

## Supporting Information

For

### **A Phosphine-Free Mn(I)-NNS Catalyst For Asymmetric Transfer**

### **Hydrogenation of Acetophenone: A Theoretical Prediction**

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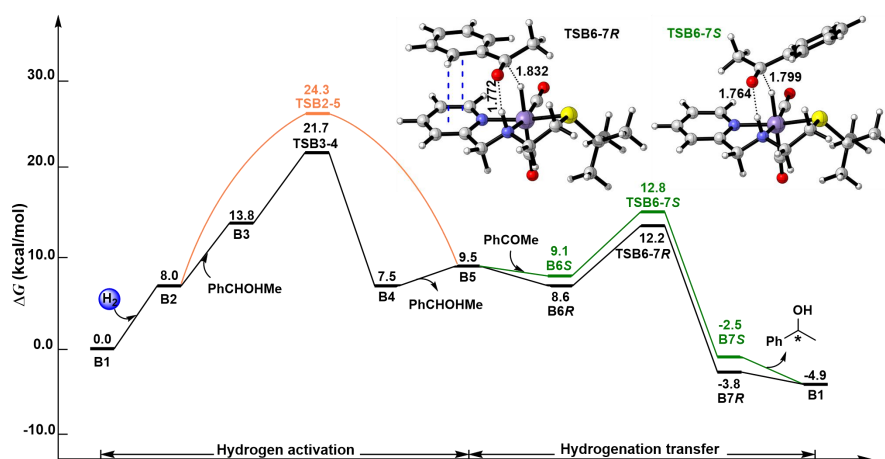
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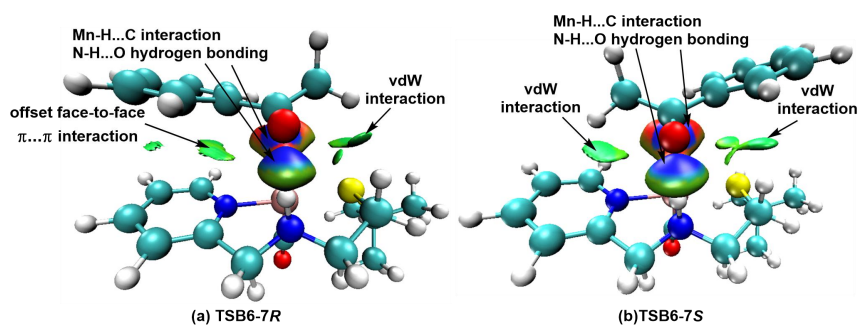
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## 1. Acetophenone hydrogenation catalyzed by complex B1



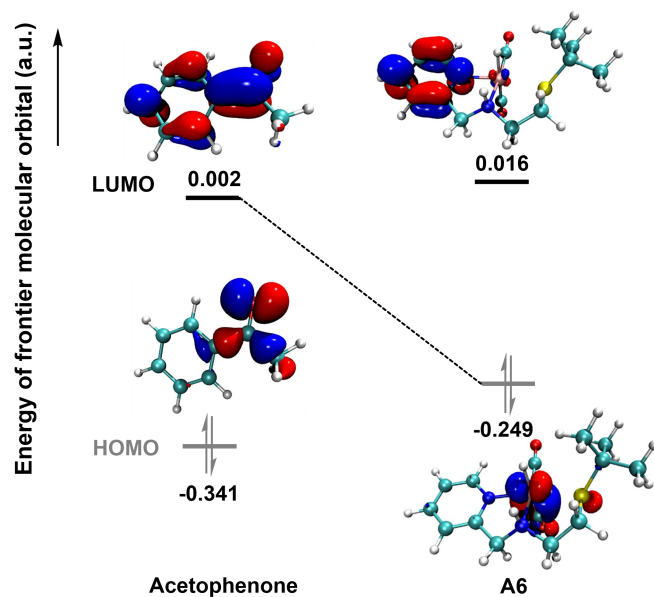
**Figure S1.** The Gibbs free energy profiles of H<sub>2</sub>-hydrogenation of acetophenone catalyzed by complex **B1** (unit: kcal/mol). Key bond lengths are given in Å. (Purple: Mn, blue: N, yellow: S, gray: C, red: O, other: H)



**Figure S2.** NCI analysis of the transition states of HT using RDG method. (Pink: Mn, blue: N, yellow: S, light blue: C, red: O, other: H)

## 2. Interaction between frontier molecular orbitals (FMOs) of acetophenone and

A6.



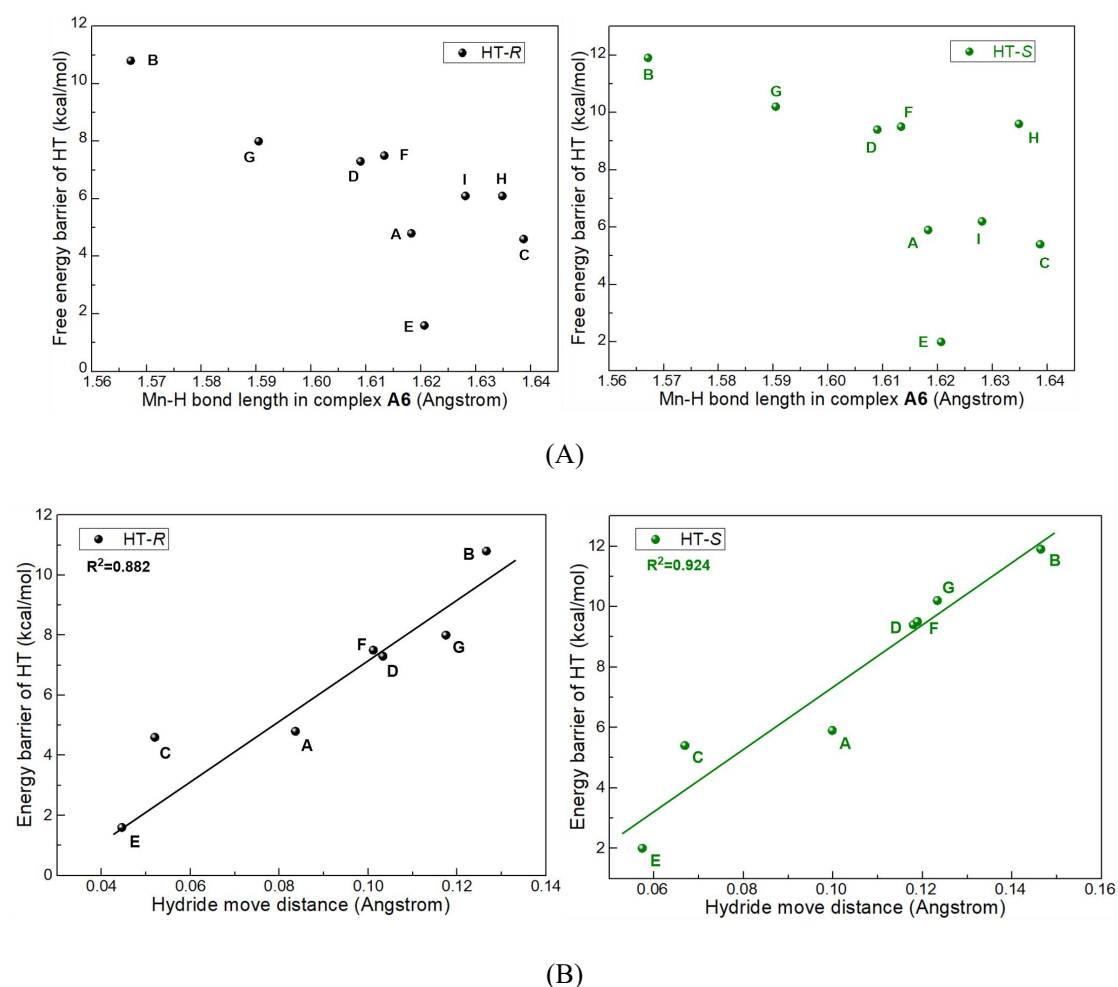
**Figure S3.** Interaction between frontier molecular orbitals (FMOs) of acetophenone and **A6**.

The calculated results about the interaction of the frontier molecular orbitals (FMOs) between acetophenone and **A6** show that the energy gap between the LUMO of acetophenone and the HOMO of **A6** is 0.251 a.u., while that between the HOMO of acetophenone and LUMO of **A6** is 0.357 a.u.. It also proves that the hydride transfer is prior to proton transfer in the HT step, which is consistent with our previous work (DOI: 10.1039/b815699a).

### 3. Key bond length and APT charge

We found that there are no good linear relationships between the energy barriers of the hydrogen transfer steps (HT) and Mn–H bond lengths, H<sup>2</sup> charges and Mn charges etc. in transition states **TSA7-8R** and **TSA7-8S**. However, if we didn't consider the solvent effect (optimization without solvent), the relationship between the energy

barrier of HT step from **A6** with different X ligands (X = CO, Cl, H, OMe, NCMe, CCMe, OPh, NCHMe, CHCHMe) to **TSA7-8** and the Mn–H bond lengths of **A6**, the hydride move distances (HMDs) were found (see Figure S4). A longer bond length of Mn–H leads to a lower HT energy barrier, and a shorter HMD leads to a lower HT energy barrier.



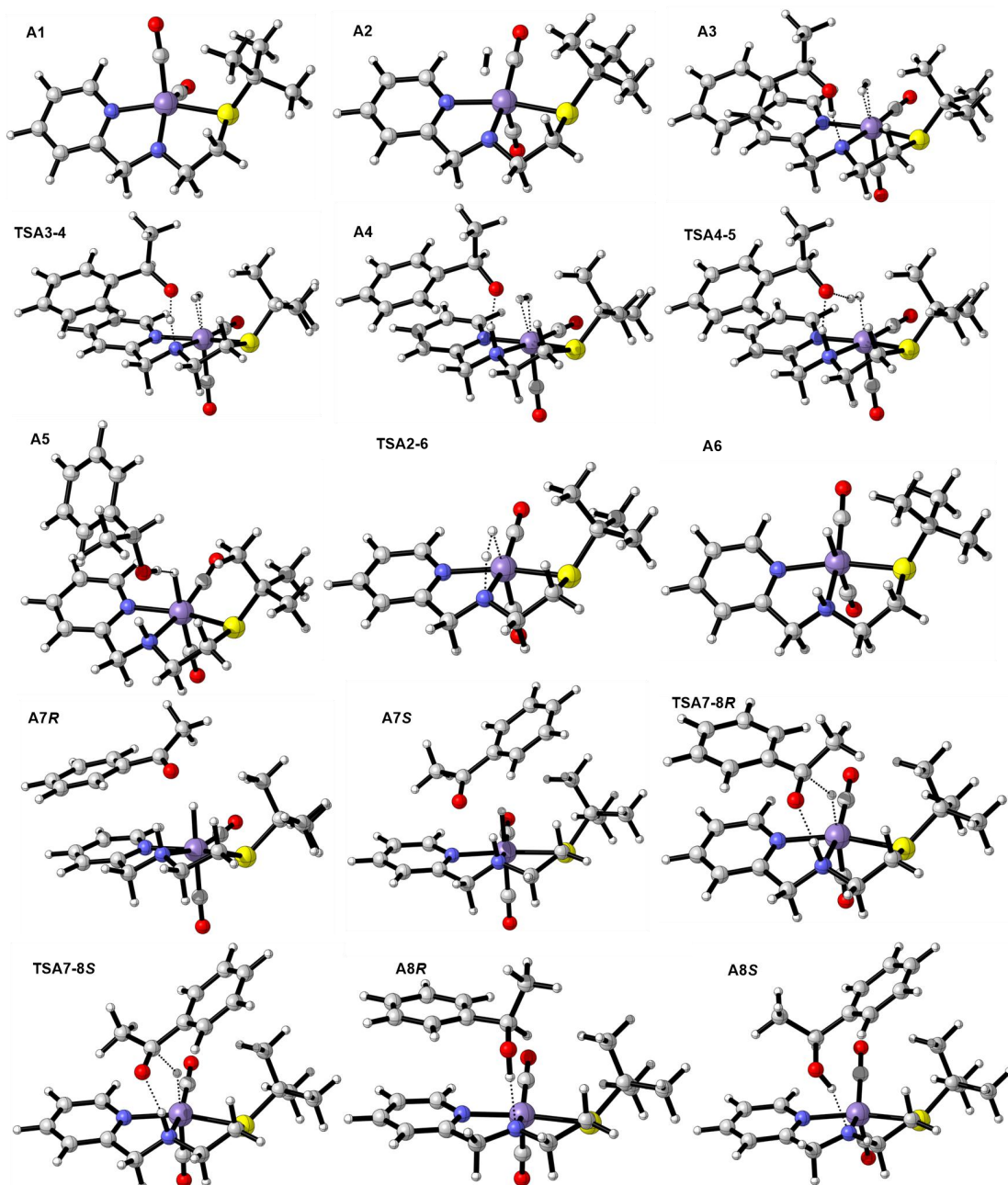
**Figure S4.** The correlation between the HT energy barrier and (A) the Mn–H bond length in complex **A6**, (B) the hydride move distance (HMD) at  $\omega$ B97X-D/BSI level (BSI denotes the LANL2DZ basis set for Mn center and the 6-31++G (d, p) basis set for all other atoms).

#### 4. The theoretical ee value is calculated with the following formulas

$$ee = \frac{R-S}{R+S} \quad (1)$$

$$ee = \frac{e^{\Delta\Delta G/RT} - 1}{e^{\Delta\Delta G/RT} + 1} \quad (2)$$

## 5. Key geometry structures



## 6. Energies of all the structures

**Table S1.** 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	$E$	$G$	$\Delta G$
<b>A1<sub>X=CO</sub></b>	-1306.81835574	-1306.538048	0.0
<b>H<sub>2</sub></b>	-1.17454544	-1.162403	/
<b>PhCOMe</b>	-384.80362867	-384.684375	/
<b>A2<sub>X=CO</sub></b>	-1307.99585861	-1307.706098	-3.5
<b>A3<sub>X=CO</sub></b>	-1694.0200745	-1693.572608	-3.5
<b>TSA3-4<sub>X=CO</sub></b>	-1694.01735631	-1693.570493	-2.2
<b>A4<sub>X=CO</sub></b>	-1694.02057026	-1693.568019	-0.6
<b>TSA4-5<sub>X=CO</sub></b>	-1694.02050611	-1693.566774	0.2
<b>A5<sub>X=CO</sub></b>	-1694.03953795	-1693.587623	-12.9
<b>TSA2-6<sub>X=CO</sub></b>	-1307.97443915	-1307.678177	14.0
<b>A6<sub>X=CO</sub></b>	-1308.01587571	-1307.7149	-9.1
<b>A7<sub>RX=CO</sub></b>	-1692.83119537	-1692.399632	-9.3
<b>A7<sub>SX=CO</sub></b>	-1692.83154333	-1692.400565	-9.9
<b>TSA7-8<sub>RX=CO</sub></b>	-1692.8202112	-1692.388684	-2.4
<b>TSA7-8<sub>SX=CO</sub></b>	-1692.81901615	-1692.38722	-1.5
<b>A8<sub>RX=CO</sub></b>	-1692.84999069	-1692.415404	-19.2
<b>A8<sub>SX=CO</sub></b>	-1692.84642212	-1692.412511	-17.4
<b>R-PhCHOHMe</b>	-386.00963145	-385.866615	/
<b>S-PhCHOHMe</b>	-386.00963145	-385.866615	/
<b>A1<sub>X=Cl</sub></b>	-1653.835864	-1653.566141	0.0
<b>A2<sub>X=Cl</sub></b>	-1655.010604	-1654.723048	3.4
<b>TSA2-6<sub>X=Cl</sub></b>	-1654.999039	-1654.713551	9.4
<b>A6<sub>X=Cl</sub></b>	-1655.035182	-1654.743521	-9.4

<b>A7R<sub>X=Cl</sub></b>	-2039.847045	-2039.426333	-8.4
<b>A7S<sub>X=Cl</sub></b>	-2039.848247	-2039.42681	-8.7
<b>TSA7-8R<sub>X=Cl</sub></b>	-2039.840207	-2039.419173	-3.9
<b>TSA7-8S<sub>X=Cl</sub></b>	-2039.839572	-2039.41748	-2.9
<b>A8R<sub>X=Cl</sub></b>	-2039.868251	-2039.445642	-20.5
<b>A8S<sub>X=Cl</sub></b>	-2039.865821	-2039.443099	-18.9
<b>A1<sub>X=H</sub></b>	-1194.162353	-1193.884274	0.0
<b>A2<sub>X=H</sub></b>	-1195.335622	-1195.04063	3.8
<b>TSA2-6<sub>X=H</sub></b>	-1195.321833	-1195.028916	11.1
<b>A6<sub>X=H</sub></b>	-1195.355432	-1195.055844	-5.8
<b>A7R<sub>X=H</sub></b>	-1580.166718	-1579.737668	-4.2
<b>A7S<sub>X=H</sub></b>	-1580.167702	-1579.739084	-5.0
<b>TSA7-8R<sub>X=H</sub></b>	-1580.160423	-1579.729812	0.8
<b>TSA7-8S<sub>X=H</sub></b>	-1580.160143	-1579.727007	2.5
<b>A8R<sub>X=H</sub></b>	-1580.196181	-1579.76296	-20.0
<b>A8S<sub>X=H</sub></b>	-1580.193742	-1579.761702	-19.2
<b>A1<sub>X=OMe</sub></b>	-1308.679725	-1308.372322	0.0
<b>A2<sub>X=OMe</sub></b>	-1309.856051	-1309.531049	2.3
<b>TSA2-6<sub>X=OMe</sub></b>	-1309.843197	-1309.51878	10.0
<b>A6<sub>X=OMe</sub></b>	-1309.880415	-1309.550153	-9.7
<b>A7R<sub>X=OMe</sub></b>	-1694.691344	-1694.232058	-8.1
<b>A7S<sub>X=OMe</sub></b>	-1694.691945	-1694.232786	-8.6
<b>TSA7-8R<sub>X=OMe</sub></b>	-1694.684796	-1694.22279	-2.3
<b>TSA7-8S<sub>X=OMe</sub></b>	-1694.68424	-1694.223293	-2.6
<b>A8R<sub>X=OMe</sub></b>	-1694.714487	-1694.251265	-20.2
<b>A8S<sub>X=OMe</sub></b>	-1694.711262	-1694.251663	-20.4
<b>A1<sub>X=CHCHMe</sub></b>	-1310.840043	-1310.505301	0.0
<b>A2<sub>X=CHCHMe</sub></b>	-1312.014082	-1311.662444	3.3
<b>TSA2-6<sub>X=CHCHMe</sub></b>	-1312.000219	-1311.648786	11.9

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<b>A6<sub>X</sub>=CHCHMe</b>	-1312.042219	-1311.650786	-4.2
<b>A7R<sub>X</sub>=CHCHMe</b>	-1696.843356	-1696.357301	-3.3
<b>A7S<sub>X</sub>=CHCHMe</b>	-1696.844347	-1696.357984	-3.7
<b>TSA7-8R<sub>X</sub>=CHCHMe</b>	-1696.837863	-1696.350006	1.3
<b>TSA7-8S<sub>X</sub>=CHCHMe</b>	-1696.837196	-1696.348706	2.1
<b>A8R<sub>X</sub>=CHCHMe</b>	-1696.874972	-1696.385845	-21.2
<b>A8S<sub>X</sub>=CHCHMe</b>	-1696.873362	-1696.385727	-21.1
<b>A1<sub>X</sub>=NCMe</b>	-1326.223192	-1325.907409	0.0
<b>A2<sub>X</sub>=NCMe</b>	-1327.399265	-1327.067352	1.5
<b>TSA2-6<sub>X</sub>=NCMe</b>	-1327.386877	-1327.056333	8.5
<b>A6<sub>X</sub>=NCMe</b>	-1327.42242	-1327.085404	-9.8
<b>A7R<sub>X</sub>=NCMe</b>	-1712.235581	-1711.76865	-9.1
<b>A7S<sub>X</sub>=NCMe</b>	-1712.23652	-1711.770403	-10.2
<b>TSA7-8R<sub>X</sub>=NCMe</b>	-1712.228367	-1711.760831	-4.2
<b>TSA7-8S<sub>X</sub>=NCMe</b>	-1712.226913	-1711.759485	-3.3
<b>A8R<sub>X</sub>=NCMe</b>	-1712.256541	-1711.78756	-20.9
<b>A8S<sub>X</sub>=NCMe</b>	-1712.253447	-1711.784826	-19.2
<b>A1<sub>X</sub>=CCMe</b>	-1309.624582	-1309.311039	0.0
<b>A2<sub>X</sub>=CCMe</b>	-1310.802875	-1310.476517	-1.9
<b>TSA2-6<sub>X</sub>=CCMe</b>	-1310.784956	-1310.457656	9.9
<b>A6<sub>X</sub>=CCMe</b>	-1310.818075	-1310.483022	-6.0
<b>A7R<sub>X</sub>=CCMe</b>	-1695.629266	-1695.166029	-5.2
<b>A7S<sub>X</sub>=CCMe</b>	-1695.630512	-1695.164648	-4.3
<b>TSA7-8R<sub>X</sub>=CCMe</b>	-1695.623637	-1695.156855	0.6
<b>TSA7-8S<sub>X</sub>=CCMe</b>	-1695.622672	-1695.156789	0.7
<b>A8R<sub>X</sub>=CCMe</b>	-1695.658446	-1695.188942	-19.5
<b>A8S<sub>X</sub>=CCMe</b>	-1695.654356	-1695.186242	-18.7

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## 7. Imaginary frequencies of transition states

**Table S2.** Calculated imaginary frequencies of transition states at  $\omega$  B97X-D/BSI (LANL2DZ & 6-31++G\*\*) level.

<b>TSA2-6<sub>X=CO</sub></b>	1244.29 <i>i</i>
<b>TSA3-4<sub>X=CO</sub></b>	1006.91 <i>i</i>
<b>TSA4-5<sub>X=CO</sub></b>	176.74 <i>i</i>
<b>TSA7-8<sub>R<sub>X=CO</sub></sub></b>	583.04 <i>i</i>
<b>TSA7-8<sub>S<sub>X=CO</sub></sub></b>	644.34 <i>i</i>
<b>TSA2-6<sub>X=Cl</sub></b>	1122.78 <i>i</i>
<b>TSA3-4<sub>X=Cl</sub></b>	686.20 <i>i</i>
<b>TSA4-5<sub>X=Cl</sub></b>	744.68 <i>i</i>
<b>TSA7-8<sub>R<sub>X=Cl</sub></sub></b>	480.09 <i>i</i>
<b>TSA7-8<sub>S<sub>X=Cl</sub></sub></b>	459.90 <i>i</i>
<b>TSA2-6<sub>X=H</sub></b>	1287.12 <i>i</i>
<b>TSA3-4<sub>X=H</sub></b>	571.31 <i>i</i>
<b>TSA4-5<sub>X=H</sub></b>	845.56 <i>i</i>
<b>TSA7-8<sub>R<sub>X=H</sub></sub></b>	465.53 <i>i</i>
<b>TSA7-8<sub>S<sub>X=H</sub></sub></b>	390.91 <i>i</i>
<b>TSA2-6<sub>X=OMe</sub></b>	1194.24 <i>i</i>
<b>TSA3-4<sub>X=OMe</sub></b>	678.52 <i>i</i>
<b>TSA4-5<sub>X=OMe</sub></b>	810.99 <i>i</i>
<b>TSA7-8<sub>R<sub>X=OMe</sub></sub></b>	429.39 <i>i</i>
<b>TSA7-8<sub>S<sub>X=OMe</sub></sub></b>	296.52 <i>i</i>
<b>TSA2-6<sub>X=CHCHMe</sub></b>	1251.36 <i>i</i>
<b>TSA3-4<sub>X=CHCHMe</sub></b>	332.69 <i>i</i>
<b>TSA4-5<sub>X=CHCHMe</sub></b>	860.38 <i>i</i>
<b>TSA7-8<sub>R<sub>X=CHCHMe</sub></sub></b>	390.08 <i>i</i>
<b>TSA7-8<sub>S<sub>X=CHCHMe</sub></sub></b>	412.43 <i>i</i>

<b>TSA2-6<sub>X=NCMe</sub></b>	1243.33 <i>i</i>
<b>TSA3-4<sub>X=NCMe</sub></b>	969.71 <i>i</i>
<b>TSA4-5<sub>X=NCMe</sub></b>	697.74 <i>i</i>
<b>TSA7-8<sub>RX=NCMe</sub></b>	499.57 <i>i</i>
<b>TSA7-8<sub>SX=NCMe</sub></b>	546.15 <i>i</i>
<b>TSA2-6<sub>X=CCMe</sub></b>	1199.83 <i>i</i>
<b>TSA3-4<sub>X=CCMe</sub></b>	437.70 <i>i</i>
<b>TSA4-5<sub>X=CCMe</sub></b>	836.90 <i>i</i>
<b>TSA7-8<sub>RX=CCMe</sub></b>	339.95 <i>i</i>
<b>TSA7-8<sub>SX=CCMe</sub></b>	375.70 <i>i</i>

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## 8. Cartesian coordinates of all the structures

**Table S3.** Atomic cartesian coordinates of intermediates and transition states

(presented in Å).

**A1**<sub>x=co</sub>

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Coordinates (Angstroms)			
	X	Y	Z
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25	-0.204562000	-0.196964000	0.164364000
7	-0.517282000	1.636078000	0.065221000
6	0.070850000	-1.542470000	-0.952804000
8	0.178601000	-2.412830000	-1.722331000
6	1.839619000	2.187804000	-0.130894000
6	-1.869775000	2.134949000	0.003738000
6	0.457534000	2.698336000	0.246946000
1	2.631683000	2.846927000	0.231876000
1	1.915301000	2.084486000	-1.215835000
1	0.224830000	3.566455000	-0.389197000
1	0.459451000	3.061375000	1.288725000
1	-2.018474000	2.824801000	-0.844115000
1	-2.139280000	2.707374000	0.909027000
6	-2.813393000	0.980472000	-0.124712000
6	-4.191032000	1.133033000	-0.285496000
1	-4.615045000	2.130757000	-0.335350000
6	-3.018076000	-1.326618000	-0.145675000
1	-2.512321000	-2.283674000	-0.078529000
6	-4.991521000	0.004626000	-0.377455000
1	-6.065139000	0.099757000	-0.505191000
6	-4.391077000	-1.253358000	-0.302732000
1	-4.974208000	-2.165207000	-0.365521000
7	-2.235964000	-0.232730000	-0.062287000
16	1.995013000	0.535309000	0.619771000
6	3.425923000	-0.247177000	-0.277188000
6	3.505870000	-1.671782000	0.278525000
6	4.693356000	0.534733000	0.077682000
1	2.604545000	-2.247848000	0.048751000
1	4.361299000	-2.183664000	-0.175735000
1	3.650128000	-1.672266000	1.364241000
1	4.646948000	1.565272000	-0.288877000
1	4.862687000	0.555871000	1.158874000
1	5.557282000	0.052719000	-0.394332000
6	3.219686000	-0.267051000	-1.790673000

1	4.035396000	-0.837601000	-2.249707000
1	2.275667000	-0.741267000	-2.067779000
1	3.242834000	0.737756000	-2.221765000
6	-0.192234000	-1.334953000	1.515890000
8	-0.197526000	-2.055866000	2.431524000

A2<sub>x=CO</sub>

Coordinates (Angstroms)

	X	Y	Z
25	0.199308000	-0.236010000	-0.182868000
1	0.336569000	2.694330000	2.847621000
6	0.199426000	-1.410380000	-1.500423000
8	0.218641000	-2.152789000	-2.398413000
7	0.517038000	1.601232000	-0.181841000
6	-0.087499000	-1.549266000	0.970310000
8	-0.211397000	-2.397728000	1.761490000
6	-1.836942000	2.167571000	-0.007171000
6	1.870982000	2.096665000	-0.168523000
6	-0.455052000	2.654868000	-0.415301000
1	-2.628745000	2.808781000	-0.401043000
1	-1.907483000	2.123451000	1.082059000
1	-0.218129000	3.552570000	0.177846000
1	-0.457819000	2.966939000	-1.473377000
1	2.028453000	2.843890000	0.628767000
1	2.134314000	2.604040000	-1.113189000
6	2.810478000	0.950028000	0.036129000
6	4.188900000	1.108114000	0.184555000
1	4.616999000	2.105026000	0.160230000
6	3.005992000	-1.350480000	0.223450000
1	2.496609000	-2.307908000	0.227046000
6	4.984678000	-0.013867000	0.359278000
1	6.058629000	0.085910000	0.480489000
6	4.379040000	-1.271429000	0.377451000
1	4.957815000	-2.178640000	0.509287000
7	2.228429000	-0.262526000	0.059884000
16	-1.999787000	0.477760000	-0.667928000
6	-3.427855000	-0.252433000	0.276288000
6	-3.519109000	-1.700916000	-0.211871000
6	-4.694480000	0.517860000	-0.105606000
1	-2.616619000	-2.269604000	0.031091000
1	-4.369780000	-2.189414000	0.275988000
1	-3.677432000	-1.750965000	-1.294399000
1	-4.641606000	1.564442000	0.211109000
1	-4.871570000	0.488555000	-1.185357000

1	-5.556814000	0.061932000	0.394372000
6	-3.209856000	-0.201461000	1.787488000
1	-4.028459000	-0.738969000	2.280155000
1	-2.269324000	-0.672690000	2.080708000
1	-3.218430000	0.823451000	2.169052000
1	0.318267000	2.204913000	2.282850000

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**A3**<sub>x=CO</sub>

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Coordinates (Angstroms)

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	X	Y	Z
25	-1.197234000	0.970626000	-0.063093000
1	-0.791030000	-0.086141000	-1.486713000
6	-1.619704000	2.279580000	1.059192000
8	-1.915689000	3.153671000	1.759713000
7	-0.167826000	-0.129409000	1.319404000
6	-2.004763000	1.885560000	-1.363640000
8	-2.532374000	2.531112000	-2.175407000
6	-2.139439000	-1.464293000	1.752029000
6	0.918410000	0.666545000	1.844864000
6	-0.972408000	-0.710666000	2.373788000
1	-2.805429000	-1.881906000	2.510084000
1	-1.765633000	-2.267129000	1.110669000
1	-0.391119000	-1.428982000	2.978421000
1	-1.355384000	0.052241000	3.080056000
1	1.692226000	0.060509000	2.344486000
1	0.572070000	1.403942000	2.598235000
6	1.541892000	1.428005000	0.710761000
6	2.865646000	1.861781000	0.712351000
1	3.500346000	1.630425000	1.561163000
6	1.194023000	2.353112000	-1.385999000
1	0.496128000	2.527874000	-2.197564000
6	3.354031000	2.560302000	-0.382936000
1	4.385472000	2.897759000	-0.405967000
6	2.502433000	2.804918000	-1.459017000
1	2.840250000	3.336640000	-2.341353000
7	0.716481000	1.682803000	-0.324347000
16	-3.066774000	-0.271456000	0.720522000
6	-3.991438000	-1.345953000	-0.490644000
6	-4.982433000	-0.404725000	-1.179716000
6	-4.743244000	-2.421817000	0.297824000
1	-4.470273000	0.413345000	-1.695875000
1	-5.548984000	-0.968992000	-1.929033000
1	-5.694413000	0.023546000	-0.466843000

1	-4.060580000	-3.154592000	0.738549000
1	-5.354150000	-1.986962000	1.095459000
1	-5.409437000	-2.959900000	-0.385855000
6	-3.064397000	-1.984156000	-1.523063000
1	-3.643869000	-2.693931000	-2.124930000
1	-2.647503000	-1.233833000	-2.199688000
1	-2.239027000	-2.533780000	-1.059417000
1	-0.707939000	-0.577757000	-0.895860000
1	1.297498000	-1.220262000	-1.616793000
1	0.447720000	-1.429732000	0.532044000
6	1.653324000	-2.031562000	-0.958943000
8	0.712498000	-2.291509000	0.048392000
6	3.008761000	-1.590662000	-0.417709000
6	3.938288000	-0.991843000	-1.276042000
6	3.359305000	-1.787408000	0.918697000
6	5.190304000	-0.597674000	-0.810104000
1	3.673898000	-0.820949000	-2.317709000
6	4.611356000	-1.389728000	1.391633000
1	2.638812000	-2.243084000	1.591090000
6	5.531277000	-0.794263000	0.529845000
1	5.896982000	-0.128579000	-1.489181000
1	4.865021000	-1.543645000	2.437053000
1	6.503874000	-0.480744000	0.898567000
6	1.790861000	-3.293839000	-1.808059000
1	0.818645000	-3.564893000	-2.231999000
1	2.499180000	-3.144182000	-2.629206000
1	2.147291000	-4.125910000	-1.190563000

**TSA3-4<sub>x=co</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	-1.191412000	0.982270000	-0.042236000
1	-0.819191000	-0.018898000	-1.486371000
6	-1.615319000	2.261633000	1.117622000
8	-1.913580000	3.118132000	1.837030000
7	-0.131545000	-0.141477000	1.314950000
6	-2.024842000	1.922087000	-1.309642000
8	-2.566468000	2.575389000	-2.103265000
6	-2.095413000	-1.495859000	1.740469000
6	0.965753000	0.658313000	1.834416000
6	-0.931830000	-0.746329000	2.371376000
1	-2.750808000	-1.929472000	2.498312000
1	-1.715098000	-2.284937000	1.086531000

1	-0.337358000	-1.465127000	2.957328000
1	-1.302786000	0.015748000	3.075129000
1	1.742630000	0.045321000	2.313263000
1	0.608594000	1.372872000	2.595316000
6	1.563798000	1.434346000	0.695812000
6	2.893258000	1.846729000	0.668765000
1	3.549686000	1.585053000	1.491884000
6	1.170205000	2.401788000	-1.372508000
1	0.454396000	2.598463000	-2.162944000
6	3.360245000	2.560522000	-0.426363000
1	4.395988000	2.881665000	-0.473322000
6	2.481794000	2.839635000	-1.471529000
1	2.801791000	3.384779000	-2.352276000
7	0.713653000	1.715792000	-0.311962000
16	-3.044126000	-0.302381000	0.727974000
6	-3.940610000	-1.381930000	-0.501291000
6	-4.947285000	-0.453541000	-1.184781000
6	-4.674970000	-2.479842000	0.273250000
1	-4.450240000	0.380807000	-1.689390000
1	-5.497286000	-1.021365000	-1.943655000
1	-5.672071000	-0.048392000	-0.471285000
1	-3.980908000	-3.204799000	0.708972000
1	-5.298243000	-2.065611000	1.072285000
1	-5.327570000	-3.022955000	-0.419449000
6	-2.993999000	-1.991840000	-1.533380000
1	-3.549113000	-2.726680000	-2.128041000
1	-2.608573000	-1.231143000	-2.217066000
1	-2.144972000	-2.504843000	-1.070249000
1	-0.665215000	-0.539709000	-0.929481000
1	1.324149000	-1.041279000	-1.659030000
1	0.334720000	-1.110634000	0.630069000
6	1.584613000	-1.897696000	-1.001510000
8	0.621183000	-2.093627000	-0.027580000
6	2.969198000	-1.570727000	-0.439168000
6	3.954061000	-1.013695000	-1.263972000
6	3.282455000	-1.821210000	0.897381000
6	5.218619000	-0.709424000	-0.765311000
1	3.721759000	-0.801568000	-2.306029000
6	4.547117000	-1.516133000	1.404785000
1	2.514232000	-2.242372000	1.539303000
6	5.520057000	-0.958435000	0.575826000
1	5.967323000	-0.270645000	-1.419562000
1	4.770294000	-1.710169000	2.450734000
1	6.503016000	-0.716801000	0.970454000

6	1.662533000	-3.137110000	-1.902717000
1	0.682849000	-3.321897000	-2.356574000
1	2.399443000	-3.016131000	-2.705299000
1	1.939427000	-4.014991000	-1.306835000

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A4<sub>x=CO</sub>

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Coordinates (Angstroms)

	X	Y	Z
25	1.109858000	-0.996999000	-0.093078000
1	0.716564000	0.172325000	-1.360357000
6	1.550996000	-2.415918000	0.889256000
8	1.844144000	-3.360063000	1.491461000
7	0.114889000	-0.017342000	1.438226000
6	1.878998000	-1.762336000	-1.509704000
8	2.377790000	-2.274709000	-2.423822000
6	2.099629000	1.300284000	1.861515000
6	-0.987420000	-0.853644000	1.906692000
6	0.973397000	0.505319000	2.503528000
1	2.780739000	1.697011000	2.616415000
1	1.679456000	2.118413000	1.268939000
1	0.408011000	1.165777000	3.174867000
1	1.366045000	-0.327808000	3.098820000
1	-1.731866000	-0.281384000	2.473423000
1	-0.594259000	-1.633924000	2.571526000
6	-1.629366000	-1.495989000	0.707853000
6	-2.963103000	-1.891721000	0.692778000
1	-3.578209000	-1.727922000	1.570813000
6	-1.334774000	-2.217618000	-1.471937000
1	-0.656143000	-2.326010000	-2.310346000
6	-3.485248000	-2.468103000	-0.457273000
1	-4.525905000	-2.773707000	-0.496090000
6	-2.655791000	-2.627864000	-1.564755000
1	-3.021233000	-3.061442000	-2.488592000
7	-0.823196000	-1.666983000	-0.359109000
16	3.010138000	0.170366000	0.747553000
6	3.909887000	1.316977000	-0.416966000
6	4.933680000	0.426268000	-1.125751000
6	4.623176000	2.387198000	0.412830000
1	4.452558000	-0.408533000	-1.645321000
1	5.467436000	1.022666000	-1.874049000
1	5.669257000	0.020944000	-0.423509000
1	3.916382000	3.087354000	0.868083000
1	5.240475000	1.946061000	1.202127000
1	5.278961000	2.964487000	-0.248575000



6	2.963613000	1.958141000	-1.429063000
1	3.514567000	2.720936000	-1.991964000
1	2.589336000	1.218223000	-2.141895000
1	2.102764000	2.436128000	-0.950140000
1	0.512794000	0.690719000	-0.786113000
1	-1.235515000	1.355423000	-1.832064000
1	-0.273259000	0.824953000	0.916048000
6	-1.427227000	2.088730000	-1.008353000
8	-0.413442000	2.086697000	-0.088385000
6	-2.786560000	1.679277000	-0.425664000
6	-3.805753000	1.181991000	-1.246210000
6	-3.042786000	1.816201000	0.940573000
6	-5.049201000	0.835954000	-0.718867000
1	-3.618795000	1.053136000	-2.310993000
6	-4.284614000	1.471834000	1.476514000
1	-2.245133000	2.186196000	1.578984000
6	-5.294489000	0.981077000	0.648093000
1	-5.824268000	0.444631000	-1.372789000
1	-4.463672000	1.583967000	2.542914000
1	-6.260300000	0.707758000	1.063951000
6	-1.570186000	3.462338000	-1.692556000
1	-0.617653000	3.736086000	-2.160189000
1	-2.349395000	3.464866000	-2.465181000
1	-1.819320000	4.226290000	-0.945684000

**TSA4-5<sub>x=co</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	1.100628000	-0.994713000	-0.098183000
1	0.714657000	0.210512000	-1.316162000
6	1.541649000	-2.425879000	0.863331000
8	1.834848000	-3.380191000	1.451062000
7	0.108306000	-0.031591000	1.449106000
6	1.861118000	-1.734392000	-1.530630000
8	2.352589000	-2.226935000	-2.460060000
6	2.095562000	1.281848000	1.875626000
6	-0.992412000	-0.874032000	1.911125000
6	0.970385000	0.483443000	2.515534000
1	2.776983000	1.674612000	2.632312000
1	1.676103000	2.104525000	1.288695000
1	0.408025000	1.137775000	3.195110000
1	1.364249000	-0.356115000	3.100521000
1	-1.734967000	-0.309067000	2.487489000

1	-0.594608000	-1.661392000	2.564301000
6	-1.637858000	-1.501119000	0.705812000
6	-2.972103000	-1.894916000	0.690607000
1	-3.584214000	-1.740146000	1.572442000
6	-1.351278000	-2.195205000	-1.483327000
1	-0.676109000	-2.292503000	-2.325841000
6	-3.498483000	-2.457635000	-0.464348000
1	-4.539465000	-2.762094000	-0.503465000
6	-2.672802000	-2.604176000	-1.576404000
1	-3.041529000	-3.026326000	-2.504256000
7	-0.835252000	-1.658751000	-0.365808000
16	3.004062000	0.157896000	0.754519000
6	3.916808000	1.310358000	-0.393839000
6	4.936763000	0.419139000	-1.107537000
6	4.634440000	2.366219000	0.450354000
1	4.451405000	-0.407509000	-1.636177000
1	5.477279000	1.018796000	-1.848340000
1	5.667259000	0.002364000	-0.406664000
1	3.930726000	3.066282000	0.910537000
1	5.244973000	1.911621000	1.237301000
1	5.297091000	2.946147000	-0.201872000
6	2.980309000	1.968979000	-1.403444000
1	3.541952000	2.727569000	-1.961569000
1	2.596162000	1.237715000	-2.119856000
1	2.124997000	2.454999000	-0.923414000
1	0.458776000	0.767460000	-0.768505000
1	-1.265941000	1.326898000	-1.879958000
1	-0.281071000	0.803278000	0.934662000
6	-1.428338000	2.065058000	-1.056082000
8	-0.386256000	2.046172000	-0.163330000
6	-2.774463000	1.677721000	-0.432608000
6	-3.821719000	1.188847000	-1.222299000
6	-2.992652000	1.827120000	0.939061000
6	-5.055161000	0.863133000	-0.659863000
1	-3.664520000	1.050759000	-2.290633000
6	-4.224032000	1.502080000	1.509918000
1	-2.176244000	2.192829000	1.555789000
6	-5.261989000	1.019610000	0.712100000
1	-5.852519000	0.478277000	-1.290326000
1	-4.373439000	1.623638000	2.579777000
1	-6.220023000	0.762695000	1.155329000
6	-1.564375000	3.440049000	-1.736114000
1	-0.618361000	3.698233000	-2.225132000
1	-2.360260000	3.453731000	-2.491180000

1	-1.785079000	4.208439000	-0.984944000
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**A5<sub>x=CO</sub>**

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Coordinates (Angstroms)

	X	Y	Z
25	-0.928461000	-1.034943000	0.418269000
1	-0.109253000	0.379719000	0.559555000
6	-1.796950000	-2.593030000	0.444153000
8	-2.358123000	-3.606704000	0.581506000
7	-0.654471000	-0.960806000	-1.688273000
1	-0.081912000	-0.144012000	-1.903221000
6	-0.971598000	-0.919760000	2.173684000
8	-0.971233000	-0.821736000	3.337570000
6	-2.692903000	0.367693000	-1.861430000
6	0.121865000	-2.146351000	-2.063466000
6	-1.918280000	-0.814400000	-2.423950000
1	-3.649186000	0.476405000	-2.377304000
1	-2.114783000	1.287988000	-1.984533000
1	-1.740702000	-0.650537000	-3.494941000
1	-2.487633000	-1.743165000	-2.312297000
1	0.548013000	-2.065227000	-3.070409000
1	-0.549524000	-3.013548000	-2.050379000
6	1.208308000	-2.351820000	-1.042298000
6	2.429836000	-2.937567000	-1.360568000
1	2.631716000	-3.229144000	-2.386060000
6	1.825962000	-2.133684000	1.172650000
1	1.557505000	-1.782803000	2.162576000
6	3.368726000	-3.137541000	-0.355043000
1	4.326960000	-3.596233000	-0.577291000
6	3.057534000	-2.728621000	0.938292000
1	3.759730000	-2.849877000	1.755460000
7	0.911307000	-1.948770000	0.208673000
16	-2.981050000	0.075821000	-0.078525000
6	-3.302146000	1.783632000	0.598467000
6	-3.704444000	1.547465000	2.057170000
6	-4.469731000	2.394922000	-0.180767000
1	-2.897653000	1.071903000	2.622516000
1	-3.921621000	2.511942000	2.529508000
1	-4.600624000	0.922663000	2.132858000
1	-4.199592000	2.608717000	-1.219796000
1	-5.345542000	1.737637000	-0.176486000
1	-4.753910000	3.343211000	0.289671000
6	-2.079208000	2.694634000	0.531620000

1	-2.354517000	3.678898000	0.928870000
1	-1.255597000	2.299451000	1.130624000
1	-1.723135000	2.834773000	-0.493087000
1	0.752242000	3.493131000	-0.406109000
1	0.186127000	1.244511000	-0.626488000
6	1.330780000	2.784125000	-1.018073000
8	0.480074000	1.731526000	-1.436716000
6	2.488311000	2.279059000	-0.171262000
6	2.950911000	3.044258000	0.901870000
6	3.127164000	1.070260000	-0.466006000
6	4.036291000	2.617120000	1.666926000
1	2.452709000	3.980257000	1.144692000
6	4.212956000	0.641249000	0.295592000
1	2.762842000	0.457932000	-1.286837000
6	4.671429000	1.413032000	1.364665000
1	4.380232000	3.220802000	2.502093000
1	4.698682000	-0.300931000	0.058943000
1	5.513826000	1.074294000	1.960918000
6	1.820473000	3.507054000	-2.265893000
1	0.968734000	3.877311000	-2.845197000
1	2.452281000	4.357952000	-1.992493000
1	2.406616000	2.828392000	-2.895354000

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**TSA2-6<sub>x=co</sub>**  
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Coordinates (Angstroms)

	X	Y	Z
25	0.165713000	0.292729000	0.156350000
1	-0.047489000	0.155879000	-1.557928000
6	0.440516000	0.307343000	1.918207000
8	0.620090000	0.342008000	3.064485000
7	0.529818000	-1.698956000	-0.289966000
1	0.195460000	-0.713194000	-1.258051000
6	-0.134235000	2.042028000	0.128526000
8	-0.312767000	3.192720000	0.100925000
6	-1.852941000	-2.137204000	-0.197001000
6	1.881603000	-2.029581000	0.075595000
6	-0.463442000	-2.631019000	0.180600000
1	-2.629596000	-2.799084000	0.191609000
1	-1.946772000	-2.071622000	-1.285016000
1	-0.330088000	-3.631929000	-0.263725000
1	-0.402776000	-2.761011000	1.279344000
1	2.255050000	-2.938736000	-0.422685000
1	1.968236000	-2.213225000	1.167380000
6	2.781104000	-0.870183000	-0.256014000

6	4.138251000	-1.016997000	-0.533649000
1	4.576746000	-2.009306000	-0.547882000
6	2.934662000	1.428680000	-0.488542000
1	2.419653000	2.382179000	-0.464548000
6	4.906843000	0.111834000	-0.788981000
1	5.966487000	0.018708000	-1.005144000
6	4.291907000	1.361288000	-0.765658000
1	4.846193000	2.272430000	-0.960712000
7	2.189584000	0.340618000	-0.236555000
16	-2.058824000	-0.463980000	0.515575000
6	-3.403981000	0.298874000	-0.524279000
6	-3.774109000	1.594439000	0.203087000
6	-4.602538000	-0.653258000	-0.543465000
1	-2.919783000	2.273218000	0.280866000
1	-4.559799000	2.109599000	-0.360928000
1	-4.154251000	1.395337000	1.210266000
1	-4.386191000	-1.572972000	-1.095383000
1	-4.920269000	-0.919357000	0.470005000
1	-5.442424000	-0.156666000	-1.042719000
6	-2.929199000	0.603067000	-1.943140000
1	-3.773428000	0.999579000	-2.519458000
1	-2.132818000	1.351579000	-1.944509000
1	-2.564830000	-0.291262000	-2.458097000

**A6<sub>x=CO</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.177793000	0.341905000	0.146762000
1	-0.055313000	0.547942000	-1.469402000
6	0.464333000	0.213719000	1.902348000
8	0.646721000	0.239316000	3.054986000
7	0.515845000	-1.699421000	-0.300486000
1	0.451563000	-1.770032000	-1.313541000
6	-0.081404000	2.079279000	0.265438000
8	-0.241866000	3.235661000	0.322665000
6	-1.879431000	-2.103722000	-0.100656000
6	1.890133000	-2.020076000	0.094507000
6	-0.492788000	-2.595522000	0.279369000
1	-2.644933000	-2.741045000	0.346755000
1	-1.998697000	-2.120074000	-1.188045000
1	-0.364945000	-3.626821000	-0.074553000
1	-0.362703000	-2.589605000	1.366816000
1	2.252008000	-2.950412000	-0.358857000

1	1.904553000	-2.150257000	1.183588000
6	2.786645000	-0.867015000	-0.268725000
6	4.136530000	-1.036985000	-0.561283000
1	4.562875000	-2.034727000	-0.565036000
6	2.955600000	1.419602000	-0.544782000
1	2.447287000	2.376965000	-0.541103000
6	4.914720000	0.079706000	-0.844525000
1	5.970530000	-0.027675000	-1.071808000
6	4.309992000	1.333285000	-0.835856000
1	4.869582000	2.235734000	-1.055364000
7	2.201590000	0.346494000	-0.261470000
16	-2.072291000	-0.386168000	0.497383000
6	-3.441608000	0.283245000	-0.577270000
6	-3.765198000	1.654253000	0.023204000
6	-4.650554000	-0.647638000	-0.450735000
1	-2.898665000	2.321726000	-0.007590000
1	-4.568593000	2.120263000	-0.558207000
1	-4.103806000	1.569492000	1.061193000
1	-4.470465000	-1.616958000	-0.926014000
1	-4.920721000	-0.817314000	0.596646000
1	-5.509137000	-0.187442000	-0.953274000
6	-3.029040000	0.431422000	-2.038581000
1	-3.894618000	0.783062000	-2.612709000
1	-2.218886000	1.155049000	-2.152402000
1	-2.703545000	-0.517464000	-2.476503000

**A7R<sub>x=CO</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	-0.742910000	-1.134931000	0.133170000
1	-0.436905000	0.196081000	1.036142000
6	-1.052323000	-2.655911000	-0.743573000
8	-1.269137000	-3.699109000	-1.222065000
7	0.071238000	-0.065038000	-1.498157000
1	0.386938000	0.821754000	-1.110554000
6	-1.312725000	-1.792913000	1.659911000
8	-1.676382000	-2.198285000	2.695094000
6	-2.141897000	0.865533000	-1.936663000
6	1.245700000	-0.798316000	-1.976614000
6	-0.905003000	0.234535000	-2.553715000
1	-2.888515000	1.067756000	-2.707447000
1	-1.873430000	1.803731000	-1.443503000
1	-0.487245000	0.921040000	-3.302217000

1	-1.157164000	-0.705177000	-3.056480000
1	1.906859000	-0.174483000	-2.590606000
1	0.893299000	-1.627111000	-2.602867000
6	1.995682000	-1.365768000	-0.801929000
6	3.349763000	-1.678344000	-0.872554000
1	3.898495000	-1.470541000	-1.785245000
6	1.877438000	-2.121288000	1.376642000
1	1.260004000	-2.275162000	2.254477000
6	3.973758000	-2.245965000	0.230926000
1	5.029139000	-2.497526000	0.198688000
6	3.222367000	-2.464390000	1.381987000
1	3.663727000	-2.892505000	2.275059000
7	1.264574000	-1.593374000	0.305855000
16	-2.826525000	-0.288163000	-0.694078000
6	-3.861798000	0.826563000	0.384790000
6	-4.617733000	-0.122307000	1.319021000
6	-4.848806000	1.585984000	-0.505557000
1	-3.932890000	-0.709597000	1.938207000
1	-5.253531000	0.468389000	1.988233000
1	-5.260394000	-0.810425000	0.759893000
1	-4.341099000	2.305774000	-1.154926000
1	-5.438087000	0.906395000	-1.130195000
1	-5.540954000	2.148646000	0.131505000
6	-3.009531000	1.799361000	1.192560000
1	-3.669453000	2.450695000	1.778402000
1	-2.346819000	1.267573000	1.878271000
1	-2.394192000	2.434800000	0.549265000
6	0.645572000	2.950487000	0.436852000
8	-0.027761000	3.149338000	-0.568496000
6	2.017297000	2.364105000	0.309305000
6	2.673838000	1.774482000	1.396638000
6	2.661120000	2.424580000	-0.933053000
6	3.957809000	1.259651000	1.242213000
1	2.182006000	1.701038000	2.361120000
6	3.950010000	1.922554000	-1.082241000
1	2.147788000	2.880484000	-1.774228000
6	4.599759000	1.341072000	0.006657000
1	4.455453000	0.791273000	2.085670000
1	4.447130000	1.984035000	-2.045584000
1	5.602311000	0.940139000	-0.110375000
6	0.137321000	3.310456000	1.805062000
1	-0.798316000	3.863361000	1.715793000
1	-0.042829000	2.395042000	2.379433000
1	0.875679000	3.906764000	2.349950000

-----  
**A7S<sub>x=CO</sub>**  
-----

Coordinates (Angstroms)

	X	Y	Z
25	0.849365000	-1.153589000	0.259387000
1	-0.002353000	0.134000000	0.789364000
6	1.812286000	-2.579411000	-0.210712000
8	2.437921000	-3.543243000	-0.421382000
7	0.815902000	-0.220887000	-1.635926000
1	0.371761000	0.684636000	-1.491725000
6	0.752526000	-1.643339000	1.943338000
8	0.662968000	-1.929224000	3.074502000
6	-1.340952000	-1.261059000	-2.058404000
6	2.202735000	0.040657000	-2.027578000
6	0.030551000	-0.950672000	-2.636958000
1	-1.945031000	-1.812178000	-2.781943000
1	-1.857225000	-0.331851000	-1.796301000
1	-0.088643000	-0.366404000	-3.559199000
1	0.564816000	-1.874055000	-2.886007000
1	2.277634000	0.766652000	-2.845583000
1	2.644744000	-0.903312000	-2.370548000
6	2.960238000	0.523911000	-0.820038000
6	4.052391000	1.381576000	-0.915412000
1	4.359133000	1.750727000	-1.888573000
6	3.171652000	0.421148000	1.477729000
1	2.780475000	0.029141000	2.409658000
6	4.726506000	1.753569000	0.241535000
1	5.580357000	2.421969000	0.192534000
6	4.276176000	1.260491000	1.463592000
1	4.763268000	1.522970000	2.396120000
7	2.521400000	0.052930000	0.362796000
16	-1.106108000	-2.263476000	-0.548125000
6	-2.721480000	-2.060570000	0.358508000
6	-2.648735000	-3.071788000	1.506725000
6	-3.864078000	-2.421472000	-0.594399000
1	-1.809267000	-2.858080000	2.175357000
1	-3.571507000	-3.011998000	2.094651000
1	-2.547942000	-4.097174000	1.135706000
1	-3.984236000	-1.674305000	-1.385375000
1	-3.711398000	-3.401348000	-1.058858000
1	-4.802314000	-2.456677000	-0.028527000
6	-2.905144000	-0.650003000	0.907111000
1	-3.891836000	-0.578126000	1.380358000
1	-2.143878000	-0.411032000	1.652364000



1	-2.856659000	0.106001000	0.118894000
6	0.056294000	2.896968000	-0.106782000
8	0.569831000	2.750358000	-1.211499000
6	-1.432902000	2.831744000	0.036700000
6	-2.063539000	2.933636000	1.282216000
6	-2.213236000	2.671199000	-1.115749000
6	-3.452783000	2.881168000	1.371304000
1	-1.479769000	3.047137000	2.189971000
6	-3.600327000	2.619504000	-1.026350000
1	-1.721035000	2.589275000	-2.079648000
6	-4.222371000	2.727246000	0.218725000
1	-3.934014000	2.958001000	2.341414000
1	-4.196142000	2.494696000	-1.925533000
1	-5.305189000	2.684403000	0.291455000
6	0.906812000	3.173201000	1.101810000
1	1.958356000	3.166586000	0.810491000
1	0.650833000	4.148156000	1.531115000
1	0.738053000	2.413878000	1.871185000

**TSA7-8R<sub>x=CO</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.598894000	-0.642575000	0.491835000
1	-0.159677000	0.863735000	-0.212328000
6	-0.968195000	-2.175593000	1.310276000
8	-1.187912000	-3.151319000	1.907518000
7	-0.439736000	-1.305719000	-1.469212000
1	-0.048169000	-0.475850000	-1.943829000
6	-0.588952000	0.272995000	2.000360000
8	-0.572435000	0.910141000	2.978309000
6	-2.732070000	-0.572353000	-1.859814000
6	0.586631000	-2.346375000	-1.544641000
6	-1.696446000	-1.651865000	-2.145364000
1	-3.682401000	-0.818366000	-2.338092000
1	-2.384478000	0.399930000	-2.222443000
1	-1.550754000	-1.741305000	-3.229701000
1	-2.042854000	-2.621069000	-1.768755000
1	0.961679000	-2.489470000	-2.565699000
1	0.147162000	-3.295195000	-1.211881000
6	1.713160000	-1.985627000	-0.613697000
6	3.003004000	-2.481938000	-0.780792000
1	3.232011000	-3.098296000	-1.644063000
6	2.321794000	-0.910251000	1.339175000

1	2.015357000	-0.270384000	2.158090000
6	3.971091000	-2.187818000	0.171217000
1	4.981377000	-2.570395000	0.065892000
6	3.620102000	-1.390375000	1.256944000
1	4.338967000	-1.128202000	2.024678000
7	1.380857000	-1.196571000	0.425726000
16	-2.929704000	-0.519586000	-0.047954000
6	-3.936043000	1.002541000	0.301049000
6	-4.223759000	0.931781000	1.803831000
6	-5.240054000	0.926103000	-0.495885000
1	-3.300940000	0.963071000	2.390990000
1	-4.834039000	1.795147000	2.091415000
1	-4.774594000	0.023139000	2.068385000
1	-5.062712000	1.008259000	-1.572841000
1	-5.778864000	-0.006803000	-0.300534000
1	-5.886858000	1.761061000	-0.202476000
6	-3.169362000	2.274609000	-0.034107000
1	-3.767664000	3.145163000	0.260809000
1	-2.214976000	2.310993000	0.497048000
1	-2.975980000	2.353933000	-1.106839000
6	0.788608000	1.699670000	-1.453275000
8	0.783832000	0.955523000	-2.462783000
6	2.060006000	1.803496000	-0.637999000
6	2.106702000	2.442737000	0.605684000
6	3.243700000	1.309945000	-1.190605000
6	3.316737000	2.592786000	1.277503000
1	1.192069000	2.806910000	1.063926000
6	4.457428000	1.461346000	-0.521041000
1	3.201868000	0.813577000	-2.154843000
6	4.498363000	2.107051000	0.713304000
1	3.338442000	3.086399000	2.244864000
1	5.369826000	1.071661000	-0.963647000
1	5.442699000	2.227505000	1.236362000
6	-0.095937000	2.931271000	-1.465651000
1	-1.029484000	2.704993000	-1.981448000
1	-0.311665000	3.330617000	-0.474025000
1	0.437475000	3.703443000	-2.036410000

**TSA7-8S<sub>x=CO</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	0.830125000	-0.848976000	0.312947000
1	-0.038858000	0.653184000	0.380631000

6	1.780626000	-2.350471000	0.334310000
8	2.419551000	-3.320784000	0.413065000
7	1.012971000	-0.323406000	-1.687091000
1	0.662679000	0.648879000	-1.681907000
6	0.509095000	-0.910966000	2.049204000
8	0.283464000	-0.906932000	3.193895000
6	-1.195585000	-1.280141000	-2.083028000
6	2.433472000	-0.235895000	-2.028280000
6	0.207809000	-1.093674000	-2.643336000
1	-1.804497000	-1.871637000	-2.769913000
1	-1.676287000	-0.312268000	-1.912550000
1	0.149244000	-0.582928000	-3.613131000
1	0.687493000	-2.066067000	-2.800863000
1	2.607915000	0.336743000	-2.947651000
1	2.819817000	-1.250718000	-2.185808000
6	3.164150000	0.388311000	-0.869641000
6	4.369997000	1.065514000	-1.026968000
1	4.784285000	1.197410000	-2.021095000
6	3.234597000	0.685644000	1.421805000
1	2.744612000	0.526074000	2.375385000
6	5.024092000	1.556181000	0.096457000
1	5.967493000	2.083591000	-0.002301000
6	4.446219000	1.356471000	1.347636000
1	4.916002000	1.719776000	2.254644000
7	2.596055000	0.213519000	0.339330000
16	-1.005239000	-2.155914000	-0.495896000
6	-2.675650000	-2.082879000	0.315415000
6	-2.567751000	-3.053688000	1.495708000
6	-3.732223000	-2.566616000	-0.679521000
1	-1.780246000	-2.752136000	2.193946000
1	-3.517287000	-3.056075000	2.042384000
1	-2.364671000	-4.076494000	1.162063000
1	-3.871609000	-1.854824000	-1.499253000
1	-3.475804000	-3.543382000	-1.102438000
1	-4.692018000	-2.663351000	-0.159132000
6	-2.998013000	-0.679258000	0.808063000
1	-3.977911000	-0.686110000	1.300035000
1	-2.253578000	-0.330482000	1.527359000
1	-3.039688000	0.036463000	-0.015683000
6	-0.104364000	2.303224000	-0.154649000
8	0.396809000	2.329539000	-1.306758000
6	-1.612954000	2.398169000	-0.040688000
6	-2.263261000	2.583159000	1.183715000
6	-2.376400000	2.364291000	-1.211678000

6	-3.648581000	2.725821000	1.235147000
1	-1.696908000	2.602951000	2.109546000
6	-3.762135000	2.502206000	-1.162800000
1	-1.867650000	2.235666000	-2.161834000
6	-4.403367000	2.685340000	0.062669000
1	-4.139583000	2.865493000	2.193994000
1	-4.340411000	2.472769000	-2.082151000
1	-5.482939000	2.797674000	0.104633000
6	0.705599000	2.875945000	0.994079000
1	1.765981000	2.746569000	0.778583000
1	0.494793000	3.951830000	1.053065000
1	0.476306000	2.424937000	1.961103000

**A8R** <sub>X=CO</sub>

Coordinates (Angstroms)

	X	Y	Z
25	0.660451000	-0.940310000	-0.361511000
1	0.166891000	1.648038000	0.271322000
6	1.030007000	-2.426540000	-1.211459000
8	1.247734000	-3.433845000	-1.753043000
7	0.484469000	-1.130566000	1.539409000
1	-0.177647000	0.505072000	1.982722000
6	0.596568000	-0.087301000	-1.928150000
8	0.551883000	0.445301000	-2.963142000
6	2.694347000	-0.245809000	1.968157000
6	-0.649445000	-1.900473000	2.003702000
6	1.622498000	-1.216355000	2.439117000
1	3.636809000	-0.388895000	2.500787000
1	2.351018000	0.784074000	2.099152000
1	1.340608000	-0.944742000	3.469578000
1	2.032036000	-2.240621000	2.482214000
1	-1.047281000	-1.531007000	2.964178000
1	-0.386050000	-2.960436000	2.170512000
6	-1.727143000	-1.840805000	0.964237000
6	-3.045259000	-2.222518000	1.211064000
1	-3.323748000	-2.564702000	2.202610000
6	-2.236781000	-1.330600000	-1.236390000
1	-1.876616000	-0.967940000	-2.192216000
6	-3.974387000	-2.154306000	0.184198000
1	-5.007555000	-2.440316000	0.354285000
6	-3.559728000	-1.700157000	-1.067702000
1	-4.251061000	-1.622946000	-1.899071000
7	-1.331552000	-1.393857000	-0.242240000
16	2.932162000	-0.568283000	0.188494000

6	3.784174000	0.960837000	-0.445064000
6	4.161357000	0.627403000	-1.890994000
6	5.043765000	1.199593000	0.391069000
1	3.281159000	0.385669000	-2.494313000
1	4.650268000	1.497062000	-2.343587000
1	4.856693000	-0.216977000	-1.937976000
1	4.801576000	1.478662000	1.421261000
1	5.689624000	0.315684000	0.410981000
1	5.610647000	2.025966000	-0.052436000
6	2.870389000	2.182746000	-0.392742000
1	3.419726000	3.055525000	-0.764449000
1	1.984440000	2.048682000	-1.017585000
1	2.548113000	2.405358000	0.628460000
6	-0.571864000	2.093201000	0.958157000
8	-0.512644000	1.414539000	2.192154000
6	-1.932764000	1.973550000	0.285144000
6	-2.060830000	2.281097000	-1.074182000
6	-3.068722000	1.586658000	0.996570000
6	-3.300098000	2.215655000	-1.707136000
1	-1.179300000	2.568721000	-1.643117000
6	-4.312761000	1.521417000	0.366608000
1	-2.968590000	1.329460000	2.046534000
6	-4.434110000	1.838771000	-0.985369000
1	-3.380694000	2.450508000	-2.764990000
1	-5.188004000	1.214591000	0.932958000
1	-5.400891000	1.780317000	-1.477101000
6	-0.202882000	3.556904000	1.181280000
1	0.787360000	3.630877000	1.641120000
1	-0.188301000	4.106055000	0.234489000
1	-0.931293000	4.033715000	1.846902000

-----  
**A8S<sub>x=co</sub>**  
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Coordinates (Angstroms)

	X	Y	Z
25	-0.795875000	-1.092796000	-0.279083000
1	-0.528145000	1.726297000	-0.353885000
6	-1.537588000	-2.517144000	-0.984184000
8	-2.053674000	-3.458308000	-1.435016000
7	-1.084112000	-0.746983000	1.570753000
1	-0.463743000	0.997419000	1.621130000
6	-0.168716000	-0.657562000	-1.889775000
8	0.213091000	-0.365376000	-2.950819000
6	1.097714000	-1.578160000	2.208707000

6	-2.430687000	-0.388090000	1.965128000
6	-0.346225000	-1.390301000	2.645573000
1	1.650967000	-2.219438000	2.897905000
1	1.599101000	-0.609844000	2.126120000
1	-0.356232000	-0.776600000	3.560892000
1	-0.790002000	-2.365184000	2.911238000
1	-2.449139000	0.327705000	2.802712000
1	-3.002658000	-1.271065000	2.300443000
6	-3.130552000	0.212706000	0.784957000
6	-4.320209000	0.933411000	0.886418000
1	-4.772861000	1.081043000	1.861497000
6	-3.092906000	0.507471000	-1.512230000
1	-2.576721000	0.314369000	-2.445724000
6	-4.899416000	1.450966000	-0.262466000
1	-5.824157000	2.016538000	-0.207097000
6	-4.271104000	1.233544000	-1.489208000
1	-4.684489000	1.619682000	-2.414030000
7	-2.524654000	0.006789000	-0.399228000
16	1.026566000	-2.350158000	0.558501000
6	2.729195000	-2.091130000	-0.147503000
6	2.731933000	-2.877954000	-1.461087000
6	3.753573000	-2.678751000	0.826090000
1	1.969839000	-2.511517000	-2.155847000
1	3.708640000	-2.763065000	-1.944050000
1	2.560019000	-3.945544000	-1.289671000
1	3.793709000	-2.115550000	1.763645000
1	3.538860000	-3.727604000	1.055026000
1	4.747296000	-2.627483000	0.366886000
6	3.014693000	-0.613795000	-0.401332000
1	4.015338000	-0.511449000	-0.836949000
1	2.295513000	-0.182065000	-1.099853000
1	2.994321000	-0.028295000	0.521831000
6	-0.132668000	2.455693000	0.370004000
8	-0.349814000	1.976819000	1.679714000
6	1.347455000	2.633108000	0.065329000
6	1.777116000	2.702109000	-1.264165000
6	2.293733000	2.747154000	1.085078000
6	3.124855000	2.876621000	-1.570208000
1	1.048888000	2.604202000	-2.066385000
6	3.645021000	2.924797000	0.783132000
1	1.965273000	2.677944000	2.117593000
6	4.065846000	2.988143000	-0.544816000
1	3.442656000	2.917242000	-2.608471000
1	4.372004000	3.005745000	1.586805000

1	5.118311000	3.119265000	-0.779456000
6	-0.894207000	3.767159000	0.195072000
1	-1.964457000	3.602738000	0.356399000
1	-0.541112000	4.508788000	0.920643000
1	-0.751780000	4.174460000	-0.811083000

**PhCOMe**

Coordinates (Angstroms)

	X	Y	Z
6	1.697046000	-0.202738000	0.000058000
8	2.211879000	-1.306215000	0.000124000
6	0.203093000	-0.058471000	0.000000000
6	-0.427771000	1.189942000	0.000018000
6	-0.577318000	-1.220064000	-0.000056000
6	-1.817595000	1.275742000	-0.000025000
1	0.157669000	2.103818000	0.000073000
6	-1.964098000	-1.134511000	-0.000101000
1	-0.073348000	-2.180810000	-0.000061000
6	-2.586341000	0.114126000	-0.000087000
1	-2.299538000	2.248100000	-0.000010000
1	-2.562067000	-2.040381000	-0.000146000
1	-3.669907000	0.181945000	-0.000124000
6	2.550811000	1.046880000	0.000041000
1	3.600758000	0.754945000	-0.000137000
1	2.342089000	1.658461000	-0.883735000
1	2.342340000	1.658205000	0.884060000

**R-PhCHOHMe**

Coordinates (Angstroms)

	X	Y	Z
1	-1.848087000	-1.272051000	-0.797469000
1	-1.887846000	0.873247000	-1.747889000
6	-1.654644000	-0.345057000	-0.236133000
8	-2.293204000	0.747545000	-0.884604000
6	-0.151238000	-0.154459000	-0.139673000
6	0.711986000	-1.237590000	-0.312268000
6	0.387773000	1.099718000	0.160246000
6	2.089973000	-1.076895000	-0.179740000
1	0.302424000	-2.216207000	-0.552044000
6	1.764294000	1.264601000	0.287072000
1	-0.281614000	1.945552000	0.288209000
6	2.619616000	0.176021000	0.119795000
1	2.749756000	-1.928159000	-0.317240000

1	2.172155000	2.244156000	0.517355000
1	3.692628000	0.305495000	0.220350000
6	-2.298408000	-0.467669000	1.139060000
1	-3.376014000	-0.619236000	1.035329000
1	-1.868776000	-1.311601000	1.685466000
1	-2.125104000	0.446430000	1.714607000

### S-PhCHOHMe

Coordinates (Angstroms)			
	X	Y	Z
1	1.848087000	-1.272044000	-0.797480000
1	1.887839000	0.873272000	-1.747874000
6	1.654644000	-0.345055000	-0.236136000
8	2.293206000	0.747552000	-0.884596000
6	0.151238000	-0.154456000	-0.139675000
6	-0.711984000	-1.237588000	-0.312272000
6	-0.387774000	1.099718000	0.160248000
6	-2.089971000	-1.076896000	-0.179743000
1	-0.302422000	-2.216204000	-0.552053000
6	-1.764295000	1.264600000	0.287075000
1	0.281611000	1.945553000	0.288214000
6	-2.619616000	0.176019000	0.119797000
1	-2.749753000	-1.928161000	-0.317245000
1	-2.172157000	2.244154000	0.517362000
1	-3.692628000	0.305491000	0.220353000
6	2.298406000	-0.467680000	1.139057000
1	3.376012000	-0.619242000	1.035326000
1	2.125097000	0.446411000	1.714615000
1	1.868776000	-1.311620000	1.685452000

### Al<sub>X=Cl</sub>

Coordinates (Angstroms)			
	X	Y	Z
25	0.198778000	-0.209731000	-0.043116000
7	0.513693000	1.653791000	-0.156640000
6	-0.078911000	-1.142338000	1.394098000
8	-0.196768000	-1.657451000	2.458632000
6	-1.853143000	2.162409000	0.039205000
6	1.862348000	2.151621000	-0.107138000
6	-0.474411000	2.696013000	-0.339630000
1	-2.655550000	2.805618000	-0.332795000
1	-1.924100000	2.082757000	1.126503000



1	-0.269764000	3.577138000	0.295075000
1	-0.488897000	3.064924000	-1.382291000
1	2.028258000	2.860114000	0.727707000
1	2.140369000	2.707334000	-1.022667000
6	2.811969000	0.996437000	0.046711000
6	4.196571000	1.157595000	0.123301000
1	4.622233000	2.155083000	0.070786000
6	3.022442000	-1.301564000	0.234349000
1	2.505718000	-2.254534000	0.267742000
6	5.004860000	0.037816000	0.261246000
1	6.083796000	0.140933000	0.324922000
6	4.403355000	-1.220601000	0.318716000
1	4.991089000	-2.125727000	0.426617000
7	2.235165000	-0.218568000	0.103346000
16	-1.983170000	0.482042000	-0.661913000
6	-3.473633000	-0.243665000	0.183368000
6	-3.427132000	-1.737864000	-0.148570000
6	-4.735553000	0.392678000	-0.405690000
1	-2.539394000	-2.212830000	0.280058000
1	-4.317138000	-2.225643000	0.265519000
1	-3.419131000	-1.910476000	-1.230354000
1	-4.761728000	1.473378000	-0.229397000
1	-4.806323000	0.216069000	-1.483737000
1	-5.621985000	-0.044104000	0.070408000
6	-3.434530000	-0.039509000	1.697910000
1	-4.239729000	-0.626983000	2.155339000
1	-2.485014000	-0.371747000	2.124652000
1	-3.598109000	1.006306000	1.974173000
17	0.288436000	-1.942832000	-1.873117000

A2<sub>X=Cl</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.140630000	-0.343891000	-0.020710000
7	-0.480976000	1.657572000	-0.410469000
6	0.089822000	-2.062037000	0.303382000
8	0.228015000	-3.208888000	0.531726000
6	1.889380000	2.112889000	-0.198164000
6	-1.822270000	2.004503000	-0.030006000
6	0.477637000	2.580608000	0.133535000
1	2.649359000	2.758441000	0.249947000
1	2.031775000	2.089119000	-1.283278000
1	0.365058000	3.605396000	-0.275555000

1	0.388964000	2.686833000	1.238115000
1	-2.208018000	2.921440000	-0.517798000
1	-1.919113000	2.185473000	1.064170000
6	-2.743833000	0.860808000	-0.348483000
6	-4.113417000	1.022365000	-0.565840000
1	-4.544033000	2.018414000	-0.534681000
6	-2.932843000	-1.429070000	-0.629416000
1	-2.422250000	-2.386189000	-0.648491000
6	-4.904193000	-0.091056000	-0.817644000
1	-5.971106000	0.016876000	-0.988083000
6	-4.299468000	-1.346641000	-0.852307000
1	-4.869776000	-2.248208000	-1.047745000
7	-2.163780000	-0.356296000	-0.379305000
16	2.052397000	0.411749000	0.457842000
6	3.459000000	-0.297213000	-0.531640000
6	3.797704000	-1.623752000	0.154320000
6	4.657444000	0.652269000	-0.455393000
1	2.937694000	-2.300638000	0.162686000
1	4.610774000	-2.117923000	-0.390403000
1	4.125863000	-1.468622000	1.187454000
1	4.468117000	1.591719000	-0.983976000
1	4.918441000	0.884440000	0.582572000
1	5.525896000	0.176146000	-0.926027000
6	3.068260000	-0.549450000	-1.987450000
1	3.949291000	-0.895704000	-2.541439000
1	2.296204000	-1.319661000	-2.059346000
1	2.699135000	0.356469000	-2.479183000
17	-0.685609000	-0.000336000	2.524304000
1	0.089964000	-0.888015000	-1.630926000
1	0.160332000	-0.093956000	-1.673655000

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### A3<sub>x=Cl</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
25	-1.144366000	0.809702000	-0.214652000
1	-0.784843000	-0.224810000	-1.506119000
7	-0.189514000	-0.218002000	1.312781000
6	-1.904017000	1.719261000	-1.522101000
8	-2.406170000	2.340016000	-2.385145000
6	-2.254529000	-1.405576000	1.782266000
6	0.892837000	0.583098000	1.832881000
6	-1.046644000	-0.693633000	2.376730000
1	-2.949592000	-1.738764000	2.557141000

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1	-1.925032000	-2.268947000	1.196801000
1	-0.527688000	-1.411016000	3.041495000
1	-1.394780000	0.134747000	3.023218000
1	1.661206000	-0.011575000	2.361405000
1	0.530687000	1.339540000	2.554811000
6	1.547122000	1.330573000	0.707081000
6	2.848280000	1.828065000	0.790778000
1	3.428214000	1.648122000	1.690448000
6	1.311633000	2.191289000	-1.425911000
1	0.665946000	2.313883000	-2.289120000
6	3.381475000	2.531680000	-0.278915000
1	4.392753000	2.924276000	-0.233375000
6	2.597624000	2.710123000	-1.418533000
1	2.970403000	3.242460000	-2.286728000
7	0.784170000	1.521862000	-0.387022000
16	-3.084987000	-0.211813000	0.671077000
6	-4.098629000	-1.301383000	-0.446113000
6	-4.962086000	-0.339967000	-1.267808000
6	-4.988309000	-2.202163000	0.414964000
1	-4.345531000	0.326471000	-1.878801000
1	-5.603986000	-0.919729000	-1.941176000
1	-5.606081000	0.272810000	-0.628044000
1	-4.400894000	-2.924906000	0.989776000
1	-5.596824000	-1.616091000	1.111683000
1	-5.665261000	-2.768769000	-0.235186000
6	-3.231925000	-2.144042000	-1.381299000
1	-3.880782000	-2.793997000	-1.980938000
1	-2.658138000	-1.514264000	-2.065545000
1	-2.534823000	-2.786441000	-0.834490000
1	-0.821881000	-0.709612000	-0.866385000
1	1.276767000	-1.203636000	-1.451720000
1	0.439356000	-1.480205000	0.640226000
6	1.678215000	-2.040444000	-0.855882000
8	0.811064000	-2.353497000	0.193968000
6	3.062073000	-1.601274000	-0.384528000
6	3.941168000	-0.979067000	-1.279013000
6	3.482558000	-1.811219000	0.929486000
6	5.210077000	-0.574726000	-0.870642000
1	3.621409000	-0.793342000	-2.302657000
6	4.752391000	-1.405615000	1.344882000
1	2.796820000	-2.281347000	1.627783000
6	5.620968000	-0.785819000	0.447383000
1	5.874836000	-0.083784000	-1.576344000
1	5.060397000	-1.570176000	2.374092000

1	6.606995000	-0.464538000	0.771275000
6	1.782442000	-3.256567000	-1.777176000
1	0.789636000	-3.517592000	-2.158264000
1	2.440367000	-3.058729000	-2.630108000
1	2.180249000	-4.115802000	-1.225076000
17	-1.600531000	2.827498000	1.383348000

**TSA3-4<sub>X=Cl</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
25	-1.157110000	0.840058000	-0.198801000
1	-0.793218000	-0.140430000	-1.535404000
7	-0.170527000	-0.232049000	1.288991000
6	-1.919559000	1.795403000	-1.472680000
8	-2.403438000	2.453834000	-2.316851000
6	-2.223208000	-1.450724000	1.741842000
6	0.914671000	0.570191000	1.816124000
6	-1.023110000	-0.737820000	2.350082000
1	-2.908831000	-1.810122000	2.513216000
1	-1.882811000	-2.296519000	1.137791000
1	-0.489957000	-1.460404000	2.994564000
1	-1.371206000	0.078938000	3.004608000
1	1.687306000	-0.033776000	2.322764000
1	0.544469000	1.303148000	2.552402000
6	1.550591000	1.342293000	0.695965000
6	2.863347000	1.810538000	0.755978000
1	3.467602000	1.588580000	1.629866000
6	1.270932000	2.268955000	-1.403598000
1	0.603426000	2.428821000	-2.243679000
6	3.380385000	2.532396000	-0.309945000
1	4.401874000	2.899506000	-0.284909000
6	2.567043000	2.761984000	-1.418996000
1	2.925277000	3.311892000	-2.282326000
7	0.761102000	1.577989000	-0.370301000
16	-3.078531000	-0.248554000	0.658263000
6	-4.071497000	-1.334151000	-0.480490000
6	-4.945938000	-0.371463000	-1.289139000
6	-4.950978000	-2.259784000	0.364711000
1	-4.337094000	0.308256000	-1.893143000
1	-5.582903000	-0.949455000	-1.968615000
1	-5.595102000	0.227535000	-0.641661000
1	-4.354877000	-2.981061000	0.932370000
1	-5.570264000	-1.691769000	1.066832000

1	-5.617050000	-2.828023000	-0.295122000
6	-3.190735000	-2.149867000	-1.426199000
1	-3.829456000	-2.798842000	-2.037680000
1	-2.623553000	-1.502283000	-2.099226000
1	-2.486362000	-2.791455000	-0.888156000
1	-0.799578000	-0.653523000	-0.919090000
1	1.290027000	-1.142452000	-1.447523000
1	0.381283000	-1.321337000	0.686433000
6	1.659069000	-1.995713000	-0.846938000
8	0.795582000	-2.275975000	0.200923000
6	3.063064000	-1.595091000	-0.390466000
6	3.956660000	-0.999282000	-1.289077000
6	3.482378000	-1.808237000	0.923407000
6	5.235221000	-0.621571000	-0.884872000
1	3.640166000	-0.811260000	-2.313529000
6	4.762373000	-1.431398000	1.335284000
1	2.782539000	-2.256125000	1.622598000
6	5.643635000	-0.835448000	0.433767000
1	5.910758000	-0.151146000	-1.594497000
1	5.068579000	-1.598283000	2.364834000
1	6.637756000	-0.536087000	0.754147000
6	1.733532000	-3.206320000	-1.784554000
1	0.732283000	-3.438566000	-2.163196000
1	2.393148000	-3.021636000	-2.640181000
1	2.109027000	-4.080660000	-1.239839000
17	-1.645143000	2.739419000	1.489325000

A4<sub>x=Cl</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
25	-1.106868000	0.898878000	-0.223913000
1	-0.724652000	-0.200919000	-1.462326000
7	-0.139141000	-0.028286000	1.401211000
6	-1.873423000	1.724464000	-1.581062000
8	-2.384871000	2.295561000	-2.469105000
6	-2.178958000	-1.248952000	1.875061000
6	0.961158000	0.816009000	1.850740000
6	-1.029061000	-0.456896000	2.478503000
1	-2.880794000	-1.570839000	2.647457000
1	-1.781527000	-2.122501000	1.349349000
1	-0.502059000	-1.094279000	3.204374000
1	-1.403073000	0.426324000	3.008758000
1	1.711207000	0.257804000	2.427416000
1	0.560090000	1.608099000	2.493796000

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6	1.606681000	1.457505000	0.653584000
6	2.932258000	1.886186000	0.668326000
1	3.529716000	1.737824000	1.561666000
6	1.349689000	2.169534000	-1.529088000
1	0.687025000	2.260637000	-2.382817000
6	3.469329000	2.476927000	-0.467029000
1	4.502598000	2.809621000	-0.479838000
6	2.661036000	2.616869000	-1.593256000
1	3.035402000	3.062460000	-2.508180000
7	0.820671000	1.604970000	-0.431144000
16	-3.031794000	-0.169681000	0.665661000
6	-3.911956000	-1.397447000	-0.423342000
6	-4.839445000	-0.552508000	-1.301433000
6	-4.737787000	-2.335717000	0.461052000
1	-4.272998000	0.168445000	-1.899313000
1	-5.381690000	-1.210073000	-1.990577000
1	-5.575334000	-0.005975000	-0.702275000
1	-4.103290000	-3.000716000	1.055052000
1	-5.388543000	-1.775804000	1.140944000
1	-5.371094000	-2.964112000	-0.176107000
6	-2.942763000	-2.193478000	-1.298506000
1	-3.489074000	-3.010260000	-1.785767000
1	-2.512829000	-1.562135000	-2.080767000
1	-2.115630000	-2.625786000	-0.725896000
1	-0.646677000	-0.662919000	-0.810718000
1	1.214557000	-1.458447000	-1.661393000
1	0.247796000	-0.907574000	0.943918000
6	1.488863000	-2.193493000	-0.861435000
8	0.539282000	-2.275996000	0.111298000
6	2.860597000	-1.712442000	-0.356836000
6	3.821510000	-1.199505000	-1.236963000
6	3.183540000	-1.791652000	0.999249000
6	5.071886000	-0.787034000	-0.778581000
1	3.582453000	-1.110404000	-2.295625000
6	4.432941000	-1.380683000	1.467634000
1	2.425200000	-2.168488000	1.680255000
6	5.384537000	-0.877742000	0.579821000
1	5.799980000	-0.385215000	-1.478771000
1	4.661802000	-1.448101000	2.528485000
1	6.355287000	-0.550309000	0.942177000
6	1.683278000	-3.541854000	-1.590252000
1	0.727072000	-3.862430000	-2.019839000
1	2.424926000	-3.484850000	-2.397988000
1	2.009566000	-4.305574000	-0.872712000

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17	-1.618499000	2.902212000	1.274669000
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**TSA4-5<sub>X=Cl</sub>**

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Coordinates (Angstroms)			
	X	Y	Z
25	1.058122000	-0.868168000	-0.264045000
1	0.721633000	0.464202000	-1.286085000
7	0.118062000	-0.024135000	1.445270000
6	1.762724000	-1.576035000	-1.704642000
8	2.223039000	-2.052037000	-2.679355000
6	2.189037000	1.149312000	1.941104000
6	-0.976505000	-0.892958000	1.864548000
6	1.025523000	0.361250000	2.525506000
1	2.897066000	1.427825000	2.724747000
1	1.818494000	2.054944000	1.451458000
1	0.517255000	0.978177000	3.280965000
1	1.387952000	-0.548030000	3.017123000
1	-1.713559000	-0.372687000	2.490778000
1	-0.554624000	-1.720728000	2.444989000
6	-1.645253000	-1.461738000	0.642502000
6	-2.966971000	-1.902298000	0.667685000
1	-3.540808000	-1.814006000	1.584385000
6	-1.441673000	-2.036189000	-1.583825000
1	-0.802453000	-2.067261000	-2.459449000
6	-3.529225000	-2.431658000	-0.485961000
1	-4.558782000	-2.775921000	-0.491160000
6	-2.750539000	-2.492797000	-1.639689000
1	-3.145066000	-2.887108000	-2.569714000
7	-0.885395000	-1.535920000	-0.468389000
16	3.013704000	0.094065000	0.692896000
6	3.982625000	1.326506000	-0.312625000
6	4.883997000	0.473320000	-1.210035000
6	4.834674000	2.180789000	0.629747000
1	4.292632000	-0.190583000	-1.848443000
1	5.475410000	1.129725000	-1.858891000
1	5.576427000	-0.137262000	-0.620990000
1	4.219466000	2.842276000	1.247860000
1	5.451914000	1.561331000	1.289108000
1	5.502683000	2.813024000	0.032909000
6	3.080041000	2.213752000	-1.168729000
1	3.692396000	2.988786000	-1.646049000
1	2.586324000	1.633974000	-1.952427000
1	2.300156000	2.706648000	-0.580638000

1	0.363280000	1.053656000	-0.732099000
1	-1.346790000	1.378981000	-1.877522000
1	-0.271861000	0.836690000	1.018479000
6	-1.498794000	2.122066000	-1.058966000
8	-0.417032000	2.126788000	-0.207945000
6	-2.807755000	1.714148000	-0.377286000
6	-3.882801000	1.220156000	-1.125616000
6	-2.967528000	1.848344000	1.003946000
6	-5.086536000	0.875025000	-0.513537000
1	-3.769165000	1.091308000	-2.200482000
6	-4.169049000	1.503037000	1.624235000
1	-2.129384000	2.216279000	1.589311000
6	-5.235207000	1.016162000	0.867599000
1	-5.905485000	0.484050000	-1.111688000
1	-4.272677000	1.611213000	2.700949000
1	-6.169663000	0.742175000	1.349393000
6	-1.684254000	3.489412000	-1.740461000
1	-0.761716000	3.761074000	-2.265443000
1	-2.507055000	3.483879000	-2.466258000
1	-1.891718000	4.259817000	-0.987470000
17	1.534678000	-2.981326000	1.143198000

**A5**  $x=Cl$

-----			
Coordinates (Angstroms)			
	X	Y	Z
25	0.943140000	-0.949942000	-0.313569000
1	0.527892000	0.378853000	-1.224994000
7	-0.028344000	-0.050692000	1.391149000
1	-0.445282000	0.801678000	1.017877000
6	1.650234000	-1.677740000	-1.727244000
8	2.104737000	-2.149983000	-2.715106000
6	2.069312000	1.100902000	1.892010000
6	-1.109133000	-0.936770000	1.824295000
6	0.885075000	0.339829000	2.471330000
1	2.766022000	1.375152000	2.687819000
1	1.725278000	2.010845000	1.390931000
1	0.380579000	0.967595000	3.219536000
1	1.228837000	-0.574175000	2.965491000
1	-1.867879000	-0.414448000	2.421562000
1	-0.666219000	-1.725525000	2.440728000
6	-1.745770000	-1.580906000	0.621974000
6	-3.047719000	-2.074519000	0.664362000
1	-3.629368000	-1.963265000	1.573684000



6	-1.503890000	-2.263291000	-1.568156000
1	-0.857519000	-2.312399000	-2.437654000
6	-3.581038000	-2.690178000	-0.460665000
1	-4.593451000	-3.081901000	-0.450159000
6	-2.791941000	-2.778473000	-1.605170000
1	-3.162167000	-3.238171000	-2.515101000
7	-0.973568000	-1.682573000	-0.478627000
16	2.894782000	0.010691000	0.675995000
6	3.944553000	1.194833000	-0.304779000
6	4.792582000	0.295138000	-1.209054000
6	4.844572000	1.982606000	0.650431000
1	4.162929000	-0.321892000	-1.857851000
1	5.429903000	0.919433000	-1.846166000
1	5.440336000	-0.366256000	-0.623645000
1	4.264949000	2.657790000	1.288154000
1	5.433568000	1.318469000	1.291930000
1	5.540089000	2.596662000	0.065704000
6	3.108228000	2.148797000	-1.154181000
1	3.780539000	2.808778000	-1.716570000
1	2.484429000	1.598733000	-1.862557000
1	2.451928000	2.777832000	-0.545595000
1	-1.241815000	2.323890000	-2.071909000
1	0.205596000	1.670163000	-0.635630000
6	-1.368531000	2.743225000	-1.063301000
8	-0.183735000	2.531257000	-0.316246000
6	-2.571538000	2.062392000	-0.426789000
6	-3.507746000	1.390471000	-1.216685000
6	-2.786638000	2.141154000	0.953056000
6	-4.646947000	0.824113000	-0.645212000
1	-3.340062000	1.304023000	-2.287859000
6	-3.921760000	1.572788000	1.528949000
1	-2.056520000	2.649108000	1.578418000
6	-4.859531000	0.917497000	0.729573000
1	-5.360678000	0.297178000	-1.272351000
1	-4.074857000	1.641241000	2.602535000
1	-5.742008000	0.469863000	1.177708000
6	-1.594600000	4.246453000	-1.183778000
1	-0.744614000	4.715710000	-1.688986000
1	-2.503379000	4.457956000	-1.756756000
1	-1.702053000	4.696703000	-0.190335000
17	1.433454000	-3.031142000	1.266041000

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.141055000	0.335454000	0.009547000
1	-0.093666000	0.234490000	-1.669590000
7	0.501153000	-1.678736000	-0.456902000
1	0.149238000	-0.651518000	-1.364538000
6	-0.166874000	2.058450000	0.071659000
8	-0.377732000	3.220818000	0.062288000
6	-1.883388000	-2.110826000	-0.277192000
6	1.857667000	-2.021403000	-0.127033000
6	-0.478780000	-2.621786000	0.017203000
1	-2.640955000	-2.786786000	0.126714000
1	-2.029499000	-2.016413000	-1.357715000
1	-0.375106000	-3.612269000	-0.463229000
1	-0.376490000	-2.792233000	1.106987000
1	2.242654000	-2.892376000	-0.687142000
1	1.950478000	-2.279348000	0.947298000
6	2.762404000	-0.842273000	-0.365267000
6	4.133443000	-0.985649000	-0.579248000
1	4.566558000	-1.980207000	-0.619125000
6	2.942802000	1.459537000	-0.476537000
1	2.429373000	2.413835000	-0.434391000
6	4.923781000	0.146025000	-0.734109000
1	5.993105000	0.054152000	-0.897906000
6	4.313819000	1.397698000	-0.680516000
1	4.882264000	2.313782000	-0.798075000
7	2.173644000	0.369606000	-0.318024000
16	-2.044678000	-0.455245000	0.490343000
6	-3.461485000	0.304818000	-0.447840000
6	-3.790107000	1.594621000	0.310064000
6	-4.662133000	-0.644341000	-0.407134000
1	-2.932289000	2.273167000	0.336752000
1	-4.614497000	2.111298000	-0.195307000
1	-4.099456000	1.386923000	1.339845000
1	-4.476953000	-1.562052000	-0.974087000
1	-4.920761000	-0.917837000	0.621365000
1	-5.530620000	-0.147368000	-0.855584000
6	-3.083044000	0.630368000	-1.892180000
1	-3.955232000	1.055729000	-2.403729000
1	-2.269022000	1.358927000	-1.931144000
1	-2.773097000	-0.260174000	-2.448365000
17	0.700712000	0.047046000	2.528928000
-----			

A6<sub>x=Cl</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.150396000	0.413868000	-0.034399000
1	-0.067572000	0.647832000	-1.671620000
7	0.480219000	-1.657252000	-0.513787000
1	0.376116000	-1.665424000	-1.525212000
6	-0.068303000	2.109112000	0.284007000
8	-0.199192000	3.275122000	0.461471000
6	-1.913816000	-2.064055000	-0.229251000
6	1.863598000	-2.003105000	-0.183187000
6	-0.510597000	-2.576272000	0.059078000
1	-2.655214000	-2.720156000	0.233025000
1	-2.090045000	-2.042865000	-1.308787000
1	-0.405274000	-3.591194000	-0.349538000
1	-0.334909000	-2.617961000	1.137872000
1	2.226184000	-2.875375000	-0.741829000
1	1.895463000	-2.245209000	0.884282000
6	2.763028000	-0.816485000	-0.409388000
6	4.126957000	-0.972480000	-0.648839000
1	4.545104000	-1.970848000	-0.731520000
6	2.968976000	1.481010000	-0.439358000
1	2.468770000	2.439488000	-0.356172000
6	4.931292000	0.153978000	-0.775432000
1	5.996465000	0.054791000	-0.959655000
6	4.336919000	1.408429000	-0.663028000
1	4.915039000	2.321728000	-0.752719000
7	2.183110000	0.397516000	-0.315432000
16	-2.057279000	-0.366306000	0.442369000
6	-3.513478000	0.326263000	-0.487680000
6	-3.676438000	1.746740000	0.061531000
6	-4.751831000	-0.513723000	-0.163746000
1	-2.798440000	2.359726000	-0.162669000
1	-4.550791000	2.216570000	-0.403500000
1	-3.831062000	1.744895000	1.146124000
1	-4.661939000	-1.532899000	-0.554234000
1	-4.925954000	-0.570713000	0.915814000
1	-5.634340000	-0.058087000	-0.628864000
6	-3.278978000	0.378087000	-1.995756000
1	-4.131338000	0.876234000	-2.473770000
1	-2.368178000	0.933843000	-2.231776000
1	-3.194817000	-0.619959000	-2.437593000
17	0.686443000	-0.288121000	2.494910000

-----  
**A7R<sub>X=Cl</sub>**  
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Coordinates (Angstroms)

	X	Y	Z
25	-0.831515000	-0.679389000	0.499020000
1	-0.264539000	0.869845000	0.419185000
7	-0.554948000	-0.764183000	-1.634292000
1	-0.103851000	0.124691000	-1.842643000
6	-0.970101000	-0.565665000	2.227112000
8	-1.042756000	-0.448518000	3.407248000
6	-2.782267000	0.202624000	-1.890453000
6	0.400318000	-1.828085000	-1.942516000
6	-1.799489000	-0.838949000	-2.405698000
1	-3.722183000	0.143022000	-2.444620000
1	-2.362730000	1.206185000	-2.011760000
1	-1.623910000	-0.671708000	-3.477992000
1	-2.213109000	-1.844191000	-2.278426000
1	0.883770000	-1.690485000	-2.918467000
1	-0.149467000	-2.774886000	-1.962478000
6	1.435134000	-1.918209000	-0.851907000
6	2.678237000	-2.508747000	-1.074306000
1	2.926834000	-2.869780000	-2.067648000
6	1.955828000	-1.541631000	1.364641000
1	1.633545000	-1.127762000	2.313787000
6	3.575087000	-2.629605000	-0.020573000
1	4.545904000	-3.091995000	-0.170038000
6	3.204154000	-2.130922000	1.226232000
1	3.871966000	-2.183840000	2.079274000
7	1.072708000	-1.441653000	0.355748000
16	-3.069973000	-0.122394000	-0.113533000
6	-3.808552000	1.477097000	0.488192000
6	-4.211431000	1.190914000	1.938126000
6	-5.047667000	1.807105000	-0.348428000
1	-3.344616000	0.899395000	2.539292000
1	-4.643733000	2.096159000	2.380183000
1	-4.959960000	0.393484000	1.997042000
1	-4.787888000	2.051436000	-1.383692000
1	-5.760743000	0.975977000	-0.356950000
1	-5.550669000	2.682126000	0.080515000
6	-2.814867000	2.636965000	0.446876000
1	-3.319020000	3.549889000	0.787834000
1	-1.960004000	2.444324000	1.098641000
1	-2.438403000	2.822757000	-0.563952000

6	1.636018000	2.130811000	-1.487828000
8	1.532759000	1.324530000	-2.406990000
6	2.743703000	1.993659000	-0.492939000
6	2.826916000	2.816798000	0.636577000
6	3.720844000	1.013038000	-0.701568000
6	3.870431000	2.657660000	1.544795000
1	2.074446000	3.575838000	0.821795000
6	4.767288000	0.860163000	0.201473000
1	3.645704000	0.372925000	-1.574562000
6	4.842413000	1.681251000	1.327639000
1	3.922432000	3.293182000	2.423514000
1	5.520238000	0.096069000	0.033846000
1	5.654606000	1.557521000	2.038077000
6	0.678929000	3.285711000	-1.367370000
1	-0.064378000	3.224690000	-2.163499000
1	0.173094000	3.264716000	-0.397982000
1	1.220919000	4.234933000	-1.444977000
17	-1.638042000	-3.235330000	0.319234000

A7S<sub>X=Cl</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.880001000	-0.980748000	0.376920000
1	-0.065881000	0.254852000	0.895213000
7	0.788140000	-0.066164000	-1.563843000
1	0.260207000	0.786544000	-1.392204000
6	0.958398000	-1.637039000	1.983625000
8	0.996104000	-2.048325000	3.098134000
6	-1.264666000	-1.305105000	-1.992084000
6	2.139662000	0.326984000	-1.961539000
6	0.065304000	-0.846444000	-2.571976000
1	-1.812599000	-1.903882000	-2.723528000
1	-1.873221000	-0.437155000	-1.716748000
1	-0.118823000	-0.261019000	-3.484244000
1	0.683876000	-1.709501000	-2.837475000
1	2.142562000	1.096428000	-2.743911000
1	2.644389000	-0.564382000	-2.348574000
6	2.890682000	0.806732000	-0.748204000
6	3.936333000	1.722767000	-0.845005000
1	4.198573000	2.131861000	-1.815692000
6	3.167095000	0.656780000	1.537633000
1	2.819879000	0.218460000	2.466822000
6	4.620796000	2.102002000	0.303445000

1	5.437473000	2.815403000	0.251247000
6	4.225746000	1.553755000	1.521974000
1	4.722064000	1.816066000	2.450091000
7	2.502390000	0.280351000	0.431387000
16	-0.914086000	-2.293935000	-0.492915000
6	-2.553546000	-2.294704000	0.391382000
6	-2.366546000	-3.280254000	1.548563000
6	-3.639164000	-2.800033000	-0.562429000
1	-1.553152000	-2.965966000	2.210003000
1	-3.289060000	-3.323706000	2.139509000
1	-2.148147000	-4.290407000	1.185579000
1	-3.838162000	-2.083342000	-1.365816000
1	-3.366991000	-3.760682000	-1.012168000
1	-4.574251000	-2.937192000	-0.006106000
6	-2.924239000	-0.915790000	0.933249000
1	-3.906942000	-0.974786000	1.417903000
1	-2.190941000	-0.567431000	1.663506000
1	-2.988279000	-0.167785000	0.138201000
6	-0.316934000	3.014395000	-0.137177000
8	0.205971000	2.942436000	-1.244313000
6	-1.788315000	2.772028000	0.006380000
6	-2.432591000	2.832013000	1.247066000
6	-2.535532000	2.475319000	-1.140750000
6	-3.804840000	2.609100000	1.336357000
1	-1.870210000	3.045889000	2.150134000
6	-3.905698000	2.253229000	-1.051607000
1	-2.029696000	2.420097000	-2.099594000
6	-4.542980000	2.322575000	0.188494000
1	-4.296535000	2.655272000	2.303171000
1	-4.476266000	2.022334000	-1.946351000
1	-5.612229000	2.146390000	0.261354000
6	0.498781000	3.372599000	1.074325000
1	1.548342000	3.460349000	0.788362000
1	0.153200000	4.324885000	1.492857000
1	0.394447000	2.607291000	1.847972000
17	2.494995000	-2.807698000	-0.763504000

**TSA7-8R<sub>X=Cl</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.596996000	-0.546090000	0.482598000
1	-0.158961000	0.963344000	-0.166442000
7	-0.466720000	-1.154246000	-1.542820000

1	-0.092530000	-0.301062000	-1.973695000
6	-0.576189000	0.128382000	2.085704000
8	-0.522110000	0.639796000	3.155092000
6	-2.779669000	-0.428015000	-1.846579000
6	0.557839000	-2.187474000	-1.674922000
6	-1.737282000	-1.483908000	-2.195004000
1	-3.739494000	-0.678879000	-2.304672000
1	-2.460130000	0.556015000	-2.204320000
1	-1.628461000	-1.542331000	-3.287434000
1	-2.062817000	-2.465012000	-1.833065000
1	0.956240000	-2.260422000	-2.696024000
1	0.104072000	-3.150750000	-1.417035000
6	1.671033000	-1.922793000	-0.695819000
6	2.948781000	-2.446218000	-0.885264000
1	3.167572000	-3.007459000	-1.788547000
6	2.293248000	-1.002830000	1.326751000
1	1.996869000	-0.408507000	2.183577000
6	3.918358000	-2.247849000	0.089863000
1	4.918204000	-2.652369000	-0.034381000
6	3.579430000	-1.512818000	1.222971000
1	4.299615000	-1.321190000	2.010813000
7	1.346712000	-1.198985000	0.393857000
16	-2.921617000	-0.407316000	-0.024741000
6	-3.895766000	1.129209000	0.343977000
6	-4.135659000	1.071819000	1.856087000
6	-5.227410000	1.079942000	-0.408447000
1	-3.189592000	1.071967000	2.406536000
1	-4.710726000	1.952201000	2.165637000
1	-4.701429000	0.178329000	2.141248000
1	-5.082810000	1.150018000	-1.491431000
1	-5.778958000	0.159238000	-0.190637000
1	-5.849033000	1.930196000	-0.102593000
6	-3.123032000	2.393532000	-0.014242000
1	-3.710451000	3.273493000	0.277241000
1	-2.162256000	2.426017000	0.504742000
1	-2.938569000	2.462155000	-1.089904000
6	0.890557000	1.871740000	-1.437830000
8	0.869313000	1.168991000	-2.468839000
6	2.143436000	1.886498000	-0.590830000
6	2.192639000	2.479916000	0.675775000
6	3.315006000	1.352525000	-1.132548000
6	3.391050000	2.541028000	1.381375000
1	1.286616000	2.870932000	1.128351000
6	4.517800000	1.416559000	-0.429615000

1	3.272073000	0.889881000	-2.113483000
6	4.560632000	2.014147000	0.828503000
1	3.412662000	2.997536000	2.366844000
1	5.419763000	0.995269000	-0.864761000
1	5.495845000	2.064263000	1.378862000
6	0.020868000	3.111778000	-1.385438000
1	-0.914595000	2.922886000	-1.913109000
1	-0.194549000	3.455196000	-0.373195000
1	0.562286000	3.910530000	-1.911400000
17	-1.172782000	-3.043582000	1.140535000

---

**TSA7-8S<sub>X=Cl</sub>**

---

Coordinates (Angstroms)

	X	Y	Z
25	0.806414000	-0.739070000	0.379630000
1	-0.169842000	0.679849000	0.430780000
7	0.955662000	-0.215590000	-1.670547000
1	0.528254000	0.717438000	-1.656427000
6	0.611832000	-0.950862000	2.096234000
8	0.446985000	-1.032107000	3.268033000
6	-1.169280000	-1.365175000	-2.027079000
6	2.362360000	-0.026004000	-2.015174000
6	0.208902000	-1.063363000	-2.603230000
1	-1.731601000	-2.008483000	-2.708250000
1	-1.727761000	-0.437346000	-1.866927000
1	0.094738000	-0.583508000	-3.585762000
1	0.768026000	-1.994743000	-2.743797000
1	2.498626000	0.586369000	-2.916737000
1	2.804782000	-1.011147000	-2.199114000
6	3.075933000	0.595874000	-0.843721000
6	4.258531000	1.315614000	-1.003792000
1	4.656037000	1.475719000	-2.001195000
6	3.166778000	0.860659000	1.446750000
1	2.692679000	0.667298000	2.402531000
6	4.912319000	1.812089000	0.117373000
1	5.837571000	2.370723000	0.015377000
6	4.353753000	1.575502000	1.371568000
1	4.820849000	1.941271000	2.279487000
7	2.528033000	0.376917000	0.368360000
16	-0.905924000	-2.200275000	-0.422953000
6	-2.584363000	-2.190901000	0.372957000
6	-2.444900000	-3.136126000	1.570611000
6	-3.623997000	-2.732479000	-0.610639000



1	-1.664911000	-2.794392000	2.258882000
1	-3.392870000	-3.164163000	2.120497000
1	-2.205432000	-4.157057000	1.254641000
1	-3.792296000	-2.041147000	-1.442629000
1	-3.327355000	-3.704411000	-1.019070000
1	-4.580757000	-2.860201000	-0.090282000
6	-2.969625000	-0.794547000	0.848850000
1	-3.952612000	-0.833587000	1.334691000
1	-2.237279000	-0.410313000	1.563339000
1	-3.032092000	-0.090260000	0.015964000
6	-0.282363000	2.441142000	-0.130879000
8	0.252501000	2.494012000	-1.258823000
6	-1.793948000	2.420707000	-0.061376000
6	-2.496826000	2.600968000	1.134689000
6	-2.515825000	2.276379000	-1.250756000
6	-3.890585000	2.625179000	1.141042000
1	-1.964007000	2.710139000	2.073928000
6	-3.908789000	2.293321000	-1.246525000
1	-1.969002000	2.151162000	-2.180107000
6	-4.602246000	2.468461000	-0.048294000
1	-4.420352000	2.761904000	2.079545000
1	-4.452628000	2.172759000	-2.179389000
1	-5.688471000	2.483866000	-0.041284000
6	0.469614000	2.999861000	1.060176000
1	1.539212000	2.884748000	0.884335000
1	0.242892000	4.072233000	1.135302000
1	0.208611000	2.520334000	2.004665000
17	2.420355000	-2.788603000	-0.048094000

**A8R<sub>x=Cl</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.895719000	-0.966572000	-0.174154000
1	-0.404282000	1.447127000	-0.902824000
7	0.358334000	-0.324336000	1.593327000
1	-0.038347000	1.334605000	1.198644000
6	1.014410000	-0.684443000	-1.901221000
8	0.984931000	-0.379657000	-3.045152000
6	2.549200000	0.600265000	2.087814000
6	-0.896490000	-0.828263000	2.099774000
6	1.322336000	-0.102195000	2.653481000
1	3.376946000	0.599488000	2.801058000
1	2.297432000	1.634420000	1.839056000

1	0.915617000	0.536410000	3.459229000
1	1.618515000	-1.053622000	3.132473000
1	-1.483733000	-0.068835000	2.649279000
1	-0.740028000	-1.658590000	2.814737000
6	-1.723001000	-1.365500000	0.966728000
6	-3.070659000	-1.698300000	1.111420000
1	-3.564439000	-1.521413000	2.061808000
6	-1.734707000	-2.085601000	-1.230157000
1	-1.166595000	-2.217676000	-2.144392000
6	-3.752084000	-2.256921000	0.040614000
1	-4.800865000	-2.522383000	0.132105000
6	-3.065312000	-2.463062000	-1.156074000
1	-3.551626000	-2.897971000	-2.022386000
7	-1.068541000	-1.540803000	-0.196193000
16	3.046811000	-0.259007000	0.548269000
6	3.839183000	1.113593000	-0.430009000
6	4.464733000	0.425734000	-1.646413000
6	4.930196000	1.775655000	0.415369000
1	3.715057000	-0.122178000	-2.225522000
1	4.912388000	1.182658000	-2.300771000
1	5.251422000	-0.275273000	-1.347736000
1	4.512802000	2.314697000	1.271512000
1	5.652037000	1.040412000	0.786507000
1	5.472409000	2.502145000	-0.201365000
6	2.802164000	2.146032000	-0.874992000
1	3.308842000	2.966330000	-1.398767000
1	2.071407000	1.703178000	-1.556171000
1	2.256381000	2.572411000	-0.028579000
6	-0.905579000	2.218682000	-0.293883000
8	-0.300744000	2.275627000	0.975128000
6	-2.381211000	1.844848000	-0.214719000
6	-3.026320000	1.285867000	-1.322761000
6	-3.122816000	2.081959000	0.944868000
6	-4.385890000	0.982076000	-1.278537000
1	-2.454983000	1.074911000	-2.224559000
6	-4.483878000	1.778026000	0.994168000
1	-2.621229000	2.498405000	1.813160000
6	-5.121473000	1.229924000	-0.118530000
1	-4.867777000	0.538080000	-2.145349000
1	-5.045161000	1.965402000	1.905759000
1	-6.179884000	0.987966000	-0.079598000
6	-0.724624000	3.568411000	-0.983168000
1	0.341009000	3.798046000	-1.083500000
1	-1.174670000	3.561022000	-1.981159000

1	-1.200916000	4.362094000	-0.395852000
17	1.575248000	-3.381527000	-0.038097000

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**A8S<sub>X=Cl</sub>**

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Coordinates (Angstroms)

	X	Y	Z
25	1.165659000	0.773415000	-0.343431000
1	-0.597641000	-1.160454000	-0.333575000
7	1.153993000	0.255544000	1.578943000
1	-0.007510000	-0.936861000	1.640554000
6	0.757286000	0.825371000	-2.050908000
8	0.438354000	0.787568000	-3.189601000
6	-0.459051000	1.975690000	2.129892000
6	2.324746000	-0.500418000	1.961790000
6	0.787759000	1.230285000	2.584416000
1	-0.703620000	2.803645000	2.799825000
1	-1.305973000	1.284814000	2.089491000
1	0.564982000	0.759550000	3.559972000
1	1.603839000	1.954626000	2.770047000
1	2.158910000	-1.155781000	2.836198000
1	3.164009000	0.167632000	2.236300000
6	2.768517000	-1.336931000	0.795319000
6	3.561856000	-2.476466000	0.934168000
1	3.869250000	-2.794330000	1.925551000
6	2.717742000	-1.599605000	-1.501769000
1	2.355741000	-1.218055000	-2.450274000
6	3.939974000	-3.187030000	-0.197220000
1	4.553775000	-4.078380000	-0.110688000
6	3.508288000	-2.737132000	-1.444607000
1	3.772279000	-3.257150000	-2.358980000
7	2.347894000	-0.907782000	-0.410444000
16	-0.130059000	2.605488000	0.442192000
6	-1.836176000	2.777733000	-0.280825000
6	-1.631247000	3.487913000	-1.622036000
6	-2.697980000	3.638759000	0.645251000
1	-0.983165000	2.908187000	-2.285852000
1	-2.601319000	3.611635000	-2.117433000
1	-1.189640000	4.481003000	-1.486454000
1	-2.881309000	3.146561000	1.605418000
1	-2.231899000	4.611079000	0.836648000
1	-3.671313000	3.814351000	0.171901000
6	-2.477839000	1.408386000	-0.499904000
1	-3.468048000	1.533586000	-0.955049000

1	-1.867717000	0.792886000	-1.166221000
1	-2.614291000	0.864390000	0.439316000
6	-0.989236000	-1.974237000	0.306782000
8	-0.670987000	-1.708399000	1.646135000
6	-2.494645000	-2.010545000	0.091676000
6	-3.015721000	-2.017318000	-1.208057000
6	-3.382191000	-2.025867000	1.168756000
6	-4.391117000	-2.037711000	-1.426464000
1	-2.335898000	-1.988089000	-2.057090000
6	-4.762029000	-2.050349000	0.954523000
1	-2.979980000	-2.002987000	2.176324000
6	-5.272394000	-2.055347000	-0.342660000
1	-4.777785000	-2.032513000	-2.441974000
1	-5.439779000	-2.060172000	1.804116000
1	-6.345578000	-2.068991000	-0.510480000
6	-0.332566000	-3.279665000	-0.154294000
1	0.749430000	-3.222758000	0.000912000
1	-0.721176000	-4.125034000	0.425063000
1	-0.519276000	-3.471269000	-1.216545000
17	3.234953000	2.200877000	-0.424179000

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**Al<sub>X=H</sub>**

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Coordinates (Angstroms)

	X	Y	Z
25	0.222127000	-0.295737000	-0.391943000
7	0.542239000	1.508764000	0.105364000
6	-0.072128000	-1.840546000	0.358338000
8	-0.224674000	-2.847471000	0.978925000
6	-1.822324000	2.018323000	0.362312000
6	1.895522000	1.975715000	0.260252000
6	-0.424262000	2.587202000	0.145428000
1	-2.598339000	2.751126000	0.125618000
1	-1.929301000	1.701713000	1.402691000
1	-0.217497000	3.294150000	0.968944000
1	-0.405356000	3.186117000	-0.785004000
1	2.069852000	2.465806000	1.237141000
1	2.171211000	2.731807000	-0.499995000
6	2.839841000	0.815984000	0.123823000
6	4.220391000	0.935187000	0.296579000
1	4.645579000	1.902120000	0.547879000
6	3.047134000	-1.440711000	-0.339783000
1	2.533841000	-2.361819000	-0.594828000
6	5.025757000	-0.184180000	0.141559000

1	6.101224000	-0.113687000	0.272238000
6	4.422960000	-1.400796000	-0.184104000
1	5.006048000	-2.305604000	-0.317731000
7	2.259266000	-0.358116000	-0.189177000
16	-1.981280000	0.541940000	-0.703675000
6	-3.422237000	-0.366335000	0.046993000
6	-3.524244000	-1.662795000	-0.761837000
6	-4.691536000	0.471570000	-0.126131000
1	-2.612391000	-2.259617000	-0.663504000
1	-4.370027000	-2.254943000	-0.393905000
1	-3.690685000	-1.460570000	-1.825670000
1	-4.629144000	1.418697000	0.420261000
1	-4.882804000	0.693243000	-1.181213000
1	-5.552407000	-0.082172000	0.267903000
6	-3.190750000	-0.686463000	1.524262000
1	-3.993522000	-1.345382000	1.876974000
1	-2.235360000	-1.194628000	1.675432000
1	-3.209790000	0.211672000	2.149131000
1	0.308291000	-0.863336000	-1.955848000

A2<sub>X=H</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.203597000	0.362794000	-0.306406000
7	-0.530770000	-1.660123000	0.097632000
6	0.002373000	2.055323000	-0.698354000
8	0.119517000	3.195874000	-1.000897000
6	1.846783000	-2.099576000	-0.139594000
6	-1.859464000	-1.990473000	-0.334345000
6	0.433619000	-2.543227000	-0.496798000
1	2.603287000	-2.712775000	-0.636733000
1	1.992475000	-2.163885000	0.942912000
1	0.324802000	-3.594484000	-0.158615000
1	0.343545000	-2.576293000	-1.608549000
1	-2.254772000	-2.939225000	0.079698000
1	-1.921749000	-2.104147000	-1.445961000
6	-2.795289000	-0.871141000	0.025478000
6	-4.152082000	-1.056786000	0.291994000
1	-4.567657000	-2.059471000	0.268885000
6	-3.007370000	1.412777000	0.332150000
1	-2.510062000	2.377323000	0.337273000
6	-4.950655000	0.042280000	0.584697000
1	-6.008481000	-0.083832000	0.794738000

6	-4.363536000	1.306070000	0.607106000
1	-4.939647000	2.196739000	0.833870000
7	-2.230761000	0.354878000	0.044014000
16	2.026095000	-0.351619000	-0.658187000
6	3.357210000	0.284392000	0.480080000
6	3.676866000	1.693108000	-0.029460000
6	4.590706000	-0.614340000	0.357548000
1	2.789331000	2.333928000	-0.005882000
1	4.439896000	2.147570000	0.613462000
1	4.063414000	1.673772000	-1.054034000
1	4.410667000	-1.609484000	0.776720000
1	4.901127000	-0.729916000	-0.686283000
1	5.423757000	-0.166620000	0.912791000
6	2.896514000	0.359035000	1.935627000
1	3.746426000	0.647019000	2.566652000
1	2.111441000	1.107889000	2.064170000
1	2.520909000	-0.600332000	2.305859000
1	-0.464487000	0.017808000	-1.925062000
1	-0.036455000	0.944474000	1.328436000
1	0.025157000	0.155057000	1.405679000

### A3<sub>X=H</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	1.225374000	1.154096000	-0.176748000
1	0.964862000	0.461879000	1.376801000
7	0.247066000	-0.254327000	-1.377676000
6	1.990954000	2.413385000	0.763625000
8	2.504478000	3.299949000	1.358225000
6	2.347487000	-1.437284000	-1.676339000
6	-0.876575000	0.392123000	-2.011020000
6	1.098929000	-0.890576000	-2.356198000
1	3.035324000	-1.887192000	-2.396938000
1	2.061372000	-2.187132000	-0.933410000
1	0.597411000	-1.740135000	-2.860686000
1	1.398408000	-0.186140000	-3.158270000
1	-1.628632000	-0.314455000	-2.409290000
1	-0.552760000	1.015299000	-2.872019000
6	-1.540492000	1.314353000	-1.028095000
6	-2.887339000	1.669143000	-1.106767000
1	-3.505530000	1.242584000	-1.890273000
6	-1.254389000	2.645532000	0.840239000
1	-0.568106000	3.011664000	1.597080000

6	-3.419352000	2.546580000	-0.171789000
1	-4.467138000	2.828364000	-0.212598000
6	-2.584379000	3.040722000	0.829225000
1	-2.950839000	3.722260000	1.589299000
7	-0.729597000	1.806642000	-0.069181000
16	3.168615000	-0.044119000	-0.817320000
6	4.156364000	-0.903732000	0.507469000
6	5.027064000	0.196090000	1.122621000
6	5.037479000	-1.973925000	-0.142241000
1	4.413189000	1.015569000	1.510720000
1	5.605426000	-0.220023000	1.955710000
1	5.730895000	0.608009000	0.391377000
1	4.443560000	-2.809250000	-0.526766000
1	5.628316000	-1.560231000	-0.966208000
1	5.731390000	-2.377141000	0.605246000
6	3.269116000	-1.526129000	1.585637000
1	3.895671000	-2.110056000	2.271005000
1	2.754634000	-0.757735000	2.167601000
1	2.516306000	-2.202175000	1.167624000
1	0.890010000	-0.162193000	0.881931000
1	-1.016208000	-0.890309000	1.601796000
1	-0.254389000	-1.409306000	-0.480864000
6	-1.389547000	-1.818954000	1.137453000
8	-0.533607000	-2.232513000	0.115187000
6	-2.804026000	-1.513176000	0.652033000
6	-3.676704000	-0.777340000	1.462121000
6	-3.258588000	-1.960561000	-0.589450000
6	-4.974375000	-0.495213000	1.042667000
1	-3.327853000	-0.405550000	2.423691000
6	-4.557381000	-1.677717000	-1.016322000
1	-2.577129000	-2.519687000	-1.223455000
6	-5.419822000	-0.943987000	-0.202619000
1	-5.634240000	0.088091000	1.679239000
1	-4.894289000	-2.027491000	-1.988785000
1	-6.428959000	-0.718655000	-0.536146000
6	-1.416580000	-2.900706000	2.218707000
1	-0.405538000	-3.061708000	2.607375000
1	-2.068464000	-2.619170000	3.052726000
1	-1.782127000	-3.844343000	1.797142000
1	1.466916000	2.072396000	-1.549859000

TSA3-4<sub>X=H</sub>

Coordinates (Angstroms)

	X	Y	Z
25	-1.291458000	1.136368000	0.241614000
1	-1.071506000	0.568015000	-1.367771000
7	-0.237741000	-0.306626000	1.338068000
6	-2.113482000	2.442245000	-0.578582000
8	-2.652169000	3.365892000	-1.086846000
6	-2.289085000	-1.577981000	1.612678000
6	0.885715000	0.343216000	1.977108000
6	-1.049666000	-1.022515000	2.300327000
1	-2.948606000	-2.083927000	2.322178000
1	-1.988021000	-2.285896000	0.835220000
1	-0.506654000	-1.875222000	2.750494000
1	-1.352545000	-0.363883000	3.135043000
1	1.662905000	-0.363244000	2.318086000
1	0.559318000	0.910561000	2.870376000
6	1.494650000	1.325727000	1.018045000
6	2.843171000	1.677430000	1.044186000
1	3.503716000	1.205867000	1.765178000
6	1.109213000	2.753631000	-0.758212000
1	0.386179000	3.152677000	-1.462239000
6	3.325074000	2.606129000	0.131151000
1	4.374225000	2.885680000	0.128996000
6	2.437621000	3.153777000	-0.793520000
1	2.763639000	3.876226000	-1.533871000
7	0.634622000	1.861486000	0.127538000
16	-3.173961000	-0.180698000	0.824294000
6	-4.121895000	-1.023746000	-0.540302000
6	-5.040022000	0.060899000	-1.111091000
6	-4.955278000	-2.158576000	0.061526000
1	-4.461133000	0.914258000	-1.479873000
1	-5.609927000	-0.351138000	-1.951932000
1	-5.751742000	0.422630000	-0.361308000
1	-4.325564000	-2.978411000	0.421565000
1	-5.572533000	-1.804632000	0.894022000
1	-5.623402000	-2.566096000	-0.706694000
6	-3.207335000	-1.558455000	-1.642548000
1	-3.806293000	-2.144792000	-2.350048000
1	-2.733878000	-0.742631000	-2.193779000
1	-2.419056000	-2.210035000	-1.252732000
1	-0.893530000	-0.077109000	-0.929069000
1	1.188434000	-0.467370000	-1.469556000
1	0.237802000	-1.244212000	0.445333000
6	1.471551000	-1.505647000	-1.209683000
8	0.582041000	-2.039396000	-0.288077000



6	2.905233000	-1.413422000	-0.681044000
6	3.884011000	-0.708485000	-1.393450000
6	3.260642000	-2.000205000	0.533707000
6	5.181891000	-0.588935000	-0.902076000
1	3.620473000	-0.226832000	-2.333225000
6	4.560264000	-1.884652000	1.032327000
1	2.495877000	-2.533361000	1.090381000
6	5.526185000	-1.177528000	0.317556000
1	5.923619000	-0.028127000	-1.464725000
1	4.815650000	-2.343872000	1.983826000
1	6.535485000	-1.079648000	0.707627000
6	1.422478000	-2.326929000	-2.502190000
1	0.406627000	-2.303998000	-2.911431000
1	2.110625000	-1.941021000	-3.262694000
1	1.686029000	-3.370453000	-2.292997000
1	-1.539170000	1.940110000	1.671216000

**A4<sub>X=H</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	1.214482000	1.205667000	-0.187932000
1	0.913914000	0.460106000	1.340846000
7	0.196173000	-0.144571000	-1.455385000
6	2.009084000	2.420561000	0.788518000
8	2.538468000	3.278130000	1.405443000
6	2.253609000	-1.397062000	-1.729527000
6	-0.943972000	0.548731000	-2.040449000
6	1.050356000	-0.799542000	-2.441991000
1	2.929442000	-1.879680000	-2.439045000
1	1.907578000	-2.128583000	-0.993442000
1	0.515879000	-1.608467000	-2.964525000
1	1.367295000	-0.065419000	-3.192407000
1	-1.691416000	-0.138677000	-2.460339000
1	-0.586198000	1.194756000	-2.853847000
6	-1.573996000	1.415063000	-0.985996000
6	-2.930954000	1.727268000	-0.986366000
1	-3.573740000	1.314409000	-1.756940000
6	-1.233795000	2.664573000	0.926176000
1	-0.524617000	3.012740000	1.669822000
6	-3.442630000	2.541766000	0.015433000
1	-4.499697000	2.787569000	0.041467000
6	-2.573899000	3.018665000	0.994540000
1	-2.922727000	3.651796000	1.803092000

7	-0.730426000	1.881123000	-0.042426000
16	3.126347000	-0.050305000	-0.846768000
6	4.049254000	-0.980647000	0.479229000
6	5.005548000	0.049741000	1.087175000
6	4.844243000	-2.116229000	-0.171561000
1	4.460289000	0.918070000	1.471830000
1	5.546802000	-0.407517000	1.923622000
1	5.740920000	0.398975000	0.354555000
1	4.189558000	-2.908743000	-0.547136000
1	5.460707000	-1.752070000	-1.000350000
1	5.511157000	-2.563478000	0.575128000
6	3.111891000	-1.528120000	1.556960000
1	3.673465000	-2.213386000	2.203759000
1	2.719987000	-0.720543000	2.180998000
1	2.255877000	-2.067886000	1.137282000
1	0.811551000	-0.156129000	0.843559000
1	-1.072218000	-0.840727000	1.804457000
1	-0.141764000	-0.903537000	-0.789710000
6	-1.302076000	-1.788579000	1.252673000
8	-0.359520000	-2.079977000	0.315246000
6	-2.707397000	-1.552741000	0.667994000
6	-3.718312000	-0.935387000	1.416228000
6	-3.002338000	-1.949132000	-0.637691000
6	-4.986558000	-0.724261000	0.877202000
1	-3.504227000	-0.601651000	2.430350000
6	-4.269503000	-1.741327000	-1.186059000
1	-2.206245000	-2.408160000	-1.217718000
6	-5.268503000	-1.127067000	-0.430613000
1	-5.753522000	-0.234828000	1.472266000
1	-4.475009000	-2.050706000	-2.208021000
1	-6.253437000	-0.957585000	-0.857035000
6	-1.393960000	-2.886271000	2.336265000
1	-0.409583000	-3.014950000	2.801185000
1	-2.120804000	-2.649263000	3.124371000
1	-1.680469000	-3.839803000	1.874143000
1	1.479296000	2.135462000	-1.535293000

**TSA4-5<sub>X=H</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	1.132562000	1.227424000	-0.143882000
1	0.779235000	0.155431000	1.200067000
7	0.161514000	-0.062817000	-1.538305000

6	1.857293000	2.332782000	0.992769000
8	2.334952000	3.110236000	1.750487000
6	2.240842000	-1.292573000	-1.794302000
6	-0.964847000	0.658971000	-2.117519000
6	1.045102000	-0.690999000	-2.518549000
1	2.933032000	-1.747857000	-2.506260000
1	1.895606000	-2.051249000	-1.085338000
1	0.529765000	-1.487464000	-3.076593000
1	1.370612000	0.067897000	-3.238761000
1	-1.687071000	-0.002182000	-2.615873000
1	-0.576407000	1.362427000	-2.865421000
6	-1.642006000	1.438914000	-1.024399000
6	-3.004744000	1.723042000	-1.048735000
1	-3.612783000	1.354492000	-1.868486000
6	-1.388066000	2.558287000	0.977535000
1	-0.710730000	2.866918000	1.766486000
6	-3.565052000	2.458793000	-0.012063000
1	-4.627029000	2.683856000	-0.004971000
6	-2.736943000	2.882439000	1.024857000
1	-3.124295000	3.450894000	1.863393000
7	-0.835967000	1.852650000	-0.023991000
16	3.075725000	0.044586000	-0.864328000
6	4.085222000	-0.900447000	0.384648000
6	4.964285000	0.161531000	1.053232000
6	4.957212000	-1.924169000	-0.347599000
1	4.355050000	0.943743000	1.518026000
1	5.567237000	-0.309007000	1.838570000
1	5.646209000	0.631919000	0.336511000
1	4.358933000	-2.737629000	-0.770497000
1	5.531723000	-1.458616000	-1.155580000
1	5.665737000	-2.369110000	0.361495000
6	3.215222000	-1.590958000	1.433065000
1	3.856322000	-2.199783000	2.083144000
1	2.689545000	-0.860238000	2.052087000
1	2.458724000	-2.243548000	0.987941000
1	0.474708000	-0.616475000	0.843237000
1	-1.154062000	-0.885455000	2.133498000
1	-0.189550000	-0.802292000	-0.904583000
6	-1.247157000	-1.759114000	1.447526000
8	-0.170886000	-1.809996000	0.588885000
6	-2.585747000	-1.576886000	0.728152000
6	-3.684919000	-1.012809000	1.385424000
6	-2.746080000	-1.997031000	-0.594993000
6	-4.913749000	-0.875067000	0.741113000

1	-3.572146000	-0.665695000	2.410967000
6	-3.972324000	-1.861002000	-1.246632000
1	-1.889602000	-2.422185000	-1.111393000
6	-5.062531000	-1.300300000	-0.580356000
1	-5.753129000	-0.424708000	1.264412000
1	-4.076469000	-2.188428000	-2.278060000
1	-6.016662000	-1.187127000	-1.087544000
6	-1.306950000	-3.012274000	2.337303000
1	-0.362474000	-3.114053000	2.883030000
1	-2.126339000	-2.966891000	3.065480000
1	-1.443139000	-3.907046000	1.717264000
1	1.428070000	2.272924000	-1.431722000

**A5S<sub>X=H</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	1.115905000	-1.256332000	0.066371000
1	0.732450000	-0.124533000	-1.179379000
7	0.086859000	0.037075000	1.465614000
1	-0.301531000	0.794607000	0.903686000
6	1.870889000	-2.365187000	-1.036066000
8	2.364447000	-3.146521000	-1.786082000
6	2.184374000	1.245139000	1.804583000
6	-1.019873000	-0.735689000	2.026027000
6	0.960742000	0.638859000	2.476232000
1	2.851871000	1.674363000	2.555860000
1	1.876399000	2.035080000	1.112870000
1	0.440085000	1.422162000	3.046822000
1	1.261571000	-0.146124000	3.177336000
1	-1.771210000	-0.106223000	2.521229000
1	-0.602608000	-1.422825000	2.772507000
6	-1.655097000	-1.549261000	0.932333000
6	-3.004207000	-1.890494000	0.954809000
1	-3.631983000	-1.531040000	1.763569000
6	-1.339388000	-2.705814000	-1.037844000
1	-0.644743000	-3.003702000	-1.815607000
6	-3.527216000	-2.675556000	-0.065818000
1	-4.578223000	-2.947373000	-0.072367000
6	-2.672623000	-3.090579000	-1.084172000
1	-3.027033000	-3.699940000	-1.908687000
7	-0.822693000	-1.951649000	-0.052177000
16	3.044230000	-0.071821000	0.869789000
6	4.120406000	0.898569000	-0.301120000

6	4.943818000	-0.168452000	-1.029921000
6	5.039469000	1.819787000	0.505176000
1	4.295755000	-0.851123000	-1.588716000
1	5.620984000	0.317609000	-1.741918000
1	5.550569000	-0.758277000	-0.333935000
1	4.480340000	2.620832000	1.000031000
1	5.596811000	1.265149000	1.267687000
1	5.763969000	2.291731000	-0.169716000
6	3.310316000	1.703822000	-1.313919000
1	3.999381000	2.248932000	-1.971087000
1	2.685258000	1.049262000	-1.926297000
1	2.658080000	2.439530000	-0.834052000
1	-1.268986000	1.355836000	-2.345066000
1	0.271914000	1.223719000	-0.908795000
6	-1.362908000	2.100460000	-1.540997000
8	-0.177027000	2.108083000	-0.770645000
6	-2.584239000	1.730275000	-0.710704000
6	-3.672833000	1.091284000	-1.312130000
6	-2.670304000	2.074979000	0.641070000
6	-4.828627000	0.812782000	-0.584511000
1	-3.611641000	0.806881000	-2.360449000
6	-3.821944000	1.790859000	1.375187000
1	-1.826749000	2.564715000	1.120330000
6	-4.907752000	1.164099000	0.763617000
1	-5.663600000	0.311871000	-1.066591000
1	-3.871306000	2.058987000	2.427158000
1	-5.804593000	0.941355000	1.334710000
6	-1.543182000	3.480111000	-2.170429000
1	-0.691398000	3.712107000	-2.817569000
1	-2.459445000	3.522078000	-2.768559000
1	-1.606080000	4.245703000	-1.388648000
1	1.402921000	-2.264349000	1.429079000

**TSA2-6<sub>X=H</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.204455000	0.346141000	-0.316664000
1	-0.034548000	0.225764000	1.403045000
7	-0.582161000	-1.681906000	0.180917000
1	-0.270585000	-0.664068000	1.075301000
6	0.091823000	2.063151000	-0.385311000
8	0.289958000	3.233573000	-0.373321000
6	1.809209000	-2.102804000	0.093228000

6	-1.921197000	-2.011938000	-0.217324000
6	0.418067000	-2.618454000	-0.255587000
1	2.582995000	-2.783151000	-0.270783000
1	1.907031000	-2.000919000	1.178756000
1	0.301259000	-3.610775000	0.218637000
1	0.355306000	-2.786905000	-1.350121000
1	-2.330893000	-2.901691000	0.293555000
1	-1.964908000	-2.234949000	-1.306117000
6	-2.833901000	-0.838914000	0.025756000
6	-4.202243000	-0.987260000	0.248435000
1	-4.631655000	-1.983334000	0.290363000
6	-3.019247000	1.461765000	0.144830000
1	-2.508638000	2.417643000	0.102670000
6	-4.996102000	0.141850000	0.410784000
1	-6.064066000	0.046557000	0.581129000
6	-4.389124000	1.394649000	0.356758000
1	-4.958846000	2.309166000	0.481111000
7	-2.246510000	0.375151000	-0.023427000
16	2.009359000	-0.451586000	-0.675525000
6	3.387217000	0.306344000	0.321380000
6	3.757104000	1.583145000	-0.439766000
6	4.581549000	-0.650861000	0.351028000
1	2.897275000	2.253746000	-0.533327000
1	4.545601000	2.116259000	0.104490000
1	4.131095000	1.357053000	-1.444016000
1	4.366176000	-1.554388000	0.930278000
1	4.880329000	-0.949586000	-0.659498000
1	5.435235000	-0.150465000	0.823757000
6	2.942387000	0.656343000	1.740402000
1	3.794829000	1.073870000	2.290429000
1	2.140524000	1.399189000	1.729425000
1	2.588609000	-0.221761000	2.290181000
1	-0.472726000	0.111217000	-1.987794000

**A6<sub>X=H</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.216525000	0.407806000	-0.231703000
1	-0.018049000	0.553731000	1.474774000
7	-0.544212000	-1.700294000	0.127733000
1	-0.493187000	-1.809648000	1.137727000
6	-0.028186000	2.100352000	-0.568542000
8	0.076570000	3.258977000	-0.822919000

6	1.863061000	-2.068109000	-0.121417000
6	-1.906279000	-2.005563000	-0.310165000
6	0.471523000	-2.564321000	-0.482357000
1	2.620133000	-2.684876000	-0.612046000
1	2.010452000	-2.132074000	0.960563000
1	0.366050000	-3.609112000	-0.156311000
1	0.326872000	-2.530646000	-1.566545000
1	-2.290366000	-2.944382000	0.110422000
1	-1.881570000	-2.111391000	-1.401958000
6	-2.823495000	-0.861084000	0.027368000
6	-4.186944000	-1.051646000	0.238393000
1	-4.597261000	-2.056302000	0.207781000
6	-3.043951000	1.417788000	0.305751000
1	-2.547761000	2.381658000	0.338136000
6	-5.001599000	0.049468000	0.477840000
1	-6.067787000	-0.075048000	0.638853000
6	-4.412600000	1.311324000	0.511515000
1	-4.997132000	2.205630000	0.699196000
7	-2.249401000	0.360622000	0.059936000
16	2.022801000	-0.321927000	-0.648943000
6	3.431976000	0.285156000	0.414321000
6	3.589971000	1.759094000	0.028318000
6	4.696519000	-0.498182000	0.053017000
1	2.692330000	2.330923000	0.283573000
1	4.438601000	2.189361000	0.572772000
1	3.781453000	1.878284000	-1.043948000
1	4.605448000	-1.557248000	0.316749000
1	4.918259000	-0.426762000	-1.016900000
1	5.551362000	-0.090964000	0.606712000
6	3.147267000	0.175098000	1.910598000
1	3.978392000	0.628200000	2.464889000
1	2.224947000	0.697689000	2.174328000
1	3.060822000	-0.863877000	2.244536000
1	-0.474530000	-0.007826000	-1.895814000

**A7R<sub>X=H</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	-0.843287000	-1.159144000	0.365736000
1	-0.434320000	0.446471000	0.706621000
7	-0.442916000	-0.708235000	-1.720678000
1	-0.058036000	0.235287000	-1.728180000
6	-1.058517000	-1.564980000	2.037597000

8	-1.170129000	-1.853476000	3.188738000
6	-2.745504000	0.091172000	-1.913642000
6	0.603558000	-1.627055000	-2.163621000
6	-1.636230000	-0.717962000	-2.570520000
1	-3.643783000	0.074699000	-2.536351000
1	-2.421720000	1.128584000	-1.790719000
1	-1.429811000	-0.298595000	-3.566235000
1	-1.950149000	-1.758751000	-2.700839000
1	1.094567000	-1.299767000	-3.090498000
1	0.131628000	-2.598885000	-2.355043000
6	1.617588000	-1.801193000	-1.064630000
6	2.935158000	-2.166703000	-1.330191000
1	3.257681000	-2.286847000	-2.359983000
6	2.018673000	-1.803474000	1.206454000
1	1.616541000	-1.634638000	2.199467000
6	3.812399000	-2.375648000	-0.272897000
1	4.842916000	-2.664065000	-0.455245000
6	3.341048000	-2.181482000	1.023512000
1	3.985781000	-2.311316000	1.886160000
7	1.152885000	-1.629901000	0.191418000
16	-3.092680000	-0.624390000	-0.267178000
6	-4.021785000	0.749222000	0.584498000
6	-4.284228000	0.209920000	1.993968000
6	-5.343546000	0.987448000	-0.150344000
1	-3.344640000	0.056133000	2.533061000
1	-4.889219000	0.931993000	2.554656000
1	-4.828719000	-0.740603000	1.969467000
1	-5.179200000	1.373930000	-1.161876000
1	-5.932621000	0.067227000	-0.223860000
1	-5.938064000	1.730999000	0.394774000
6	-3.219400000	2.044855000	0.673701000
1	-3.779057000	2.770035000	1.277604000
1	-2.249029000	1.871600000	1.144691000
1	-3.051571000	2.498714000	-0.308074000
6	1.093553000	2.506459000	-0.935323000
8	0.911950000	2.020492000	-2.047904000
6	2.305127000	2.134554000	-0.139461000
6	2.457378000	2.526017000	1.196421000
6	3.318096000	1.388649000	-0.754175000
6	3.604920000	2.177061000	1.903742000
1	1.678470000	3.091303000	1.696996000
6	4.469776000	1.051737000	-0.051159000
1	3.194710000	1.081262000	-1.787653000
6	4.614576000	1.444817000	1.279704000



1	3.710353000	2.474308000	2.942663000
1	5.251857000	0.476854000	-0.537527000
1	5.511362000	1.176473000	1.830866000
6	0.132101000	3.517839000	-0.373488000
1	-0.673306000	3.686652000	-1.089329000
1	-0.290825000	3.159683000	0.569432000
1	0.650138000	4.462020000	-0.172242000
1	-1.259675000	-2.748624000	-0.214081000

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**A7S<sub>X=H</sub>**

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Coordinates (Angstroms)

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	X	Y	Z
25	0.699546000	-1.498917000	0.158315000
1	0.073299000	-0.101227000	0.857408000
7	0.755881000	-0.358830000	-1.673322000
1	0.471626000	0.583651000	-1.416914000
6	0.755200000	-2.403917000	1.638591000
8	0.825789000	-3.014869000	2.660117000
6	-1.551830000	-1.027311000	-2.104826000
6	2.152959000	-0.301832000	-2.101260000
6	-0.164320000	-0.846789000	-2.702412000
1	-2.242547000	-1.407134000	-2.861971000
1	-1.924651000	-0.063977000	-1.742067000
1	-0.229260000	-0.150425000	-3.551648000
1	0.220324000	-1.801913000	-3.074772000
1	2.339511000	0.482889000	-2.845850000
1	2.398738000	-1.270150000	-2.555465000
6	3.031760000	-0.107204000	-0.895881000
6	4.256933000	0.551473000	-0.969162000
1	4.578088000	0.978580000	-1.914094000
6	3.334926000	-0.531874000	1.351281000
1	2.923515000	-0.964349000	2.257035000
6	5.046852000	0.653923000	0.170202000
1	6.006346000	1.160416000	0.136032000
6	4.570794000	0.098697000	1.356436000
1	5.140189000	0.154711000	2.278128000
7	2.567163000	-0.644645000	0.252097000
16	-1.446532000	-2.188769000	-0.693692000
6	-2.999812000	-1.796211000	0.259336000
6	-2.985061000	-2.782548000	1.431034000
6	-4.213563000	-2.053796000	-0.638054000
1	-2.097152000	-2.634734000	2.053547000
1	-3.873134000	-2.620983000	2.052945000

1	-2.996614000	-3.822130000	1.085014000
1	-4.267330000	-1.333291000	-1.461216000
1	-4.191744000	-3.062973000	-1.062909000
1	-5.133763000	-1.950903000	-0.049933000
6	-3.025119000	-0.365347000	0.792879000
1	-3.965489000	-0.203823000	1.334755000
1	-2.191156000	-0.184530000	1.474138000
1	-2.975297000	0.378343000	-0.007641000
6	0.688519000	2.743871000	0.035936000
8	1.132785000	2.649003000	-1.103306000
6	-0.782839000	2.932207000	0.247224000
6	-1.344279000	3.011323000	1.526687000
6	-1.616640000	3.027888000	-0.874180000
6	-2.716966000	3.190832000	1.680930000
1	-0.717340000	2.925579000	2.408158000
6	-2.987070000	3.208106000	-0.720274000
1	-1.177166000	2.957473000	-1.864131000
6	-3.539386000	3.291599000	0.559161000
1	-3.145606000	3.247640000	2.676760000
1	-3.626046000	3.279818000	-1.595417000
1	-4.609515000	3.430354000	0.681814000
6	1.608073000	2.699505000	1.225486000
1	2.629700000	2.526884000	0.882753000
1	1.560138000	3.645782000	1.776088000
1	1.310640000	1.895281000	1.904455000
1	1.322876000	-2.785947000	-0.834513000

**TSA7-8R<sub>X=H</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.657335000	0.620484000	-0.806564000
1	-0.314448000	-0.704722000	0.256475000
7	-0.484947000	1.733547000	0.995128000
1	-0.143768000	1.021897000	1.650371000
6	-0.680962000	-0.460090000	-2.161560000
8	-0.661789000	-1.250302000	-3.054179000
6	-2.835333000	1.227940000	1.448184000
6	0.581284000	2.718168000	0.833169000
6	-1.736148000	2.281515000	1.526022000
1	-3.776103000	1.638641000	1.824053000
1	-2.564342000	0.353522000	2.048658000
1	-1.622849000	2.608142000	2.570073000
1	-2.011799000	3.157652000	0.928753000

1	0.974271000	3.085085000	1.791838000
1	0.170079000	3.577831000	0.288509000
6	1.689726000	2.123180000	0.004640000
6	2.997093000	2.598796000	0.076562000
1	3.244523000	3.373011000	0.796257000
6	2.264908000	0.646071000	-1.671178000
1	1.938201000	-0.140561000	-2.341622000
6	3.960345000	2.082760000	-0.782831000
1	4.983621000	2.443831000	-0.748748000
6	3.580600000	1.086836000	-1.678734000
1	4.291164000	0.643239000	-2.367847000
7	1.322409000	1.148806000	-0.854525000
16	-2.998311000	0.734835000	-0.304772000
6	-4.035219000	-0.806812000	-0.238480000
6	-4.338469000	-1.117694000	-1.707975000
6	-5.331909000	-0.526037000	0.522733000
1	-3.415916000	-1.265017000	-2.278480000
1	-4.929233000	-2.039088000	-1.771115000
1	-4.911390000	-0.312134000	-2.179789000
1	-5.145949000	-0.342858000	1.585985000
1	-5.859665000	0.339877000	0.109106000
1	-5.995834000	-1.395972000	0.448736000
6	-3.272147000	-1.966242000	0.391500000
1	-3.876081000	-2.880746000	0.334681000
1	-2.326252000	-2.129625000	-0.131934000
1	-3.053210000	-1.777598000	1.446261000
6	0.739887000	-1.262841000	1.827911000
8	0.714971000	-0.295980000	2.611621000
6	2.002325000	-1.539035000	1.047170000
6	2.048514000	-2.433424000	-0.028389000
6	3.185791000	-0.929122000	1.470279000
6	3.256728000	-2.721988000	-0.656017000
1	1.131277000	-2.879316000	-0.401178000
6	4.398106000	-1.217905000	0.844174000
1	3.147329000	-0.229800000	2.299556000
6	4.438461000	-2.120701000	-0.216347000
1	3.275967000	-3.412415000	-1.494557000
1	5.309849000	-0.735843000	1.185696000
1	5.380855000	-2.345117000	-0.707885000
6	-0.182184000	-2.435575000	2.080324000
1	-1.117996000	-2.074287000	2.508750000
1	-0.391039000	-3.028967000	1.189767000
1	0.311699000	-3.083985000	2.817852000
1	-0.972685000	2.092865000	-1.648466000

-----  
**TSA7-8S<sub>X=H</sub>**  
-----

Coordinates (Angstroms)

	X	Y	Z
25	0.819543000	-1.158905000	0.326503000
1	0.048937000	0.396506000	0.480150000
7	1.004953000	-0.514441000	-1.690524000
1	0.755823000	0.477097000	-1.607999000
6	0.642701000	-1.442364000	2.029594000
8	0.506765000	-1.561087000	3.207707000
6	-1.292375000	-1.263208000	-2.057247000
6	2.416128000	-0.559712000	-2.061223000
6	0.104066000	-1.149000000	-2.655088000
1	-1.963226000	-1.764688000	-2.759417000
1	-1.690554000	-0.269207000	-1.829782000
1	0.051682000	-0.581657000	-3.595767000
1	0.494910000	-2.145728000	-2.887352000
1	2.645158000	0.045281000	-2.949681000
1	2.676730000	-1.602280000	-2.285092000
6	3.240306000	-0.102423000	-0.888248000
6	4.502969000	0.463149000	-1.049844000
1	4.891210000	0.625561000	-2.050587000
6	3.421610000	0.022000000	1.407761000
1	2.950547000	-0.157766000	2.367765000
6	5.247349000	0.806098000	0.073093000
1	6.234000000	1.246992000	-0.029882000
6	4.692168000	0.574691000	1.329770000
1	5.226356000	0.822198000	2.240916000
7	2.693926000	-0.314906000	0.327633000
16	-1.141516000	-2.223923000	-0.510921000
6	-2.778845000	-1.958126000	0.330007000
6	-2.762716000	-2.935612000	1.510389000
6	-3.919989000	-2.304178000	-0.628953000
1	-1.922196000	-2.730973000	2.181448000
1	-3.691056000	-2.825147000	2.082834000
1	-2.692397000	-3.975354000	1.172920000
1	-3.994189000	-1.580240000	-1.447149000
1	-3.798011000	-3.303857000	-1.059826000
1	-4.871120000	-2.283229000	-0.083106000
6	-2.921916000	-0.529258000	0.841346000
1	-3.875538000	-0.426162000	1.374436000
1	-2.106459000	-0.272369000	1.521859000
1	-2.916385000	0.194406000	0.022869000

6	0.285259000	2.249102000	0.008930000
8	0.858062000	2.257518000	-1.098579000
6	-1.208130000	2.477461000	0.041031000
6	-1.904763000	2.739281000	1.225752000
6	-1.910496000	2.486883000	-1.169036000
6	-3.274235000	2.998583000	1.200301000
1	-1.386902000	2.730960000	2.179398000
6	-3.279939000	2.738163000	-1.196471000
1	-1.366917000	2.295507000	-2.088995000
6	-3.967767000	2.997014000	-0.009761000
1	-3.800272000	3.196634000	2.129928000
1	-3.810771000	2.736159000	-2.144482000
1	-5.035605000	3.195386000	-0.028275000
6	1.080630000	2.581386000	1.253897000
1	2.120481000	2.295817000	1.092542000
1	1.038963000	3.668654000	1.407933000
1	0.706799000	2.086373000	2.151190000
1	1.572815000	-2.645098000	-0.095410000

**A8R<sub>X=H</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.677756000	-0.899262000	0.845805000
1	-0.272129000	1.277876000	-0.621394000
7	-0.505816000	-1.704350000	-0.945608000
1	0.046768000	-0.360993000	-1.859407000
6	-0.637329000	0.382189000	2.029556000
8	-0.586475000	1.308608000	2.776430000
6	-2.782062000	-1.128237000	-1.538340000
6	0.637347000	-2.568851000	-1.122836000
6	-1.658310000	-2.143096000	-1.707746000
1	-3.719204000	-1.488685000	-1.970219000
1	-2.502235000	-0.184652000	-2.016077000
1	-1.435122000	-2.224893000	-2.787750000
1	-2.009328000	-3.142313000	-1.386885000
1	1.029785000	-2.568618000	-2.157252000
1	0.395314000	-3.624791000	-0.895429000
6	1.727819000	-2.127239000	-0.187547000
6	3.058560000	-2.517994000	-0.340934000
1	3.333866000	-3.158216000	-1.173568000
6	2.258565000	-0.895971000	1.694967000
1	1.898783000	-0.246624000	2.485360000
6	4.007737000	-2.078438000	0.570830000

1	5.049711000	-2.365659000	0.467319000
6	3.596527000	-1.246951000	1.612257000
1	4.300010000	-0.866034000	2.344563000
7	1.329545000	-1.325350000	0.820544000
16	-2.973014000	-0.847840000	0.258665000
6	-3.890284000	0.768547000	0.346957000
6	-4.224127000	0.948814000	1.830869000
6	-5.176309000	0.675287000	-0.477938000
1	-3.317440000	0.957595000	2.443600000
1	-4.739831000	1.905751000	1.972441000
1	-4.881625000	0.151661000	2.194043000
1	-4.966729000	0.584852000	-1.548707000
1	-5.790439000	-0.178532000	-0.172244000
1	-5.764725000	1.588875000	-0.331272000
6	-3.027812000	1.931682000	-0.141330000
1	-3.599091000	2.864988000	-0.063620000
1	-2.121567000	2.030789000	0.461391000
1	-2.737651000	1.808745000	-1.188884000
6	0.415286000	1.497541000	-1.457042000
8	0.363512000	0.441131000	-2.381484000
6	1.799676000	1.679244000	-0.847764000
6	1.950642000	2.428859000	0.324403000
6	2.935484000	1.128581000	-1.442290000
6	3.210757000	2.639346000	0.880338000
1	1.069048000	2.836284000	0.814125000
6	4.200419000	1.337427000	-0.889342000
1	2.817508000	0.525768000	-2.337462000
6	4.343948000	2.097210000	0.270753000
1	3.308091000	3.215112000	1.796783000
1	5.074541000	0.896876000	-1.361615000
1	5.326774000	2.252805000	0.706771000
6	-0.047060000	2.784749000	-2.137628000
1	-1.044182000	2.644290000	-2.566760000
1	-0.088476000	3.615266000	-1.425172000
1	0.641950000	3.056817000	-2.945751000
1	-0.969465000	-2.103554000	1.934029000

-----  
**A8S<sub>X=H</sub>**

-----  
Coordinates (Angstroms)

	X	Y	Z
25	1.026688000	-1.306973000	0.508831000
1	0.042201000	1.127239000	0.345045000
7	1.259371000	-1.013617000	-1.420212000

1	0.516171000	0.523346000	-1.574884000
6	0.478341000	-0.891164000	2.112156000
8	0.088844000	-0.502686000	3.168404000
6	-0.853640000	-2.055545000	-1.977116000
6	2.590814000	-0.631398000	-1.831912000
6	0.581980000	-1.811916000	-2.422378000
1	-1.357337000	-2.784083000	-2.617184000
1	-1.409565000	-1.113400000	-1.997237000
1	0.550555000	-1.302237000	-3.402957000
1	1.090632000	-2.779615000	-2.590943000
1	2.600163000	0.015154000	-2.728766000
1	3.209529000	-1.512439000	-2.088822000
6	3.255993000	0.093910000	-0.697617000
6	4.366885000	0.920118000	-0.872153000
1	4.777604000	1.058212000	-1.867653000
6	3.244880000	0.513197000	1.575666000
1	2.765373000	0.325077000	2.530136000
6	4.926080000	1.553780000	0.228978000
1	5.788818000	2.202939000	0.115135000
6	4.349761000	1.344834000	1.482233000
1	4.746183000	1.817461000	2.374290000
7	2.696868000	-0.105001000	0.513070000
16	-0.786865000	-2.663200000	-0.253067000
6	-2.489864000	-2.277095000	0.391076000
6	-2.553492000	-2.950916000	1.764201000
6	-3.540611000	-2.881451000	-0.542874000
1	-1.778243000	-2.565425000	2.433606000
1	-3.528835000	-2.750990000	2.222924000
1	-2.432915000	-4.036434000	1.682619000
1	-3.548682000	-2.387527000	-1.519498000
1	-3.373655000	-3.952863000	-0.696284000
1	-4.534682000	-2.751730000	-0.098328000
6	-2.696697000	-0.769942000	0.532949000
1	-3.697928000	-0.574492000	0.936732000
1	-1.959378000	-0.338784000	1.213859000
1	-2.620812000	-0.253133000	-0.428299000
6	-0.087220000	1.947675000	-0.384370000
8	0.158663000	1.459408000	-1.679467000
6	-1.516984000	2.445023000	-0.244399000
6	-2.052587000	2.681200000	1.027396000
6	-2.324788000	2.662297000	-1.362093000
6	-3.366129000	3.119106000	1.179679000
1	-1.441040000	2.497385000	1.908194000
6	-3.640564000	3.106549000	-1.214438000

1	-1.917570000	2.463314000	-2.348159000
6	-4.167555000	3.334569000	0.055950000
1	-3.769430000	3.283259000	2.175235000
1	-4.255797000	3.268883000	-2.095522000
1	-5.193540000	3.672124000	0.172571000
6	0.921472000	3.045480000	-0.035288000
1	1.938709000	2.646145000	-0.106507000
1	0.827217000	3.881306000	-0.738395000
1	0.768819000	3.425914000	0.980553000
1	1.889892000	-2.632374000	0.981445000

Al<sub>X=OMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	0.226498000	-0.190821000	-0.074286000
7	0.527744000	1.699120000	-0.148334000
6	-0.047532000	-1.170895000	1.318384000
8	-0.170297000	-1.740233000	2.362970000
6	-1.841797000	2.203554000	0.001147000
6	1.873063000	2.200384000	-0.064985000
6	-0.456852000	2.737125000	-0.353495000
1	-2.637247000	2.846333000	-0.386829000
1	-1.931663000	2.130262000	1.087666000
1	-0.269794000	3.622431000	0.282806000
1	-0.456053000	3.107576000	-1.397394000
1	2.030198000	2.878771000	0.797641000
1	2.163416000	2.791696000	-0.955687000
6	2.828126000	1.042661000	0.049199000
6	4.213933000	1.197560000	0.120505000
1	4.643131000	2.195056000	0.113027000
6	3.034119000	-1.263924000	0.108670000
1	2.510316000	-2.213349000	0.085378000
6	5.020227000	0.069150000	0.192394000
1	6.100062000	0.166525000	0.252205000
6	4.416963000	-1.190057000	0.181587000
1	5.005978000	-2.099866000	0.228010000
7	2.251621000	-0.172647000	0.057540000
16	-1.972557000	0.517042000	-0.689554000
6	-3.482509000	-0.168449000	0.155550000
6	-3.502303000	-1.655245000	-0.207833000
6	-4.727485000	0.529269000	-0.397855000
1	-2.641929000	-2.175161000	0.223336000
1	-4.416802000	-2.111894000	0.188338000



1	-3.491393000	-1.807965000	-1.292697000
1	-4.708489000	1.606367000	-0.200319000
1	-4.823565000	0.377623000	-1.477920000
1	-5.622911000	0.118520000	0.084739000
6	-3.412825000	-0.008220000	1.674811000
1	-4.228595000	-0.582383000	2.130934000
1	-2.465748000	-0.381966000	2.073149000
1	-3.538291000	1.033546000	1.984403000
8	0.405311000	-1.521764000	-1.583293000
6	0.023010000	-2.827858000	-1.476542000
1	0.264353000	-3.410747000	-2.394363000
1	0.518185000	-3.375542000	-0.637624000
1	-1.069186000	-2.977659000	-1.309870000

A2<sub>X=OMe</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.178043000	-0.306707000	-0.067450000
7	-0.538090000	1.743700000	-0.348714000
6	0.062020000	-2.038002000	0.085768000
8	0.211318000	-3.210272000	0.163406000
6	1.846277000	2.149640000	-0.097494000
6	-1.847849000	2.006732000	0.191117000
6	0.439048000	2.591224000	0.283636000
1	2.610688000	2.769144000	0.380072000
1	1.976675000	2.193647000	-1.183888000
1	0.337001000	3.659337000	-0.001564000
1	0.355823000	2.560348000	1.392131000
1	-2.286815000	2.973889000	-0.127581000
1	-1.829298000	2.019223000	1.301850000
6	-2.786113000	0.898447000	-0.193160000
6	-4.164290000	1.074613000	-0.334610000
1	-4.593504000	2.061370000	-0.189445000
6	-2.987051000	-1.351386000	-0.694487000
1	-2.475878000	-2.298603000	-0.833930000
6	-4.966347000	-0.011952000	-0.660714000
1	-6.039446000	0.108309000	-0.775751000
6	-4.363487000	-1.254991000	-0.846534000
1	-4.942196000	-2.135137000	-1.105588000
7	-2.208546000	-0.306616000	-0.372866000
16	2.011354000	0.415097000	0.457543000
6	3.429064000	-0.226217000	-0.557484000
6	3.782064000	-1.578983000	0.069156000

6	4.619412000	0.729541000	-0.442558000
1	2.922844000	-2.257466000	0.064518000
1	4.588196000	-2.049927000	-0.505878000
1	4.125060000	-1.463501000	1.102905000
1	4.423237000	1.686058000	-0.937116000
1	4.874577000	0.926895000	0.604155000
1	5.494614000	0.279578000	-0.926674000
6	3.038881000	-0.419715000	-2.022811000
1	3.919600000	-0.737791000	-2.594514000
1	2.268442000	-1.188534000	-2.124938000
1	2.663352000	0.504473000	-2.474377000
8	-0.563354000	0.066085000	1.905236000
6	-0.136493000	-0.822413000	2.849592000
1	-0.296012000	-0.438155000	3.882580000
1	-0.656768000	-1.809726000	2.813685000
1	0.951978000	-1.066644000	2.789036000
1	0.133559000	0.064894000	-1.714998000
1	-0.004391000	-0.720882000	-1.743716000

**A3<sub>X=OMe</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	1.101467000	0.804402000	0.196871000
1	0.568096000	-0.219049000	1.447010000
7	0.165386000	-0.223478000	-1.401892000
6	1.820670000	1.686197000	1.532922000
8	2.294057000	2.277645000	2.435440000
6	2.278394000	-1.377693000	-1.783868000
6	-0.874735000	0.651303000	-1.931881000
6	1.107696000	-0.656158000	-2.432646000
1	2.996928000	-1.708244000	-2.537854000
1	1.915579000	-2.244865000	-1.224210000
1	0.631351000	-1.333911000	-3.157751000
1	1.465864000	0.230083000	-2.967428000
1	-1.619820000	0.105747000	-2.529059000
1	-0.396147000	1.404152000	-2.567593000
6	-1.551851000	1.378841000	-0.804782000
6	-2.850912000	1.872534000	-0.918617000
1	-3.408380000	1.699797000	-1.833495000
6	-1.374489000	2.207697000	1.343000000
1	-0.755255000	2.311372000	2.227930000
6	-3.412768000	2.563707000	0.145531000
1	-4.423975000	2.953134000	0.078715000

6	-2.659138000	2.730216000	1.305869000
1	-3.056448000	3.249143000	2.171277000
7	-0.819027000	1.553440000	0.310753000
16	3.075206000	-0.202609000	-0.628961000
6	4.048846000	-1.321460000	0.492801000
6	4.891049000	-0.378023000	1.356851000
6	4.961941000	-2.210901000	-0.355629000
1	4.259818000	0.281271000	1.960714000
1	5.511719000	-0.970933000	2.038652000
1	5.555311000	0.242404000	0.745670000
1	4.389961000	-2.922832000	-0.958868000
1	5.591714000	-1.614933000	-1.024782000
1	5.618620000	-2.790012000	0.304310000
6	3.147741000	-2.175455000	1.384385000
1	3.772912000	-2.835350000	1.998304000
1	2.549357000	-1.553206000	2.054667000
1	2.469419000	-2.807484000	0.802609000
1	0.791372000	-0.729279000	0.862479000
1	-1.251291000	-1.531111000	1.476274000
1	-0.289054000	-1.091493000	-0.986274000
6	-1.693712000	-2.245689000	0.738124000
8	-0.884290000	-2.458628000	-0.333800000
6	-3.057000000	-1.624462000	0.384220000
6	-3.822858000	-0.957474000	1.348172000
6	-3.570850000	-1.730585000	-0.910423000
6	-5.073144000	-0.426647000	1.035084000
1	-3.426859000	-0.842853000	2.356252000
6	-4.823113000	-1.203893000	-1.232472000
1	-2.957295000	-2.224005000	-1.659438000
6	-5.582063000	-0.551879000	-0.259609000
1	-5.646776000	0.095753000	1.796652000
1	-5.206670000	-1.297265000	-2.245719000
1	-6.553580000	-0.133832000	-0.508757000
6	-1.952703000	-3.546581000	1.534074000
1	-0.993464000	-3.969362000	1.854961000
1	-2.573590000	-3.384347000	2.425437000
1	-2.453017000	-4.282568000	0.891278000
8	1.450882000	2.185017000	-1.254131000
6	2.362374000	3.181835000	-1.034411000
1	2.557523000	3.771995000	-1.956042000
1	2.040869000	3.921944000	-0.264491000
1	3.359290000	2.817266000	-0.692106000

TSA3-4<sub>X=OMe</sub>

-----  
 Coordinates (Angstroms)  
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	X	Y	Z
25	-1.138768000	0.906778000	-0.047410000
1	-0.859943000	-0.159975000	-1.492014000
7	-0.099167000	-0.210499000	1.323352000
6	-1.969877000	1.864315000	-1.340969000
8	-2.487588000	2.464225000	-2.182270000
6	-2.091247000	-1.526439000	1.753006000
6	0.965275000	0.626219000	1.847185000
6	-0.931670000	-0.765410000	2.379252000
1	-2.756368000	-1.942221000	2.512594000
1	-1.712590000	-2.330018000	1.115632000
1	-0.363597000	-1.468990000	3.009652000
1	-1.312656000	0.032176000	3.034147000
1	1.748194000	0.046888000	2.358835000
1	0.564560000	1.357131000	2.566213000
6	1.571464000	1.393686000	0.709388000
6	2.883954000	1.860322000	0.716327000
1	3.518908000	1.649612000	1.570124000
6	1.219820000	2.293599000	-1.403703000
1	0.526173000	2.440015000	-2.224307000
6	3.362313000	2.560808000	-0.381680000
1	4.385570000	2.922566000	-0.399429000
6	2.516036000	2.776546000	-1.468835000
1	2.850034000	3.308406000	-2.352254000
7	0.753407000	1.621816000	-0.337921000
16	-3.031543000	-0.347821000	0.713701000
6	-3.941321000	-1.437008000	-0.494052000
6	-4.936915000	-0.507600000	-1.192687000
6	-4.687239000	-2.512627000	0.300532000
1	-4.429734000	0.310820000	-1.713494000
1	-5.495630000	-1.081636000	-1.940281000
1	-5.654949000	-0.079825000	-0.485739000
1	-4.000061000	-3.235442000	0.750403000
1	-5.306730000	-2.077142000	1.091128000
1	-5.344269000	-3.062361000	-0.382568000
6	-3.005475000	-2.077195000	-1.518578000
1	-3.572862000	-2.810575000	-2.103235000
1	-2.608475000	-1.332275000	-2.213635000
1	-2.165290000	-2.598230000	-1.048628000
1	-0.614070000	-0.625011000	-0.915584000
1	1.331339000	-1.134770000	-1.650406000
1	0.391444000	-1.219588000	0.643684000
6	1.625495000	-1.967108000	-0.977858000

8	0.672882000	-2.177536000	0.007085000
6	3.000159000	-1.581075000	-0.431772000
6	3.953716000	-0.996583000	-1.273942000
6	3.337198000	-1.805801000	0.903723000
6	5.212374000	-0.641933000	-0.793822000
1	3.701504000	-0.802987000	-2.314971000
6	4.596120000	-1.450458000	1.392041000
1	2.593141000	-2.246854000	1.560495000
6	5.538350000	-0.866864000	0.545706000
1	5.936713000	-0.182365000	-1.461014000
1	4.838168000	-1.625576000	2.437079000
1	6.516347000	-0.585167000	0.925859000
6	1.735848000	-3.222167000	-1.851826000
1	0.759674000	-3.447245000	-2.294706000
1	2.463701000	-3.094711000	-2.661359000
1	2.044061000	-4.077779000	-1.239481000
8	-1.457353000	2.091292000	1.346265000
6	-2.066174000	3.326706000	1.159114000
1	-2.107806000	3.870070000	2.116887000
1	-1.516909000	3.970014000	0.447237000
1	-3.106146000	3.242045000	0.793222000

**A4<sub>X=OMe</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	-1.127352000	0.802204000	-0.189958000
1	-0.690916000	-0.208616000	-1.500419000
7	-0.140241000	-0.236815000	1.371808000
6	-1.880491000	1.700621000	-1.496671000
8	-2.373080000	2.305517000	-2.380210000
6	-2.221834000	-1.438638000	1.774301000
6	0.893169000	0.651483000	1.892339000
6	-1.049713000	-0.710422000	2.413387000
1	-2.916130000	-1.800913000	2.536510000
1	-1.856316000	-2.285227000	1.185731000
1	-0.543425000	-1.394134000	3.112031000
1	-1.410753000	0.157399000	2.975834000
1	1.653044000	0.117730000	2.481051000
1	0.408211000	1.397012000	2.531688000
6	1.544930000	1.386099000	0.754983000
6	2.846425000	1.878740000	0.838807000
1	3.425102000	1.704306000	1.740088000
6	1.317151000	2.217842000	-1.386829000

1	0.676545000	2.324917000	-2.255976000
6	3.384562000	2.568898000	-0.238579000
1	4.397741000	2.956581000	-0.195679000
6	2.604190000	2.736234000	-1.381006000
1	2.981443000	3.255010000	-2.255459000
7	0.785384000	1.563275000	-0.342424000
16	-3.065803000	-0.251389000	0.666345000
6	-4.059785000	-1.358456000	-0.448143000
6	-4.928044000	-0.406559000	-1.276364000
6	-4.945789000	-2.267181000	0.408296000
1	-4.314074000	0.262652000	-1.887133000
1	-5.563794000	-0.992679000	-1.950062000
1	-5.578700000	0.203578000	-0.640563000
1	-4.354224000	-2.980168000	0.991074000
1	-5.566897000	-1.685518000	1.097790000
1	-5.610561000	-2.845384000	-0.244308000
6	-3.176343000	-2.191821000	-1.375921000
1	-3.813511000	-2.838292000	-1.991876000
1	-2.590364000	-1.555144000	-2.043420000
1	-2.487400000	-2.836691000	-0.821972000
1	-0.721301000	-0.721782000	-0.882345000
1	1.374502000	-1.228661000	-1.537968000
1	0.314643000	-1.079576000	0.911438000
6	1.747135000	-2.069404000	-0.898861000
8	0.879021000	-2.387488000	0.098123000
6	3.118530000	-1.575322000	-0.400823000
6	4.026358000	-0.946877000	-1.263398000
6	3.484192000	-1.736993000	0.936705000
6	5.262767000	-0.495592000	-0.804771000
1	3.753914000	-0.791973000	-2.306255000
6	4.721486000	-1.289071000	1.405067000
1	2.764899000	-2.205900000	1.602631000
6	5.617027000	-0.665578000	0.536124000
1	5.947182000	-0.001042000	-1.489526000
1	4.983291000	-1.420842000	2.452228000
1	6.576912000	-0.308076000	0.899160000
6	1.968588000	-3.252302000	-1.869171000
1	1.001724000	-3.562923000	-2.282053000
1	2.636534000	-3.003390000	-2.704529000
1	2.395713000	-4.104404000	-1.324664000
8	-1.463430000	2.156122000	1.292132000
6	-2.404448000	3.133405000	1.114470000
1	-2.580184000	3.710101000	2.048526000
1	-2.128084000	3.887709000	0.341266000

1	-3.404582000	2.748427000	0.804907000
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**TSA4-5<sub>X=OMe</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	-1.049022000	0.809333000	-0.229301000
1	-0.675967000	-0.527009000	-1.283826000
7	-0.092484000	-0.094501000	1.454030000
6	-1.743842000	1.549082000	-1.647833000
8	-2.193246000	2.028267000	-2.634330000
6	-2.169444000	-1.298729000	1.880910000
6	0.920948000	0.845887000	1.918866000
6	-1.012199000	-0.530666000	2.502850000
1	-2.869801000	-1.626083000	2.653472000
1	-1.795397000	-2.174206000	1.341382000
1	-0.511113000	-1.169440000	3.245512000
1	-1.389323000	0.362443000	3.011602000
1	1.662578000	0.383883000	2.585714000
1	0.400011000	1.644331000	2.457692000
6	1.603890000	1.466023000	0.731015000
6	2.907643000	1.953760000	0.800885000
1	3.462444000	1.861725000	1.729032000
6	1.435550000	2.087501000	-1.484573000
1	0.817323000	2.113320000	-2.375872000
6	3.477896000	2.536496000	-0.323428000
1	4.493016000	2.920396000	-0.292554000
6	2.725952000	2.598638000	-1.494854000
1	3.127692000	3.032277000	-2.404211000
7	0.871566000	1.537489000	-0.397561000
16	-3.002522000	-0.172662000	0.704705000
6	-4.032364000	-1.329282000	-0.323049000
6	-4.905459000	-0.408594000	-1.181491000
6	-4.911583000	-2.183000000	0.594072000
1	-4.292919000	0.247251000	-1.808520000
1	-5.536775000	-1.017036000	-1.839654000
1	-5.560244000	0.215577000	-0.563743000
1	-4.316664000	-2.876207000	1.197249000
1	-5.511248000	-1.562355000	1.268497000
1	-5.596949000	-2.782160000	-0.017399000
6	-3.177170000	-2.220796000	-1.222350000
1	-3.831245000	-2.902069000	-1.780575000
1	-2.606434000	-1.624760000	-1.938521000
1	-2.469082000	-2.827287000	-0.649458000

1	-0.239243000	-1.122869000	-0.780715000
1	1.502402000	-1.311436000	-1.941208000
1	0.357008000	-0.918829000	1.023289000
6	1.681142000	-2.067049000	-1.139982000
8	0.591804000	-2.148291000	-0.304007000
6	2.959324000	-1.615819000	-0.427690000
6	4.017995000	-1.044929000	-1.143741000
6	3.108253000	-1.787604000	0.950777000
6	5.195384000	-0.661738000	-0.503433000
1	3.911527000	-0.886558000	-2.215418000
6	4.283429000	-1.405497000	1.599079000
1	2.281361000	-2.215335000	1.510919000
6	5.333809000	-0.841603000	0.874151000
1	6.001383000	-0.210435000	-1.076217000
1	4.378656000	-1.544461000	2.673024000
1	6.247508000	-0.537901000	1.377439000
6	1.940910000	-3.406897000	-1.852605000
1	1.039333000	-3.707662000	-2.397789000
1	2.773224000	-3.347292000	-2.565252000
1	2.171461000	-4.184778000	-1.114157000
8	-1.410899000	2.296265000	1.147937000
6	-2.379768000	3.221935000	0.883191000
1	-2.550648000	3.907235000	1.743797000
1	-2.146190000	3.883881000	0.015335000
1	-3.378399000	2.779555000	0.651696000

**A5<sub>X=OMe</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	-0.912250000	-0.909349000	0.275602000
1	-0.488503000	0.415297000	1.250425000
7	0.079028000	0.041091000	-1.405081000
1	0.532699000	0.880421000	-1.048185000
6	-1.625003000	-1.699416000	1.643586000
8	-2.088580000	-2.219457000	2.609467000
6	-2.040740000	1.181305000	-1.868001000
6	1.100529000	-0.898739000	-1.866587000
6	-0.856159000	0.435742000	-2.463768000
1	-2.734897000	1.474963000	-2.659899000
1	-1.700433000	2.079358000	-1.343339000
1	-0.370050000	1.069661000	-3.219992000
1	-1.204179000	-0.484068000	-2.941713000
1	1.871053000	-0.418771000	-2.485327000



1	0.585029000	-1.660720000	-2.458132000
6	1.733315000	-1.596988000	-0.693871000
6	3.011116000	-2.147356000	-0.775699000
1	3.581113000	-2.033952000	-1.692413000
6	1.501354000	-2.334731000	1.478576000
1	0.868637000	-2.379536000	2.358724000
6	3.536363000	-2.823239000	0.318583000
1	4.529087000	-3.260668000	0.275707000
6	2.764266000	-2.911120000	1.475066000
1	3.128423000	-3.415600000	2.363667000
7	0.977725000	-1.698086000	0.417851000
16	-2.867449000	0.060956000	-0.680697000
6	-3.927391000	1.230082000	0.303333000
6	-4.764115000	0.318396000	1.206562000
6	-4.841429000	2.014332000	-0.641939000
1	-4.126162000	-0.293578000	1.852208000
1	-5.409682000	0.931663000	1.846337000
1	-5.403878000	-0.349571000	0.619281000
1	-4.272492000	2.699026000	-1.279264000
1	-5.425554000	1.347147000	-1.285015000
1	-5.541848000	2.618223000	-0.052105000
6	-3.100895000	2.190085000	1.157097000
1	-3.777932000	2.834835000	1.731768000
1	-2.460663000	1.643892000	1.853907000
1	-2.459307000	2.835598000	0.549932000
1	1.299410000	2.261556000	2.122595000
1	-0.147675000	1.695960000	0.655787000
6	1.445130000	2.712438000	1.130106000
8	0.259578000	2.563989000	0.370891000
6	2.629744000	2.013979000	0.477177000
6	3.522115000	1.259894000	1.243310000
6	2.868026000	2.151000000	-0.894376000
6	4.641408000	0.668998000	0.657282000
1	3.335365000	1.127825000	2.306646000
6	3.982424000	1.557528000	-1.485218000
1	2.172173000	2.724353000	-1.502004000
6	4.876482000	0.818861000	-0.708744000
1	5.320296000	0.078106000	1.265818000
1	4.153289000	1.671565000	-2.552219000
1	5.742981000	0.352028000	-1.168388000
6	1.720072000	4.201851000	1.307184000
1	0.883014000	4.680023000	1.825633000
1	2.632062000	4.361585000	1.891754000
1	1.847725000	4.685350000	0.331923000

8	-1.273565000	-2.314170000	-1.244716000
6	-2.120396000	-3.344718000	-0.960793000
1	-2.297202000	-4.003700000	-1.842650000
1	-1.754186000	-4.022819000	-0.152314000
1	-3.136312000	-3.020091000	-0.625770000

**TSA2-6<sub>X=OMe</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.183032000	0.297166000	-0.063956000
1	-0.023977000	0.004521000	-1.755585000
7	0.561271000	-1.783140000	-0.354171000
1	0.234170000	-0.842880000	-1.335379000
6	-0.120090000	2.009853000	-0.164765000
8	-0.332228000	3.171564000	-0.290532000
6	-1.840304000	-2.154027000	-0.132584000
6	1.886626000	-2.036538000	0.148423000
6	-0.441802000	-2.640071000	0.225907000
1	-2.603366000	-2.793619000	0.318528000
1	-1.976117000	-2.151816000	-1.218920000
1	-0.351652000	-3.687829000	-0.118145000
1	-0.346606000	-2.662537000	1.328650000
1	2.328563000	-2.978420000	-0.225088000
1	1.869585000	-2.108998000	1.253234000
6	2.807690000	-0.895344000	-0.189207000
6	4.188292000	-1.058872000	-0.310302000
1	4.621385000	-2.047956000	-0.196952000
6	2.998544000	1.371955000	-0.591960000
1	2.484019000	2.320501000	-0.703779000
6	4.988650000	0.046698000	-0.571010000
1	6.064749000	-0.060829000	-0.667812000
6	4.379071000	1.291485000	-0.714086000
1	4.955195000	2.187004000	-0.920746000
7	2.220637000	0.308925000	-0.333763000
16	-2.001006000	-0.441573000	0.492771000
6	-3.438834000	0.219679000	-0.481608000
6	-3.768360000	1.563027000	0.176899000
6	-4.630737000	-0.732294000	-0.352342000
1	-2.912056000	2.243937000	0.144995000
1	-4.599375000	2.038259000	-0.357670000
1	-4.067487000	1.432689000	1.222488000
1	-4.449864000	-1.683975000	-0.861979000

1	-4.864854000	-0.940614000	0.697236000
1	-5.513878000	-0.273085000	-0.812725000
6	-3.082172000	0.433637000	-1.952183000
1	-3.963243000	0.811300000	-2.485824000
1	-2.273007000	1.160637000	-2.059378000
1	-2.771219000	-0.496785000	-2.438106000
8	0.571911000	0.064249000	1.933004000
6	0.120359000	1.017900000	2.797743000
1	-0.980759000	1.201366000	2.739343000
1	0.320164000	0.753175000	3.861581000
1	0.587523000	2.022431000	2.648806000

A6<sub>X=OMe</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.187395000	0.371761000	-0.121110000
1	-0.007316000	0.465422000	-1.828376000
7	0.520657000	-1.764103000	-0.357976000
1	0.481552000	-1.962965000	-1.354038000
6	-0.004841000	2.081882000	0.093479000
8	-0.118955000	3.259618000	0.228349000
6	-1.890829000	-2.091832000	-0.034414000
6	1.875779000	-2.022772000	0.135366000
6	-0.494744000	-2.570642000	0.330185000
1	-2.639329000	-2.690440000	0.491560000
1	-2.058677000	-2.191034000	-1.111096000
1	-0.400814000	-3.638603000	0.085272000
1	-0.328398000	-2.432506000	1.401529000
1	2.282209000	-2.979418000	-0.219159000
1	1.809140000	-2.044653000	1.226979000
6	2.796290000	-0.889968000	-0.231232000
6	4.168576000	-1.083150000	-0.384439000
1	4.583164000	-2.081237000	-0.280439000
6	3.018473000	1.368167000	-0.644870000
1	2.517824000	2.324037000	-0.756461000
6	4.985471000	0.005690000	-0.667024000
1	6.056450000	-0.122821000	-0.789394000
6	4.393997000	1.259996000	-0.799198000
1	4.980877000	2.144036000	-1.024575000
7	2.222689000	0.323021000	-0.362787000
16	-2.033193000	-0.331895000	0.445207000
6	-3.495213000	0.239376000	-0.550651000
6	-3.687561000	1.701125000	-0.133313000

6	-4.725957000	-0.586352000	-0.166192000
1	-2.804700000	2.299237000	-0.379625000
1	-4.548154000	2.123599000	-0.664981000
1	-3.876191000	1.792292000	0.942113000
1	-4.622692000	-1.633321000	-0.470023000
1	-4.905471000	-0.556572000	0.913812000
1	-5.611761000	-0.181076000	-0.670346000
6	-3.251192000	0.163893000	-2.057382000
1	-4.123336000	0.572439000	-2.582830000
1	-2.367384000	0.740964000	-2.341513000
1	-3.111654000	-0.864983000	-2.404721000
8	0.494680000	-0.221972000	1.875773000
6	0.268812000	0.708349000	2.848187000
1	0.374310000	0.282155000	3.873075000
1	0.968567000	1.577970000	2.814371000
1	-0.753581000	1.157596000	2.814685000

**A7R<sub>X=OMe</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.754799000	-0.784873000	0.387006000
1	-0.123069000	0.768603000	0.640163000
7	-0.384105000	-0.491189000	-1.728286000
1	0.078984000	0.410006000	-1.828778000
6	-0.972188000	-1.043561000	2.086637000
8	-1.088537000	-1.200245000	3.263194000
6	-2.634609000	0.456854000	-1.908228000
6	0.546203000	-1.544230000	-2.135920000
6	-1.611343000	-0.479765000	-2.530369000
1	-3.546313000	0.473058000	-2.511360000
1	-2.231803000	1.472531000	-1.849910000
1	-1.416895000	-0.168897000	-3.567632000
1	-2.001175000	-1.501338000	-2.534039000
1	1.053603000	-1.320310000	-3.084455000
1	-0.043175000	-2.458948000	-2.250704000
6	1.550888000	-1.803623000	-1.047065000
6	2.801867000	-2.355780000	-1.321243000
1	3.082771000	-2.552377000	-2.351575000
6	1.998008000	-1.790385000	1.214053000
1	1.644694000	-1.535113000	2.207313000
6	3.664024000	-2.650793000	-0.272414000
1	4.639517000	-3.088265000	-0.461716000
6	3.250524000	-2.357705000	1.025387000

1	3.885875000	-2.555177000	1.882171000
7	1.148419000	-1.522321000	0.207951000
16	-2.994582000	-0.150698000	-0.221370000
6	-3.797702000	1.325123000	0.575339000
6	-4.204857000	0.833973000	1.968394000
6	-5.038543000	1.726682000	-0.226431000
1	-3.332441000	0.506850000	2.543145000
1	-4.689103000	1.651143000	2.516061000
1	-4.914234000	0.000946000	1.909909000
1	-4.774789000	2.099650000	-1.221623000
1	-5.730080000	0.885657000	-0.344627000
1	-5.568512000	2.532115000	0.297078000
6	-2.839408000	2.508487000	0.703902000
1	-3.342062000	3.326672000	1.234981000
1	-1.941729000	2.222665000	1.256858000
1	-2.527652000	2.892347000	-0.272598000
6	1.476350000	2.606336000	-1.090630000
8	1.301252000	2.069483000	-2.180164000
6	2.608616000	2.173437000	-0.213829000
6	2.804100000	2.720781000	1.059619000
6	3.496883000	1.200349000	-0.686605000
6	3.873379000	2.301745000	1.847248000
1	2.118480000	3.466282000	1.448563000
6	4.568471000	0.787268000	0.097388000
1	3.336543000	0.772177000	-1.670817000
6	4.758382000	1.337351000	1.366086000
1	4.014086000	2.727291000	2.836202000
1	5.253959000	0.032915000	-0.276073000
1	5.592482000	1.010994000	1.980684000
6	0.582250000	3.726930000	-0.635005000
1	-0.168979000	3.923698000	-1.400989000
1	0.083576000	3.455893000	0.300433000
1	1.167171000	4.635197000	-0.453689000
8	-1.417997000	-2.636213000	-0.392016000
6	-2.124125000	-3.454138000	0.438786000
1	-3.042292000	-2.984237000	0.869948000
1	-2.480572000	-4.377165000	-0.076350000
1	-1.544538000	-3.813523000	1.323809000

A7S<sub>X=OMe</sub>

-----  
Coordinates (Angstroms)

	X	Y	Z
25	0.827686000	-0.973151000	0.342942000

-----

1	-0.118254000	0.332761000	0.826231000
7	0.803679000	-0.092881000	-1.635902000
1	0.323732000	0.801007000	-1.561889000
6	0.912556000	-1.639054000	1.939511000
8	0.975857000	-2.075895000	3.047820000
6	-1.253824000	-1.334805000	-2.065233000
6	2.201925000	0.164108000	-1.980542000
6	0.100659000	-0.919888000	-2.619222000
1	-1.796424000	-1.935399000	-2.800024000
1	-1.849436000	-0.447872000	-1.823927000
1	-0.043034000	-0.388660000	-3.571886000
1	0.717244000	-1.805514000	-2.795220000
1	2.313489000	0.854590000	-2.827341000
1	2.644676000	-0.803164000	-2.237697000
6	2.927722000	0.687624000	-0.771086000
6	4.001426000	1.570321000	-0.873600000
1	4.305688000	1.928880000	-1.852237000
6	3.130628000	0.630394000	1.526213000
1	2.741065000	0.243204000	2.461790000
6	4.663515000	1.979954000	0.278577000
1	5.501621000	2.667846000	0.221840000
6	4.217222000	1.494222000	1.505847000
1	4.694532000	1.780391000	2.437039000
7	2.486247000	0.227546000	0.418097000
16	-0.963561000	-2.300638000	-0.539151000
6	-2.631603000	-2.265516000	0.282132000
6	-2.489403000	-3.220088000	1.472246000
6	-3.693840000	-2.787581000	-0.689085000
1	-1.694808000	-2.891031000	2.149964000
1	-3.430050000	-3.244818000	2.035118000
1	-2.263697000	-4.241191000	1.145333000
1	-3.859027000	-2.092889000	-1.519147000
1	-3.417196000	-3.763044000	-1.103295000
1	-4.648223000	-2.900594000	-0.160324000
6	-3.005477000	-0.870072000	0.780075000
1	-3.993432000	-0.908863000	1.256532000
1	-2.275444000	-0.504651000	1.505654000
1	-3.057363000	-0.142259000	-0.034930000
6	-0.179429000	3.088030000	-0.309021000
8	0.209207000	2.939531000	-1.463184000
6	-1.633321000	2.925690000	0.014698000
6	-2.108098000	2.951193000	1.331075000
6	-2.538241000	2.729603000	-1.035884000
6	-3.465486000	2.778011000	1.590418000

1	-1.421111000	3.084479000	2.160244000
6	-3.895143000	2.565554000	-0.777442000
1	-2.163889000	2.704057000	-2.054406000
6	-4.360910000	2.587662000	0.538200000
1	-3.823518000	2.786294000	2.615468000
1	-4.590105000	2.414579000	-1.598161000
1	-5.418688000	2.450294000	0.742753000
6	0.784547000	3.458898000	0.783323000
1	1.788959000	3.542890000	0.364839000
1	0.494544000	4.411978000	1.239484000
1	0.780028000	2.696880000	1.567445000
8	1.957192000	-2.402403000	-0.733861000
6	2.195804000	-3.599074000	-0.125117000
1	2.665099000	-4.340040000	-0.814494000
1	2.884778000	-3.533603000	0.752055000
1	1.278166000	-4.101208000	0.267992000

**TSA7-8R<sub>X=OMe</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	-0.594536000	-0.579491000	0.397919000
1	-0.161564000	1.036023000	-0.033350000
7	-0.416757000	-0.946993000	-1.693985000
1	-0.031550000	-0.068483000	-2.054783000
6	-0.630812000	-0.147435000	2.074909000
8	-0.623086000	0.210057000	3.212947000
6	-2.759972000	-0.259868000	-1.919659000
6	0.577455000	-2.002756000	-1.871319000
6	-1.684885000	-1.238805000	-2.367626000
1	-3.707460000	-0.492849000	-2.413041000
1	-2.472626000	0.765418000	-2.173022000
1	-1.584725000	-1.191077000	-3.462162000
1	-1.976290000	-2.256421000	-2.090163000
1	0.997932000	-2.028333000	-2.886476000
1	0.073551000	-2.954508000	-1.674066000
6	1.674284000	-1.862897000	-0.851031000
6	2.940622000	-2.407357000	-1.060633000
1	3.163160000	-2.891754000	-2.006639000
6	2.272246000	-1.156300000	1.259923000
1	1.971077000	-0.634977000	2.161936000
6	3.893577000	-2.328365000	-0.052239000
1	4.884512000	-2.749593000	-0.191880000
6	3.547515000	-1.690083000	1.136061000

1	4.254137000	-1.592679000	1.953190000
7	1.342848000	-1.234064000	0.293656000
16	-2.919787000	-0.415841000	-0.105602000
6	-3.914869000	1.081400000	0.358251000
6	-4.147718000	0.929281000	1.865212000
6	-5.250868000	1.063816000	-0.388674000
1	-3.198968000	0.904433000	2.410733000
1	-4.732576000	1.780769000	2.232403000
1	-4.701367000	0.012400000	2.095907000
1	-5.113400000	1.210035000	-1.465126000
1	-5.785225000	0.120486000	-0.233042000
1	-5.886066000	1.880063000	-0.023339000
6	-3.162132000	2.378864000	0.078275000
1	-3.754621000	3.230402000	0.436167000
1	-2.194918000	2.383212000	0.585988000
1	-2.989183000	2.525260000	-0.992075000
6	0.957084000	2.098297000	-1.228827000
8	0.886726000	1.549781000	-2.343951000
6	2.221218000	1.935717000	-0.413498000
6	2.326623000	2.348339000	0.920383000
6	3.350351000	1.412875000	-1.049053000
6	3.540980000	2.255933000	1.594572000
1	1.450382000	2.716216000	1.445291000
6	4.567230000	1.317593000	-0.375343000
1	3.262604000	1.086648000	-2.080610000
6	4.668288000	1.745966000	0.946874000
1	3.606776000	2.573298000	2.631500000
1	5.435136000	0.905562000	-0.882627000
1	5.614904000	1.671761000	1.474553000
6	0.121196000	3.333815000	-0.967564000
1	-0.839937000	3.234460000	-1.473469000
1	-0.045659000	3.538135000	0.090243000
1	0.657579000	4.188453000	-1.403571000
8	-1.102069000	-2.608898000	0.408434000
6	-1.614876000	-3.115959000	1.565488000
1	-2.535300000	-2.590541000	1.922945000
1	-1.904830000	-4.188228000	1.467897000
1	-0.905912000	-3.075434000	2.428294000

TSA7-8S<sub>X=OMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	-0.831577000	0.742680000	0.314612000



1	0.131204000	-0.714708000	0.474582000
7	-0.947927000	0.100062000	-1.708361000
1	-0.544148000	-0.841364000	-1.681716000
6	-0.708581000	1.144574000	1.997452000
8	-0.603689000	1.397068000	3.157809000
6	1.172004000	1.265130000	-2.078666000
6	-2.366564000	-0.029739000	-2.030375000
6	-0.196989000	0.926056000	-2.654811000
1	1.739006000	1.875425000	-2.786695000
1	1.734596000	0.350761000	-1.862751000
1	-0.069513000	0.423270000	-3.624899000
1	-0.765208000	1.847470000	-2.816692000
1	-2.548724000	-0.627931000	-2.934277000
1	-2.756350000	0.982345000	-2.180693000
6	-3.090542000	-0.619946000	-0.850475000
6	-4.271178000	-1.346685000	-0.995039000
1	-4.663449000	-1.536908000	-1.989402000
6	-3.188985000	-0.822943000	1.445759000
1	-2.715123000	-0.604491000	2.396891000
6	-4.930116000	-1.812501000	0.137125000
1	-5.853837000	-2.375889000	0.047011000
6	-4.376026000	-1.540815000	1.386316000
1	-4.846389000	-1.881808000	2.302325000
7	-2.547203000	-0.367731000	0.357573000
16	0.884403000	2.178246000	-0.521979000
6	2.555781000	2.200316000	0.286087000
6	2.400004000	3.183938000	1.450854000
6	3.607424000	2.713898000	-0.700001000
1	1.614658000	2.859472000	2.141329000
1	3.342128000	3.238676000	2.009139000
1	2.155974000	4.191611000	1.097142000
1	3.787028000	1.998489000	-1.509139000
1	3.313021000	3.671907000	-1.141969000
1	4.558676000	2.860352000	-0.174044000
6	2.944794000	0.822778000	0.815049000
1	3.924836000	0.883693000	1.305271000
1	2.210450000	0.458114000	1.537905000
1	3.016401000	0.088565000	0.008649000
6	0.277642000	-2.537999000	-0.092135000
8	-0.217431000	-2.603982000	-1.234711000
6	1.783597000	-2.489982000	0.032864000
6	2.443297000	-2.631220000	1.258599000
6	2.548402000	-2.362484000	-1.131740000
6	3.835628000	-2.629220000	1.318709000

1	1.876635000	-2.725985000	2.179365000
6	3.940349000	-2.355449000	-1.073917000
1	2.036019000	-2.265720000	-2.083726000
6	4.590071000	-2.488789000	0.153602000
1	4.331949000	-2.734306000	2.279304000
1	4.517489000	-2.247418000	-1.988151000
1	5.675273000	-2.483461000	0.203048000
6	-0.520328000	-3.072074000	1.078925000
1	-1.581719000	-2.926530000	0.875442000
1	-0.325491000	-4.150604000	1.159292000
1	-0.271480000	-2.600722000	2.030138000
8	-2.031271000	2.290424000	-0.412556000
6	-2.182551000	3.397985000	0.367663000
1	-2.774228000	4.195617000	-0.139217000
1	-2.708967000	3.204124000	1.333747000
1	-1.219495000	3.885626000	0.659272000

**A8R<sub>X=OMe</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.740882000	-1.013488000	-0.023359000
1	-0.121991000	1.795324000	-0.999743000
7	0.238407000	-0.205089000	1.689938000
1	-0.042969000	1.471464000	1.163040000
6	0.712118000	-0.589152000	-1.703165000
8	0.565497000	-0.193104000	-2.820725000
6	2.456166000	0.715823000	2.081507000
6	-1.055636000	-0.550947000	2.227129000
6	1.199360000	0.135718000	2.720954000
1	3.281593000	0.765475000	2.796088000
1	2.244793000	1.720346000	1.707865000
1	0.810004000	0.894616000	3.426206000
1	1.462756000	-0.745553000	3.335975000
1	-1.632372000	0.325173000	2.582894000
1	-0.968291000	-1.222838000	3.101961000
6	-1.862539000	-1.278179000	1.185226000
6	-3.200410000	-1.629326000	1.374419000
1	-3.708685000	-1.325525000	2.284562000
6	-1.827125000	-2.337112000	-0.871518000
1	-1.234416000	-2.591701000	-1.743292000
6	-3.853665000	-2.369131000	0.398450000
1	-4.894487000	-2.651519000	0.525042000
6	-3.147616000	-2.739305000	-0.746869000

1	-3.613244000	-3.320424000	-1.535686000
7	-1.195421000	-1.610439000	0.065802000
16	2.920259000	-0.335646000	0.655010000
6	3.851028000	0.854915000	-0.431954000
6	4.378919000	0.002821000	-1.589588000
6	5.015094000	1.460122000	0.356606000
1	3.561132000	-0.498281000	-2.117419000
1	4.902484000	0.647950000	-2.304792000
1	5.084918000	-0.757739000	-1.239388000
1	4.663049000	2.102801000	1.170061000
1	5.659776000	0.683890000	0.782007000
1	5.624889000	2.079670000	-0.312176000
6	2.939333000	1.960235000	-0.969056000
1	3.537797000	2.655426000	-1.570888000
1	2.152325000	1.547340000	-1.603408000
1	2.465646000	2.534293000	-0.167135000
6	-0.727589000	2.454642000	-0.361248000
8	-0.219189000	2.431428000	0.954284000
6	-2.162532000	1.952683000	-0.422962000
6	-2.592725000	1.177906000	-1.503243000
6	-3.079136000	2.276680000	0.581954000
6	-3.916270000	0.746587000	-1.588628000
1	-1.876131000	0.892038000	-2.270258000
6	-4.402942000	1.846367000	0.501601000
1	-2.744046000	2.859710000	1.435252000
6	-4.827297000	1.083853000	-0.587731000
1	-4.232173000	0.134753000	-2.429219000
1	-5.104576000	2.103521000	1.290678000
1	-5.856638000	0.741443000	-0.648259000
6	-0.616218000	3.879467000	-0.892319000
1	0.431269000	4.199320000	-0.888322000
1	-0.996270000	3.944696000	-1.917168000
1	-1.195495000	4.567289000	-0.265299000
8	1.244962000	-2.948487000	-0.082566000
6	2.267392000	-3.372835000	-0.885435000
1	3.241893000	-2.866238000	-0.695158000
1	2.467093000	-4.459986000	-0.760632000
1	2.066855000	-3.220171000	-1.972468000

A8S<sub>X=OMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	1.149175000	0.879599000	-0.123238000

1	-0.251823000	-1.723324000	-0.911340000
7	1.030781000	-0.010061000	1.622854000
1	0.215902000	-1.504818000	1.145476000
6	0.580018000	0.597681000	-1.734377000
8	0.170971000	0.255956000	-2.802911000
6	-1.080903000	1.061282000	2.137710000
6	2.225055000	-0.681383000	2.078192000
6	0.194644000	0.453494000	2.709901000
1	-1.656231000	1.583303000	2.906866000
1	-1.697525000	0.272598000	1.697635000
1	-0.100563000	-0.366133000	3.392582000
1	0.716498000	1.202643000	3.335852000
1	2.023195000	-1.622096000	2.624933000
1	2.806867000	-0.049909000	2.777097000
6	3.103539000	-0.982167000	0.893822000
6	4.197669000	-1.846637000	0.959065000
1	4.420577000	-2.356193000	1.891588000
6	3.545277000	-0.515193000	-1.328983000
1	3.245047000	0.040721000	-2.210708000
6	4.981797000	-2.038068000	-0.170863000
1	5.834520000	-2.709882000	-0.144324000
6	4.651235000	-1.351499000	-1.340103000
1	5.234027000	-1.464664000	-2.247917000
7	2.775650000	-0.338563000	-0.241896000
16	-0.573729000	2.219162000	0.816584000
6	-2.151828000	2.538476000	-0.113771000
6	-1.757049000	3.490004000	-1.246288000
6	-3.161501000	3.210895000	0.819134000
1	-1.021581000	3.028150000	-1.912843000
1	-2.647800000	3.737368000	-1.835514000
1	-1.336348000	4.424372000	-0.859580000
1	-3.467335000	2.543159000	1.631195000
1	-2.753430000	4.127102000	1.258573000
1	-4.062396000	3.476145000	0.252383000
6	-2.734067000	1.251605000	-0.695657000
1	-3.604891000	1.498634000	-1.315690000
1	-2.002269000	0.734088000	-1.319340000
1	-3.073307000	0.563451000	0.083473000
6	-0.681717000	-2.515530000	-0.278587000
8	-0.122705000	-2.434373000	1.009809000
6	-2.192114000	-2.305619000	-0.259788000
6	-2.895595000	-2.160482000	-1.461913000
6	-2.901266000	-2.242976000	0.940593000
6	-4.272958000	-1.954194000	-1.464128000

1	-2.357076000	-2.190699000	-2.406567000
6	-4.283157000	-2.038296000	0.943610000
1	-2.357999000	-2.343711000	1.874912000
6	-4.974332000	-1.892289000	-0.257801000
1	-4.798425000	-1.832062000	-2.407377000
1	-4.817375000	-1.987138000	1.888711000
1	-6.047870000	-1.725728000	-0.256726000
6	-0.316127000	-3.869876000	-0.883873000
1	0.772473000	-3.963710000	-0.951882000
1	-0.697450000	-4.681381000	-0.253250000
1	-0.736698000	-3.987250000	-1.887785000
8	2.397887000	2.423972000	-0.336986000
6	2.035701000	3.546565000	-1.028808000
1	1.127988000	4.055007000	-0.631243000
1	2.838180000	4.316514000	-1.017810000
1	1.815254000	3.350022000	-2.104302000

Al<sub>X=CHCHMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	-0.166761000	0.044787000	0.107059000
7	-0.419500000	-1.736774000	-0.563540000
6	0.123380000	0.963074000	1.547626000
8	0.288835000	1.526137000	2.589263000
6	1.962882000	-2.179350000	-0.733519000
6	-1.755789000	-2.241257000	-0.728029000
6	0.569875000	-2.556298000	-1.226502000
1	2.744278000	-2.578064000	-1.386249000
1	2.108425000	-2.562106000	0.280198000
1	0.421527000	-3.633437000	-1.025409000
1	0.524820000	-2.443209000	-2.328252000
1	-1.903464000	-3.240447000	-0.273204000
1	-2.032028000	-2.363669000	-1.794753000
6	-2.729474000	-1.278226000	-0.109183000
6	-4.099267000	-1.534978000	-0.025020000
1	-4.490788000	-2.471237000	-0.411611000
6	-3.008651000	0.781562000	0.902848000
1	-2.530958000	1.689348000	1.255213000
6	-4.937999000	-0.589066000	0.547882000
1	-6.005741000	-0.769364000	0.626410000
6	-4.376799000	0.597614000	1.022742000
1	-4.986794000	1.370577000	1.477974000
7	-2.187649000	-0.134522000	0.353692000

16	2.033652000	-0.354072000	-0.680686000
6	3.488823000	-0.012844000	0.424607000
6	3.579658000	1.514774000	0.479918000
6	4.754157000	-0.598860000	-0.206724000
1	2.667507000	1.948789000	0.900579000
1	4.425427000	1.806967000	1.113228000
1	3.736752000	1.944043000	-0.515859000
1	4.707636000	-1.691330000	-0.266431000
1	4.917299000	-0.203283000	-1.214697000
1	5.624769000	-0.337139000	0.407235000
6	3.281343000	-0.579338000	1.829562000
1	4.114783000	-0.265988000	2.470446000
1	2.350067000	-0.214698000	2.269459000
1	3.261216000	-1.673635000	1.832603000
6	-0.394221000	1.584869000	-1.138707000
1	-0.517386000	1.219068000	-2.185556000
6	-0.495901000	2.933074000	-1.087794000
1	-0.388777000	3.434569000	-0.116907000
6	-0.749267000	3.875329000	-2.245699000
1	-1.683191000	4.442313000	-2.120037000
1	0.051150000	4.621252000	-2.356268000
1	-0.823114000	3.325666000	-3.192802000

A2<sub>X=CHCHMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	-0.029344000	-0.270516000	-0.273951000
7	-0.300281000	1.796377000	0.052911000
6	0.132438000	-1.985288000	-0.520927000
8	0.207269000	-3.167923000	-0.607055000
6	2.045379000	2.022813000	0.616796000
6	-1.663334000	2.017545000	0.440288000
6	0.612437000	2.384140000	0.992209000
1	2.766744000	2.409461000	1.342073000
1	2.280628000	2.425123000	-0.373609000
1	0.549584000	3.492127000	1.023602000
1	0.426680000	2.050682000	2.040413000
1	-2.007635000	3.065230000	0.323476000
1	-1.845114000	1.765734000	1.511538000
6	-2.565669000	1.119030000	-0.360400000
6	-3.902786000	1.423562000	-0.620694000
1	-4.312702000	2.363450000	-0.263316000
6	-2.772287000	-0.897614000	-1.473413000

1	-2.281376000	-1.810626000	-1.794362000
6	-4.689687000	0.523268000	-1.327986000
1	-5.732541000	0.742893000	-1.536170000
6	-4.109016000	-0.665479000	-1.766521000
1	-4.675613000	-1.402388000	-2.325620000
7	-2.007561000	-0.034544000	-0.783740000
16	2.137378000	0.195485000	0.558601000
6	3.623976000	-0.126732000	-0.509947000
6	3.861401000	-1.636276000	-0.405594000
6	4.825504000	0.638699000	0.050314000
1	2.982900000	-2.197590000	-0.739946000
1	4.708672000	-1.918880000	-1.041482000
1	4.092006000	-1.935504000	0.622410000
1	4.704545000	1.720528000	-0.064728000
1	4.982898000	0.419278000	1.111661000
1	5.730867000	0.346857000	-0.495481000
6	3.380643000	0.258452000	-1.969191000
1	4.307149000	0.112110000	-2.537976000
1	2.603960000	-0.365860000	-2.417649000
1	3.087573000	1.307784000	-2.078086000
6	-1.716470000	-1.224863000	2.157223000
1	-2.518902000	-1.535064000	1.474652000
6	-2.031599000	-1.465259000	3.618221000
1	-2.931371000	-0.922488000	3.943824000
1	-2.221926000	-2.527848000	3.829730000
1	-1.201408000	-1.144452000	4.260513000
1	0.303857000	-0.156472000	-2.004814000
1	0.449154000	0.577663000	-1.748855000
6	-0.589111000	-0.687038000	1.642118000
1	0.132744000	-0.429793000	2.446631000

**A3<sub>X=CHCHMe</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	1.158939000	0.631659000	0.283065000
1	0.819356000	-0.725275000	1.555042000
7	0.145230000	-0.193644000	-1.277514000
6	1.941322000	1.421592000	1.681145000
8	2.448285000	1.999908000	2.551452000
6	2.074920000	-1.543346000	-1.853628000
6	-0.886782000	0.721846000	-1.706223000
6	0.937248000	-0.681472000	-2.387196000
1	2.741294000	-1.877063000	-2.651820000

1	1.677235000	-2.412540000	-1.322438000
1	0.337984000	-1.305589000	-3.073464000
1	1.353717000	0.140402000	-2.999979000
1	-1.680779000	0.235179000	-2.297239000
1	-0.487807000	1.539257000	-2.338836000
6	-1.500150000	1.349057000	-0.488514000
6	-2.778176000	1.904742000	-0.477657000
1	-3.375033000	1.881641000	-1.383151000
6	-1.207668000	1.881177000	1.753961000
1	-0.548724000	1.852705000	2.614802000
6	-3.270483000	2.456459000	0.695583000
1	-4.266499000	2.886798000	0.725578000
6	-2.473770000	2.433929000	1.840711000
1	-2.822801000	2.841111000	2.782702000
7	-0.723390000	1.358771000	0.613902000
16	3.017106000	-0.504143000	-0.677772000
6	3.989546000	-1.711097000	0.356296000
6	4.912455000	-0.841420000	1.213542000
6	4.808842000	-2.588396000	-0.593293000
1	4.339223000	-0.179857000	1.870514000
1	5.528729000	-1.490714000	1.845297000
1	5.580372000	-0.230697000	0.597762000
1	4.170910000	-3.242507000	-1.195590000
1	5.427310000	-1.985426000	-1.265876000
1	5.472592000	-3.226140000	0.001243000
6	3.097082000	-2.571623000	1.248583000
1	3.718521000	-3.334524000	1.731508000
1	2.625180000	-1.976007000	2.033939000
1	2.315951000	-3.089125000	0.683278000
1	0.651292000	-1.108466000	0.907864000
1	-1.461758000	-1.495432000	1.455366000
1	-0.573946000	-1.541199000	-0.672815000
6	-1.855987000	-2.215083000	0.717381000
8	-0.917632000	-2.431011000	-0.302697000
6	-3.173328000	-1.639483000	0.209600000
6	-4.088648000	-1.093385000	1.116965000
6	-3.501171000	-1.653987000	-1.146675000
6	-5.303832000	-0.572674000	0.678930000
1	-3.841117000	-1.063793000	2.176272000
6	-4.715610000	-1.128110000	-1.591437000
1	-2.790447000	-2.068261000	-1.855295000
6	-5.621642000	-0.586323000	-0.680926000
1	-6.000403000	-0.147885000	1.396655000
1	-4.951160000	-1.140058000	-2.652296000



1	-6.565074000	-0.173637000	-1.026880000
6	-2.084121000	-3.545106000	1.432850000
1	-1.139216000	-3.914285000	1.844798000
1	-2.802850000	-3.437867000	2.251537000
1	-2.471318000	-4.288656000	0.727029000
6	1.667664000	2.209744000	-0.815448000
1	2.079995000	1.984084000	-1.810301000
6	1.471736000	3.513127000	-0.564945000
1	1.060618000	3.818379000	0.402426000
6	1.733108000	4.645469000	-1.524633000
1	2.152621000	4.278511000	-2.468236000
1	0.810359000	5.194600000	-1.754629000
1	2.435083000	5.376258000	-1.101634000

**TSA3-4<sub>X</sub>=CHCHMe**

Coordinates (Angstroms)			
	X	Y	Z
25	-1.199190000	0.618365000	-0.358582000
1	-0.746713000	-0.562246000	-1.539856000
7	-0.152425000	-0.231135000	1.268254000
6	-2.018157000	1.386930000	-1.689231000
8	-2.583583000	1.970975000	-2.552385000
6	-2.148806000	-1.472424000	1.874663000
6	0.880449000	0.690992000	1.677834000
6	-0.984124000	-0.631495000	2.382932000
1	-2.820269000	-1.763302000	2.686592000
1	-1.766896000	-2.371006000	1.381513000
1	-0.426858000	-1.239786000	3.120932000
1	-1.376625000	0.242855000	2.934403000
1	1.679455000	0.214841000	2.275529000
1	0.470368000	1.507795000	2.300183000
6	1.493225000	1.321423000	0.458863000
6	2.785960000	1.845600000	0.455406000
1	3.389658000	1.773982000	1.354737000
6	1.196718000	1.926616000	-1.750489000
1	0.529766000	1.937404000	-2.606505000
6	3.284395000	2.433239000	-0.699027000
1	4.289155000	2.843996000	-0.722563000
6	2.471859000	2.468051000	-1.831557000
1	2.814737000	2.906155000	-2.762689000
7	0.702536000	1.369753000	-0.632099000
16	-3.053978000	-0.461531000	0.645927000
6	-3.998928000	-1.730620000	-0.332596000

6	-4.924740000	-0.912868000	-1.238580000
6	-4.823497000	-2.593862000	0.625715000
1	-4.349255000	-0.254493000	-1.897088000
1	-5.515824000	-1.590818000	-1.865338000
1	-5.617820000	-0.298642000	-0.653849000
1	-4.187169000	-3.227591000	1.251809000
1	-5.452074000	-1.979526000	1.279218000
1	-5.478918000	-3.253151000	0.044153000
6	-3.082674000	-2.607394000	-1.185832000
1	-3.684773000	-3.381319000	-1.677415000
1	-2.583472000	-2.021199000	-1.961362000
1	-2.316990000	-3.113088000	-0.588836000
1	-0.791798000	-0.998614000	-0.872786000
1	1.407604000	-1.327451000	-1.247775000
1	0.485794000	-1.406793000	0.811065000
6	1.810791000	-2.126136000	-0.599436000
8	0.960602000	-2.357518000	0.475041000
6	3.202108000	-1.649114000	-0.180103000
6	4.095085000	-1.147533000	-1.135457000
6	3.606068000	-1.683524000	1.155012000
6	5.358820000	-0.692945000	-0.766293000
1	3.789540000	-1.093423000	-2.178735000
6	4.870763000	-1.226937000	1.532380000
1	2.906386000	-2.057119000	1.896448000
6	5.752790000	-0.729891000	0.573722000
1	6.035037000	-0.300004000	-1.521017000
1	5.164333000	-1.255449000	2.578649000
1	6.735304000	-0.369453000	0.865669000
6	1.912095000	-3.396289000	-1.450226000
1	0.914534000	-3.683896000	-1.799302000
1	2.556236000	-3.252610000	-2.324790000
1	2.319884000	-4.219359000	-0.851572000
6	-1.641074000	2.261426000	0.770679000
1	-2.327383000	2.108278000	1.630978000
6	-1.234882000	3.547220000	0.697838000
1	-0.551373000	3.844945000	-0.108607000
6	-1.601084000	4.676635000	1.636670000
1	-2.295803000	4.333561000	2.413984000
1	-0.718873000	5.096779000	2.141762000
1	-2.081396000	5.514518000	1.110535000

A4<sub>x</sub>= CHCHMe

Coordinates (Angstroms)

	X	Y	Z
25	1.165923000	0.639944000	0.347147000
1	0.720374000	-0.568055000	1.504093000
7	0.116093000	-0.128183000	-1.340635000
6	1.991846000	1.370878000	1.694398000
8	2.565816000	1.933583000	2.561802000
6	2.075249000	-1.440303000	-1.908877000
6	-0.907256000	0.837728000	-1.712612000
6	0.966846000	-0.547896000	-2.449932000
1	2.747404000	-1.759264000	-2.708780000
1	1.630774000	-2.317453000	-1.429021000
1	0.397446000	-1.111318000	-3.205297000
1	1.388938000	0.335864000	-2.943060000
1	-1.690404000	0.406383000	-2.352301000
1	-0.436599000	1.659308000	-2.267706000
6	-1.519930000	1.403801000	-0.460665000
6	-2.814024000	1.919264000	-0.436679000
1	-3.415996000	1.889334000	-1.339160000
6	-1.226420000	1.902775000	1.774086000
1	-0.560641000	1.875507000	2.630439000
6	-3.316036000	2.446973000	0.745623000
1	-4.323084000	2.850196000	0.787803000
6	-2.504544000	2.433519000	1.878129000
1	-2.850492000	2.825809000	2.828261000
7	-0.729825000	1.401341000	0.631475000
16	3.001050000	-0.480920000	-0.652974000
6	3.875698000	-1.804603000	0.319872000
6	4.823165000	-1.038375000	1.248355000
6	4.675235000	-2.687327000	-0.642155000
1	4.267820000	-0.362063000	1.906060000
1	5.371348000	-1.750012000	1.876576000
1	5.553964000	-0.450676000	0.682630000
1	4.021175000	-3.298124000	-1.272740000
1	5.324136000	-2.089007000	-1.290554000
1	5.308389000	-3.369491000	-0.062558000
6	2.910437000	-2.652162000	1.148189000
1	3.466557000	-3.475480000	1.612863000
1	2.449913000	-2.062523000	1.944627000
1	2.110490000	-3.087273000	0.540987000
1	0.619837000	-0.974426000	0.824220000
1	-1.429938000	-1.592141000	1.473296000
1	-0.349062000	-1.006196000	-0.959537000
6	-1.765421000	-2.292847000	0.666300000
8	-0.838883000	-2.421823000	-0.321958000

6	-3.106112000	-1.702931000	0.190897000
6	-4.047423000	-1.203948000	1.100566000
6	-3.409596000	-1.645387000	-1.170538000
6	-5.257794000	-0.668233000	0.663703000
1	-3.822411000	-1.221966000	2.165892000
6	-4.618939000	-1.109000000	-1.617573000
1	-2.663330000	-2.012614000	-1.869792000
6	-5.549815000	-0.618324000	-0.701743000
1	-5.970722000	-0.279266000	1.386487000
1	-4.831684000	-1.066084000	-2.683145000
1	-6.488567000	-0.193551000	-1.046881000
6	-2.040646000	-3.637728000	1.376168000
1	-1.102153000	-4.025618000	1.789146000
1	-2.768041000	-3.548430000	2.193962000
1	-2.422054000	-4.367975000	0.650491000
6	1.650052000	2.296113000	-0.743189000
1	2.172568000	2.132336000	-1.710559000
6	1.417241000	3.609130000	-0.532779000
1	0.910912000	3.915526000	0.392223000
6	1.765722000	4.759127000	-1.452518000
1	2.262999000	4.399512000	-2.362305000
1	0.873466000	5.322439000	-1.762511000
1	2.437250000	5.485273000	-0.972054000

**TSA4-5<sub>X</sub>=CHCHMe**

Coordinates (Angstroms)			
	X	Y	Z
25	1.085627000	0.635861000	0.366585000
1	0.597109000	-0.833284000	1.227406000
7	0.088853000	-0.042027000	-1.405938000
6	1.822192000	1.238023000	1.815158000
8	2.320603000	1.712531000	2.783453000
6	2.074382000	-1.332157000	-1.959898000
6	-0.917836000	0.950338000	-1.758195000
6	0.968485000	-0.436840000	-2.503797000
1	2.760249000	-1.623679000	-2.758799000
1	1.638366000	-2.229735000	-1.510930000
1	0.421584000	-0.979183000	-3.289709000
1	1.394893000	0.464811000	-2.957477000
1	-1.679441000	0.562915000	-2.449700000
1	-0.414403000	1.793813000	-2.246445000
6	-1.569265000	1.446812000	-0.495353000
6	-2.862015000	1.964293000	-0.489602000

1	-3.429470000	1.989161000	-1.414467000
6	-1.357843000	1.809889000	1.772505000
1	-0.728959000	1.724864000	2.652151000
6	-3.406091000	2.428230000	0.701331000
1	-4.412307000	2.834691000	0.729392000
6	-2.636518000	2.343224000	1.859208000
1	-3.015165000	2.681516000	2.817756000
7	-0.816750000	1.374530000	0.622371000
16	2.966466000	-0.393260000	-0.666253000
6	3.909289000	-1.717538000	0.239009000
6	4.849977000	-0.943206000	1.168521000
6	4.718135000	-2.545460000	-0.762869000
1	4.286662000	-0.288235000	1.841266000
1	5.422823000	-1.649542000	1.780647000
1	5.558896000	-0.330334000	0.601558000
1	4.071863000	-3.159753000	-1.398279000
1	5.337385000	-1.910680000	-1.405713000
1	5.382246000	-3.223900000	-0.214083000
6	2.992602000	-2.621895000	1.060604000
1	3.591110000	-3.422294000	1.513068000
1	2.501962000	-2.061371000	1.860434000
1	2.210873000	-3.084141000	0.449968000
1	0.177840000	-1.408656000	0.654044000
1	-1.529458000	-1.788944000	1.795339000
1	-0.378084000	-0.891953000	-1.048282000
6	-1.716125000	-2.372416000	0.864624000
8	-0.611563000	-2.320328000	0.040515000
6	-2.971615000	-1.763990000	0.236543000
6	-4.002983000	-1.264107000	1.039316000
6	-3.133343000	-1.727373000	-1.150990000
6	-5.169372000	-0.750138000	0.474667000
1	-3.884837000	-1.268445000	2.121447000
6	-4.296759000	-1.211654000	-1.723578000
1	-2.327735000	-2.097564000	-1.779440000
6	-5.321786000	-0.723112000	-0.912583000
1	-5.954031000	-0.358880000	1.116961000
1	-4.402038000	-1.186079000	-2.805275000
1	-6.225319000	-0.314719000	-1.356728000
6	-2.016000000	-3.816330000	1.302108000
1	-1.133906000	-4.237385000	1.796649000
1	-2.862748000	-3.869323000	1.997739000
1	-2.247655000	-4.434027000	0.425495000
6	1.589385000	2.352647000	-0.633135000
1	2.120775000	2.236147000	-1.604991000

6	1.356535000	3.659036000	-0.375473000
1	0.842316000	3.931284000	0.556260000
6	1.713677000	4.845168000	-1.246236000
1	2.220764000	4.521434000	-2.164299000
1	0.824513000	5.420290000	-1.544217000
1	2.379506000	5.553002000	-0.731411000

**A5<sub>X=</sub> CHCHMe**

Coordinates (Angstroms)			
	X	Y	Z
25	-0.869715000	0.709395000	-0.372913000
1	-0.188957000	-0.743124000	-0.797333000
7	-0.326765000	0.335278000	1.649292000
1	0.221915000	-0.525570000	1.643213000
6	-1.246017000	1.042247000	-2.064216000
8	-1.492929000	1.300564000	-3.173378000
6	-2.409936000	-0.922699000	1.912811000
6	0.555346000	1.420340000	2.082512000
6	-1.482833000	0.116120000	2.529518000
1	-3.290242000	-1.063690000	2.543002000
1	-1.894017000	-1.880617000	1.801567000
1	-1.170771000	-0.230700000	3.523404000
1	-2.002294000	1.071844000	2.649940000
1	1.158177000	1.145388000	2.956491000
1	-0.064950000	2.280261000	2.353805000
6	1.445680000	1.823726000	0.938080000
6	2.649912000	2.490217000	1.144167000
1	2.977727000	2.698949000	2.157175000
6	1.749651000	1.881732000	-1.357032000
1	1.358512000	1.610309000	-2.330792000
6	3.413490000	2.866535000	0.047043000
1	4.356501000	3.385762000	0.185356000
6	2.960121000	2.544904000	-1.229620000
1	3.529779000	2.799085000	-2.116184000
7	0.996438000	1.541392000	-0.299736000
16	-2.930938000	-0.318032000	0.265504000
6	-3.535498000	-1.839905000	-0.621408000
6	-4.067327000	-1.322285000	-1.960587000
6	-4.670338000	-2.443504000	0.210256000
1	-3.264600000	-0.896181000	-2.569487000
1	-4.500950000	-2.161111000	-2.515919000
1	-4.846678000	-0.564806000	-1.826956000
1	-4.306811000	-2.841483000	1.162973000

1	-5.455706000	-1.708553000	0.414176000
1	-5.117135000	-3.274621000	-0.347008000
6	-2.434549000	-2.869749000	-0.857865000
1	-2.872826000	-3.734640000	-1.369755000
1	-1.639324000	-2.461847000	-1.486576000
1	-1.988396000	-3.224482000	0.075144000
1	1.111387000	-3.727552000	-0.595174000
1	0.103068000	-1.845408000	0.215891000
6	1.480227000	-3.225190000	0.311149000
8	0.420355000	-2.484243000	0.898616000
6	2.638003000	-2.324734000	-0.088352000
6	3.234984000	-2.448861000	-1.344130000
6	3.143241000	-1.378556000	0.809935000
6	4.322628000	-1.648683000	-1.698740000
1	2.842857000	-3.173655000	-2.054082000
6	4.229920000	-0.580986000	0.461145000
1	2.677048000	-1.263046000	1.785407000
6	4.823975000	-0.713411000	-0.795285000
1	4.774227000	-1.754264000	-2.681128000
1	4.610896000	0.150271000	1.167767000
1	5.666966000	-0.085257000	-1.068941000
6	1.913344000	-4.285024000	1.314515000
1	1.070204000	-4.935957000	1.566496000
1	2.716390000	-4.900598000	0.897638000
1	2.279466000	-3.814909000	2.233793000
6	-1.717156000	2.516838000	0.138609000
1	-2.799792000	2.494830000	0.349033000
6	-1.202506000	3.757931000	0.206962000
1	-0.137297000	3.916397000	0.003461000
6	-1.951526000	5.020352000	0.564093000
1	-3.010875000	4.814604000	0.758093000
1	-1.532954000	5.499579000	1.460042000
1	-1.896806000	5.767043000	-0.239938000

**TSA2-6<sub>x=CHCHMe</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.031867000	0.321604000	-0.217004000
7	0.328293000	-1.806846000	-0.332566000
6	-0.212588000	2.033381000	-0.368189000
8	-0.361740000	3.211401000	-0.433494000
6	-2.027762000	-2.107926000	0.187077000

6	1.707775000	-2.096538000	-0.062072000
6	-0.600594000	-2.569567000	0.457398000
1	-2.741561000	-2.655317000	0.807710000
1	-2.275477000	-2.270181000	-0.866404000
1	-0.554701000	-3.653008000	0.238094000
1	-0.384431000	-2.461364000	1.540152000
1	2.047296000	-3.066310000	-0.469864000
1	1.893737000	-2.145834000	1.030820000
6	2.592786000	-1.001916000	-0.599386000
6	3.941830000	-1.213849000	-0.883440000
1	4.361299000	-2.208258000	-0.764780000
6	2.784817000	1.232712000	-1.152683000
1	2.283947000	2.189360000	-1.253959000
6	4.731034000	-0.149592000	-1.302083000
1	5.785101000	-0.293749000	-1.518748000
6	4.136486000	1.103087000	-1.439556000
1	4.703252000	1.968680000	-1.765312000
7	2.018078000	0.211342000	-0.734010000
16	-2.123867000	-0.315037000	0.550406000
6	-3.615071000	0.219466000	-0.425192000
6	-3.850831000	1.674774000	-0.008417000
6	-4.818113000	-0.641845000	-0.032193000
1	-2.981362000	2.298158000	-0.238997000
1	-4.712502000	2.074899000	-0.555439000
1	-4.060975000	1.757094000	1.063427000
1	-4.700300000	-1.679474000	-0.360245000
1	-4.978112000	-0.636611000	1.051261000
1	-5.720882000	-0.243708000	-0.510891000
6	-3.373489000	0.145688000	-1.932293000
1	-4.282542000	0.465214000	-2.456850000
1	-2.550340000	0.799569000	-2.231557000
1	-3.139561000	-0.871005000	-2.263958000
6	0.548359000	0.559155000	1.754746000
1	-0.285061000	0.754084000	2.463960000
6	1.729358000	0.543170000	2.415680000
1	2.658071000	0.372018000	1.855489000
6	1.945934000	0.735069000	3.902388000
1	2.429505000	-0.137487000	4.365937000
1	2.594905000	1.596063000	4.119901000
1	0.992890000	0.898628000	4.421602000
1	-0.358215000	-0.180289000	-1.856351000
1	-0.089045000	-0.984977000	-1.363098000

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**A6<sub>X=CHCHMe</sub>**



-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.027668000	0.361903000	0.064885000
1	-0.394022000	1.158751000	-1.298903000
7	0.323877000	-1.351961000	-1.173389000
1	0.117249000	-0.986999000	-2.099258000
6	-0.185930000	1.872677000	0.960857000
8	-0.304922000	2.884447000	1.521634000
6	-2.031509000	-1.906824000	-0.859797000
6	1.736259000	-1.710272000	-1.080422000
6	-0.602570000	-2.436558000	-0.845375000
1	-2.732434000	-2.699815000	-0.589329000
1	-2.286694000	-1.540362000	-1.858576000
1	-0.521521000	-3.277510000	-1.550724000
1	-0.338105000	-2.795496000	0.154414000
1	2.067264000	-2.370388000	-1.894230000
1	1.874227000	-2.230292000	-0.125460000
6	2.570987000	-0.456119000	-1.034263000
6	3.889111000	-0.422681000	-1.478196000
1	4.330411000	-1.309246000	-1.921390000
6	2.683517000	1.751930000	-0.360034000
1	2.159513000	2.590371000	0.082840000
6	4.620750000	0.751291000	-1.339491000
1	5.651639000	0.800529000	-1.675301000
6	4.006411000	1.859711000	-0.766801000
1	4.533535000	2.797688000	-0.637409000
7	1.978827000	0.621102000	-0.488141000
16	-2.165969000	-0.526686000	0.333716000
6	-3.598719000	0.466716000	-0.318505000
6	-3.716138000	1.643400000	0.656515000
6	-4.853896000	-0.409489000	-0.252620000
1	-2.845889000	2.300600000	0.593200000
1	-4.605765000	2.229256000	0.400302000
1	-3.820979000	1.301148000	1.690933000
1	-4.789502000	-1.262089000	-0.936835000
1	-5.025059000	-0.787263000	0.759826000
1	-5.725058000	0.184801000	-0.551035000
6	-3.365822000	0.983003000	-1.737026000
1	-4.176863000	1.672029000	-1.999506000
1	-2.408289000	1.504918000	-1.806897000
1	-3.376785000	0.176138000	-2.477393000
6	0.588876000	-0.706158000	1.736727000
1	-0.230139000	-1.052211000	2.389371000
6	1.798077000	-0.997677000	2.246545000

1	2.706146000	-0.677230000	1.720487000
6	2.073066000	-1.715546000	3.546947000
1	2.652247000	-2.636446000	3.392065000
1	2.656311000	-1.089379000	4.235129000
1	1.137985000	-1.986096000	4.049376000

**A7R<sub>X=CHCHMe</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	0.854044000	0.592413000	0.447943000
1	0.140293000	-0.969479000	0.686530000
7	0.483628000	0.337788000	-1.684523000
1	0.015439000	-0.561348000	-1.781099000
6	1.121025000	0.910516000	2.124463000
8	1.312064000	1.210804000	3.262666000
6	2.680104000	-0.710489000	-1.887924000
6	-0.447682000	1.380682000	-2.103358000
6	1.712527000	0.302780000	-2.479653000
1	3.610462000	-0.725671000	-2.461169000
1	2.232687000	-1.708106000	-1.919191000
1	1.514101000	0.039542000	-3.529462000
1	2.153558000	1.304563000	-2.461100000
1	-0.976229000	1.129378000	-3.032993000
1	0.130074000	2.293556000	-2.283854000
6	-1.430746000	1.672272000	-1.002000000
6	-2.658097000	2.276609000	-1.268264000
1	-2.934357000	2.486090000	-2.297408000
6	-1.864154000	1.673045000	1.260388000
1	-1.516682000	1.402963000	2.251624000
6	-3.501994000	2.606684000	-0.215398000
1	-4.459082000	3.085403000	-0.398174000
6	-3.093671000	2.289615000	1.078261000
1	-3.716286000	2.508183000	1.939399000
7	-1.025324000	1.377812000	0.250418000
16	3.006059000	-0.247417000	-0.148226000
6	3.669945000	-1.829497000	0.573945000
6	3.921649000	-1.499233000	2.048264000
6	4.984250000	-2.183804000	-0.126293000
1	2.986667000	-1.244427000	2.556983000
1	4.359964000	-2.371696000	2.546761000
1	4.616741000	-0.659744000	2.161617000
1	4.827256000	-2.414118000	-1.185446000
1	5.710636000	-1.367328000	-0.055511000

1	5.423509000	-3.072434000	0.343589000
6	2.680715000	-2.988256000	0.467373000
1	3.092772000	-3.860672000	0.989592000
1	1.722492000	-2.725981000	0.921293000
1	2.501083000	-3.284292000	-0.570874000
6	-1.689357000	-2.568035000	-1.150821000
8	-1.474234000	-1.983761000	-2.208509000
6	-2.808008000	-2.125166000	-0.261322000
6	-3.022651000	-2.705035000	0.994920000
6	-3.673651000	-1.120551000	-0.709822000
6	-4.087063000	-2.286384000	1.788988000
1	-2.356232000	-3.476693000	1.365370000
6	-4.742457000	-0.709436000	0.079820000
1	-3.499905000	-0.668775000	-1.680997000
6	-4.950414000	-1.291442000	1.331016000
1	-4.241627000	-2.737200000	2.764536000
1	-5.412094000	0.067137000	-0.276728000
1	-5.782421000	-0.967464000	1.949658000
6	-0.875392000	-3.772527000	-0.762058000
1	-0.096319000	-3.936489000	-1.507622000
1	-0.414626000	-3.633573000	0.219485000
1	-1.520632000	-4.656892000	-0.707496000
6	1.649517000	2.483959000	0.041633000
1	2.735578000	2.556283000	-0.192602000
6	1.102330000	3.720890000	0.097706000
1	0.032749000	3.822060000	0.328473000
6	1.794051000	5.047932000	-0.137100000
1	1.360465000	5.596576000	-0.986672000
1	1.714389000	5.717725000	0.731877000
1	2.862077000	4.904967000	-0.346441000

A7S<sub>X</sub>=CHCHMe

Coordinates (Angstroms)

	X	Y	Z
25	-0.976475000	0.710260000	0.462782000
1	0.331278000	-0.272923000	1.036372000
7	-0.571397000	-0.186651000	-1.476745000
1	0.188229000	-0.843272000	-1.320360000
6	-1.413431000	1.419158000	1.978333000
8	-1.795386000	1.927949000	2.987671000
6	1.011551000	1.614224000	-1.923797000
6	-1.750727000	-0.955210000	-1.863860000
6	-0.137673000	0.786234000	-2.479146000

1	1.325605000	2.362263000	-2.655975000
1	1.861972000	0.961622000	-1.703192000
1	0.191971000	0.297876000	-3.408803000
1	-0.991750000	1.428370000	-2.717912000
1	-1.533799000	-1.704617000	-2.635816000
1	-2.488639000	-0.250846000	-2.262526000
6	-2.348087000	-1.609789000	-0.648101000
6	-3.078149000	-2.793260000	-0.734267000
1	-3.180020000	-3.287134000	-1.695775000
6	-2.731456000	-1.480876000	1.621882000
1	-2.559177000	-0.934062000	2.542711000
6	-3.659648000	-3.325242000	0.410697000
1	-4.230421000	-4.247710000	0.366284000
6	-3.482792000	-2.647982000	1.615585000
1	-3.911075000	-3.017023000	2.541514000
7	-2.165673000	-0.957539000	0.519405000
16	0.464324000	2.422814000	-0.375095000
6	2.083301000	2.810851000	0.457805000
6	1.687697000	3.569472000	1.728552000
6	2.917498000	3.711188000	-0.458004000
1	1.061239000	2.949043000	2.377659000
1	2.591798000	3.844424000	2.284401000
1	1.140313000	4.489693000	1.495336000
1	3.242959000	3.181939000	-1.359871000
1	2.359438000	4.603080000	-0.762892000
1	3.818568000	4.038965000	0.074735000
6	2.870397000	1.554795000	0.826615000
1	3.808528000	1.849621000	1.313679000
1	2.301647000	0.921718000	1.509244000
1	3.129410000	0.956920000	-0.051794000
6	1.235588000	-2.916856000	-0.144552000
8	0.642484000	-2.952264000	-1.217263000
6	2.606314000	-2.314436000	-0.071980000
6	3.313750000	-2.222481000	1.131833000
6	3.191853000	-1.831467000	-1.249174000
6	4.587759000	-1.659643000	1.156698000
1	2.872479000	-2.580492000	2.056147000
6	4.464688000	-1.271085000	-1.224918000
1	2.638719000	-1.899799000	-2.180609000
6	5.165469000	-1.185531000	-0.020568000
1	5.125198000	-1.584422000	2.097065000
1	4.909340000	-0.895150000	-2.141560000
1	6.156271000	-0.741244000	0.001314000
6	0.615443000	-3.503200000	1.093992000

1	-0.403414000	-3.821626000	0.866744000
1	1.201173000	-4.365516000	1.433488000
1	0.594641000	-2.769244000	1.903253000
6	-2.521253000	1.812218000	-0.400408000
1	-2.302473000	2.877859000	-0.635492000
6	-3.815670000	1.532477000	-0.679520000
1	-4.198282000	0.519409000	-0.493665000
6	-4.857381000	2.476920000	-1.243583000
1	-4.429377000	3.471532000	-1.423757000
1	-5.273776000	2.116340000	-2.196221000
1	-5.713418000	2.603863000	-0.564337000

**TSA7-8R<sub>X=CHCHMe</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	0.657156000	0.503468000	0.369217000
1	0.145173000	-1.168042000	0.109931000
7	0.451514000	0.574913000	-1.757206000
1	0.057902000	-0.348219000	-1.966571000
6	0.734334000	0.357882000	2.091900000
8	0.775828000	0.283808000	3.281716000
6	2.738203000	-0.252626000	-1.952375000
6	-0.562480000	1.567945000	-2.092235000
6	1.703282000	0.722064000	-2.500582000
1	3.684854000	-0.140434000	-2.487194000
1	2.383760000	-1.281860000	-2.066433000
1	1.563801000	0.535148000	-3.575775000
1	2.056106000	1.752777000	-2.380506000
1	-0.998268000	1.412894000	-3.089320000
1	-0.087865000	2.555642000	-2.081309000
6	-1.641306000	1.562064000	-1.042310000
6	-2.917161000	2.056752000	-1.304105000
1	-3.161503000	2.394924000	-2.306698000
6	-2.195557000	1.156457000	1.158782000
1	-1.873227000	0.774047000	2.120856000
6	-3.850729000	2.121279000	-0.276635000
1	-4.847654000	2.512303000	-0.455251000
6	-3.476840000	1.659870000	0.983244000
1	-4.168203000	1.672911000	1.819036000
7	-1.277355000	1.113598000	0.177205000
16	2.951879000	0.128556000	-0.179026000
6	3.881327000	-1.337658000	0.479765000
6	4.204376000	-0.958449000	1.929054000

6	5.172774000	-1.536245000	-0.316466000
1	3.289279000	-0.773971000	2.500796000
1	4.747540000	-1.781191000	2.408514000
1	4.830672000	-0.060946000	1.981321000
1	4.970249000	-1.840290000	-1.348688000
1	5.776094000	-0.622161000	-0.337811000
1	5.770165000	-2.328545000	0.150811000
6	3.027474000	-2.600672000	0.452797000
1	3.573439000	-3.425879000	0.927008000
1	2.087713000	-2.438343000	0.987035000
1	2.791356000	-2.902567000	-0.571913000
6	-1.009779000	-2.355118000	-1.017148000
8	-0.912462000	-1.899947000	-2.171499000
6	-2.269036000	-2.087755000	-0.228396000
6	-2.380610000	-2.371991000	1.137443000
6	-3.391016000	-1.616067000	-0.914552000
6	-3.593498000	-2.198721000	1.797898000
1	-1.510256000	-2.703106000	1.695473000
6	-4.608266000	-1.445881000	-0.256227000
1	-3.298660000	-1.392810000	-1.972726000
6	-4.714463000	-1.741403000	1.101412000
1	-3.664016000	-2.413689000	2.860427000
1	-5.471905000	-1.078622000	-0.803518000
1	-5.660792000	-1.607321000	1.617686000
6	-0.212546000	-3.585714000	-0.642867000
1	0.743603000	-3.573678000	-1.167183000
1	-0.038594000	-3.688512000	0.428537000
1	-0.785022000	-4.460436000	-0.983027000
6	1.216580000	2.505614000	0.483755000
1	2.296543000	2.704572000	0.658339000
6	0.529173000	3.672144000	0.455966000
1	-0.557713000	3.654532000	0.299003000
6	1.090799000	5.070296000	0.615913000
1	2.177324000	5.044412000	0.769803000
1	0.895211000	5.699173000	-0.265506000
1	0.647683000	5.598828000	1.472933000

**TSA7-8S<sub>X=CHCHMe</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	-0.824952000	0.567672000	0.370181000
1	0.445027000	-0.672234000	0.469264000
7	-0.800297000	-0.076860000	-1.665917000

1	-0.176420000	-0.888340000	-1.616469000
6	-0.824425000	0.989596000	2.048141000
8	-0.875862000	1.305582000	3.196884000
6	1.045466000	1.464268000	-2.056737000
6	-2.121728000	-0.587195000	-2.007564000
6	-0.244531000	0.880522000	-2.620766000
1	1.466999000	2.193838000	-2.753195000
1	1.779356000	0.669443000	-1.885119000
1	-0.035160000	0.412517000	-3.594253000
1	-0.982132000	1.675325000	-2.781822000
1	-2.112471000	-1.240608000	-2.891187000
1	-2.774599000	0.266736000	-2.222715000
6	-2.682689000	-1.319544000	-0.817786000
6	-3.638873000	-2.323341000	-0.955435000
1	-3.949427000	-2.630855000	-1.949401000
6	-2.772897000	-1.479593000	1.481438000
1	-2.391823000	-1.122808000	2.431987000
6	-4.185218000	-2.909419000	0.180963000
1	-4.936120000	-3.688970000	0.097335000
6	-3.743967000	-2.469779000	1.427176000
1	-4.136886000	-2.888683000	2.347514000
7	-2.238664000	-0.906443000	0.388544000
16	0.629002000	2.258737000	-0.464736000
6	2.285329000	2.556395000	0.325522000
6	1.989200000	3.524511000	1.475721000
6	3.239719000	3.203739000	-0.679897000
1	1.256575000	3.100773000	2.171164000
1	2.913041000	3.719924000	2.032809000
1	1.603000000	4.481216000	1.107657000
1	3.516333000	2.509454000	-1.479836000
1	2.804546000	4.101338000	-1.132525000
1	4.162026000	3.497432000	-0.164201000
6	2.878986000	1.262665000	0.871911000
1	3.846067000	1.474328000	1.345692000
1	2.214260000	0.809543000	1.611017000
1	3.044102000	0.530549000	0.077881000
6	0.940042000	-2.479710000	-0.152761000
8	0.458794000	-2.585665000	-1.297050000
6	2.408130000	-2.154185000	-0.017809000
6	3.074051000	-2.166117000	1.212772000
6	3.140882000	-1.880741000	-1.177984000
6	4.440147000	-1.900755000	1.280872000
1	2.528777000	-2.363700000	2.129970000
6	4.505798000	-1.609574000	-1.111670000

1	2.623371000	-1.883417000	-2.132188000
6	5.161169000	-1.618615000	0.119974000
1	4.941408000	-1.907587000	2.244567000
1	5.058363000	-1.393985000	-2.022060000
1	6.225481000	-1.408740000	0.176190000
6	0.254664000	-3.186507000	0.996147000
1	-0.812637000	-3.254501000	0.781444000
1	0.663037000	-4.204811000	1.060252000
1	0.395749000	-2.694912000	1.959250000
6	-2.328919000	1.959321000	0.062753000
1	-2.018482000	3.027143000	0.069944000
6	-3.671703000	1.866146000	-0.085263000
1	-4.143940000	0.875119000	-0.104395000
6	-4.659742000	3.004838000	-0.237365000
1	-5.200420000	2.959612000	-1.194529000
1	-5.428415000	2.993290000	0.549285000
1	-4.152905000	3.977198000	-0.189238000

**A8R<sub>X=CHCHMe</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	-0.943481000	0.724698000	-0.092338000
1	0.702358000	-1.427764000	-1.016036000
7	-0.239779000	0.021584000	1.615292000
1	0.331316000	-1.524898000	1.095556000
6	-1.197469000	0.691904000	-1.807081000
8	-1.294559000	0.600976000	-2.994684000
6	-2.252516000	-1.245229000	2.085070000
6	0.928544000	0.696687000	2.124548000
6	-1.139464000	-0.387963000	2.674248000
1	-3.047290000	-1.433317000	2.811120000
1	-1.839878000	-2.200866000	1.751363000
1	-0.627624000	-0.989310000	3.449150000
1	-1.574989000	0.483833000	3.200539000
1	1.632797000	0.025399000	2.652142000
1	0.656346000	1.478623000	2.861149000
6	1.650193000	1.379175000	0.996826000
6	2.950931000	1.868888000	1.123396000
1	3.486420000	1.719592000	2.055981000
6	1.515430000	2.171125000	-1.170383000
1	0.909104000	2.266557000	-2.064633000
6	3.534805000	2.539243000	0.058787000
1	4.545860000	2.927317000	0.136079000



6	2.796564000	2.695635000	-1.114760000
1	3.207371000	3.207249000	-1.978498000
7	0.941765000	1.518016000	-0.141361000
16	-2.923069000	-0.365326000	0.624896000
6	-3.536488000	-1.767276000	-0.435819000
6	-4.320551000	-1.096952000	-1.567620000
6	-4.464306000	-2.667151000	0.383980000
1	-3.692247000	-0.398555000	-2.128280000
1	-4.679298000	-1.863841000	-2.264377000
1	-5.190522000	-0.553341000	-1.183696000
1	-3.926478000	-3.195847000	1.177375000
1	-5.279463000	-2.095399000	0.840272000
1	-4.907679000	-3.423167000	-0.275393000
6	-2.364933000	-2.568572000	-1.002867000
1	-2.748072000	-3.408267000	-1.596290000
1	-1.744152000	-1.939931000	-1.646697000
1	-1.723066000	-2.971667000	-0.214112000
6	1.284646000	-2.185388000	-0.461278000
8	0.681824000	-2.417486000	0.787053000
6	2.706143000	-1.652724000	-0.321118000
6	3.319326000	-0.989285000	-1.389150000
6	3.431396000	-1.842383000	0.857231000
6	4.632409000	-0.534442000	-1.286009000
1	2.758896000	-0.817662000	-2.305948000
6	4.745984000	-1.386663000	0.965675000
1	2.949769000	-2.339843000	1.693446000
6	5.352581000	-0.733802000	-0.106819000
1	5.090658000	-0.013666000	-2.122407000
1	5.294100000	-1.537867000	1.891900000
1	6.373490000	-0.371967000	-0.021941000
6	1.270672000	-3.483980000	-1.264184000
1	0.241342000	-3.828230000	-1.405977000
1	1.728260000	-3.342335000	-2.248709000
1	1.828808000	-4.263964000	-0.733111000
6	-1.748721000	2.501931000	0.273646000
1	-1.628805000	2.761198000	1.352851000
6	-2.386166000	3.490216000	-0.394800000
1	-2.572917000	3.365489000	-1.468834000
6	-2.894790000	4.797022000	0.175091000
1	-2.417983000	5.667687000	-0.298249000
1	-3.976997000	4.920958000	0.024890000
1	-2.700650000	4.860333000	1.253376000

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**A8S**<sub>X=CHCHMe</sub>

-----  
Coordinates (Angstroms)  
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	X	Y	Z
25	1.179105000	0.459207000	-0.173075000
1	-0.917357000	-1.098995000	-0.366845000
7	0.980399000	-0.111514000	1.725568000
1	-0.447627000	-1.000809000	1.655116000
6	0.832118000	0.640317000	-1.863193000
8	0.553314000	0.718716000	-3.021479000
6	-0.281934000	1.868802000	2.300051000
6	1.931459000	-1.125427000	2.114574000
6	0.774710000	0.874846000	2.763014000
1	-0.384788000	2.704747000	2.996508000
1	-1.245399000	1.359642000	2.202930000
1	0.423388000	0.422544000	3.709601000
1	1.711228000	1.414252000	3.008308000
1	1.587709000	-1.759570000	2.952810000
1	2.888914000	-0.677298000	2.450203000
6	2.226083000	-1.995171000	0.925367000
6	2.738276000	-3.288092000	1.035106000
1	2.924311000	-3.706687000	2.019411000
6	2.211091000	-2.147329000	-1.381703000
1	1.984042000	-1.656975000	-2.322033000
6	2.994969000	-4.021074000	-0.116487000
1	3.392959000	-5.029253000	-0.053367000
6	2.724982000	-3.435043000	-1.352818000
1	2.904133000	-3.963790000	-2.282836000
7	1.959433000	-1.431098000	-0.270744000
16	0.231197000	2.472283000	0.649946000
6	-1.377328000	3.033359000	-0.099645000
6	-0.981106000	3.769876000	-1.382677000
6	-2.090402000	3.987879000	0.860148000
1	-0.408566000	3.120587000	-2.052114000
1	-1.886280000	4.091801000	-1.910771000
1	-0.380188000	4.659289000	-1.164030000
1	-2.426428000	3.476058000	1.767494000
1	-1.443724000	4.822504000	1.151466000
1	-2.977888000	4.401485000	0.366323000
6	-2.264622000	1.835297000	-0.430072000
1	-3.198562000	2.181948000	-0.889902000
1	-1.762875000	1.160527000	-1.128006000
1	-2.529374000	1.263893000	0.464594000
6	-1.532882000	-1.794504000	0.234076000
8	-1.277768000	-1.581935000	1.598177000
6	-2.986040000	-1.508497000	-0.107705000

6	-3.369000000	-1.359072000	-1.446160000
6	-3.959118000	-1.382559000	0.885126000
6	-4.692467000	-1.087466000	-1.785181000
1	-2.616728000	-1.435222000	-2.228545000
6	-5.288179000	-1.114191000	0.549787000
1	-3.663917000	-1.481210000	1.924802000
6	-5.660196000	-0.963858000	-0.785599000
1	-4.967209000	-0.961740000	-2.828986000
1	-6.033473000	-1.017503000	1.334967000
1	-6.692788000	-0.748825000	-1.045766000
6	-1.147557000	-3.221878000	-0.169611000
1	-0.090882000	-3.398446000	0.055260000
1	-1.747610000	-3.948264000	0.390933000
1	-1.305697000	-3.392828000	-1.240172000
6	2.980978000	1.296209000	-0.229382000
1	3.385005000	1.468457000	0.796855000
6	3.872731000	1.670579000	-1.175444000
1	3.597153000	1.554982000	-2.231238000
6	5.256816000	2.242549000	-0.954975000
1	6.042213000	1.597193000	-1.374733000
1	5.378725000	3.225609000	-1.432447000
1	5.467332000	2.365915000	0.115030000

**Al<sub>X=NCMe</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	-0.201415000	0.020669000	0.084955000
7	-0.513589000	-1.689973000	-0.635002000
6	0.060982000	0.443342000	1.756305000
8	0.167678000	0.602271000	2.922077000
6	1.850590000	-2.238564000	-0.601481000
6	-1.864599000	-2.169827000	-0.774782000
6	0.476768000	-2.618255000	-1.144711000
1	2.660187000	-2.724144000	-1.152898000
1	1.911186000	-2.511092000	0.454491000
1	0.266141000	-3.656141000	-0.833697000
1	0.497079000	-2.623346000	-2.249628000
1	-2.037448000	-3.116565000	-0.229785000
1	-2.127750000	-2.382129000	-1.827437000
6	-2.814914000	-1.132788000	-0.248476000
6	-4.199522000	-1.307404000	-0.231525000
1	-4.625863000	-2.229951000	-0.612978000
6	-3.023636000	0.969321000	0.702406000

1	-2.509669000	1.852106000	1.068451000
6	-5.006251000	-0.296989000	0.271636000
1	-6.085312000	-0.413308000	0.295734000
6	-4.404253000	0.868299000	0.749776000
1	-4.992172000	1.684152000	1.155681000
7	-2.237328000	-0.007449000	0.212509000
16	1.977227000	-0.423414000	-0.722041000
6	3.469881000	0.009511000	0.299111000
6	3.404379000	1.531340000	0.457258000
6	4.725682000	-0.395158000	-0.476598000
1	2.520798000	1.833085000	1.027945000
1	4.296377000	1.876317000	0.992129000
1	3.377836000	2.037203000	-0.514351000
1	4.757138000	-1.475245000	-0.655037000
1	4.781938000	0.117471000	-1.442097000
1	5.616718000	-0.127583000	0.104296000
6	3.446770000	-0.668515000	1.668312000
1	4.248061000	-0.246479000	2.286212000
1	2.496728000	-0.505561000	2.183364000
1	3.625137000	-1.745281000	1.593136000
6	-0.183846000	2.916879000	-1.121104000
6	-0.193007000	4.235955000	-1.734395000
1	-1.219836000	4.519237000	-1.978867000
1	0.226661000	4.969785000	-1.041666000
1	0.402324000	4.223159000	-2.650802000
7	-0.177380000	1.869017000	-0.627567000

**A2**<sub>X=NCMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	-0.098128000	-0.399891000	0.087938000
7	-0.441443000	0.963910000	-1.426960000
6	0.150806000	-1.623603000	1.337046000
8	0.307206000	-2.430689000	2.177058000
6	1.915303000	1.528459000	-1.468007000
6	-1.800511000	1.426384000	-1.357297000
6	0.487360000	2.058841000	-1.504193000
1	2.652256000	2.335330000	-1.469033000
1	2.093045000	0.874958000	-2.327475000
1	0.376376000	2.645859000	-2.436779000
1	0.359268000	2.792726000	-0.674128000
1	-2.174005000	1.869878000	-2.299482000
1	-1.944973000	2.221115000	-0.587169000

6	-2.697780000	0.282759000	-0.967699000
6	-4.055427000	0.234177000	-1.287049000
1	-4.495678000	1.040337000	-1.865439000
6	-2.849530000	-1.741703000	0.147523000
1	-2.329100000	-2.508331000	0.711862000
6	-4.820767000	-0.844337000	-0.862813000
1	-5.878531000	-0.899831000	-1.101297000
6	-4.203391000	-1.857036000	-0.130154000
1	-4.754679000	-2.722457000	0.220557000
7	-2.105709000	-0.698164000	-0.256132000
16	2.077831000	0.546286000	0.067134000
6	3.528064000	-0.568806000	-0.268585000
6	3.843093000	-1.226740000	1.077908000
6	4.713905000	0.282248000	-0.729294000
1	2.981126000	-1.779561000	1.463983000
1	4.668109000	-1.936659000	0.949394000
1	4.144697000	-0.485984000	1.825662000
1	4.542998000	0.721786000	-1.716956000
1	4.926990000	1.089496000	-0.020880000
1	5.605172000	-0.352362000	-0.798969000
6	3.196497000	-1.638217000	-1.308328000
1	4.104794000	-2.208678000	-1.536754000
1	2.443282000	-2.335737000	-0.932462000
1	2.831144000	-1.204613000	-2.244624000
6	-0.864357000	1.834049000	2.193847000
6	-1.215802000	2.877308000	3.143865000
1	-1.922764000	3.571229000	2.682496000
1	-1.673683000	2.431763000	4.030095000
1	-0.315953000	3.422674000	3.438732000
7	-0.584661000	1.010524000	1.432882000
1	0.240795000	-1.783906000	-0.923814000
1	0.227463000	-1.173411000	-1.425732000

A3<sub>X=NCMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	-1.150035000	0.586992000	-0.437793000
1	-0.755089000	-0.684005000	-1.535019000
7	-0.140547000	-0.101192000	1.238196000
6	-1.932065000	1.182833000	-1.906053000
8	-2.438227000	1.609608000	-2.875136000
6	-2.126421000	-1.325953000	1.907513000
6	0.881396000	0.851236000	1.602676000

6	-0.971426000	-0.447443000	2.370349000
1	-2.798978000	-1.579507000	2.730422000
1	-1.740634000	-2.245025000	1.457154000
1	-0.411041000	-1.007288000	3.142386000
1	-1.379443000	0.450112000	2.877980000
1	1.673049000	0.420697000	2.241088000
1	0.469926000	1.707741000	2.174590000
6	1.510563000	1.402230000	0.353303000
6	2.788411000	1.960502000	0.334958000
1	3.369933000	1.986211000	1.250822000
6	1.256255000	1.806830000	-1.910937000
1	0.613401000	1.728138000	-2.781193000
6	3.300769000	2.454997000	-0.855622000
1	4.295357000	2.888554000	-0.891436000
6	2.520215000	2.368569000	-2.007801000
1	2.879061000	2.730680000	-2.964917000
7	0.749658000	1.338874000	-0.757797000
16	-3.035390000	-0.378240000	0.633633000
6	-3.999269000	-1.675918000	-0.287269000
6	-4.960058000	-0.887991000	-1.182792000
6	-4.785875000	-2.521252000	0.717756000
1	-4.416494000	-0.227891000	-1.865853000
1	-5.549965000	-1.587114000	-1.786356000
1	-5.652393000	-0.280670000	-0.590529000
1	-4.126761000	-3.136269000	1.338455000
1	-5.402377000	-1.898080000	1.374032000
1	-5.450823000	-3.198082000	0.168866000
6	-3.092690000	-2.561882000	-1.140190000
1	-3.697449000	-3.354111000	-1.597291000
1	-2.619871000	-1.988987000	-1.941881000
1	-2.308108000	-3.042393000	-0.547016000
1	-0.681601000	-1.028994000	-0.824387000
1	1.489571000	-1.490725000	-1.287991000
1	0.573850000	-1.459560000	0.790084000
6	1.893535000	-2.190657000	-0.536514000
8	0.972606000	-2.370591000	0.502232000
6	3.219861000	-1.597287000	-0.067824000
6	4.143045000	-1.123651000	-1.008175000
6	3.540926000	-1.509490000	1.287281000
6	5.356536000	-0.572514000	-0.604116000
1	3.901869000	-1.173383000	-2.068222000
6	4.753859000	-0.952790000	1.698008000
1	2.822842000	-1.867311000	2.018747000
6	5.666166000	-0.482119000	0.754945000

1	6.057641000	-0.203161000	-1.347708000
1	4.982828000	-0.882472000	2.758134000
1	6.607910000	-0.044615000	1.074036000
6	2.114233000	-3.539366000	-1.220591000
1	1.165686000	-3.915147000	-1.618061000
1	2.829006000	-3.457690000	-2.045886000
1	2.501586000	-4.267437000	-0.498520000
7	-1.571163000	2.285654000	0.549850000
6	-1.808817000	3.268214000	1.109241000
6	-2.096213000	4.503402000	1.820439000
1	-3.176184000	4.663485000	1.861915000
1	-1.701084000	4.439625000	2.837313000
1	-1.626385000	5.343210000	1.302934000

**TSA3-4<sub>X=NCMe</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	1.140042000	0.593363000	0.430109000
1	0.741558000	-0.660060000	1.540945000
7	0.121842000	-0.110282000	-1.243379000
6	1.927105000	1.199845000	1.892481000
8	2.435599000	1.629020000	2.857423000
6	2.108006000	-1.352961000	-1.889664000
6	-0.900961000	0.849718000	-1.613550000
6	0.963415000	-0.472632000	-2.372463000
1	2.778622000	-1.623212000	-2.708499000
1	1.709742000	-2.261326000	-1.428952000
1	0.399146000	-1.033270000	-3.137260000
1	1.369477000	0.424008000	-2.870793000
1	-1.689808000	0.410484000	-2.244963000
1	-0.472808000	1.687824000	-2.189432000
6	-1.522863000	1.410258000	-0.364415000
6	-2.803527000	1.960884000	-0.346344000
1	-3.390528000	1.972073000	-1.258947000
6	-1.258867000	1.835711000	1.893824000
1	-0.612493000	1.766457000	2.762135000
6	-3.312169000	2.463712000	0.842552000
1	-4.309114000	2.891528000	0.879721000
6	-2.524822000	2.392908000	1.990897000
1	-2.880774000	2.762062000	2.946334000
7	-0.755882000	1.359075000	0.742790000
16	3.024119000	-0.397981000	-0.626012000
6	3.972149000	-1.695527000	0.312380000

6	4.936156000	-0.905982000	1.202910000
6	4.755052000	-2.556277000	-0.682367000
1	4.395722000	-0.236442000	1.879194000
1	5.519809000	-1.604062000	1.813605000
1	5.634076000	-0.308583000	0.607164000
1	4.093196000	-3.172215000	-1.299158000
1	5.378162000	-1.943777000	-1.342403000
1	5.413131000	-3.232568000	-0.124729000
6	3.055304000	-2.565725000	1.170510000
1	3.651809000	-3.361149000	1.632783000
1	2.588731000	-1.983124000	1.968819000
1	2.265531000	-3.041998000	0.580927000
1	0.665931000	-1.019460000	0.836477000
1	-1.477336000	-1.434039000	1.283078000
1	-0.471588000	-1.210016000	-0.857847000
6	-1.843237000	-2.137912000	0.508722000
8	-0.934067000	-2.253738000	-0.528736000
6	-3.202878000	-1.585533000	0.073035000
6	-4.119534000	-1.126837000	1.027255000
6	-3.556835000	-1.519679000	-1.275194000
6	-5.355575000	-0.610903000	0.644740000
1	-3.854022000	-1.157850000	2.082533000
6	-4.793453000	-1.001775000	-1.665920000
1	-2.839148000	-1.863752000	-2.013979000
6	-5.697802000	-0.544332000	-0.708178000
1	-6.049897000	-0.250765000	1.399397000
1	-5.047736000	-0.949834000	-2.721576000
1	-6.657646000	-0.135070000	-1.010809000
6	-2.026608000	-3.499304000	1.191678000
1	-1.062940000	-3.851825000	1.575517000
1	-2.735429000	-3.448572000	2.026202000
1	-2.398030000	-4.233028000	0.466183000
7	1.577856000	2.277939000	-0.574701000
6	1.847889000	3.251938000	-1.134300000
6	2.189238000	4.475838000	-1.840855000
1	1.425479000	4.692830000	-2.591361000
1	2.245464000	5.304852000	-1.131455000
1	3.156707000	4.355535000	-2.334236000

**A4**<sub>X=NCMe</sub>

Coordinates (Angstroms)			
	X	Y	Z
25	1.079462000	0.650714000	0.429432000



1	0.592449000	-0.648055000	1.443726000
7	0.110252000	0.080804000	-1.344602000
6	1.829138000	1.148064000	1.951024000
8	2.319159000	1.507557000	2.951324000
6	2.073537000	-1.200930000	-1.959631000
6	-0.914576000	1.065939000	-1.670051000
6	1.003642000	-0.240360000	-2.456959000
1	2.772323000	-1.458570000	-2.758030000
1	1.597656000	-2.107611000	-1.574341000
1	0.458505000	-0.716517000	-3.284860000
1	1.456489000	0.681652000	-2.842612000
1	-1.676055000	0.670479000	-2.355242000
1	-0.446484000	1.926877000	-2.164580000
6	-1.563305000	1.532473000	-0.394341000
6	-2.854614000	2.052713000	-0.366941000
1	-3.426055000	2.109099000	-1.287366000
6	-1.344859000	1.821936000	1.888885000
1	-0.713835000	1.708269000	2.763515000
6	-3.393511000	2.470906000	0.842017000
1	-4.400412000	2.873652000	0.887387000
6	-2.623866000	2.346994000	1.996633000
1	-3.003486000	2.647685000	2.966729000
7	-0.812896000	1.427256000	0.720494000
16	2.968495000	-0.377754000	-0.590618000
6	3.760456000	-1.799872000	0.314719000
6	4.749916000	-1.149443000	1.285314000
6	4.509597000	-2.672311000	-0.696230000
1	4.245345000	-0.457558000	1.967198000
1	5.223848000	-1.930725000	1.890233000
1	5.538362000	-0.604679000	0.755441000
1	3.824148000	-3.223492000	-1.347072000
1	5.183936000	-2.077520000	-1.321288000
1	5.111858000	-3.408732000	-0.152071000
6	2.730522000	-2.625741000	1.085331000
1	3.216054000	-3.530689000	1.469763000
1	2.336986000	-2.064967000	1.937512000
1	1.884440000	-2.927834000	0.459033000
1	0.476427000	-0.981594000	0.728401000
1	-1.393790000	-1.857471000	1.442806000
1	-0.349728000	-0.834483000	-1.041300000
6	-1.678133000	-2.367925000	0.487536000
8	-0.693542000	-2.284405000	-0.452493000
6	-2.995937000	-1.696335000	0.069099000
6	-3.930644000	-1.273870000	1.021870000

6	-3.299189000	-1.511169000	-1.281849000
6	-5.139309000	-0.694305000	0.637721000
1	-3.704712000	-1.394325000	2.080249000
6	-4.506385000	-0.931557000	-1.675264000
1	-2.561262000	-1.819819000	-2.017306000
6	-5.433590000	-0.521661000	-0.716372000
1	-5.847939000	-0.365991000	1.393744000
1	-4.721135000	-0.792155000	-2.731996000
1	-6.371201000	-0.063751000	-1.019303000
6	-1.976706000	-3.833042000	0.872828000
1	-1.054479000	-4.308971000	1.225521000
1	-2.734482000	-3.915582000	1.663005000
1	-2.331670000	-4.382804000	-0.008138000
7	1.615083000	2.362285000	-0.461760000
6	1.934068000	3.359503000	-0.950630000
6	2.335828000	4.613901000	-1.565412000
1	1.589515000	4.916547000	-2.303610000
1	2.418758000	5.387376000	-0.798033000
1	3.302667000	4.487397000	-2.058390000

**TSA4-5<sub>X</sub>=NCMe**

Coordinates (Angstroms)			
	X	Y	Z
25	1.039515000	0.633379000	0.442009000
1	0.565919000	-0.806311000	1.244268000
7	0.081153000	0.146702000	-1.383424000
6	1.750946000	0.993186000	2.010152000
8	2.213795000	1.222508000	3.064698000
6	2.045571000	-1.137030000	-2.008612000
6	-0.925707000	1.161610000	-1.676296000
6	0.978099000	-0.167257000	-2.496753000
1	2.742386000	-1.383119000	-2.812545000
1	1.574385000	-2.052914000	-1.639425000
1	0.435729000	-0.625343000	-3.335858000
1	1.435150000	0.760389000	-2.861041000
1	-1.678795000	0.813977000	-2.395345000
1	-0.431441000	2.036915000	-2.115082000
6	-1.592021000	1.565598000	-0.386954000
6	-2.882480000	2.087782000	-0.356347000
1	-3.436029000	2.196505000	-1.283079000
6	-1.412404000	1.735576000	1.910220000
1	-0.797561000	1.572451000	2.788593000
6	-3.441508000	2.445361000	0.863256000

1	-4.447898000	2.849105000	0.911844000
6	-2.692453000	2.258370000	2.022625000
1	-3.088953000	2.507943000	3.000478000
7	-0.860095000	1.399349000	0.733144000
16	2.937501000	-0.330795000	-0.629532000
6	3.798957000	-1.746247000	0.219011000
6	4.788197000	-1.080566000	1.180159000
6	4.553716000	-2.571445000	-0.826364000
1	4.274723000	-0.426371000	1.891874000
1	5.310024000	-1.856395000	1.751962000
1	5.538350000	-0.490913000	0.642833000
1	3.871984000	-3.127373000	-1.477328000
1	5.199682000	-1.943983000	-1.449539000
1	5.186251000	-3.303212000	-0.310774000
6	2.819705000	-2.624248000	0.995381000
1	3.357704000	-3.495641000	1.387938000
1	2.386272000	-2.078703000	1.837439000
1	1.995791000	-2.980887000	0.369949000
1	0.217074000	-1.264626000	0.581020000
1	-1.505124000	-1.840085000	1.634943000
1	-0.388998000	-0.735776000	-1.096583000
6	-1.681559000	-2.346896000	0.657045000
8	-0.585217000	-2.206150000	-0.163743000
6	-2.951960000	-1.708090000	0.089575000
6	-3.983483000	-1.289112000	0.937514000
6	-3.122019000	-1.554230000	-1.288829000
6	-5.157505000	-0.739498000	0.424688000
1	-3.860011000	-1.388431000	2.014502000
6	-4.293870000	-1.003802000	-1.809548000
1	-2.316660000	-1.862801000	-1.950044000
6	-5.317958000	-0.594867000	-0.954533000
1	-5.942270000	-0.412343000	1.101692000
1	-4.406603000	-0.887779000	-2.884482000
1	-6.228102000	-0.160100000	-1.358237000
6	-1.955333000	-3.826570000	0.976884000
1	-1.064168000	-4.270947000	1.433770000
1	-2.799057000	-3.951984000	1.666812000
1	-2.178016000	-4.374464000	0.052901000
7	1.589956000	2.392379000	-0.354082000
6	1.918627000	3.408962000	-0.796529000
6	2.334273000	4.685928000	-1.354343000
1	1.602408000	5.020242000	-2.093579000
1	2.406151000	5.430336000	-0.557555000
1	3.309120000	4.575925000	-1.835544000

A5<sub>X=NCMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	0.909002000	0.712020000	0.475108000
1	0.356963000	-0.689521000	1.182704000
7	-0.058972000	0.101162000	-1.344178000
1	-0.566004000	-0.743241000	-1.081769000
6	1.575343000	1.118686000	2.035597000
8	1.987031000	1.347142000	3.119136000
6	1.960006000	-1.165625000	-1.905395000
6	-1.040344000	1.125155000	-1.706727000
6	0.857431000	-0.258268000	-2.434245000
1	2.656747000	-1.417234000	-2.708186000
1	1.531850000	-2.087063000	-1.500227000
1	0.330081000	-0.767187000	-3.252823000
1	1.287736000	0.664936000	-2.837073000
1	-1.812573000	0.744306000	-2.387256000
1	-0.515554000	1.934716000	-2.226298000
6	-1.675783000	1.678745000	-0.457261000
6	-2.922666000	2.297662000	-0.486796000
1	-3.466670000	2.356668000	-1.423846000
6	-1.482942000	2.057716000	1.811523000
1	-0.881077000	1.933997000	2.705163000
6	-3.451780000	2.819164000	0.686761000
1	-4.422582000	3.304573000	0.687192000
6	-2.717656000	2.689319000	1.863021000
1	-3.090460000	3.067854000	2.808451000
7	-0.956145000	1.568084000	0.677036000
16	2.830272000	-0.260418000	-0.576298000
6	3.804025000	-1.580798000	0.299535000
6	4.732885000	-0.804231000	1.238730000
6	4.622910000	-2.370613000	-0.723996000
1	4.162084000	-0.176835000	1.930793000
1	5.323853000	-1.511443000	1.831732000
1	5.425363000	-0.165723000	0.679988000
1	3.984637000	-2.979895000	-1.371910000
1	5.232084000	-1.711926000	-1.352084000
1	5.297599000	-3.051191000	-0.191509000
6	2.904737000	-2.515892000	1.103042000
1	3.526811000	-3.283410000	1.579920000
1	2.365144000	-1.970520000	1.881433000
1	2.168868000	-3.022160000	0.471548000

1	-1.461950000	-2.834295000	1.720166000
1	0.012663000	-1.908355000	0.419014000
6	-1.596797000	-2.992566000	0.640612000
8	-0.381468000	-2.702616000	-0.031814000
6	-2.729212000	-2.089137000	0.174790000
6	-3.577212000	-1.472538000	1.097964000
6	-2.965556000	-1.895436000	-1.190881000
6	-4.652533000	-0.693662000	0.669409000
1	-3.393266000	-1.601636000	2.162036000
6	-4.035726000	-1.114555000	-1.623203000
1	-2.302850000	-2.357753000	-1.918605000
6	-4.887098000	-0.516056000	-0.693163000
1	-5.299648000	-0.216936000	1.400310000
1	-4.205510000	-0.970998000	-2.686802000
1	-5.718644000	0.096941000	-1.028848000
6	-1.929059000	-4.460171000	0.399919000
1	-1.124214000	-5.096601000	0.780574000
1	-2.859986000	-4.733760000	0.906937000
1	-2.051199000	-4.653924000	-0.671604000
7	1.464997000	2.419007000	-0.464418000
6	1.786068000	3.409686000	-0.969935000
6	2.191276000	4.654716000	-1.604176000
1	3.259800000	4.818646000	-1.444232000
1	1.992208000	4.604518000	-2.677597000
1	1.632720000	5.488849000	-1.172628000

**TSA2-6<sub>X=NCMe</sub>**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.090532000	0.369183000	0.002425000
7	0.434490000	-1.294588000	-1.217995000
6	-0.209009000	1.949947000	0.706599000
8	-0.405052000	3.030689000	1.130282000
6	-1.938903000	-1.805005000	-1.136387000
6	1.807131000	-1.710890000	-1.113352000
6	-0.523124000	-2.364805000	-1.101530000
1	-2.680155000	-2.596238000	-1.002660000
1	-2.120453000	-1.303022000	-2.091445000
1	-0.432031000	-3.100633000	-1.920095000
1	-0.378158000	-2.929962000	-0.158699000
1	2.159006000	-2.286607000	-1.986607000
1	1.957434000	-2.372636000	-0.235000000
6	2.697105000	-0.510786000	-0.921808000

6	4.052074000	-0.523326000	-1.252599000
1	4.485228000	-1.413665000	-1.697154000
6	2.860608000	1.664163000	-0.151232000
1	2.347915000	2.516679000	0.279916000
6	4.825006000	0.604392000	-1.007136000
1	5.882054000	0.614125000	-1.254459000
6	4.215317000	1.723153000	-0.443249000
1	4.771690000	2.630642000	-0.236172000
7	2.108957000	0.574438000	-0.380038000
16	-2.083055000	-0.577321000	0.213962000
6	-3.536116000	0.462713000	-0.305410000
6	-3.859839000	1.330075000	0.914725000
6	-4.718904000	-0.453262000	-0.630654000
1	-3.003191000	1.945029000	1.208197000
1	-4.688125000	2.003444000	0.666432000
1	-4.161704000	0.720424000	1.772870000
1	-4.542082000	-1.036768000	-1.539451000
1	-4.932878000	-1.144476000	0.191376000
1	-5.611500000	0.160230000	-0.799316000
6	-3.194838000	1.347088000	-1.503612000
1	-4.089750000	1.908504000	-1.798676000
1	-2.404850000	2.060423000	-1.256122000
1	-2.868796000	0.761478000	-2.369062000
6	0.921537000	-1.120370000	2.669881000
6	1.349957000	-1.811829000	3.875714000
1	2.121608000	-2.543525000	3.624930000
1	1.755292000	-1.090064000	4.589207000
1	0.498864000	-2.325726000	4.328759000
1	-0.215093000	0.919094000	-1.580772000
1	0.047572000	-0.021241000	-1.654864000
7	0.587995000	-0.565709000	1.711302000

A6<sub>X=NCMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	0.105240000	0.463784000	0.010204000
7	0.469530000	-1.177461000	-1.327138000
6	-0.177214000	1.901737000	0.955342000
8	-0.383410000	2.908527000	1.540720000
6	-1.919037000	-1.684474000	-1.244573000
6	1.859136000	-1.611619000	-1.172678000
6	-0.512187000	-2.263190000	-1.221786000
1	-2.657463000	-2.484570000	-1.154586000

1	-2.090816000	-1.149508000	-2.183731000
1	-0.405586000	-2.989939000	-2.038560000
1	-0.332297000	-2.790467000	-0.278940000
1	2.227147000	-2.165310000	-2.045192000
1	1.908194000	-2.287865000	-0.311498000
6	2.738839000	-0.417831000	-0.898860000
6	4.101276000	-0.433751000	-1.190112000
1	4.537832000	-1.308347000	-1.661897000
6	2.895845000	1.712615000	-0.025608000
1	2.377007000	2.549831000	0.427829000
6	4.878556000	0.672916000	-0.869313000
1	5.942600000	0.682462000	-1.083824000
6	4.260332000	1.769102000	-0.272933000
1	4.818492000	2.659932000	-0.006257000
7	2.138209000	0.644781000	-0.326793000
16	-2.075762000	-0.516322000	0.154161000
6	-3.580688000	0.482772000	-0.295719000
6	-3.889171000	1.302115000	0.961413000
6	-4.740168000	-0.467812000	-0.605175000
1	-3.042826000	1.937359000	1.241765000
1	-4.749319000	1.952136000	0.764586000
1	-4.137457000	0.656733000	1.810666000
1	-4.578652000	-1.014558000	-1.539610000
1	-4.895731000	-1.192550000	0.201032000
1	-5.661974000	0.114598000	-0.719048000
6	-3.321307000	1.414138000	-1.477629000
1	-4.246718000	1.953584000	-1.714195000
1	-2.541558000	2.141971000	-1.243915000
1	-3.015656000	0.865903000	-2.374407000
6	0.854020000	-1.464926000	2.432282000
6	1.198799000	-2.335859000	3.545397000
1	2.177182000	-2.790643000	3.371136000
1	1.232224000	-1.757260000	4.471951000
1	0.448655000	-3.124627000	3.642767000
7	0.578379000	-0.770371000	1.547645000
1	0.367037000	-0.745601000	-2.241821000
1	-0.216877000	1.350829000	-1.357964000

**A7R<sub>X</sub>**=NCMe

Coordinates (Angstroms)

	X	Y	Z
25	-0.752531000	0.571593000	-0.467778000
1	-0.124864000	-0.947219000	-0.553998000

7	-0.371363000	0.472620000	1.643078000
1	0.135810000	-0.403020000	1.762025000
6	-0.928971000	0.510670000	-2.197716000
8	-1.013801000	0.407605000	-3.374247000
6	-2.536928000	-0.632930000	1.902521000
6	0.530982000	1.566377000	2.003699000
6	-1.582127000	0.406976000	2.469699000
1	-3.447907000	-0.676088000	2.503961000
1	-2.064087000	-1.619352000	1.903260000
1	-1.347815000	0.153309000	3.512859000
1	-2.053513000	1.395569000	2.464454000
1	1.062583000	1.379373000	2.945706000
1	-0.067376000	2.474148000	2.143320000
6	1.513636000	1.811812000	0.886928000
6	2.724490000	2.461835000	1.116674000
1	2.990385000	2.751788000	2.128513000
6	1.964698000	1.656266000	-1.369784000
1	1.631997000	1.305527000	-2.340289000
6	3.568137000	2.728287000	0.046006000
1	4.514895000	3.236329000	0.200331000
6	3.178947000	2.311685000	-1.224684000
1	3.804791000	2.480967000	-2.094013000
7	1.131563000	1.414287000	-0.343395000
16	-2.932996000	-0.153945000	0.182674000
6	-3.653193000	-1.709938000	-0.540008000
6	-4.166338000	-1.291474000	-1.921494000
6	-4.816385000	-2.179959000	0.337229000
1	-3.354898000	-0.909995000	-2.548893000
1	-4.601274000	-2.163501000	-2.423006000
1	-4.941221000	-0.520846000	-1.847585000
1	-4.471431000	-2.534225000	1.314017000
1	-5.551789000	-1.383921000	0.494786000
1	-5.323239000	-3.017818000	-0.156244000
6	-2.608634000	-2.813564000	-0.682180000
1	-3.089317000	-3.708900000	-1.095515000
1	-1.801530000	-2.508309000	-1.351566000
1	-2.166750000	-3.087262000	0.280374000
6	1.591262000	-2.556823000	1.250160000
8	1.344568000	-1.979779000	2.305752000
6	2.708624000	-2.082216000	0.376488000
6	2.918230000	-2.613124000	-0.901859000
6	3.571571000	-1.090233000	0.857647000
6	3.974698000	-2.157808000	-1.686227000
1	2.253363000	-3.373420000	-1.297736000



6	4.633556000	-0.644259000	0.078208000
1	3.404339000	-0.678597000	1.847786000
6	4.836236000	-1.176999000	-1.195679000
1	4.125064000	-2.569605000	-2.679487000
1	5.301341000	0.121992000	0.459609000
1	5.662220000	-0.824632000	-1.806750000
6	0.804164000	-3.769929000	0.836397000
1	0.059777000	-3.997998000	1.600123000
1	0.301020000	-3.589562000	-0.118499000
1	1.471332000	-4.628600000	0.704177000
6	-1.892198000	3.516073000	-0.047215000
6	-2.423079000	4.860658000	0.119153000
1	-1.744079000	5.455181000	0.735438000
1	-2.533288000	5.338778000	-0.857370000
1	-3.399886000	4.812700000	0.606572000
7	-1.475607000	2.444463000	-0.185468000

A7S<sub>X=NCMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	-0.974820000	0.655692000	0.477511000
1	0.286016000	-0.290480000	0.944888000
7	-0.699842000	-0.137167000	-1.503036000
1	0.040776000	-0.826215000	-1.395443000
6	-1.146897000	1.183808000	2.127600000
8	-1.235105000	1.507494000	3.263016000
6	0.935446000	1.619905000	-1.924305000
6	-1.915266000	-0.859106000	-1.880448000
6	-0.253059000	0.853884000	-2.486420000
1	1.276140000	2.370607000	-2.641009000
1	1.758377000	0.929062000	-1.716149000
1	0.037461000	0.380787000	-3.434800000
1	-1.086091000	1.534605000	-2.692627000
1	-1.745635000	-1.568344000	-2.699630000
1	-2.655280000	-0.126247000	-2.221944000
6	-2.461880000	-1.577356000	-0.673329000
6	-3.210906000	-2.746258000	-0.789910000
1	-3.380490000	-3.176936000	-1.771614000
6	-2.687000000	-1.600832000	1.623805000
1	-2.444600000	-1.119734000	2.565001000
6	-3.719171000	-3.346749000	0.355479000
1	-4.303011000	-4.259427000	0.288628000
6	-3.452622000	-2.757596000	1.589334000

1	-3.822551000	-3.186406000	2.514225000
7	-2.194665000	-1.011780000	0.520962000
16	0.416166000	2.418064000	-0.362331000
6	2.035411000	2.788343000	0.478305000
6	1.647900000	3.561785000	1.742200000
6	2.885006000	3.667353000	-0.443384000
1	1.009759000	2.958176000	2.394932000
1	2.556757000	3.820157000	2.297667000
1	1.121652000	4.492191000	1.502257000
1	3.205356000	3.125382000	-1.339248000
1	2.343811000	4.566781000	-0.755477000
1	3.788581000	3.982219000	0.092043000
6	2.796101000	1.518918000	0.853242000
1	3.741975000	1.798600000	1.333258000
1	2.219300000	0.901966000	1.544346000
1	3.037229000	0.909946000	-0.022705000
6	1.126690000	-2.911352000	-0.288596000
8	0.548391000	-2.896955000	-1.370591000
6	2.501571000	-2.329601000	-0.172107000
6	3.185743000	-2.287072000	1.047875000
6	3.114740000	-1.812922000	-1.320735000
6	4.465852000	-1.742206000	1.116379000
1	2.723278000	-2.672276000	1.950610000
6	4.394124000	-1.271627000	-1.252822000
1	2.578635000	-1.841744000	-2.264130000
6	5.072288000	-1.236725000	-0.033023000
1	4.986932000	-1.708010000	2.068186000
1	4.861570000	-0.871710000	-2.147654000
1	6.068800000	-0.808501000	0.022819000
6	0.475590000	-3.524141000	0.920224000
1	-0.526492000	-3.864920000	0.654369000
1	1.067585000	-4.372192000	1.282070000
1	0.408519000	-2.790857000	1.728987000
6	-3.437931000	2.336423000	-0.640660000
6	-4.576163000	3.110760000	-1.112421000
1	-5.305145000	2.447113000	-1.584035000
1	-5.049362000	3.621516000	-0.270053000
1	-4.242182000	3.853530000	-1.841000000
7	-2.534852000	1.720361000	-0.258547000

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**TSA7-8R<sub>X=NCMe</sub>**

-----  
Coordinates (Angstroms)

X

Y

Z  
-----

25	-0.590830000	0.446239000	-0.346444000
1	-0.081163000	-1.140008000	0.034833000
7	-0.428535000	0.725191000	1.742107000
1	0.018486000	-0.158579000	2.019676000
6	-0.581775000	-0.019253000	-2.030809000
8	-0.544520000	-0.394054000	-3.150582000
6	-2.678046000	-0.195954000	1.968511000
6	0.528640000	1.795751000	2.013947000
6	-1.690470000	0.845059000	2.480067000
1	-3.631400000	-0.105299000	2.494226000
1	-2.277709000	-1.203875000	2.115034000
1	-1.540676000	0.704088000	3.559274000
1	-2.091351000	1.853558000	2.326665000
1	0.946161000	1.740784000	3.027918000
1	0.009373000	2.757570000	1.923853000
6	1.634462000	1.752536000	0.990031000
6	2.875838000	2.338335000	1.229369000
1	3.077039000	2.787619000	2.196795000
6	2.263792000	1.171741000	-1.153434000
1	1.986487000	0.684465000	-2.081009000
6	3.829299000	2.348211000	0.219053000
1	4.800547000	2.805507000	0.380077000
6	3.513360000	1.754269000	-1.000062000
1	4.224085000	1.728476000	-1.818621000
7	1.333107000	1.166133000	-0.185184000
16	-2.897789000	0.114746000	0.183109000
6	-3.808149000	-1.378961000	-0.440641000
6	-4.146303000	-1.038404000	-1.895501000
6	-5.089972000	-1.574044000	0.371639000
1	-3.240084000	-0.857546000	-2.481724000
1	-4.679892000	-1.881786000	-2.348172000
1	-4.787835000	-0.153285000	-1.964066000
1	-4.875414000	-1.851693000	1.408646000
1	-5.707490000	-0.669539000	0.374905000
1	-5.676574000	-2.386113000	-0.073787000
6	-2.935862000	-2.628161000	-0.382416000
1	-3.479595000	-3.472555000	-0.823291000
1	-2.004039000	-2.480766000	-0.934008000
1	-2.689003000	-2.893370000	0.649136000
6	1.023515000	-2.170102000	1.118447000
8	0.961899000	-1.659720000	2.257217000
6	2.275046000	-1.958385000	0.295728000
6	2.366191000	-2.328736000	-1.050623000
6	3.405038000	-1.440584000	0.932903000

6	3.567450000	-2.191280000	-1.740892000
1	1.489613000	-2.702295000	-1.571212000
6	4.609895000	-1.304514000	0.244942000
1	3.328203000	-1.152911000	1.976679000
6	4.695906000	-1.683483000	-1.093608000
1	3.622894000	-2.474454000	-2.788292000
1	5.479959000	-0.898331000	0.753147000
1	5.633057000	-1.576366000	-1.632384000
6	0.241737000	-3.439290000	0.849535000
1	-0.698918000	-3.410310000	1.400536000
1	0.041518000	-3.619154000	-0.207193000
1	0.842847000	-4.275717000	1.232072000
6	-1.391636000	3.488192000	-0.797088000
6	-1.725509000	4.881833000	-1.049162000
1	-2.119727000	5.341486000	-0.139685000
1	-0.830241000	5.422011000	-1.366841000
1	-2.480359000	4.941433000	-1.837197000
7	-1.119877000	2.378186000	-0.615114000

**TSA7-8S<sub>X</sub>=NCMe**

Coordinates (Angstroms)

	X	Y	Z
25	-0.811797000	0.500765000	0.392422000
1	0.370515000	-0.740109000	0.477140000
7	-0.848948000	-0.048040000	-1.644858000
1	-0.285979000	-0.907585000	-1.620718000
6	-0.644131000	0.705943000	2.118959000
8	-0.497053000	0.780646000	3.288711000
6	1.070817000	1.426053000	-1.999979000
6	-2.205741000	-0.456500000	-2.006879000
6	-0.234384000	0.898115000	-2.582100000
1	1.515578000	2.159921000	-2.676607000
1	1.780210000	0.608589000	-1.839391000
1	-0.036168000	0.429346000	-3.555712000
1	-0.934674000	1.725086000	-2.746021000
1	-2.231288000	-1.077514000	-2.911804000
1	-2.798571000	0.443884000	-2.208966000
6	-2.822443000	-1.195423000	-0.847185000
6	-3.857217000	-2.111488000	-1.023705000
1	-4.206745000	-2.337084000	-2.026173000
6	-2.886330000	-1.485691000	1.442631000
1	-2.459035000	-1.221357000	2.403677000
6	-4.423497000	-2.720698000	0.089452000

1	-5.229619000	-3.438843000	-0.023706000
6	-3.929089000	-2.396324000	1.350756000
1	-4.334697000	-2.844047000	2.251339000
7	-2.332874000	-0.893363000	0.371565000
16	0.660400000	2.198863000	-0.397373000
6	2.302161000	2.487979000	0.420086000
6	1.969925000	3.337137000	1.651357000
6	3.216282000	3.263084000	-0.530202000
1	1.275101000	2.815789000	2.317275000
1	2.891923000	3.533649000	2.210243000
1	1.529175000	4.299965000	1.371811000
1	3.506004000	2.659100000	-1.396150000
1	2.740786000	4.181941000	-0.889189000
1	4.134180000	3.540276000	0.001473000
6	2.950388000	1.175958000	0.844673000
1	3.899546000	1.386510000	1.352592000
1	2.302237000	0.620747000	1.526866000
1	3.164441000	0.535699000	-0.014764000
6	0.760118000	-2.435049000	-0.059680000
8	0.187796000	-2.609195000	-1.158374000
6	2.249261000	-2.160895000	-0.074019000
6	3.034397000	-2.204064000	1.083025000
6	2.873116000	-1.916461000	-1.301929000
6	4.412072000	-2.003718000	1.012971000
1	2.575520000	-2.381382000	2.050249000
6	4.248554000	-1.708788000	-1.374158000
1	2.265332000	-1.898705000	-2.201287000
6	5.024462000	-1.753203000	-0.214763000
1	5.006333000	-2.037810000	1.921780000
1	4.717538000	-1.518528000	-2.335569000
1	6.097590000	-1.593986000	-0.268734000
6	0.179816000	-3.091609000	1.177390000
1	-0.900928000	-3.170843000	1.058401000
1	0.595533000	-4.105755000	1.252331000
1	0.401557000	-2.556308000	2.101907000
6	-3.099570000	2.652082000	-0.064658000
6	-4.156068000	3.632305000	-0.265345000
1	-5.057568000	3.135479000	-0.631899000
1	-4.380093000	4.131663000	0.680574000
1	-3.833362000	4.377139000	-0.996739000
7	-2.257493000	1.875696000	0.100478000

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**A8R<sub>x</sub>**=NCMe

-----  
Coordinates (Angstroms)  
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	X	Y	Z
25	-0.677938000	0.645830000	-0.294812000
1	0.091018000	-1.840413000	0.167929000
7	-0.467759000	0.653345000	1.677745000
1	0.332125000	-0.813587000	1.968867000
6	-0.636373000	0.184717000	-1.999163000
8	-0.585681000	-0.142241000	-3.128870000
6	-2.627768000	-0.396468000	1.985440000
6	0.524636000	1.593669000	2.145456000
6	-1.637890000	0.623076000	2.531569000
1	-3.574747000	-0.374230000	2.529581000
1	-2.199248000	-1.401650000	2.043800000
1	-1.388412000	0.334770000	3.568519000
1	-2.126869000	1.614700000	2.595357000
1	0.983613000	1.303362000	3.107403000
1	0.088624000	2.598605000	2.312144000
6	1.601749000	1.728852000	1.106006000
6	2.864756000	2.249506000	1.387886000
1	3.101745000	2.552186000	2.403031000
6	2.169736000	1.435612000	-1.117683000
1	1.856256000	1.090301000	-2.096529000
6	3.795981000	2.367580000	0.365993000
1	4.785102000	2.769350000	0.563052000
6	3.440210000	1.950359000	-0.915998000
1	4.136720000	2.010057000	-1.744878000
7	1.261167000	1.324132000	-0.132746000
16	-2.902944000	0.033819000	0.230136000
6	-3.598517000	-1.525153000	-0.509097000
6	-4.074075000	-1.122072000	-1.907793000
6	-4.782507000	-1.998228000	0.336989000
1	-3.252380000	-0.725273000	-2.511485000
1	-4.474125000	-2.004506000	-2.419700000
1	-4.865950000	-0.367371000	-1.859522000
1	-4.465478000	-2.337487000	1.328020000
1	-5.530846000	-1.208443000	0.460841000
1	-5.264462000	-2.846209000	-0.163561000
6	-2.533884000	-2.616172000	-0.604015000
1	-2.981359000	-3.523186000	-1.027992000
1	-1.707416000	-2.307212000	-1.250082000
1	-2.128438000	-2.872906000	0.378784000
6	0.882970000	-2.267718000	0.809099000
8	0.797986000	-1.702368000	2.090252000
6	2.209255000	-1.975055000	0.118524000

6	2.330659000	-2.165213000	-1.262897000
6	3.322063000	-1.534879000	0.835959000
6	3.543148000	-1.938577000	-1.910801000
1	1.463883000	-2.487230000	-1.836563000
6	4.538600000	-1.305245000	0.190782000
1	3.222107000	-1.363714000	1.903244000
6	4.655594000	-1.510901000	-1.183157000
1	3.619652000	-2.088778000	-2.984278000
1	5.394972000	-0.958162000	0.762835000
1	5.601278000	-1.329117000	-1.685885000
6	0.646067000	-3.773909000	0.907863000
1	-0.317437000	-3.968813000	1.388939000
1	0.642419000	-4.242350000	-0.081740000
1	1.434499000	-4.241957000	1.508489000
6	-1.570515000	3.607888000	-0.700542000
6	-1.955633000	5.004134000	-0.832695000
1	-1.345287000	5.620112000	-0.167660000
1	-1.804702000	5.331866000	-1.864176000
1	-3.009178000	5.124094000	-0.569183000
7	-1.260570000	2.498006000	-0.601696000

**A8S<sub>X=NCMe</sub>**

Coordinates (Angstroms)

	X	Y	Z
25	1.128627000	0.437949000	-0.335397000
1	-0.918795000	-1.169404000	-0.275932000
7	1.103459000	-0.011167000	1.591171000
1	-0.375423000	-0.870137000	1.714394000
6	0.718325000	0.595315000	-2.046058000
8	0.412358000	0.663781000	-3.181028000
6	0.010087000	2.072824000	2.162937000
6	2.073627000	-1.023098000	1.944759000
6	1.064120000	1.055383000	2.571053000
1	0.024763000	2.956321000	2.805306000
1	-0.980987000	1.613255000	2.205992000
1	0.804647000	0.682797000	3.578139000
1	2.046963000	1.555923000	2.670187000
1	1.805295000	-1.588238000	2.854609000
1	3.067847000	-0.577834000	2.147995000
6	2.227185000	-1.976594000	0.794813000
6	2.733659000	-3.268437000	0.938038000
1	3.023769000	-3.621906000	1.922414000
6	1.954334000	-2.286482000	-1.482177000

1	1.629671000	-1.859738000	-2.424597000
6	2.849774000	-4.081734000	-0.180923000
1	3.240197000	-5.090739000	-0.091467000
6	2.448407000	-3.579893000	-1.418500000
1	2.513331000	-4.176523000	-2.321619000
7	1.843152000	-1.491992000	-0.402826000
16	0.357859000	2.552730000	0.430574000
6	-1.312896000	3.081028000	-0.201098000
6	-1.045444000	3.733059000	-1.559863000
6	-1.919549000	4.102207000	0.763538000
1	-0.549538000	3.041697000	-2.247406000
1	-1.999725000	4.029024000	-2.010146000
1	-0.425411000	4.629904000	-1.458753000
1	-2.173892000	3.651172000	1.727412000
1	-1.239208000	4.942033000	0.939531000
1	-2.844391000	4.498830000	0.328715000
6	-2.230190000	1.869857000	-0.360345000
1	-3.213618000	2.197300000	-0.719159000
1	-1.820712000	1.160305000	-1.084093000
1	-2.381449000	1.342211000	0.585726000
6	-1.529170000	-1.774160000	0.418000000
8	-1.213670000	-1.432027000	1.744146000
6	-2.983202000	-1.473825000	0.096249000
6	-3.388949000	-1.366805000	-1.238927000
6	-3.936285000	-1.311424000	1.102877000
6	-4.717801000	-1.102860000	-1.562841000
1	-2.650968000	-1.473962000	-2.031523000
6	-5.270138000	-1.049640000	0.782823000
1	-3.623249000	-1.377983000	2.140119000
6	-5.666132000	-0.943762000	-0.550184000
1	-5.012035000	-1.012076000	-2.604927000
1	-6.001224000	-0.925208000	1.577276000
1	-6.703016000	-0.735608000	-0.798243000
6	-1.206826000	-3.247599000	0.150350000
1	-0.151428000	-3.443317000	0.365201000
1	-1.817556000	-3.890507000	0.794795000
1	-1.403821000	-3.515103000	-0.893593000
6	4.046407000	1.528714000	-0.512858000
6	5.412106000	2.028307000	-0.545668000
1	6.090437000	1.282707000	-0.123695000
1	5.702900000	2.235386000	-1.578527000
1	5.481280000	2.949591000	0.037911000
7	2.958495000	1.136173000	-0.493661000

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A1<sub>X=CCMe</sub>

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Coordinates (Angstroms)

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	X	Y	Z
25	-0.188720000	0.053390000	0.097130000
7	-0.481208000	-1.656982000	-0.697483000
6	0.083667000	0.579001000	1.724744000
8	0.208399000	0.872402000	2.871509000
6	1.885931000	-2.190890000	-0.701386000
6	-1.823594000	-2.149079000	-0.856355000
6	0.514302000	-2.536854000	-1.273219000
1	2.696700000	-2.643346000	-1.279409000
1	1.941155000	-2.532593000	0.335204000
1	0.311646000	-3.598468000	-1.042076000
1	0.541508000	-2.462086000	-2.377182000
1	-1.976294000	-3.136990000	-0.379290000
1	-2.101575000	-2.291138000	-1.918474000
6	-2.787510000	-1.171014000	-0.245839000
6	-4.165637000	-1.391923000	-0.202561000
1	-4.573727000	-2.303941000	-0.627688000
6	-3.034123000	0.862792000	0.828857000
1	-2.536815000	1.743927000	1.220825000
6	-4.989629000	-0.442451000	0.384859000
1	-6.063298000	-0.596134000	0.434057000
6	-4.408828000	0.711828000	0.913542000
1	-5.008793000	1.483770000	1.383319000
7	-2.229358000	-0.057729000	0.264930000
16	2.006752000	-0.370802000	-0.711468000
6	3.485184000	-0.009707000	0.354681000
6	3.444980000	1.506040000	0.565948000
6	4.755543000	-0.412147000	-0.398186000
1	2.540935000	1.800970000	1.106112000
1	4.319925000	1.815169000	1.149522000
1	3.466147000	2.045406000	-0.387424000
1	4.777845000	-1.487764000	-0.603963000
1	4.843337000	0.123790000	-1.348680000
1	5.635599000	-0.172403000	0.211488000
6	3.410764000	-0.732949000	1.699309000
1	4.203664000	-0.353362000	2.355059000
1	2.448917000	-0.563882000	2.190494000
1	3.565057000	-1.810911000	1.591621000
6	-0.326495000	2.980965000	-1.261354000
6	-0.424058000	4.284144000	-1.940330000
1	-1.204831000	4.285764000	-2.711023000

1	-0.664407000	5.092973000	-1.238964000
1	0.515863000	4.558008000	-2.435538000
6	-0.247464000	1.883090000	-0.695535000

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**A2<sub>X=CCMe</sub>**

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Coordinates (Angstroms)

	X	Y	Z
25	-0.192676000	0.085584000	0.058554000
7	-0.501730000	-1.601990000	-0.779493000
6	0.065346000	0.390770000	1.736742000
8	0.171797000	0.495403000	2.918639000
6	1.854920000	-2.176593000	-0.710935000
6	-1.844786000	-2.092773000	-0.916737000
6	0.488738000	-2.522054000	-1.296669000
1	2.670900000	-2.653667000	-1.261592000
1	1.887509000	-2.489866000	0.335262000
1	0.262137000	-3.568882000	-1.020545000
1	0.538453000	-2.500641000	-2.401939000
1	-1.997516000	-3.061412000	-0.398190000
1	-2.129154000	-2.278881000	-1.969769000
6	-2.804301000	-1.094015000	-0.334064000
6	-4.186991000	-1.288927000	-0.328437000
1	-4.600274000	-2.191797000	-0.767855000
6	-3.040796000	0.941227000	0.739707000
1	-2.537466000	1.813228000	1.143349000
6	-5.008270000	-0.325591000	0.239581000
1	-6.085739000	-0.458325000	0.257325000
6	-4.419872000	0.815603000	0.787890000
1	-5.017593000	1.597813000	1.243273000
7	-2.238898000	0.008071000	0.193121000
16	1.997616000	-0.359938000	-0.761032000
6	3.492716000	0.001385000	0.284487000
6	3.459613000	1.515717000	0.507207000
6	4.750480000	-0.395912000	-0.492436000
1	2.580452000	1.809428000	1.087505000
1	4.358434000	1.820204000	1.055967000
1	3.441212000	2.062385000	-0.441974000
1	4.766486000	-1.469145000	-0.710695000
1	4.825034000	0.150732000	-1.437959000
1	5.640405000	-0.165284000	0.106348000
6	3.444084000	-0.729270000	1.626481000
1	4.250435000	-0.352483000	2.267297000
1	2.493396000	-0.561929000	2.139144000

1	3.596414000	-1.806638000	1.510857000
6	-0.213658000	3.145120000	-1.014660000
6	-0.243436000	4.515100000	-1.554169000
1	-1.002253000	4.629003000	-2.338417000
1	-0.472478000	5.255176000	-0.777186000
1	0.719397000	4.800957000	-1.995566000
1	-0.662867000	-3.132245000	2.036910000
1	-0.509774000	-2.593533000	1.537201000
6	-0.185530000	1.993449000	-0.562422000

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**A3<sub>X=CCMe</sub>**

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Coordinates (Angstroms)

	X	Y	Z
25	1.202625000	0.655046000	0.434641000
1	0.751549000	-0.557182000	1.586860000
7	0.122470000	-0.084109000	-1.210465000
6	2.041927000	1.317088000	1.819848000
8	2.609127000	1.824179000	2.723710000
6	2.070019000	-1.356872000	-1.900219000
6	-0.886287000	0.885552000	-1.565597000
6	0.937464000	-0.441813000	-2.349543000
1	2.734828000	-1.614390000	-2.728885000
1	1.652751000	-2.274866000	-1.476334000
1	0.359626000	-0.984892000	-3.122888000
1	1.361977000	0.450504000	-2.847884000
1	-1.694906000	0.469559000	-2.193777000
1	-0.454738000	1.731472000	-2.134803000
6	-1.485825000	1.456840000	-0.311573000
6	-2.778259000	1.978710000	-0.260450000
1	-3.397175000	1.953196000	-1.151800000
6	-1.153317000	1.953980000	1.921487000
1	-0.471868000	1.926343000	2.765538000
6	-3.259363000	2.502026000	0.931524000
1	-4.265192000	2.906411000	0.992662000
6	-2.428888000	2.484687000	2.051111000
1	-2.757595000	2.874878000	3.008267000
7	-0.679883000	1.452416000	0.769149000
16	3.013153000	-0.482450000	-0.596118000
6	3.837754000	-1.875282000	0.321950000
6	4.801827000	-1.187836000	1.293492000
6	4.618076000	-2.737664000	-0.674425000
1	4.264997000	-0.523422000	1.978323000
1	5.319265000	-1.946777000	1.891923000

1	5.558262000	-0.600286000	0.762366000
1	3.950558000	-3.302885000	-1.332648000
1	5.284226000	-2.129759000	-1.295788000
1	5.231153000	-3.461601000	-0.124534000
6	2.842076000	-2.732271000	1.103570000
1	3.371449000	-3.585638000	1.544761000
1	2.381579000	-2.164206000	1.915512000
1	2.045287000	-3.129569000	0.466825000
1	0.640215000	-0.927127000	0.891141000
1	-1.517020000	-1.422314000	1.278478000
1	-0.559634000	-1.366099000	-0.786086000
6	-1.906582000	-2.132351000	0.527092000
8	-0.984370000	-2.302789000	-0.505417000
6	-3.242631000	-1.559024000	0.055812000
6	-4.173553000	-1.089224000	0.990665000
6	-3.561896000	-1.482765000	-1.300407000
6	-5.392117000	-0.553907000	0.580270000
1	-3.933535000	-1.127465000	2.051537000
6	-4.780581000	-0.943701000	-1.718118000
1	-2.834940000	-1.834088000	-2.026280000
6	-5.700329000	-0.476801000	-0.780157000
1	-6.098526000	-0.186418000	1.319860000
1	-5.007418000	-0.881961000	-2.779304000
1	-6.646030000	-0.051497000	-1.104249000
6	-2.116701000	-3.478465000	1.223105000
1	-1.164441000	-3.841634000	1.623848000
1	-2.833801000	-3.400441000	2.047247000
1	-2.494383000	-4.215590000	0.504759000
6	1.716712000	2.296527000	-0.606658000
6	2.024436000	3.324760000	-1.218378000
6	2.379241000	4.542721000	-1.966244000
1	3.454236000	4.592751000	-2.179055000
1	1.857138000	4.596953000	-2.929868000
1	2.120656000	5.452333000	-1.409925000

**TSA3-4<sub>x=CCMe</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	1.202598000	0.656537000	0.432287000
1	0.754593000	-0.545233000	1.593210000
7	0.115059000	-0.091992000	-1.207819000
6	2.047423000	1.328060000	1.810307000
8	2.617817000	1.839151000	2.709032000

6	2.062236000	-1.370223000	-1.891510000
6	-0.895424000	0.879768000	-1.563570000
6	0.932520000	-0.455330000	-2.347204000
1	2.724122000	-1.635692000	-2.719878000
1	1.641179000	-2.283152000	-1.460662000
1	0.352569000	-0.998889000	-3.117027000
1	1.355212000	0.437046000	-2.841822000
1	-1.704154000	0.459495000	-2.186725000
1	-0.459424000	1.718096000	-2.136097000
6	-1.489353000	1.455923000	-0.309022000
6	-2.782548000	1.975043000	-0.255069000
1	-3.405644000	1.943239000	-1.143277000
6	-1.147907000	1.963111000	1.920105000
1	-0.463104000	1.939813000	2.761523000
6	-3.259147000	2.503220000	0.936610000
1	-4.265510000	2.905797000	1.000361000
6	-2.423667000	2.492687000	2.052453000
1	-2.748888000	2.886737000	3.009184000
7	-0.678757000	1.457068000	0.768019000
16	3.010856000	-0.489898000	-0.595431000
6	3.834036000	-1.879169000	0.329374000
6	4.800600000	-1.187400000	1.295386000
6	4.611412000	-2.747931000	-0.663744000
1	4.265839000	-0.518356000	1.977303000
1	5.317790000	-1.943643000	1.897382000
1	5.557109000	-0.603963000	0.759859000
1	3.942059000	-3.315263000	-1.318272000
1	5.277879000	-2.144233000	-1.288844000
1	5.223881000	-3.470087000	-0.110890000
6	2.838180000	-2.730166000	1.117270000
1	3.366774000	-3.582899000	1.560561000
1	2.381701000	-2.157480000	1.928219000
1	2.038432000	-3.128070000	0.484671000
1	0.643161000	-0.923085000	0.901180000
1	-1.516891000	-1.390305000	1.276356000
1	-0.520801000	-1.270860000	-0.806407000
6	-1.890841000	-2.106399000	0.519850000
8	-0.972677000	-2.256753000	-0.511188000
6	-3.240379000	-1.552914000	0.057498000
6	-4.172227000	-1.089180000	0.994593000
6	-3.569420000	-1.488372000	-1.297044000
6	-5.399632000	-0.570699000	0.588479000
1	-3.925483000	-1.117492000	2.054369000
6	-4.797207000	-0.967290000	-1.711109000

1	-2.840431000	-1.834566000	-2.023454000
6	-5.717164000	-0.505598000	-0.770563000
1	-6.106042000	-0.207001000	1.330046000
1	-5.031297000	-0.915202000	-2.771338000
1	-6.669934000	-0.093665000	-1.091402000
6	-2.085630000	-3.453539000	1.223242000
1	-1.127436000	-3.804547000	1.621290000
1	-2.800982000	-3.383574000	2.050294000
1	-2.455971000	-4.197174000	0.507504000
6	1.715583000	2.291332000	-0.622076000
6	2.024956000	3.315377000	-1.239703000
6	2.385310000	4.530402000	-1.989657000
1	3.141685000	4.325886000	-2.757393000
1	1.517866000	4.966754000	-2.500390000
1	2.795994000	5.307509000	-1.333227000

A4<sub>X=CCMe</sub>

Coordinates (Angstroms)			
	X	Y	Z
25	1.121468000	0.683255000	0.444140000
1	0.578074000	-0.599271000	1.459310000
7	0.134987000	0.095085000	-1.343308000
6	1.874655000	1.213187000	1.932905000
8	2.374969000	1.625175000	2.917123000
6	2.101567000	-1.178936000	-1.961450000
6	-0.885704000	1.082894000	-1.664347000
6	1.037880000	-0.207002000	-2.450171000
1	2.808467000	-1.418485000	-2.758902000
1	1.617095000	-2.095272000	-1.611319000
1	0.503310000	-0.669095000	-3.294493000
1	1.495208000	0.722222000	-2.809648000
1	-1.649890000	0.694730000	-2.352575000
1	-0.407980000	1.944525000	-2.146945000
6	-1.533575000	1.551600000	-0.389824000
6	-2.827892000	2.066032000	-0.363264000
1	-3.401161000	2.112552000	-1.283341000
6	-1.310358000	1.866766000	1.886768000
1	-0.674038000	1.767697000	2.759677000
6	-3.366086000	2.497048000	0.841713000
1	-4.374120000	2.897547000	0.885149000
6	-2.590943000	2.389946000	1.994255000
1	-2.966344000	2.703359000	2.962239000
7	-0.779276000	1.458947000	0.723082000

16	2.984650000	-0.411621000	-0.551519000
6	3.686726000	-1.896824000	0.327370000
6	4.651498000	-1.318500000	1.366969000
6	4.454582000	-2.757189000	-0.680328000
1	4.135666000	-0.635712000	2.050108000
1	5.074223000	-2.136221000	1.962159000
1	5.478738000	-0.778611000	0.893905000
1	3.782141000	-3.255325000	-1.385655000
1	5.178157000	-2.163594000	-1.249104000
1	5.003950000	-3.538573000	-0.141984000
6	2.601487000	-2.721506000	1.021148000
1	3.038988000	-3.663680000	1.373776000
1	2.202162000	-2.190592000	1.889363000
1	1.761283000	-2.955512000	0.357935000
1	0.495144000	-0.939781000	0.742952000
1	-1.377471000	-1.883606000	1.382435000
1	-0.327068000	-0.818469000	-1.061468000
6	-1.692289000	-2.383466000	0.430637000
8	-0.733358000	-2.312102000	-0.532723000
6	-3.011134000	-1.688159000	0.051025000
6	-3.919954000	-1.263896000	1.027882000
6	-3.340791000	-1.483659000	-1.290942000
6	-5.128997000	-0.664752000	0.676167000
1	-3.672818000	-1.397460000	2.079983000
6	-4.549037000	-0.885546000	-1.652270000
1	-2.619430000	-1.791498000	-2.043118000
6	-5.450734000	-0.474937000	-0.669542000
1	-5.816726000	-0.334983000	1.450757000
1	-4.783812000	-0.731146000	-2.702672000
1	-6.388617000	-0.001405000	-0.946703000
6	-2.009714000	-3.845542000	0.818733000
1	-1.087927000	-4.339349000	1.147461000
1	-2.750376000	-3.919041000	1.626245000
1	-2.394747000	-4.385222000	-0.056067000
6	1.700483000	2.388684000	-0.442051000
6	2.029967000	3.451678000	-0.976645000
6	2.409405000	4.715956000	-1.628672000
1	2.953246000	4.544177000	-2.565688000
1	1.530525000	5.324972000	-1.874471000
1	3.055918000	5.328609000	-0.988503000

TSA4-5<sub>X=CCMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	1.089603000	0.659651000	0.460336000
1	0.540599000	-0.808113000	1.240536000
7	0.085182000	0.144150000	-1.355756000
6	1.834917000	1.051080000	1.986407000
8	2.342507000	1.328393000	3.018678000
6	2.028685000	-1.159106000	-2.003790000
6	-0.911559000	1.169612000	-1.637166000
6	0.967376000	-0.174708000	-2.476008000
1	2.713282000	-1.407527000	-2.818110000
1	1.547751000	-2.074390000	-1.644602000
1	0.415285000	-0.622442000	-3.315895000
1	1.432345000	0.750528000	-2.833918000
1	-1.674757000	0.837041000	-2.354017000
1	-0.401834000	2.040527000	-2.065103000
6	-1.561691000	1.577895000	-0.342501000
6	-2.857818000	2.085468000	-0.295184000
1	-3.429844000	2.171902000	-1.213319000
6	-1.341800000	1.786785000	1.945221000
1	-0.706276000	1.647201000	2.813183000
6	-3.399927000	2.457347000	0.927919000
1	-4.409887000	2.850833000	0.988618000
6	-2.624830000	2.300080000	2.074640000
1	-3.002425000	2.566209000	3.055916000
7	-0.807035000	1.432596000	0.765480000
16	2.945360000	-0.389788000	-0.618646000
6	3.760520000	-1.854961000	0.191508000
6	4.733908000	-1.245981000	1.205601000
6	4.531897000	-2.650926000	-0.864881000
1	4.208935000	-0.615221000	1.930286000
1	5.233086000	-2.052004000	1.756163000
1	5.504275000	-0.642782000	0.713329000
1	3.858660000	-3.167567000	-1.556238000
1	5.201515000	-2.008820000	-1.446929000
1	5.140509000	-3.414658000	-0.366250000
6	2.755510000	-2.754330000	0.908349000
1	3.275628000	-3.643710000	1.285430000
1	2.298148000	-2.236405000	1.755010000
1	1.947075000	-3.083395000	0.248749000
1	0.135908000	-1.321967000	0.617470000
1	-1.629741000	-1.741053000	1.676870000
1	-0.393119000	-0.726047000	-1.065212000
6	-1.790035000	-2.288258000	0.719145000
8	-0.664928000	-2.205391000	-0.072122000



6	-3.028352000	-1.652061000	0.082040000
6	-4.105200000	-1.232438000	0.871934000
6	-3.123017000	-1.498250000	-1.303100000
6	-5.246634000	-0.677134000	0.296054000
1	-4.041726000	-1.331695000	1.954159000
6	-4.262001000	-0.942117000	-1.887195000
1	-2.283156000	-1.808658000	-1.918637000
6	-5.330123000	-0.529838000	-1.089970000
1	-6.066654000	-0.348378000	0.929193000
1	-4.313761000	-0.824011000	-2.966617000
1	-6.214823000	-0.090112000	-1.541982000
6	-2.100748000	-3.747970000	1.093285000
1	-1.234845000	-4.185495000	1.602042000
1	-2.971592000	-3.830003000	1.755467000
1	-2.298404000	-4.332070000	0.185907000
6	1.690956000	2.400822000	-0.363956000
6	2.058561000	3.475947000	-0.851932000
6	2.494804000	4.748583000	-1.452073000
1	2.723917000	4.637385000	-2.519327000
1	1.723824000	5.524820000	-1.369780000
1	3.398211000	5.140915000	-0.969069000

**A5<sub>X=CCMe</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	0.922215000	0.651257000	0.480633000
1	-0.015973000	-0.755629000	0.784455000
7	0.422932000	0.427976000	-1.628697000
1	-0.233548000	-0.350568000	-1.678019000
6	1.227187000	0.885277000	2.173047000
8	1.424838000	1.084343000	3.327279000
6	2.344720000	-1.068119000	-1.865434000
6	-0.279195000	1.643176000	-2.038335000
6	1.576645000	0.098737000	-2.470870000
1	3.217119000	-1.301964000	-2.480982000
1	1.700301000	-1.950731000	-1.815666000
1	1.271382000	-0.166560000	-3.493777000
1	2.215868000	0.985256000	-2.529299000
1	-0.850661000	1.509927000	-2.966977000
1	0.472377000	2.420380000	-2.213825000
6	-1.184792000	2.104906000	-0.926879000
6	-2.316183000	2.878254000	-1.177570000
1	-2.576038000	3.126048000	-2.202201000

6	-1.584394000	2.161878000	1.343461000
1	-1.263635000	1.843062000	2.329353000
6	-3.094184000	3.314525000	-0.111662000
1	-3.981082000	3.916668000	-0.283229000
6	-2.721023000	2.940992000	1.176925000
1	-3.299564000	3.239423000	2.044611000
7	-0.814303000	1.753912000	0.321136000
16	2.870161000	-0.611929000	-0.172434000
6	3.239333000	-2.264199000	0.601881000
6	3.744263000	-1.916908000	2.005919000
6	4.342151000	-2.957171000	-0.203372000
1	2.975181000	-1.388798000	2.578792000
1	3.996521000	-2.840111000	2.540652000
1	4.641910000	-1.289673000	1.970639000
1	3.995576000	-3.241772000	-1.202515000
1	5.223267000	-2.316125000	-0.312443000
1	4.649585000	-3.874703000	0.312989000
6	2.012468000	-3.168557000	0.707066000
1	2.309772000	-4.115218000	1.175287000
1	1.234432000	-2.706588000	1.318899000
1	1.578240000	-3.398977000	-0.269727000
1	-1.525696000	-3.490061000	0.422461000
1	-0.381090000	-1.655956000	-0.291957000
6	-1.858221000	-2.923798000	-0.461714000
8	-0.759131000	-2.233807000	-1.018919000
6	-2.965944000	-1.980333000	-0.014589000
6	-3.699753000	-2.256941000	1.141544000
6	-3.296732000	-0.850325000	-0.768841000
6	-4.749185000	-1.427111000	1.537436000
1	-3.441069000	-3.125591000	1.743452000
6	-4.348588000	-0.022870000	-0.380456000
1	-2.720416000	-0.614470000	-1.659673000
6	-5.078446000	-0.307242000	0.774812000
1	-5.302139000	-1.650855000	2.445633000
1	-4.593390000	0.852556000	-0.974477000
1	-5.890319000	0.345855000	1.082207000
6	-2.368517000	-3.912961000	-1.503238000
1	-1.573206000	-4.611497000	-1.782421000
1	-3.214208000	-4.485896000	-1.109941000
1	-2.698693000	-3.380787000	-2.402490000
6	1.991379000	2.312251000	-0.007328000
6	2.629241000	3.343524000	-0.258343000
6	3.389618000	4.569074000	-0.560250000
1	4.406218000	4.529896000	-0.149138000

1	3.487999000	4.736922000	-1.640358000
1	2.909889000	5.462114000	-0.140420000

**TSA2-6<sub>X=CCMe</sub>**

Coordinates (Angstroms)			
	X	Y	Z
25	-0.101725000	-0.380553000	0.096632000
7	-0.441554000	1.042676000	-1.467478000
6	0.190724000	-1.776676000	1.098823000
8	0.389630000	-2.742792000	1.755688000
6	1.935313000	1.560701000	-1.441831000
6	-1.808978000	1.477427000	-1.401397000
6	0.517372000	2.113538000	-1.524899000
1	2.671214000	2.368431000	-1.442651000
1	2.129449000	0.903400000	-2.295059000
1	0.442721000	2.695826000	-2.462367000
1	0.360488000	2.834762000	-0.697140000
1	-2.181615000	1.914508000	-2.345340000
1	-1.935939000	2.264436000	-0.628585000
6	-2.700689000	0.328818000	-1.007132000
6	-4.054556000	0.287270000	-1.340933000
1	-4.480775000	1.087439000	-1.938146000
6	-2.878377000	-1.670530000	0.137779000
1	-2.369791000	-2.432680000	0.718043000
6	-4.836409000	-0.773992000	-0.901794000
1	-5.892962000	-0.822718000	-1.147094000
6	-4.233300000	-1.775579000	-0.143769000
1	-4.795310000	-2.627602000	0.223018000
7	-2.118118000	-0.644370000	-0.278094000
16	2.077535000	0.587573000	0.102028000
6	3.542093000	-0.507989000	-0.237688000
6	3.833065000	-1.189941000	1.103283000
6	4.736375000	0.351942000	-0.658672000
1	2.967418000	-1.759032000	1.455977000
1	4.671049000	-1.886566000	0.984161000
1	4.104080000	-0.459281000	1.872742000
1	4.580731000	0.816202000	-1.637758000
1	4.937767000	1.142294000	0.072234000
1	5.630236000	-0.279476000	-0.730403000
6	3.235893000	-1.560326000	-1.301665000
1	4.131182000	-2.170912000	-1.472041000
1	2.423233000	-2.216961000	-0.981660000
1	2.955027000	-1.109557000	-2.258837000

6	-0.581686000	0.865893000	1.611810000
6	-0.922415000	1.652909000	2.502853000
6	-1.321849000	2.600049000	3.557509000
1	-0.573686000	3.389463000	3.701923000
1	-2.271080000	3.097359000	3.322021000
1	-1.453236000	2.102785000	4.526588000
1	0.199592000	-1.202558000	-1.402483000
1	-0.062037000	-0.283804000	-1.625555000

A6<sub>X=CCMe</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	-0.113038000	-0.458470000	0.097475000
1	0.188762000	-1.540905000	-1.220622000
7	-0.437469000	1.025976000	-1.455386000
1	-0.315252000	0.500563000	-2.316717000
6	0.095159000	-1.692433000	1.298566000
8	0.225541000	-2.529558000	2.132036000
6	1.947994000	1.547588000	-1.376432000
6	-1.828135000	1.467292000	-1.369868000
6	0.538603000	2.117918000	-1.439043000
1	2.679539000	2.358510000	-1.338779000
1	2.144561000	0.941588000	-2.266599000
1	0.451360000	2.759395000	-2.328030000
1	0.336804000	2.731500000	-0.555890000
1	-2.184632000	1.934812000	-2.297244000
1	-1.889539000	2.216000000	-0.572351000
6	-2.711422000	0.305123000	-0.995232000
6	-4.061173000	0.275443000	-1.340613000
1	-4.479438000	1.086161000	-1.929278000
6	-2.898864000	-1.705863000	0.116896000
1	-2.395259000	-2.479576000	0.686614000
6	-4.850614000	-0.789848000	-0.922595000
1	-5.905380000	-0.832188000	-1.175936000
6	-4.252872000	-1.801583000	-0.174940000
1	-4.818738000	-2.657702000	0.176389000
7	-2.128622000	-0.678116000	-0.278867000
16	2.095215000	0.493444000	0.112021000
6	3.589643000	-0.544181000	-0.283761000
6	3.873409000	-1.307266000	1.014561000
6	4.768559000	0.370277000	-0.627305000
1	3.014147000	-1.918901000	1.308959000
1	4.730658000	-1.974070000	0.865935000

1	4.110862000	-0.624458000	1.837413000
1	4.620181000	0.883335000	-1.583134000
1	4.933152000	1.124616000	0.149681000
1	5.681722000	-0.230992000	-0.714394000
6	3.332784000	-1.533647000	-1.417685000
1	4.249295000	-2.105737000	-1.608824000
1	2.532410000	-2.228538000	-1.155288000
1	3.053452000	-1.032154000	-2.350024000
6	-0.574872000	0.958164000	1.487959000
6	-0.894726000	1.784414000	2.352649000
6	-1.267554000	2.769743000	3.382506000
1	-1.980284000	3.512582000	3.001916000
1	-1.737247000	2.294281000	4.252785000
1	-0.395813000	3.323122000	3.753702000

**A7R<sub>x</sub>=CCMe**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.886321000	0.520793000	0.498640000
1	0.170690000	-1.021980000	0.539324000
7	0.549937000	0.448097000	-1.647709000
1	0.050164000	-0.424079000	-1.807122000
6	1.088463000	0.593298000	2.218377000
8	1.226662000	0.677955000	3.396957000
6	2.718113000	-0.652051000	-1.891046000
6	-0.345344000	1.547578000	-1.998995000
6	1.786472000	0.421998000	-2.431779000
1	3.654271000	-0.657958000	-2.455055000
1	2.246173000	-1.634301000	-1.987801000
1	1.591601000	0.224628000	-3.496342000
1	2.257771000	1.406143000	-2.349969000
1	-0.854686000	1.388072000	-2.958807000
1	0.258789000	2.457260000	-2.087953000
6	-1.353968000	1.767711000	-0.902003000
6	-2.562933000	2.416267000	-1.148482000
1	-2.808407000	2.716432000	-2.162764000
6	-1.851120000	1.587905000	1.341509000
1	-1.535146000	1.228906000	2.315055000
6	-3.430319000	2.670893000	-0.093740000
1	-4.375253000	3.178256000	-0.261961000
6	-3.065330000	2.240343000	1.179617000
1	-3.709567000	2.396933000	2.038156000
7	-0.993352000	1.360949000	0.331642000

16	3.045203000	-0.312702000	-0.122370000
6	3.644719000	-1.965799000	0.494532000
6	3.977969000	-1.720510000	1.968928000
6	4.907898000	-2.355304000	-0.277879000
1	3.086686000	-1.421316000	2.529092000
1	4.369339000	-2.642982000	2.413572000
1	4.737635000	-0.939739000	2.086298000
1	4.693094000	-2.552468000	-1.333508000
1	5.670021000	-1.570792000	-0.222003000
1	5.331055000	-3.272757000	0.149427000
6	2.590977000	-3.066055000	0.380328000
1	2.994364000	-3.991073000	0.810979000
1	1.680473000	-2.795225000	0.919229000
1	2.324552000	-3.278061000	-0.659951000
6	-1.922331000	-2.203906000	-1.297456000
8	-1.704240000	-1.532956000	-2.301315000
6	-3.039257000	-1.828490000	-0.374991000
6	-3.185480000	-2.411144000	0.890010000
6	-3.969539000	-0.873971000	-0.801534000
6	-4.244279000	-2.038918000	1.714827000
1	-2.468828000	-3.144517000	1.244273000
6	-5.033893000	-0.512227000	0.017111000
1	-3.849450000	-0.421235000	-1.780142000
6	-5.171803000	-1.093079000	1.278219000
1	-4.345120000	-2.488406000	2.698007000
1	-5.752244000	0.227144000	-0.323777000
1	-5.998668000	-0.806501000	1.921674000
6	-1.114737000	-3.439390000	-1.005278000
1	-0.341834000	-3.553184000	-1.766791000
1	-0.644055000	-3.370597000	-0.021148000
1	-1.766784000	-4.320526000	-1.008201000
6	1.669942000	2.382718000	0.238678000
6	2.110833000	3.532583000	0.107310000
6	2.634303000	4.899818000	-0.060124000
1	2.427145000	5.299230000	-1.061289000
1	2.191807000	5.599825000	0.660005000
1	3.721523000	4.943354000	0.081908000

A7S<sub>X=CCMe</sub>

Coordinates (Angstroms)

	X	Y	Z
25	-1.008057000	0.618035000	0.481895000
1	0.360712000	-0.314682000	0.810231000

7	-0.749457000	-0.128205000	-1.536243000
1	0.025801000	-0.781700000	-1.459277000
6	-1.152087000	1.112708000	2.135852000
8	-1.238121000	1.438720000	3.277975000
6	0.776862000	1.721027000	-1.959118000
6	-1.943444000	-0.894392000	-1.879306000
6	-0.381076000	0.900178000	-2.508970000
1	1.058700000	2.500568000	-2.671179000
1	1.641717000	1.072544000	-1.785482000
1	-0.084499000	0.462074000	-3.473542000
1	-1.254998000	1.536725000	-2.680731000
1	-1.787911000	-1.567522000	-2.732720000
1	-2.732492000	-0.181651000	-2.144369000
6	-2.391404000	-1.673568000	-0.670416000
6	-3.074123000	-2.882326000	-0.785729000
1	-3.254427000	-3.301078000	-1.771012000
6	-2.534984000	-1.753533000	1.629969000
1	-2.289181000	-1.276306000	2.572704000
6	-3.508398000	-3.535378000	0.362166000
1	-4.041487000	-4.478659000	0.294721000
6	-3.235064000	-2.952005000	1.597198000
1	-3.549818000	-3.416055000	2.525804000
7	-2.109853000	-1.115106000	0.526020000
16	0.264456000	2.462671000	-0.367268000
6	1.899749000	2.901488000	0.409637000
6	1.524402000	3.715798000	1.652324000
6	2.709736000	3.764947000	-0.561065000
1	0.885630000	3.134084000	2.324746000
1	2.435572000	3.988316000	2.197922000
1	0.998658000	4.639141000	1.385592000
1	3.046119000	3.192314000	-1.431593000
1	2.130943000	4.625168000	-0.914487000
1	3.603359000	4.143804000	-0.050446000
6	2.700315000	1.668201000	0.823030000
1	3.677177000	1.986126000	1.209357000
1	2.179857000	1.110354000	1.604105000
1	2.875477000	0.986125000	-0.014439000
6	1.279257000	-2.870258000	-0.397020000
8	0.761087000	-2.847185000	-1.508527000
6	2.626004000	-2.245817000	-0.189326000
6	3.224637000	-2.176849000	1.073687000
6	3.295622000	-1.706551000	-1.294695000
6	4.472317000	-1.576912000	1.227728000
1	2.717292000	-2.575941000	1.945764000

6	4.544496000	-1.113032000	-1.142185000
1	2.823801000	-1.756456000	-2.270871000
6	5.134896000	-1.046612000	0.121021000
1	4.924952000	-1.518300000	2.212857000
1	5.054393000	-0.695163000	-2.005123000
1	6.105963000	-0.575835000	0.243850000
6	0.587062000	-3.539019000	0.759132000
1	-0.376559000	-3.927308000	0.424787000
1	1.200665000	-4.359097000	1.148431000
1	0.429487000	-2.821055000	1.569330000
6	-2.671499000	1.627608000	-0.155155000
6	-3.691724000	2.235649000	-0.506940000
6	-4.904519000	2.955252000	-0.934972000
1	-4.699953000	4.012265000	-1.147121000
1	-5.337741000	2.524494000	-1.846909000
1	-5.687831000	2.930360000	-0.167067000

**TSA7-8R<sub>X</sub>=CCMe**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
25	0.626691000	0.481951000	0.388815000
1	0.081824000	-1.121603000	0.007856000
7	0.493467000	0.720457000	-1.730330000
1	0.071315000	-0.170170000	-2.012759000
6	0.583138000	0.114510000	2.082141000
8	0.511917000	-0.162192000	3.236995000
6	2.762106000	-0.164893000	-1.916518000
6	-0.473209000	1.772847000	-2.027421000
6	1.773686000	0.877346000	-2.421950000
1	3.727170000	-0.041528000	-2.414600000
1	2.381917000	-1.170175000	-2.122328000
1	1.663459000	0.768776000	-3.511102000
1	2.151401000	1.885636000	-2.220403000
1	-0.877636000	1.702117000	-3.046707000
1	0.035981000	2.739509000	-1.935916000
6	-1.589517000	1.737648000	-1.017447000
6	-2.836608000	2.298674000	-1.286068000
1	-3.032512000	2.716783000	-2.268764000
6	-2.232591000	1.212159000	1.132844000
1	-1.958269000	0.755307000	2.076795000
6	-3.801365000	2.329697000	-0.286393000
1	-4.776179000	2.771093000	-0.469595000
6	-3.487389000	1.776481000	0.952317000



1	-4.203767000	1.767034000	1.766622000
7	-1.289176000	1.189131000	0.176425000
16	2.939782000	0.054066000	-0.110097000
6	3.774824000	-1.518520000	0.424141000
6	4.016913000	-1.327446000	1.924970000
6	5.109578000	-1.663799000	-0.310757000
1	3.073997000	-1.190537000	2.463210000
1	4.515836000	-2.216196000	2.328474000
1	4.656936000	-0.460668000	2.122783000
1	4.966276000	-1.825277000	-1.384221000
1	5.739977000	-0.778937000	-0.173737000
1	5.649492000	-2.532548000	0.085110000
6	2.895050000	-2.742726000	0.190574000
1	3.381896000	-3.629570000	0.615066000
1	1.917890000	-2.614452000	0.662368000
1	2.738697000	-2.931463000	-0.875660000
6	-1.124706000	-2.168820000	-1.140892000
8	-1.050089000	-1.637258000	-2.263718000
6	-2.351604000	-1.924618000	-0.293975000
6	-2.414514000	-2.257728000	1.064055000
6	-3.493152000	-1.418553000	-0.919718000
6	-3.600745000	-2.099990000	1.774956000
1	-1.525482000	-2.612795000	1.576479000
6	-4.683445000	-1.262087000	-0.210413000
1	-3.437595000	-1.155642000	-1.971486000
6	-4.742327000	-1.607690000	1.138177000
1	-3.633441000	-2.352416000	2.831124000
1	-5.562612000	-0.865425000	-0.710457000
1	-5.667735000	-1.484402000	1.693591000
6	-0.366296000	-3.453516000	-0.883918000
1	0.584518000	-3.431624000	-1.417294000
1	-0.189631000	-3.655377000	0.172926000
1	-0.976110000	-4.272340000	-1.291076000
6	1.203689000	2.411942000	0.609768000
6	1.508299000	3.603145000	0.755913000
6	1.866538000	5.021660000	0.933234000
1	2.921835000	5.210965000	0.699945000
1	1.271221000	5.677762000	0.285530000
1	1.702775000	5.358464000	1.964786000

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**TSA7-8S<sub>x=CCMe</sub>**

-----  
Coordinates (Angstroms)

X

Y

Z  
-----

25	-0.880855000	0.513250000	0.398369000
1	0.387130000	-0.719177000	0.445925000
7	-0.889707000	-0.067105000	-1.648759000
1	-0.263069000	-0.878969000	-1.638145000
6	-0.803014000	0.838218000	2.101150000
8	-0.763558000	1.063588000	3.267374000
6	0.942796000	1.496167000	-2.028288000
6	-2.218054000	-0.572361000	-1.978065000
6	-0.353413000	0.918905000	-2.586941000
1	1.352991000	2.238972000	-2.717437000
1	1.681059000	0.700672000	-1.879619000
1	-0.156425000	0.475590000	-3.574157000
1	-1.096726000	1.713578000	-2.717126000
1	-2.225503000	-1.191749000	-2.885899000
1	-2.880948000	0.284535000	-2.146771000
6	-2.744670000	-1.357496000	-0.804549000
6	-3.691541000	-2.367991000	-0.959803000
1	-4.027147000	-2.636342000	-1.956808000
6	-2.766622000	-1.620521000	1.487796000
1	-2.361615000	-1.301584000	2.441946000
6	-4.196548000	-3.010156000	0.165109000
1	-4.940273000	-3.795031000	0.068127000
6	-3.726084000	-2.621023000	1.417178000
1	-4.088321000	-3.084569000	2.328493000
7	-2.271819000	-0.995786000	0.406190000
16	0.544220000	2.262923000	-0.418233000
6	2.203837000	2.564669000	0.360809000
6	1.900557000	3.479301000	1.552529000
6	3.126512000	3.273896000	-0.632039000
1	1.188859000	3.010512000	2.240744000
1	2.827865000	3.674438000	2.103881000
1	1.486700000	4.440212000	1.228535000
1	3.405961000	2.618155000	-1.463167000
1	2.663120000	4.177717000	-1.042073000
1	4.049919000	3.568805000	-0.119039000
6	2.837090000	1.267630000	0.848951000
1	3.807618000	1.485517000	1.312362000
1	2.199313000	0.772895000	1.585506000
1	3.004096000	0.567037000	0.027224000
6	0.921814000	-2.448824000	-0.221266000
8	0.440702000	-2.536475000	-1.368802000
6	2.388551000	-2.111804000	-0.084488000
6	3.055983000	-2.135980000	1.144832000
6	3.117305000	-1.820296000	-1.242329000

6	4.420959000	-1.865313000	1.214005000
1	2.512508000	-2.346628000	2.060228000
6	4.481522000	-1.545221000	-1.175177000
1	2.597725000	-1.814185000	-2.195343000
6	5.138874000	-1.567016000	0.055161000
1	4.924034000	-1.881860000	2.176630000
1	5.031979000	-1.317266000	-2.083821000
1	6.202658000	-1.354663000	0.112043000
6	0.259807000	-3.210568000	0.907332000
1	-0.805924000	-3.302281000	0.695092000
1	0.696818000	-4.218346000	0.937286000
1	0.392105000	-2.745818000	1.884944000
6	-2.399103000	1.822202000	0.100679000
6	-3.336566000	2.615284000	-0.057536000
6	-4.442066000	3.568507000	-0.258831000
1	-4.955647000	3.406087000	-1.215059000
1	-5.201673000	3.490109000	0.529086000
1	-4.089345000	4.607689000	-0.258997000

**A8R<sub>x</sub>**= CCMc

Coordinates (Angstroms)

	X	Y	Z
25	-0.951505000	0.760287000	-0.165561000
1	0.652803000	-1.575708000	-0.986738000
7	-0.304747000	0.156218000	1.574245000
1	0.248870000	-1.452378000	1.130871000
6	-1.109744000	0.538169000	-1.886991000
8	-1.127549000	0.330662000	-3.056806000
6	-2.335041000	-1.072526000	2.082835000
6	0.899503000	0.780771000	2.066735000
6	-1.208561000	-0.215957000	2.646682000
1	-3.141733000	-1.207741000	2.807330000
1	-1.942398000	-2.052126000	1.798608000
1	-0.699995000	-0.806184000	3.431319000
1	-1.627027000	0.674162000	3.151471000
1	1.574802000	0.077178000	2.589324000
1	0.673704000	1.578612000	2.799597000
6	1.640790000	1.414355000	0.924663000
6	2.943654000	1.898021000	1.051363000
1	3.463943000	1.782918000	1.997187000
6	1.544380000	2.118885000	-1.274512000
1	0.950268000	2.185862000	-2.179498000
6	3.548181000	2.518798000	-0.031169000

1	4.561019000	2.902291000	0.045779000
6	2.829112000	2.634168000	-1.221315000
1	3.256819000	3.108514000	-2.097919000
7	0.952183000	1.514208000	-0.227913000
16	-2.972006000	-0.250501000	0.574992000
6	-3.596874000	-1.690387000	-0.426650000
6	-4.338006000	-1.060181000	-1.608925000
6	-4.567996000	-2.517585000	0.419556000
1	-3.681701000	-0.403792000	-2.188262000
1	-4.697157000	-1.852802000	-2.275831000
1	-5.204042000	-0.478729000	-1.274818000
1	-4.061924000	-3.019478000	1.250314000
1	-5.372260000	-1.896647000	0.828214000
1	-5.022385000	-3.293102000	-0.208656000
6	-2.440884000	-2.559324000	-0.925135000
1	-2.845018000	-3.428846000	-1.458295000
1	-1.799514000	-1.999552000	-1.610257000
1	-1.814595000	-2.924088000	-0.105722000
6	1.223759000	-2.264807000	-0.341212000
8	0.590516000	-2.368137000	0.911153000
6	2.641688000	-1.717809000	-0.223834000
6	3.260425000	-1.115318000	-1.323933000
6	3.360985000	-1.839463000	0.967235000
6	4.572821000	-0.653241000	-1.239474000
1	2.705380000	-0.997748000	-2.252452000
6	4.674038000	-1.376141000	1.057150000
1	2.876879000	-2.290443000	1.828176000
6	5.286376000	-0.783897000	-0.047031000
1	5.034432000	-0.179140000	-2.101328000
1	5.216889000	-1.474549000	1.993503000
1	6.305993000	-0.415552000	0.023598000
6	1.228511000	-3.643017000	-0.996316000
1	0.202681000	-4.006200000	-1.115736000
1	1.701827000	-3.605007000	-1.982693000
1	1.782266000	-4.355892000	-0.374492000
6	-1.740382000	2.574659000	-0.109035000
6	-2.185417000	3.721722000	0.019194000
6	-2.725938000	5.082421000	0.178217000
1	-1.936395000	5.842923000	0.136568000
1	-3.451023000	5.329331000	-0.607268000
1	-3.239752000	5.207672000	1.139574000

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Coordinates (Angstroms)

	X	Y	Z
25	1.210302000	0.465111000	-0.211614000
1	-0.899598000	-1.109882000	-0.380632000
7	1.064028000	-0.062806000	1.681026000
1	-0.403730000	-0.974882000	1.623145000
6	0.665286000	0.521364000	-1.866639000
8	0.263040000	0.493479000	-2.983425000
6	-0.230350000	1.895949000	2.263412000
6	1.965852000	-1.112780000	2.094604000
6	0.826419000	0.905400000	2.731786000
1	-0.331560000	2.736184000	2.954666000
1	-1.194378000	1.387513000	2.170791000
1	0.456810000	0.429964000	3.659035000
1	1.751330000	1.446231000	3.007408000
1	1.563195000	-1.740844000	2.910382000
1	2.922593000	-0.703323000	2.473156000
6	2.271925000	-1.983420000	0.909698000
6	2.789427000	-3.273999000	1.029014000
1	2.974310000	-3.685767000	2.016311000
6	2.268806000	-2.148394000	-1.396336000
1	2.047437000	-1.662648000	-2.340378000
6	3.052766000	-4.011453000	-0.117174000
1	3.454628000	-5.017601000	-0.046970000
6	2.786897000	-3.433503000	-1.358573000
1	2.973762000	-3.966204000	-2.284684000
7	2.007053000	-1.429648000	-0.289644000
16	0.275457000	2.491045000	0.609334000
6	-1.336316000	3.059051000	-0.128242000
6	-0.949077000	3.758119000	-1.434609000
6	-2.011055000	4.050103000	0.822461000
1	-0.405176000	3.082822000	-2.102241000
1	-1.857100000	4.089963000	-1.951220000
1	-0.323850000	4.637593000	-1.246701000
1	-2.338496000	3.566093000	1.748026000
1	-1.342010000	4.877681000	1.080995000
1	-2.900195000	4.469612000	0.336806000
6	-2.255719000	1.872960000	-0.413749000
1	-3.189398000	2.232096000	-0.864155000
1	-1.785261000	1.171492000	-1.106283000
1	-2.518172000	1.328280000	0.498050000
6	-1.506618000	-1.794406000	0.238706000
8	-1.218079000	-1.565311000	1.596160000
6	-2.965462000	-1.503040000	-0.070731000

6	-3.376754000	-1.352458000	-1.400451000
6	-3.916350000	-1.373293000	0.943085000
6	-4.706266000	-1.076530000	-1.710764000
1	-2.642058000	-1.432238000	-2.198842000
6	-5.251412000	-1.100860000	0.636424000
1	-3.598984000	-1.472438000	1.976260000
6	-5.651769000	-0.949719000	-0.690631000
1	-5.003270000	-0.950372000	-2.748387000
1	-5.979476000	-1.001755000	1.437300000
1	-6.689116000	-0.731871000	-0.928449000
6	-1.136027000	-3.228310000	-0.152703000
1	-0.074420000	-3.405201000	0.048718000
1	-1.724894000	-3.945026000	0.431496000
1	-1.320278000	-3.412078000	-1.216899000
6	2.955415000	1.314470000	-0.599178000
6	4.072036000	1.811859000	-0.789260000
6	5.398231000	2.412430000	-1.012312000
1	6.032888000	1.776845000	-1.642440000
1	5.324606000	3.386871000	-1.510826000
1	5.938424000	2.572965000	-0.071021000

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