

Supporting Information for

# A Comprehensive Model for the Electronic Structures of 1,2,4-Cyclohexatriene and Related Compounds

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**Table 1 Absolute energies in a.u.,  $\langle S^2 \rangle$  and imaginary frequencies**

	B3LYP	MRCI	CASPT2	CCSD(T)	$\Delta G_{298}^{\text{corr}}$	$\langle S^2 \rangle$	Imag. Freq. (cm <sup>-1</sup> )
<b>1a</b>	-218.29791	-217.6838	-217.657613	-217.84152	0.052924		
<b>1b</b>	-218.27854	-217.6646	-217.639384		0.051735	1.0416	-544
<b>1d</b>	-218.29547	-217.6797	-217.654676	-217.838105	0.051811		
<b>1<sup>2</sup>b</b>	-218.09210	-217.5662	-217.551535		0.043346	1.0161	-504
<b>1<sup>2</sup>c</b>	-218.18034	-217.5916	-217.578046		0.049459		
<b>2a</b>	-232.12975	-231.5087	-231.483800	-231.67254	0.068345		
<b>2b</b>	-232.12359	-231.4914	-231.466183		0.066315	1.0594	-215
<b>2c</b>	-232.09730	-231.4667	-231.434814	-231.629949	0.07197		
<b>2b</b>	-231.51942	-230.8884	-230.882618		0.05219	1.0221	
<b>2c</b>	-231.59640	-230.9690	-230.957735		0.057206		
<b>3b</b>	-248.16809	-247.5170	-247.504089		0.057445	1.0360	-212
<b>3c</b>	-248.20478	-247.5572	-247.540560		0.059112		
<b>3<sup>+</sup>a</b>	-248.50463	-247.8643	-247.845950	-248.038744	0.071098		
<b>3<sup>+</sup>b</b>	-248.49761	-247.8500	-247.827383		0.069249	1.0607	-166
<b>3<sup>+</sup>c</b>	-248.45985	-247.8033	-247.784587	-247.983391	0.071174		
<b>4a</b>	-268.04714	-267.3805	-267.367063	-267.56104	0.046259		
<b>4b</b>	-268.02347	-267.3534	-267.345488		0.048183	1.0449	
<b>4c</b>	-268.04544	-267.3749	-267.360815	-267.558014	0.046171		-251
<b>5a</b>	-435.89359	-434.9089	-434.882448	-435.063723	0.045158		
<b>5b</b>	-435.86619	-434.8788	-434.855248		0.043326	1.0476	-756
<b>5d</b>	-435.88411	-434.8967	-434.870203	-435.051829	0.043773		-596
<b>6a</b>	-483.54929	-482.5549	-482.520712	-482.715546	0.056109		
<b>6b</b>	-483.53064	-482.5329	-482.499501		0.054169	1.0573	-291
<b>6c</b>	-483.51277	-482.5076	-482.475275	-482.671514	0.052771		-1334
<b>6d</b>	-483.47214				0.055699		
<b>7a</b>	-534.79711	-533.7785		-533.954044	0.049092		
<b>7b</b>	-534.78202	-533.7570			0.047077	1.0909	-235
<b>7c</b>	-534.77296	-533.7506		-533.929066	0.047284		
<b>8a</b>	-837.46037	-836.0531		-836.237247	0.032131		

<b>8b</b>	-837.43319	-836.0169			0.029958	0.9668	-311
<b>8c</b>	-837.42292	-836.0183		-836.199886	0.030154		
<b>9a</b>	-591.04306	-590.0079	-589.984812	-590.191967	0.041582		
<b>9b</b>	-591.02568	-589.9840	-589.964944		0.03927	1.0452	-741
<b>9c</b>	-591.03223	-589.9915	-589.971802	-590.175527	0.04129		-432

**Table 2** Energies and characters of the electronic states of 1,2,4-cyclohexatriene and its hetero analogues as indicated in Scheme 1.<sup>a)</sup>

<i>X</i>	<i>B3LYP</i> <sup>b</sup>		<i>CASPT2</i> <sup>c</sup>		<i>MRCI+Q</i> <sup>d</sup>		<i>CCSD(T)</i> <sup>e</sup>
	<i>diradical</i>	<i>zwitterion</i>	<i>diradical</i>	<i>zwitterion</i>	<i>diradical</i>	<i>zwitterion</i>	<i>zwitterion</i>
BH ( <b>1</b> ) <sup>f</sup>	+11	+1	+11	+1	+11	+2	+1
CH <sub>2</sub> ( <b>2</b> ) <sup>g</sup>	+3	+23	+10	+33	+10	+29	+29
NH ( <b>3</b> ) <sup>g,h</sup>	+22	0	+22	0	+24	0 <sup>g</sup>	n.a. <sup>h</sup>
O ( <b>4</b> ) <sup>g</sup>	+16	+1	+15	+4	+18	+3	+2
AlH( <b>5</b> ) <sup>f</sup>	+16	+5	+16	+7	+18	+7	+7
SiH <sub>2</sub> ( <b>6</b> ) <sup>f</sup>	+10	+21 <sup>i</sup>	+12	+26	+13	+28	+26
PH ( <b>7</b> ) <sup>g</sup>	+8	+14	n.a.	n.a.	+12	+16	+15
PH ( <b>8</b> ) <sup>g</sup>	+16	+22	n.a.	n.a.	+21	+21	+22
S ( <b>9</b> ) <sup>g</sup>	+9	+7	+11	+8	+14	+10	+10

a) All values are given in kcal·mol<sup>-1</sup> with respect to the allene structure except for **3**.

b) (U)B3LYP/cc-pVDZ/(U)B3LYP/cc-pVDZ

c) CASPT2/ano-l/(U)B3LYP/cc-pVDZ

d) MRCI+Q/ano-l/(U)B3LYP/cc-pVDZ

e) CCSD(T)/cc-pVTZ(f/p)//B3LYP/cc-pVDZ

f) zwitterion of type d (see Scheme 1)

g) zwitterion of type c (see Scheme 1)

h) zwitterion is ground state

i) zwitterion **c** 48 kcal·mol<sup>-1</sup> higher than allene **a**

**Table 3** Absolute orbital and single determinant energies

	X=CH <sub>2</sub>		X=CH <sup>-</sup>		X=NH		X=O	
	<b>2b</b>	<b>2c</b>	<b>2b<sup>-</sup></b>	<b>2c<sup>-</sup></b>	<b>3b</b>	<b>3c</b>	<b>4b</b>	<b>4c</b>
$\epsilon_{\pi}^*$	-0.091	-0.076	+0.207	+0.230	-0.038	-0.018	-0.073	-0.056
$\epsilon_{\sigma}$	-0.132	-0.175	+0.073	+0.028	-0.134	-0.172	-0.156	-0.194
$E_{\sigma\pi}^{\text{det}*}(\mathbf{b})$	-230.580		-229.964		-246.576		-266.392	
$E_{\sigma\pi}^{\text{det}*}(\mathbf{c})$	-230.553		-229.934		-246.554		-266.372	
$E_{\sigma}^{\text{det}*}(\mathbf{c})$	-230.548		-230.046		-246.611		-266.409	

**Geometries optimized with (U)B3LYP/cc-pVDZ in cartesian coordinates**

The labelling is according to the manuscript (Figure 1 and Scheme 1)

**1a**

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Atom      Coordinates (Angstroms)
          X           Y           Z
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B   -0.886268    1.079363   -0.047894
C   -1.639424   -0.334523   -0.097396
C    0.621195    1.235333   -0.043056
C    1.426119    0.113009    0.055725
C    0.786635   -1.173531    0.016033
C   -0.553389   -1.037283    0.061459
H   -2.656813   -0.435103    0.270962
H    1.101136    2.218548   -0.041763
H    2.520889    0.153501    0.067188
H    1.295088   -2.095123   -0.264015
H   -1.675777    1.943331    0.250505
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**1b**

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Atom      Coordinates (Angstroms)
          X           Y           Z
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B   -1.308355    0.000000    0.726272
C   -1.313159    0.000000   -0.838385
C    0.088425    0.000000    1.411223
C    1.240108    0.000000    0.651302
C    1.166893    0.000000   -0.775414
C   -0.085585    0.000000   -1.413450
H   -2.225437    0.000000   -1.445670
H    0.200311    0.000000    2.500814
H    2.234536    0.000000    1.110581
H    2.089195    0.000000   -1.364416
H   -2.336916    0.000000    1.355673
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**1c**

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Atom	Coordinates (Angstroms)		
	X	Y	Z
B	1.284094	-0.544235	0.000000
C	1.285942	1.077456	0.000000
C	0.043817	-1.382730	0.000000
C	-1.204124	-0.764012	0.000000
C	-1.261574	0.659164	0.000000
C	0.000000	1.157249	0.000000
H	2.192297	1.663231	0.000000
H	0.080878	-2.475333	0.000000
H	-2.150619	-1.315244	0.000000
H	-2.165643	1.261855	0.000000
H	2.438252	-0.896095	0.000000

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**1<sup>2</sup>-b**

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Atom	Coordinates (Angstroms)		
	X	Y	Z
B	1.338722	-0.699942	0.000000
C	1.306102	0.893761	0.000000
C	0.022065	-1.416347	0.000000
C	-1.254368	-0.709603	0.000000
C	-1.219638	0.763831	0.000000
C	0.000000	1.412010	0.000000
H	2.186038	1.567083	0.000000
H	-0.044404	-2.528066	0.000000
H	-2.232291	-1.229845	0.000000
H	-2.169028	1.336814	0.000000
H	2.441110	-1.308192	0.000000

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**1<sup>2</sup>-c**

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Atom	Coordinates (Angstroms)		
	X	Y	Z
B	1.274348	-0.795756	0.000000
C	-0.097841	-1.459477	0.000000
C	1.259210	0.726488	0.000000
C	0.000000	1.362856	0.000000
C	-1.213922	0.637462	0.000000
C	-1.371599	-0.790840	0.000000
H	-0.152151	-2.584646	0.000000
H	2.155955	1.383288	0.000000
H	-0.057277	2.480187	0.000000
H	-2.133757	1.278045	0.000000
H	2.360397	-1.437032	0.000000

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**2a**

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.155061	-0.867191	-0.182352
C	1.253229	0.588107	0.245748
C	-0.067246	1.301714	-0.056757
C	-1.241503	0.651232	-0.215865
C	-1.244852	-0.782199	0.166455
C	-0.064392	-1.380819	-0.023237
H	-2.167849	1.193697	-0.424222
H	2.061198	1.048669	-0.349165
H	1.530430	0.783547	1.302738
H	-0.037176	2.395323	-0.097915
H	-2.060769	-1.179225	0.778740
H	1.932392	-1.307078	-0.814134

**2b**

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.128601	-0.928476	0.000000
C	-1.303431	0.579814	0.000000
C	0.000000	1.330493	0.000000
C	1.219532	0.709195	0.000000
C	1.332205	-0.718345	0.000000
C	0.126357	-1.429664	0.000000
H	2.133305	1.311200	0.000000
H	-1.921064	0.887559	0.873073
H	-1.921064	0.887559	-0.873073
H	-0.051727	2.422896	0.000000
H	2.307036	-1.208849	0.000000
H	-2.022859	-1.558468	0.000000

**2c**

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.266734	0.587128	0.000000
C	0.000000	1.372468	0.000000
C	1.253385	0.591704	0.000000
C	1.179982	-0.767855	0.000000
C	-0.109651	-1.410534	0.000000
C	-1.401330	-0.807227	0.000000
H	2.091230	-1.374161	0.000000
H	-0.004356	2.075348	0.863015
H	-0.004356	2.075348	-0.863015
H	2.211464	1.119160	0.000000
H	-0.059688	-2.512170	0.000000
H	-2.168206	1.222365	0.000000

**2<sup>-</sup>b**

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Atom	Coordinates (Angstroms)		
	X	Y	Z
C	0.000000	-1.405502	0.000000
C	1.246329	-0.808910	0.000000
C	1.234525	0.668224	0.000000
C	0.000000	1.329166	0.000000
C	-1.234532	0.668227	0.000000
C	-1.246323	-0.808910	0.000000
H	2.185084	-1.372477	0.000000
H	2.175606	1.230514	0.000000
H	0.000002	2.430169	0.000000
H	-2.175610	1.230511	0.000000
H	-2.185077	-1.372481	0.000000

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**2<sup>-</sup>c**

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Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.375598	-0.746792	0.000000
C	-1.222473	0.671547	0.000000
C	0.000000	1.366893	0.000000
C	1.208001	0.655800	0.000000
C	1.146312	-0.744581	0.000000
C	-0.102736	-1.390972	0.000000
H	-2.130854	1.306068	0.000000
H	0.021129	2.469027	0.000000
H	2.172185	1.179267	0.000000
H	2.082032	-1.327339	0.000000
H	-0.065530	-2.498390	0.000000

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**3b**

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Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-1.195186	0.590322	0.000000
C	0.000000	1.303971	0.000000
C	-1.172889	-0.826900	0.000000
C	0.054306	-1.409658	0.000000
C	1.294263	-0.774007	0.000000
C	1.208311	0.666619	0.000000
H	-2.077471	1.081729	0.000000
H	-0.095760	2.389679	0.000000
H	2.118388	1.271030	0.000000
H	2.250392	-1.295276	0.000000
H	-2.133191	-1.339571	0.000000

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**3c**

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.000000	1.283999	0.000000
C	-1.207198	0.635380	0.000000
C	-1.363749	-0.756171	0.000000
C	-0.101130	-1.411836	0.000000
C	1.146888	-0.761468	0.000000
C	1.179447	0.622741	0.000000
H	0.019843	2.303612	0.000000
H	2.088928	1.222718	0.000000
H	2.091983	-1.312148	0.000000
H	-0.074735	-2.511451	0.000000
H	-2.051572	1.337404	0.000000

**3<sup>+</sup>a**

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	1.176734	0.543192	0.268098
C	-1.249552	-0.784662	0.201402
C	-0.088687	-1.376567	-0.068943
C	1.123044	-0.879316	-0.221801
C	-0.094678	1.294430	-0.084207
C	-1.255083	0.636105	-0.230533
H	1.972753	-1.202035	-0.822057
H	1.353361	0.640066	1.285840
H	0.045172	2.374620	-0.135333
H	-2.166379	1.189375	-0.469425
H	-2.024090	-1.156160	0.878866
H	1.971778	1.011846	-0.190089

**3<sup>+</sup>b**

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-1.253327	0.523578	0.000000
C	1.376187	-0.702368	0.000000
C	0.180464	-1.423118	0.000000
C	-1.081276	-0.969602	0.000000
C	0.000000	1.322984	0.000000
C	1.218018	0.719196	0.000000
H	-2.014487	-1.531961	0.000000
H	2.099482	1.365247	0.000000
H	2.360675	-1.171136	0.000000
H	-0.174322	2.398026	0.000000
H	-1.829210	0.796116	0.817877
H	-1.829210	0.796116	-0.817877



**3<sup>+</sup>c**

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.000000	1.329304	0.000000
C	-0.090137	-1.453575	0.000000
C	-1.373493	-0.833659	0.000000
C	-1.309109	0.518234	0.000000
C	1.243835	0.578571	0.000000
C	1.184031	-0.771555	0.000000
H	-2.139680	1.234223	0.000000
H	2.118996	-1.337671	0.000000
H	-0.035086	-2.551555	0.000000
H	2.155470	1.179419	0.000000
H	-0.015232	1.971176	0.817466
H	-0.015232	1.971176	-0.817466

**4a**

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	1.126203	0.703053	0.128124
C	-0.071366	1.284330	0.006559
C	-1.230108	0.567287	-0.148193
C	-1.138047	-0.833769	0.085873
C	0.092728	-1.481648	-0.009573
C	1.181218	-0.667587	-0.095394
H	-0.016459	2.368846	0.108514
H	-2.174922	1.103364	-0.265860
H	-2.039510	-1.367146	0.415629
H	2.214713	-0.941165	-0.318903

**4b**

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	-1.218123	0.641974	0.000000
C	0.000000	1.280289	0.000000
C	1.200606	0.636957	0.000000
C	1.267602	-0.797612	0.000000
C	0.007268	-1.393356	0.000000
C	-1.186709	-0.760856	0.000000
H	-0.124097	2.362178	0.000000
H	2.111307	1.240609	0.000000
H	2.210797	-1.341643	0.000000
H	-2.185621	-1.189474	0.000000

**4c**

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	-1.150974	0.656792	0.000000
C	0.000000	1.313690	0.000000
C	1.198373	0.639030	0.000000
C	1.169037	-0.770912	0.000000
C	-0.023543	-1.544358	0.000000
C	-1.136290	-0.726070	0.000000
H	-0.127704	2.397163	0.000000
H	2.129031	1.212519	0.000000
H	2.142377	-1.282881	0.000000
H	-2.181378	-1.049422	0.000000

**5a**

Atom	Coordinates (Angstroms)		
	X	Y	Z
Al	-1.278952	-0.633073	-0.095899
C	-1.103725	1.370032	-0.023662
C	0.491131	-1.422722	0.041188
C	1.569607	-0.578197	0.092712
C	1.439131	0.871243	-0.054903
C	0.196880	1.359215	0.049688
H	-1.787483	1.891982	0.658293
H	0.706079	-2.496554	0.089831
H	2.595976	-0.966125	0.140005
H	2.261009	1.461067	-0.466094
H	-2.707350	-1.257851	0.194512

**5b**

Atom	Coordinates (Angstroms)		
	X	Y	Z
Al	0.000000	1.485188	0.000000
C	1.621396	0.374604	0.000000
C	-1.494560	0.223636	0.000000
C	-1.215915	-1.130389	0.000000
C	0.102638	-1.686708	0.000000
C	1.290965	-0.932957	0.000000
H	2.675495	0.684141	0.000000
H	-2.558716	0.491409	0.000000
H	-2.034281	-1.863571	0.000000
H	0.187887	-2.779138	0.000000
H	-0.097531	3.070607	0.000000

**5c**

Atom	Coordinates (Angstroms)		
	X	Y	Z
Al	-1.154515	-0.832017	0.000000
C	-1.265311	1.253958	0.000000
C	0.665777	-1.358942	0.000000
C	1.619654	-0.350297	0.000000
C	1.326768	1.047880	0.000000
C	0.000000	1.362950	0.000000
H	-2.264871	1.658223	0.000000
H	1.036688	-2.388412	0.000000
H	2.688629	-0.600838	0.000000
H	2.094993	1.818495	0.000000
H	-2.628068	-1.404535	0.000000

**6a**

Atom	Coordinates (Angstroms)		
	X	Y	Z
Si	1.313493	-0.360085	0.169944
C	-0.265793	-1.384836	-0.179836
C	0.764652	1.416428	-0.237054
C	-0.533138	1.350794	-0.019286
C	-1.613824	0.627671	0.236439
C	-1.486485	-0.801121	-0.174253
H	-2.401477	-1.379064	-0.348775
H	1.842124	-0.636934	1.546714
H	2.376770	-0.701606	-0.828549
H	-0.198911	-2.459151	-0.388741
H	-2.418321	0.935936	0.908590
H	1.218444	2.028397	-1.024520

**6b**

Atom	Coordinates (Angstroms)		
	X	Y	Z
Si	0.000000	1.411568	0.000000
C	1.417524	0.180078	0.000000
C	-1.537729	0.310954	0.000000
C	-1.278986	-1.012433	0.000000
C	-0.105034	-1.780132	0.000000
C	1.193275	-1.177515	0.000000
H	2.047501	-1.865565	0.000000
H	0.049069	2.312527	1.202732
H	0.049069	2.312527	-1.202732
H	2.457709	0.524047	0.000000
H	-0.174635	-2.871739	0.000000
H	-2.563017	0.700534	0.000000

**6c**

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Atom	Coordinates (Angstroms)		
	X	Y	Z
Si	0.000000	1.383889	0.000000
C	1.405101	0.182791	0.000000
C	-1.653143	0.266493	0.000000
C	-1.083625	-0.884604	0.000000
C	-0.096815	-1.810841	0.000000
C	1.199181	-1.174361	0.000000
H	2.055599	-1.859126	0.000000
H	-0.123641	2.289855	1.198180
H	-0.123641	2.289855	-1.198180
H	2.435314	0.550552	0.000000
H	-0.254066	-2.884821	0.000000
H	-2.613762	0.762364	0.000000

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**6d**

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Atom	Coordinates (Angstroms)		
	X	Y	Z
Si	0.000000	1.398983	0.000000
C	-1.443902	-1.156570	0.000000
C	-1.498556	0.243289	0.000000
C	1.475917	0.235533	0.000000
C	1.220996	-1.102094	0.000000
C	-0.114192	-1.689789	0.000000
H	2.055591	-1.815550	0.000000
H	0.071334	2.275109	1.216621
H	0.071334	2.275109	-1.216621
H	2.517315	0.576070	0.000000
H	-0.060278	-2.792389	0.000000
H	-2.496877	0.713668	0.000000

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**7a**

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Atom	Coordinates (Angstroms)		
	X	Y	Z
P	-1.382332	-0.320473	0.049974
C	0.144097	-1.336843	-0.107595
C	-0.690477	1.381052	-0.179198
C	0.617935	1.345369	0.006585
C	1.660748	0.540136	0.208797
C	1.412521	-0.852562	-0.186403
H	-1.673823	-0.563052	1.440283
H	-1.213146	2.055252	-0.862869
H	2.530604	0.794444	0.819735
H	2.252213	-1.529111	-0.379776
H	-0.029808	-2.413345	-0.220094

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**7b**

Atom	Coordinates (Angstroms)		
	X	Y	Z
P	1.408924	-0.233207	-0.097299
C	-0.782454	1.403788	0.029010
C	0.566094	1.395895	-0.016917
C	-1.740325	0.391159	0.029221
C	-1.320556	-0.968172	-0.028278
C	-0.001705	-1.360882	0.018906
H	1.185627	2.297389	-0.009221
H	-2.806298	0.626265	0.072823
H	-2.097095	-1.741239	-0.048583
H	0.238332	-2.428099	0.047791
H	2.019249	-0.426942	1.205027

**7c**

Atom	Coordinates (Angstroms)		
	X	Y	Z
P	1.363679	-0.162994	-0.100821
C	-0.864856	1.405905	0.052227
C	0.477000	1.456644	0.011186
C	-1.715659	0.293004	0.022742
C	-1.250838	-1.033200	-0.060502
C	0.097345	-1.360223	0.051640
H	1.116882	2.341070	0.035783
H	-2.800295	0.445279	0.065850
H	-1.985977	-1.845888	-0.083724
H	0.391200	-2.401460	0.206806
H	2.365045	-0.666877	0.823850

**8a**

Atom	Coordinates (Angstroms)		
	X	Y	Z
P	1.580208	-0.576530	0.072437
P	-1.662929	-0.526837	-0.161086
C	0.026117	1.521878	0.009036
C	1.268183	1.208168	-0.299185
C	-1.219600	1.221346	0.302659
C	-0.136285	-1.257613	-0.011408
H	1.856729	1.680574	-1.089093
H	-1.858795	1.752262	1.012481
H	-0.150804	-2.354888	-0.094847
H	1.763190	-0.690116	1.494594

**8b**

Atom	Coordinates (Angstroms)		
	X	Y	Z
P	-1.632753	-0.597520	-0.033753
P	1.565580	-0.551904	-0.110969
C	-0.061752	-1.289294	0.067649
C	-1.311307	1.158842	0.043012
C	-0.038493	1.690098	0.037041
C	1.235397	1.244997	-0.016067
H	2.102945	1.912124	-0.005435
H	-2.189779	1.811070	0.096296
H	-0.045036	-2.383608	0.152129
H	2.196400	-0.926084	1.138032

**8c**

Atom	Coordinates (Angstroms)		
	X	Y	Z
P	1.557997	-0.539513	-0.126558
P	-1.622745	-0.608894	-0.057888
C	-0.054387	1.650249	0.057242
C	1.220857	1.321394	0.005820
C	-1.326781	1.141099	0.052481
C	-0.035082	-1.271436	0.101791
H	2.110415	1.950537	0.027436
H	-2.213955	1.779454	0.115683
H	-0.013528	-2.337095	0.361012
H	2.260650	-1.214617	0.958553

**9a**

Atom	Coordinates (Angstroms)		
	X	Y	Z
S	1.368061	-0.237797	-0.164998
C	-0.000372	-1.307361	0.118495
C	-1.306878	-0.924684	0.202330
C	-1.661311	0.421224	-0.215824
C	-0.733966	1.380674	-0.003013
C	0.581814	1.304528	0.241247
H	-2.065350	-1.684130	0.413123
H	1.186948	2.017636	0.806637
H	-2.577905	0.585133	-0.792432
H	0.291614	-2.360161	0.153238

**9b**

Atom	Coordinates (Angstroms)		
	X	Y	Z
S	-1.404742	0.263680	0.000000
C	0.000000	1.333705	0.000000
C	1.309955	0.933658	0.000000
C	1.736922	-0.428040	0.000000
C	0.746182	-1.404350	0.000000
C	-0.598617	-1.344668	0.000000
H	-0.276587	2.389413	0.000000
H	2.072970	1.718781	0.000000
H	2.798650	-0.677132	0.000000
H	-1.285816	-2.191780	0.000000

**9c**

Atom	Coordinates (Angstroms)		
	X	Y	Z
S	-1.354605	0.328720	0.000000
C	-0.600550	-1.273751	0.000000
C	0.000000	1.358671	0.000000
C	1.300570	0.887454	0.000000
C	1.634711	-0.481762	0.000000
C	0.746750	-1.590808	0.000000
H	2.101022	1.634424	0.000000
H	-1.400592	-2.025060	0.000000
H	2.713848	-0.694018	0.000000
H	-0.229476	2.426311	0.000000