

Supporting Information (data in Å)**COT (1)**

C	-1.703000	-0.013416	-0.384977
C	-0.011314	1.706322	0.379599
C	1.705964	0.013077	-0.386335
C	0.015117	-1.699831	0.393800
C	-1.184119	1.226150	-0.384248
C	1.228748	1.188352	0.374796
C	1.187322	-1.226555	-0.374369
C	-1.225442	-1.182810	0.384476
H	-2.602235	-0.177437	-0.956564
H	-0.171237	2.608497	0.948879
H	2.606721	0.172800	-0.958366
H	0.180409	-2.597568	0.969746
H	-1.695906	1.982899	-0.957771
H	1.988768	1.702957	0.941513
H	1.703280	-1.988744	-0.936922
H	-1.985295	-1.694540	0.954686

SBV (2)

C	-1.567448	.020800	-.674303
C	.005765	.841698	.885405
C	1.569011	-.003889	-.671119
C	-.006813	-.737168	.980589
C	-1.196668	1.127665	-.006989
C	1.214200	1.108786	-.004779
C	.789732	-1.178759	-.197555
C	-.807764	-1.166242	-.199205
H	-2.285634	-.015548	-1.472820
H	.008926	1.361213	1.835838
H	2.287990	-.051546	-1.468331
H	-.011839	-1.242003	1.930688
H	-1.538627	2.125212	-.217189
H	1.571991	2.100858	-.214571
H	1.230424	-2.160130	-.226627
H	-1.263702	-2.140587	-.229338

C	.234205	1.859205	.096147
C	.045328	.028435	-1.741928
C	.204306	-1.819218	.082059
C	.351809	1.314549	1.388921
C	.107205	1.326486	-1.200673
C	.085604	-1.274550	-1.210618
C	.331122	-1.286488	1.378900
H	.492767	.006644	2.992146
H	.243519	2.935799	.100219
H	-.056669	.033383	-2.813716
H	.196119	-2.895821	.077884
H	.429272	2.072328	2.149791
H	.042121	2.091240	-1.955700
H	.007240	-2.032320	-1.971406
H	.397110	-2.051245	2.133849

DIR' (7)

C	1.637111	-.078244	-.250020
C	.002975	-1.632102	.921643
C	-1.636860	-.084069	-.249766
C	-.003256	1.831505	.020785
C	.799153	-1.282548	-.263609
C	-.794625	-1.285383	-.263485
C	-1.280980	1.231884	-.054228
C	1.276581	1.236434	-.054427
H	2.694155	-.272042	-.330639
H	.002008	-1.048970	1.826063
H	-2.693220	-.281626	-.330221
H	-.005150	2.901138	.136983
H	1.177178	-2.105101	-.847839
H	-1.169811	-2.109276	-.847657
H	-2.105350	1.922814	.007052
H	2.098497	1.930293	.006726

CI_b

C	-1.569016	.001955	-.648954
C	.007163	1.457934	.652634
C	1.575058	-.011012	-.642106
C	-.009217	-1.426898	.691812

C	0.469330	1.067395	1.316729
H	0.362084	2.854451	0.224150
H	1.705529	-0.562929	-1.478096
H	-1.836610	-2.195900	-0.397547
H	0.557770	-0.570471	2.642483
H	0.295808	1.967650	-2.006590
H	-1.042585	-1.106689	-2.385046
H	-0.967722	-2.018355	1.738121
H	0.639192	1.672774	2.192501

TS_{st}

C	0.307122	1.803206	0.170670
C	0.722230	-0.140851	-1.399048
C	-1.091796	-1.475548	-0.231258
C	0.417684	-0.369325	1.475339
C	0.552727	1.243481	-1.077906
C	-0.414600	-1.008970	-1.351697
C	-0.668581	-1.206059	1.065261
C	0.287644	1.049136	1.337980
H	0.198322	2.870215	0.244769
H	1.344578	-0.301023	-2.267026
H	-1.933979	-2.128621	-0.373068
H	0.846005	-0.667081	2.420951
H	0.730995	1.942672	-1.882328
H	-0.721025	-1.432273	-2.297494
H	-1.153447	-1.772032	1.847745
H	0.277398	1.610584	2.261191

DIR

C	-1.716570	.011077	-.597811
C	.005408	.803900	.847398
C	1.717701	-.015738	-.594321
C	-.007149	-.800199	.852044
C	-1.139662	1.154824	-.058576
C	1.157961	1.136862	-.055848
C	1.139657	-1.156370	-.049663
C	-1.157841	-1.138406	-.051612
H	-2.484297	.014873	-1.349811
H	.007892	1.268438	1.826203
H	2.486919	-.023892	-1.344760

H	-2.092870	1.931507	-.034089
H	2.075197	1.898403	.061274

DIR''

C	1.642757	.022457	-.108774
C	.002934	-1.608983	1.020791
C	-1.642841	.016609	-.108518
C	-.003467	1.938177	-.248187
C	.776109	-1.187722	-.161758
C	-.771902	-1.190480	-.161651
C	-1.292586	1.335319	-.164795
C	1.287804	1.339912	-.165005
H	2.692645	-.193724	-.000863
H	.004580	-2.509309	1.602541
H	-2.691934	-.203306	-.000430
H	-.005384	3.011951	-.313133
H	1.198955	-1.985260	-.755498
H	-1.191993	-1.989510	-.755339
H	-2.110738	2.035538	-.125835
H	2.103464	2.043038	-.126187

TS'

C	1.643989	-.011430	-.163875
C	.002928	-1.595333	.930460
C	-1.643971	-.017273	-.163618
C	-.003412	1.910469	-.176839
C	.786811	-1.223486	-.238686
C	-.782497	-1.226273	-.238534
C	-1.287575	1.305049	-.133219
C	1.282898	1.309619	-.133405
H	2.697402	-.223050	-.079150
H	.003863	-2.065340	1.886372
H	-2.696615	-.232635	-.078759
H	-.005325	2.986347	-.177293
H	1.196409	-2.023288	-.839736
H	-1.189355	-2.027541	-.839493
H	-2.107547	2.000697	-.063290
H	2.100402	2.008175	-.063574

C	.036314	1.024480	.672485
C	1.775967	-.145336	-.603699
C	-.037713	-1.021795	.678332
C	-1.282177	1.242594	.176026
C	1.139426	1.024273	-.347204
C	1.281754	-1.242782	.185727
C	-1.138845	-1.027501	-.343473
H	-2.622031	.211280	-1.266248
H	.300145	1.528505	1.595224
H	2.624598	-.219765	-1.259668
H	-.303345	-1.520443	1.603477
H	-1.953712	1.965993	.604558
H	1.393279	1.950500	-.833039
H	1.952402	-1.963737	.619730
H	-1.391762	-1.956532	-.824419

TS_{RI}

C	0.392970	0.044184	1.925489
C	0.230853	1.864530	0.063712
C	0.044897	-0.004185	-1.747223
C	0.207017	-1.824529	0.114555
C	0.354397	1.295009	1.415437
C	0.109024	1.353127	-1.181209
C	0.083471	-1.255008	-1.237170
C	0.328846	-1.313127	1.359475
H	0.494258	0.017684	2.997526
H	0.241635	2.941309	0.089310
H	-0.056383	0.022315	-2.819260
H	0.196230	-2.901308	0.088957
H	0.431012	2.068303	2.161340
H	0.041916	2.102908	-1.951631
H	0.006846	-2.028302	-1.983072
H	0.395965	-2.062908	2.129895