

Supplementary Material

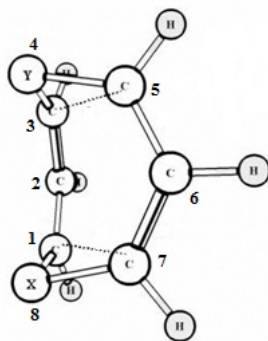
Cope Rearrangement in Bicyclo[5.1.0]octa-2,5-diene and its Mono- and Di-Hetero Analogues: A DFT Study

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Table S1 Total energies and entropies of different species

Re ac. No.	Entry		5				TS				6			
	X	Y	HF	ZPE	TE	S	HF	ZPE	TE	S	HF	ZPE	TE	S
1	CH ₂	CH ₂	-310.8080445	0.156924	-310.651121	81.845	-310.7856765	0.156002	-310.629675	78.486	-310.8080445	0.156924	-310.651121	81.846
2	CH ₂	NH	-326.8581565	0.146049	-326.712108	80.236	-326.8160602	0.143956	-326.672105	77.752	-326.8352739	0.145301	-326.689973	82.626
3	CH ₂	O	-346.7121354	0.133340	-346.578796	79.631	-346.682378	0.130946	-346.551432	77.349	-346.7065158	0.132631	-346.573885	82.887
4	CH ₂	PH	-613.4419365	0.138246	-613.303691	84.220	-613.4136625	0.137084	-613.276576	81.278	-613.4539638	0.139054	-613.314910	84.598
5	NH	CH ₂	-326.8354792	0.145710	-326.689769	79.206	-326.8160603	0.143954	-326.672107	77.762	-326.858157	0.146050	-326.712107	80.234
6	NH	NH	-342.8867065	0.134623	-342.752084	79.751	-342.8346432	0.131572	-342.703071	77.624	-342.8867057	0.134628	-342.752077	79.755
7	NH	O	-362.7395002	0.121791	-362.617709	79.287	-362.7026797	0.118810	-362.583869	77.008	-362.759068	0.122047	-362.637021	79.515
8	NH	PH	-629.4687587	0.126854	-629.341905	82.258	-629.4449554	0.125014	-629.319942	80.765	-629.5044708	0.128128	-629.376342	83.522
9	O	CH ₂	-346.7064897	0.132642	-346.573847	82.548	-346.6823779	0.130946	-346.551432	77.350	-346.7121358	0.133335	-346.578801	79.624
10	O	NH	-362.759068	0.122047	-362.637021	79.515	-362.7026798	0.118811	-362.583869	77.010	-362.7395003	0.121792	-362.617708	79.284
11	O	O	-382.6106081	0.109135	-382.501473	79.106	-382.5706679	0.105947	-382.464721	76.446	-382.6106043	0.109129	-382.501416	79.129
12	O	PH	-649.3398325	0.113978	-649.225854	83.459	-649.3089202	0.112134	-649.196786	80.327	-649.3577724	0.115418	-649.242355	82.811
13	PH	CH ₂	-613.453963	0.139056	-613.314907	84.600	-613.4136627	0.137087	-613.276576	81.278	-613.4366802	0.138244	-613.298436	85.105
14	PH	NH	-629.5044709	0.128128	-629.376343	83.522	-629.4449555	0.125016	-629.319939	80.764	-629.4687589	0.126855	-629.341904	82.265
15	PH	O	-649.3577724	0.115416	-649.242357	82.810	-649.3089202	0.112134	-649.196786	80.327	-649.3411292	0.114211	-649.226918	81.894
16	PH	PH	-916.0825733	0.120283	-915.962290	87.964	-916.0401977	0.117991	-915.922207	84.746	-916.0825567	0.120231	-915.962325	87.994

Table S2 NLMO occupancies and second order perturbation interactions in the transition structures



Species	Orbitals	Occupancy	Second Order Perturbations	
			Donor \rightarrow Acceptor	E _{ij} (kcal mol ⁻¹)
TSAa	σ C1C7	1.55	π C2C3 \rightarrow σ^* C1C7	22.23
	π C2C3	1.70	π C5C6 \rightarrow σ^* C1C7	22.23
	π C5C6	1.70		
TSAb	σ C3C5	1.63	π C1C2 \rightarrow σ^* C3C5	19.69
	π C1C2	1.73	π C6C7 \rightarrow σ^* C3C5	19.69
	π C6C7	1.73		
TSAc	σ C1C7	1.61	π C2C3 \rightarrow σ^* C1C7	16.82
	π C2C3	1.75	π C5C6 \rightarrow σ^* C1C7	16.82
	π C5C6	1.75		
TSA d	σ C3C5	1.63	π C1C2 \rightarrow σ^* C3C5	20.43
	π C1C2	1.72	π C6C7 \rightarrow σ^* C3C5	20.43
	π C6C7	1.72		
TSBa	σ C3C5	1.56	π C1C2 \rightarrow σ^* C3C5	20.49
	π C1C2	1.71	π C6C7 \rightarrow σ^* C3C5	20.49
	π C6C7	1.71		
TSBb	σ C3C5	1.59	π C1C2 \rightarrow σ^* C3C5	20.42
	π C1C2	1.70	π C6C7 \rightarrow σ^* C3C5	20.42
	π C6C7	1.70		
TSBc	σ C1C7	1.63	π C2C3 \rightarrow σ^* C1C7	17.00
	π C2C3	1.73	π C5C6 \rightarrow σ^* C1C7	16.99
	π C5C6	1.73		
TSBd	σ C3C5	1.61	π C1C2 \rightarrow σ^* C3C5	19.88
	π C1C2	1.71	π C6C7 \rightarrow σ^* C3C5	19.88
	π C6C7	1.71		
TSCa	σ C3C5	1.61	π C1C2 \rightarrow σ^* C3C5	16.82
	π C1C2	1.75	π C6C7 \rightarrow σ^* C3C5	16.82
	π C6C7	1.75		
TSCb	σ C3C5	1.63	π C1C2 \rightarrow σ^* C3C5	16.99
	π C1C2	1.73	π C6C7 \rightarrow σ^* C3C5	16.99
	π C6C7	1.73		
TSCc	σ C3C5	1.64	π C1C2 \rightarrow σ^* C3C5	16.98
	π C1C2	1.68	π C6C7 \rightarrow σ^* C3C5	16.98

	πC6C7	1.68		
TSCd	σC3C5	1.65	$\pi\text{C1C2} \rightarrow \sigma^*\text{C3C5}$	16.35
	πC1C2	1.73	$\pi\text{C6C7} \rightarrow \sigma^*\text{C3C5}$	16.35
	πC6C7	1.73		
TSDa	σC3C5	1.77	$\pi\text{C1C2} \rightarrow \sigma^*\text{C3C5}$	9.61
	πC1C2	1.89	$\pi\text{C6C7} \rightarrow \sigma^*\text{C3C5}$	9.61
	πC6C7	1.89		
TSDb	σC1C7	1.61	$\pi\text{C2C3} \rightarrow \sigma^*\text{C1C7}$	19.88
	πC2C3	1.71	$\pi\text{C5C6} \rightarrow \sigma^*\text{C1C7}$	19.88
	πC5C6	1.71		
TSDc	σC1C7	1.65	$\pi\text{C2C3} \rightarrow \sigma^*\text{C1C7}$	16.35
	πC2C3	1.73	$\pi\text{C5C6} \rightarrow \sigma^*\text{C1C7}$	16.35
	πC5C6	1.73		
TSDd	σC3C5	1.58	$\pi\text{C1C2} \rightarrow \sigma^*\text{C3C5}$	21.34
	πC1C2	1.70	$\pi\text{C6C7} \rightarrow \sigma^*\text{C3C5}$	21.34
	πC6C7	1.70		

Cartesian coordinate of the optimized geometries of different species

5Aa

C	-1.967413000	-0.000014000	0.676361000
C	-1.206179000	0.753430000	-0.406920000
C	-0.051790000	1.622919000	-0.070747000
C	1.242916000	1.317655000	0.094191000
C	1.968224000	0.000008000	-0.004794000
C	1.242935000	-1.317642000	0.094222000
C	-0.051762000	-1.622914000	-0.070767000
C	-1.206157000	-0.753440000	-0.406932000
H	-1.852943000	-1.197530000	-1.164891000
H	-3.055102000	-0.000035000	0.653131000
H	-0.322966000	-2.673601000	0.049554000
H	-1.852968000	1.197515000	-1.164880000
H	-0.322997000	2.673600000	0.049595000
H	1.907972000	2.150713000	0.326974000
H	2.546057000	-0.000008000	-0.947335000
H	1.907991000	-2.150690000	0.327032000
H	2.746701000	0.000030000	0.773571000
H	-1.526390000	-0.000005000	1.669561000

TSAa

C	-1.559800000	0.000000000	0.849961000
C	-1.258484000	-1.068492000	-0.157583000
C	-0.000001000	-1.520765000	-0.554672000
C	1.258483000	-1.068525000	-0.157576000
C	1.559805000	0.000000000	0.849938000
C	1.258482000	1.068526000	-0.157574000
C	-0.000001000	1.520765000	-0.554672000
C	-1.258485000	1.068491000	-0.157584000
H	-2.115767000	1.459377000	-0.700953000
H	-0.000010000	2.237465000	-1.375098000
H	2.115761000	1.459437000	-0.700931000
H	2.612227000	0.000000000	1.142937000
H	2.115761000	-1.459432000	-0.700936000
H	-0.000010000	-2.237465000	-1.375097000
H	-2.115766000	-1.459381000	-0.700948000
H	-2.612218000	0.000000000	1.142973000
H	-0.954991000	0.000002000	1.753320000
H	0.955016000	-0.000003000	1.753311000

6Aa

C	1.968214000	0.000001000	-0.004843000
C	1.242916000	1.317676000	0.094222000
C	-0.051791000	1.622928000	-0.070707000
C	-1.206164000	0.753443000	-0.406932000
C	-1.967389000	-0.000002000	0.676317000
C	-1.206162000	-0.753443000	-0.406933000
C	-0.051789000	-1.622929000	-0.070707000
C	1.242918000	-1.317674000	0.094223000
H	1.908007000	-2.150725000	0.326922000
H	-0.323041000	-2.673608000	0.049583000
H	-1.852920000	-1.197506000	-1.164928000
H	-3.055082000	-0.000003000	0.653289000
H	-1.852925000	1.197509000	-1.164922000
H	-0.323044000	2.673607000	0.049586000
H	1.908004000	2.150727000	0.326921000
H	2.546097000	0.000001000	-0.947337000
H	2.746624000	0.000002000	0.773592000
H	-1.526229000	-0.000002000	1.669452000

5Ab

C	-1.979310000	0.000086000	0.667564000
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C	-1.192440000	-0.751677000	-0.402107000
C	-0.024833000	-1.595939000	-0.062163000
C	1.273801000	-1.254737000	0.065871000
N	1.868020000	-0.000306000	-0.000057000
C	1.274339000	1.254324000	0.065924000
C	-0.024128000	1.596063000	-0.062049000
C	-1.192040000	0.752205000	-0.401647000
H	-1.822389000	-1.194435000	-1.175063000
H	-3.067260000	0.000730000	0.619530000
H	-0.243296000	-2.652349000	0.086705000
H	-1.822274000	1.195219000	-1.174232000
H	-0.242162000	2.652622000	0.086414000
H	1.998728000	-2.038718000	0.271402000
H	2.870119000	-0.000500000	0.116541000
H	-1.559508000	-0.000535000	1.669874000
H	1.999569000	2.038148000	0.270867000

TSAb

C	1.528414000	0.000000000	0.854397000
C	1.235395000	-1.050442000	-0.175522000
C	-0.028482000	-1.508656000	-0.550783000
C	-1.255657000	-1.009637000	-0.124578000
N	-1.352617000	0.000000000	0.891668000
C	-1.255657000	1.009637000	-0.124578000
C	-0.028482000	1.508656000	-0.550783000
C	1.235395000	1.050442000	-0.175522000
H	2.088418000	-1.435846000	-0.729348000
H	-0.070424000	-2.212316000	-1.380467000
H	-2.174855000	-1.369139000	-0.587689000
H	-2.256869000	0.000000000	1.355502000
H	-2.174855000	1.369139000	-0.587689000
H	-0.070424000	2.212316000	-1.380467000
H	2.088418000	1.435846000	-0.729348000
H	2.577038000	0.000000000	1.160281000
H	0.876308000	0.000000000	1.721768000

6Ab

C	1.952051000	0.000000000	0.109364000
C	1.241758000	1.312213000	-0.123109000
C	-0.057856000	1.616826000	-0.023106000
C	-1.185987000	0.742792000	0.386268000
N	-1.923279000	0.000000000	-0.671209000
C	-1.185987000	-0.742792000	0.386268000
C	-0.057855000	-1.616826000	-0.023106000
C	1.241759000	-1.312212000	-0.123109000
H	1.912539000	2.125402000	-0.402889000
H	-0.349824000	2.645284000	-0.240717000
H	-1.814865000	1.201343000	1.153790000
H	-2.925304000	0.000001000	-0.470321000
H	-1.814864000	-1.201344000	1.153789000
H	-0.349822000	-2.645285000	-0.240717000
H	1.912540000	-2.125401000	-0.402889000
H	2.357020000	0.000001000	1.137727000
H	2.848237000	0.000001000	-0.526120000

5Ac

C	1.966169000	0.000000000	0.671391000
C	1.189309000	0.750743000	-0.404100000
C	0.002581000	1.566905000	-0.067579000
C	-1.285287000	1.220100000	0.073903000
O	-1.901310000	-0.000001000	0.008050000
C	-1.285286000	-1.220101000	0.073903000
C	0.002582000	-1.566905000	-0.067580000
C	1.189310000	-0.750743000	-0.404101000

H	1.817174000	1.207633000	-1.169259000
H	3.053526000	0.000001000	0.626724000
H	0.191028000	2.630561000	0.075411000
H	1.817176000	-1.207632000	-1.169259000
H	0.191030000	-2.630560000	0.075412000
H	-2.039288000	-1.971736000	0.284783000
H	-2.039290000	1.971735000	0.284780000
H	1.542858000	-0.000001000	1.671994000

TSAc

C	-1.524329000	-0.000081000	0.846405000
C	-1.214461000	-1.002967000	-0.218165000
C	0.062393000	-1.491930000	-0.539686000
C	1.263786000	-0.983459000	-0.087948000
O	1.330449000	0.000053000	0.909012000
C	1.263709000	0.983538000	-0.087984000
C	0.062262000	1.491937000	-0.539673000
C	-1.214565000	1.002907000	-0.218111000
H	-2.057128000	1.389768000	-0.785156000
H	0.133120000	2.228754000	-1.337323000
H	2.226614000	1.375076000	-0.407148000
H	2.226722000	-1.374988000	-0.407033000
H	0.133324000	-2.228722000	-1.337354000
H	-2.056992000	-1.389783000	-0.785285000
H	-2.573460000	-0.000176000	1.146252000
H	-0.868566000	-0.000026000	1.711921000

6Ac

C	0.780478000	-1.772377000	0.000000000
C	0.307342000	-1.189670000	1.309789000
C	-0.052231000	0.064005000	1.612615000
C	-0.052231000	1.261338000	0.735517000
O	-1.261428000	1.578363000	0.000000000
C	-0.052231000	1.261338000	-0.735517000
C	-0.052231000	0.064005000	-1.612615000
C	0.307342000	-1.189670000	-1.309789000
H	0.276300000	-1.915379000	-2.123255000
H	-0.358164000	0.266720000	-2.639282000
H	0.371928000	2.147237000	-1.216022000
H	0.371928000	2.147237000	1.216022000
H	-0.358164000	0.266720000	2.639282000
H	0.276300000	-1.915379000	2.123255000
H	1.885497000	-1.781490000	0.000000000
H	0.508373000	-2.836383000	0.000000000

5Ad

C	2.330748000	-0.000002000	0.515833000
C	1.418966000	-0.757300000	-0.438109000
C	0.367647000	-1.672512000	0.078309000
C	-0.948110000	-1.458317000	0.236357000
P	-1.931200000	-0.000002000	-0.244890000
C	-0.948111000	1.458318000	0.236356000
C	0.367645000	1.672514000	0.078311000
C	1.418966000	0.757302000	-0.438105000
H	1.952144000	1.188372000	-1.288100000
H	3.403583000	0.000000000	0.335973000
H	0.747724000	2.663860000	0.336088000
H	1.952141000	-1.188367000	-1.288108000
H	0.747727000	-2.663857000	0.336089000
H	-1.557260000	2.289480000	0.594430000
H	-2.807283000	-0.000002000	0.875725000
H	2.039984000	-0.000005000	1.563095000
H	-1.557256000	-2.289478000	0.594437000

TSAd

C	0.934651000	1.114700000	-0.546918000
P	1.609288000	0.000011000	0.743143000
C	0.935016000	-1.114276000	-0.547101000
C	-0.396275000	-1.532469000	-0.681030000
C	-1.517341000	-1.077820000	0.001516000
C	-1.544004000	-0.000193000	1.047062000
C	-1.517685000	1.077496000	0.001591000
C	-0.396738000	1.532552000	-0.680844000
H	-2.486628000	1.439186000	-0.334856000
H	-0.594056000	2.194828000	-1.524047000
H	1.635414000	1.463299000	-1.301807000
H	2.942941000	0.000686000	0.242551000
H	1.636188000	-1.463022000	-1.301549000
H	-0.593426000	-2.194852000	-1.524190000
H	-2.486173000	-1.439793000	-0.334948000
H	-2.472516000	-0.000336000	1.622924000
H	-0.706817000	-0.000100000	1.743123000

6Ad

C	2.262736000	0.000000000	-0.221609000
C	1.539768000	1.316052000	-0.137665000
C	0.282343000	1.616305000	0.222190000
C	-0.825019000	0.744038000	0.672386000
P	-1.988775000	0.000000000	-0.655283000
C	-0.825019000	-0.744038000	0.672386000
C	0.282343000	-1.616305000	0.222190000
C	1.539768000	-1.316052000	-0.137665000
H	2.170503000	2.161366000	-0.415967000
H	0.006172000	2.670778000	0.191592000
H	-1.391591000	1.187092000	1.491248000
H	-3.163091000	0.000000000	0.161702000
H	-1.391591000	-1.187092000	1.491248000
H	0.006172000	-2.670778000	0.191592000
H	2.170503000	-2.161366000	-0.415967000
H	3.055477000	0.000000000	0.548512000
H	2.827550000	0.000000000	-1.167997000

5Ba

C	1.627931000	0.000047000	0.621312000
C	1.212206000	-1.249002000	-0.137355000
C	1.212080000	1.249149000	-0.137367000
C	-0.042158000	-1.558102000	-0.504744000
C	-0.042335000	1.558080000	-0.504726000
C	-1.263920000	0.761823000	-0.227291000
C	-1.263771000	-0.761935000	-0.227362000
N	-1.353693000	-0.000047000	1.030414000
H	-2.309334000	-0.000216000	1.384607000
H	-2.186722000	-1.215785000	-0.588548000
H	-2.186857000	1.215642000	-0.588553000
H	-0.202770000	2.457417000	-1.098303000
H	-0.202513000	-2.457480000	-1.098267000
H	2.010123000	1.924006000	-0.444688000
H	2.010370000	-1.923736000	-0.444651000
H	2.715578000	0.000134000	0.746204000
H	1.187778000	-0.000008000	1.624504000

TSBa

C	1.528989000	-0.000004000	0.854231000
C	1.235310000	-1.050171000	-0.175687000
C	-0.028713000	-1.508915000	-0.550520000
C	-1.255839000	-1.010369000	-0.124270000
N	-1.352650000	0.000003000	0.891109000
C	-1.255834000	1.010373000	-0.124272000
C	-0.028706000	1.508915000	-0.550520000

C	1.235315000	1.050168000	-0.175684000
H	2.088132000	-1.435449000	-0.729918000
H	-0.070500000	-2.212729000	-1.380091000
H	-2.174956000	-1.369845000	-0.587628000
H	-2.255585000	0.000006000	1.356427000
H	-2.174949000	1.369847000	-0.587636000
H	-0.070488000	2.212730000	-1.380091000
H	2.088140000	1.435446000	-0.729911000
H	2.577896000	-0.000008000	1.159176000
H	0.877720000	-0.000003000	1.722232000

6Ba

C	1.980847000	-0.000069000	0.666040000
C	1.191844000	-0.751988000	-0.401909000
C	0.024381000	-1.595796000	-0.060512000
C	-1.274310000	-1.254301000	0.066072000
N	-1.868334000	0.000051000	-0.001430000
C	-1.274219000	1.254362000	0.066066000
C	0.024495000	1.595786000	-0.060505000
C	1.191938000	0.751948000	-0.401908000
H	1.820369000	-1.194842000	-1.176038000
H	0.242506000	-2.652183000	0.089010000
H	-1.999587000	-2.038134000	0.270886000
H	-2.870176000	0.000087000	0.116910000
H	-1.999444000	2.038238000	0.270899000
H	0.242674000	2.652153000	0.089070000
H	1.820533000	1.194857000	-1.175949000
H	3.068688000	-0.000114000	0.615998000
H	1.562922000	-0.000066000	1.669159000

5Bb

N	-1.855403000	0.000001000	0.017274000
C	-1.265044000	1.253883000	-0.061239000
C	0.034005000	1.597406000	0.042256000
C	1.193987000	0.741336000	0.369251000
N	1.878669000	0.000000000	-0.732052000
C	1.193986000	-0.741338000	0.369251000
C	0.034003000	-1.597406000	0.042256000
C	-1.265046000	-1.253882000	-0.061239000
H	2.890889000	0.000000000	-0.577803000
H	1.863640000	-1.195981000	1.102980000
H	1.863641000	1.195979000	1.102981000
H	0.257433000	2.649775000	-0.121447000
H	0.257430000	-2.649775000	-0.121447000
H	-1.995744000	2.035866000	-0.253126000
H	-1.995747000	-2.035864000	-0.253127000
H	-2.859747000	0.000002000	-0.078786000

TSBb

N	-1.406374000	0.000000000	0.879174000
C	-1.245329000	-0.997293000	-0.139129000
C	0.000002000	-1.494548000	-0.518526000
C	1.245301000	-0.997340000	-0.139111000
N	1.406377000	0.000000000	0.879124000
C	1.245301000	0.997340000	-0.139111000
C	0.000001000	1.494548000	-0.518526000
C	-1.245329000	0.997293000	-0.139129000
H	-2.136668000	1.373294000	-0.642987000
H	-0.000012000	2.196004000	-1.350423000
H	2.136689000	1.373369000	-0.642857000
H	2.347178000	0.000000000	1.262662000
H	2.136690000	-1.373369000	-0.642857000
H	-0.000012000	-2.196004000	-1.350423000
H	-2.136668000	-1.373294000	-0.642987000

H	-2.346904000	0.000000000	1.262976000
6Bb			
N	1.879379000	0.000000000	-0.730507000
C	1.193887000	-0.741378000	0.368656000
C	0.033853000	-1.597891000	0.041481000
C	-1.265099000	-1.254110000	-0.061416000
N	-1.855148000	-0.000002000	0.017980000
C	-1.265101000	1.254108000	-0.061416000
C	0.033850000	1.597891000	0.041481000
C	1.193886000	0.741382000	0.368655000
H	1.862090000	1.196306000	1.103697000
H	0.257611000	2.650130000	-0.122642000
H	-1.996279000	2.035736000	-0.252946000
H	-2.859638000	-0.000003000	-0.077301000
H	-1.996275000	-2.035740000	-0.252945000
H	0.257618000	-2.650128000	-0.122642000
H	1.862091000	-1.196300000	1.103700000
H	2.891512000	-0.000005000	-0.575879000
5Bc			
O	1.887240000	0.000000000	0.025087000
C	1.277283000	-1.220024000	-0.071007000
C	-0.011646000	-1.569595000	0.036436000
C	-1.188448000	-0.740047000	0.372256000
N	-1.872222000	0.000000000	-0.726033000
C	-1.188448000	0.740047000	0.372256000
C	-0.011645000	1.569595000	0.036436000
C	1.277283000	1.220024000	-0.071007000
H	-2.883707000	0.000000000	-0.572027000
H	-1.847982000	1.208396000	1.105262000
H	-1.847981000	-1.208396000	1.105263000
H	-0.208350000	-2.627122000	-0.132113000
H	-0.208350000	2.627122000	-0.132113000
H	2.038867000	-1.966643000	-0.272480000
H	2.038867000	1.966642000	-0.272481000
TSBc			
C	-1.255094000	-0.963921000	-0.105271000
C	-0.035907000	-1.480741000	-0.511178000
C	1.221709000	-0.958559000	-0.181783000
N	1.401058000	-0.000073000	0.871331000
C	1.221850000	0.958466000	-0.181747000
C	-0.035731000	1.480727000	-0.511178000
C	-1.254982000	0.964037000	-0.105297000
O	-1.375649000	0.000069000	0.900102000
H	-2.198452000	1.367272000	-0.467912000
H	-0.070090000	2.213048000	-1.314673000
H	2.104424000	1.347596000	-0.688686000
H	2.355583000	-0.000233000	1.221243000
H	2.104225000	-1.347642000	-0.688859000
H	-0.070355000	-2.213054000	-1.314676000
H	-2.198611000	-1.367083000	-0.467848000
6Bc			
O	1.866706000	0.000000000	0.714789000
C	1.213858000	0.733845000	-0.360194000
C	0.054841000	1.594198000	-0.043533000
C	-1.245784000	1.252614000	0.050981000
N	-1.835983000	0.000000000	-0.025556000
C	-1.245784000	-1.252614000	0.050981000
C	0.054842000	-1.594198000	-0.043533000
C	1.213858000	-0.733845000	-0.360195000
H	1.939944000	-1.213560000	-1.020668000
H	0.280460000	-2.646912000	0.109998000

H	-1.977831000	-2.036488000	0.229268000
H	-2.841897000	0.000000000	0.056330000
H	-1.977831000	2.036488000	0.229268000
H	0.280460000	2.646912000	0.109998000
H	1.939944000	1.213561000	-1.020668000

5Bd

P	-1.638971000	0.000000000	0.554512000
C	-0.886768000	-1.395683000	-0.395829000
C	0.423130000	-1.598128000	-0.612470000
C	1.538916000	-0.762967000	-0.095821000
N	1.300563000	0.000000000	1.131486000
C	1.538916000	0.762967000	-0.095821000
C	0.423131000	1.598128000	-0.612470000
C	-0.886767000	1.395684000	-0.395829000
H	2.102503000	-0.000001000	1.759147000
H	2.526809000	1.207400000	-0.221342000
H	2.526808000	-1.207401000	-0.221342000
H	0.727995000	-2.446452000	-1.225825000
H	0.727996000	2.446452000	-1.225825000
H	-1.591595000	-2.106228000	-0.826121000
H	-1.591594000	2.106229000	-0.826121000
H	-2.851633000	0.000000000	-0.201218000

TSBd

P	1.569917000	0.000000000	0.727716000
C	0.891250000	1.114823000	-0.570167000
C	-0.437793000	1.532619000	-0.675388000
C	-1.496763000	1.017847000	0.059506000
N	-1.252386000	0.000000000	1.035294000
C	-1.496763000	-1.017847000	0.059506000
C	-0.437793000	-1.532619000	-0.675388000
C	0.891250000	-1.114823000	-0.570167000
H	1.586030000	-1.473495000	-1.325360000
H	-0.695207000	-2.192586000	-1.502995000
H	-2.521117000	-1.339526000	-0.130243000
H	-1.890196000	0.000000000	1.825585000
H	-2.521117000	1.339526000	-0.130243000
H	-0.695207000	2.192586000	-1.502995000
H	1.586030000	1.473495000	-1.325360000
H	2.888401000	0.000000000	0.161403000

6Bd

P	-1.995563000	0.000000000	-0.640635000
C	-0.809526000	0.743876000	0.665886000
C	0.308115000	1.590229000	0.202356000
C	1.572254000	1.252381000	-0.132035000
N	2.165269000	0.000000000	-0.195465000
C	1.572253000	-1.252381000	-0.132035000
C	0.308114000	-1.590228000	0.202357000
C	-0.809526000	-0.743875000	0.665887000
H	-1.359385000	-1.186319000	1.496837000
H	0.077331000	-2.650714000	0.130403000
H	2.260345000	-2.045457000	-0.412228000
H	3.134321000	-0.000001000	-0.475756000
H	2.260346000	2.045456000	-0.412227000
H	0.077333000	2.650715000	0.130403000
H	-1.359385000	1.186321000	1.496836000
H	-3.164457000	0.000001000	0.189006000

5Ca

O	-1.914884000	0.000000000	-0.645461000
C	-1.203267000	0.735483000	0.382571000
C	-0.077981000	1.612301000	-0.026938000
C	1.223108000	1.309827000	-0.118148000

C	1.932840000	0.000000000	0.126380000
C	1.223108000	-1.309828000	-0.118148000
C	-0.077982000	-1.612301000	-0.026938000
C	-1.203267000	-0.735483000	0.382571000
H	-1.890810000	1.216519000	1.083602000
H	-0.373034000	2.639166000	-0.244336000
H	-1.890810000	-1.216519000	1.083602000
H	-0.373035000	-2.639166000	-0.244336000
H	1.894161000	-2.123562000	-0.395348000
H	2.319804000	0.000000000	1.161484000
H	1.894162000	2.123561000	-0.395348000
H	2.839276000	0.000000000	-0.493729000

TSCa

C	1.263873000	-0.983642000	-0.087769000
C	0.062550000	-1.492003000	-0.539652000
C	-1.214378000	-1.003118000	-0.218244000
C	-1.524323000	-0.000340000	0.846358000
C	-1.214708000	1.002880000	-0.217935000
C	0.062038000	1.492108000	-0.539581000
C	1.263539000	0.983865000	-0.088013000
O	1.330633000	0.000244000	0.908821000
H	2.226834000	-1.375000000	-0.407011000
H	0.133597000	-2.228724000	-1.337380000
H	-2.056807000	-1.389731000	-0.785659000
H	-2.573453000	-0.000531000	1.146232000
H	-2.057380000	1.389689000	-0.784864000
H	0.132844000	2.228921000	-1.337230000
H	2.226357000	1.375317000	-0.407560000
H	-0.868604000	-0.000387000	1.711916000

6Ca

C	1.285275000	-1.220328000	0.074272000
C	-0.002606000	-1.567216000	-0.065469000
C	-1.188478000	-0.750669000	-0.404474000
C	-1.967489000	0.000000000	0.669506000
C	-1.188477000	0.750671000	-0.404471000
C	-0.002603000	1.567216000	-0.065469000
C	1.285277000	1.220327000	0.074271000
O	1.901212000	-0.000001000	0.005603000
H	2.039819000	-1.971099000	0.286522000
H	-0.191906000	-2.630299000	0.080470000
H	-1.815200000	-1.206847000	-1.171006000
H	-3.054774000	0.000002000	0.623426000
H	-1.815201000	1.206851000	-1.171000000
H	-0.191902000	2.630300000	0.080469000
H	2.039823000	1.971096000	0.286521000
H	-1.545743000	-0.000001000	1.670772000

5Cb

O	1.866722000	0.000001000	0.714774000
C	1.213857000	-0.733836000	-0.360201000
C	0.054854000	-1.594197000	-0.043520000
C	-1.245776000	-1.252622000	0.050978000
N	-1.835984000	-0.000011000	-0.025558000
C	-1.245795000	1.252607000	0.050974000
C	0.054831000	1.594202000	-0.043513000
C	1.213845000	0.733857000	-0.360186000
H	1.939929000	1.213574000	-1.020662000
H	0.280434000	2.646920000	0.110008000
H	1.939937000	-1.213537000	-1.020694000
H	0.280476000	-2.646910000	0.110013000
H	-1.977851000	2.036477000	0.229237000
H	-2.841895000	-0.000019000	0.056361000

H -1.977819000 -2.036500000 0.229259000

TSCb

C -1.255047000 -0.964104000 -0.105263000
C -0.035849000 -1.480773000 -0.511194000
C 1.221740000 -0.958543000 -0.181728000
N 1.401045000 -0.000018000 0.871247000
C 1.221806000 0.958500000 -0.181787000
C -0.035806000 1.480801000 -0.511155000
C -1.255021000 0.964131000 -0.105230000
O -1.375621000 -0.000001000 0.900020000
H -2.198515000 1.367385000 -0.467762000
H -0.070182000 2.213213000 -1.314567000
H 2.104372000 1.347726000 -0.688663000
H 2.355507000 -0.000052000 1.221282000
H 2.104305000 -1.347792000 -0.688559000
H -0.070216000 -2.213123000 -1.314660000
H -2.198553000 -1.367303000 -0.467823000

6Cb

C 1.277249000 1.219963000 -0.070913000
O 1.887408000 0.000000000 0.024868000
C 1.277249000 -1.219963000 -0.070913000
C -0.011741000 -1.569341000 0.036717000
C -1.188536000 -0.740124000 0.372383000
N -1.871810000 0.000000000 -0.726385000
C -1.188536000 0.740124000 0.372383000
C -0.011741000 1.569341000 0.036717000
H 2.038597000 1.966739000 -0.272614000
H -0.208180000 2.626927000 -0.132047000
H -1.848869000 1.207933000 1.104970000
H -2.883354000 0.000000000 -0.573115000
H -1.848869000 -1.207933000 1.104971000
H -0.208180000 -2.626927000 -0.132047000
H 2.038597000 -1.966739000 -0.272614000

5Cc

C 0.032555000 -0.034428000 1.566611000
C 0.032555000 1.259744000 1.218936000
O 0.176410000 1.860107000 0.000000000
C 0.032555000 1.259744000 -1.218936000
C 0.032555000 -0.034428000 -1.566611000
C 0.272538000 -1.231442000 -0.732807000
C 0.272538000 -1.231442000 0.732807000
O -0.841759000 -1.805946000 0.000000000
H 0.878657000 -1.994144000 1.225457000
H -0.143495000 -0.220846000 2.624104000
H 0.878657000 -1.994144000 -1.225457000
H -0.143495000 -0.220846000 -2.624104000
H -0.099645000 2.035102000 -1.966853000
H -0.099645000 2.035102000 1.966853000

TSCc

C -1.234089000 -0.925946000 -0.149151000
C 0.000047000 -1.467315000 -0.503407000
C 1.234135000 -0.925910000 -0.149121000
O 1.374658000 0.000029000 0.890772000
C 1.234084000 0.925983000 -0.149139000
C -0.000046000 1.467332000 -0.503388000
C -1.234147000 0.925898000 -0.149115000
O -1.374643000 -0.000055000 0.890798000
H -2.167819000 1.345935000 -0.517389000
H -0.000072000 2.226610000 -1.281475000
H 2.167730000 1.346029000 -0.517469000
H 2.167792000 -1.346025000 -0.517335000

H	0.000084000	-2.226583000	-1.281501000
H	-2.167736000	-1.346001000	-0.517469000

6Cc

C	1.258723000	-1.218997000	0.060626000
O	1.868176000	0.000000000	-0.037601000
C	1.258723000	1.218997000	0.060626000
C	-0.031942000	1.566592000	-0.034999000
C	-1.207900000	0.732791000	-0.362990000
O	-1.863467000	0.000000000	0.705647000
C	-1.207900000	-0.732791000	-0.362990000
C	-0.031943000	-1.566592000	-0.034999000
H	2.022150000	-1.966977000	0.249682000
H	-0.230877000	-2.624142000	0.126427000
H	-1.923389000	-1.225540000	-1.024114000
H	-1.923389000	1.225541000	-1.024114000
H	-0.230877000	2.624142000	0.126427000
H	2.022150000	1.966976000	0.249682000

5Cd

C	0.392924000	1.645474000	-0.171243000
C	-0.928980000	1.443052000	-0.269552000
P	-1.888257000	0.000000000	0.312258000
C	-0.928979000	-1.443052000	-0.269552000
C	0.392924000	-1.645474000	-0.171243000
C	1.411612000	-0.738541000	0.420713000
C	1.411611000	0.738541000	0.420713000
O	2.273742000	0.000000000	-0.476945000
H	1.981900000	-1.210397000	1.226877000
H	0.797545000	-2.600892000	-0.508856000
H	1.981899000	1.210397000	1.226877000
H	0.797544000	2.600892000	-0.508856000
H	-1.543103000	-2.253934000	-0.662934000
H	-2.845428000	0.000000000	-0.737500000
H	-1.543103000	2.253934000	-0.662934000

TSCd

C	-1.499219000	0.967077000	-0.090389000
O	-1.257453000	0.000000000	-1.078441000
C	-1.499219000	-0.967077000	-0.090389000
C	-0.462684000	-1.502563000	0.649320000
C	0.866472000	-1.056539000	0.605325000
P	1.584284000	0.000000000	-0.716531000
C	0.866472000	1.056539000	0.605325000
C	-0.462684000	1.502563000	0.649320000
H	-2.522413000	-1.330267000	-0.039611000
H	-0.746257000	-2.195442000	1.439945000
H	1.541056000	-1.421067000	1.375353000
H	2.895746000	0.000000000	-0.146952000
H	1.541056000	1.421067000	1.375353000
H	-0.746257000	2.195442000	1.439945000
H	-2.522413000	1.330267000	-0.039611000

6Cd

C	1.581107000	1.217981000	-0.146578000
C	0.329302000	1.560535000	0.198837000
C	-0.804495000	0.742901000	0.670595000
P	-1.989324000	-0.000032000	-0.634593000
C	-0.804634000	-0.742436000	0.671072000
C	0.328816000	-1.560437000	0.199108000
C	1.580659000	-1.218297000	-0.146544000
O	2.195825000	-0.000264000	-0.216506000
H	2.296258000	1.979038000	-0.440151000
H	0.127503000	2.627499000	0.124273000
H	-1.343399000	1.199495000	1.500123000

H	-3.150243000	0.000398000	0.203099000
H	-1.343404000	-1.198473000	1.500968000
H	0.126529000	-2.627282000	0.124037000
H	2.295481000	-1.979564000	-0.440354000

5Da

C	-2.262540000	-0.000004000	-0.221824000
C	-1.539942000	1.316195000	-0.136817000
C	-0.282272000	1.616797000	0.221727000
C	0.824742000	0.744067000	0.671842000
P	1.989041000	0.000000000	-0.654740000
C	0.824752000	-0.744057000	0.671831000
C	-0.282264000	-1.616794000	0.221729000
C	-1.539938000	-1.316200000	-0.136810000
H	3.163325000	-0.000003000	0.162026000
H	1.390999000	-1.186276000	1.491421000
H	1.390992000	1.186288000	1.491429000
H	-0.006019000	2.671172000	0.190027000
H	-0.006007000	-2.671168000	0.190035000
H	-2.170882000	2.161276000	-0.415553000
H	-2.170877000	-2.161287000	-0.415532000
H	-3.056850000	-0.000003000	0.546588000
H	-2.825532000	-0.000009000	-1.169411000

TSDa

C	0.934673000	-1.114399000	-0.547113000
P	1.609581000	-0.000007000	0.743040000
C	0.934704000	1.114387000	-0.547143000
C	-0.396645000	1.532312000	-0.680939000
C	-1.517635000	1.077490000	0.001643000
C	-1.543884000	-0.000011000	1.047288000
C	-1.517665000	-1.077449000	0.001597000
C	-0.396677000	-1.532300000	-0.680963000
H	-2.486558000	1.439193000	-0.334830000
H	-0.593952000	2.194672000	-1.524076000
H	1.635748000	1.464147000	-1.301224000
H	2.943016000	-0.000061000	0.242007000
H	1.635731000	-1.464190000	-1.301167000
H	-0.593980000	-2.194611000	-1.524140000
H	-2.486603000	-1.439063000	-0.334936000
H	-2.472049000	-0.000108000	1.623697000
H	-0.706286000	-0.000055000	1.742841000

6Da

C	0.920151000	-1.425340000	-0.327319000
P	1.733901000	0.000000000	0.496339000
C	0.920151000	1.425340000	-0.327320000
C	-0.391437000	1.629378000	-0.537822000
C	-1.557863000	0.768985000	-0.196815000
C	-1.668631000	0.000000000	1.102640000
C	-1.557863000	-0.768985000	-0.196816000
C	-0.391437000	-1.629378000	-0.537822000
H	-2.497027000	1.186861000	-0.552372000
H	-0.670329000	2.568632000	-1.017520000
H	1.605266000	2.219304000	-0.624424000
H	2.904568000	0.000000000	-0.312309000
H	1.605266000	-2.219304000	-0.624424000
H	-0.670329000	-2.568632000	-1.017520000
H	-2.497027000	-1.186860000	-0.552374000
H	-2.623545000	0.000000000	1.622376000
H	-0.803780000	0.000000000	1.761129000

5Db

C	1.572229000	-1.252396000	-0.131975000
C	0.308200000	-1.590276000	0.202830000

C	-0.809594000	-0.743907000	0.665845000
C	-0.809594000	0.743907000	0.665845000
C	0.308200000	1.590276000	0.202830000
C	1.572229000	1.252396000	-0.131975000
N	2.165125000	0.000000000	-0.196011000
P	-1.995475000	0.000000000	-0.640855000
H	-3.164414000	0.000000000	0.188846000
H	-1.359710000	1.186189000	1.496706000
H	-1.359710000	-1.186189000	1.496706000
H	0.077601000	-2.650835000	0.131298000
H	0.077602000	2.650835000	0.131298000
H	2.260346000	-2.045513000	-0.411978000
H	2.260346000	2.045513000	-0.411978000
H	3.134151000	0.000000000	-0.476390000

TSDb

C	0.891012000	-1.114939000	-0.570189000
P	1.570066000	-0.000124000	0.727477000
C	0.891123000	1.114983000	-0.569931000
C	-0.437903000	1.532704000	-0.675350000
C	-1.496769000	1.017892000	0.059584000
N	-1.251920000	0.000103000	1.035255000
C	-1.496859000	-1.017858000	0.059725000
C	-0.438094000	-1.532651000	-0.675331000
H	-2.521236000	1.339153000	-0.130236000
H	-0.695261000	2.192657000	-1.502972000
H	1.585964000	1.473828000	-1.324942000
H	2.888238000	-0.000057000	0.160425000
H	1.585699000	-1.473665000	-1.325441000
H	-0.695590000	-2.192567000	-1.502953000
H	-2.521343000	-1.339169000	-0.129934000
H	-1.889080000	0.000187000	1.826072000

6Db

C	-0.886754000	1.395720000	-0.394893000
C	0.423057000	1.598081000	-0.612010000
C	1.539256000	0.762886000	-0.096395000
N	1.301840000	0.000000000	1.131519000
C	1.539256000	-0.762886000	-0.096395000
C	0.423057000	-1.598081000	-0.612010000
C	-0.886754000	-1.395720000	-0.394893000
P	-1.639964000	0.000000000	0.553837000
H	2.526916000	-1.207548000	-0.222670000
H	0.727594000	-2.447128000	-1.224524000
H	-1.591252000	-2.107284000	-0.824135000
H	-2.851351000	0.000000000	-0.204148000
H	-1.591252000	2.107284000	-0.824135000
H	0.727594000	2.447128000	-1.224523000
H	2.526916000	1.207548000	-0.222670000
H	2.104698000	0.000000000	1.758194000

5Dc

C	1.580763000	-1.218178000	-0.146576000
C	0.329018000	-1.560600000	0.199189000
C	-0.804532000	-0.742678000	0.671017000
C	-0.804532000	0.742678000	0.671017000
C	0.329018000	1.560600000	0.199189000
C	1.580763000	1.218178000	-0.146576000
O	2.195576000	0.000000000	-0.216783000
P	-1.989062000	0.000000000	-0.634817000
H	-3.150347000	0.000000000	0.202542000
H	-1.343512000	1.198835000	1.500722000
H	-1.343512000	-1.198835000	1.500722000
H	0.127059000	-2.627539000	0.124763000

H	0.127059000	2.627539000	0.124763000
H	2.295792000	-1.979304000	-0.440276000
H	2.295792000	1.979304000	-0.440276000

TSDc

C	-1.499219000	0.967077000	-0.090389000
O	-1.257453000	0.000000000	-1.078441000
C	-1.499219000	-0.967077000	-0.090389000
C	-0.462684000	-1.502563000	0.649320000
C	0.866472000	-1.056539000	0.605325000
P	1.584284000	0.000000000	-0.716531000
C	0.866472000	1.056539000	0.605325000
C	-0.462684000	1.502563000	0.649320000
H	-2.522413000	-1.330267000	-0.039611000
H	-0.746257000	-2.195442000	1.439945000
H	1.541056000	-1.421067000	1.375353000
H	2.895746000	0.000000000	-0.146952000
H	1.541056000	1.421067000	1.375353000
H	-0.746257000	2.195442000	1.439945000
H	-2.522413000	1.330267000	-0.039611000

6Dc

C	-0.865109000	1.393137000	-0.410752000
C	0.450201000	1.589989000	-0.597339000
C	1.545039000	0.750614000	-0.050317000
O	1.276502000	0.000000000	1.143098000
C	1.545039000	-0.750614000	-0.050317000
C	0.450201000	-1.589989000	-0.597339000
C	-0.865109000	-1.393137000	-0.410752000
P	-1.628977000	0.000000000	0.530695000
H	2.527542000	-1.225750000	-0.048641000
H	0.780464000	-2.443155000	-1.189507000
H	-1.558185000	-2.108605000	-0.851448000
H	-2.838568000	0.000000000	-0.225129000
H	-1.558185000	2.108605000	-0.851448000
H	0.780464000	2.443155000	-1.189507000
H	2.527542000	1.225750000	-0.048641000

5Dd

C	0.409054000	-1.175161000	1.477270000
C	0.409054000	0.154335000	1.682847000
C	0.361228000	1.299812000	0.746303000
C	0.361228000	1.299812000	-0.746303000
C	0.409054000	0.154335000	-1.682847000
C	0.409054000	-1.175161000	-1.477270000
P	0.122782000	-2.193206000	0.000000000
P	-1.323729000	1.835832000	0.000000000
H	-1.051462000	3.239036000	0.000000000
H	0.890654000	2.158177000	-1.157570000
H	0.890654000	2.158177000	1.157570000
H	0.447640000	0.481440000	2.723532000
H	0.447640000	0.481440000	-2.723532000
H	0.441186000	-1.797536000	2.373521000
H	0.441186000	-1.797536000	-2.373521000
H	1.354682000	-2.910406000	0.000000000

TSDd

C	-1.257561000	1.143042000	0.460143000
C	-0.000006000	1.550412000	0.906442000
C	1.257556000	1.143041000	0.460158000
P	1.589566000	0.000000000	-0.939662000
C	1.257556000	-1.143041000	0.460158000
C	-0.000006000	-1.550412000	0.906442000
C	-1.257561000	-1.143042000	0.460143000
P	-1.589555000	0.000000000	-0.939681000

H	-2.115060000	-1.466605000	1.045538000
H	-0.000011000	-2.150879000	1.817514000
H	2.115047000	-1.466604000	1.045564000
H	3.005873000	0.000000000	-0.773984000
H	2.115047000	1.466604000	1.045564000
H	-0.000011000	2.150879000	1.817514000
H	-2.115060000	1.466605000	1.045538000
H	-3.005864000	0.000000000	-0.774020000

6Dd

C	-1.240190000	-1.476860000	0.099917000
P	-2.148175000	0.000000000	-0.442619000
C	-1.240190000	1.476860000	0.099917000
C	0.045090000	1.682782000	0.439689000
C	1.166186000	0.746391000	0.680416000
P	2.107109000	0.000000000	-0.816886000
C	1.166186000	-0.746391000	0.680416000
C	0.045090000	-1.682782000	0.439689000
H	1.864648000	1.157406000	1.408021000
H	0.350480000	2.723303000	0.564215000
H	-1.851422000	2.372639000	-0.024893000
H	-3.161943000	0.000000000	0.559467000
H	-1.851422000	-2.372639000	-0.024893000
H	0.350480000	-2.723303000	0.564215000
H	1.864648000	-1.157406000	1.408021000
H	3.397495000	0.000000000	-0.201842000