615424	3.553685	1.509688
H	2.440446	5.425507	0.347829
H	0.283427	4.989169	-0.796832
H	-1.424736	-1.508318	-1.394161

1B-OFF

B3LYP/6-31G(d): -1913.386611 a.u.

C	7.076892	-1.802723	-0.182221
C	6.854459	-0.940124	0.899269
C	5.577315	-0.453933	1.158252
C	4.485963	-0.813943	0.346065
C	4.722259	-1.681710	-0.737641
C	5.997114	-2.168979	-0.998577
C	3.175234	-0.312930	0.613134
C	2.062026	0.112333	0.840280
C	0.714874	0.596997	1.136151
C	0.265581	1.840842	0.365339
C	-0.983179	2.396074	0.622526
C	-1.424741	3.553518	-0.097320
C	-0.553334	4.140709	-1.073670
C	0.715524	3.552512	-1.300632
C	1.110274	2.436072	-0.603490
C	-1.885954	1.771251	1.654194
C	-2.603328	0.603933	1.255501
C	-3.191220	-0.389224	0.867007
C	-3.889652	-1.548886	0.428801
C	-4.696456	-2.286681	1.317007
C	-5.377678	-3.420369	0.889782
C	-5.271723	-3.850439	-0.440241
C	-4.471350	-3.123131	-1.334167
C	-3.791348	-1.990561	-0.906317
S	-6.113698	-5.294356	-1.062824
S	8.685839	-2.466198	-0.580954
C	-2.004115	2.284828	2.894819
C	-2.702541	4.148645	0.105064
H	2.084407	1.993041	-0.783776
H	1.377175	3.998502	-2.039640
H	0.636637	0.800362	2.213231
H	-0.004495	-0.213327	0.949673
H	-1.453357	3.175271	3.182016
H	-2.651759	1.830037	3.638333
H	-4.783942	-1.961375	2.349027
H	-3.174841	-1.433334	-1.604693
H	-5.992894	-3.970353	1.596631
H	-4.380719	-3.444967	-2.367978
H	5.415253	0.214141	1.998565
H	3.892500	-1.971439	-1.374908
H	7.678017	-0.644117	1.543427

H	6.154211	-2.837934	-1.840332
H	9.356726	-1.886232	0.435117
H	-6.716544	-5.640951	0.092634
C	-3.089365	5.260889	-0.608176
H	-3.376884	3.712731	0.833935
H	-4.070753	5.695732	-0.438027
C	-2.221751	5.843599	-1.563165
C	-0.982430	5.291789	-1.788294
H	-2.539232	6.723016	-2.116916
H	-0.307840	5.727905	-2.521563

1B-ON@S---S(OFF)

B3LYP/6-31G(d): -1913.373058 a.u.

C	1.021705	5.882694	0.601959
C	0.698179	4.517377	0.580199
C	-0.423433	4.066909	-0.169011
C	-1.102853	5.006585	-0.962154
C	-0.750821	6.355991	-0.955577
C	0.298725	6.803205	-0.150059
C	1.541357	3.539248	1.241269
C	1.411773	2.222582	0.970914
C	0.346619	1.710993	0.120061
C	-0.794018	2.630097	-0.109086
C	0.448359	0.457718	-0.436628
C	1.588800	-0.356091	-0.291992
C	2.629890	-0.992243	-0.220573
C	3.900945	-1.623258	-0.147824
C	4.163669	-2.855044	-0.781170
C	5.432873	-3.423493	-0.744898
C	6.481488	-2.781066	-0.070911
C	6.228628	-1.563067	0.578704
C	4.962965	-0.995557	0.540193
S	8.146847	-3.424739	-0.005481
C	-2.107988	2.211575	-0.134525
C	-3.310184	3.149627	-0.144213
C	-2.532196	0.858681	-0.067775
C	-3.157893	-0.189825	-0.021256
C	-4.004221	-1.331300	0.029221
C	-5.402797	-1.144397	-0.017711
C	-6.275175	-2.222974	0.027091
C	-5.778781	-3.530637	0.124606
C	-4.390407	-3.731475	0.173691
C	-3.516896	-2.650338	0.125454
S	-6.848609	-4.959201	0.191252
H	2.123580	1.503472	1.363107
H	2.347606	3.897792	1.876665
H	-0.344317	0.095315	-1.084147
H	-3.069383	4.133169	0.263513

H	-4.110158	2.708998	0.458027
H	-5.797298	-0.135699	-0.090978
H	-2.445416	-2.820122	0.165823
H	-7.346195	-2.043725	-0.011819
H	-3.990411	-4.738851	0.250160
H	3.363544	-3.359155	-1.314429
H	4.782760	-0.047190	1.036635
H	5.605632	-4.369149	-1.251541
H	7.028123	-1.054449	1.110603
H	7.909603	-4.560889	-0.692519
H	-8.015181	-4.286810	0.118476
H	-1.895840	4.675760	-1.622483
H	-1.293482	7.054756	-1.586332
H	0.567360	7.855820	-0.130738
H	1.870458	6.210478	1.197806
H	-3.712664	3.288416	-1.156139

1B-ON

B3LYP/6-31G(d): -1913.377947 a.u.

C	-8.702240	-0.798748	-0.082253
C	-8.007625	-1.727960	0.707364
C	-6.626946	-1.653733	0.829362
C	-5.892494	-0.647345	0.166174
C	-6.602755	0.280261	-0.623698
C	-7.984714	0.206156	-0.746372
C	-4.481135	-0.572605	0.291070
C	-3.266110	-0.508432	0.397596
C	-1.868997	-0.476840	0.551185
C	-1.031648	0.477272	0.020647
C	-1.569998	1.618369	-0.700112
C	-0.835442	2.735368	-0.896630
C	0.482542	2.877922	-0.306735
C	1.100038	1.750873	0.302817
C	0.440083	0.428165	0.170830
C	1.152063	-0.748904	0.029818
C	2.568750	-0.796095	0.036497
C	3.774759	-0.973702	-0.023293
C	5.189914	-1.080095	-0.073506
C	5.829287	-2.336119	-0.123167
C	7.213680	-2.430290	-0.170486
C	8.004485	-1.271155	-0.172228
C	7.380613	-0.016155	-0.125592
C	5.995270	0.077631	-0.077111
S	9.775740	-1.471777	-0.236545
S	-10.475413	-0.958352	-0.190229
C	0.536406	-2.108855	-0.261753
H	-1.259433	3.590098	-1.418362
H	-2.603249	1.563845	-1.029097

C	2.297674	1.953426	1.007350
H	-1.443690	-1.254789	1.178666
H	0.381943	-2.689817	0.656897
H	-0.429748	-2.021753	-0.765189
H	1.216903	-2.687020	-0.893652
H	5.225802	-3.238520	-0.122741
H	5.517957	1.052336	-0.046868
H	7.684290	-3.408934	-0.207579
H	7.976551	0.892507	-0.129131
H	-6.098730	-2.377136	1.442539
H	-6.056910	1.062451	-1.142157
H	-8.550822	-2.512149	1.227634
H	-8.504560	0.935095	-1.362098
H	10.086926	-0.159649	-0.226632
H	-10.682409	0.088658	-1.014583
C	2.904390	3.207542	1.057449
H	2.747267	1.127397	1.543467
H	3.822318	3.335725	1.625146
C	2.329635	4.296196	0.395876
C	1.122600	4.127494	-0.272931
H	2.807338	5.271766	0.423532
H	0.644522	4.974090	-0.760420

1-TS@S---S(OFF)

B3LYP/6-31G(d): -1759.692855 a.u.

C	-0.042452	-0.844685	2.261193
C	-0.008801	0.332884	1.483438
C	1.249890	0.889740	1.175040
C	2.422921	0.302426	1.631873
C	2.375105	-0.865047	2.407102
C	1.129356	-1.434835	2.712883
C	-1.207000	0.947589	1.040477
C	-2.242865	1.489118	0.684371
C	-3.426763	2.133663	0.278013
C	-3.373784	3.474898	-0.204270
S	3.834235	-1.671094	3.038216
C	-4.704317	1.555429	0.628464
C	-5.799087	2.419713	0.980845
C	-6.884298	1.855047	1.691240
C	-6.974087	0.495948	1.924620
C	-5.937988	-0.361253	1.504834
C	-4.820493	0.165464	0.894303
C	-5.773418	3.867412	0.718072
C	-6.393201	4.747526	1.641287
C	-6.843472	5.525269	2.467633
C	-7.351379	6.414154	3.450651
C	-7.775083	7.715747	3.112928
C	-8.255183	8.586606	4.083875

C	-8.329048	8.182627	5.424209
C	-7.915558	6.887957	5.772910
C	-7.434598	6.019319	4.803260
S	-8.924920	9.243122	6.728870
H	-6.011763	-1.431650	1.676983
H	-3.995012	-0.480169	0.610138
H	-7.687498	2.515531	2.003686
H	-7.853058	0.088375	2.416829
H	-5.901631	4.163694	-0.325421
H	-4.326368	4.027812	0.546534
H	-2.401208	3.965617	-0.165703
H	1.296426	1.793806	0.575893
H	-1.002120	-1.286571	2.510343
H	3.378244	0.756535	1.383295
H	1.078536	-2.339783	3.312154
H	-7.720483	8.038993	2.077949
H	-7.112130	5.021176	5.082733
H	-8.571751	9.584930	3.794116
H	-7.967693	6.561132	6.807933
H	-9.194628	10.315722	5.957138
H	4.733671	-0.811508	2.517650
H	-3.912435	3.696127	-1.128499

1-TS@S---S(ON)

B3LYP/6-31G(d): -1759.685916 a.u.

C	0.603602	3.392295	0.660666
H	1.122472	4.295459	0.970994
C	1.320125	2.240656	0.405252
H	2.401070	2.234772	0.505685
C	-0.796440	3.405219	0.490539
H	-1.359299	4.316524	0.673826
C	-1.450685	2.255313	0.111214
H	-2.532185	2.246158	0.021763
C	0.692332	1.063991	-0.067702
C	1.492524	-0.115367	-0.418225
H	1.382240	-0.422064	-1.462721
C	-0.747654	1.045557	-0.147882
C	-1.468291	-0.203805	-0.245006
C	-0.776537	-1.411238	-0.569090
H	-0.328519	-1.490630	-1.560241
H	0.523494	-1.118920	-0.075067
H	-1.277794	-2.336224	-0.280906
C	2.878284	-0.202799	-0.042156
C	4.084084	-0.297247	0.144226
C	-2.847360	-0.265141	0.106512
C	-4.062011	-0.308302	0.263961
C	-5.487367	-0.338389	0.383961
C	-6.233044	-1.493876	0.056729

C	-6.216689	0.798508	0.797254
C	-7.623574	-1.508271	0.130052
H	-5.707204	-2.388697	-0.261895
C	-7.608678	0.788395	0.860655
H	-5.679807	1.704219	1.063002
C	-8.337922	-0.364158	0.525267
H	-8.157263	-2.419004	-0.128056
H	-8.126182	1.691792	1.172369
C	5.509302	-0.362721	0.284242
C	6.298313	-1.057488	-0.660513
C	6.193688	0.287984	1.333051
C	7.687408	-1.089916	-0.568875
H	5.807219	-1.574176	-1.479493
C	7.585350	0.261008	1.422667
H	5.623798	0.830025	2.081801
C	8.357298	-0.424463	0.470969
H	8.254215	-1.637502	-1.317149
H	8.068081	0.786947	2.242175
S	-10.140447	-0.438801	0.556271
H	-10.333061	0.776817	1.107542
S	10.162662	-0.472723	0.503366
H	10.309671	0.131979	1.699884

2-ON

B3LYP/6-31G(d): -1831.59855322 a.u.

O	-1.23248200	-1.32372300	-0.00023700
C	-0.74141100	-0.08218500	-0.00022700
C	0.65554700	0.18261000	-0.00028400
C	-1.66420500	1.00054300	-0.00015200
C	-1.16464300	2.31035300	-0.00016800
H	-1.87658300	3.13016700	-0.00012700
C	1.59657100	-0.94781900	-0.00032900
C	1.10653900	1.51735400	-0.00029000
H	2.17601000	1.70260900	-0.00032300
C	0.20895600	2.57297600	-0.00024100
H	0.56560400	3.59809500	-0.00023900
C	3.01173800	-0.67475000	-0.00023200
C	4.21870800	-0.51698700	-0.00013900
C	-3.06116400	0.74340900	-0.00008300
C	-4.25902600	0.53308400	-0.00001900
C	-5.65413600	0.25714300	0.00005600
C	-6.60479100	1.29753100	0.00008400
C	-6.12121900	-1.07210900	0.00010400
C	-7.96577200	1.02015000	0.00015400
H	-6.26351300	2.32812100	0.00005400
C	-7.48299200	-1.35044700	0.00016700

H	-5.40165300	-1.88479900	0.00008900
C	-8.41921300	-0.30716900	0.00019200
H	-8.68042100	1.83866600	0.00018700
H	-7.81494200	-2.38514700	0.00019900
C	5.63058500	-0.35918200	-0.00002700
C	6.22004400	0.92125200	0.00007500
C	6.47307800	-1.48872400	-0.00000800
C	7.59990800	1.06631500	0.00020000
H	5.58360800	1.80056100	0.00006400
C	7.85417700	-1.34407700	0.00010900
H	6.03127400	-2.48007100	-0.00008600
C	8.43158700	-0.06522200	0.00021800
H	8.03610400	2.06114300	0.00029800
H	8.48302000	-2.22977500	0.00011000
S	-10.18229900	-0.58500500	0.00025200
H	-10.13388500	-1.93271300	0.00033200
S	10.19100200	0.20195500	0.00035300
H	10.55243900	-1.09723700	0.00049600
O	1.21238200	-2.13453200	-0.00043300
H	-0.44872200	-1.93906900	-0.00032100

2-OFF

B3LYP/6-31G(d): -1831.59848405 a.u.

C	-1.10798500	1.51270200	0.00010700
C	-0.65612300	0.17827900	0.00024000
C	0.74101000	-0.08555000	0.00018800
C	1.66306300	0.99785500	-0.00004000
C	1.16262200	2.30731500	-0.00015000
C	-0.21115800	2.56897100	-0.00008100
H	-2.17759900	1.69711700	0.00012100
H	1.87401200	3.12760600	-0.00032000
H	-0.56849100	3.59386600	-0.00017800
O	1.23297800	-1.32668500	0.00032800
C	-1.59644900	-0.95287100	0.00037300
C	-3.01174000	-0.68045900	0.00025300
C	-4.21865700	-0.52227900	0.00024000
C	3.06020400	0.74180400	-0.00017400
C	4.25829000	0.53274100	-0.00036100
O	-1.21132100	-2.13918900	0.00050600
C	-5.63027400	-0.36208700	0.00015900
C	-6.21569800	0.91903900	0.00048500
C	-6.47656400	-1.49012600	-0.00027300

C	-7.59632700	1.06946200	0.00037500
H	-5.57705000	1.79684300	0.00088100
C	-7.85581000	-1.34042300	-0.00041800
H	-6.03724500	-2.48248400	-0.00051300
C	-8.43028200	-0.05883700	-0.00011000
H	-8.02432500	2.06783500	0.00066400
H	-8.49195100	-2.22099200	-0.00068700
C	5.65366500	0.25815700	-0.00029800
C	6.60330900	1.29945500	-0.00002200
C	6.12202900	-1.07065400	-0.00041800
C	7.96455600	1.02339000	0.00002400
H	6.26106000	2.32972400	0.00009500
C	7.48406600	-1.34766900	-0.00030300
H	5.40324900	-1.88403500	-0.00057700
C	8.41928900	-0.30347900	-0.00011900
H	8.67839100	1.84262200	0.00014900
H	7.81700800	-2.38204900	-0.00032300
S	10.18260900	-0.57957500	0.00018600
H	10.13548400	-1.92732000	-0.00101100
S	-10.20636800	0.05114700	-0.00036400
H	-10.28560400	1.39738900	-0.00058400
H	0.44973800	-1.94269900	0.00041000

3-ON

B3LYP/6-31G(d): -1682.28954222 a.u.

C	-4.90463500	-1.12620700	0.66846400
C	-4.28787600	0.20831000	1.12167200
C	-2.79657000	0.19196600	0.68548700
C	-2.79657000	0.19196600	-0.68548700
C	-4.90463500	-1.12620700	-0.66846400
C	-4.28787600	0.20831000	-1.12167200
C	-4.84619200	1.13042900	0.00000000
H	-5.20201600	-1.92453000	1.33904000
H	-4.45395400	0.49661000	2.16026700
H	-5.20201600	-1.92453000	-1.33904000
H	-4.45395400	0.49661000	-2.16026700
H	-4.40527700	2.13269300	0.00000000
H	-5.93908800	1.19246500	0.00000000
C	-1.71894000	0.14096400	1.57439700
C	-0.81169300	0.10497400	2.39075800
C	-1.71894000	0.14096400	-1.57439700
C	-0.81169300	0.10497400	-2.39075800

C	0.25690800	0.06072700	3.32302500
C	0.00857400	0.05019500	4.71106500
C	1.59912700	0.02620500	2.88864400
C	1.05407100	0.00690000	5.62526400
H	-1.01721800	0.07634800	5.06557000
C	2.64408100	-0.01678400	3.80141000
H	1.80951900	0.03367300	1.82379400
C	2.38305700	-0.02706700	5.18021400
H	0.83187000	-0.00033400	6.68891600
H	3.66947900	-0.04272600	3.44266400
C	0.25690800	0.06072700	-3.32302500
C	0.00857400	0.05019500	-4.71106500
C	1.59912700	0.02620500	-2.88864400
C	1.05407100	0.00690000	-5.62526400
H	-1.01721800	0.07634800	-5.06557000
C	2.64408100	-0.01678400	-3.80141000
H	1.80951900	0.03367300	-1.82379400
C	2.38305700	-0.02706700	-5.18021400
H	0.83187000	-0.00033400	-6.68891600
H	3.66947900	-0.04272600	-3.44266400
S	3.77782900	-0.08349400	-6.29100000
H	3.07118800	-0.07809500	-7.43970800
S	3.77782900	-0.08349400	6.29100000
H	3.07118800	-0.07809500	7.43970800

3-OFF

B3LYP/6-31G(d): -1682.24291315 a.u.

C	-4.27484700	1.06854900	0.77012800
C	-4.49045300	-0.37486000	1.15245100
C	-3.08088500	0.10133700	0.78614200
C	-3.08088500	0.10133700	-0.78614200
C	-4.27484700	1.06854900	-0.77012800
C	-4.49045300	-0.37486000	-1.15245100
C	-5.10175800	-1.15048200	0.00000000
C	-1.94649000	0.06660600	-1.63626500
C	-1.94649000	0.06660600	1.63626500
C	-0.96928600	0.04394200	-2.35958500
C	0.17366900	0.01665100	-3.20940300
C	0.17366900	0.01665100	3.20940300
C	-0.96928600	0.04394200	2.35958500
C	0.04253400	-0.19668900	4.59511400
C	1.15801100	-0.22100100	5.42524900

C	2.44106700	-0.03739400	4.89333500
C	2.58480300	0.17377400	3.51445500
C	1.46918600	0.20251200	2.68713100
C	1.46918600	0.20251200	-2.68713100
C	2.58480300	0.17377400	-3.51445500
C	2.44106700	-0.03739400	-4.89333500
C	1.15801100	-0.22100100	-5.42524900
C	0.04253400	-0.19668900	-4.59511400
H	-4.43777500	1.91968500	1.41989300
H	-4.68138700	-0.63183900	2.18937100
H	-4.43777500	1.91968500	-1.41989300
H	-4.68138700	-0.63183900	-2.18937100
H	-4.80285700	-2.20516100	0.00000000
H	-6.19786100	-1.09415700	0.00000000
H	-0.94650100	-0.34356700	5.01822700
H	1.02446200	-0.38574700	6.49106900
H	3.57334900	0.31733400	3.08663800
H	1.59058000	0.36868300	1.62122600
H	1.59058000	0.36868300	-1.62122600
H	3.57334900	0.31733400	-3.08663800
H	1.02446200	-0.38574700	-6.49106900
H	-0.94650100	-0.34356700	-5.01822700
S	3.92026500	-0.05602000	-5.89393000
H	3.31481500	-0.30768400	-7.07241800
S	3.92026500	-0.05602000	5.89393000
H	3.31481500	-0.30768400	7.07241800

4-ON

B3LYP/6-31G(d): -1720.38265605 a.u.

C	-0.67499100	4.88448300	-0.53639200
C	-1.58624500	3.74211400	-0.52674800
C	1.58217900	2.67325800	0.31015800
C	-1.58210600	2.67317700	0.31016000
C	0.66800000	2.51114500	1.47421600
C	-0.66792000	2.51110100	1.47419900
H	-2.39978200	3.79557500	-1.25024500
H	-1.16290600	5.84992000	-0.67944000
H	1.17701800	2.31887200	2.41860700
H	-1.17693800	2.31879000	2.41858600
C	0.67496500	4.88452600	-0.53637600
H	1.16283300	5.84998900	-0.67938300
C	1.58626700	3.74218100	-0.52675800

H	2.39979000	3.79567900	-1.25026900
C	-2.58468500	1.66839700	0.18978700
C	-3.42347400	0.78677000	0.13363100
C	2.58473500	1.66845300	0.18975400
C	3.42352300	0.78682500	0.13358600
C	-4.41362400	-0.22936700	0.04009900
C	-4.46052800	-1.28620900	0.97218100
C	-5.37640000	-0.20722800	-0.98859000
C	-5.42876700	-2.27726700	0.87907700
H	-3.72603000	-1.32106100	1.77070200
C	-6.34585400	-1.19860800	-1.08266800
H	-5.35606200	0.59819900	-1.71616600
C	-6.38219300	-2.24411300	-0.14959600
H	-5.44411300	-3.08252400	1.60843500
H	-7.07568900	-1.15543800	-1.88654000
C	4.41365000	-0.22933500	0.04005000
C	4.46055800	-1.28612700	0.97219800
C	5.37639300	-0.20727800	-0.98866400
C	5.42875600	-2.27722300	0.87911500
H	3.72606600	-1.32091800	1.77072600
C	6.34581700	-1.19869200	-1.08271300
H	5.35606600	0.59811100	-1.71628200
C	6.38215100	-2.24415100	-0.14959200
H	5.44409500	-3.08244600	1.60851100
H	7.07562600	-1.15559500	-1.88661400
S	-7.59577800	-3.55085700	-0.20280100
H	-8.23846000	-3.12973400	-1.31106100
S	7.59571500	-3.55092000	-0.20276600
H	8.23824600	-3.12995600	-1.31117400

4-OFF

B3LYP/6-31G(d): -1720.34893595 a.u.

C	5.31859500	0.29652400	-1.36006500
C	5.19413200	-1.15547300	-1.34213700
C	4.27488600	-1.79204800	-0.59759900
C	3.34011500	-1.07386700	0.34980100
C	3.48271000	0.57095700	0.33114400
C	4.52360700	1.09746800	-0.63142000
C	4.02825000	0.38121300	1.75001700
C	3.91277300	-0.94911200	1.76456400
C	1.98485900	-1.60067500	0.26428900
C	2.23350600	1.31356900	0.22941100
C	1.19912700	1.94306700	0.14546100

C	0.86418400	-2.06192600	0.19359100
C	-0.03715900	2.64919000	0.05156000
C	-0.46066300	-2.58620400	0.11691700
C	-1.38653100	-2.36470200	1.15581000
C	-2.67836300	-2.87164800	1.08127900
C	-3.08372100	-3.61862200	-0.03435800
C	-2.17122000	-3.84635300	-1.07330800
C	-0.87968400	-3.33623800	-0.99803100
C	-1.25924200	1.95042600	-0.00420300
C	-2.46627300	2.63285500	-0.09231900
C	-2.48844300	4.03471600	-0.12757500
C	-1.27888800	4.73961400	-0.07388400
C	-0.07114200	4.05521000	0.01403800
H	6.06450800	0.73710900	-2.01734400
H	5.85488900	-1.73250500	-1.98480100
H	4.17066500	-2.87349400	-0.64298000
H	4.60228700	2.17954100	-0.70512100
H	4.40656900	1.11861900	2.45181900
H	4.15854800	-1.72569200	2.48290700
H	-1.07989600	-1.79051600	2.02465800
H	-3.37492400	-2.68726300	1.89465700
H	-2.46644300	-4.42229600	-1.94616400
H	-0.18076100	-3.51562800	-1.80914000
H	-1.25105300	0.86518800	0.02185500
H	-3.39650100	2.07282400	-0.13472400
H	-1.27511300	5.82596200	-0.10053400
H	0.86087700	4.61064800	0.05521800
S	-4.75719700	-4.23937100	-0.05771500
H	-4.68926100	-4.84388000	-1.26130300
S	-4.07785000	4.84097300	-0.24001200
H	-3.61613200	6.10810800	-0.24327200

***cis*-5-OFF@S---S(ON)**

B3LYP/6-31G(d): -1833.749673 a.u.

C	15.067750	4.612129	1.332695
C	14.151389	4.940621	2.357557
C	14.725707	5.440228	3.550538
C	16.108825	5.590838	3.710555
C	17.011718	5.249457	2.686576
C	16.452431	4.760199	1.491440
C	12.715483	4.736158	2.223336
C	11.507531	4.548966	2.143456
C	10.106551	4.072367	2.279523
C	9.760834	2.728614	1.649246
C	8.374045	2.594916	1.456751
C	7.848613	1.441607	0.883816
C	8.720197	0.414833	0.508743
C	10.098465	0.547706	0.700065

C	10.627926	1.709551	1.269619
C	7.625507	3.833191	1.935121
C	6.249743	4.042099	1.413606
C	5.052221	3.997537	1.159604
C	3.621506	3.925665	0.895930
C	2.663465	4.277671	1.876191
C	1.285727	4.162156	1.653035
C	0.773282	3.684242	0.432671
C	1.715770	3.339652	-0.553992
C	3.094166	3.457929	-0.329259
S	-1.049300	3.531298	0.205007
S	18.823207	5.446866	2.963331
H	9.941887	3.981009	3.369894
H	8.321932	-0.490785	0.059302
H	6.777759	1.352610	0.725146
H	10.765688	-0.255191	0.398528
H	11.698815	1.827039	1.408242
H	7.503860	3.746004	3.031464
H	14.074584	5.714340	4.375420
H	14.691686	4.226399	0.389518
H	16.480821	5.979421	4.654890
H	17.096299	4.482078	0.661007
H	3.004425	4.647513	2.838737
H	3.776164	3.174096	-1.125574
H	0.606724	4.449500	2.451494
H	1.383916	2.967395	-1.519827
H	19.191521	5.058048	1.725447
H	-0.990135	3.112415	-1.075705
C	8.813212	4.898737	1.830995
O	8.746733	6.048764	1.511521

cis-5-OFF

B3LYP/6-31G(d): -1833.772156 a.u.

C	1.397787	3.582184	1.778381
C	1.604212	4.015144	0.460394
C	2.888170	4.071772	-0.067168
C	4.004435	3.699370	0.706266
C	3.786019	3.268214	2.027823
C	2.501481	3.209108	2.557157
C	5.323387	3.757695	0.164344
C	6.445121	3.809175	-0.293139
C	7.793552	3.860339	-0.840777
C	8.729600	2.732235	-0.436671
C	8.437479	1.373198	-0.347229
C	9.445946	0.488940	0.041750
C	10.726615	0.962941	0.346859
C	11.014459	2.327132	0.267074
C	10.010212	3.206554	-0.130747

C	10.102450	4.715438	-0.289386
C	10.819752	5.435405	0.754125
C	11.418199	6.034243	1.621948
C	12.110348	6.756112	2.640483
C	11.882629	8.133484	2.825481
C	12.556209	8.839985	3.814067
C	13.478621	8.190360	4.647282
C	13.711882	6.819885	4.472337
C	13.036204	6.113879	3.482687
S	14.305712	9.165292	5.892991
S	-0.279787	3.532218	2.385411
C	8.605069	5.133922	-0.438494
H	9.231642	-0.573773	0.115402
H	7.435125	1.013723	-0.563181
H	11.500986	0.266040	0.655778
H	12.000918	2.703254	0.524169
H	11.168951	8.642921	2.185711
H	13.222960	5.051892	3.355987
H	12.364000	9.902019	3.939424
H	14.421738	6.298464	5.108688
H	3.038690	4.409912	-1.087639
H	4.635513	2.979850	2.639169
H	0.757901	4.310194	-0.153904
H	2.362085	2.872150	3.580703
H	15.050834	8.167863	6.411257
H	0.011565	3.105011	3.630958
O	8.161406	6.238567	-0.288601
H	10.558935	4.956108	-1.267157
H	7.725741	3.907429	-1.942674

trans-5-OFF@S---S(ON)

C	-6.05779	0.28085	-0.86821
C	-5.31595	-0.52908	0.02359
C	-6.09366	-1.34940	0.87651
C	-7.49605	-1.35466	0.84548
C	-8.22270	-0.53636	-0.04048
C	-7.46067	0.27937	-0.89883
C	-3.85623	-0.49161	0.09162
C	-2.63288	-0.45098	0.17077
C	-1.19736	-0.20424	0.51327
C	-0.66276	1.19438	0.23019
C	0.66275	1.19439	-0.23021
C	1.33085	2.39742	-0.44946
C	0.66350	3.60235	-0.22020
C	-0.66349	3.60234	0.22043
C	-1.33084	2.39740	0.44957
C	1.19732	-0.20428	-0.51327
C	2.63288	-0.45095	-0.17092

C	3.85624	-0.49139	-0.09165
C	5.31596	-0.52890	-0.02362
C	6.09365	-1.34778	-0.87796
C	7.49603	-1.35312	-0.84695
C	8.22271	-0.53637	0.04042
C	7.46070	0.27789	0.90018
C	6.05781	0.27947	0.86957
S	10.07710	-0.56726	0.02527
S	-10.07710	-0.56714	-0.02537
H	-1.14049	-0.36816	1.60503
H	1.17799	4.54431	-0.38980
H	2.36094	2.39037	-0.79511
H	-1.17795	4.54430	0.39014
H	-2.36093	2.39031	0.79524
H	1.14027	-0.36832	-1.60500
H	-5.59045	-2.00040	1.58550
H	-5.52765	0.93517	-1.55440
H	-8.02248	-2.01272	1.53182
H	-7.95564	0.93527	-1.61053
H	5.59041	-1.99752	-1.58808
H	5.52770	0.93262	1.55688
H	8.02245	-2.00997	-1.53446
H	7.95570	0.93253	1.61303
H	-10.22892	0.29423	-1.05221
H	10.22900	0.29364	1.05249
C	-0.00001	-1.12494	0.00010
O	0.00000	-2.32451	0.00018

***trans*-5-OFF**

B3LYP/6-31G(d): -1833.772228 a.u.

C	1.083764	3.419943	-0.078347
C	1.334056	3.980613	1.182775
C	2.611649	3.943656	1.727178
C	3.677930	3.346173	1.027534
C	3.415954	2.787537	-0.237266
C	2.137549	2.822997	-0.783348
C	4.990172	3.308391	1.587045
C	6.103563	3.272877	2.067833
C	7.455341	3.248786	2.625454
C	8.453651	2.462817	1.791499
C	8.515028	1.081716	1.614876
C	9.531034	0.544626	0.821851
C	10.474930	1.381625	0.216213
C	10.411932	2.765216	0.392933
C	9.392235	3.299634	1.177506
C	9.128825	4.766528	1.483334
C	10.295113	5.576820	1.805699
C	11.274130	6.241660	2.070156

C	12.425451	7.023978	2.385085
C	12.548169	8.348603	1.923281
C	13.669040	9.109860	2.230278
C	14.702927	8.568213	3.007977
C	14.591593	7.250839	3.472602
C	13.468064	6.491106	3.165579
S	16.112416	9.605500	3.358199
S	-0.582798	3.503999	-0.711138
C	8.069031	4.686456	2.625805
H	9.591541	-0.530758	0.678409
H	7.782848	0.432856	2.088397
H	11.264881	0.951914	-0.393781
H	11.150061	3.418410	-0.064301
H	11.752002	8.776842	1.322402
H	13.389352	5.472137	3.531797
H	13.740712	10.130794	1.865370
H	15.381583	6.813588	4.077083
H	2.796783	4.380941	2.703288
H	4.226135	2.322802	-0.790757
H	0.526849	4.448079	1.739970
H	1.963642	2.383602	-1.761805
H	16.784827	8.714606	4.115062
H	-0.342369	2.880517	-1.882483
O	7.776606	5.567316	3.387256
H	8.597245	5.229253	0.633066
H	7.418980	2.903689	3.668864

5-ON@S---S(*cis*-OFF)

C	5.37709	-0.97514	1.45207
C	4.84572	-0.08294	0.49434
C	5.29811	-0.19299	-0.83871
C	6.22617	-1.15974	-1.20107
C	6.74006	-2.04470	-0.24168
C	6.30757	-1.93960	1.08932
C	3.82146	0.82870	0.84147
C	2.83129	1.50209	1.09400
C	1.55236	2.01102	1.33374
C	0.80321	2.72990	0.41374
C	-0.67558	2.69624	0.39697
C	-1.35448	3.50629	-0.59211
C	-0.66965	4.21842	-1.52696
C	0.76832	4.18049	-1.56316
C	1.46339	3.45648	-0.64559
C	-1.37991	1.79677	1.17598
C	-2.69432	1.35395	0.96801
C	-3.72356	0.72353	0.78504
C	-4.81816	-0.11914	0.45914
C	-5.11423	-0.39571	-0.89177

C	-6.10889	-1.29944	-1.23517
C	-6.84669	-1.95078	-0.23675
C	-6.57722	-1.67094	1.11201
C	-5.57740	-0.77245	1.45415
S	-8.12535	-3.12792	-0.61420
S	7.91197	-3.32720	-0.63879
H	-1.20394	4.82181	-2.25505
H	-2.43912	3.52459	-0.56501
H	1.29754	4.75493	-2.31887
H	2.54865	3.45347	-0.65015
H	5.03795	-0.91044	2.48143
H	4.89021	0.47530	-1.59080
H	6.69588	-2.62009	1.84196
H	6.53843	-1.23453	-2.23925
H	-5.36414	-0.57298	2.50035
H	-4.53275	0.08979	-1.67041
H	-7.14487	-2.16913	1.89326
H	-6.30484	-1.50819	-2.28369
H	8.12133	-2.96025	-1.91903
H	-7.92654	-3.15904	-1.94592
H	1.07906	1.65761	2.24774
H	-0.84670	1.23722	1.93934

5-ON@S---S(*trans*-5-OFF)

C	6.10365	0.29128	-0.60012
C	5.25695	-0.18621	0.42167
C	5.63934	-1.35740	1.11293
C	6.79307	-2.04352	0.76731
C	7.60595	-1.57994	-0.27858
C	7.26019	-0.39601	-0.94557
C	4.01038	0.42254	0.69990
C	2.86873	0.82492	0.87823
C	1.50798	1.09455	1.03616
C	0.77904	2.07900	0.39032
C	-0.69329	2.03259	0.34584
C	-1.39391	3.22359	-0.07639
C	-0.72081	4.28995	-0.58571
C	0.71457	4.26302	-0.70359
C	1.42922	3.19738	-0.25019
C	-1.36163	0.84299	0.56951
C	-2.73508	0.60234	0.49502
C	-3.89734	0.23586	0.39100
C	-5.18244	-0.33084	0.21971
C	-6.30905	0.43740	-0.13657
C	-7.54061	-0.16687	-0.35920
C	-7.68225	-1.55570	-0.22826
C	-6.57290	-2.32901	0.14686
C	-5.34479	-1.72714	0.36652

S	-9.20985	-2.41595	-0.53168
S	9.02372	-2.56333	-0.71422
H	1.22624	5.11751	-1.13807
H	2.51435	3.19345	-0.29412
H	-1.26406	5.16645	-0.92834
H	-2.47878	3.21804	-0.02638
H	-4.48668	-2.33057	0.64491
H	-6.20586	1.51215	-0.24969
H	-6.67285	-3.40529	0.25777
H	-8.39167	0.44586	-0.64362
H	5.00373	-1.73157	1.90925
H	5.83008	1.19397	-1.13749
H	7.05906	-2.95223	1.30037
H	7.88502	-0.01794	-1.75009
H	-9.95622	-1.33138	-0.82484
H	9.49640	-1.75250	-1.68281
H	-0.76635	-0.04913	0.75030
H	0.97607	0.40301	1.68641

5-ON

B3LYP/6-31G(d): -1720.419794 a.u.

C	0.725342	3.450997	0.356226
C	1.419135	4.652232	0.571176
C	2.800681	4.652666	0.698975
C	3.538573	3.451106	0.616547
C	2.828549	2.250811	0.400342
C	1.445553	2.250558	0.272282
C	4.948797	3.454319	0.746893
C	6.166956	3.462114	0.860922
C	7.556801	3.526831	0.999891
C	8.428841	2.455303	0.900933
C	7.929292	1.148611	0.529666
C	8.763259	0.108052	0.270739
C	10.189708	0.273802	0.372541
C	10.718105	1.461097	0.768059
C	9.884130	2.592618	1.113020
C	10.453292	3.729385	1.662785
C	11.822000	3.948064	1.847057
C	13.008937	4.183557	2.027888
C	14.381448	4.461753	2.238994
C	14.789915	5.661722	2.862083
C	16.133851	5.936397	3.070421
C	17.117892	5.021658	2.663696
C	16.726333	3.826177	2.043768
C	15.381025	3.551128	1.835021
S	18.823207	5.446866	2.963331
S	-1.049300	3.531297	0.205007
H	9.804559	4.532038	2.005530

H	8.358967	-0.854992	-0.028948
H	6.854638	1.036597	0.426823
H	10.841158	-0.565009	0.142908
H	11.791476	1.582467	0.873650
H	7.959191	4.520046	1.184748
H	14.036293	6.374936	3.180869
H	15.088982	2.623022	1.353498
H	16.422899	6.866177	3.552688
H	17.473321	3.106027	1.721196
H	3.328343	5.586759	0.864167
H	3.376160	1.315758	0.334516
H	0.873942	5.589775	0.637513
H	0.926302	1.310480	0.107076
H	19.363696	4.321149	2.454007
H	-1.254816	2.214735	-0.002861