

*Supporting Information*

**Production of Carbon Monoxide and Hydrogen from Methanol using a  
Ruthenium Pincer Complex: A DFT Study**

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## 1. Computational details

### Distortion-interaction analysis

In distortion-interaction analysis, the transition state was divided into two fragments, followed by single point energy calculations on each fragment. The activation energy  $\Delta E^\ddagger$  was divided into  $\Delta E_{\text{dist}}^\ddagger$  and  $\Delta E_{\text{int}}^\ddagger$ , where  $\Delta E_{\text{dist}}^\ddagger$  and  $\Delta E_{\text{int}}^\ddagger$  are distortion energy and interaction energy, respectively. The distortion energy  $\Delta E_{\text{dist}}^\ddagger$  of each fragment is the energy difference between the distorted fragment and the corresponding optimized structure without the other fragment. The interaction energy  $\Delta E_{\text{int}}^\ddagger$  can be calculated using  $\Delta E_{\text{int}}^\ddagger = \Delta E^\ddagger - \Delta E_{\text{dist}}^\ddagger$ .

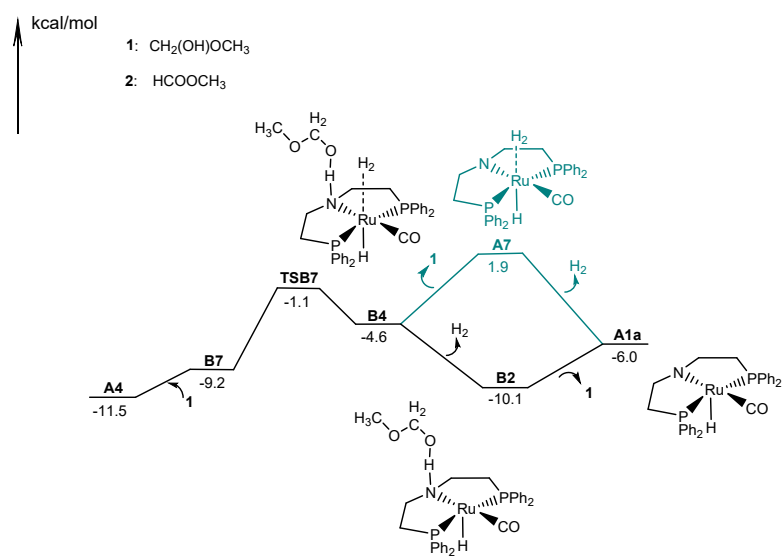
## 2. Test results of different functionals

**Table S1.** The relative Gibbs free energies (in kcal/mol) of key intermediates and transition states with different DFT functionals.

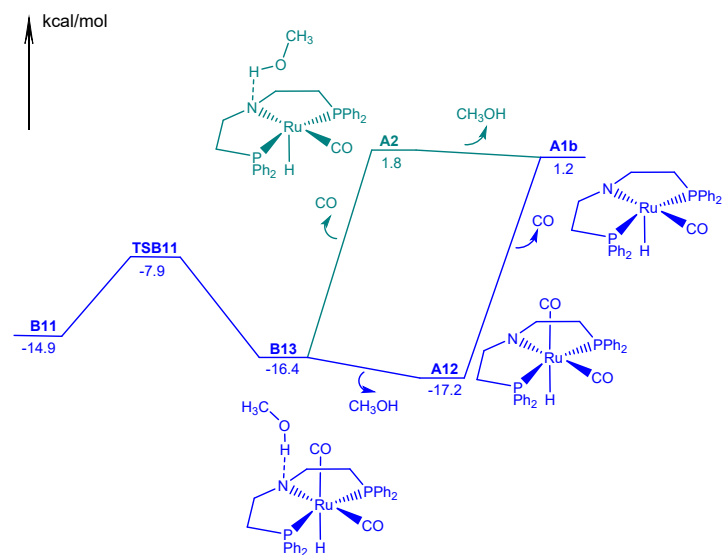
Complex	M06L	M06	B3LYP- D3(BJ)	$\omega$ B97X-D	M06-2X-D3
<b>A1</b>	0.0	0.0	0.0	0.0	0.0
<b>A4</b>	-11.5	-7.4	-5.9	-12.1	-8.6
<b>A1a</b>	-6.0	-3.5	-5.2	-2.8	-1.3
<b>TSB8</b>	14.4	15.9	16.3	13.6	11.1
<b>TSB9</b>	17.0	21.6	19.0	21.0	16.2

### 3. Other possible pathways

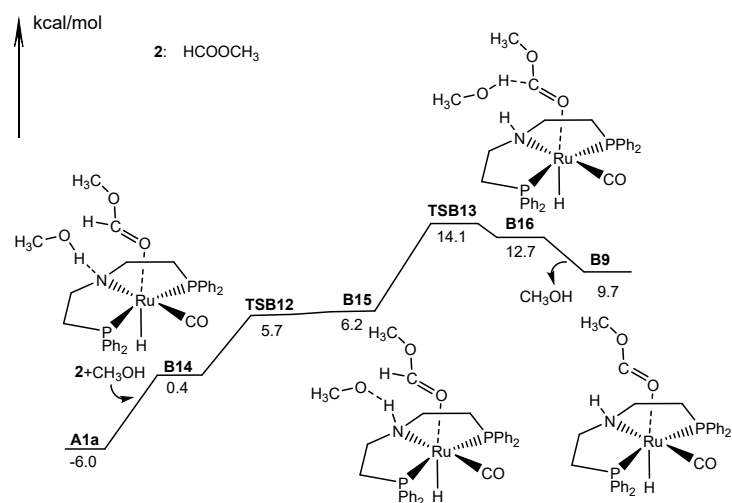
**Fig. S1** Other possible pathway for the transformation of **B4** → **A1a**.



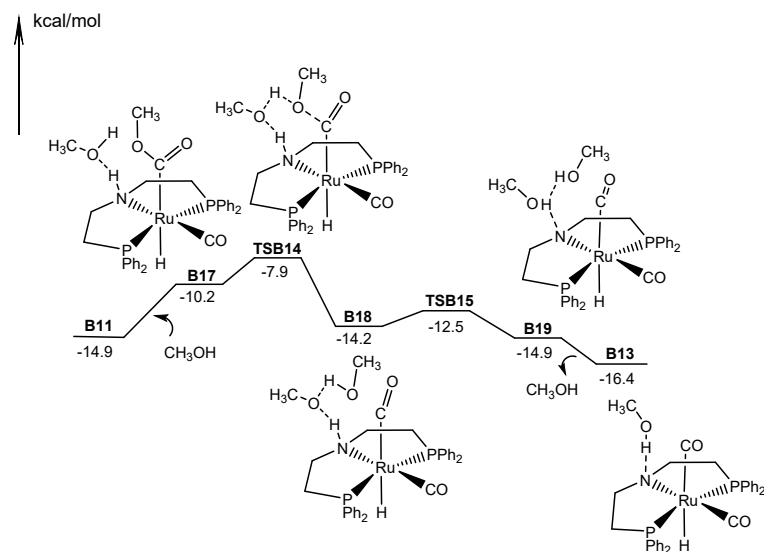
**Fig. S2** Other possible pathway for the transformation of **B13** → **A1b**.



**Fig. S3** The CH<sub>3</sub>OH acts at the co-catalyst for the transformation of **A1a** → **B9**.



**Fig. S4** The CH<sub>3</sub>OH acts at the co-catalyst for the transformation of **B11** → **B13**.



#### 4. IRC results of key transition states

Fig. S5 IRC result of TSA2.

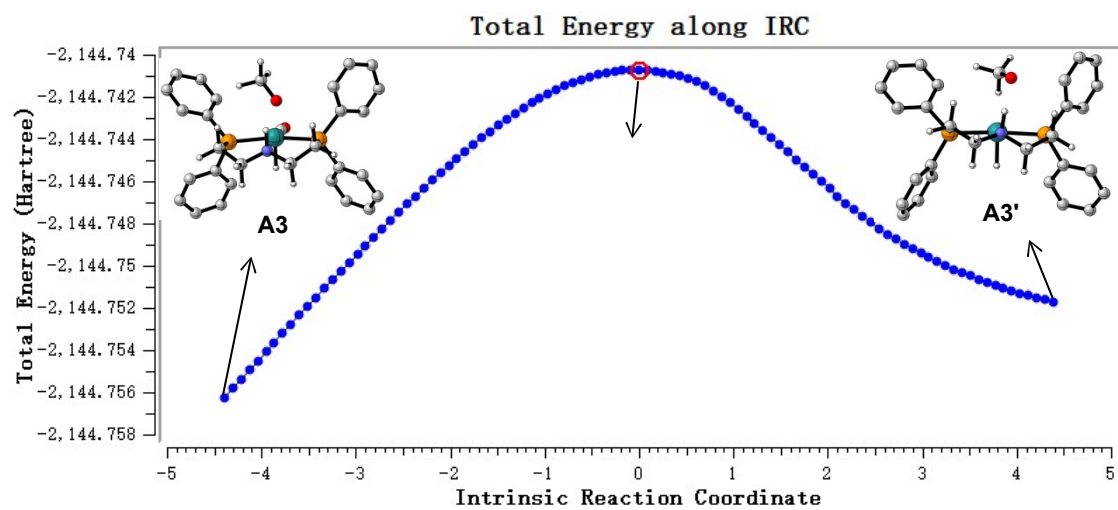
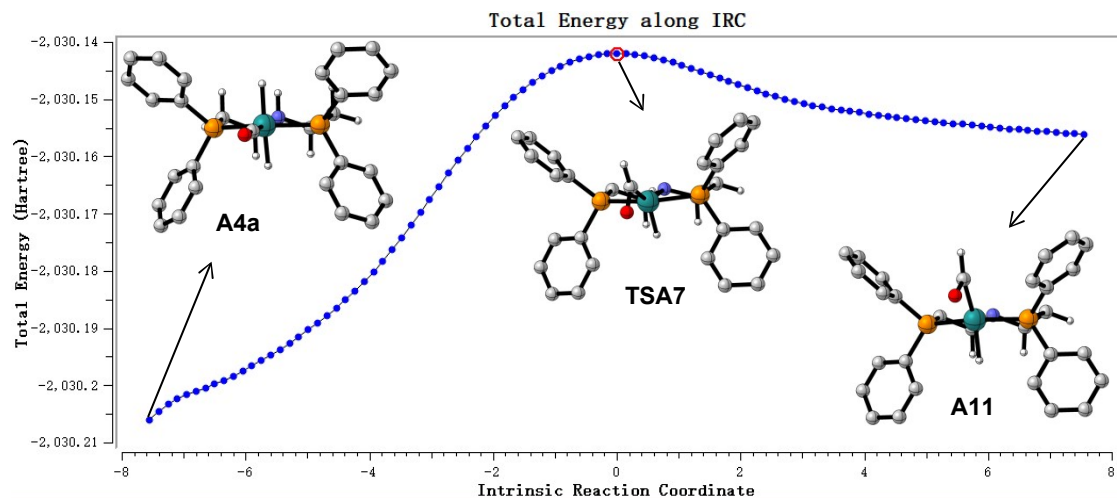
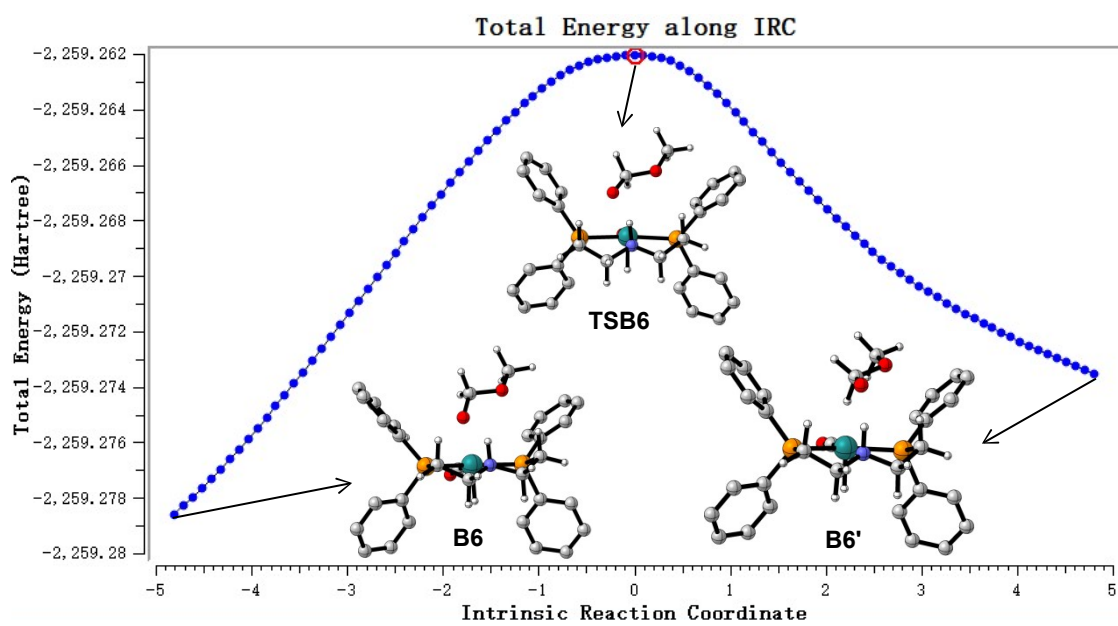


Fig. S6 IRC result of TSA7.





**Fig. S7** IRC results of TSB6.



## 5. Energies of all the structures

**Table S2.** The calculated absolute electronic energies ( $E$ , in a.u.), thermal free energies ( $G$ , in a.u.), and relative Gibbs energies ( $\Delta G$ , in kcal/mol) (Calculated at 298.15 K and 1 atm).

Complex	$E$	$G_{corr}$	$G$	$\Delta G$
<b>A1</b>	0.439306	-2030.493005	-2030.053699	0.0
<b>A2</b>	0.48869	-2146.254819	-2145.766129	0.6
<b>A3</b>	0.492676	-2146.266795	-2145.774119	-4.4
<b>A3'</b>	0.487841	-2146.250666	-2145.762825	2.7
<b>A4</b>	0.461194	-2031.696334	-2031.23514	8.5
<b>A5</b>	0.509413	-2147.456378	-2146.946965	9.5
<b>A6</b>	0.500252	-2147.432515	-2146.932263	18.7
<b>A7</b>	0.453534	-2031.6673	-2031.213766	21.9
<b>A8</b>	0.465967	-2145.028532	-2144.562565	20.0
<b>A9</b>	0.465428	-2145.003392	-2144.537964	35.4
<b>A10</b>	0.469041	-2145.051378	-2144.582337	7.6
<b>A11</b>	0.458587	-2031.614122	-2031.155535	62.2
<b>A12</b>	0.44369	-2143.866494	-2143.422804	-0.6
<b>TSA1</b>	0.484787	-2146.250182	-2145.765395	1.1
<b>TSA2</b>	0.488126	-2146.237112	-2145.748986	11.4
<b>TSA2'</b>	0.485692	-2146.237781	-2145.752089	9.4
<b>TSA3</b>	0.451122	-2031.651377	-2031.200255	30.4
<b>TSA4</b>	0.501149	-2147.421332	-2146.920183	26.3
<b>TSA5</b>	0.463788	-2144.998574	-2144.534786	37.4
<b>TSA6</b>	0.462882	-2144.985257	-2144.522375	45.2
<b>TSA7</b>	0.456465	-2031.59837	-2031.141905	70.8
<b>TSA8</b>	0.456719	-2145.017122	-2144.560403	21.4
<b>B1</b>	0.522497	-2260.818437	-2260.29594	-6.5
<b>B2</b>	0.523742	-2260.811672	-2260.28793	-1.5
<b>B3</b>	0.536737	-2261.990263	-2261.453526	17.0
<b>B4</b>	0.532638	-2261.984511	-2261.451873	18.0
<b>B5</b>	0.518244	-2260.798919	-2260.280675	05
<b>B6</b>	0.523588	-2260.819083	-2260.295495	-8.8
<b>B6'</b>	0.522191	-2260.810006	-2260.287815	-4.0
<b>B7</b>	0.541185	-2262.000454	-2261.459269	-9.2
<b>B8</b>	0.498936	-2259.605703	-2259.106767	1.3
<b>B9</b>	0.495623	-2259.588999	-2259.093376	9.7
<b>B10</b>	0.501732	-2259.614852	-2259.11312	-2.7
<b>B11</b>	0.502654	-2259.635229	-2259.132575	-14.9
<b>B12</b>	0.491885	-2146.219348	-2145.727463	26.1
<b>B13</b>	0.497288	-2259.632162	-2259.134874	-16.4
<b>B14</b>	0.550477	-2375.37201	-2374.821533	0.4

<b>B15</b>	0.551037	-2375.3634	-2374.812363	6.2
<b>B16</b>	0.547301	-2375.34931	-2374.802009	12.7
<b>B17</b>	0.552909	-2375.391396	-2374.838487	-10.2
<b>B18</b>	0.544135	-2375.389019	-2374.844884	-14.2
<b>B19</b>	0.54513	-2375.391043	-2374.845913	-14.9
<b>TSB1</b>	0.051724	-230.216243	-230.164519	42.3
<b>TSB2</b>	0.098969	-345.994047	-345.895078	31.5
<b>TSB3</b>	0.520535	-2260.810709	-2260.290174	-2.9
<b>TSB4</b>	0.53579	-2261.970208	-2261.434418	29.0
<b>TSB5</b>	0.516189	-2260.796336	-2260.280147	0.8
<b>TSB6</b>	0.522943	-2260.79253	-2260.269587	7.5
<b>TSB6'</b>	0.517583	-2260.807072	-2260.289489	-5.0
<b>TSB7</b>	0.531033	-2261.977349	-2261.446316	-1.1
<b>TSB8</b>	0.493709	-2259.579618	-2259.085909	14.4
<b>TSB9</b>	0.495977	-2259.577728	-2259.081751	17.0
<b>TSB10</b>	0.490174	-2146.215283	-2145.725109	27.6
<b>TSB11</b>	0.499062	-2259.620468	-2259.121406	-7.9
<b>TSB12</b>	0.547433	-2375.360528	-2374.813095	5.7
<b>TSB13</b>	0.548557	-2375.34836	-2374.799803	14.1
<b>TSB14</b>	0.547189	-2375.381994	-2374.834805	-7.9
<b>TSB15</b>	0.544961	-2375.387123	-2374.842162	-12.5
CH <sub>3</sub> OH	0.028782	-115.742197	-115.713415	/
HCHO	0.004972	-114.523453	-114.518481	/
H <sub>2</sub>	-0.00159	-1.17107	-1.17266	/
CO	-0.014114	-113.325645	-113.339759	/
<b>1</b>	0.057559	-230.285322	-230.227763	/
<b>2</b>	0.034252	-229.098943	-229.064691	/

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## 6. Imaginary frequencies of transition states

**Table S3.** Calculated imaginary frequencies of transition states at M06L level.

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<b>TSA1</b>	871.64 <i>i</i>
<b>TSA2</b>	279.21 <i>i</i>
<b>TSA2'</b>	-110.91 <i>i</i>
<b>TSA3</b>	1826.59 <i>i</i>
<b>TSA4</b>	1105.63 <i>i</i>
<b>TSA5</b>	1055.13 <i>i</i>
<b>TSA6</b>	329.94 <i>i</i>
<b>TSA7</b>	355.81 <i>i</i>
<b>TSA8</b>	912.82 <i>i</i>
<b>TSB1</b>	1700.04 <i>i</i>
<b>TSB2</b>	1329.75 <i>i</i>
<b>TSB3</b>	508.74 <i>i</i>
<b>TSB4</b>	1030.65 <i>i</i>
<b>TSB5</b>	848.91 <i>i</i>
<b>TSB6</b>	262.94 <i>i</i>
<b>TSB6'</b>	-458.15 <i>i</i>
<b>TSB7</b>	1009.71 <i>i</i>
<b>TSB8</b>	903.77 <i>i</i>
<b>TSB9</b>	165.47 <i>i</i>
<b>TSB10</b>	226.69 <i>i</i>
<b>TSB11</b>	112.21 <i>i</i>
<b>TSB12</b>	-1154.70 <i>i</i>
<b>TSB13</b>	-206.65 <i>i</i>
<b>TSB14</b>	-468.75 <i>i</i>
<b>TSB15</b>	-912.22 <i>i</i>

## 7. Cartesian coordinates of all the structures

**Table S4.** Atomic cartesian coordinates of intermediates and transition states at M06L (Lan12DZ & 6-31G(d)) level (presented in Å).

**A1**

-----			
	Coordinates (Angstroms)		
	X	Y	Z
-----			
N	0.03230200	-0.98115800	-1.07839200
C	2.47124200	-0.98861100	-1.15815100
H	2.55523900	-0.36648700	-2.05927200
H	3.37131600	-1.61289800	-1.07920700
C	-2.33991200	-0.72216000	-1.56930900
C	0.06229400	2.50892700	0.55410600
O	0.08817800	3.66659800	0.75326500
P	-2.27899600	0.43300000	-0.13711700
P	2.28438400	0.15968600	0.27406800
C	2.76825800	-0.89946400	1.69054400
C	4.06429100	-0.90959500	2.21811700
C	1.80977100	-1.77261500	2.22312600
C	4.39386600	-1.77272700	3.25997700
H	4.82054300	-0.23408000	1.81889500
C	2.14623900	-2.64474400	3.25360200
H	0.79156100	-1.74703800	1.82884800
C	3.43773800	-2.64335700	3.77692100
H	5.40272900	-1.76305800	3.66991000
H	1.39333900	-3.31968400	3.65735800
H	3.69720600	-3.31605000	4.59292400
C	3.65465300	1.35225600	0.13082100
C	4.68102300	1.19374800	-0.80691000
C	3.67920200	2.46483100	0.98342600
C	5.70809000	2.12997300	-0.89619600
H	4.68573500	0.33191300	-1.47213800
C	4.71161300	3.39299100	0.89949100
H	2.88391500	2.59987800	1.71676500
C	5.72530200	3.23001800	-0.04353800
H	6.49754400	1.99634500	-1.63387900
H	4.71994500	4.25238900	1.56760700
H	6.52718300	3.96302400	-0.11426700
C	-3.14721800	-0.41150600	1.23007000
C	-3.07866500	0.16594400	2.50635200
C	-3.85488700	-1.60770900	1.06847500
C	-3.71451400	-0.43121600	3.58837400
H	-2.51173800	1.08702100	2.64597500

C	-4.48026800	-2.21268100	2.15745600
H	-3.92236400	-2.08019800	0.08984100
C	-4.41449500	-1.62505100	3.41671700
H	-3.65547300	0.03148300	4.57202400
H	-5.02126000	-3.14718600	2.01656900
H	-4.90446300	-2.09834000	4.26595700
C	-3.40171000	1.79667200	-0.60691800
C	-2.86711100	2.86661200	-1.33526200
C	-4.76658500	1.79656900	-0.29714300
C	-3.68416700	3.90996100	-1.75833800
H	-1.79992600	2.87722800	-1.56268100
C	-5.58107000	2.84525600	-0.71602200
H	-5.19309800	0.97467900	0.27805800
C	-5.04237900	3.90116100	-1.44772400
H	-3.25595600	4.73778300	-2.32094400
H	-6.64087900	2.83829800	-0.46672300
H	-5.68039300	4.72261600	-1.76971000
H	-3.31162400	-1.21816500	-1.69249700
H	-2.18640500	-0.08967700	-2.45394100
Ru	0.01764400	0.69146900	0.13094500
H	-0.12750700	0.51315300	1.71512800
C	1.20495200	-1.82309200	-1.23744700
H	1.24182800	-2.62560900	-0.47151600
H	1.17009800	-2.34572200	-2.21147900
C	-1.18095100	-1.69496200	-1.43875200
H	-1.03769700	-2.22873000	-2.39685500
H	-1.42954300	-2.47950000	-0.69347300

A2

Coordinates (Angstroms)

	X	Y	Z
C	3.21252400	1.42224300	-0.92271100
H	3.25175000	0.56712900	-1.61531800
H	3.74247500	2.26949700	-1.38429300
H	3.74015600	1.13842000	-0.00639400
O	1.88978900	1.78072300	-0.57472000
H	1.29760300	1.76406300	-1.39300100
N	-0.25631700	1.08757900	-1.97150200
C	0.86567500	-0.75758200	-3.10551600
H	1.78971200	-0.18444100	-3.27042400
H	0.79423900	-1.50631000	-3.90489800
C	-1.29810800	2.96341800	-0.81773100
C	0.49770400	-0.60331400	1.61990500
O	0.66710500	-1.10732000	2.66834700

P	-1.19448200	1.93291000	0.71014400
P	0.99891500	-1.51093800	-1.42490800
C	0.10574500	-3.11023600	-1.53103900
C	-0.69667800	-3.53128800	-0.46583600
C	0.26220800	-3.95484500	-2.63733400
C	-1.33764800	-4.76731100	-0.51057400
H	-0.81815300	-2.87856800	0.39830600
C	-0.38564300	-5.18473200	-2.68585500
H	0.90250400	-3.65518400	-3.46772700
C	-1.18796000	-5.59280700	-1.62144300
H	-1.95909600	-5.08276900	0.32575100
H	-0.26128000	-5.82833000	-3.55520400
H	-1.69377600	-6.55614100	-1.65840500
C	2.74009400	-2.06945500	-1.31000000
C	3.51795200	-2.34516000	-2.44162500
C	3.31327600	-2.21550700	-0.04092300
C	4.84203000	-2.75425500	-2.30516100
H	3.09196200	-2.23413100	-3.43895700
C	4.63446900	-2.63136900	0.09429300
H	2.71915500	-1.98670600	0.84478500
C	5.40191400	-2.89858700	-1.03764700
H	5.43805300	-2.96036400	-3.19279700
H	5.06827200	-2.73794600	1.08701700
H	6.43821100	-3.21501800	-0.93255400
C	-2.92115000	1.56102000	1.18037800
C	-3.21168300	0.33462700	1.78946300
C	-3.95548600	2.48873700	1.00128300
C	-4.50636500	0.04176700	2.20901500
H	-2.41214800	-0.39326200	1.92684700
C	-5.25210900	2.19120700	1.41139300
H	-3.74885800	3.45865900	0.54947200
C	-5.52917400	0.96744800	2.01700700
H	-4.71676400	-0.91509800	2.68357900
H	-6.04734700	2.91924100	1.26004700
H	-6.54332900	0.73534200	2.33780500
C	-0.62974500	3.09408600	2.00804600
C	0.69126000	3.55967400	1.92624100
C	-1.43001900	3.50375200	3.08038200
C	1.18705200	4.43780200	2.88372300
H	1.32732700	3.21617400	1.10926300
C	-0.92505300	4.37708600	4.04169900
H	-2.45232700	3.13965500	3.17075000
C	0.38044300	4.84942700	3.94390900
H	2.21276900	4.79552200	2.80741200

H	-1.55810800	4.68705700	4.87170200
H	0.77240700	5.53180500	4.69634300
H	-2.13201800	3.67629200	-0.79621600
H	-0.37046300	3.55218300	-0.85424300
Ru	0.12321000	0.15087200	-0.04354000
H	-1.22920600	-0.69713800	-0.08421600
C	-0.32772500	0.18412000	-3.10384200
H	-1.26492800	-0.41263200	-3.09959900
H	-0.34023400	0.75232100	-4.05483200
C	-1.36497000	2.02414700	-2.00970800
H	-1.33957500	2.61806400	-2.94473400
H	-2.34783800	1.50437700	-2.01291000

### TSA1

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
C	3.08391200	1.57700300	-1.00795700
H	3.20979000	0.72221600	-1.69876700
H	3.57712300	2.44959200	-1.47216700
H	3.63961500	1.32964600	-0.09115900
O	1.74876300	1.85384900	-0.70386800
H	0.98876600	1.68248800	-1.58339300
N	-0.19495300	1.15646700	-2.00261100
C	0.96730000	-0.68024100	-3.11315200
H	1.89638100	-0.11314200	-3.26717500
H	0.90626400	-1.42900800	-3.91299600
C	-1.18899000	3.04365000	-0.82920800
C	0.53864000	-0.52472300	1.61485600
O	0.72505100	-0.99986600	2.67311000
P	-1.13128100	2.00514900	0.69751300
P	1.08094400	-1.44288400	-1.42986500
C	0.21756700	-3.05634600	-1.56994700
C	-0.59491200	-3.49990000	-0.52159800
C	0.40104500	-3.88689200	-2.68283900
C	-1.21985600	-4.74299800	-0.58937400
H	-0.73779100	-2.85808200	0.34719600
C	-0.23072600	-5.12407800	-2.75445300
H	1.04949300	-3.57170800	-3.50100200
C	-1.04396700	-5.55384000	-1.70709500
H	-1.84972900	-5.07526100	0.23401800
H	-0.08517800	-5.75600700	-3.62906900
H	-1.53784600	-6.52244400	-1.76293500
C	2.83238700	-1.96116700	-1.29728100
C	3.60307100	-2.29329600	-2.41877600



C	3.41896400	-2.02283700	-0.02814100
C	4.93292600	-2.67772300	-2.27179600
H	3.16657900	-2.24592000	-3.41671000
C	4.74689600	-2.41380300	0.11813600
H	2.83015800	-1.74793900	0.84754100
C	5.50650200	-2.73899100	-1.00336400
H	5.52380400	-2.92780600	-3.15150600
H	5.19163300	-2.45439100	1.11084400
H	6.54756500	-3.03646900	-0.89017900
C	-2.86750000	1.68847700	1.16628500
C	-3.19040900	0.47453900	1.78423100
C	-3.87624100	2.64210400	0.97795500
C	-4.49275100	0.21942700	2.20421500
H	-2.41028500	-0.27323100	1.92747500
C	-5.18084800	2.38163700	1.38825900
H	-3.64328700	3.60296200	0.51932000
C	-5.49049300	1.17028000	2.00306900
H	-4.72915600	-0.72779800	2.68572400
H	-5.95666000	3.12896700	1.23035000
H	-6.51089200	0.96752600	2.32390500
C	-0.51785100	3.13936900	1.99460100
C	0.82550400	3.53748600	1.91531500
C	-1.30199000	3.58685800	3.06339400
C	1.35995200	4.38899200	2.87607300
H	1.43962400	3.16430700	1.09314100
C	-0.75723700	4.43315100	4.02720100
H	-2.34161300	3.27397300	3.14951700
C	0.57084700	4.83900000	3.93401600
H	2.40231300	4.69593200	2.80403500
H	-1.37674900	4.77402300	4.85530400
H	0.99355200	5.50014000	4.68885500
H	-1.99683700	3.78545900	-0.81100500
H	-0.23884000	3.59512900	-0.84885200
Ru	0.15953000	0.20152800	-0.04929100
H	-1.18607600	-0.67749200	-0.06261100
C	-0.22437100	0.26296100	-3.14852500
H	-1.16310200	-0.32210900	-3.16031700
H	-0.20714300	0.83874900	-4.09283900
C	-1.27761500	2.12909300	-2.03998800
H	-1.22369200	2.73425800	-2.96443600
H	-2.26103900	1.62137000	-2.05951500

A3

Coordinates (Angstroms)

	<b>X</b>	<b>Y</b>	<b>Z</b>
C	2.91106900	1.38703500	-0.24877900
H	3.42263100	0.59967000	-0.84846000
H	3.49103900	2.31932100	-0.42787600
H	3.09258000	1.11817400	0.81602800
O	1.58393800	1.56968200	-0.55728900
H	0.44546400	1.45102600	-2.04054900
N	-0.46135000	0.95057500	-2.04976000
C	0.77540100	-0.85341400	-3.09618900
H	1.65310100	-0.20870000	-3.24825800
H	0.77813400	-1.61380700	-3.88726200
C	-1.33145400	2.87503200	-0.86040600
C	0.43667700	-0.63464200	1.60068000
O	0.67992100	-1.07502100	2.66257900
P	-1.22473600	1.89851400	0.70551600
P	0.94057200	-1.59631100	-1.40453600
C	0.12882600	-3.23559000	-1.58471800
C	-0.93879100	-3.60615300	-0.76339000
C	0.58303000	-4.13799200	-2.55681700
C	-1.54868900	-4.85000700	-0.91940700
H	-1.29027400	-2.90662400	-0.00559300
C	-0.02832300	-5.37607500	-2.71490900
H	1.43143700	-3.87344200	-3.19010400
C	-1.09875400	-5.73352100	-1.89582000
H	-2.38086900	-5.12662300	-0.27403300
H	0.33372600	-6.06658500	-3.47501100
H	-1.57760600	-6.70373300	-2.01797400
C	2.70698900	-2.05470200	-1.29521400
C	3.53150700	-2.18968000	-2.41874600
C	3.25766100	-2.25378100	-0.02279500
C	4.87876500	-2.50989600	-2.27158000
H	3.12538400	-2.03613600	-3.41846800
C	4.60130600	-2.58123900	0.12209500
H	2.63155800	-2.12939200	0.86104400
C	5.41582800	-2.70456300	-1.00178700
H	5.51100600	-2.60324800	-3.15319500
H	5.01711400	-2.72637200	1.11750800
H	6.47063200	-2.94897400	-0.88757200
C	-2.95067500	1.64080400	1.24535700
C	-3.28027100	0.45754200	1.91643000
C	-3.93865100	2.61816900	1.07018300
C	-4.56873000	0.25810900	2.40459800
H	-2.51615900	-0.30879400	2.04724400
C	-5.23033200	2.41185800	1.54573800

H	-3.69874900	3.55823400	0.57349000
C	-5.54632400	1.23223200	2.21613900
H	-4.81032100	-0.66387600	2.93078400
H	-5.98988500	3.17781500	1.39838000
H	-6.55536500	1.07348900	2.59314200
C	-0.55699900	3.08099600	1.92671000
C	0.75133200	3.55013800	1.73137800
C	-1.26886500	3.48361800	3.06220800
C	1.31914400	4.42896200	2.64767500
H	1.30628100	3.18591500	0.86386600
C	-0.68980500	4.35934900	3.97785500
H	-2.27788600	3.11408300	3.23887000
C	0.60063900	4.83767000	3.77075100
H	2.33441200	4.79000400	2.48840800
H	-1.25267400	4.66592800	4.85813600
H	1.04966000	5.52335600	4.48772200
H	-2.09166400	3.66454800	-0.82675200
H	-0.35127200	3.36208300	-0.96245000
Ru	0.01339500	0.05587500	-0.05078800
H	-1.37949200	-0.81262900	-0.03744600
C	-0.48637200	-0.00887500	-3.15870600
H	-1.38575300	-0.63118900	-3.05605500
H	-0.55232300	0.51331200	-4.12754000
C	-1.54969300	1.93502400	-2.03416100
H	-1.57820900	2.49946400	-2.98083900
H	-2.50266400	1.39531200	-1.94189500

**TSA2**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
C	2.79465000	1.67597900	-0.49798100
H	3.19737500	0.88600900	-1.18805200
H	3.70580900	2.23262200	-0.15994200
H	2.50070900	1.10724100	0.43982300
O	1.82565800	2.46309100	-1.03046000
H	0.74875400	1.66790300	-1.88723600
N	-0.13933800	1.07150100	-2.00775500
C	1.18523100	-0.68647800	-3.05161700
H	2.07486300	-0.04400700	-3.12193000
H	1.23422800	-1.41227200	-3.87323000
C	-1.20659200	2.94538500	-0.87188800
C	0.42519600	-0.69833800	1.62319100
O	0.46090700	-1.26651400	2.64837100
P	-1.00388200	1.99385800	0.69992600

P	1.24040700	-1.48945600	-1.38658200
C	0.36102700	-3.08184200	-1.60783900
C	-0.59810400	-3.48529300	-0.67344400
C	0.65229500	-3.92466300	-2.68872100
C	-1.26177900	-4.70108600	-0.82278400
H	-0.82333800	-2.83801200	0.17357600
C	-0.01563100	-5.13467800	-2.84121600
H	1.41475800	-3.63944500	-3.41453300
C	-0.97635700	-5.52357300	-1.90871000
H	-2.00614700	-5.00379700	-0.08855200
H	0.21633300	-5.77711000	-3.68892400
H	-1.49899300	-6.47086400	-2.02930700
C	2.98431600	-1.98939100	-1.18249600
C	3.81099600	-2.28181500	-2.27470300
C	3.50704300	-2.08635600	0.11258400
C	5.13240100	-2.66932400	-2.07266800
H	3.42583500	-2.20018600	-3.29126000
C	4.82697500	-2.47894200	0.31235400
H	2.87627000	-1.84004200	0.96700300
C	5.64115800	-2.77055000	-0.77953700
H	5.76754400	-2.88955300	-2.92893600
H	5.22220100	-2.54744500	1.32407500
H	6.67593700	-3.07034800	-0.62373700
C	-2.71189100	1.69378400	1.27970900
C	-3.09548700	0.42528200	1.72687100
C	-3.65227400	2.73385500	1.30464500
C	-4.39331000	0.19683200	2.17934300
H	-2.36805700	-0.38573700	1.71692300
C	-4.94881400	2.50453600	1.75229500
H	-3.36356600	3.73562100	0.98540200
C	-5.32163000	1.23391000	2.18874300
H	-4.67838400	-0.79558500	2.52386000
H	-5.67032300	3.31974400	1.76303700
H	-6.33730500	1.05455700	2.53723900
C	-0.31732800	3.18316400	1.90197900
C	0.89445300	3.81520000	1.58097200
C	-0.91242300	3.41454800	3.14790600
C	1.47645900	4.68891700	2.49435500
H	1.36994100	3.58718100	0.61618800
C	-0.31574900	4.28601900	4.05593500
H	-1.84421400	2.91700000	3.41363800
C	0.87590100	4.92810800	3.72978400
H	2.41384900	5.18234700	2.24094000
H	-0.78735600	4.46160300	5.02158000

H	1.33967600	5.60944400	4.44159100
H	-2.08006800	3.60801500	-0.83796300
H	-0.30536000	3.56099700	-0.97504600
Ru	0.24682500	0.14184600	-0.01647900
H	-1.12560500	-0.62127200	-0.20129800
C	-0.07167800	0.16092100	-3.14974100
H	-0.96892700	-0.47745900	-3.14858900
H	-0.07538100	0.72582700	-4.09682700
C	-1.29724600	1.97095200	-2.03365800
H	-1.32878800	2.52403900	-2.98754400
H	-2.21785500	1.36991500	-1.97419500

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**A3'**

<b>Coordinates (Angstroms)</b>			
	<b>X</b>	<b>Y</b>	<b>Z</b>
C	2.35792500	1.85528800	-0.55119100
H	3.15018700	1.15326500	-0.92473500
H	2.76550900	2.34661600	0.36823600
H	1.60930400	1.08798600	-0.01900600
O	1.79344300	2.64240100	-1.43656800
H	0.55703000	1.70471900	-1.92499700
N	-0.25256100	1.00949400	-1.98218000
C	1.22821600	-0.66715500	-2.94184400
H	2.08339400	0.01019400	-2.80646300
H	1.46444300	-1.30555700	-3.80238000
C	-1.53953500	2.75974400	-0.89897700
C	0.17659400	-0.85273100	1.61531800
O	0.27634000	-1.40148700	2.64647700
P	-1.28610200	1.82724300	0.68365800
P	1.06113800	-1.60006300	-1.35711500
C	0.16422100	-3.13913700	-1.76148900
C	-0.27014900	-3.93463900	-0.69154700
C	-0.11495200	-3.55393400	-3.06780600
C	-0.95035500	-5.12383700	-0.92476800
H	-0.07847100	-3.61105000	0.33225400
C	-0.80826100	-4.74101700	-3.29981100
H	0.20263100	-2.95243900	-3.91825800
C	-1.22262500	-5.52937500	-2.23090400
H	-1.27675600	-5.73286600	-0.08370100
H	-1.02290700	-5.04794600	-4.32208400
H	-1.76319800	-6.45640600	-2.41344700
C	2.75304800	-2.17331600	-0.97674200
C	3.36871700	-3.18642200	-1.72310100
C	3.45869500	-1.56528000	0.06771900

C	4.67293200	-3.57498900	-1.43535000
H	2.81974100	-3.67869600	-2.52694500
C	4.76426300	-1.95695100	0.35389300
H	2.97533800	-0.78407900	0.65667300
C	5.37171100	-2.95945100	-0.39737400
H	5.14492000	-4.36336400	-2.01925100
H	5.30472100	-1.47935300	1.16893900
H	6.39117200	-3.26709300	-0.17097500
C	-2.96238300	1.55532500	1.35666600
C	-3.34934000	0.28291900	1.78728500
C	-3.86811500	2.61974100	1.47209900
C	-4.62138700	0.07488800	2.31686000
H	-2.64674700	-0.54521600	1.69962400
C	-5.13924300	2.40924300	1.99490800
H	-3.57121900	3.62272200	1.16314200
C	-5.51752700	1.13504600	2.41757000
H	-4.91144400	-0.92020100	2.64923000
H	-5.83631000	3.24153500	2.07638300
H	-6.51262100	0.97162800	2.82783800
C	-0.55764700	3.07032100	1.80761500
C	0.53470300	3.83050400	1.36114200
C	-0.99576700	3.21156700	3.13016800
C	1.15050200	4.73400000	2.22229400
H	0.91407400	3.70440800	0.34203500
C	-0.36872700	4.11300200	3.98643000
H	-1.83349100	2.61799300	3.49450000
C	0.70147600	4.88013000	3.53348100
H	1.99301800	5.32379000	1.86425700
H	-0.72125000	4.21538600	5.01145600
H	1.18947800	5.58607900	4.20356300
H	-2.47383600	3.33351500	-0.88164400
H	-0.70707900	3.46937700	-0.98984500
Ru	-0.01712800	-0.01254100	-0.02353800
H	-1.40451000	-0.81369000	-0.25553800
C	-0.03208400	0.15170300	-3.15840900
H	-0.91032300	-0.49727500	-3.28869300
H	0.06062900	0.77021200	-4.06565700
C	-1.49234400	1.79963800	-2.07138000
H	-1.51809200	2.36099700	-3.01997800
H	-2.34932200	1.11260000	-2.06706900

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**TSA2'**

-----  
**Coordinates (Angstroms)**

**X**

**Y**

**Z**  
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C	0.51729700	5.88670500	-5.04524000
H	-0.72321100	4.86965900	-4.11513000
H	1.24010900	5.09386700	-4.76151700
H	0.33886900	6.64586200	-4.25434400
O	0.19198400	6.07978800	-6.21994000
H	-1.60321700	5.61488500	-6.34358400
N	-2.47119400	5.06435300	-6.26293000
C	-1.23433800	3.18955000	-7.19560700
H	-0.33310800	3.81632500	-7.25154900
H	-1.18062900	2.43781800	-7.99312300
C	-3.50296100	6.98308400	-5.18013400
C	-2.18787600	3.27016900	-2.59874500
O	-2.14939600	2.73421000	-1.55314700
P	-3.35719200	6.04627700	-3.58741800
P	-1.26603700	2.43017700	-5.50954300
C	-2.06323300	0.79645600	-5.75523200
C	-1.54994700	-0.12290000	-6.68011600
C	-3.18583900	0.44783400	-5.00025200
C	-2.15967000	-1.35946700	-6.85807500
H	-0.65924300	0.12769800	-7.25888300
C	-3.79147100	-0.79538200	-5.17307600
H	-3.58305500	1.16728800	-4.28436400
C	-3.28302500	-1.69714000	-6.10334700
H	-1.75535100	-2.06479900	-7.58230500
H	-4.66506400	-1.05771200	-4.57867700
H	-3.75823600	-2.66725400	-6.23996400
C	0.47286600	1.96818500	-5.18910000
C	1.43717800	1.86206400	-6.19822500
C	0.84936000	1.71446000	-3.86384600
C	2.74905800	1.51063700	-5.88644200
H	1.17222100	2.06192700	-7.23618200
C	2.15628800	1.35419900	-3.55560000
H	0.11150200	1.81644300	-3.06775900
C	3.11016600	1.25369600	-4.56693100
H	3.49118200	1.43814700	-6.67993100
H	2.43295900	1.16069200	-2.52064300
H	4.13607000	0.98144000	-4.32512200
C	-5.06565100	5.99225200	-2.92121400
C	-5.59053200	4.77620600	-2.47475200
C	-5.84640500	7.15089700	-2.81460600
C	-6.87259400	4.71862000	-1.93294500
H	-4.98652000	3.87373100	-2.56759400
C	-7.13034700	7.09091700	-2.28443800
H	-5.44572900	8.11143300	-3.14191000

C	-7.64469300	5.87310600	-1.84073000
H	-7.26940800	3.76631800	-1.58547700
H	-7.73066500	7.99662400	-2.21430200
H	-8.64902800	5.82667800	-1.42269700
C	-2.53670100	7.23765800	-2.46585800
C	-1.77894700	6.73856800	-1.39983900
C	-2.63854400	8.62445300	-2.63297400
C	-1.14930600	7.60663300	-0.51330600
H	-1.67108100	5.66071200	-1.27724400
C	-2.00028400	9.49222100	-1.75061900
H	-3.21428700	9.03581300	-3.46248600
C	-1.25760000	8.98458800	-0.68772500
H	-0.56316700	7.20431900	0.31120800
H	-2.08188600	10.56815300	-1.89662500
H	-0.75814100	9.66346000	0.00147100
H	-4.35032000	7.68038900	-5.18089400
H	-2.58479100	7.57845000	-5.29104600
Ru	-2.28721400	4.09148100	-4.24301200
H	-3.80716200	3.42740000	-4.57853900
C	-2.45547900	4.07497100	-7.35698200
H	-3.38496800	3.49365500	-7.29682400
H	-2.43642900	4.58509300	-8.33371900
C	-3.60870000	5.99779100	-6.32908900
H	-3.61591600	6.52874000	-7.29491100
H	-4.53138200	5.40736000	-6.26106700

A4

-----			
<b>Coordinates (Angstroms)</b>			
	<b>X</b>	<b>Y</b>	<b>Z</b>
-----			
N	-0.13068700	-1.10870900	-1.27073400
C	2.29787700	-1.25496400	-1.12007100
H	2.41295300	-0.62679100	-2.01458200
H	3.16712400	-1.92304700	-1.09437400
C	-2.53531300	-0.71468400	-1.37264600
C	0.03714500	1.74985400	1.67656300
O	0.09804200	2.58946200	2.49783100
P	-2.33544000	0.43231400	0.07031000
P	2.21342100	-0.09943900	0.32748500
C	2.92198900	-1.04008000	1.73395700
C	2.52251100	-0.66944700	3.02423200
C	3.85228800	-2.07616800	1.59124500
C	3.05520800	-1.30281600	4.14153500
H	1.77252800	0.11233900	3.14373800
C	4.37468200	-2.72153800	2.70994600



H	4.17944800	-2.39313100	0.60123100
C	3.98113700	-2.33267800	3.98709600
H	2.73611500	-0.99922200	5.13714800
H	5.09208400	-3.53054200	2.58054100
H	4.39114700	-2.83583500	4.86140200
C	3.52798200	1.13023200	-0.02103800
C	4.87906900	0.76825700	-0.10081800
C	3.17084600	2.46998900	-0.20153700
C	5.85160200	1.72678000	-0.36499500
H	5.17606000	-0.26869200	0.05982400
C	4.14740900	3.43043700	-0.45717700
H	2.11798100	2.74715100	-0.14509300
C	5.48657100	3.06091400	-0.54111300
H	6.89865300	1.43388400	-0.42551600
H	3.85834700	4.47203800	-0.58831900
H	6.24977700	3.81249400	-0.73673300
C	-3.39325700	-0.27117300	1.39524600
C	-3.03219000	-0.00731100	2.72232000
C	-4.55444900	-1.01344800	1.15051200
C	-3.82306600	-0.45438200	3.77551900
H	-2.10969900	0.53822500	2.92194900
C	-5.33870600	-1.47450300	2.20521300
H	-4.85883000	-1.24244800	0.12956600
C	-4.97783000	-1.19068000	3.51940500
H	-3.52978000	-0.23599300	4.80091300
H	-6.23445100	-2.05765200	1.99673000
H	-5.59251200	-1.54884600	4.34370800
C	-3.28326100	1.92268700	-0.42150700
C	-2.64295800	3.16535600	-0.42766200
C	-4.63786400	1.85263400	-0.77293300
C	-3.34542500	4.31740500	-0.77565500
H	-1.58667800	3.21582300	-0.16296000
C	-5.33542900	3.00174000	-1.12846400
H	-5.15790500	0.89417200	-0.75784100
C	-4.68984800	4.23741300	-1.12748900
H	-2.83800500	5.28082600	-0.77053500
H	-6.38736800	2.93499100	-1.40190700
H	-5.23883600	5.13806600	-1.39783800
H	-3.52742600	-1.17904400	-1.42687400
H	-2.42367400	-0.10367300	-2.27944600
Ru	-0.03947600	0.45677200	0.37555400
H	-0.24752900	-0.85706600	1.45965900
C	1.00443200	-2.04491500	-1.20214900
H	0.86224300	-2.65901400	-0.30301300

H	1.00782500	-2.71751100	-2.07562800
C	-1.44578100	-1.77006700	-1.31723700
H	-1.51027100	-2.44940700	-2.18312500
H	-1.53429900	-2.37377100	-0.40445000
H	-0.02793000	-0.55080200	-2.11951000
H	0.16442200	1.60222100	-0.90075500

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**TSA3**

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**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	-0.12646200	-1.09175200	-1.18693800
C	2.30497900	-1.16610500	-1.18843300
H	2.36214400	-0.48290600	-2.04681500
H	3.19907200	-1.80081000	-1.22899600
C	-2.54489600	-0.79938400	-1.25573700
C	0.12906100	1.90463400	1.58506900
O	0.24261300	2.77187400	2.36835200
P	-2.33778000	0.40590000	0.13136200
P	2.24289300	-0.08364200	0.30406400
C	2.91456200	-1.05761500	1.69676300
C	2.72184100	-0.54880900	2.98871700
C	3.61306900	-2.25927800	1.54190000
C	3.23410500	-1.21489900	4.09568600
H	2.15548900	0.37371300	3.12178000
C	4.11464100	-2.93369600	2.65419200
H	3.76816700	-2.68402800	0.55104600
C	3.93062600	-2.41148500	3.93071800
H	3.08016400	-0.80429900	5.09201400
H	4.65045900	-3.87171900	2.51853700
H	4.32433000	-2.93834800	4.79820700
C	3.53837600	1.17223900	0.00619600
C	4.90045900	0.86390900	0.11592500
C	3.15786400	2.46636300	-0.36615200
C	5.86330900	1.83203500	-0.14961800
H	5.20818200	-0.13699000	0.42076800
C	4.12415400	3.43365800	-0.63213500
H	2.09721600	2.70860800	-0.44387800
C	5.47602600	3.11795100	-0.52425100
H	6.91961900	1.58352100	-0.06059900
H	3.81818500	4.43853000	-0.91787500
H	6.23087100	3.87619100	-0.72591800
C	-3.37194000	-0.23437800	1.50219100
C	-2.87290000	-0.23244000	2.80798200
C	-4.68035800	-0.68005400	1.27423700

C	-3.66427000	-0.67683200	3.86508200
H	-1.85525100	0.11425200	2.98655000
C	-5.46677000	-1.13116700	2.32872700
H	-5.09341900	-0.66677600	0.26476700
C	-4.95830600	-1.13104100	3.62698300
H	-3.26425300	-0.67115000	4.87747000
H	-6.48012600	-1.48064500	2.13804600
H	-5.57437700	-1.48300400	4.45272700
C	-3.28657600	1.87039800	-0.41821800
C	-2.92870500	3.13099700	0.07281500
C	-4.37424300	1.76768400	-1.29465800
C	-3.64930700	4.26350800	-0.29494800
H	-2.07497900	3.22205200	0.74456900
C	-5.08949100	2.90213200	-1.66810100
H	-4.66627100	0.79548800	-1.69197800
C	-4.72922000	4.15134400	-1.16765200
H	-3.35962300	5.23785000	0.09451900
H	-5.92978300	2.80960700	-2.35429200
H	-5.28892400	5.03784400	-1.46076500
H	-3.51186900	-1.31653500	-1.21950100
H	-2.51190600	-0.21691100	-2.18657500
Ru	-0.01388300	0.49738000	0.38510300
H	-0.14103400	-0.48658700	1.67215400
C	1.01633800	-1.97191200	-1.25132800
H	0.99908900	-2.70546400	-0.41646300
H	1.00058700	-2.56791500	-2.18435700
C	-1.38984400	-1.78836600	-1.22663900
H	-1.45016000	-2.44059600	-2.11942300
H	-1.49973300	-2.45737500	-0.34668200
H	-0.00363500	0.27997700	-1.59972300
H	0.08849900	1.23774500	-1.44274300

A5

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	0.08800200	-1.12549500	-1.34313900
C	2.52480700	-1.16404000	-1.22002400
H	2.59271800	-0.46189800	-2.06320800
H	3.42638600	-1.78832900	-1.25252100
C	-2.32434600	-0.85447900	-1.40734600
C	0.19835300	1.63433900	1.71072500
O	0.24350900	2.41458500	2.58828400
P	-2.15090300	0.36977400	-0.02218900
P	2.40007800	-0.13982900	0.31579600

C	3.03360600	-1.22462800	1.65192500
C	2.53362600	-1.02207600	2.94433000
C	3.98186600	-2.23473200	1.44898100
C	2.98000400	-1.79859700	4.00797900
H	1.76963400	-0.26107300	3.10325500
C	4.41816200	-3.02284400	2.51178800
H	4.38512700	-2.42112800	0.45377900
C	3.92066200	-2.80410900	3.79329600
H	2.58025500	-1.62772800	5.00605900
H	5.14815800	-3.81136400	2.33544000
H	4.25966400	-3.42196900	4.62322200
C	3.72286900	1.11365600	0.12513800
C	5.07595200	0.75629500	0.05775500
C	3.37201000	2.46487500	0.03997900
C	6.05577300	1.73009700	-0.10349900
H	5.37004000	-0.29027900	0.14095700
C	4.35557900	3.43948200	-0.11455800
H	2.31875300	2.74211800	0.08505600
C	5.69654000	3.07443100	-0.18817100
H	7.10370700	1.43949900	-0.15735900
H	4.07017400	4.48834200	-0.17508100
H	6.46473000	3.83650900	-0.30879200
C	-3.24407900	-0.25733100	1.31185600
C	-2.88719200	0.01380300	2.63827000
C	-4.42897200	-0.96136300	1.06620800
C	-3.70131400	-0.39382400	3.69024300
H	-1.95108200	0.53330500	2.84083500
C	-5.23682000	-1.38226800	2.11940000
H	-4.73198700	-1.19438300	0.04587500
C	-4.87699700	-1.09498600	3.43340100
H	-3.40935300	-0.17171900	4.71518300
H	-6.15014400	-1.93717600	1.91023500
H	-5.50913800	-1.42304500	4.25692300
C	-3.07080200	1.82464400	-0.65492400
C	-2.43888000	3.07143300	-0.68415900
C	-4.37800100	1.71265900	-1.14748600
C	-3.09856700	4.18404700	-1.20225700
H	-1.41574600	3.15379700	-0.31577700
C	-5.03231700	2.82171700	-1.67269800
H	-4.89063900	0.75057400	-1.12200100
C	-4.39204100	4.05989400	-1.70175100
H	-2.59585100	5.14980100	-1.21998700
H	-6.04490500	2.72057200	-2.06040100
H	-4.90479400	4.92832200	-2.11258300

H	-3.29750400	-1.35979900	-1.41436500
H	-2.24986000	-0.28471100	-2.34424700
Ru	0.14571900	0.41476300	0.33747500
H	-0.10730200	-0.91486500	1.37040200
C	1.26806900	-2.00612600	-1.33980800
H	1.17193500	-2.68387500	-0.48038000
H	1.29145000	-2.62287900	-2.25277000
C	-1.18925800	-1.85774000	-1.33678100
H	-1.23811000	-2.55863400	-2.18661300
H	-1.23271700	-2.44270200	-0.40866500
H	0.10390400	-0.56208700	-2.20168800
H	0.42871100	1.66339400	-0.84129000
C	-1.11525600	1.83926100	-3.89173100
H	-1.20348700	1.50869200	-4.93262500
H	-2.09270800	1.68525200	-3.40141900
H	-0.90866200	2.92093400	-3.89409900
O	-0.07149000	1.09969100	-3.30094400
H	0.07676800	1.45451300	-2.38870500

**TSA4**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
N	-0.01366900	-1.07954500	-1.34918600
C	2.38540800	-1.44545600	-1.08407700
H	2.61296000	-0.87825300	-1.99593200
H	3.18838300	-2.17865300	-0.93519200
C	-2.40090200	-0.61062900	-1.59926100
C	0.15093300	1.64507900	1.67825300
O	0.22123200	2.38362200	2.58454600
P	-2.26347100	0.37773000	-0.04987500
P	2.30329800	-0.21026900	0.28115600
C	2.90845900	-1.05740600	1.77982000
C	3.27757900	-0.28178200	2.88690000
C	2.93609300	-2.45119200	1.88987800
C	3.67728700	-0.88845600	4.07195900
H	3.25587800	0.80650900	2.81715200
C	3.33554300	-3.05704800	3.07904900
H	2.63996900	-3.07437300	1.04677700
C	3.70751900	-2.27855600	4.17115400
H	3.96519600	-0.27312600	4.92252700
H	3.35514400	-4.14335200	3.14969300
H	4.01968400	-2.75334900	5.09975400
C	3.62586900	1.00115500	-0.05960800
C	4.96398700	0.60399500	-0.18620100

C	3.30130100	2.35535300	-0.17866400
C	5.95424300	1.54777000	-0.43550100
H	5.23249500	-0.44783900	-0.08035400
C	4.29560800	3.29991800	-0.42258200
H	2.26110600	2.66567600	-0.07709900
C	5.62072900	2.89706300	-0.55316600
H	6.99130600	1.23120200	-0.53453900
H	4.03145000	4.35234400	-0.50994400
H	6.39878100	3.63460400	-0.74263500
C	-3.25231700	-0.50782500	1.20957000
C	-2.94485100	-0.28508700	2.55832600
C	-4.30583000	-1.37283500	0.89241900
C	-3.68093700	-0.90175100	3.56403200
H	-2.10919700	0.36547700	2.81652000
C	-5.03500900	-1.99957800	1.90052300
H	-4.56245900	-1.57208400	-0.14738600
C	-4.72663700	-1.76252700	3.23707300
H	-3.42904100	-0.71712200	4.60679900
H	-5.84694800	-2.67574500	1.63758800
H	-5.29591900	-2.25395900	4.02410200
C	-3.24630400	1.88192600	-0.39042500
C	-2.62236900	3.13314000	-0.38427100
C	-4.61337600	1.80144000	-0.68593200
C	-3.35092200	4.28416400	-0.67634600
H	-1.55915400	3.19894700	-0.15040900
C	-5.33811200	2.95052200	-0.98091400
H	-5.11649600	0.83370100	-0.67864800
C	-4.70692600	4.19366400	-0.97693400
H	-2.85572800	5.25362400	-0.66776400
H	-6.39947500	2.87741900	-1.21247400
H	-5.27596900	5.09298800	-1.20625200
H	-3.40048200	-1.03423200	-1.75830200
H	-2.22106900	0.09249100	-2.42450700
Ru	0.05439300	0.42895200	0.27124600
H	-0.17261300	-0.75495000	1.33769900
C	1.02327800	-2.10680100	-1.23292900
H	0.80750600	-2.76293400	-0.37179100
H	1.02319800	-2.74827300	-2.13250200
C	-1.32592700	-1.68308100	-1.57862500
H	-1.32917600	-2.23783000	-2.53412400
H	-1.54557700	-2.42024700	-0.78528700
H	0.33636000	-0.32530900	-2.27411900
H	0.21042500	1.91641700	-1.03373000
C	-0.10644700	1.06354800	-3.89336700

H	0.34833700	1.62929500	-4.72784600
H	-0.74045000	0.27951900	-4.36357500
H	-0.81526000	1.77282700	-3.39827800
O	0.85185800	0.55832600	-3.04250300
H	0.54397500	1.45217900	-1.62445500

**A6**

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<b>Coordinates (Angstroms)</b>			
	<b>X</b>	<b>Y</b>	<b>Z</b>
-----			
N	-0.00793600	-1.02521900	-1.36058000
C	2.40402400	-1.35227600	-1.15354200
H	2.61784000	-0.75425400	-2.04900000
H	3.22433000	-2.07268300	-1.03736900
C	-2.41164300	-0.66557400	-1.56756500
C	0.17391700	1.76103400	1.58579700
O	0.24846300	2.49771600	2.49497600
P	-2.25883500	0.38094400	-0.06159000
P	2.31019100	-0.16481100	0.24774200
C	2.85651900	-1.07636300	1.73258800
C	3.12502900	-0.34969800	2.90077500
C	2.95444100	-2.47098200	1.76561900
C	3.49101100	-1.00401900	4.07121400
H	3.04862100	0.73836000	2.89053200
C	3.31795200	-3.12508400	2.94127300
H	2.74033500	-3.05829800	0.87379400
C	3.58828200	-2.39484000	4.09451900
H	3.69983300	-0.42598000	4.96979500
H	3.39022600	-4.21138400	2.95192300
H	3.87163700	-2.90743100	5.01208200
C	3.66960600	1.02900500	-0.00543400
C	5.00728100	0.60952100	-0.01462500
C	3.37847500	2.38336300	-0.19198500
C	6.02959500	1.52980900	-0.21776500
H	5.24832700	-0.44174700	0.14704200
C	4.40425300	3.30498900	-0.39119200
H	2.33957000	2.71387600	-0.17303200
C	5.72888600	2.87875500	-0.40609700
H	7.06561800	1.19536700	-0.22590100
H	4.16570900	4.35772400	-0.53157800
H	6.53125200	3.59827300	-0.56006900
C	-3.20030400	-0.46930300	1.25701600
C	-2.84762600	-0.21452700	2.58853700
C	-4.26670100	-1.33753600	0.99581800
C	-3.55142500	-0.80455000	3.63310700

H	-2.00336200	0.44093000	2.80177000
C	-4.96382900	-1.93670000	2.04243500
H	-4.55707200	-1.56178600	-0.02991200
C	-4.60983200	-1.66925600	3.36205100
H	-3.26419000	-0.59614200	4.66210800
H	-5.78467400	-2.61746400	1.82309300
H	-5.15423300	-2.13966000	4.17899400
C	-3.27433800	1.85854700	-0.43082900
C	-2.68868600	3.12767300	-0.39712300
C	-4.62717500	1.74167300	-0.77655500
C	-3.43738600	4.26015100	-0.71073800
H	-1.63849500	3.22323100	-0.11792500
C	-5.37289800	2.87171800	-1.09380200
H	-5.10184400	0.75987600	-0.79220900
C	-4.77796500	4.13272700	-1.06256900
H	-2.97049500	5.24291700	-0.67917100
H	-6.42231600	2.76961400	-1.36504100
H	-5.36354000	5.01667500	-1.30919700
H	-3.39950600	-1.13002100	-1.67919300
H	-2.27624000	0.01309400	-2.42108600
Ru	0.06617900	0.50023300	0.20258700
H	-0.13863900	-0.65501100	1.29463900
C	1.04501400	-2.02402200	-1.29129400
H	0.88841300	-2.73377200	-0.44966700
H	1.04275700	-2.64265800	-2.21055700
C	-1.28825800	-1.68704000	-1.53170100
H	-1.29512300	-2.26921400	-2.47464000
H	-1.48974000	-2.42340300	-0.72223000
H	0.51313000	-0.05003500	-2.72943100
H	-0.05053200	1.96116200	-1.16293600
C	-0.21870900	1.16320300	-4.04638000
H	0.13903800	1.81488400	-4.85393500
H	-0.93213900	0.44587000	-4.49573300
H	-0.79727300	1.80189200	-3.34526100
O	0.87967900	0.54511600	-3.45346900
H	0.64074000	1.64240500	-1.38492100

A7

Coordinates (Angstroms)

	X	Y	Z
N	-0.13045600	-1.06611300	-1.22238700
C	2.28901500	-1.28394000	-1.18582500
H	2.38873700	-0.65361300	-2.07990600
H	3.15358800	-1.95967700	-1.16448000



C	-2.53177700	-0.75699800	-1.42248800
C	0.06069500	1.87381300	1.52197900
O	0.10034900	2.64757900	2.40750600
P	-2.34595100	0.39615400	-0.00320300
P	2.21941900	-0.12452600	0.23712100
C	2.79909100	-1.04658700	1.70627100
C	2.55594600	-0.47692600	2.96394600
C	3.47311600	-2.27021100	1.63940700
C	2.99059400	-1.10761900	4.12351800
H	2.01053000	0.46540800	3.02940300
C	3.89602600	-2.90866300	2.80406800
H	3.66567800	-2.74221000	0.67695200
C	3.66004300	-2.32791900	4.04635500
H	2.79722000	-0.64990100	5.09217400
H	4.41069600	-3.86586900	2.73629400
H	3.99090200	-2.82842200	4.95490900
C	3.57096200	1.07700300	-0.04749100
C	4.90241800	0.66450000	-0.18862800
C	3.26881000	2.43959900	-0.13192800
C	5.90674100	1.59782000	-0.42169300
H	5.15443300	-0.39379000	-0.10811300
C	4.27599800	3.37447500	-0.36106600
H	2.23472700	2.76539700	-0.00793600
C	5.59409900	2.95447200	-0.50857700
H	6.93830300	1.26694300	-0.53159800
H	4.02861100	4.43299500	-0.41997300
H	6.38257100	3.68396300	-0.68571700
C	-3.28332500	-0.33138300	1.39049100
C	-2.92007400	0.04029800	2.69134100
C	-4.36115000	-1.20664700	1.21540400
C	-3.62669700	-0.43988000	3.78870100
H	-2.06928600	0.70586400	2.83843100
C	-5.06101400	-1.69622300	2.31556800
H	-4.65983900	-1.51915400	0.21531700
C	-4.69759400	-1.31140300	3.60316700
H	-3.33317900	-0.13952400	4.79311100
H	-5.89123400	-2.38434300	2.16404600
H	-5.24543200	-1.69492600	4.46237400
C	-3.34692100	1.86361600	-0.44547500
C	-2.75799200	3.13141700	-0.41981800
C	-4.69365400	1.74591300	-0.81381500
C	-3.49914300	4.26186300	-0.75729500
H	-1.71127900	3.22543200	-0.12538300
C	-5.43153400	2.87368400	-1.15530900

H	-5.17001800	0.76466200	-0.82739900
C	-4.83497700	4.13386900	-1.12647900
H	-3.03087100	5.24435200	-0.72871300
H	-6.47695300	2.77120200	-1.44219800
H	-5.41507500	5.01635500	-1.39069200
H	-3.51819500	-1.23518000	-1.47362500
H	-2.41328200	-0.14512000	-2.32693600
Ru	-0.02327000	0.51977500	0.22955500
H	-0.19757100	-0.53879300	1.40183200
C	0.95766500	-2.01813400	-1.22929300
H	0.91027300	-2.74200600	-0.38161900
H	0.91788000	-2.64034600	-2.14610100
C	-1.39331200	-1.76074900	-1.33247100
H	-1.40236300	-2.39875800	-2.23924000
H	-1.58542100	-2.45650300	-0.48203800
H	-0.12758300	1.98330800	-1.52231300
H	0.62522800	1.87618600	-1.41707600

A8

Coordinates (Angstroms)

	X	Y	Z
C	2.58732400	1.99406600	-1.19190900
H	1.99038700	1.94944100	-2.12711600
H	3.55267000	2.53855600	-1.19357500
O	2.17433400	1.48230300	-0.16835400
N	-0.23955300	1.17844900	-2.10351500
C	0.79362700	-0.67730900	-3.28322500
H	1.70991700	-0.11254200	-3.50494700
H	0.67689100	-1.44817600	-4.05618900
C	-1.15990500	3.11560700	-0.95550200
C	0.36401700	-0.62254800	1.44836900
O	0.44237300	-1.18429800	2.47949600
P	-1.11423000	2.05990100	0.55004100
P	0.99724800	-1.41044400	-1.59966600
C	0.22640700	-3.06967800	-1.71618900
C	-0.81867200	-3.43110000	-0.86185000
C	0.67943700	-3.99428700	-2.66710300
C	-1.40798300	-4.69015300	-0.96512500
H	-1.16955400	-2.71532300	-0.11872000
C	0.09086000	-5.24908900	-2.76976900
H	1.50718300	-3.73195100	-3.32787600
C	-0.95693200	-5.59813800	-1.91858600
H	-2.22416600	-4.95958100	-0.29677000
H	0.45168600	-5.95836600	-3.51293800

H	-1.41911000	-6.58070700	-1.99907600
C	2.78266100	-1.80671300	-1.48716100
C	3.59580900	-1.96964200	-2.61612600
C	3.35655700	-1.94478400	-0.21683500
C	4.94914000	-2.26878900	-2.47716500
H	3.17141200	-1.86411000	-3.61472600
C	4.70698000	-2.24893100	-0.07896500
H	2.73741900	-1.79976300	0.66924000
C	5.50636300	-2.41009200	-1.20884800
H	5.56923200	-2.39129400	-3.36394400
H	5.13826700	-2.35333100	0.91509700
H	6.56476700	-2.64165400	-1.10079800
C	-2.85734400	1.77495700	1.03084800
C	-3.13911000	0.65702600	1.82718100
C	-3.90882900	2.62235800	0.66438300
C	-4.43620100	0.40208900	2.25827700
H	-2.32963800	-0.02091700	2.09974300
C	-5.21023500	2.35931700	1.08588500
H	-3.72111600	3.49406600	0.03850500
C	-5.47604600	1.25161700	1.88579500
H	-4.63787100	-0.46933100	2.87890700
H	-6.01942100	3.02274900	0.78437900
H	-6.49378900	1.04687200	2.21389700
C	-0.49939500	3.17276600	1.86754400
C	0.65397200	2.83248600	2.58092200
C	-1.15780600	4.37297800	2.16472300
C	1.14179200	3.68050700	3.57356800
H	1.16712900	1.89834100	2.34934500
C	-0.66809800	5.21979200	3.15222400
H	-2.06593100	4.64268100	1.62387300
C	0.48302600	4.87316700	3.85892600
H	2.03851700	3.40558000	4.12646800
H	-1.18717100	6.15073000	3.37553300
H	0.86488800	5.53503400	4.63472300
H	-1.94405700	3.88356200	-0.93377400
H	-0.19433600	3.64073400	-0.98645100
Ru	0.09772400	0.21808100	-0.19923600
H	-1.30474100	-0.53595900	-0.33272300
C	-0.38614900	0.28087100	-3.22965800
H	-1.33569500	-0.29996100	-3.20034000
H	-0.42285800	0.85438900	-4.17830600
C	-1.28139500	2.18349000	-2.14874300
H	-1.20837300	2.77423000	-3.08465700
H	-2.30602400	1.74389800	-2.16106400

## TSA5

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	Coordinates (Angstroms)		
	X	Y	Z
-----			
C	2.13720600	2.13552400	-1.43786900
H	0.83165900	1.77894400	-2.12963600
H	3.09513100	2.74035700	-1.50109500
O	2.06593500	1.51522200	-0.36015600
N	-0.24311100	1.18966100	-2.12447600
C	0.90107200	-0.64340000	-3.24476900
H	1.82007000	-0.06112200	-3.39972900
H	0.84666600	-1.39617500	-4.04155300
C	-1.20895700	3.08874500	-0.94860400
C	0.35509400	-0.60764900	1.46076000
O	0.48134300	-1.13599000	2.50297300
P	-1.14359900	2.04176700	0.56863700
P	1.02778900	-1.41462700	-1.56639900
C	0.22642100	-3.05348500	-1.75454300
C	-0.81149700	-3.43755200	-0.90110000
C	0.65271500	-3.94274000	-2.75022000
C	-1.41904300	-4.68345500	-1.04841800
H	-1.14188100	-2.74859400	-0.12399000
C	0.04427000	-5.18348200	-2.89851600
H	1.47593700	-3.66616400	-3.41061900
C	-0.99558600	-5.55507800	-2.04735500
H	-2.22836200	-4.97122500	-0.37934600
H	0.38366200	-5.86389900	-3.67795100
H	-1.47299800	-6.52675500	-2.16309500
C	2.80251100	-1.83692000	-1.42617100
C	3.60177200	-2.08922800	-2.54842300
C	3.37894500	-1.91463200	-0.15313200
C	4.94465600	-2.42391400	-2.39984900
H	3.17581600	-2.01854800	-3.54935800
C	4.72083000	-2.25243700	-0.00537600
H	2.77236900	-1.69231900	0.72498900
C	5.50482000	-2.50946900	-1.12757500
H	5.55443200	-2.61711700	-3.28093800
H	5.15729900	-2.30698800	0.99031700
H	6.55591700	-2.76870100	-1.01158600
C	-2.88041200	1.75822300	1.06993000
C	-3.15364700	0.64181500	1.87154500
C	-3.93714400	2.60199900	0.70905600
C	-4.44650800	0.38598000	2.31416100
H	-2.34165700	-0.03491100	2.13897800
C	-5.23455400	2.33774700	1.14216600

H	-3.75734900	3.47405800	0.08118900
C	-5.49153200	1.23156400	1.94681900
H	-4.64111200	-0.48426000	2.93857700
H	-6.04735900	2.99893800	0.84568300
H	-6.50608000	1.02513100	2.28339300
C	-0.50590000	3.17943400	1.84967400
C	0.74092800	2.92699200	2.43075900
C	-1.22566600	4.31732800	2.23501900
C	1.26089500	3.80471100	3.38043500
H	1.30226300	2.04332000	2.12577700
C	-0.70334000	5.19300800	3.17994100
H	-2.20598500	4.51375000	1.79919300
C	0.54138700	4.93678100	3.75359000
H	2.23173600	3.60191100	3.82928800
H	-1.26962500	6.07578900	3.47229500
H	0.94883000	5.62156700	4.49551400
H	-2.00366600	3.84511900	-0.92588700
H	-0.25589400	3.63653100	-0.97788500
Ru	0.07791300	0.20599300	-0.18187000
H	-1.33258800	-0.56767500	-0.30477900
C	-0.29982700	0.28682700	-3.27495000
H	-1.24012100	-0.28832600	-3.25797500
H	-0.29709800	0.86710700	-4.21513200
C	-1.31701700	2.18507200	-2.16429200
H	-1.24309800	2.78662200	-3.08806700
H	-2.29835000	1.68195500	-2.19077800

A9

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Coordinates (Angstroms)			
	X	Y	Z
-----			
C	2.13531200	2.19157700	-1.15369900
H	0.60031500	1.67604600	-2.02145800
H	3.11344800	2.77517100	-1.03233800
O	1.99552300	1.44520100	-0.15453500
N	-0.28393700	1.06892700	-2.01538200
C	1.05066000	-0.66825900	-3.05853900
H	1.92588600	-0.00181200	-3.05025200
H	1.17371500	-1.34534200	-3.91265100
C	-1.35539400	2.89343700	-0.83013000
C	0.42090700	-0.71300400	1.58123700
O	0.61581300	-1.23506900	2.61500800
P	-1.22431200	1.86600300	0.69895600
P	1.06120400	-1.53046100	-1.42425000
C	0.15148100	-3.09781500	-1.67576100

C	-0.45379500	-3.69144200	-0.56025700
C	0.05568400	-3.74033000	-2.91597800
C	-1.12398800	-4.90431000	-0.67943900
H	-0.40654900	-3.18536200	0.40400600
C	-0.62598800	-4.94930300	-3.03692900
H	0.51162800	-3.30030400	-3.80222200
C	-1.21317900	-5.53507200	-1.91882700
H	-1.58627100	-5.35362800	0.19759800
H	-0.69782500	-5.43331100	-4.00954300
H	-1.74564600	-6.47975500	-2.01431800
C	2.79771500	-2.06135600	-1.20935100
C	3.37510800	-3.05994100	-2.00394700
C	3.57278800	-1.43070400	-0.22951300
C	4.70806500	-3.41504700	-1.82671400
H	2.77521400	-3.57234200	-2.75677000
C	4.90761500	-1.78913900	-0.05465300
H	3.12418800	-0.65096300	0.38550900
C	5.47574000	-2.77913800	-0.85171600
H	5.14849900	-4.19368200	-2.44735100
H	5.50304000	-1.29367400	0.71010000
H	6.51808500	-3.06078600	-0.71148900
C	-2.94293800	1.50014100	1.20850200
C	-3.16182500	0.36510200	2.00034400
C	-4.03685600	2.30258500	0.86331000
C	-4.43975700	0.05034800	2.44940900
H	-2.31944600	-0.27990800	2.25151300
C	-5.31886900	1.97903600	1.30269400
H	-3.89881300	3.18730800	0.24252500
C	-5.52220000	0.85514800	2.09838700
H	-4.59264900	-0.83384700	3.06560800
H	-6.16096500	2.60812800	1.01880900
H	-6.52456500	0.60259300	2.43979200
C	-0.62453200	3.02707100	1.97674400
C	0.64278600	2.81615100	2.53078100
C	-1.38751200	4.12113600	2.40477300
C	1.14125500	3.69109000	3.49347200
H	1.23751700	1.96752700	2.19349900
C	-0.88638300	4.99397200	3.36441200
H	-2.38446700	4.28429900	1.99380400
C	0.37905700	4.77909400	3.90969100
H	2.12785900	3.51942000	3.92006600
H	-1.48632900	5.84158000	3.69163800
H	0.76808900	5.46126700	4.66379700
H	-2.18054600	3.61565900	-0.80415100

H	-0.42275900	3.47462600	-0.88250000
Ru	0.08670900	0.08593700	-0.04916700
H	-1.28895900	-0.76834100	-0.16349800
C	-0.21356200	0.16684200	-3.17355300
H	-1.11227700	-0.46670000	-3.18780700
H	-0.20375900	0.74914500	-4.11004800
C	-1.43942100	1.97743200	-2.03983100
H	-1.43732500	2.57132300	-2.96923800
H	-2.36375800	1.38193100	-2.02976300

**TSA6**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
C	1.76220500	1.85674100	-0.35593900
H	0.37284000	1.51457900	-1.96540600
H	2.10963000	2.92370500	-0.02117300
O	2.20332300	0.97885100	0.42384000
N	-0.49114100	0.93496700	-2.06225600
C	0.89294100	-0.77443200	-3.10768900
H	1.75231300	-0.09454300	-3.19166300
H	0.96070700	-1.50277900	-3.92625900
C	-1.62361700	2.74254000	-0.88097800
C	0.09256100	-0.92680800	1.56433300
O	0.14452000	-1.52668800	2.57252400
P	-1.31906400	1.79741700	0.68381600
P	1.01136000	-1.57004100	-1.44052600
C	0.24848100	-3.22055300	-1.67444100
C	-0.70321400	-3.68453100	-0.76100800
C	0.62211800	-4.04620100	-2.74324600
C	-1.27442400	-4.94590300	-0.91596500
H	-0.99599100	-3.04670700	0.07240300
C	0.04691200	-5.30216800	-2.90165100
H	1.37636000	-3.70802300	-3.45492400
C	-0.90385500	-5.75377600	-1.98703700
H	-2.01271200	-5.29603300	-0.19670500
H	0.34311200	-5.93221300	-3.73868500
H	-1.35275300	-6.73794700	-2.11007100
C	2.78649300	-1.93954300	-1.24971900
C	3.62117200	-2.20320200	-2.34288100
C	3.32363400	-1.96922200	0.04193700
C	4.96641500	-2.50153700	-2.14532600
H	3.22377600	-2.17083800	-3.35779100
C	4.66701800	-2.27425200	0.23749700
H	2.68656700	-1.72596700	0.89113700

C	5.48949000	-2.54058400	-0.85464800
H	5.60788300	-2.70103800	-3.00214300
H	5.07504700	-2.29007100	1.24638500
H	6.54243300	-2.77096200	-0.70115700
C	-2.98802300	1.52712700	1.38800200
C	-3.38193500	0.24402900	1.77920100
C	-3.87844800	2.59503000	1.56273900
C	-4.64446100	0.03081100	2.32873800
H	-2.69137900	-0.58827900	1.64644200
C	-5.13987300	2.38094000	2.10685100
H	-3.58034800	3.60481500	1.27744700
C	-5.52485100	1.09666200	2.49037500
H	-4.93908800	-0.97282000	2.63025300
H	-5.82405900	3.21801400	2.23505400
H	-6.51200200	0.92976600	2.91797600
C	-0.55357000	3.02726400	1.79329600
C	0.35365300	2.57523700	2.75855900
C	-0.81429400	4.39971600	1.69191800
C	0.97867900	3.47744700	3.61366800
H	0.58859700	1.51266600	2.81762100
C	-0.18531400	5.30066100	2.54616900
H	-1.50759400	4.77221500	0.93731400
C	0.71092200	4.84015500	3.50829300
H	1.68842400	3.11454100	4.35462000
H	-0.39161500	6.36588800	2.45596000
H	1.20798400	5.54643000	4.17105000
H	-2.53719200	3.34855800	-0.82763600
H	-0.77267400	3.42676000	-1.00477400
Ru	-0.05314500	-0.02225200	-0.03211700
H	-1.43805600	-0.77734900	-0.31527100
C	-0.40073300	0.01720200	-3.19826400
H	-1.27115700	-0.65462100	-3.16558500
H	-0.44701500	0.56677100	-4.15308800
C	-1.68543800	1.78231900	-2.05705400
H	-1.77303300	2.34440100	-3.00182700
H	-2.56681600	1.12879300	-1.98227500

**A10**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
C	2.98293900	2.15974500	-0.68448100
H	3.15283300	2.73448200	-1.68396200
H	1.66156700	2.73015600	-2.84857800
O	3.90033800	2.24758100	0.11287800



N	0.79674400	2.19339700	-2.69817700
C	1.85713200	0.27210600	-3.77656600
H	2.78486300	0.83162400	-3.96699300
H	1.76419000	-0.48588400	-4.56474000
C	-0.18251100	4.04271200	-1.43036000
C	1.39938800	0.34812000	0.91868100
O	1.57807400	-0.15616600	1.96335600
P	-0.08844400	2.98740500	0.08368300
P	2.01546300	-0.49511800	-2.09249400
C	1.20323500	-2.13168500	-2.25398700
C	0.13192900	-2.47340000	-1.42454100
C	1.65886200	-3.06104800	-3.19910600
C	-0.47815100	-3.72087400	-1.54485100
H	-0.22564300	-1.74463700	-0.69716200
C	1.04503600	-4.30203100	-3.32195000
H	2.50802200	-2.81730300	-3.83894800
C	-0.02612600	-4.63376600	-2.49332300
H	-1.31225700	-3.97712200	-0.89373900
H	1.40663300	-5.01471400	-4.06143400
H	-0.50534800	-5.60697200	-2.58727700
C	3.78896800	-0.92689300	-1.99066300
C	4.57229800	-1.19449800	-3.12096800
C	4.38423000	-0.98289500	-0.72485400
C	5.91887500	-1.52110200	-2.98692800
H	4.13214700	-1.14109500	-4.11720200
C	5.72832800	-1.31654600	-0.59206100
H	3.79538800	-0.73546200	0.15787300
C	6.49697600	-1.58721800	-1.72151300
H	6.51730900	-1.72406600	-3.87364700
H	6.17912800	-1.35140700	0.39802200
H	7.55090900	-1.83970100	-1.61689800
C	-1.81527000	2.70899900	0.61525100
C	-2.01775400	1.87855700	1.72640800
C	-2.92779500	3.26216200	-0.02450700
C	-3.30031700	1.62185800	2.19338900
H	-1.15950100	1.42316700	2.22281700
C	-4.21550000	2.99531700	0.43920100
H	-2.80384600	3.90453300	-0.89573600
C	-4.40456800	2.17971600	1.54965800
H	-3.43985300	0.97756800	3.05976600
H	-5.07235900	3.43180400	-0.07187900
H	-5.41032900	1.97444600	1.91233600
C	0.52537000	4.12040100	1.37876000
C	1.71703200	3.82695700	2.04857700

C	-0.18929300	5.27807500	1.71564100
C	2.19167300	4.68984700	3.03538300
H	2.27815300	2.93148100	1.78307500
C	0.29105400	6.13870700	2.69548300
H	-1.13279200	5.49921000	1.21393700
C	1.48314100	5.84388400	3.35690600
H	3.12062000	4.45581200	3.55257800
H	-0.26782400	7.03788600	2.95011500
H	1.85751500	6.51655300	4.12708100
H	-0.97753000	4.79787600	-1.38754100
H	0.76806900	4.59434900	-1.47391200
Ru	1.12607200	1.16369700	-0.70943500
H	-0.44169200	0.46667400	-1.03543500
C	0.67152900	1.21850800	-3.79973600
H	-0.26769000	0.67481000	-3.64069700
H	0.60523100	1.73757300	-4.76950900
C	-0.32414200	3.15515800	-2.65346700
H	-0.35222800	3.75573300	-3.57665900
H	-1.24927200	2.56641100	-2.60607900

**A11**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
C	1.81368900	0.70574100	0.82427900
H	2.76407800	1.29628000	0.90435500
H	0.39444700	1.66927300	-2.18347200
O	1.55658200	-0.07143800	1.76544700
N	-0.38142900	1.03510900	-1.98412500
C	0.84420100	-0.76205500	-3.09483500
H	1.69355200	-0.09577800	-3.30365500
H	0.81810700	-1.52303200	-3.88527000
C	-1.51829600	2.83066700	-0.77847100
P	-1.16761100	1.86179700	0.76614500
P	1.07998600	-1.49456500	-1.40344400
C	0.38965600	-3.19328400	-1.60726500
C	-0.68251100	-3.61735800	-0.81910900
C	0.92984300	-4.07783300	-2.55096600
C	-1.21075300	-4.89786100	-0.97592400
H	-1.10105100	-2.92078700	-0.09263900
C	0.39786300	-5.35243200	-2.71362000
H	1.78144400	-3.76904600	-3.15967200
C	-0.67513000	-5.76514700	-1.92379100
H	-2.04527900	-5.21694200	-0.35331900
H	0.82379900	-6.02844700	-3.45364600

H	-1.08938900	-6.76473800	-2.04667900
C	2.87817300	-1.86298700	-1.35673100
C	3.70406300	-1.86962100	-2.48810500
C	3.45077400	-2.13933300	-0.10655600
C	5.06564100	-2.14326500	-2.37319500
H	3.28642300	-1.66533200	-3.47394400
C	4.80905300	-2.41830400	0.00633700
H	2.82386700	-2.12464400	0.78438000
C	5.62111400	-2.41827600	-1.12645400
H	5.69308100	-2.14359200	-3.26342200
H	5.23637100	-2.63097400	0.98492600
H	6.68501300	-2.63154500	-1.03746600
C	-2.84968300	1.63665300	1.48898800
C	-3.37916300	0.35503300	1.65634600
C	-3.61538600	2.74440100	1.87941600
C	-4.65267900	0.18238900	2.19644200
H	-2.77803800	-0.49948400	1.34434300
C	-4.88898500	2.57245700	2.41089900
H	-3.20669700	3.75108500	1.77666900
C	-5.40986300	1.28849600	2.57142300
H	-5.05276800	-0.82235100	2.32443400
H	-5.47511400	3.44121700	2.70722400
H	-6.40470600	1.15358200	2.99334800
C	-0.46999100	3.11065500	1.91366900
C	0.08645500	2.64045300	3.11266300
C	-0.43567300	4.48577500	1.65234300
C	0.65731200	3.52210500	4.02423900
H	0.07634700	1.57146000	3.32425400
C	0.14154500	5.36788500	2.56430000
H	-0.86880600	4.88178100	0.73411000
C	0.68899000	4.88875800	3.75113700
H	1.08447800	3.13950600	4.94977400
H	0.15925700	6.43471700	2.34579000
H	1.14059100	5.57845900	4.46215700
H	-2.43033600	3.43616700	-0.70201100
H	-0.67794400	3.51697500	-0.95534800
Ru	0.11917300	0.11817700	-0.04589600
H	-1.37559300	-0.76067700	-0.24374800
C	-0.43907700	0.03983900	-3.07504400
H	-1.30182500	-0.60544100	-2.86330900
H	-0.61296100	0.54564000	-4.03867700
C	-1.61682100	1.84355900	-1.92201500
H	-1.78106100	2.35592900	-2.88386500
H	-2.44364900	1.13919600	-1.76233000

## TSA7

-----			
	Coordinates (Angstroms)		
	X	Y	Z
-----			
C	2.22027000	0.88167400	0.86735200
H	3.19470600	1.30696600	1.25936400
H	1.36595300	2.66191900	-2.78394100
O	1.65208800	0.03360000	1.56457200
N	0.55371400	2.05279800	-2.66681400
C	1.83594100	0.31052600	-3.80273100
H	2.68093900	0.97996600	-4.01870800
H	1.81842700	-0.45599100	-4.58795600
C	-0.52766500	3.89307600	-1.47851400
P	-0.14471400	2.93535400	0.06999000
P	2.09387900	-0.40997500	-2.10616500
C	1.42047400	-2.11948800	-2.26689600
C	0.35590700	-2.51107700	-1.44926600
C	1.94571900	-3.03935400	-3.18381300
C	-0.17908900	-3.79379300	-1.55109300
H	-0.04920500	-1.79354100	-0.73433100
C	1.40590300	-4.31693300	-3.29282900
H	2.79264200	-2.75631000	-3.81142600
C	0.34161900	-4.69608800	-2.47506900
H	-1.00473100	-4.08843000	-0.90521300
H	1.81988800	-5.02204900	-4.01225500
H	-0.07713600	-5.69803300	-2.55612800
C	3.89738700	-0.76030800	-2.08384200
C	4.72014900	-0.73846200	-3.21762300
C	4.47798700	-1.05769900	-0.84233200
C	6.08496900	-1.00048700	-3.11102500
H	4.29859800	-0.52201900	-4.19908300
C	5.83723400	-1.33068000	-0.73775800
H	3.85122300	-1.07446900	0.05049200
C	6.64695600	-1.29729400	-1.87244000
H	6.70989800	-0.97608300	-4.00275600
H	6.26795900	-1.56329400	0.23478300
H	7.71308700	-1.50175100	-1.79050800
C	-1.80597500	2.69719700	0.83510500
C	-2.28874100	1.39896200	1.02520400
C	-2.59985200	3.78133900	1.23205000
C	-3.54250500	1.18689200	1.59524500
H	-1.66695700	0.55748300	0.71648300
C	-3.85579900	3.57076400	1.79212100
H	-2.22583600	4.79972800	1.11265000
C	-4.32851800	2.27152400	1.97557500

H	-3.90404400	0.17059100	1.74397000
H	-4.46543600	4.42131400	2.09392300
H	-5.30846800	2.10695400	2.42102100
C	0.55729700	4.21370900	1.18533600
C	1.15008800	3.76736000	2.37610600
C	0.55426600	5.58819800	0.91542600
C	1.71638000	4.66728400	3.27162300
H	1.16547000	2.69931300	2.59895400
C	1.13338300	6.48918100	1.80761700
H	0.09112400	5.96936500	0.00563800
C	1.71463200	6.03239700	2.98709200
H	2.16768900	4.30088100	4.19226200
H	1.12451700	7.55426500	1.57990200
H	2.16654000	6.73723200	3.68283600
H	-1.43888500	4.49756400	-1.38627000
H	0.30598100	4.58491200	-1.66531200
Ru	0.96655500	1.08958500	-0.75946900
H	-0.48069400	0.44562900	-1.26528200
C	0.54710300	1.10677900	-3.80539500
H	-0.32544700	0.45625100	-3.67228200
H	0.42716500	1.66397500	-4.74874900
C	-0.64436400	2.92127800	-2.63484500
H	-0.73942600	3.45522900	-3.59440500
H	-1.51224300	2.26139300	-2.51745200

**TSA8**

**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
C	2.87482800	2.23041000	-0.57290300
H	2.68521400	3.29056200	-2.43533900
H	1.65926500	2.75592900	-2.66282800
O	3.87605300	2.58582300	-0.09803100
N	0.68776500	2.09633600	-2.63446300
C	1.95003200	0.33893700	-3.75782200
H	2.83219200	0.98568900	-3.85972700
H	1.95928600	-0.38618700	-4.58130700
C	-0.42297900	3.92807500	-1.47026700
C	1.34814600	0.27007800	0.92880000
O	1.42478100	-0.31719800	1.93744900
P	-0.18339600	2.94653500	0.06991500
P	2.08153300	-0.46807700	-2.10683500
C	1.26856000	-2.09891000	-2.28638000
C	0.34718000	-2.53784200	-1.33140900
C	1.59141500	-2.94149500	-3.35866700

C	-0.24688800	-3.79241400	-1.44966400
H	0.09004400	-1.88417400	-0.49902700
C	0.99057600	-4.18943800	-3.48110600
H	2.32347900	-2.62370700	-4.10215400
C	0.06967200	-4.61678100	-2.52549500
H	-0.96233100	-4.12362900	-0.69914300
H	1.24421500	-4.83138200	-4.32293200
H	-0.39890200	-5.59476300	-2.62093200
C	3.84834100	-0.90110600	-1.94905000
C	4.65456100	-1.14433400	-3.06805300
C	4.40943900	-1.00728100	-0.67140900
C	5.99327300	-1.49074400	-2.90962500
H	4.23978700	-1.05716800	-4.07220000
C	5.74657700	-1.35882100	-0.51458800
H	3.79575000	-0.80025200	0.20557200
C	6.54016800	-1.60086600	-1.63330900
H	6.61146200	-1.67077800	-3.78737200
H	6.17129000	-1.43317900	0.48465100
H	7.58832100	-1.86802800	-1.51133000
C	-1.86487100	2.61869900	0.71584900
C	-2.22615500	1.33234700	1.12637200
C	-2.79352700	3.66034700	0.84310700
C	-3.49565000	1.08940500	1.64586100
H	-1.50816600	0.51955000	1.02565300
C	-4.06348300	3.41503800	1.35324500
H	-2.52000900	4.67383400	0.54697700
C	-4.41621400	2.12755800	1.75592100
H	-3.76543100	0.08335400	1.96205600
H	-4.77930700	4.23062700	1.43995000
H	-5.40998600	1.93597400	2.15693500
C	0.49811400	4.14192300	1.26971600
C	1.30527500	3.67423000	2.31291800
C	0.22313600	5.51262100	1.18433500
C	1.81769600	4.55698400	3.25862000
H	1.54453200	2.61231100	2.37528200
C	0.74153600	6.39481000	2.12771200
H	-0.39300400	5.89882400	0.37247200
C	1.53662000	5.91809600	3.16737500
H	2.44727300	4.18045100	4.06254000
H	0.52638600	7.45891100	2.04729000
H	1.94393400	6.60980900	3.90253200
H	-1.31325900	4.56805100	-1.42601200
H	0.45942700	4.57522600	-1.56751000
Ru	1.12474900	1.15423300	-0.70044800

H	-0.31373700	0.33641300	-0.91890600
C	0.69437100	1.19049300	-3.78857300
H	-0.20976000	0.56192200	-3.77073300
H	0.66424900	1.77683000	-4.72213700
C	-0.48461400	2.97861700	-2.65233200
H	-0.50224200	3.55452700	-3.59286900
H	-1.40383600	2.37287500	-2.62531500

**A12**

**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
C	2.80298300	2.03779300	-0.40049600
O	3.81752400	2.57340400	-0.23404700
N	0.72109300	2.20432600	-2.55959000
C	1.85439500	0.44248300	-3.79349400
H	2.73926200	1.08437000	-3.90063200
H	1.81787000	-0.24988800	-4.64431500
C	-0.42407200	3.94456700	-1.30177700
C	1.16550100	0.03921600	0.88019600
O	1.13017600	-0.66793900	1.80779600
P	-0.19006200	2.89484200	0.19422800
P	2.01320400	-0.43532300	-2.18832400
C	1.21274200	-2.06448500	-2.42744200
C	0.15284900	-2.47314100	-1.61384900
C	1.67496400	-2.92766500	-3.43074000
C	-0.44118700	-3.71909200	-1.80570800
H	-0.21110700	-1.80314800	-0.83646800
C	1.07715300	-4.16741400	-3.62507300
H	2.51467000	-2.63018800	-4.06045100
C	0.01657100	-4.56501100	-2.81142900
H	-1.26616400	-4.02647200	-1.16549400
H	1.44118800	-4.82721900	-4.41077200
H	-0.45053800	-5.53683900	-2.96194000
C	3.78033700	-0.86756700	-2.03264900
C	4.62800800	-0.95006200	-3.14412800
C	4.30260300	-1.12877400	-0.75973000
C	5.96862900	-1.29207900	-2.98410900
H	4.24317800	-0.74074200	-4.14211200
C	5.64002600	-1.47698800	-0.60247000
H	3.65416800	-1.04910100	0.11387100
C	6.47566300	-1.55770400	-1.71468700
H	6.61921200	-1.34756700	-3.85518000
H	6.03263400	-1.67690500	0.39280800
H	7.52422600	-1.82257800	-1.59131100

C	-1.87987000	2.59409100	0.83582200
C	-2.38983100	3.29267800	1.93761100
C	-2.70645500	1.67473800	0.17627000
C	-3.69875900	3.08022500	2.36367400
H	-1.76306000	4.00492100	2.47177300
C	-4.01742700	1.47552200	0.59643300
H	-2.30768500	1.10522900	-0.66299800
C	-4.51696600	2.17621700	1.69234600
H	-4.07769600	3.62515100	3.22672900
H	-4.64770400	0.76047800	0.07039600
H	-5.54005800	2.01180800	2.02624700
C	0.57261900	3.98439000	1.44072700
C	1.39718300	3.43067200	2.42712200
C	0.35121000	5.36787100	1.43800500
C	1.98548500	4.24156100	3.39314200
H	1.58552400	2.35648000	2.42977600
C	0.94605500	6.17870000	2.40071300
H	-0.29302200	5.81451100	0.68071100
C	1.76241000	5.61647400	3.37975100
H	2.62626100	3.79860500	4.15326900
H	0.77096300	7.25302200	2.38530100
H	2.22890000	6.25171300	4.13061900
H	-1.31482700	4.58018600	-1.22345000
H	0.46204700	4.58930800	-1.37946700
Ru	1.09315800	1.11694000	-0.68137500
H	-0.37265300	0.39439000	-1.05563500
C	0.61292600	1.31094900	-3.68905600
H	-0.28922500	0.65263600	-3.63530200
H	0.50174800	1.89341800	-4.62534800
C	-0.47547500	3.00918800	-2.49570000
H	-0.57703800	3.61344200	-3.41961800
H	-1.40844800	2.39583000	-2.43891300

**B1**

**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
Ru	0.03376600	0.19271200	0.05726800
P	-2.27047500	0.34834600	0.42009800
C	0.05358800	0.31304500	-1.78252100
H	0.07570900	1.80735500	0.14935600
O	0.15578000	-2.13114400	0.14684400
P	2.34380900	0.08642400	0.42131900
N	0.00312700	0.26135000	2.30246300
O	0.07697900	0.43044000	-2.94994200



C	0.28292800	-2.81273000	-1.07645200
C	-0.83039000	-2.88006200	1.09597100
C	2.40188400	-0.17725200	2.25268400
C	-1.11510900	1.07644600	2.80457900
H	-0.23222600	-0.74499200	2.46530000
C	1.29166600	0.63090600	2.89744700
C	-2.43003200	0.55316600	2.25127200
H	1.10278700	-2.37200500	-1.65614300
H	-0.64491200	-2.76088400	-1.67418600
O	-1.20472800	-2.12479900	2.06678500
H	-0.19894700	-3.77730600	1.34862000
H	1.44757700	1.70695800	2.72942400
H	1.27856900	0.46732900	3.98743000
C	-4.59144500	3.96230200	-1.32731100
C	-5.24610900	3.03274500	-0.51923800
C	-4.54770000	1.94790700	-0.00177800
C	-3.18256200	1.78166300	-0.27603300
C	-2.53724400	2.71634000	-1.09008300
C	-3.23953300	3.80048600	-1.61438900
H	-5.13965100	4.80941600	-1.73636000
H	-6.30535000	3.15145400	-0.29688100
H	-5.06942300	1.21440900	0.61504400
H	-1.47744500	2.58882000	-1.30737500
H	-2.72591600	4.51987200	-2.25006400
C	-4.87763900	-3.20289700	-0.98241400
C	-4.10612400	-2.46730900	-1.87966000
C	-3.34086200	-1.39891900	-1.42346100
C	-3.34289700	-1.04478200	-0.06724700
C	-4.12212000	-1.78679600	0.82492100
C	-4.88411300	-2.85898900	0.36715800
H	-5.47115400	-4.04508000	-1.33412500
H	-4.09092400	-2.73071300	-2.93589100
H	-2.72800000	-0.83341600	-2.12786100
H	-4.12987100	-1.54310400	1.88463600
H	-5.48287700	-3.43168300	1.07350600
C	4.62167400	-3.41014300	-1.57151700
C	4.65149700	-2.13421000	-2.13030800
C	4.00690500	-1.07786400	-1.49441100
C	3.32211900	-1.28132500	-0.28767100
C	3.28947900	-2.57045100	0.26014200
C	3.94040300	-3.62360300	-0.37574000
H	5.12454300	-4.23723400	-2.06945800
H	5.17883500	-1.95829700	-3.06629300
H	4.03522700	-0.08356900	-1.94061900

H	2.73059700	-2.76836000	1.17222500
H	3.90649400	-4.61876900	0.06459800
C	5.03240100	3.78000800	-0.29771800
C	3.71964700	3.77193300	-0.76014200
C	2.90830700	2.65983700	-0.54159300
C	3.40691200	1.54558800	0.13946600
C	4.73429200	1.55794500	0.59142700
C	5.54051800	2.67005300	0.37737000
H	5.66483800	4.64992800	-0.46621100
H	3.32261600	4.63370400	-1.29359100
H	1.87812700	2.64588400	-0.89727000
H	5.14102000	0.68449900	1.10288600
H	6.56879300	2.67144000	0.73463900
H	-0.93947400	2.11580200	2.49314700
H	-1.13683000	1.05731300	3.90705500
H	-3.25895000	1.22194200	2.51256600
H	-2.61878600	-0.44109600	2.66572700
H	2.22943000	-1.24424700	2.44645500
H	3.38396700	0.07885000	2.67037700
H	0.51874100	-3.87662000	-0.90043600
H	-1.63102700	-3.22214500	0.38549200

**B2**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
N	1.64449700	0.40295700	-1.52398900
C	3.22408100	-0.85234500	-0.15275300
H	3.68105900	0.06159300	0.24710900
H	3.98303100	-1.64459300	-0.12907600
C	0.07940500	1.72596600	-2.83705000
C	-1.33901900	-0.61617100	1.01809900
O	-2.22263300	-1.02980400	1.67428300
P	-1.20584200	1.12944000	-1.65691900
P	1.77404600	-1.27192600	0.91088800
C	1.72882900	-3.09773600	0.95184500
C	2.87188100	-3.82992400	1.30340200
C	0.54914700	-3.78348900	0.64840800
C	2.83582200	-5.21932300	1.33952100
H	3.79332400	-3.30601200	1.56066300
C	0.51256100	-5.17603600	0.69033600
H	-0.33999000	-3.21533300	0.37643900
C	1.65474000	-5.89442100	1.03176900
H	3.73034700	-5.77818000	1.60941400
H	-0.41210200	-5.69965300	0.45386500

H	1.62686400	-6.98244700	1.06065300
C	2.24763700	-0.81419800	2.61451200
C	2.86770500	0.41958400	2.86179500
C	1.87696700	-1.61613600	3.70206700
C	3.13168700	0.82318900	4.16692100
H	3.11419300	1.08105000	2.03191800
C	2.13730300	-1.20443700	5.00628800
H	1.38305300	-2.57211300	3.52882400
C	2.76932200	0.01389200	5.24228600
H	3.62151300	1.77968600	4.34402500
H	1.84666100	-1.84147100	5.84013400
H	2.97596100	0.33401800	6.26225500
C	-2.43569900	0.25116400	-2.69385200
C	-2.84195900	-1.04509500	-2.36530500
C	-3.00962600	0.88455100	-3.80472800
C	-3.79704100	-1.70132200	-3.13933600
H	-2.40112300	-1.53612400	-1.49824100
C	-3.95708700	0.22618600	-4.58060900
H	-2.71868100	1.90518500	-4.05852800
C	-4.35166900	-1.06974800	-4.24862900
H	-4.10621700	-2.71058000	-2.87290600
H	-4.39298000	0.72576700	-5.44420300
H	-5.09557900	-1.58425400	-4.85463300
C	-2.15475400	2.60449800	-1.13716400
C	-1.88655600	3.90119000	-1.58949500
C	-3.17967100	2.41442600	-0.19795800
C	-2.62308900	4.98324700	-1.10955700
H	-1.10152400	4.07565800	-2.32409700
C	-3.91876600	3.49335500	0.27291600
H	-3.39143300	1.40970000	0.17181900
C	-3.63772300	4.78290500	-0.17829700
H	-2.40101500	5.98692700	-1.46848200
H	-4.71118400	3.32916000	1.00104200
H	-4.21033400	5.62947600	0.19630900
H	-0.33049900	1.94013100	-3.83267300
H	0.49911400	2.65957100	-2.43658900
Ru	0.04630500	-0.08177900	-0.10848400
C	2.70382700	-0.59442000	-1.55759700
H	2.35383000	-1.54884500	-2.00475900
H	3.53976000	-0.24843300	-2.19628700
C	1.17382700	0.67066800	-2.87186400
H	2.00514100	1.02916000	-3.50942700
H	0.78675500	-0.24700300	-3.36360500
H	2.22262400	1.70236100	-0.71165200

O	0.71128800	1.82683000	1.25130000
C	1.36101400	2.89433600	0.52875700
H	0.61851600	3.28864300	-0.20187100
H	1.59936100	3.69623500	1.24968800
C	-0.26776000	2.30470800	2.15255400
H	-0.65152200	1.44211300	2.70487100
H	0.18604700	3.01325000	2.86373400
H	-1.10082100	2.80459200	1.63200600
O	2.50346400	2.43289000	-0.03442900
H	-0.22233900	-1.36256300	-1.02877700

**B3**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	-0.11158000	-1.45078800	-1.57440700
C	2.32773200	-1.48755100	-1.45444300
H	2.39824300	-0.77961800	-2.29255800
H	3.23291700	-2.10604300	-1.48998200
C	-2.53375000	-1.20194800	-1.60242300
C	-0.02535200	1.24108300	1.52589400
O	0.01672100	1.98903700	2.43062100
P	-2.38505900	-0.08226800	-0.12703600
P	2.19184500	-0.46688500	0.07890200
C	2.82898500	-1.53172800	1.42983400
C	2.51642400	-1.16681400	2.74650300
C	3.60024900	-2.67915300	1.21781200
C	2.97151700	-1.92276000	3.82026600
H	1.89267800	-0.29059700	2.92583600
C	4.04268600	-3.44688600	2.29421500
H	3.85736000	-2.99398000	0.20715000
C	3.73241700	-3.06930900	3.59647700
H	2.71882700	-1.62390800	4.83618700
H	4.63104600	-4.34437000	2.10915500
H	4.07616100	-3.67020200	4.43679500
C	3.51024000	0.79210700	-0.07744500
C	4.86100900	0.43321100	-0.16834800
C	3.16119700	2.14541300	-0.09584500
C	5.84212000	1.41096600	-0.29332200
H	5.14862900	-0.61828300	-0.13312200
C	4.14609200	3.12445400	-0.21265900
H	2.10771000	2.42248000	-0.02637300
C	5.48527600	2.75873700	-0.31440600
H	6.88932300	1.12176300	-0.36666100
H	3.86389900	4.17617800	-0.22100500

H	6.25475400	3.52366600	-0.40546400
C	-3.36020200	-0.92638500	1.17310500
C	-2.85156700	-0.99356000	2.47397800
C	-4.61522400	-1.49151000	0.90704600
C	-3.57804100	-1.61440700	3.48680800
H	-1.86925500	-0.57024600	2.68033000
C	-5.33583200	-2.12195000	1.91671800
H	-5.04332900	-1.42586100	-0.09387700
C	-4.81742400	-2.18424400	3.20922600
H	-3.16843600	-1.65874500	4.49446100
H	-6.30601700	-2.56373700	1.69465700
H	-5.38090600	-2.67860900	3.99881000
C	-3.43850500	1.35197000	-0.57760300
C	-3.06425900	2.13992700	-1.67475400
C	-4.56562900	1.72538600	0.16229100
C	-3.81755300	3.24854400	-2.04323700
H	-2.15558900	1.89067100	-2.22648100
C	-5.31166300	2.84548200	-0.19859300
H	-4.86592100	1.14250600	1.03071900
C	-4.94589100	3.60469600	-1.30521800
H	-3.51641700	3.84538900	-2.90281100
H	-6.18319400	3.12292900	0.39203700
H	-5.53052700	4.47859600	-1.58744200
H	-3.50079400	-1.71867200	-1.63391000
H	-2.47864100	-0.57348600	-2.50361400
Ru	-0.07362200	0.05571800	0.12135100
H	-0.22518700	-1.30269000	1.12250600
C	1.07161200	-2.33199800	-1.57893200
H	0.97400200	-3.01834800	-0.72659300
H	1.09264000	-2.93529000	-2.50085900
C	-1.38510700	-2.19136200	-1.59915600
H	-1.43149700	-2.84210800	-2.48744600
H	-1.41630900	-2.82781900	-0.70498400
H	-0.08290000	-0.91707100	-2.44735900
H	0.02259900	1.34109700	-1.06346500
C	-0.12647500	0.60733300	-4.50154900
O	-0.17047400	-0.60349800	-4.43925600
H	0.42844300	1.14068100	-5.30260400
H	-0.71629900	1.26402200	-3.82271400
C	1.75736700	2.77664200	-3.26663500
H	2.31749100	2.90310000	-4.19934100
H	0.76257700	3.23941600	-3.39164500
H	2.28735000	3.32428700	-2.47241900
O	1.67945700	1.39456800	-2.99783700

H	1.13764700	1.29939800	-2.16699500
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**B4**

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**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	0.07584000	-1.38373500	-1.56767900
C	2.48592500	-1.69732400	-1.35024200
H	2.67824200	-1.02872900	-2.20041300
H	3.30837100	-2.42217300	-1.29286600
C	-2.34423200	-1.06156600	-1.75116900
C	0.10158800	1.14291600	1.61183200
O	0.04908400	1.74886800	2.61434000
P	-2.17710500	0.03724600	-0.28550900
P	2.36791800	-0.64764000	0.15622300
C	2.93243300	-1.71634100	1.53261300
C	2.15953900	-1.86042600	2.68793700
C	4.16578100	-2.37700200	1.45020600
C	2.60607700	-2.66068100	3.73793600
H	1.20267600	-1.34447200	2.75706000
C	4.60739200	-3.17974700	2.49574800
H	4.78955600	-2.25597000	0.56319600
C	3.82608000	-3.32353300	3.64190100
H	1.99488700	-2.76625300	4.63256000
H	5.56483200	-3.69218300	2.41846300
H	4.17245400	-3.95102200	4.46140200
C	3.72896400	0.56355000	0.02149200
C	4.79235100	0.40382400	-0.87427600
C	3.70658100	1.68870800	0.85620700
C	5.81206000	1.35093700	-0.93399900
H	4.82716300	-0.46170800	-1.53508600
C	4.73094900	2.62775700	0.80223900
H	2.87552400	1.82868400	1.54898700
C	5.78434200	2.46195100	-0.09540300
H	6.62977400	1.21865100	-1.64044800
H	4.70237000	3.49681000	1.45722100
H	6.58117400	3.20208500	-0.14402300
C	-3.22578500	-0.68392500	1.02462600
C	-3.56252400	0.10729700	2.13116700
C	-3.64749000	-2.01710400	0.99209100
C	-4.31613900	-0.42045700	3.17354800
H	-3.23581300	1.14714900	2.17273300
C	-4.40100800	-2.54433000	2.03861100
H	-3.38496400	-2.65513200	0.14894200
C	-4.73857300	-1.74831900	3.12941900

H	-4.57438100	0.20767800	4.02435900
H	-4.72485700	-3.58304800	1.99810200
H	-5.32854900	-2.16162600	3.94552600
C	-3.08003100	1.56675900	-0.71089200
C	-2.44955700	2.80795800	-0.58625300
C	-4.40586400	1.51430500	-1.16221500
C	-3.13152400	3.97994200	-0.90809300
H	-1.41687300	2.85076000	-0.23780500
C	-5.08263600	2.68380400	-1.49224200
H	-4.91261500	0.55238100	-1.25030300
C	-4.44605600	3.91842300	-1.36384700
H	-2.63202100	4.94160000	-0.80522400
H	-6.11101300	2.63353000	-1.84613300
H	-4.97876200	4.83352300	-1.61701500
H	-3.32783600	-1.54539600	-1.80938600
H	-2.24488200	-0.39632600	-2.61812000
Ru	0.12803500	0.04155300	0.09615400
H	-0.18244700	-1.21911200	1.04085700
C	1.13825800	-2.37613000	-1.52990300
H	0.98568300	-3.11814600	-0.71612100
H	1.15009400	-2.95776200	-2.47265600
C	-1.19864100	-2.06170400	-1.73163900
H	-1.20566600	-2.63818900	-2.67829200
H	-1.36985500	-2.80844900	-0.92563200
H	0.44780800	-0.41664900	-2.92063800
H	0.87271200	1.47225300	-1.05862800
C	-0.40733800	0.58738300	-4.32943200
H	-1.14208900	-0.22611400	-4.54521600
H	-0.14061500	1.06043200	-5.29311100
O	-1.06896600	1.55382000	-3.50891900
C	-2.26537700	1.97824300	-4.10503300
H	-2.98961200	1.14916200	-4.22057400
H	-2.70763200	2.74546900	-3.46219300
H	-2.09278100	2.41252000	-5.10612700
O	0.72399100	0.14450300	-3.72594100
H	0.14007900	1.42305900	-1.35948500

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**TSB1**  
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**Coordinates (Angstroms)**  
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	<b>X</b>	<b>Y</b>	<b>Z</b>
C	-0.63345600	0.80857600	0.48484400
H	-0.27402000	1.44172300	1.30545000
H	-1.67168300	1.04644100	0.17887900
O	0.14377500	1.45775800	-0.87835400

C	-0.51446700	2.62493800	-1.38042300
H	-0.43871900	3.41178600	-0.62470300
H	0.00076400	2.94055800	-2.29111900
H	-1.57101500	2.42315600	-1.60118100
O	-0.26152400	-0.42916400	0.50758400
H	-0.54737100	-0.73783100	-0.60056200
H	-0.15871800	0.59089800	-1.48458900
H	-0.68708400	-0.54421000	-1.68646700

**TSB2**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
C	0.12335300	-1.40518000	1.39335800
H	0.67953000	-2.02616000	0.67261700
H	0.48620900	-1.61622500	2.40459500
H	-0.93890300	-1.67261400	1.33907900
O	0.27670700	-0.02105100	1.13774100
H	1.43818100	0.33246100	1.09941200
C	-0.08949600	0.39089700	-0.44227100
O	0.55214400	1.46509600	-0.73577000
H	-1.19051700	0.46560900	-0.37674200
H	0.20754600	-0.56928400	-0.93105200
C	3.31152400	-0.05678700	0.05156000
H	4.15848500	0.46885300	-0.40175000
H	3.69070800	-0.73269700	0.82546700
H	2.81013100	-0.64993800	-0.72838400
O	2.43413500	0.89119200	0.65036700
H	1.75435500	1.30919500	-0.14182100

**TSB3**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
N	-1.35072000	10.14657000	4.78493400
C	0.21442500	8.85370800	6.13959500
H	0.69046400	9.75685800	6.54071600
H	0.95977100	8.04861600	6.14947900
C	-2.92729000	11.49841000	3.50812900
C	-4.34519500	9.08388900	7.31148700
O	-5.22693600	8.66810000	7.96651300
P	-4.21833400	10.86737500	4.66452700
P	-1.23099500	8.45207200	7.21774400
C	-1.29570300	6.62715800	7.27961900
C	-0.16421500	5.88466400	7.64701300
C	-2.48365100	5.95230400	6.98434000



C	-0.22155100	4.49695900	7.71036800
H	0.76403500	6.40006100	7.89739200
C	-2.54145000	4.56185000	7.05329900
H	-3.36451500	6.52601700	6.69859100
C	-1.41166700	3.83339600	7.41334400
H	0.66372200	3.93021700	7.99383800
H	-3.47332600	4.04755200	6.82408600
H	-1.45620800	2.74679300	7.46485000
C	-0.74378300	8.92810400	8.91069900
C	-0.12955500	10.16937300	9.13446300
C	-1.09822000	8.13642200	10.01074700
C	0.14762600	10.58872900	10.43162500
H	0.10025000	10.82074300	8.29143100
C	-0.82420500	8.56470300	11.30668200
H	-1.58805100	7.17546100	9.85408500
C	-0.19693700	9.78940800	11.52035800
H	0.63171600	11.55111700	10.59212600
H	-1.10113600	7.93645800	12.15179700
H	0.01969600	10.12238400	12.53426400
C	-5.42797600	9.99886100	3.59632500
C	-5.76101800	8.66491300	3.84624600
C	-6.05765200	10.67221500	2.53994200
C	-6.69925900	8.01146300	3.05030900
H	-5.27553300	8.14324300	4.67024900
C	-6.99014500	10.01781600	1.74346900
H	-5.82236300	11.72001700	2.34612100
C	-7.31269400	8.68490200	1.99824400
H	-6.95148100	6.97263000	3.25615600
H	-7.47195600	10.54944400	0.92460500
H	-8.04615300	8.17418500	1.37629300
C	-5.18440400	12.32180000	5.20502900
C	-4.89101200	13.63537200	4.82325900
C	-6.25083900	12.09532600	6.08833700
C	-5.64630600	14.69878400	5.31476900
H	-4.07155000	13.83846700	4.13506100
C	-7.00727500	13.15634400	6.57107900
H	-6.48412200	11.07640500	6.40198900
C	-6.70307200	14.46286700	6.18878700
H	-5.40502700	15.71594700	5.01045900
H	-7.83254800	12.96450000	7.25467900
H	-7.29091700	15.29504800	6.57228000
H	-3.33464500	11.73567400	2.51664800
H	-2.51340200	12.42394400	3.93169300
Ru	-2.96269500	9.64079700	6.19874400

C	-0.30409900	9.13071700	4.73816500
H	-0.68613300	8.19604300	4.28430600
H	0.53285800	9.46991300	4.09965400
C	-1.82588400	10.45251000	3.44238800
H	-0.99739000	10.82983600	2.81474200
H	-2.20607700	9.53998700	2.94336800
H	-0.85885600	11.22783900	5.47860400
O	-2.31859500	11.54541200	7.53420300
C	-1.57641700	12.56846300	6.79045100
H	-2.32218500	13.00818500	6.08063900
H	-1.30511700	13.35338400	7.52520500
C	-3.30510200	12.11705800	8.36689400
H	-3.82342000	11.30217700	8.88158400
H	-2.83233300	12.77000700	9.11849700
H	-4.03725600	12.71090000	7.79477900
O	-0.49640500	12.02835100	6.22110000
H	-3.20220600	8.35627400	5.27330200

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**TSB4**

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<b>Coordinates (Angstroms)</b>			
	<b>X</b>	<b>Y</b>	<b>Z</b>
N	-0.13311000	-0.98301100	-1.18403600
C	2.29360300	-1.00045500	-1.10774300
H	2.29729200	-0.30198900	-1.95744100
H	3.21425100	-1.59355600	-1.17101800
C	-2.54937700	-0.73449200	-1.27043500
C	-0.06547700	1.71633600	1.89337300
O	-0.03838900	2.44650200	2.80995200
P	-2.41591200	0.39622700	0.19164300
P	2.18616200	0.02985000	0.41513700
C	2.81952200	-1.01402600	1.77862200
C	2.52582100	-0.62190100	3.09202900
C	3.57016500	-2.17678300	1.57608900
C	2.98065400	-1.36739000	4.17331700
H	1.92212100	0.26970000	3.26442500
C	4.01378100	-2.93179200	2.66071200
H	3.80979200	-2.51043100	0.56721900
C	3.72279100	-2.52787300	3.95972300
H	2.74402100	-1.04825900	5.18691600
H	4.58794100	-3.84015700	2.48517400
H	4.06747300	-3.11930900	4.80623000
C	3.48060200	1.30133400	0.21588100
C	4.83543500	0.95353600	0.14501700
C	3.11279000	2.64535400	0.11178000

C	5.80314500	1.93514400	-0.03844900
H	5.13611200	-0.09059900	0.24105100
C	4.08347900	3.62769900	-0.06993700
H	2.05726400	2.91445100	0.16842700
C	5.42761900	3.27348000	-0.14641600
H	6.85403700	1.65600900	-0.09337700
H	3.78667600	4.67239100	-0.15051300
H	6.18683900	4.04106800	-0.28635600
C	-3.41947800	-0.40162000	1.49333600
C	-2.92832600	-0.46958400	2.80086900
C	-4.69349800	-0.91790200	1.21786100
C	-3.69287000	-1.04401100	3.81338300
H	-1.93535400	-0.07751700	3.01746600
C	-5.45200500	-1.49999500	2.22789500
H	-5.10381900	-0.85039000	0.20974700
C	-4.95223300	-1.56312800	3.52804400
H	-3.29903900	-1.08861200	4.82716500
H	-6.43813800	-1.90168100	2.00092600
H	-5.54741900	-2.01794900	4.31809200
C	-3.40166500	1.86391400	-0.27933000
C	-3.05450300	2.57536700	-1.43683400
C	-4.43997800	2.34741700	0.52374500
C	-3.75200000	3.72286200	-1.79615800
H	-2.22061000	2.23380000	-2.05416300
C	-5.13020800	3.50316900	0.16715900
H	-4.71431400	1.82159500	1.43654800
C	-4.79327700	4.19000100	-0.99478300
H	-3.47458900	4.25999900	-2.70193100
H	-5.93520500	3.86600900	0.80416600
H	-5.33544500	5.09183000	-1.27378500
H	-3.52072600	-1.24223200	-1.31098000
H	-2.46796800	-0.11767500	-2.17724000
Ru	-0.09992600	0.53601300	0.47241000
H	-0.24649500	-0.73120400	1.50077300
C	1.04830800	-1.86539400	-1.18175200
H	0.97648300	-2.54142300	-0.31779300
H	1.05779700	-2.47996800	-2.09571300
C	-1.40272900	-1.72588800	-1.23104600
H	-1.42775600	-2.37691700	-2.11981800
H	-1.46339900	-2.36658300	-0.34059600
H	-0.06806000	-0.45439900	-2.08226200
H	-0.06114100	1.89435900	-0.77550600
C	0.28337300	1.32965500	-3.84022100
O	0.30647500	0.08779600	-3.69445800

H	0.82868500	1.79831400	-4.69226100
H	-0.64544400	1.91579000	-3.60660900
C	1.22092200	3.51426500	-2.74436100
H	2.13428300	3.87898700	-3.23716700
H	0.35184700	3.83015300	-3.35431200
H	1.12976100	4.02120300	-1.76920600
O	1.26320600	2.12413300	-2.57783800
H	0.52434900	1.89310800	-1.48065100

**B5**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	-0.21189500	-1.27770700	-1.80032200
C	2.23008900	-1.30035600	-1.94397100
H	2.24627800	-0.49441500	-2.68772100
H	3.12980900	-1.91141100	-2.09269400
C	-2.64872500	-1.19592900	-1.69840800
C	0.03705200	1.12037600	1.44485900
O	0.13077800	1.79194900	2.40617100
P	-2.41265000	-0.24926300	-0.13055500
P	2.18028400	-0.46258200	-0.30772700
C	2.86652900	-1.66556000	0.89281000
C	3.34264200	-2.93140400	0.53869700
C	2.88552500	-1.29222000	2.24454800
C	3.82948200	-3.80302000	1.51277100
H	3.33028600	-3.25391400	-0.50136300
C	3.38134900	-2.15644500	3.21281100
H	2.49804200	-0.31484800	2.53717900
C	3.85385500	-3.41750700	2.84888700
H	4.19017000	-4.78815100	1.22088000
H	3.39220100	-1.84865100	4.25709100
H	4.23494400	-4.09866500	3.60785600
C	3.49508300	0.81049300	-0.33172900
C	4.82298200	0.47768900	-0.62607600
C	3.17580400	2.13704900	-0.02699600
C	5.81106500	1.45815800	-0.62709600
H	5.08795800	-0.55765000	-0.84550400
C	4.16669600	3.11576800	-0.01633200
H	2.13802200	2.39672100	0.18861400
C	5.48387700	2.77821400	-0.31965600
H	6.84033000	1.19018400	-0.86050000
H	3.90804600	4.14521100	0.22706000
H	6.25859100	3.54336200	-0.31262300
C	-3.28237900	-1.22153300	1.15709900

C	-2.65483600	-1.48777600	2.37764700
C	-4.59332500	-1.67274200	0.95397300
C	-3.32214900	-2.19995500	3.37232600
H	-1.63639800	-1.13571100	2.54037300
C	-5.25650200	-2.38852900	1.94452100
H	-5.10466400	-1.45447200	0.01513300
C	-4.61993300	-2.65412400	3.15647600
H	-2.82182500	-2.40155100	4.31793100
H	-6.27363000	-2.73704200	1.77280200
H	-5.13902200	-3.21349900	3.93302800
C	-3.49871400	1.21208200	-0.31408100
C	-3.21770800	2.35531000	0.44335400
C	-4.60423200	1.22344900	-1.17308800
C	-4.03198800	3.48018800	0.35474600
H	-2.34878100	2.36066800	1.10228900
C	-5.41515400	2.35185800	-1.26582400
H	-4.83626300	0.34635600	-1.77750700
C	-5.13106400	3.48126200	-0.50172500
H	-3.80188000	4.36184300	0.95054100
H	-6.26991100	2.34929800	-1.94048500
H	-5.76431500	4.36372200	-0.57640300
H	-3.57648300	-1.78274300	-1.69939400
H	-2.71994000	-0.45517200	-2.50675600
Ru	-0.09057000	-0.01760500	-0.02513200
H	-0.04647400	-1.25044000	0.98459000
C	0.94720200	-2.10800200	-2.08011300
H	0.99004200	-2.98881800	-1.40273500
H	0.88506000	-2.52475000	-3.10485900
C	-1.42390400	-2.07093100	-1.91275000
H	-1.48806100	-2.54055500	-2.91427700
H	-1.43652600	-2.91177700	-1.18682200
C	0.32092200	2.24638900	-2.69882000
H	0.25105700	3.19819100	-2.14233100
H	-0.01812900	2.42326200	-3.74038000
O	1.64447100	1.77596900	-2.71375700
C	2.52606100	2.71128200	-3.28359400
H	2.53176100	3.66170900	-2.72342500
H	3.52922200	2.27662700	-3.24917800
H	2.26671800	2.93070200	-4.33361700
O	-0.49057300	1.32966400	-2.06030700
H	-0.33815000	0.38566900	-2.41021800

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**TSB5**

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**Coordinates (Angstroms)**

	X	Y	Z
N	-0.27588400	-0.40033000	-1.46756400
C	2.17071100	-0.43217900	-1.58076100
H	2.21341200	0.37973400	-2.31579000
H	3.06529200	-1.05331400	-1.71657400
C	-2.71344300	-0.27157000	-1.38416700
C	-0.03101900	1.95697200	1.82394900
O	0.06896700	2.63380500	2.78010800
P	-2.48920400	0.62746000	0.21511100
P	2.11110900	0.40007200	0.06105600
C	2.81782400	-0.79429500	1.25759400
C	3.27522800	-2.06761300	0.90595100
C	2.86814300	-0.40833000	2.60498500
C	3.77588300	-2.93389600	1.87773700
H	3.23829300	-2.40014500	-0.13038100
C	3.37651400	-1.26777100	3.57089100
H	2.49589000	0.57520200	2.89630100
C	3.83140400	-2.53597500	3.20927800
H	4.12300600	-3.92441500	1.58769600
H	3.41164500	-0.95040400	4.61173400
H	4.22308100	-3.21295400	3.96655300
C	3.40737500	1.69040800	0.02238600
C	4.74300300	1.36802100	-0.24753800
C	3.06425300	3.02142400	0.27760200
C	5.71525300	2.36362000	-0.27593100
H	5.02595800	0.32998000	-0.42845300
C	4.03963300	4.01542800	0.26154200
H	2.02071800	3.27321600	0.47301300
C	5.36445000	3.68829200	-0.01880000
H	6.75063700	2.10414300	-0.49111200
H	3.76255400	5.04868000	0.46514900
H	6.12699100	4.46546300	-0.03318600
C	-3.38883000	-0.36857000	1.46263700
C	-2.78467600	-0.65640000	2.69018600
C	-4.69541600	-0.81625100	1.22655700
C	-3.47024900	-1.38583700	3.65943600
H	-1.76948400	-0.30747900	2.87784000
C	-5.37659100	-1.54993700	2.19159300
H	-5.18969800	-0.58147600	0.28272500
C	-4.76327200	-1.83670700	3.41069000
H	-2.98786800	-1.60384700	4.61064800
H	-6.38991500	-1.89573100	1.99408600
H	-5.29686500	-2.41003500	4.16693500
C	-3.55038900	2.10743100	0.04586100

C	-3.25113600	3.24037900	0.81127800
C	-4.65626400	2.14155900	-0.81204500
C	-4.04800900	4.37847700	0.73100700
H	-2.38178100	3.22786100	1.46925700
C	-5.44963500	3.28277300	-0.89612800
H	-4.90145200	1.27320300	-1.42377800
C	-5.14751600	4.40227000	-0.12427700
H	-3.80354300	5.25238000	1.33238600
H	-6.30447300	3.29840000	-1.57042400
H	-5.76684200	5.29502500	-0.19255600
H	-3.64939500	-0.84376600	-1.41591900
H	-2.76197500	0.49674200	-2.16715000
Ru	-0.16210000	0.83293800	0.35161000
H	-0.11853300	-0.40145600	1.36870600
C	0.88616200	-1.22733100	-1.76013000
H	0.89920100	-2.12011500	-1.10344000
H	0.83423900	-1.61242400	-2.79629300
C	-1.50599200	-1.16530400	-1.61747200
H	-1.56884200	-1.60287900	-2.63207600
H	-1.52741700	-2.01969900	-0.91322700
C	0.19293200	2.95931700	-2.36815700
H	0.11426700	3.93379800	-1.84564600
H	-0.15795400	3.10403500	-3.41348600
O	1.54789600	2.55076200	-2.40277400
C	2.37387900	3.52722400	-2.97962200
H	2.34255000	4.47701600	-2.41749600
H	3.39905600	3.14429400	-2.96314100
H	2.09092800	3.73983700	-4.02574700
O	-0.56454100	2.03144400	-1.71257700
H	-0.36646600	0.94719400	-1.96990100

**B6**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	0.06345600	-1.38364900	-1.19237100
C	2.47264100	-1.52730800	-0.90102100
H	2.62570900	-1.00703700	-1.85544900
H	3.33479400	-2.18509500	-0.73475000
C	-2.29045700	-0.94386700	-1.61426600
C	0.04572400	1.72895600	1.44550800
O	0.03254600	2.61355000	2.21753100
P	-2.21989800	0.33646700	-0.27487500
P	2.31343300	-0.22595500	0.40259500
C	2.99847200	-0.98166000	1.92321500

C	4.29410200	-1.51624000	1.94486600
C	2.24080200	-0.98397800	3.09790100
C	4.81252900	-2.05692900	3.11619400
H	4.90559100	-1.49565900	1.04139700
C	2.76476200	-1.51875500	4.27298600
H	1.23602300	-0.56218600	3.07854900
C	4.04708000	-2.05853900	4.28256600
H	5.81936000	-2.47153800	3.12299100
H	2.16706500	-1.51223800	5.18287700
H	4.45635500	-2.47697800	5.20068300
C	3.56668600	1.03708800	-0.00133100
C	4.36251700	1.01712200	-1.15030100
C	3.67462000	2.12285300	0.87985900
C	5.24411400	2.06384000	-1.41453600
H	4.29942200	0.18803800	-1.85290100
C	4.55924700	3.16125700	0.61836000
H	3.05277100	2.15567800	1.77537900
C	5.34340100	3.13668800	-0.53426300
H	5.85341100	2.03846600	-2.31640600
H	4.62922200	3.99829400	1.31085800
H	6.02972100	3.95490700	-0.74573200
C	-3.43216400	-0.21629700	0.97617400
C	-3.11792400	-0.09139600	2.33348200
C	-4.68697500	-0.72561500	0.61450400
C	-4.03626500	-0.47011600	3.30942900
H	-2.14079800	0.29796700	2.61821900
C	-5.59963800	-1.11406400	1.59007900
H	-4.96265300	-0.80440300	-0.43750800
C	-5.27511200	-0.98638000	2.93951600
H	-3.77941100	-0.36531500	4.36216300
H	-6.56926500	-1.51242500	1.29571700
H	-5.99060500	-1.28938900	3.70225600
C	-3.00845900	1.79326400	-1.04535300
C	-2.40888800	2.34641200	-2.18760500
C	-4.13158500	2.41781700	-0.49212200
C	-2.94588800	3.48810600	-2.77311200
H	-1.49684100	1.90323700	-2.59072900
C	-4.66269400	3.56125600	-1.08333000
H	-4.59700300	2.01358700	0.40560800
C	-4.07595900	4.09539900	-2.22699400
H	-2.46480600	3.90902100	-3.65566500
H	-5.53901700	4.03627300	-0.64463800
H	-4.49237500	4.99055200	-2.68676700
H	-3.29203800	-1.37777200	-1.71998300



H	-2.06665700	-0.42478800	-2.55686400
Ru	0.05344800	0.32414700	0.25975000
H	-0.30835200	-0.68858200	1.49816000
C	1.17851600	-2.31968200	-0.98293400
H	0.98425400	-2.86862600	-0.05177000
H	1.22959000	-3.05635900	-1.80099400
C	-1.25128600	-2.01977500	-1.36065300
H	-1.23130200	-2.74286400	-2.19217500
H	-1.47357200	-2.57675100	-0.44057600
C	0.80023700	2.49343900	-1.81402600
H	1.81813500	2.81145500	-1.46527600
H	0.06248400	3.11667600	-1.24028200
O	0.68648400	2.89698200	-3.19272900
C	0.93969400	4.26179400	-3.32707900
H	1.96668000	4.52995500	-3.01120900
H	0.82198700	4.52725800	-4.38409800
H	0.24123900	4.88031600	-2.73036900
O	0.58053900	1.17472800	-1.73455400
H	0.26433200	-0.80547400	-2.01838500

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**TSB6**  
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**Coordinates (Angstroms)**  
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	<b>X</b>	<b>Y</b>	<b>Z</b>
N	0.19041000	-1.16549400	-1.22556400
C	2.56010000	-1.51523900	-0.74148200
H	2.88040800	-1.04285600	-1.67637900
H	3.31393100	-2.25031400	-0.43354500
C	-2.07397700	-0.56698900	-1.87740600
C	0.02212000	1.67862800	1.70059600
O	-0.07128000	2.37562000	2.64044700
P	-2.11297700	0.52502300	-0.39272200
P	2.38084300	-0.15344800	0.49414700
C	2.96627700	-0.88476600	2.07092900
C	4.25328400	-1.43146700	2.17053400
C	2.14237600	-0.88539400	3.20033400
C	4.69984600	-1.97563000	3.36921700
H	4.91660400	-1.41818400	1.30417800
C	2.59190900	-1.42643200	4.40353900
H	1.14279800	-0.45685100	3.13155200
C	3.86810800	-1.97400600	4.48877500
H	5.70188000	-2.39669300	3.43378000
H	1.94115000	-1.41781600	5.27626600
H	4.22029100	-2.39552800	5.42875400
C	3.67476000	1.06750000	0.10561000

C	4.78233800	0.77460200	-0.69709200
C	3.55256000	2.34912700	0.65509300
C	5.74518000	1.74770200	-0.94787600
H	4.89276500	-0.21429200	-1.14065200
C	4.51700300	3.31967600	0.40448000
H	2.68829100	2.59137600	1.27483000
C	5.61480500	3.02128800	-0.39907300
H	6.59926500	1.50956700	-1.57982000
H	4.40570700	4.31418700	0.83296200
H	6.36732300	3.78183800	-0.60008900
C	-3.35992000	-0.23803000	0.71435300
C	-3.09341200	-0.38559800	2.07896500
C	-4.60669100	-0.64160200	0.21858400
C	-4.04875300	-0.93861900	2.92907000
H	-2.12996200	-0.06314000	2.47265800
C	-5.55606900	-1.20280000	1.06566100
H	-4.84264400	-0.50632400	-0.83798200
C	-5.27680700	-1.35412600	2.42317100
H	-3.82923900	-1.04642400	3.98996500
H	-6.51839900	-1.51950500	0.66693500
H	-6.02074100	-1.79112500	3.08708600
C	-2.96934800	2.03882700	-0.94102200
C	-3.68802400	2.10383800	-2.13974500
C	-2.93010300	3.16404800	-0.10819000
C	-4.35682300	3.27189700	-2.49636900
H	-3.72195900	1.24310900	-2.80668300
C	-3.60282600	4.32836900	-0.46447400
H	-2.36483600	3.12763100	0.82427300
C	-4.31528100	4.38493000	-1.66088500
H	-4.90947200	3.31179500	-3.43380000
H	-3.56394000	5.19678800	0.19059400
H	-4.83778700	5.29766000	-1.94223700
H	-3.06656100	-0.94238900	-2.15679600
H	-1.69552000	0.05794500	-2.69900600
Ru	0.12971700	0.47763100	0.30357500
H	-0.27011200	-0.66021300	1.32865600
C	1.20954200	-2.18441100	-0.94548400
H	0.90469600	-2.74287100	-0.04828600
H	1.26930300	-2.90565700	-1.77738400
C	-1.11046800	-1.71083300	-1.61584300
H	-1.01270700	-2.34242000	-2.51370900
H	-1.47781200	-2.35435500	-0.80189300
C	1.06056600	2.04360700	-2.10708000
H	1.72960400	2.87822300	-2.46489900

H	0.72427300	2.39310000	-1.06697200
O	-0.15742100	2.14223500	-2.91638600
C	-0.60267100	3.46363200	-2.98181800
H	0.14458300	4.12563000	-3.45989100
H	-1.52272600	3.49197400	-3.57601200
H	-0.82414800	3.88608400	-1.98210800
O	1.59133700	0.84595700	-2.16276600
H	0.57672700	-0.49799500	-1.94067000

**B6'**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	0.10275700	-1.76261600	-1.41155600
C	2.46348600	-2.04608200	-0.94122000
H	2.71215300	-1.53567500	-1.88236000
H	3.27335100	-2.74527800	-0.69913500
C	-2.16573200	-1.20603200	-2.05672900
C	-0.05746600	1.22027400	1.35573500
O	-0.12971700	2.03033300	2.20270600
P	-2.22558100	-0.08332800	-0.59843900
P	2.25873400	-0.72608600	0.33851000
C	2.85415400	-1.46516100	1.90274400
C	4.12646800	-2.04708900	1.98196900
C	2.04929200	-1.42833900	3.04512700
C	4.57948900	-2.59013200	3.17882500
H	4.77254000	-2.06420500	1.10296700
C	2.50716000	-1.96745800	4.24566900
H	1.05960800	-0.97569600	2.98476300
C	3.76851000	-2.55143000	4.31291000
H	5.56891200	-3.04156200	3.22945500
H	1.87338300	-1.93202400	5.12994900
H	4.12564700	-2.97299700	5.25093100
C	3.53933600	0.51016300	-0.06771100
C	4.67796900	0.20361600	-0.82209400
C	3.35942000	1.82245100	0.38824500
C	5.62012600	1.18853200	-1.10699200
H	4.83048300	-0.80743000	-1.19888400
C	4.30536000	2.80280100	0.10916800
H	2.46410500	2.07672400	0.95658100
C	5.43691000	2.48743800	-0.64041600
H	6.49804300	0.93930300	-1.70039500
H	4.15269400	3.81856900	0.46954600
H	6.17334300	3.25668000	-0.86624500
C	-3.47768200	-0.83183000	0.51439900

C	-3.22412900	-0.95172400	1.88375600
C	-4.71910300	-1.24716300	0.01419200
C	-4.18724900	-1.48884200	2.73536900
H	-2.26234400	-0.62316400	2.27697800
C	-5.67482500	-1.79550600	0.86275400
H	-4.94617000	-1.13235400	-1.04670700
C	-5.40885400	-1.91889700	2.22576000
H	-3.97807200	-1.57447700	3.80041000
H	-6.63186100	-2.12390400	0.46070900
H	-6.15804200	-2.34542300	2.89063400
C	-3.09949200	1.41700400	-1.16041500
C	-3.60932700	1.56628700	-2.45364200
C	-3.25584700	2.46214600	-0.24046200
C	-4.27260100	2.73714600	-2.81520500
H	-3.48148600	0.77588500	-3.19111300
C	-3.91905700	3.62856200	-0.60296800
H	-2.85007500	2.36062100	0.76711400
C	-4.43017800	3.76780800	-1.89271300
H	-4.66363800	2.84324300	-3.82579000
H	-4.03368900	4.43237400	0.12209500
H	-4.94880200	4.68146300	-2.17832500
H	-3.15359900	-1.57961800	-2.35389100
H	-1.75163700	-0.61912200	-2.88990900
Ru	0.02245500	-0.11922900	0.08185700
H	-0.38803000	-1.20958000	1.21319000
C	1.13876600	-2.76699800	-1.11941100
H	0.85216900	-3.31863800	-0.21373400
H	1.20923000	-3.49265700	-1.94594000
C	-1.20942200	-2.34252100	-1.74103100
H	-1.11828600	-3.01773100	-2.60680700
H	-1.56029500	-2.93987500	-0.88748800
C	0.82765400	0.97577500	-2.69062400
H	1.69157900	1.69255100	-2.64816900
H	0.63508400	0.81958800	-1.49310600
O	-0.33439100	1.72623500	-3.07998200
C	-0.41420500	2.93768300	-2.38270700
H	0.46930300	3.57507000	-2.56712100
H	-1.30861100	3.46936500	-2.72289000
H	-0.49109200	2.77538700	-1.28915800
O	0.99908200	-0.11821600	-3.32827200
H	0.42559200	-1.22782700	-2.26730200

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**TSB6'**

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Coordinates (Angstroms)

	X	Y	Z
N	0.08015200	-1.84843700	-1.33767800
C	2.43723700	-2.14319200	-0.83628300
H	2.73754700	-1.68651200	-1.78915600
H	3.22421700	-2.84601600	-0.53616500
C	-2.17495200	-1.25811200	-1.99234600
C	-0.09493100	1.11481700	1.46148800
O	-0.13264200	1.96656900	2.27039500
P	-2.24909500	-0.16546300	-0.50428200
P	2.22625700	-0.76197300	0.38782500
C	2.93176400	-1.39674900	1.95366200
C	4.24134300	-1.89024200	2.01913300
C	2.15365300	-1.37351700	3.11471300
C	4.75603500	-2.36374200	3.22091400
H	4.86723400	-1.89667100	1.12576200
C	2.67310100	-1.84147300	4.31990600
H	1.13349100	-0.99423700	3.05906600
C	3.97116100	-2.33951300	4.37372500
H	5.77398000	-2.74816100	3.26073000
H	2.05850300	-1.81793300	5.21810700
H	4.37624200	-2.70781500	5.31475600
C	3.44146300	0.49063700	-0.15981900
C	4.61245900	0.16423800	-0.85506800
C	3.16071300	1.83875600	0.09664800
C	5.48415900	1.16363600	-1.27973600
H	4.84374100	-0.87735100	-1.07966100
C	4.03684700	2.83609900	-0.31996200
H	2.23292200	2.10385500	0.60528700
C	5.19893700	2.50021900	-1.01118100
H	6.38559800	0.89653400	-1.82883800
H	3.80288500	3.87974800	-0.11623200
H	5.87848000	3.28055100	-1.34960500
C	-3.60262400	-0.90338800	0.49417800
C	-3.35716100	-1.39823900	1.77674500
C	-4.90101100	-0.97978000	-0.03007100
C	-4.38871200	-1.97104900	2.51917600
H	-2.34657800	-1.33361000	2.18085400
C	-5.92769300	-1.55549100	0.70916100
H	-5.11096400	-0.57746300	-1.02252300
C	-5.67171800	-2.05378100	1.98633100
H	-4.18672800	-2.35299500	3.51868800
H	-6.93130700	-1.61319000	0.29061600
H	-6.47620600	-2.50342100	2.56620900
C	-3.02446700	1.38757400	-1.07097000

C	-3.43074800	1.61147200	-2.39018800
C	-3.20034600	2.40686900	-0.12437600
C	-4.00378100	2.82874000	-2.75405900
H	-3.29662300	0.83990500	-3.14624300
C	-3.77508000	3.61901300	-0.48820800
H	-2.87961400	2.24753900	0.90601800
C	-4.17778800	3.83303000	-1.80614500
H	-4.31346600	2.99011200	-3.78546300
H	-3.90564200	4.40054400	0.25826700
H	-4.62502500	4.78336600	-2.09322000
H	-3.16635200	-1.61285700	-2.30192000
H	-1.74447200	-0.67019300	-2.81630200
Ru	-0.02668400	-0.23112700	0.20243500
H	-0.38648600	-1.41450400	1.33384500
C	1.10874100	-2.85496400	-1.02703900
H	0.80280300	-3.38738000	-0.11755700
H	1.18502600	-3.59250900	-1.84273300
C	-1.23596800	-2.41157000	-1.68279000
H	-1.14907800	-3.08428300	-2.55101700
H	-1.59321800	-3.00680100	-0.83102700
C	0.84350600	1.03454200	-2.66054400
H	1.75034400	1.57992800	-2.31327400
H	0.41318700	0.77940900	-1.19039400
O	-0.17063500	1.90827800	-2.99560600
C	-0.18935700	3.07351800	-2.19570800
H	0.78237400	3.59269800	-2.21965400
H	-0.95996600	3.73249600	-2.60280000
H	-0.42874700	2.82338800	-1.14884300
O	0.93133700	-0.03732200	-3.28358000
H	0.40565800	-1.31277500	-2.16454000

**B7**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	-0.03219600	-0.90363500	-1.48166400
C	2.40792200	-1.01282000	-1.36707200
H	2.49765800	-0.26690800	-2.16904100
H	3.29412300	-1.65514500	-1.44261700
C	-2.46592400	-0.62495700	-1.46621200
C	0.17262800	1.64696700	1.73993600
O	0.25254300	2.37990600	2.65448100
P	-2.22516500	0.54652000	-0.04243400
P	2.31742300	-0.07082700	0.22317400
C	2.95833900	-1.21046200	1.50721600

C	2.65600700	-0.91061100	2.84258000
C	3.72543700	-2.34785300	1.23230300
C	3.11749400	-1.71930100	3.87411700
H	2.03585000	-0.04301200	3.06932600
C	4.17431000	-3.16825100	2.26594000
H	3.97465500	-2.61135800	0.20514800
C	3.87458300	-2.85443900	3.58784700
H	2.87352700	-1.46984400	4.90518600
H	4.76053900	-4.05588100	2.03315700
H	4.22473300	-3.49619000	4.39468300
C	3.65562200	1.17020700	0.07993100
C	5.00488800	0.79429400	0.04268600
C	3.32131900	2.52539300	-0.00502800
C	5.99924200	1.75716800	-0.09347000
H	5.28032100	-0.25781700	0.12952700
C	4.31976200	3.48819700	-0.13539900
H	2.27055300	2.81496800	0.02319100
C	5.65713800	3.10619900	-0.18164400
H	7.04496500	1.45557200	-0.12463400
H	4.04853200	4.54064300	-0.19798700
H	6.43682800	3.85948400	-0.28273500
C	-3.33516000	-0.09219100	1.27428200
C	-2.87282200	-0.11820100	2.59413800
C	-4.63964900	-0.52701200	1.00835600
C	-3.69790000	-0.56187200	3.62451100
H	-1.85129200	0.19561900	2.80431300
C	-5.45951300	-0.98285700	2.03561300
H	-5.02697100	-0.51285200	-0.01039000
C	-4.99007700	-0.99842900	3.34760400
H	-3.32372800	-0.57394000	4.64676500
H	-6.46856400	-1.32490700	1.81065800
H	-5.63234300	-1.35279100	4.15229000
C	-3.08889400	2.06855200	-0.59047000
C	-2.51383200	3.30681800	-0.28384000
C	-4.30866200	2.04001800	-1.28021600
C	-3.15912300	4.49099300	-0.63033500
H	-1.54695400	3.33334500	0.21865500
C	-4.94899300	3.22418500	-1.63360500
H	-4.76562000	1.08572000	-1.54588100
C	-4.37890200	4.45228500	-1.30099200
H	-2.70004800	5.44687300	-0.38290900
H	-5.89605900	3.18835700	-2.17012900
H	-4.88347800	5.37811400	-1.57344700
H	-3.42687100	-1.15171500	-1.41275300

H	-2.48074900	-0.02542500	-2.38762300
Ru	0.07213900	0.51498700	0.29659500
H	-0.18103400	-0.88318200	1.23795100
C	1.12879900	-1.81171700	-1.53563200
H	1.01229900	-2.53840900	-0.71997100
H	1.13578800	-2.37086000	-2.48526200
C	-1.32045500	-1.61883700	-1.50628700
H	-1.39260100	-2.25727900	-2.40228500
H	-1.34329500	-2.27004800	-0.62329200
H	0.01629600	-0.28742300	-2.30151700
H	0.31308200	1.85436200	-0.78082300
C	-0.67588000	2.11901300	-3.67652600
H	-1.56086800	1.82193600	-3.06762400
H	-0.85569400	1.80597000	-4.72162700
O	-0.52910400	3.51232300	-3.59246900
C	-1.70130100	4.15949100	-4.01114100
H	-2.59152700	3.79137300	-3.47192300
H	-1.58215300	5.22685100	-3.80342600
H	-1.87989700	4.02567700	-5.09328900
O	0.48324200	1.50089700	-3.25523800
H	0.55547000	1.69800100	-2.27885800

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**TSB7**  
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**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	0.03174800	-0.94727500	-1.36989100
C	2.43369500	-1.26402900	-1.14453400
H	2.59997900	-0.62468700	-2.02149800
H	3.25908900	-1.98396800	-1.07420900
C	-2.37392400	-0.54153300	-1.60909000
C	0.06197600	1.53166500	1.85709700
O	0.02021500	2.11641000	2.87029000
P	-2.21661700	0.54017200	-0.12761000
P	2.33985000	-0.16326800	0.33076700
C	2.99044900	-1.17278700	1.71197800
C	2.22345500	-1.40926200	2.85610700
C	4.27839400	-1.71998700	1.62815600
C	2.73188700	-2.18891200	3.89366900
H	1.22367100	-0.98195100	2.92843300
C	4.78175600	-2.50087700	2.66123500
H	4.89482000	-1.52465700	0.74939900
C	4.00711000	-2.73778900	3.79634600
H	2.12628200	-2.36803300	4.78038100
H	5.78217400	-2.92331500	2.58350300



H	4.40177500	-3.34840400	4.60685300
C	3.65383500	1.08058300	0.08556000
C	4.64682400	0.93834000	-0.88973600
C	3.66728300	2.21419000	0.90926900
C	5.63488800	1.90886000	-1.03695900
H	4.65195600	0.06804600	-1.54432100
C	4.65869300	3.17877300	0.76501000
H	2.89067800	2.34199800	1.66474000
C	5.64379000	3.02800100	-0.20963500
H	6.39842200	1.78848400	-1.80343700
H	4.65805500	4.05510600	1.41067400
H	6.41473200	3.78736100	-0.32779400
C	-3.31294900	-0.17802700	1.14545700
C	-3.63751300	0.59646200	2.26727800
C	-3.79229800	-1.48922300	1.06706200
C	-4.43637700	0.07504900	3.27829600
H	-3.26647400	1.61962600	2.34284800
C	-4.59143000	-2.01063300	2.08198900
H	-3.54296700	-2.11504600	0.21102600
C	-4.91720100	-1.23040600	3.18733300
H	-4.68573600	0.69054300	4.14084800
H	-4.96126800	-3.03188300	2.00511700
H	-5.54428900	-1.63803200	3.97840200
C	-3.07649300	2.09297300	-0.55423500
C	-2.44412700	3.31999900	-0.33536500
C	-4.37085700	2.07466200	-1.08989300
C	-3.09551500	4.51199200	-0.64385200
H	-1.43265000	3.33716600	0.07291200
C	-5.01640700	3.26533100	-1.40634000
H	-4.87870300	1.12351500	-1.25545400
C	-4.37940900	4.48561300	-1.18194200
H	-2.59465800	5.46256300	-0.46885400
H	-6.02055200	3.24206200	-1.82659000
H	-4.88801300	5.41687700	-1.42631700
H	-3.36843800	-0.99632600	-1.69961400
H	-2.23080100	0.12584400	-2.46815300
Ru	0.08409700	0.48369900	0.31288800
H	-0.24311100	-0.78210800	1.23949400
C	1.09112600	-1.95599100	-1.29641600
H	0.90699400	-2.64351900	-0.45224700
H	1.09329800	-2.56773200	-2.21607100
C	-1.26923300	-1.58399700	-1.57431500
H	-1.26577100	-2.15411200	-2.52072400
H	-1.45478100	-2.31437800	-0.76623100

H	0.32976100	-0.19437000	-2.30876400
H	0.59113800	2.16705500	-0.65226700
C	-0.18545500	1.11280400	-3.92699000
H	-0.90177800	0.34022000	-4.32923700
H	0.19306400	1.67615400	-4.81255600
O	-1.00750400	2.04397100	-3.16663000
C	-2.06962300	2.52746700	-3.93313100
H	-2.78068100	1.72696800	-4.22136100
H	-2.60968900	3.27449600	-3.34043500
H	-1.72037600	3.00628400	-4.86727800
O	0.79401300	0.62535100	-3.17296600
H	0.51254000	1.77665100	-1.33147300

**B8**

**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	-0.21720300	-1.61076900	-0.91211600
C	2.15177400	-2.02632000	-0.53800400
H	2.45686100	-1.79047300	-1.56720400
H	2.89756900	-2.71543900	-0.12088000
C	-2.57287800	-1.18492700	-1.36049600
C	-0.11885200	1.67436900	1.42008200
O	-0.10696600	2.57839600	2.17307400
P	-2.46905200	0.02953500	0.01504900
P	2.08159400	-0.42864500	0.39521300
C	2.91467800	-0.75849500	1.99210200
C	4.20682000	-1.29796100	2.03521100
C	2.25907600	-0.46823100	3.19221500
C	4.82665800	-1.55009400	3.25375300
H	4.73609900	-1.51907600	1.10717500
C	2.88273800	-0.71811600	4.41311100
H	1.25260700	-0.05158200	3.16189000
C	4.16345600	-1.26078000	4.44587500
H	5.83063000	-1.97117800	3.27479200
H	2.36158600	-0.48838300	5.34101300
H	4.64916900	-1.45716800	5.40043500
C	3.27663500	0.64666600	-0.49064400
C	4.34533500	0.14511800	-1.24657900
C	3.08560200	2.03343700	-0.43183900
C	5.20496700	1.01054100	-1.91905300
H	4.51192100	-0.93066900	-1.31181000
C	3.94382700	2.89752100	-1.10467800
H	2.23872100	2.42934700	0.13023000
C	5.00507000	2.38762600	-1.84961200

H	6.03325900	0.60700500	-2.49993100
H	3.77709200	3.97202800	-1.05384900
H	5.67423300	3.06325500	-2.38003400
C	-3.45943600	-0.65845500	1.38961000
C	-3.30316500	-0.07012200	2.65231000
C	-4.36247500	-1.71678200	1.24587900
C	-4.04602600	-0.51668600	3.73877200
H	-2.58297500	0.73939700	2.77978100
C	-5.09750600	-2.17278600	2.33916600
H	-4.49569400	-2.19827900	0.27798200
C	-4.94484900	-1.57130900	3.58470600
H	-3.91608600	-0.04678100	4.71216200
H	-5.79234400	-3.00186400	2.21348300
H	-5.52102300	-1.92699800	4.43731600
C	-3.47402300	1.45828300	-0.52906100
C	-2.84894000	2.68974500	-0.74953600
C	-4.85530200	1.34497400	-0.73540700
C	-3.59247800	3.78882300	-1.17431600
H	-1.77481900	2.77838100	-0.58773700
C	-5.59487600	2.44239600	-1.16224800
H	-5.35604500	0.39380100	-0.54769700
C	-4.96342000	3.66649700	-1.38165300
H	-3.09755800	4.74445700	-1.33949700
H	-6.66817900	2.34524900	-1.31869500
H	-5.54480600	4.52694000	-1.70909500
H	-3.57590500	-1.60867200	-1.50231900
H	-2.32255000	-0.62494500	-2.27267000
Ru	-0.16922300	0.15866900	0.32949100
H	-0.36804600	-0.74810700	1.62757900
C	0.75313000	-2.62317600	-0.55099500
H	0.54046200	-3.08996200	0.43665000
H	0.73204600	-3.45833600	-1.28080500
C	-1.51042200	-2.23789600	-1.09519900
H	-1.47908200	-2.95206400	-1.94337200
H	-1.81877200	-2.84704200	-0.21240600
C	0.82074100	0.88032200	-2.56239400
O	0.09712500	1.44692900	-1.76713400
H	1.05747500	-0.20062100	-2.48832400
O	1.35028400	1.52749900	-3.59481500
C	2.19229500	0.76845200	-4.46742900
H	1.66153500	0.59028400	-5.40768000
H	3.08909700	1.36271400	-4.65582300
H	2.47297100	-0.18984400	-4.01374400

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**TSB8**

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.14635800	-1.36892900	-1.18077300
C	2.27048800	-1.60187500	-1.06661500
H	2.41338100	-1.06283000	-2.01420500
H	3.12745600	-2.27972500	-0.96190800
C	-2.52613600	-0.94082100	-1.41427600
C	0.09483100	1.79297100	1.36075800
O	0.16252000	2.69954300	2.10325700
P	-2.34023100	0.25034900	-0.01732200
P	2.21780700	-0.30176900	0.24204000
C	2.84749800	-1.07883400	1.77008400
C	2.92161400	-0.27642000	2.91772500
C	3.22978900	-2.42039300	1.85832400
C	3.38897000	-0.79898400	4.11719500
H	2.60621400	0.76653900	2.86636900
C	3.69092400	-2.94552100	3.06495200
H	3.17016300	-3.07003600	0.98647600
C	3.77504700	-2.13686000	4.19364900
H	3.44490500	-0.16206900	4.99815200
H	3.98469300	-3.99257000	3.11863600
H	4.13722900	-2.54762800	5.13441700
C	3.56428400	0.84590400	-0.21725900
C	4.91236600	0.48500600	-0.09190500
C	3.23446100	2.10330800	-0.73465300
C	5.91335800	1.36569500	-0.48704900
H	5.17866700	-0.48773000	0.32387100
C	4.24063000	2.98260000	-1.12905600
H	2.18555400	2.38158300	-0.83606000
C	5.57777900	2.61584000	-1.00573900
H	6.95894500	1.07844700	-0.38666800
H	3.97569600	3.95954800	-1.52983400
H	6.36317000	3.30559900	-1.31118300
C	-3.30159900	-0.44340100	1.37577000
C	-2.98758800	-0.00193000	2.66818700
C	-4.34354500	-1.36329000	1.21276300
C	-3.71239300	-0.45255000	3.76585500
H	-2.16209600	0.69593500	2.81002100
C	-5.06079300	-1.82433000	2.31476600
H	-4.60408400	-1.73025100	0.22041700
C	-4.74923000	-1.36732200	3.59188100
H	-3.45775700	-0.09726700	4.76293300
H	-5.86386000	-2.54577200	2.17260400

H	-5.31075100	-1.72717800	4.45241500
C	-3.32539000	1.70441400	-0.52579200
C	-2.66415600	2.90042900	-0.82484300
C	-4.72112500	1.64688000	-0.63108800
C	-3.38976100	4.02058600	-1.22470800
H	-1.57809300	2.94399400	-0.74927100
C	-5.44219400	2.76586900	-1.03305900
H	-5.24836600	0.72497800	-0.38154700
C	-4.77630400	3.95463700	-1.32916200
H	-2.86679800	4.94801500	-1.45208600
H	-6.52707300	2.71328000	-1.10914000
H	-5.34262000	4.83249900	-1.63595600
H	-3.53406900	-1.36726100	-1.49335400
H	-2.35882500	-0.35455000	-2.32930300
Ru	-0.02335600	0.33608000	0.21925600
H	-0.20895500	-0.61586700	1.49906600
C	0.94001000	-2.34010800	-1.09516900
H	0.82481300	-2.97348900	-0.19739500
H	0.91348500	-3.02183800	-1.96636800
C	-1.45298300	-2.01103500	-1.28553300
H	-1.48298200	-2.67766800	-2.16798400
H	-1.64658800	-2.64813900	-0.40376500
C	0.24611900	0.67336000	-2.80247500
O	0.20881500	1.51214900	-1.88694600
H	0.04283400	-0.62062000	-2.21223200
O	0.44125700	1.20550200	-4.03854800
C	0.48481500	0.25824300	-5.09546500
H	-0.33965900	0.45509300	-5.79070900
H	1.43506000	0.36600800	-5.63025900
H	0.39801900	-0.76567700	-4.70655700

**B9**

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Coordinates (Angstroms)			
	X	Y	Z
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N	-0.16483300	-1.47629300	-1.14872300
C	2.25259300	-1.64550600	-1.04263000
H	2.32959400	-1.11699700	-2.00441800
H	3.13012400	-2.29972300	-0.97235300
C	-2.54223200	-1.02983600	-1.35395900
C	0.07555800	1.79195100	1.29506400
O	0.13438100	2.71859100	2.01131300
P	-2.35815400	0.22481900	-0.00883900
P	2.22161300	-0.32461500	0.24802900
C	2.80282700	-1.10917200	1.79329400

C	2.57493500	-0.42396000	2.99462100
C	3.46805500	-2.33907800	1.83664900
C	3.01715700	-0.94692100	4.20413300
H	2.03547400	0.52344000	2.97863800
C	3.89804100	-2.86994600	3.05160800
H	3.65991500	-2.89621000	0.92066900
C	3.67749500	-2.17417900	4.23596300
H	2.83530700	-0.39915400	5.12716100
H	4.40946500	-3.83114900	3.06842200
H	4.01599300	-2.58825100	5.18407200
C	3.60340400	0.77512100	-0.22440500
C	4.93242200	0.46701200	0.09305800
C	3.31969300	1.93835300	-0.95117900
C	5.96364800	1.30498000	-0.31858900
H	5.16015700	-0.42787300	0.67312500
C	4.35711300	2.77143100	-1.36277300
H	2.28627700	2.17907200	-1.20157000
C	5.67690400	2.45745800	-1.04808600
H	6.99391800	1.05952300	-0.06602100
H	4.12890800	3.67282100	-1.92896600
H	6.48517700	3.11367300	-1.36731900
C	-3.27982700	-0.43869900	1.42344300
C	-2.92884700	0.01927600	2.70025500
C	-4.32681900	-1.35976100	1.30235800
C	-3.61783400	-0.42126200	3.82499000
H	-2.10030600	0.71919300	2.80889700
C	-5.00810000	-1.81048100	2.43103000
H	-4.62349300	-1.73124000	0.32202500
C	-4.65677200	-1.34047800	3.69316500
H	-3.33416800	-0.05295500	4.80936100
H	-5.81589800	-2.53215000	2.32071200
H	-5.18998800	-1.69235600	4.57474800
C	-3.36749400	1.64179400	-0.56876200
C	-2.72879700	2.67128000	-1.27330900
C	-4.74353400	1.72711300	-0.32288200
C	-3.46422900	3.75978600	-1.73478300
H	-1.65631900	2.60799400	-1.46188700
C	-5.47158700	2.81978300	-0.78357800
H	-5.24740900	0.94239200	0.24130800
C	-4.83325600	3.83692800	-1.49034000
H	-2.96001800	4.55550800	-2.28035800
H	-6.54039200	2.87976700	-0.58378300
H	-5.40372200	4.69438800	-1.84398100
H	-3.55462300	-1.44690000	-1.42188500

H	-2.35553900	-0.48957100	-2.29397500
Ru	-0.02963600	0.31799700	0.19284900
H	-0.21104100	-0.61260800	1.50315400
C	0.94876400	-2.42423500	-1.00256500
H	0.82874800	-2.95991900	-0.04984700
H	0.92274500	-3.17303100	-1.81113700
C	-1.48973900	-2.11070300	-1.17621700
H	-1.54734300	-2.84381800	-1.99748200
H	-1.63445300	-2.65785800	-0.23337900
C	0.25511000	0.77269600	-2.86935100
O	0.21902700	1.45376700	-1.81179700
H	-0.03047700	-0.95919800	-2.05648200
O	0.44352400	1.61250400	-3.95076300
C	0.50900900	0.94934200	-5.19644100
H	-0.26484000	1.34716700	-5.86543300
H	1.49118400	1.12114000	-5.65630300
H	0.35512700	-0.13039600	-5.06015800

**TSB9**

**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	0.09635000	-1.55553600	-1.15190900
C	2.52635100	-1.57062200	-0.93287000
H	2.65827600	-1.04341300	-1.88814800
H	3.41178000	-2.19923500	-0.77208900
C	-2.32243000	-1.30672400	-1.41685500
C	-0.04587200	1.54356200	1.54110800
O	-0.11384100	2.35499900	2.38432900
P	-2.24357800	0.03410500	-0.14262500
P	2.33633800	-0.27045400	0.37115500
C	2.99374300	-1.06152700	1.88909700
C	4.25324000	-1.67607100	1.89353100
C	2.24939400	-1.03286900	3.07247300
C	4.74981000	-2.26256700	3.05221900
H	4.85706500	-1.68757800	0.98513100
C	2.75043400	-1.61507100	4.23516000
H	1.27120200	-0.55341800	3.07471700
C	3.99720000	-2.23347000	4.22586600
H	5.72825500	-2.73987000	3.04161600
H	2.16125300	-1.58500100	5.15001700
H	4.38698300	-2.69091400	5.13365600
C	3.60935300	0.96676700	-0.04265800
C	4.77543500	0.63627600	-0.74357300
C	3.41816900	2.28668000	0.38032600

C	5.73724600	1.60787600	-1.00748700
H	4.93614800	-0.38413000	-1.09217600
C	4.38333300	3.25405000	0.12169500
H	2.49544900	2.55783400	0.89155500
C	5.54368800	2.91641300	-0.57169700
H	6.63828700	1.34144400	-1.55757700
H	4.22109400	4.27884500	0.45038300
H	6.29461100	3.67643100	-0.78084500
C	-3.29357800	-0.53262100	1.24047400
C	-3.65410600	0.40104200	2.22199900
C	-3.69114900	-1.86424700	1.39587700
C	-4.40566000	0.01210300	3.32475600
H	-3.34542500	1.44209600	2.11774300
C	-4.44272200	-2.25269500	2.50325400
H	-3.41726300	-2.61254400	0.65287700
C	-4.80274300	-1.31675200	3.46813700
H	-4.68193500	0.74979100	4.07598100
H	-4.74831700	-3.29237100	2.60878900
H	-5.39044000	-1.62110000	4.33233300
C	-3.22069300	1.39312100	-0.86454900
C	-2.61931400	2.63734500	-1.07626100
C	-4.55965600	1.19819200	-1.23328300
C	-3.34862200	3.67182900	-1.66031800
H	-1.57184700	2.78256900	-0.81142700
C	-5.28070700	2.23125900	-1.82047000
H	-5.03961500	0.23549000	-1.05167000
C	-4.67328400	3.46922600	-2.03520700
H	-2.87153700	4.63509300	-1.83045400
H	-6.31888700	2.07377600	-2.10836200
H	-5.23872800	4.27791900	-2.49563100
H	-3.29078100	-1.82355800	-1.42244100
H	-2.22607600	-0.79850600	-2.38637300
Ru	0.04069000	0.21743200	0.26338400
H	-0.21513000	-0.87517900	1.40681500
C	1.26891100	-2.42029000	-0.98129600
H	1.13980600	-2.97944800	-0.04305900
H	1.33285300	-3.15758400	-1.79822800
C	-1.17369300	-2.28469600	-1.23492900
H	-1.15350500	-3.00959000	-2.06557700
H	-1.28622200	-2.85746100	-0.30313800
C	0.28556900	1.28739500	-2.12658300
O	0.77633900	2.11494500	-1.34302300
H	0.21597800	-0.94245100	-1.97944600
O	-0.43201300	1.94498300	-3.17102900



C	-1.07405700	1.09529100	-4.08028900
H	-2.16810800	1.11891700	-3.93903200
H	-0.85730300	1.41837700	-5.10760100
H	-0.72395100	0.05380300	-3.96159900

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**B10**

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**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	-0.00783300	-1.10876000	-1.40600500
C	2.43403000	-1.10558100	-1.22896100
H	2.50310800	-0.44514200	-2.10561300
H	3.33925900	-1.72694400	-1.21364300
C	-2.47030500	-1.00004600	-1.32871100
C	-0.03279100	1.42657300	1.85362600
O	-0.05778800	2.02668700	2.85735600
P	-2.30006500	0.32377800	-0.01934400
P	2.29741800	-0.03235800	0.27369100
C	3.02920300	-1.06499400	1.60384100
C	4.32834400	-1.57287100	1.46702000
C	2.31210000	-1.33803700	2.77123800
C	4.88996800	-2.35627700	2.46842600
H	4.91046700	-1.34169400	0.57322500
C	2.88100000	-2.11301400	3.78054100
H	1.30035800	-0.94759700	2.87614500
C	4.16507800	-2.62774700	3.62836400
H	5.89782200	-2.75054600	2.34799600
H	2.31452300	-2.31676800	4.68777200
H	4.60667500	-3.23663700	4.41573000
C	3.59589800	1.22769200	0.03715800
C	4.57516600	1.12116100	-0.95676300
C	3.62244300	2.32869500	0.90279300
C	5.56335900	2.09428400	-1.08319500
H	4.57834600	0.27236300	-1.63963900
C	4.61426600	3.29522600	0.77883300
H	2.84676100	2.43835500	1.65908800
C	5.58515900	3.18120300	-0.21452400
H	6.31821100	1.99958000	-1.86222900
H	4.61886500	4.15042200	1.45222800
H	6.35495600	3.94456500	-0.31489000
C	-3.40030000	-0.26048400	1.32813000
C	-4.53405500	0.45772500	1.72392000
C	-3.10253200	-1.46558200	1.97846900
C	-5.35860700	-0.02552900	2.73746900
H	-4.77994200	1.40152100	1.24071000

C	-3.93618600	-1.95347600	2.97883700
H	-2.19629800	-2.00899200	1.70753300
C	-5.06736000	-1.23379300	3.36165700
H	-6.23391400	0.54851800	3.03670800
H	-3.69503500	-2.89495600	3.47030000
H	-5.71477300	-1.61274900	4.15082700
C	-3.23718300	1.71703100	-0.74418400
C	-2.78074900	3.02378600	-0.54374200
C	-4.38856300	1.50738400	-1.51647200
C	-3.45709200	4.10046500	-1.11231700
H	-1.88029700	3.19622300	0.04565900
C	-5.05803400	2.58352000	-2.09026500
H	-4.76979800	0.49613400	-1.66437100
C	-4.59099300	3.88170500	-1.88997500
H	-3.08647900	5.11155000	-0.95471900
H	-5.94745800	2.40828500	-2.69361000
H	-5.11266000	4.72295600	-2.34340900
H	-3.37937900	-1.59462900	-1.17427800
H	-2.58223100	-0.49442000	-2.29808400
Ru	0.00101200	0.43643100	0.30540000
H	-0.21736700	-1.02259200	1.16957600
C	1.19141600	-1.96616400	-1.32647600
H	1.08203400	-2.58489800	-0.42593900
H	1.24260100	-2.64087400	-2.19596100
C	-1.25266100	-1.90124500	-1.34388800
H	-1.30341400	-2.60663700	-2.18945900
H	-1.19930200	-2.48841500	-0.41902300
C	0.42809200	2.34164100	-0.73143000
O	0.91892900	3.28083200	-0.13261000
H	0.01700100	-0.62961800	-2.30754300
O	0.17945300	2.66781800	-2.09178000
C	-0.44540900	1.73658900	-2.92227900
H	-1.17925300	1.12642800	-2.37757500
H	-0.98226100	2.28666700	-3.70513500
H	0.28259100	1.07154600	-3.42298900

**B11**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	0.18597100	-1.14113900	-1.24457000
C	2.56650300	-1.26718200	-0.72883500
H	2.84903500	-0.71540700	-1.63576600
H	3.40672100	-1.92845000	-0.48395700
C	-2.19174000	-0.81337500	-1.67933200

C	-0.19211100	1.60243300	1.78353100
O	-0.30981800	2.35871700	2.66969000
P	-2.27820800	0.20698800	-0.13538800
P	2.27373600	-0.01586200	0.61543300
C	2.90968000	-0.80942100	2.13540800
C	4.17507500	-1.41217600	2.16630000
C	2.13955600	-0.78746700	3.30179100
C	4.65366600	-1.98787200	3.33872300
H	4.79938700	-1.41576300	1.27172600
C	2.62467300	-1.35332600	4.47839700
H	1.15024000	-0.33256500	3.27333300
C	3.87796300	-1.95810100	4.49730800
H	5.63579600	-2.45791700	3.34991500
H	2.01700100	-1.32572200	5.38106800
H	4.25522500	-2.40480700	5.41586800
C	3.53272300	1.26427100	0.25232600
C	3.54713900	1.83823400	-1.02697000
C	4.41570800	1.75702400	1.21974700
C	4.43859500	2.85727900	-1.33804900
H	2.83597200	1.49768500	-1.78022700
C	5.30320400	2.78476800	0.90789400
H	4.41251200	1.33972900	2.22562200
C	5.32157300	3.33367800	-0.37042200
H	4.43675400	3.28977100	-2.33765100
H	5.98240100	3.15799200	1.67262600
H	6.01451800	4.13803700	-0.61131400
C	-3.41742100	-0.73893400	0.94276400
C	-3.05381700	-1.04500200	2.25667500
C	-4.66977200	-1.15465000	0.46849600
C	-3.92060200	-1.76214200	3.07909700
H	-2.07785800	-0.72586000	2.62112300
C	-5.53021200	-1.87824300	1.28689100
H	-4.98119900	-0.89748900	-0.54493900
C	-5.15476900	-2.18468400	2.59473800
H	-3.62654300	-1.99387400	4.10140500
H	-6.49718700	-2.20233500	0.90540900
H	-5.82850000	-2.75117400	3.23568000
C	-3.28472000	1.65698500	-0.61145800
C	-2.97209700	2.37340200	-1.77434900
C	-4.30587700	2.13277100	0.21958900
C	-3.68262000	3.52057100	-2.10987500
H	-2.15526000	2.04006300	-2.41440300
C	-5.01083300	3.28552500	-0.11459200
H	-4.55412400	1.59904900	1.13594400

C	-4.70514700	3.97945700	-1.28171900
H	-3.42868400	4.06507100	-3.01828000
H	-5.80162000	3.64203500	0.54351600
H	-5.25731600	4.88069400	-1.54258700
H	-3.15034300	-1.29565500	-1.90765400
H	-1.95406300	-0.13477000	-2.50957300
Ru	-0.01613800	0.39646000	0.40018100
H	-0.19583900	-0.96705000	1.42404500
C	1.30235100	-2.06221800	-0.98241200
H	1.03082200	-2.65670700	-0.10046000
H	1.44365800	-2.75545900	-1.82815300
C	-1.08130200	-1.83442800	-1.52636800
H	-0.99102400	-2.45301600	-2.43390200
H	-1.28279000	-2.50805000	-0.68247900
C	0.23176200	1.95663500	-1.04731000
O	0.28282200	3.16407100	-0.94282000
H	0.41666600	-0.54480500	-2.04588100
O	0.35334900	1.42567400	-2.38939300
C	0.54167700	2.40712300	-3.40115800
H	0.66509100	1.86655800	-4.34472600
H	-0.32054400	3.08377300	-3.47446000
H	1.42825600	3.02389200	-3.20552100

**B12**

**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	0.05349500	-1.93362500	-1.81442500
C	2.47693000	-1.99614100	-1.39870200
H	2.70603500	-1.58276800	-2.39174900
H	3.31696000	-2.64759600	-1.12308100
C	-2.39039700	-1.68575200	-1.92723400
P	-2.25661000	-0.29811100	-0.69367900
P	2.26558100	-0.56155500	-0.22963900
C	2.91667000	-1.20048200	1.36597600
C	4.12998100	-1.89515300	1.45283800
C	2.18624200	-0.95752300	2.53505200
C	4.59850200	-2.35187000	2.68035400
H	4.72189300	-2.07784800	0.55477100
C	2.66182800	-1.40942600	3.76506000
H	1.24830500	-0.40387100	2.47307200
C	3.86336300	-2.10835600	3.84004200
H	5.54144300	-2.89411700	2.73389700
H	2.08764300	-1.21168600	4.66882300
H	4.23097700	-2.46310700	4.80172900

C	3.60685900	0.57290000	-0.76909000
C	4.79620300	0.12814800	-1.36197900
C	3.42132900	1.94784000	-0.57615400
C	5.78021300	1.03573100	-1.74397300
H	4.95953200	-0.93670900	-1.53109700
C	4.40878000	2.85424000	-0.95452500
H	2.48468200	2.30273800	-0.14379500
C	5.58960900	2.40071800	-1.53737100
H	6.69911900	0.67586900	-2.20464600
H	4.25064100	3.92039200	-0.79888300
H	6.35956400	3.10967500	-1.83741400
C	-3.27971900	-0.87505800	0.71993900
C	-2.78591100	-0.70711700	2.01901400
C	-4.54437700	-1.44966800	0.54012000
C	-3.54542800	-1.11520900	3.11442400
H	-1.80957700	-0.24152400	2.16334400
C	-5.29568000	-1.86530600	1.63454500
H	-4.95428500	-1.56727300	-0.46410100
C	-4.79499700	-1.69911800	2.92530900
H	-3.15475000	-0.97579100	4.12117700
H	-6.27490000	-2.31666500	1.48138100
H	-5.38374800	-2.02186100	3.78273300
C	-3.32562700	0.99405300	-1.44150600
C	-3.02465000	2.33308900	-1.16276700
C	-4.41870900	0.70418500	-2.26868900
C	-3.80966400	3.35763900	-1.68565700
H	-2.15620100	2.56433100	-0.54392900
C	-5.19935400	1.72936900	-2.79552200
H	-4.66550800	-0.33120900	-2.50674300
C	-4.89814300	3.05796300	-2.50144400
H	-3.56478400	4.39435100	-1.45998900
H	-6.04597500	1.49029800	-3.43752600
H	-5.50949700	3.85902300	-2.91372600
H	-3.34535000	-2.22403000	-1.86166900
H	-2.34207100	-1.24223000	-2.93241300
Ru	0.01530800	-0.06346000	-0.38100200
H	-0.17031300	-1.15087500	0.76286000
C	1.19030700	-2.79766900	-1.45000500
H	0.96530100	-3.21410500	-0.45887900
H	1.28692200	-3.64582200	-2.14963700
C	-1.23368800	-2.64542100	-1.72223100
H	-1.28163000	-3.47705400	-2.44605600
H	-1.28142100	-3.08359600	-0.71607900
C	-0.03258100	1.43699800	0.94371300

O	-0.19752200	1.50450700	2.15659400
H	0.18078400	-1.63587600	-2.78302200
O	0.17714600	2.65495600	0.24465300
C	0.16367600	3.82902500	1.04851100
H	-0.81007100	3.97298000	1.53477700
H	0.93184000	3.79007200	1.83128500
H	0.36515800	4.66776500	0.37497500

**TSB10**

**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	0.10478000	-1.33231500	-1.40916300
C	2.52136900	-1.47335200	-1.00711000
H	2.75222700	-1.04397700	-1.99256100
H	3.34821100	-2.14717900	-0.74681200
C	-2.31851800	-1.00414800	-1.57138200
P	-2.18112400	0.27785400	-0.23795700
P	2.34577600	-0.06074500	0.18625300
C	2.97310700	-0.73026500	1.77726300
C	4.19001200	-1.41896400	1.85577300
C	2.24306800	-0.50566500	2.94881500
C	4.65719400	-1.89284400	3.07721400
H	4.78546400	-1.57727700	0.95514100
C	2.71627200	-0.97138300	4.17390700
H	1.30017500	0.03844400	2.88396000
C	3.91969700	-1.66845700	4.23927300
H	5.60245100	-2.43133300	3.12499800
H	2.14174100	-0.78751500	5.08031500
H	4.28749200	-2.03499700	5.19629800
C	3.70736700	1.06679100	-0.29069200
C	4.81114300	0.66325800	-1.05271100
C	3.63968200	2.39361000	0.15432800
C	5.82511600	1.56635400	-1.36272400
H	4.88783200	-0.36452000	-1.40801100
C	4.65708700	3.29231800	-0.15091200
H	2.77241600	2.72286900	0.72458400
C	5.75006200	2.88190900	-0.91136000
H	6.67704200	1.24005000	-1.95757900
H	4.58974300	4.32115900	0.19849900
H	6.54228300	3.58790500	-1.15516200
C	-3.19180300	-0.41856500	1.13102300
C	-2.66816300	-0.49074300	2.42494300
C	-4.50753200	-0.84487300	0.90530600
C	-3.44121900	-0.99108300	3.47124800

H	-1.64766000	-0.14880900	2.59841500
C	-5.27476700	-1.35502200	1.94689400
H	-4.94047200	-0.76376900	-0.09310400
C	-4.74091000	-1.42917200	3.23323800
H	-3.02406900	-1.03805000	4.47579800
H	-6.29416300	-1.68792900	1.75784000
H	-5.34290900	-1.82324700	4.05044600
C	-3.28099000	1.63450200	-0.79349500
C	-3.43533700	2.72225200	0.07954600
C	-3.92140100	1.67443000	-2.03658600
C	-4.20659900	3.81955100	-0.28304300
H	-2.92943300	2.71200000	1.04627700
C	-4.69003800	2.77908800	-2.40178800
H	-3.82929300	0.84168500	-2.73238700
C	-4.83299000	3.85312500	-1.52860700
H	-4.31140900	4.65641500	0.40528600
H	-5.18092200	2.79589700	-3.37370800
H	-5.43107200	4.71595400	-1.81650500
H	-3.29765100	-1.50124800	-1.58208200
H	-2.19796900	-0.49981400	-2.54039400
Ru	0.10200800	0.48829700	0.03990500
H	-0.09441000	-0.69413000	1.12659100
C	1.21520100	-2.24111100	-1.07369500
H	0.97913200	-2.68031100	-0.09530800
H	1.28589800	-3.06674800	-1.80202800
C	-1.20128700	-2.01409900	-1.38850900
H	-1.25200400	-2.79837200	-2.16224100
H	-1.28741300	-2.50789500	-0.41094800
C	0.12563300	2.17182000	0.95244300
O	-0.02319000	3.01051800	1.78495500
H	0.26119100	-0.97386700	-2.35258900
O	0.55805000	2.72863600	-0.59446500
C	-0.30040800	3.73392200	-1.05135400
H	-1.12357100	3.34875900	-1.67879200
H	-0.74610200	4.29731600	-0.21315700
H	0.27604000	4.44989300	-1.65940600

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**TSB11**  
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**Coordinates (Angstroms)**  
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	<b>X</b>	<b>Y</b>	<b>Z</b>
N	0.15641700	-1.14843700	-1.14109700
C	2.56440300	-1.11306300	-0.83093500
H	2.67785100	-0.45172200	-1.70039700
H	3.48575400	-1.69930000	-0.72920400

C	-2.23862500	-0.98847300	-1.53256100
C	-0.22157500	1.42225100	2.00405500
O	-0.33081700	2.06436200	2.97339200
P	-2.32365600	0.13476900	-0.06204600
P	2.28314000	-0.03138700	0.64374100
C	3.01991000	-0.93460300	2.04645300
C	4.34567200	-1.38745600	1.97593000
C	2.27859700	-1.17278700	3.20698300
C	4.91304300	-2.07240100	3.04431900
H	4.94104000	-1.18903600	1.08385100
C	2.85093500	-1.85551000	4.27858000
H	1.24668500	-0.82732500	3.25929400
C	4.16476900	-2.30752200	4.19768600
H	5.94201100	-2.42155200	2.97874300
H	2.26560000	-2.03554100	5.17843100
H	4.61019900	-2.84305100	5.03430300
C	3.42157100	1.36531900	0.35219400
C	3.37765500	2.00961300	-0.89296700
C	4.27284200	1.85775800	1.34762800
C	4.19147500	3.10935700	-1.14056200
H	2.68310900	1.66314900	-1.66197600
C	5.08141700	2.96344200	1.09517600
H	4.30828000	1.37595700	2.32381700
C	5.04680400	3.58712600	-0.14891700
H	4.14916400	3.59969200	-2.11159900
H	5.74044100	3.33745800	1.87685900
H	5.67911500	4.45146400	-0.34441700
C	-3.50945000	-0.64592100	1.08258100
C	-3.17332500	-0.83056100	2.42675400
C	-4.77368400	-1.05293900	0.63167900
C	-4.08186700	-1.41699200	3.30517600
H	-2.18943000	-0.52047400	2.77671900
C	-5.67650000	-1.64401800	1.50857600
H	-5.05767300	-0.89534400	-0.40948200
C	-5.33052900	-1.82717800	2.84714100
H	-3.80973000	-1.55559800	4.34991500
H	-6.65363000	-1.96052700	1.14796700
H	-6.03830000	-2.28937500	3.53303400
C	-3.20649700	1.59052300	-0.72344800
C	-2.71197900	2.18022600	-1.89660200
C	-4.29992500	2.17304700	-0.07315300
C	-3.31954200	3.31656200	-2.41810300
H	-1.82981900	1.76169400	-2.38823600
C	-4.90018200	3.31568600	-0.59811900



H	-4.68774200	1.73457200	0.84550500
C	-4.41574500	3.88568900	-1.77201100
H	-2.92717900	3.76350400	-3.32991700
H	-5.75076700	3.76066700	-0.08451900
H	-4.88637900	4.77834200	-2.18049800
H	-3.17957500	-1.53336300	-1.67516600
H	-2.08505700	-0.35336300	-2.41477100
Ru	-0.04385500	0.32443400	0.51441000
H	-0.25605800	-1.01041100	1.51573000
C	1.35367900	-1.99430600	-1.04234900
H	1.21050600	-2.68895200	-0.20282100
H	1.47096600	-2.59445600	-1.95892700
C	-1.06279600	-1.92874900	-1.39002100
H	-0.94591100	-2.53657200	-2.30176700
H	-1.20051200	-2.61700900	-0.54454400
C	0.22101300	1.89705300	-0.78875700
O	0.30210200	3.04293900	-0.98636700
H	0.29201500	-0.44653300	-1.89127300
O	0.50542900	1.00275800	-2.78758800
C	0.67437700	2.15243900	-3.49863500
H	0.89234100	1.94258600	-4.56908300
H	-0.21371300	2.82894300	-3.50319100
H	1.51294000	2.79770900	-3.14502900

**B13**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
N	0.21894000	-0.80798300	-1.22087600
C	2.62327900	-0.83306500	-0.86010200
H	2.76858500	-0.12495300	-1.68739800
H	3.53274700	-1.44082900	-0.77275800
C	-2.18378100	-0.75411600	-1.57063900
C	-0.23329200	1.43923100	2.15589900
O	-0.38299400	1.88965800	3.22067700
P	-2.28013900	0.28960600	-0.05931700
P	2.31469100	0.14926700	0.66591200
C	2.96904000	-0.86487000	2.03457600
C	4.28199800	-1.35433400	1.97207800
C	2.18917900	-1.15372700	3.15778000
C	4.79766600	-2.12432200	3.00801500
H	4.90913600	-1.11856700	1.11165100
C	2.70983400	-1.92029300	4.19825600
H	1.16623100	-0.78324500	3.20884900
C	4.01070800	-2.40867100	4.12344700

H	5.81674800	-2.50217800	2.94654000
H	2.09301400	-2.13924700	5.06793300
H	4.41451500	-3.01126300	4.93537900
C	3.47493800	1.55686700	0.56921300
C	3.52418500	2.31847900	-0.60700400
C	4.25267500	1.95034700	1.66436700
C	4.35461800	3.43027700	-0.69230000
H	2.90037900	2.05016000	-1.46061300
C	5.07747100	3.06876000	1.57779800
H	4.21767400	1.37838800	2.59051400
C	5.13479700	3.80727800	0.39946000
H	4.38554600	4.00856300	-1.61392600
H	5.67760600	3.36169800	2.43747400
H	5.78109500	4.68067200	0.33304000
C	-3.39852700	-0.60131000	1.07479300
C	-3.01380000	-0.90002800	2.38441100
C	-4.67519500	-0.98228000	0.63605800
C	-3.88711600	-1.56843400	3.24009700
H	-2.02100300	-0.61387300	2.72907100
C	-5.54358800	-1.65265900	1.48944100
H	-4.99529400	-0.73976600	-0.37794500
C	-5.14983600	-1.94627900	2.79460800
H	-3.57652600	-1.79449800	4.25858200
H	-6.53086200	-1.94575900	1.13630700
H	-5.83082300	-2.46957700	3.46372700
C	-3.23296600	1.76505000	-0.55387900
C	-2.85781400	2.46359500	-1.71184800
C	-4.26606700	2.27031500	0.24338000
C	-3.53031700	3.62670700	-2.07275000
H	-2.02345500	2.10921900	-2.32318400
C	-4.92943600	3.43889100	-0.11960700
H	-4.55777200	1.74777600	1.15325000
C	-4.56795700	4.11577300	-1.28070500
H	-3.23467500	4.15821700	-2.97572600
H	-5.73237900	3.81982800	0.50941900
H	-5.08890700	5.02819000	-1.56620800
H	-3.10636800	-1.32847500	-1.72071400
H	-2.05762200	-0.07732600	-2.42569900
Ru	-0.00265300	0.55356400	0.50038900
H	-0.18008900	-0.89040600	1.33305100
C	1.38257300	-1.66538300	-1.11437300
H	1.27147000	-2.42036900	-0.30403000
H	1.51495700	-2.24326500	-2.04967200
C	-0.95623100	-1.63282500	-1.43227300

H	-0.83244400	-2.23434100	-2.35406400
H	-1.10858100	-2.36352500	-0.60757500
C	0.20026400	2.26181200	-0.47630700
O	0.30301600	3.33531800	-0.89791500
H	0.21452900	0.39756400	-2.46050000
O	0.12666100	1.07319900	-3.20435400
C	0.18585800	0.33835400	-4.39235900
H	0.18910500	1.03849600	-5.23742600
H	1.10058900	-0.27863600	-4.47264400
H	-0.67816500	-0.34020300	-4.53288100

**B14**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
N	-0.41994100	-1.61847900	-0.94303300
C	1.97210000	-2.00867600	-0.70544100
H	2.17387700	-1.72344100	-1.74863100
H	2.75575800	-2.71125400	-0.39294100
C	-2.80630200	-1.19338800	-1.19249100
C	-0.14170000	1.72713500	1.31939200
O	-0.08804200	2.64911800	2.04689800
P	-2.58403400	0.10626100	0.08694500
P	1.97432900	-0.46015900	0.30234900
C	2.74384100	-0.91683400	1.90148300
C	3.99592900	-1.54484400	1.93461800
C	2.10135000	-0.61923400	3.10662300
C	4.58944400	-1.87463900	3.14733800
H	4.51540900	-1.77132900	1.00223300
C	2.69863800	-0.94738700	4.32208100
H	1.12790300	-0.13028900	3.08577500
C	3.93948000	-1.57674400	4.34449700
H	5.56192400	-2.36434000	3.15985700
H	2.18788300	-0.71061000	5.25398100
H	4.40513800	-1.83358900	5.29473700
C	3.27276000	0.57750300	-0.47333300
C	4.31173100	0.04084800	-1.24536600
C	3.19103400	1.96823200	-0.32407900
C	5.25182900	0.87587500	-1.84469700
H	4.38749800	-1.03720300	-1.38723700
C	4.13127200	2.80160700	-0.92241400
H	2.37253500	2.39725900	0.25575000
C	5.16360700	2.25693800	-1.68414600
H	6.05424200	0.44473800	-2.44151900
H	4.05300700	3.88026600	-0.79896600

H	5.89677200	2.90911300	-2.15574100
C	-3.49424900	-0.46890400	1.56551300
C	-3.29601500	0.22999800	2.76431900
C	-4.38158200	-1.54965900	1.55435900
C	-3.98449500	-0.13047600	3.91661000
H	-2.59129800	1.06232100	2.78953200
C	-5.06261900	-1.91795000	2.71365000
H	-4.54779100	-2.11715200	0.63973600
C	-4.86851100	-1.20846100	3.89431000
H	-3.82290500	0.42572700	4.83857100
H	-5.74577500	-2.76564900	2.69092000
H	-5.40308900	-1.49540100	4.79833400
C	-3.59699500	1.52224100	-0.47192700
C	-2.97412600	2.74004000	-0.76153000
C	-4.98774500	1.41423200	-0.60639500
C	-3.73021500	3.83239200	-1.18152100
H	-1.89273200	2.82327900	-0.65959000
C	-5.73965700	2.50459100	-1.02939500
H	-5.48572100	0.47392600	-0.36428900
C	-5.11074600	3.71601300	-1.31603000
H	-3.23653000	4.77766500	-1.40106900
H	-6.81993900	2.41240000	-1.12955400
H	-5.70135700	4.57147300	-1.63978400
H	-3.81994000	-1.61302400	-1.22653000
H	-2.63367900	-0.69208500	-2.15521800
Ru	-0.26292600	0.20205900	0.25364200
H	-0.44213300	-0.68869200	1.56742700
C	0.58329200	-2.62023000	-0.61525900
H	0.42890100	-3.05159300	0.39591900
H	0.52172700	-3.47115000	-1.32260900
C	-1.73412100	-2.24316700	-0.95316700
H	-1.78737200	-3.01559200	-1.74697900
H	-1.94861000	-2.77620500	-0.00131800
C	0.76392900	1.11553600	-2.64879300
O	-0.13191600	1.38347300	-1.86785400
H	1.60805000	0.44942000	-2.41224300
O	0.81377700	1.66902400	-3.85343600
C	1.89926900	1.20478600	-4.67135600
H	1.95921500	0.11209900	-4.62662400
H	1.66914800	1.52540200	-5.68845300
H	2.84099600	1.66001600	-4.34418500
C	-0.93566800	-0.95409000	-4.35018800
H	-0.63153900	-0.80062800	-5.39427100
H	-1.70442800	-1.74731100	-4.34572000

H	-1.41522700	-0.01816900	-4.00909100
O	0.19894100	-1.29564800	-3.60436400
H	-0.07458000	-1.35980700	-2.63052000

**TSB12**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	-0.45242100	-1.64115600	-0.91271500
C	1.90467900	-2.10921100	-0.57072700
H	2.10319000	-1.90238200	-1.63052300
H	2.66070100	-2.81582900	-0.20681500
C	-2.80149800	-1.06279000	-1.22405800
C	-0.12759400	1.60636800	1.54255700
O	-0.03683400	2.46873000	2.33322100
P	-2.59826300	0.17481300	0.12274300
P	1.95741900	-0.50736400	0.34529200
C	2.81581500	-0.87639500	1.91793200
C	4.11288700	-1.40686300	1.90872600
C	2.18746700	-0.63186700	3.14206500
C	4.76446400	-1.69439300	3.10224300
H	4.61830900	-1.58773900	0.95869500
C	2.84437900	-0.91619900	4.33784700
H	1.17750400	-0.22335700	3.15231200
C	4.12955100	-1.44862700	4.31961800
H	5.77184700	-2.10711800	3.08404600
H	2.34654000	-0.72110800	5.28616000
H	4.64171500	-1.67131900	5.25433500
C	3.16746900	0.52626100	-0.55807600
C	4.05841200	0.02040200	-1.51334000
C	3.16762500	1.90333100	-0.29424200
C	4.93528900	0.87312400	-2.18116100
H	4.07380300	-1.04477900	-1.74219100
C	4.04344100	2.75206000	-0.96087900
H	2.46131700	2.31183500	0.42963900
C	4.93003000	2.23833800	-1.90639900
H	5.62340900	0.46623200	-2.92061500
H	4.02785300	3.81941500	-0.74819800
H	5.61240000	2.90362300	-2.43300300
C	-3.57016300	-0.45726600	1.53711500
C	-3.35974500	0.13838600	2.78829800
C	-4.51783800	-1.48032100	1.42816100
C	-4.09456000	-0.26451100	3.89726800
H	-2.60692100	0.92094900	2.89108600
C	-5.24507100	-1.89238200	2.54360200

H	-4.69428500	-1.96883800	0.47078100
C	-5.03949200	-1.28253400	3.77724800
H	-3.92328900	0.21204200	4.86094000
H	-5.97575100	-2.69346900	2.44390700
H	-5.61039500	-1.60273400	4.64706000
C	-3.55806800	1.63571100	-0.40716200
C	-2.91215900	2.86447100	-0.57576800
C	-4.93731400	1.54658600	-0.63851200
C	-3.63575100	3.98642000	-0.97502600
H	-1.83925900	2.93561300	-0.40066300
C	-5.65529300	2.66658300	-1.04131600
H	-5.45278300	0.59659700	-0.48867600
C	-5.00419300	3.88855300	-1.20895600
H	-3.12606700	4.93990800	-1.10242400
H	-6.72668800	2.58902800	-1.21938600
H	-5.56863600	4.76660900	-1.51840400
H	-3.83174200	-1.42317400	-1.34128900
H	-2.53500000	-0.54230600	-2.15580300
Ru	-0.27621400	0.18744000	0.35840200
H	-0.48902000	-0.79894400	1.60299600
C	0.49664500	-2.67084900	-0.46311500
H	0.26635400	-2.98060000	0.56894900
H	0.41162300	-3.56334100	-1.10684900
C	-1.81401900	-2.18551300	-0.95825200
H	-1.88448700	-2.95467900	-1.74758800
H	-2.05559100	-2.68371600	-0.00262100
C	0.71292200	1.23565600	-2.45651200
O	0.03899400	1.64634100	-1.52099000
H	0.94505100	0.16033100	-2.63625600
O	1.18736800	2.08389600	-3.36241400
C	1.91986000	1.48291700	-4.44118000
H	2.03345000	0.40299600	-4.28572100
H	1.37226000	1.66708000	-5.37036000
H	2.90077900	1.96313200	-4.48644900
C	-0.45008100	-1.11938100	-4.20943900
H	-0.05070000	-1.21905400	-5.24041900
H	-1.42730700	-1.65474800	-4.21578000
H	-0.72095500	-0.03212900	-4.10789500
O	0.43548700	-1.57212700	-3.26941900
H	-0.09888100	-1.50992400	-2.07862500

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**B15**

-----  
**Coordinates (Angstroms)**

**X**

**Y**

**Z**  
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N	-0.28875500	-1.91368800	-0.91994100
C	2.06595600	-2.37914300	-0.57489400
H	2.25093400	-2.19377200	-1.64075900
H	2.82167800	-3.08104100	-0.20238000
C	-2.61481200	-1.27568900	-1.27946900
C	0.05640200	1.33897200	1.54077900
O	0.15711100	2.19472400	2.33586600
P	-2.42417400	-0.04067800	0.07478800
P	2.13318300	-0.76315100	0.31768100
C	3.02363200	-1.10283600	1.87717900
C	4.35438000	-1.54221200	1.84442300
C	2.38868800	-0.93628600	3.11097500
C	5.03219800	-1.82023700	3.02537800
H	4.86258000	-1.65995600	0.88613000
C	3.07204100	-1.21184200	4.29407400
H	1.35481800	-0.59342300	3.13790800
C	4.39035400	-1.65500000	4.25264600
H	6.06505400	-2.16247900	2.99008400
H	2.57031700	-1.07781300	5.25085600
H	4.92283500	-1.87027900	5.17764700
C	3.30157300	0.28208400	-0.62065500
C	4.05203100	-0.16668500	-1.71374900
C	3.38130500	1.63342000	-0.25216800
C	4.86795700	0.71814900	-2.41718600
H	4.00310400	-1.20759500	-2.02948000
C	4.19749200	2.51211900	-0.95308400
H	2.78001500	1.99911400	0.58155900
C	4.94128300	2.05610500	-2.04087000
H	5.44296500	0.35668600	-3.26851900
H	4.24343400	3.55864300	-0.65789000
H	5.57347700	2.74569700	-2.59789200
C	-3.43400100	-0.66413600	1.46554700
C	-3.21762300	-0.09847700	2.72948400
C	-4.41841300	-1.64822400	1.32551400
C	-3.98242800	-0.49224700	3.82140900
H	-2.43779500	0.65366700	2.85542200
C	-5.17539600	-2.05183100	2.42388800
H	-4.60036000	-2.11216500	0.35684700
C	-4.96328100	-1.47139700	3.67074300
H	-3.80717500	-0.03894800	4.79541500
H	-5.93421900	-2.82279500	2.30098000
H	-5.55753300	-1.78478700	4.52722200
C	-3.34884200	1.43112400	-0.48165200
C	-2.69175900	2.66015100	-0.59599700

C	-4.71453700	1.34959500	-0.78492700
C	-3.39196900	3.79078300	-1.01172900
H	-1.62846600	2.72483200	-0.36860700
C	-5.40873300	2.47866800	-1.20328300
H	-5.23877100	0.39847700	-0.68076200
C	-4.74721800	3.70123500	-1.31579600
H	-2.87387800	4.74420300	-1.09824700
H	-6.46959400	2.40757200	-1.43766000
H	-5.29315300	4.58626000	-1.63839500
H	-3.64928300	-1.61272400	-1.42445200
H	-2.31263600	-0.76343400	-2.20504200
Ru	-0.10163800	-0.06121600	0.34481200
H	-0.32538900	-1.05517700	1.58614500
C	0.66096700	-2.94418400	-0.45655500
H	0.41342200	-3.22150300	0.57742200
H	0.57125300	-3.84337200	-1.08667900
C	-1.66664400	-2.42693700	-0.99476700
H	-1.73835500	-3.19730000	-1.77903200
H	-1.91768300	-2.90654000	-0.03612000
C	0.81766000	0.98673200	-2.49301500
O	0.20798800	1.39487000	-1.50736500
H	1.02529300	-0.09802700	-2.71576400
O	1.27742000	1.86236100	-3.38239400
C	1.95006900	1.27830400	-4.51034000
H	2.10696800	0.20345600	-4.35468600
H	1.33624600	1.44051300	-5.40175500
H	2.90751000	1.79413400	-4.62238900
C	-0.04456500	-1.43574900	-4.32473800
H	0.35697800	-1.55964200	-5.36128500
H	-0.99386400	-2.03114700	-4.31545500
H	-0.40203400	-0.35936400	-4.29956500
O	0.83843800	-1.75345200	-3.34807800
H	0.04074600	-1.73468400	-1.92688800

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**TSB13**  
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**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	-0.31517300	-1.89985300	-0.98105100
C	2.08361000	-2.25390100	-0.73068700
H	2.24802200	-2.00044800	-1.78660300
H	2.87377800	-2.94995500	-0.42232700
C	-2.68119400	-1.35187200	-1.21465800
C	0.02285100	1.40778600	1.41123300
O	0.11127000	2.28935600	2.17923500



P	-2.45724700	-0.04764000	0.07598400
P	2.12184900	-0.68579400	0.24836500
C	2.93375700	-1.13378300	1.82662300
C	4.21109200	-1.71078200	1.82899500
C	2.29743200	-0.88537800	3.04605200
C	4.83299200	-2.04184500	3.02706300
H	4.72703300	-1.89206300	0.88476100
C	2.92490500	-1.21208200	4.24660000
H	1.30389700	-0.43836000	3.04866000
C	4.18944100	-1.79225000	4.23898100
H	5.82488400	-2.49080100	3.01673000
H	2.42063400	-1.01184200	5.19047400
H	4.67911000	-2.04797400	5.17731800
C	3.36885400	0.36115700	-0.57718800
C	4.30680600	-0.13467100	-1.49001600
C	3.36386100	1.73051800	-0.28310300
C	5.22789100	0.72251900	-2.08769900
H	4.32188700	-1.19430100	-1.74303900
C	4.28760800	2.58332500	-0.87577700
H	2.61664900	2.13098400	0.40253800
C	5.22187400	2.08055500	-1.77976100
H	5.95036500	0.32569100	-2.79914000
H	4.26927600	3.64588900	-0.64101100
H	5.94064700	2.74967000	-2.24988600
C	-3.37903600	-0.64827600	1.53682600
C	-2.99143600	-0.17791300	2.79860200
C	-4.45736900	-1.53708100	1.45270400
C	-3.67372400	-0.57459700	3.94369500
H	-2.13898600	0.49649500	2.87944000
C	-5.13179900	-1.94478400	2.60169000
H	-4.78278300	-1.92009500	0.48617300
C	-4.74306500	-1.46271500	3.84811400
H	-3.36107000	-0.19649000	4.91543400
H	-5.96371900	-2.64234500	2.51962700
H	-5.27113200	-1.78093400	4.74537300
C	-3.44115100	1.36816000	-0.52639000
C	-2.76822300	2.41259600	-1.17305500
C	-4.83250100	1.43116500	-0.37775400
C	-3.48420700	3.49741900	-1.67349100
H	-1.68467000	2.36329200	-1.28788700
C	-5.54101500	2.51872800	-0.87790900
H	-5.36387900	0.63314200	0.14084900
C	-4.86776500	3.55267700	-1.52641900
H	-2.95465800	4.30543700	-2.17507600

H	-6.62213700	2.56221200	-0.75577800
H	-5.42414900	4.40555200	-1.91218800
H	-3.70861200	-1.73234400	-1.27398700
H	-2.46905300	-0.86726100	-2.17931200
Ru	-0.12269900	-0.01976200	0.25564800
H	-0.33196300	-0.99856100	1.52675500
C	0.71132300	-2.88938500	-0.59605500
H	0.51211300	-3.20329200	0.43732900
H	0.64202100	-3.77760800	-1.24391900
C	-1.67840400	-2.46066500	-0.95623000
H	-1.77368300	-3.26099300	-1.70760200
H	-1.84386400	-2.91212900	0.03247200
C	0.85948100	0.87467500	-2.59538400
O	0.22702300	1.29788800	-1.60386300
H	0.93809000	-0.56766600	-3.16252300
O	1.28893400	1.90871300	-3.38909400
C	2.04399000	1.50849600	-4.52183800
H	2.27766000	0.43623300	-4.48657600
H	1.48096800	1.72487400	-5.43961700
H	2.97852300	2.08048500	-4.53682300
C	-0.15353200	-1.37527700	-4.63014000
H	0.31726300	-1.46012900	-5.62759400
H	-0.97825300	-2.10969100	-4.60251300
H	-0.61727200	-0.36749700	-4.58114200
O	0.75361000	-1.58093800	-3.59344000
H	-0.09721600	-1.66793100	-1.97052900

**B16**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
N	-0.14952700	-1.29512800	-1.19397100
C	2.22587900	-1.75650000	-0.79773800
H	2.55558400	-1.38612800	-1.77607800
H	2.95648000	-2.51053200	-0.47759100
C	-2.48687800	-0.65248700	-1.52292100
C	0.11790000	1.71318000	1.55169800
O	0.23056600	2.53318800	2.38094800
P	-2.36179200	0.37033000	0.01315700
P	2.20005200	-0.29819700	0.34507000
C	2.81031800	-0.91069700	1.95155000
C	3.33513400	0.00149100	2.87582600
C	2.67151800	-2.25112800	2.32632500
C	3.72090800	-0.42209900	4.14317200
H	3.44457500	1.05128900	2.60051200

C	3.05995800	-2.67349600	3.59503500
H	2.25082900	-2.97453200	1.62789800
C	3.58467100	-1.76063200	4.50600300
H	4.12942500	0.29735500	4.85053200
H	2.95047900	-3.72101400	3.87169800
H	3.88678800	-2.09087100	5.49842300
C	3.56198100	0.76846500	-0.23785000
C	4.87802300	0.29005000	-0.30244700
C	3.28624800	2.07936600	-0.63953700
C	5.89878500	1.10944100	-0.77118600
H	5.10398400	-0.72605900	0.02366800
C	4.31186800	2.89647300	-1.11097400
H	2.26376500	2.45167700	-0.59074500
C	5.61519500	2.41276100	-1.17880700
H	6.91889600	0.73174700	-0.81833200
H	4.08704100	3.91412100	-1.42528600
H	6.41585500	3.05259200	-1.54673900
C	-3.33113300	-0.53536400	1.26990200
C	-2.95962200	-0.40598200	2.61430300
C	-4.43983100	-1.32867800	0.94818500
C	-3.68167800	-1.05199100	3.61276000
H	-2.08779000	0.19513300	2.87204800
C	-5.15436200	-1.98484800	1.94755800
H	-4.75881600	-1.43359900	-0.08854200
C	-4.77742000	-1.84587500	3.28085800
H	-3.38114200	-0.94163200	4.65316000
H	-6.01019500	-2.60316100	1.68211400
H	-5.33585800	-2.35909300	4.06177500
C	-3.34295800	1.87287700	-0.33160700
C	-2.71470000	2.92130500	-1.01990700
C	-4.67253600	2.02135400	0.08090100
C	-3.41950100	4.08629400	-1.30697700
H	-1.67150100	2.81798400	-1.32346100
C	-5.36818900	3.19314200	-0.20380900
H	-5.16710700	1.22486600	0.63514500
C	-4.74441500	4.22583500	-0.89939900
H	-2.92398000	4.89421100	-1.84258300
H	-6.40100100	3.29963600	0.12459900
H	-5.28982600	5.14277800	-1.11777200
H	-3.50616600	-0.99942000	-1.73250400
H	-2.19899100	0.00720300	-2.35432200
Ru	-0.02640500	0.38084800	0.28351800
H	-0.22601000	-0.67243600	1.49406000
C	0.83933900	-2.36084500	-0.94079200

H	0.52730600	-2.88142500	-0.02563500
H	0.83206800	-3.08382300	-1.77111200
C	-1.51279800	-1.81221400	-1.41239200
H	-1.54131200	-2.44166600	-2.31605600
H	-1.76770000	-2.45160700	-0.55576300
C	0.70886500	1.31848000	-2.66646100
O	0.17405000	1.69653100	-1.59528000
H	0.14994400	-0.81779500	-2.05503000
O	0.82940600	2.40061900	-3.51789900
C	1.42333300	2.11342900	-4.77136100
H	0.65314100	2.00821000	-5.54897000
H	2.07375100	2.95341600	-5.03890200
H	2.02166000	1.19382500	-4.73269000
C	0.42604500	-1.33323700	-4.81798600
H	0.09746900	-2.38095400	-4.87664300
H	-0.45981000	-0.71589500	-4.57345900
H	0.75854900	-1.03588200	-5.82922800
O	1.43823100	-1.21226700	-3.85837500
H	1.32326100	-0.29268400	-3.44953900

**B17**

**Coordinates (Angstroms)**

	<b>X</b>	<b>Y</b>	<b>Z</b>
N	0.25879100	-1.37283600	-1.12746500
C	2.66463300	-1.33387200	-0.73058300
H	2.79779100	-0.71588800	-1.62906900
H	3.57364900	-1.93231500	-0.58971900
C	-2.15667600	-1.21677600	-1.45398700
C	-0.15653700	1.28405300	1.97911300
O	-0.29757200	1.95574000	2.92864600
P	-2.19326400	0.02493900	-0.07537300
P	2.35745100	-0.17954900	0.68214100
C	3.09080700	-1.02363500	2.13563600
C	4.45586400	-1.34109500	2.16322100
C	2.29664100	-1.33756700	3.24194600
C	5.01145500	-1.97163900	3.27026600
H	5.09293600	-1.08041600	1.31658600
C	2.85672000	-1.96378500	4.35399100
H	1.23502800	-1.09205600	3.21721500
C	4.21089700	-2.28399400	4.36888000
H	6.07246900	-2.21562400	3.27962900
H	2.23015100	-2.20173500	5.21195400
H	4.64773100	-2.77275700	5.23840100
C	3.51741000	1.20479900	0.40789500

C	4.60646500	1.13379100	-0.46862500
C	3.28666400	2.39538400	1.10845500
C	5.44956400	2.23026000	-0.63611900
H	4.80468200	0.22020900	-1.02956100
C	4.13393100	3.48607300	0.94616500
H	2.42405900	2.47172200	1.77106100
C	5.21567800	3.40660400	0.07125900
H	6.29059400	2.16403900	-1.32469800
H	3.93881900	4.40582000	1.49460100
H	5.87346500	4.26369200	-0.06312000
C	-3.42662300	-0.63836400	1.09962100
C	-3.08673800	-0.81985400	2.44270900
C	-4.72164900	-0.96839000	0.67410600
C	-4.02222600	-1.32136600	3.34530400
H	-2.07609100	-0.57749200	2.76895000
C	-5.65351700	-1.47193700	1.57497300
H	-5.00592600	-0.81654000	-0.36827700
C	-5.30381900	-1.64890500	2.91341300
H	-3.74553600	-1.45727500	4.38950100
H	-6.65568700	-1.72661800	1.23355500
H	-6.03367000	-2.04318700	3.61849200
C	-3.04058800	1.45961600	-0.83276600
C	-2.50968100	1.99259500	-2.01497700
C	-4.12369400	2.10655600	-0.22988200
C	-3.06425500	3.12685900	-2.59436600
H	-1.63789700	1.51959400	-2.47131800
C	-4.67727900	3.24613700	-0.80914200
H	-4.53871200	1.72142000	0.70015000
C	-4.15366000	3.75589600	-1.99322900
H	-2.63688800	3.52952400	-3.51202000
H	-5.52024400	3.73860200	-0.32711500
H	-4.58532500	4.64870900	-2.44265500
H	-3.10212800	-1.77040900	-1.51340900
H	-2.03347200	-0.67187600	-2.39968300
Ru	0.05545000	0.17869000	0.52125900
H	-0.21429700	-1.21561000	1.48293300
C	1.44598600	-2.21895200	-0.90574500
H	1.25701800	-2.81390500	-0.00246500
H	1.58553600	-2.91521300	-1.74831200
C	-0.98307800	-2.15756700	-1.26654400
H	-0.90384400	-2.84849300	-2.12134700
H	-1.09317600	-2.75359700	-0.35150600
C	0.48565100	1.83966800	-0.75935300
O	0.32434600	3.03141400	-0.61609400

H	0.39525100	-0.87760100	-2.01006000
O	1.20711600	1.43904000	-1.96609500
C	1.70083700	2.52691300	-2.74884800
H	2.32690000	3.19358300	-2.14560100
H	2.30050500	2.08613600	-3.55258500
H	0.88398400	3.12408500	-3.17915400
C	-0.62710400	0.52589600	-5.01480600
H	0.12192500	1.06742300	-5.61492100
H	-1.06011900	-0.25785600	-5.64481000
H	-1.43460700	1.23106000	-4.75438000
O	-0.06250900	-0.09962300	-3.88664900
H	0.32687300	0.58883900	-3.30820000

### TSB14

#### Coordinates (Angstroms)

	X	Y	Z
N	0.13154600	-1.23549200	-1.21713400
C	2.57173500	-1.27267600	-0.89949300
H	2.72748000	-0.62490200	-1.77297600
H	3.44735700	-1.91594300	-0.74555000
C	-2.29233500	-1.11438700	-1.48203800
C	-0.18963800	1.27349300	1.99859800
O	-0.30437600	1.83330000	3.01585800
P	-2.31812500	0.08599700	-0.07676300
P	2.31189600	-0.11972300	0.51369000
C	3.01230700	-0.99207800	1.96651100
C	4.36279900	-1.36985600	1.96945800
C	2.22577500	-1.28709400	3.08392200
C	4.90953400	-2.03557200	3.05987700
H	4.99623000	-1.13059500	1.11439200
C	2.77587000	-1.95188000	4.17840600
H	1.17554900	-0.99909700	3.08996100
C	4.11524800	-2.32843700	4.16790300
H	5.95918700	-2.32364100	3.04739500
H	2.15245000	-2.17590900	5.04224200
H	4.54445700	-2.84743600	5.02337600
C	3.48129300	1.25041000	0.24663200
C	4.65526000	1.08680900	-0.49721900
C	3.21191400	2.49359300	0.82840500
C	5.54587900	2.14600800	-0.64728300
H	4.86788500	0.13308300	-0.98075100
C	4.10053200	3.55288200	0.67233400
H	2.29250800	2.63746700	1.39758000
C	5.27097400	3.37985700	-0.06201200

H	6.45308700	2.00880600	-1.23361600
H	3.87431200	4.51754900	1.12316600
H	5.96541600	4.20892200	-0.18641800
C	-3.46478700	-0.64662900	1.13824600
C	-3.06027900	-0.90422200	2.45070000
C	-4.77596800	-0.96594000	0.75330800
C	-3.94837600	-1.47086100	3.36283600
H	-2.04125000	-0.66669700	2.75303100
C	-5.65956100	-1.53276400	1.66403200
H	-5.10866000	-0.75726900	-0.26431000
C	-5.24609200	-1.78593200	2.97149800
H	-3.62200900	-1.66664200	4.38264700
H	-6.67405000	-1.77731100	1.35403500
H	-5.93890300	-2.22887800	3.68474300
C	-3.20963500	1.52898000	-0.74912800
C	-2.79242700	2.04994400	-1.98341800
C	-4.21968100	2.18404500	-0.03440700
C	-3.39669800	3.19240600	-2.49628600
H	-1.98270800	1.57660200	-2.54629800
C	-4.81656900	3.33014300	-0.55417600
H	-4.54474700	1.79703000	0.93081900
C	-4.40965500	3.83399100	-1.78638400
H	-3.06570100	3.58651700	-3.45550900
H	-5.60305000	3.82950900	0.00920600
H	-4.87661800	4.73088900	-2.19025400
H	-3.23367400	-1.67486100	-1.53564700
H	-2.18100600	-0.53708600	-2.40853900
Ru	-0.01634800	0.28775200	0.42900600
H	-0.21778600	-1.09877500	1.34574500
C	1.31862700	-2.10151100	-1.08754800
H	1.14673500	-2.75834900	-0.22260800
H	1.41092600	-2.74282900	-1.97897000
C	-1.10188200	-2.03714200	-1.33135900
H	-1.02938800	-2.71167800	-2.20026900
H	-1.18508300	-2.65898300	-0.42930300
C	0.23700400	1.97349500	-0.67320700
O	0.19981100	3.08662200	-0.98952000
H	0.18193800	-0.66654600	-2.08604800
O	1.80555000	1.20939600	-2.35425600
C	2.36093100	2.32903200	-2.93321700
H	1.92437700	3.27793600	-2.55200500
H	3.45040600	2.39146800	-2.74403600
H	2.22835600	2.35505200	-4.03669400
C	0.13762100	-0.21705800	-4.61481400

H	1.10745800	-0.75045900	-4.52912000
H	-0.62249600	-0.97543500	-4.87550600
H	0.22779600	0.45512800	-5.49063300
O	-0.21429000	0.45492300	-3.45065400
H	0.74077200	0.89453800	-2.98990300

**B18**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	0.14355600	-1.21717000	-1.21826700
C	2.58735300	-1.25383400	-0.89920300
H	2.77695300	-0.60978300	-1.76854700
H	3.45675200	-1.90421000	-0.73897500
C	-2.27723200	-1.12380800	-1.49804800
C	-0.18782900	1.29086600	1.99257500
O	-0.30109600	1.85246200	3.00738400
P	-2.31912100	0.06698900	-0.08830300
P	2.31426200	-0.12216700	0.52739400
C	2.98293200	-1.00726600	1.98540300
C	4.30558000	-1.47199300	1.97356700
C	2.20302200	-1.21208500	3.12676600
C	4.83052600	-2.13776900	3.07508800
H	4.93373900	-1.30466600	1.09776400
C	2.73230400	-1.87355800	4.23319100
H	1.17329400	-0.85853400	3.14124000
C	4.04329000	-2.33943700	4.20818100
H	5.85771900	-2.49726000	3.05101700
H	2.11451200	-2.02569300	5.11641300
H	4.45525600	-2.85823700	5.07198900
C	3.48998000	1.24952300	0.29113800
C	4.67541900	1.08650500	-0.43508300
C	3.20462400	2.49512000	0.85939900
C	5.56159100	2.14950700	-0.58050900
H	4.90036400	0.13124400	-0.90895500
C	4.09036300	3.55838800	0.70983900
H	2.27531400	2.63690600	1.41277300
C	5.27076500	3.38661800	-0.00864900
H	6.47745300	2.01341200	-1.15322100
H	3.85285300	4.52470800	1.15075800
H	5.96154100	4.21906500	-0.13018000
C	-3.45163100	-0.67326400	1.13450900
C	-3.04382200	-0.91421400	2.44908400
C	-4.75778500	-1.01417700	0.75121900
C	-3.92298600	-1.48872400	3.36502000



H	-2.02895500	-0.65893300	2.75020700
C	-5.63220400	-1.59012000	1.66549200
H	-5.09361600	-0.81492800	-0.26713100
C	-5.21481300	-1.82845200	2.97468300
H	-3.59427600	-1.67134700	4.38641900
H	-6.64262100	-1.85213100	1.35688900
H	-5.90028400	-2.27867000	3.69049100
C	-3.21699400	1.50880900	-0.75098300
C	-2.80035600	2.03631900	-1.98364500
C	-4.23893100	2.14426600	-0.03564800
C	-3.42680200	3.16892100	-2.49464100
H	-1.96969200	1.57547100	-2.53495300
C	-4.85431900	3.28065700	-0.55484200
H	-4.56047900	1.75014400	0.92770200
C	-4.45360000	3.79122800	-1.78669100
H	-3.10213300	3.57103500	-3.45291000
H	-5.65011000	3.76619400	0.00756600
H	-4.93688700	4.67883000	-2.19183500
H	-3.21438700	-1.68967100	-1.56384700
H	-2.15307500	-0.52819300	-2.41105700
Ru	-0.01315200	0.29260100	0.41793000
H	-0.20603100	-1.08444100	1.35026500
C	1.33384500	-2.07726000	-1.11330700
H	1.17261700	-2.76710300	-0.27109100
H	1.43160400	-2.68862900	-2.02492800
C	-1.07767400	-2.03258900	-1.34276800
H	-0.98951700	-2.69506300	-2.21970200
H	-1.16498100	-2.66825300	-0.44971500
C	0.18676900	1.92958400	-0.70093000
O	0.22512100	2.98128900	-1.17498200
H	0.16151200	-0.58481300	-2.08180200
O	2.23062300	1.22196000	-2.64811600
C	2.63321500	2.44510300	-3.18356900
H	2.09281500	3.30632000	-2.75021300
H	3.70198900	2.58830500	-2.97027500
H	2.50297600	2.49332300	-4.28075000
C	-0.15190700	-0.17114500	-4.43057100
H	0.71543400	-0.87290500	-4.52632800
H	-1.05589300	-0.80211800	-4.61392800
H	-0.08028400	0.49567200	-5.32029600
O	-0.19290500	0.50937900	-3.24117100
H	1.27406900	1.03279900	-2.94356800

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**TSB15**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	0.10431600	-1.22583400	-1.17545000
C	2.54215000	-1.21888300	-0.91854300
H	2.67314300	-0.54640800	-1.77988900
H	3.44355700	-1.83790000	-0.82270500
C	-2.32231500	-1.18943300	-1.40940700
C	-0.19339200	1.27226600	2.03887700
O	-0.29521100	1.82800300	3.05794700
P	-2.33986100	0.04686200	-0.03961400
P	2.29079700	-0.14992100	0.55311100
C	3.00908800	-1.05665300	1.97002800
C	4.37388800	-1.37874100	1.96503100
C	2.22577600	-1.42794200	3.06583900
C	4.93778600	-2.07000400	3.03059400
H	5.00166600	-1.07826200	1.12482200
C	2.79440900	-2.11695100	4.13541400
H	1.16536300	-1.17929200	3.07225700
C	4.14771500	-2.43998500	4.11861300
H	5.99777300	-2.31716300	3.01504300
H	2.17540600	-2.39990900	4.98496500
H	4.59180400	-2.97736600	4.95483000
C	3.42220000	1.26254500	0.33671500
C	4.49369500	1.23473600	-0.56376100
C	3.19988600	2.41812800	1.09665200
C	5.32827800	2.34206500	-0.69336200
H	4.66867800	0.35820900	-1.18545400
C	4.03564000	3.52137000	0.96556800
H	2.35768000	2.45603900	1.78882200
C	5.10199800	3.48464500	0.06926700
H	6.15260800	2.31292700	-1.40414100
H	3.84755300	4.41471400	1.55824300
H	5.75209600	4.35090400	-0.04029700
C	-3.49207200	-0.62662200	1.20244200
C	-3.09001800	-0.83939700	2.52350100
C	-4.80805600	-0.94205100	0.83043600
C	-3.98541600	-1.35653000	3.45752300
H	-2.06681400	-0.60762100	2.81575400
C	-5.69936000	-1.45846300	1.76338500
H	-5.13820300	-0.76929900	-0.19462800
C	-5.28852100	-1.66596500	3.07954400
H	-3.66046500	-1.51786200	4.48380400
H	-6.71773700	-1.69949300	1.46375100
H	-5.98718800	-2.07036200	3.80976700

C	-3.20138200	1.48819900	-0.75542000
C	-2.72239600	1.99306800	-1.97450300
C	-4.24932400	2.14587800	-0.10225100
C	-3.30686600	3.12369000	-2.53462000
H	-1.87316100	1.51335900	-2.47521400
C	-4.82705900	3.27916400	-0.67002100
H	-4.61919700	1.77318700	0.85200300
C	-4.36074100	3.76705900	-1.88754900
H	-2.93003900	3.50768900	-3.48107400
H	-5.64376400	3.78207600	-0.15493200
H	-4.81337200	4.65352200	-2.32917600
H	-3.24792200	-1.77766400	-1.41813600
H	-2.26812200	-0.62797200	-2.34991700
Ru	-0.03362400	0.26226400	0.45809200
H	-0.25129600	-1.10653000	1.39934600
C	1.29901200	-2.06883900	-1.09310900
H	1.19544000	-2.77469200	-0.24936600
H	1.38912700	-2.67841500	-2.00882600
C	-1.09371400	-2.06374100	-1.26525300
H	-1.01351500	-2.73493800	-2.13889700
H	-1.17350000	-2.70398400	-0.37004500
C	0.22973200	1.86022900	-0.68309900
O	0.38244200	2.86837300	-1.22672600
H	0.09860000	-0.47546500	-2.15754000
O	2.56622800	1.05976400	-3.25027300
C	2.79653900	2.43384100	-3.36602200
H	2.11081800	2.91632400	-4.08535600
H	2.70719000	2.97870700	-2.40915700
H	3.82092200	2.58426600	-3.73540200
C	-0.15147700	-0.31282600	-4.29589200
H	0.52187000	-1.19429300	-4.37707800
H	-1.18266000	-0.69373200	-4.46271000
H	0.08416600	0.33057700	-5.16344900
O	-0.01371900	0.37810300	-3.10210000
H	1.58094800	0.91149800	-3.17023400

**B19**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
N	0.23207300	-0.78900000	-1.02329500
C	2.62660500	-0.55398700	-0.60359200
H	2.71313400	0.17466700	-1.42194500
H	3.59199700	-1.06645000	-0.50490800
C	-2.16326200	-0.99379400	-1.40325400

C	-0.45185100	1.55557400	2.24556800
O	-0.61505000	2.04640600	3.28982700
P	-2.38071200	0.21550300	-0.02297900
P	2.17928700	0.34393800	0.93650400
C	2.81924300	-0.69666400	2.29361300
C	4.18555600	-1.01368500	2.32354500
C	1.98650100	-1.17626300	3.30714400
C	4.70166300	-1.80870300	3.33961200
H	4.84979400	-0.62787200	1.54919700
C	2.50701400	-1.96936400	4.32798500
H	0.92567100	-0.93027600	3.28528400
C	3.86114800	-2.28938400	4.34331100
H	5.76226500	-2.05347900	3.34989700
H	1.84874100	-2.33937600	5.11214600
H	4.26543600	-2.91288800	5.13913100
C	3.21313600	1.84165500	1.03500700
C	3.50976300	2.57628300	-0.12052100
C	3.61286200	2.33696800	2.28341800
C	4.20868600	3.77641200	-0.02231000
H	3.19758300	2.21947700	-1.10417700
C	4.30650400	3.53986400	2.37335500
H	3.38275100	1.77749200	3.19021600
C	4.60814900	4.26133100	1.22071100
H	4.44123200	4.33538700	-0.92778500
H	4.61359400	3.91305900	3.34897100
H	5.15174300	5.20201100	1.29209900
C	-3.54958500	-0.57605900	1.13141900
C	-3.22311200	-0.76215100	2.47727500
C	-4.79831500	-1.01346000	0.66535800
C	-4.12706600	-1.37533700	3.34238100
H	-2.25156400	-0.43323400	2.84339100
C	-5.69802000	-1.62698500	1.52926100
H	-5.07008400	-0.86046300	-0.37992300
C	-5.36207300	-1.80911400	2.87032100
H	-3.86167300	-1.51554000	4.38877900
H	-6.66322000	-1.96457400	1.15587300
H	-6.06645900	-2.28922100	3.54746200
C	-3.32302000	1.59201100	-0.76817400
C	-2.82052300	2.15960100	-1.94885600
C	-4.45427500	2.15663800	-0.16858200
C	-3.45449900	3.25329100	-2.52641300
H	-1.91653000	1.75834900	-2.41494000
C	-5.08186300	3.25658900	-0.74991700
H	-4.84962000	1.73593500	0.75535200

C	-4.58740000	3.80401100	-1.93036200
H	-3.05552300	3.68124800	-3.44454400
H	-5.96202000	3.68624100	-0.27406300
H	-5.08055000	4.66296200	-2.38245900
H	-3.02476300	-1.66952300	-1.47236300
H	-2.11560100	-0.41592000	-2.33518000
Ru	-0.14280800	0.61589400	0.63345800
H	-0.34289600	-0.80143300	1.50627300
C	1.48350600	-1.51507400	-0.87789000
H	1.42674400	-2.26352900	-0.05807800
H	1.69862000	-2.08879100	-1.79948800
C	-0.85859100	-1.73619200	-1.18455900
H	-0.66292700	-2.39032000	-2.05672800
H	-0.95155600	-2.40924700	-0.30681600
C	0.07656500	2.26914600	-0.42257800
O	0.17869400	3.30292100	-0.93486500
H	0.18498100	0.20181600	-2.31819300
O	0.11526900	0.82521900	-3.14115800
C	0.15383700	-0.00065500	-4.28084900
H	0.24800300	0.63481200	-5.17024200
H	1.01256300	-0.69357400	-4.27170600
H	-0.76548000	-0.60043200	-4.39358700
C	2.70414600	3.10210200	-3.67820300
H	3.75531600	3.39115200	-3.80165400
H	2.20755800	3.22710700	-4.65635900
H	2.23860100	3.81477100	-2.97541400
O	2.67289200	1.77420100	-3.22653000
H	1.72338100	1.50808500	-3.16679100

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 CH<sub>3</sub>OH

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 Coordinates (Angstroms)

	X	Y	Z
C	2.83870800	-0.02091200	-0.01656600
H	3.21012100	-1.05052200	-0.02880400
H	3.19462000	0.45525000	0.91226700
H	1.73715700	-0.06000600	0.01938900
O	3.32832100	0.60510400	-1.17847300
H	3.00044200	1.51447600	-1.17064400

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 HCHO

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 Coordinates (Angstroms)

	X	Y	Z
C	-2.82869200	0.45762700	0.00001000

O	-1.62433400	0.45762700	-0.00000300
H	-3.42993900	1.39659700	-0.00000300
H	-3.42993900	-0.48134300	0.00003600

H<sub>2</sub>

Coordinates (Angstroms)

	X	Y	Z
H	-3.29950100	0.35849100	0.00000000
H	-4.04389500	0.35849100	0.00000000

CO

Coordinates (Angstroms)

	X	Y	Z
O	-3.25691800	-0.11320800	0.00000000
C	-4.39770900	-0.11320800	0.00000000

1

Coordinates (Angstroms)

	X	Y	Z
C	-0.67502800	0.81998600	0.26288100
H	-0.32910700	1.37524300	1.15123700
H	-1.78388500	0.89601600	0.21971600
O	-0.13260700	1.36142900	-0.91576500
C	-0.65677300	2.63633400	-1.18118100
H	-0.42347500	3.35675800	-0.37850100
H	-0.20157500	2.98950700	-2.11055900
H	-1.75369900	2.61318800	-1.30920200
O	-0.23735700	-0.47855100	0.41801300
H	-0.56161700	-0.97949600	-0.34615400

2

Coordinates (Angstroms)

	X	Y	Z
C	-2.81591700	0.47156500	-0.00003900
O	-1.61512900	0.52222700	0.00026900
H	-3.40101400	-0.47415800	-0.00038500
O	-3.58728000	1.56869400	-0.00000600
C	-4.99782700	1.32324300	-0.00024200
H	-5.30260600	0.77230700	0.89707500
H	-5.47535300	2.30374900	-0.00042300
H	-5.30231800	0.77212600	-0.89754800

