

Supporting Information
For
Asymmetric Induction with a Chiral Amine Catalyzed by
a Ru-PNP Pincer Complex: Insight from Theoretical
Investigation

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1. Transition states for the asymmetric imine hydrogenation with *tran*- and *cis*-imine.

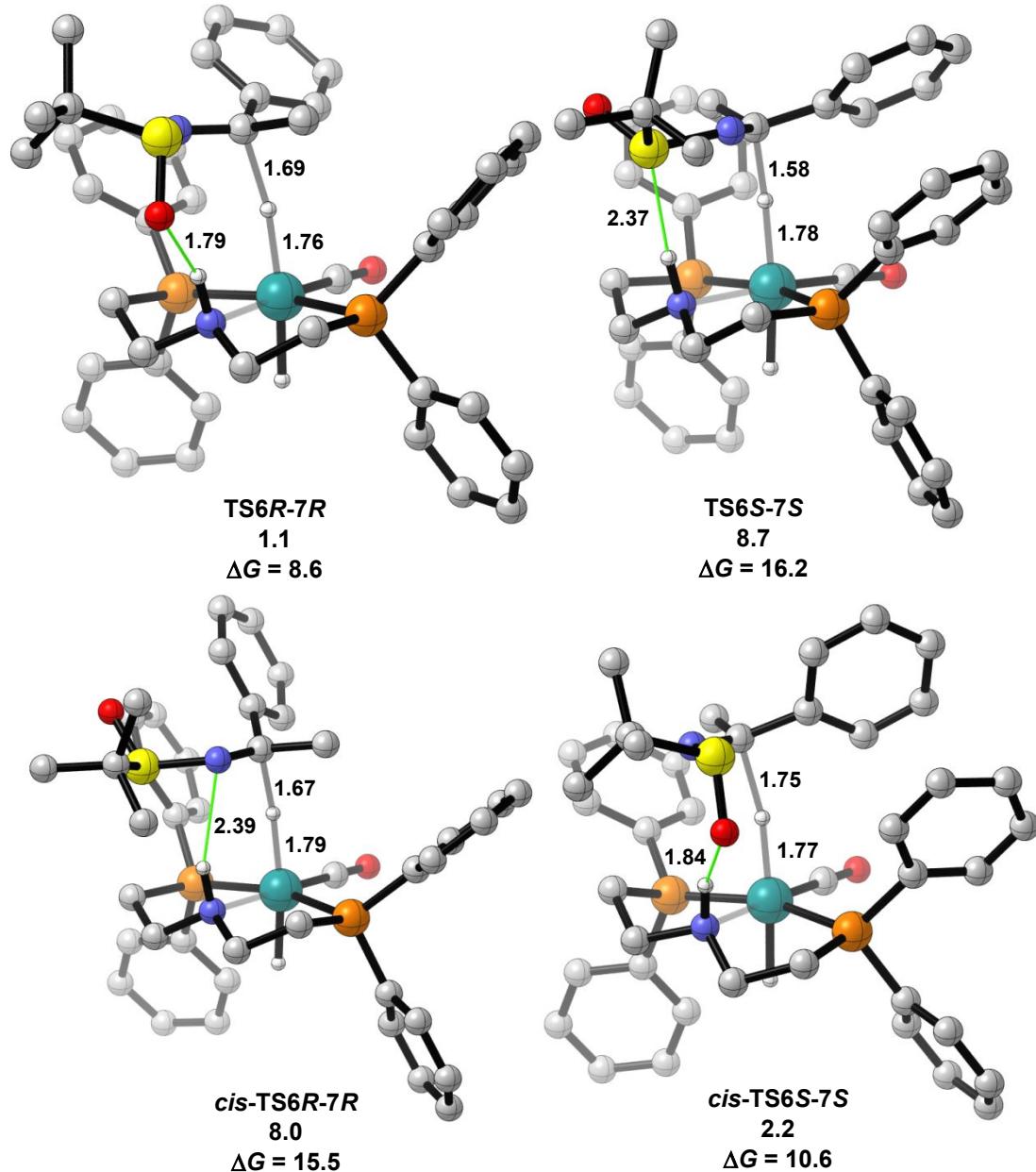


Figure S1. Transition states for the asymmetric imine hydrogenation with *trans*- and *cis*-imine. Free energies and energy barriers (ΔG) are denoted in kcal/mol, and distances are shown in angstroms. Trivial hydrogen atoms are omitted for clarity.

2. Transition states of hydride transfer and structure changes along IRC path

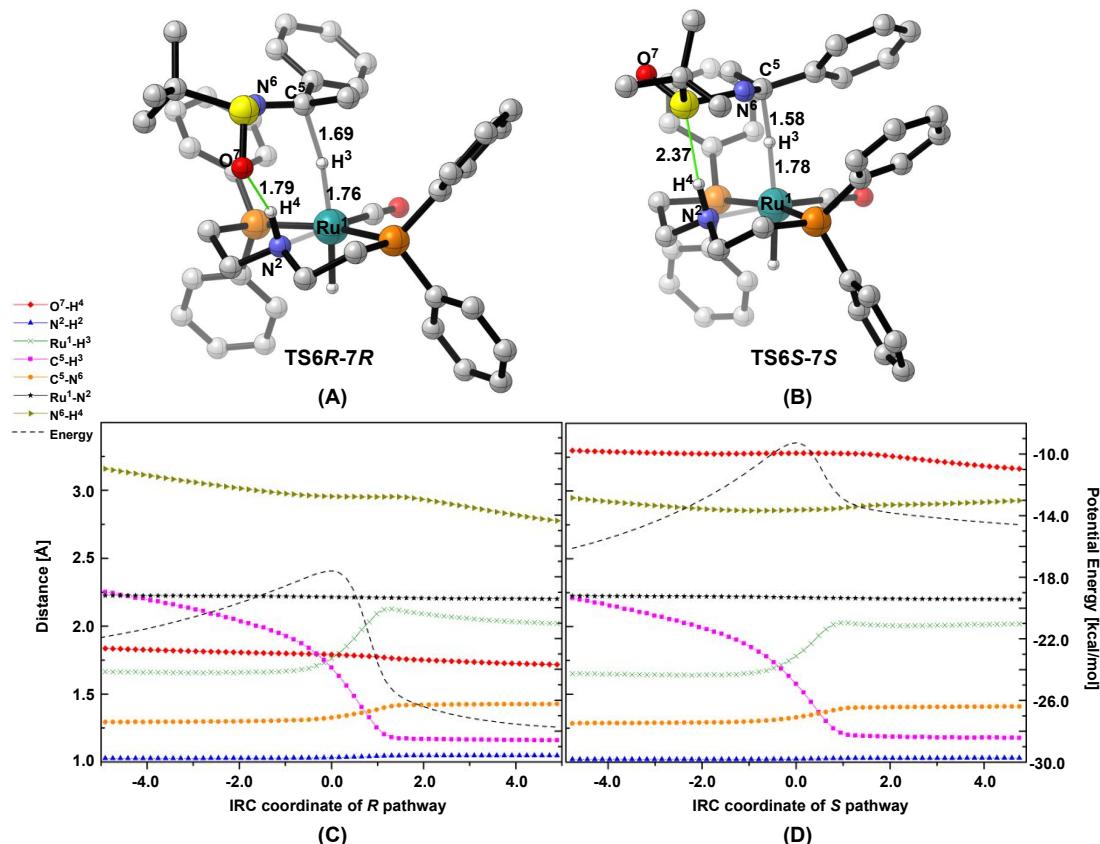


Figure S2. Transition states of hydride transfer in *R* path (A) and in *S* path (B). Less relevant hydrogen atoms are omitted for clarity. All distances are shown in angstroms. The structure changes in the hydride transfer along IRC path of *R* and *S* pathways are shown in (C) and (D), respectively. The potential energies along the IRC are relative to (PNP)RuH(CO) (structure 1).

As shown in Figure S2, in this *R* pathway of hydride transfer, the hydride H³ transfers from Ru¹ to the carbonyl C⁵, and meanwhile the distance of the imine bond C⁵-N⁶ increases slightly. The O⁷-H⁴ distance in **TS6R-7R** is much shorter than that in **TS6S-7S** along the *S* pathway, which shows that the *R* pathway involves N-H \cdots O hydrogen bonding interaction but no such interaction in the *S* pathway.

3. SAPT analysis of **6R** and **6S**

Table S1. SAPT analysis of **6R** and **6S**. All values are given in kcal/mol.

Complex	Electrostatics	Induction	Dispersion	Exchange	Total
6R	-24.7	-8.9	-32.3	35.4	-30.5
6S	-13.0	-4.8	-27.9	24.6	-21.0

Symmetry adapted perturbation theory (SAPT)¹ was calculated by using PSI4 package² at the SPAT0/def2-tzvp level of theory. The total interaction energy for **6R** is calculated to be -30.5 kcal/mol, 9.5 kcal/mol lower than **6S**. And the electrostatics energy, induction energy and dispersion for **6R** are all lower than these for **6S**.

4. Optimized structure of **7R**

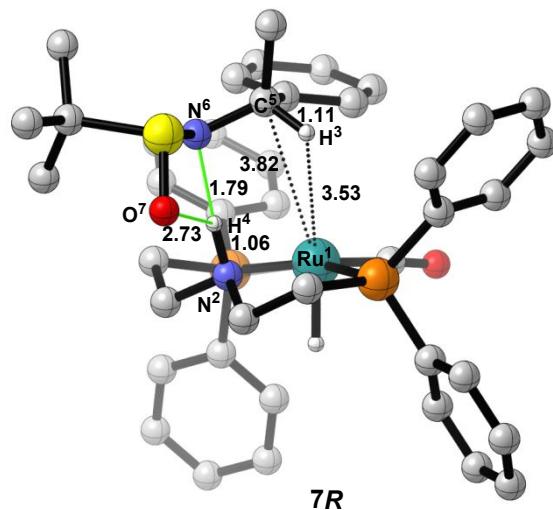


Figure S3. Optimized structure of **7R**. Trivial hydrogen atoms are omitted for clarity.

All distances are shown in angstroms.

7R is stabilized by two noncovalent interactions: strong ionic N-H...N⁻ hydrogen bonding ($d_{N^2-H^4}=1.06 \text{ \AA}$, $d_{H^4...N^6}=1.79 \text{ \AA}$, $d_{N^2-N^6}=2.85 \text{ \AA}$, $\angle N^2-H^4-N^6=176^\circ$) and weak C-H...Ru interaction in **7R** ($d_{C^5-H^3}=1.11 \text{ \AA}$, $d_{H^3-Ru^1}=3.53 \text{ \AA}$, $d_{C^5-Ru^1}=3.82 \text{ \AA}$, $\angle C^5-H^3-Ru^1=97^\circ$) (see Figure S3).

5. Free energy profiles for the alcohol dehydrogenation and the hydrogenation of imine at 393.15 K

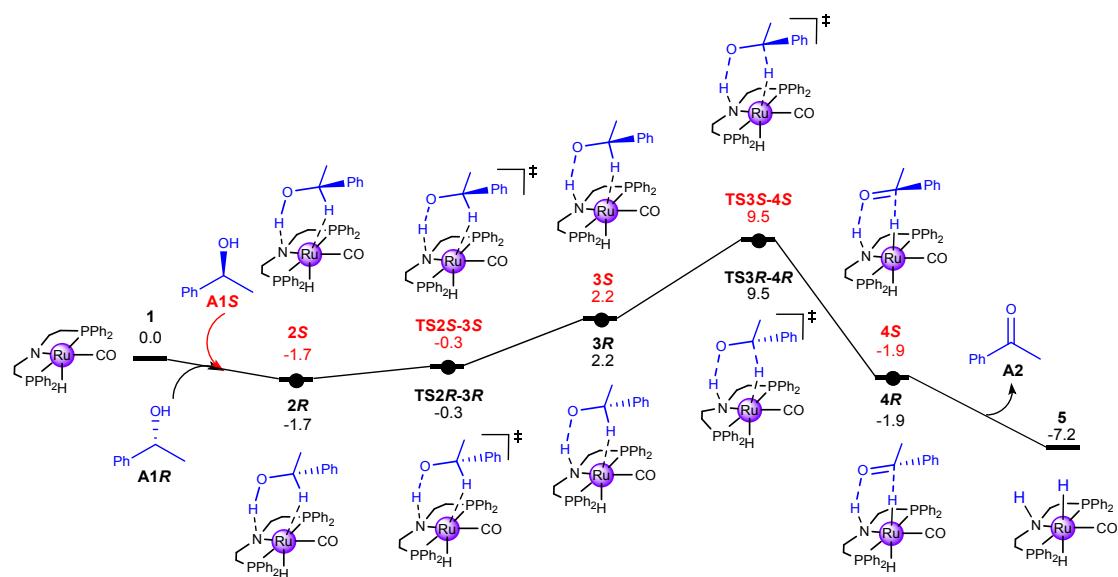


Figure S4. Free energy profiles for the alcohol dehydrogenation (in kcal/mol, calculated at 393.15 K). The energies of stationary points are free energies relative to (PNP)RuH(CO) (structure 1). The *S* path indicates that alcohol is *S*-chiral (in red) while *R* path means *R*-chiral alcohol (in black).

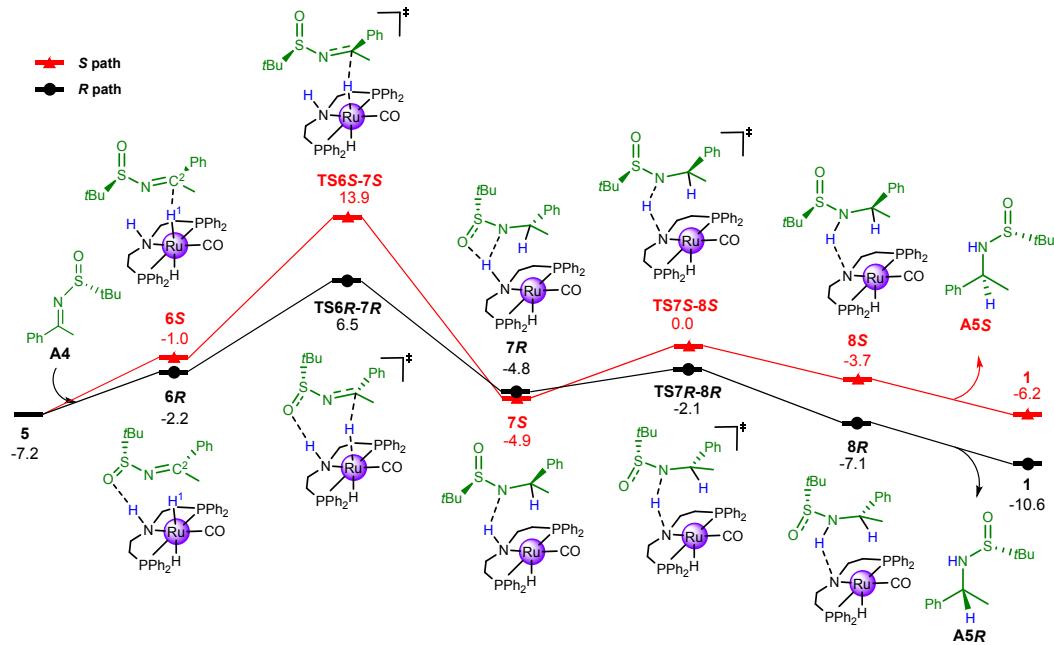


Figure S5. Free energies for the hydrogenation of imine (in kcal/mol, calculated at 393.15 K). The energies of stationary points are free energies relative to (PNP)RuH(CO) (structure **1**). *S* path indicates that final product is (*R,S*)-amine (in red) while *R* path means (*R,R*)-amine (in black).

The free energy profiles of the alcohol dehydrogenation and the hydrogenation of imine calculated at 393.15 K were shown in Figure S4 and Figure S5. Compared with the results at 298.15 K, most of the energy barriers have increased (see Table S3). The energy barriers of the chirality-determining step, the hydride transfer step, in *R/S* rise from 8.6/16.2 kcal/mol to 13.7/21.1 kcal/mol.

6. Formation of imine from acetophenone and Ellman's sulfinamide

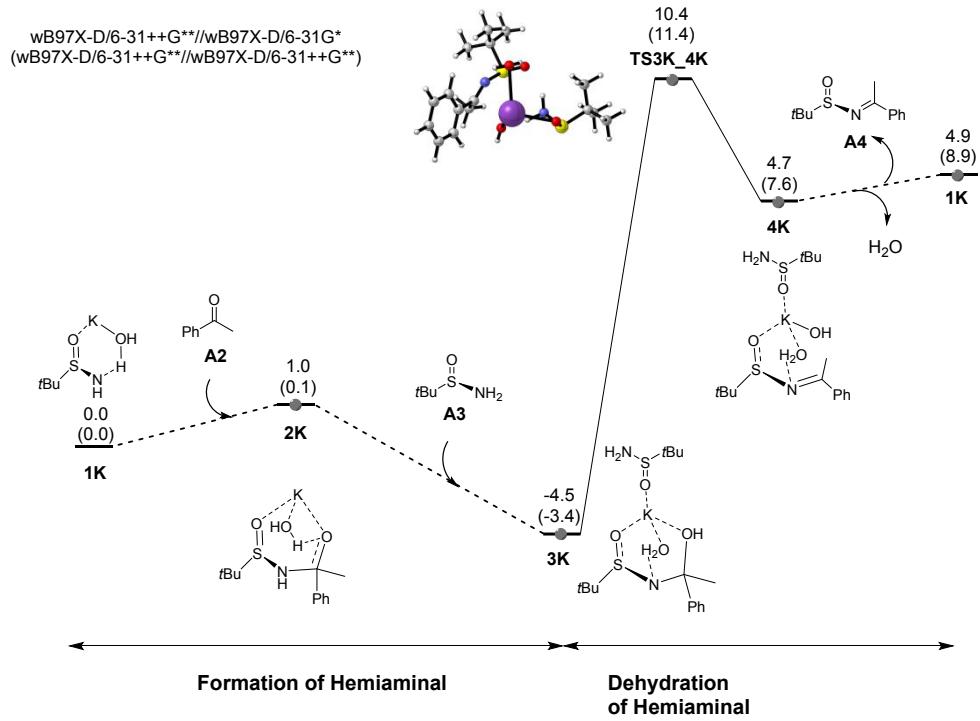


Figure S6. Free energy profiles (in kcal/mol) for the formation of imine (the energies of stationary points are free energies relative to **1K** at ω B97X-D/6-31++G**// ω B97X-D/6-31G* level, the energies in parentheses are free energies relative to **1K** at ω B97X-D/6-31++G** level, less relevant stationary points are omitted (dashed line)).

The geometry optimizations were performed in continuum solvent reaction field of implicit toluene at the ω B97X-D/6-31G* level using Gaussian 09 program. The single-point energies were calculated using ω B97X-D/6-31++G**// ω B97X-D/6-31G*. The SMD polarizable continuum model was employed in the calculations. Free energies were calculated at 298.15 K. Meanwhile, we also investigate the same pathway using DFT method in continuum solvent reaction field of implicit toluene at ω B97X-D/6-31++G** level (see the energies in parentheses in Figure S6 and the following

paragraph).

The mechanism of imine formation involves two steps: formation of hemiaminal and dehydration of hemiaminal. As shown in Figure S6, complex **1K** couple with acetophenone **A2** to form **2K**, then the K ion is coordinated by the O atom of the amine **A3** and proton transfer from the NH moiety to the O atom of C=O moiety to form **3K**, which lies 4.5 (3.4) kcal/mol below **1K**. From the resulting intermediate **3K**, the imine is formed via the transition state **TS3K-4K**, with an energy barrier of 14.9 (14.8) kcal/mol. Finally, the imine **A4** and water are released with the regeneration of **1K**, and the whole process is endergonic, by 4.9 (8.9) kcal/mol. It is obvious that the calculated results at different level are similar, which implies that the method used for the formation of imines are reliable at ω B97X-D/6-31++G**// ω B97X-D/6-31G* level.

7. Comparison of the calculated free energies using different functionals

Table S2. Comparison of free energies (in kcal/mol, relative to **5**) for chirality-determining step calculated using ω B97X-D and M06-L functionals

Complex	ω B97X-D	M06-L
5	0.0	0.0
6R	0.8	2.8
6S	2.6	4.9
TS6R-7R	8.6	8.5
TS6S-7S	16.2	15.1

Both methods using basis sets BS-II for the single point energy calculations and basis sets BS-I for the geometry optimizations. All calculations were performed in continuum solvent reaction field of implicit toluene using Gaussian 09 program. BS-I denotes the LANL2DZ basis set for Ru and the 6-31G* basis set for the other atoms. BS-II denotes the LANL2DZ basis set for Ru and the 6-31++G** basis set for the other atoms. The SMD polarizable continuum model was employed in the calculations. Free energies were calculated at 298.15 K.

The free energies of *6R* and *6S* calculated using M06-L are 2.8 kcal/mol and 4.9 kcal/mol, both are higher than those calculated using ω B97X-D. In the *R*- and *S*-determining steps, M06-L gives lower energy barriers (8.5 kcal/mol and 15.1 kcal/mol) compared with ω B97X-D (8.6 kcal/mol and 16.2 kcal/mol). The computed $\Delta\Delta G$ using ω B97X-D and M06-L are 7.6 kcal/mol and 6.6 kcal/mol, respectively.

8. Energies of all the structures

Table S3. The calculated absolute electronic energies (E , in a.u.), thermal free energies (G , in a.u.), and relative Gibbs energies (ΔG , in kcal/mol) (Calculated at 298.15 K and 1 atm).

Complex	E	G	ΔG
1	-2028.83469026	-2028.38653526	0.0
A1R	-386.00734467	-385.87684667	/
A1S	-386.00734542	-385.87685142	/
2R	-2414.87442881	-2414.27290381	-6.0
2S	-2414.87442879	-2414.27290379	-6.0
TS2R-3R	-2414.87097136	-2414.27152636	-5.1
TS2S-3S	-2414.87097136	-2414.27152636	-5.1
3R	-2414.87153261	-2414.26761861	-2.7
3S	-2414.87153331	-2414.26764431	-2.7
TS3R-4R	-2414.85998618	-2414.25656218	4.3
TS3S-4S	-2414.85998563	-2414.25657163	4.3
4R	-2414.87380183	-2414.27327983	-6.2
4S	-2414.8738009	-2414.2732719	-6.2
5	-2030.05207952	-2029.58205052	-7.5
A2	-384.800798056	-384.693279056	/
A3	-687.105154478	-686.982199478	/
H₂O	-76.4138154704	-76.4104694704	/
A4	-995.486580683	-995.257332683	/
A4_B	-920.317085015	-920.091861015	/
A4_C	-1070.68458884	-1070.45166584	/
cis-A4	-995.479535577	-995.251952577	/
6R	-3025.56050361	-3024.83805561	-6.7

6S	-3025.5537414	-3024.8352354	-4.9
6_{B1}	-2950.38592559	-2949.66427359	-1.5
6_{B2}	-2950.38592554	-2949.66427554	-1.5
6_{C1}	-3100.75146635	-3100.02502535	-0.7
6_{C2}	-3100.75364732	-3100.02804732	-2.6
cis-6R	-3025.54824919	-3024.82712419	-3.2
cis-6S	-3025.55740982	-3024.83551782	-8.4
TS6R-7R	-3025.55053554	-3024.82569954	1.1
TS6S-7S	-3025.53782431	-3024.81355331	8.7
TS6-7_{B1}	-2950.35803737	-2949.63619337	16.2
TS6-7_{B2}	-2950.35803737	-2949.63619337	16.2
TS6-7_{C1}	-3100.75021469	-3100.02047069	0.8
TS6-7_{C2}	-3100.75021459	-3100.02046759	0.8
cis-TS6R-7R	-3025.53170348	-3024.80937948	8.0
cis-TS6S-7S	-3025.54232961	-3024.81857861	2.2
7R	-3025.57119082	-3024.84284382	-9.7
7S	-3025.5710891	-3024.8429941	-9.8
TS7R-8R	-3025.56423136	-3024.83921836	-7.4
TS7S-8S	-3025.55830069	-3024.83513369	-4.8
8R	-3025.57320935	-3024.84626235	-11.8
8S	-3025.56771913	-3024.84071513	-8.3
A5R	-996.710196316	-996.457696316	/
A5S	-996.703688988	-996.450840988	/
1K	-1362.88084621	-1362.75111821	0.0
2K	-1747.70531007	-1747.44282307	1.0
3K	-2434.84199585	-2434.43380185	-4.5
TS3K-4K	-2434.81523766	-2434.41005566	10.4
4K	-2434.82207835	-2434.41904035	4.7
A4 (M06-L)	-995.599774542	-995.374195542	/

5 (M06-L)	-2030.3259627	-2029.8624947	0.0
6R (M06-L)	-3025.94463519	-3025.23228319	2.8
6S (M06-L)	-3025.9414553	-3025.2289603	4.9
TS6R-7R (M06-L)	-3025.93547575	-3025.22322175	8.5
TS6S-7S (M06-L)	-3025.92503165	-3025.21268265	15.1

Table S4. The calculated absolute electronic energies (E , in a.u.), thermal free energies (G , in a.u.), and relative Gibbs energies (ΔG , in kcal/mol) (Calculated at 393.15 K 1 atm).

Complex	E	G	ΔG
1	-2028.83469026	-2028.42026326	0.0
A1R	-386.00734467	-385.89111067	/
A1S	-386.00734542	-385.89111542	/
2R	-2414.87442881	-2414.31415281	-1.7
2S	-2414.87442879	-2414.31415279	-1.7
TS2R-3R	-2414.87097136	-2414.31192036	-0.3
TS2S-3S	-2414.87097136	-2414.31192036	-0.3
3R	-2414.87153261	-2414.30780861	2.2
3S	-2414.87153331	-2414.30784231	2.2
TS3R-4R	-2414.85998618	-2414.29621118	9.5
TS3S-4S	-2414.85998563	-2414.29622163	9.5
4R	-2414.87380183	-2414.31434583	-1.9
4S	-2414.8738009	-2414.3143349	-1.9
5	-2030.05207952	-2029.61564652	-7.2
A2	-384.800798056	-384.707133056	/
A3	-687.105154478	-686.996714478	/
H₂O	-76.4138154704	-76.4177450026	/
A4	-995.486580683	-995.277762683	/
6R	-3025.56050361	-3024.88556561	-2.2

6S	-3025.5537414	-3024.8836794	-1.0
TS6R-7R	-3025.55053554	-3024.87169454	6.5
TS6S-7S	-3025.53782431	-3024.85985631	13.9
7R	-3025.57119082	-3024.88961082	-4.8
7S	-3025.5710891	-3024.8898621	-4.9
TS7R-8R	-3025.56423136	-3024.88538036	-2.1
TS7S-8S	-3025.55830069	-3024.88202269	0.0
8R	-3025.57320935	-3024.89327935	-7.1
8S	-3025.56771913	-3024.88791213	-3.7
A5R	-996.710196316	-996.478567316	/
A5S	-996.703688988	-996.471585988	/

Table S5. The calculated energy barriers at 298.15 K and 393.15 K.

Fundamental step	ΔG (298.15 K) (kcal/mol)	ΔG (393.15 K) (kcal/mol)
2R→3R	0.9	1.4
2S→3S	0.9	1.4
3R→4R	7.0	7.3
3S→4S	7.0	7.3
6R→7R	8.6	13.7
6S→7S	16.2	21.1
7R→8R	2.3	2.7
7S→8S	5.0	4.9

9. Imaginary frequencies of transition states

Table S6. Calculated imaginary frequencies of transition states at ωB97X-D/BSI level.

TS2R-3R	889.79 <i>i</i>
TS2S-3S	889.79 <i>i</i>
TS3R-4R	527.55 <i>i</i>
TS3S-4S	527.83 <i>i</i>
TS6R-7R	513.90 <i>i</i>
TS6S-7S	627.45 <i>i</i>
TS6-7_{B1}	121.10 <i>i</i>
TS6-7_{B2}	121.10 <i>i</i>
TS6-7_{C1}	524.48 <i>i</i>
TS6-7_{C2}	524.71 <i>i</i>
cis-TS6R-7R	598.53 <i>i</i>
cis-TS6S-7S	469.71 <i>i</i>
TS7R-8R	1340.90 <i>i</i>
TS7S-8S	1245.47 <i>i</i>
TS3K-4K	183.89 <i>i</i>
TS6R-7R (M06-L)	560.16 <i>i</i>
TS6S-7S (M06-L)	608.57 <i>i</i>

10. Cartesian coordinates of all the structures

Table S7. Atomic cartesian coordinates of intermediates and transition states (presented in Å).

1

Coordinates (Angstroms)			
	X	Y	Z
44	-0.012080000	0.003272000	-0.015649000
1	0.116789000	1.425337000	-0.714836000
15	-2.285551000	0.302639000	0.353657000
15	2.290970000	-0.188778000	0.334012000
6	-2.265826000	0.959169000	2.077842000
6	2.286426000	-0.942326000	2.017251000
1	-2.021776000	2.022850000	1.976696000
1	-3.235959000	0.868156000	2.578106000
6	-1.160387000	0.246209000	2.858589000
1	3.255730000	-0.907713000	2.524968000
6	1.177756000	-0.274700000	2.825424000
1	2.037800000	-1.997029000	1.849874000
1	-1.570741000	-0.666423000	3.326132000
7	-0.017355000	-0.082719000	2.013173000
1	-0.851625000	0.900900000	3.690126000
1	1.543055000	0.688365000	3.226454000
1	0.948295000	-0.905056000	3.700954000
6	-0.099826000	-0.597651000	-1.781203000
8	-0.163939000	-1.014892000	-2.865502000
6	-3.255692000	-1.252652000	0.460245000
6	-4.549007000	-1.398358000	-0.048081000
6	-2.640920000	-2.349268000	1.080602000
6	-5.219233000	-2.614387000	0.070441000
1	-5.037784000	-0.566357000	-0.545616000
6	-3.316600000	-3.557782000	1.208147000
1	-1.623780000	-2.251116000	1.454620000
6	-4.607722000	-3.693595000	0.701303000
1	-6.221062000	-2.717053000	-0.336784000
1	-2.830569000	-4.398591000	1.694736000
1	-5.131558000	-4.640725000	0.792815000
6	-3.336470000	1.453148000	-0.592057000
6	-4.487132000	2.026252000	-0.036733000
6	-2.984170000	1.765848000	-1.907636000

6	-5.272669000	2.894428000	-0.788268000
1	-4.775812000	1.791197000	0.984180000
6	-3.775199000	2.629494000	-2.661152000
1	-2.083400000	1.337496000	-2.337203000
6	-4.918463000	3.194427000	-2.102520000
1	-6.161573000	3.336868000	-0.348120000
1	-3.494284000	2.863784000	-3.683631000
1	-5.533214000	3.870528000	-2.689692000
6	3.366909000	-1.299369000	-0.649261000
6	4.720000000	-1.039270000	-0.883354000
6	2.798344000	-2.468560000	-1.168024000
6	5.491154000	-1.935176000	-1.619570000
1	5.176359000	-0.132599000	-0.497571000
6	3.571524000	-3.365536000	-1.897838000
1	1.742412000	-2.671792000	-1.005978000
6	4.919720000	-3.099050000	-2.126708000
1	6.540600000	-1.720274000	-1.799160000
1	3.117075000	-4.266643000	-2.299045000
1	5.521854000	-3.793430000	-2.705556000
6	3.242039000	1.369610000	0.458995000
6	4.190644000	1.603783000	1.459876000
6	3.023097000	2.354948000	-0.510524000
6	4.903077000	2.800258000	1.492712000
1	4.386041000	0.854306000	2.220222000
6	3.742576000	3.545247000	-0.483467000
1	2.277196000	2.188447000	-1.282670000
6	4.682472000	3.771185000	0.519952000
1	5.633338000	2.970283000	2.278559000
1	3.563575000	4.300310000	-1.243157000
1	5.237730000	4.704320000	0.546028000

A1R

Coordinates (Angstroms)

	X	Y	Z
1	-1.887412000	1.139504000	-1.572136000
1	-1.856871000	-1.119191000	-0.990501000
6	-1.657590000	-0.297268000	-0.284741000
8	-2.296398000	0.888060000	-0.733493000
6	-0.151793000	-0.130361000	-0.163717000
6	0.698628000	-1.218767000	-0.365356000
6	0.400203000	1.103375000	0.185614000
6	2.075526000	-1.081038000	-0.214110000
1	0.278459000	-2.182635000	-0.645567000
6	1.777185000	1.244988000	0.333105000

1	-0.259375000	1.953036000	0.336989000
6	2.618865000	0.153079000	0.134977000
1	2.725560000	-1.936154000	-0.376749000
1	2.194752000	2.210795000	0.603605000
1	3.693123000	0.264275000	0.249902000
6	-2.290024000	-0.647046000	1.055991000
1	-3.371520000	-0.770125000	0.941377000
1	-1.868946000	-1.577579000	1.449297000
1	-2.102595000	0.151820000	1.781148000

A1S

Coordinates (Angstroms)

	X	Y	Z
1	1.886975000	1.138947000	-1.572546000
1	1.856724000	-1.119630000	-0.990043000
6	1.657569000	-0.297395000	-0.284635000
6	2.290214000	-0.646536000	1.056150000
1	2.102923000	0.152656000	1.780983000
1	1.869183000	-1.576887000	1.449949000
1	3.371688000	-0.769681000	0.941406000
6	0.151787000	-0.130426000	-0.163546000
6	-0.698654000	-1.218832000	-0.365162000
6	-0.400179000	1.103336000	0.185690000
6	-2.075556000	-1.081050000	-0.214039000
1	-0.278489000	-2.182736000	-0.645247000
6	-1.777179000	1.245009000	0.333032000
1	0.259374000	1.953012000	0.337085000
6	-2.618888000	0.153125000	0.134878000
1	-2.725610000	-1.936153000	-0.376662000
1	-2.194730000	2.210854000	0.603418000
1	-3.693148000	0.264377000	0.249661000
8	2.296298000	0.887732000	-0.734027000

2R

Coordinates (Angstroms)

	X	Y	Z
44	-0.301219000	0.406944000	-0.013193000
1	-0.592692000	1.942581000	-0.020671000
15	1.957183000	0.942543000	0.343978000
15	-2.605109000	0.120528000	0.331120000
6	2.153397000	0.486091000	2.114607000
6	-2.699860000	-0.134627000	2.153977000
1	3.014939000	0.961007000	2.594324000

1	2.290014000	-0.601627000	2.144999000
6	0.847110000	0.858861000	2.810122000
1	-3.658249000	0.168462000	2.586167000
6	-1.531174000	0.617162000	2.787343000
1	-2.559646000	-1.208279000	2.319315000
1	0.877364000	0.482783000	3.846561000
7	-0.287896000	0.283583000	2.097385000
1	0.771097000	1.959610000	2.879111000
1	-1.728061000	1.703819000	2.767225000
1	-1.466685000	0.329455000	3.850284000
6	-0.288855000	0.447058000	-1.887582000
8	-0.288347000	0.529997000	-3.048260000
6	3.352851000	0.167534000	-0.548395000
6	3.290189000	0.104395000	-1.944539000
6	4.497747000	-0.296096000	0.103775000
6	4.360708000	-0.397625000	-2.676302000
1	2.400577000	0.451328000	-2.462400000
6	5.567467000	-0.803181000	-0.629949000
1	4.561446000	-0.274194000	1.187568000
6	5.503012000	-0.850879000	-2.019233000
1	4.300054000	-0.439532000	-3.759931000
1	6.450019000	-1.167805000	-0.112605000
1	6.338761000	-1.245931000	-2.589560000
6	2.421765000	2.718394000	0.242542000
6	3.597837000	3.184353000	0.842811000
6	1.637547000	3.612228000	-0.489648000
6	3.966840000	4.520416000	0.733592000
1	4.241206000	2.500755000	1.390543000
6	2.010919000	4.949479000	-0.606385000
1	0.730704000	3.258899000	-0.969907000
6	3.171506000	5.406832000	0.008881000
1	4.878769000	4.869835000	1.208865000
1	1.390652000	5.631954000	-1.179992000
1	3.460119000	6.450246000	-0.079345000
6	-3.467513000	-1.326543000	-0.387860000
6	-4.516036000	-1.973262000	0.275953000
6	-3.046431000	-1.813870000	-1.628076000
6	-5.124767000	-3.090023000	-0.289189000
1	-4.855094000	-1.616557000	1.244787000
6	-3.658954000	-2.927181000	-2.196075000
1	-2.225430000	-1.328657000	-2.146538000
6	-4.695646000	-3.569540000	-1.525131000
1	-5.932611000	-3.589096000	0.238058000
1	-3.316252000	-3.298805000	-3.157271000

1	-5.166657000	-4.445164000	-1.962052000
6	-3.717131000	1.522934000	-0.067576000
6	-4.980592000	1.651085000	0.520750000
6	-3.313970000	2.465413000	-1.016994000
6	-5.816385000	2.707816000	0.175060000
1	-5.322893000	0.922292000	1.250271000
6	-4.153870000	3.518795000	-1.369624000
1	-2.336707000	2.374370000	-1.480165000
6	-5.403617000	3.644316000	-0.770966000
1	-6.791505000	2.800490000	0.644203000
1	-3.826515000	4.242908000	-2.109771000
1	-6.057416000	4.468515000	-1.041183000
1	-0.212225000	-1.429352000	2.224188000
1	-0.396781000	-1.921806000	0.153644000
6	-0.111866000	-2.769731000	0.825887000
6	-1.023507000	-3.940855000	0.462425000
1	-0.767112000	-4.809100000	1.080288000
1	-0.911525000	-4.220223000	-0.589999000
1	-2.069558000	-3.677280000	0.647187000
6	1.340895000	-3.103949000	0.516559000
6	1.805685000	-3.065732000	-0.800098000
6	2.211509000	-3.503650000	1.529731000
6	3.108826000	-3.444188000	-1.103652000
1	1.138982000	-2.726677000	-1.591594000
6	3.521704000	-3.873400000	1.229973000
1	1.846556000	-3.518267000	2.552243000
6	3.971255000	-3.852291000	-0.087664000
1	3.459407000	-3.400582000	-2.130517000
1	4.191769000	-4.182248000	2.028153000
1	4.993326000	-4.135556000	-0.322454000
8	-0.322392000	-2.429810000	2.161511000

2S

Coordinates (Angstroms)

	X	Y	Z
44	0.301219000	0.406945000	-0.013193000
1	0.592692000	1.942582000	-0.020671000
15	-1.957184000	0.942543000	0.343978000
15	2.605109000	0.120528000	0.331120000
6	-2.153398000	0.486091000	2.114606000
6	2.699860000	-0.134626000	2.153977000
1	-3.014940000	0.961006000	2.594323000
1	-2.290015000	-0.601627000	2.144999000
6	-0.847111000	0.858860000	2.810122000

1	3.658249000	0.168464000	2.586167000
6	1.531173000	0.617163000	2.787343000
1	2.559646000	-1.208278000	2.319316000
1	-0.877365000	0.482782000	3.846561000
7	0.287896000	0.283583000	2.097385000
1	-0.771098000	1.959610000	2.879112000
1	1.728060000	1.703820000	2.767225000
1	1.466684000	0.329455000	3.850284000
6	0.288856000	0.447060000	-1.887583000
8	0.288348000	0.529999000	-3.048260000
6	-3.352851000	0.167534000	-0.548395000
6	-3.290188000	0.104394000	-1.944539000
6	-4.497747000	-0.296096000	0.103774000
6	-4.360707000	-0.397627000	-2.676303000
1	-2.400576000	0.451326000	-2.462400000
6	-5.567467000	-0.803182000	-0.629950000
1	-4.561446000	-0.274194000	1.187567000
6	-5.503011000	-0.850880000	-2.019234000
1	-4.300053000	-0.439534000	-3.759932000
1	-6.450019000	-1.167806000	-0.112607000
1	-6.338760000	-1.245933000	-2.589562000
6	-2.421766000	2.718393000	0.242542000
6	-3.597839000	3.184352000	0.842810000
6	-1.637549000	3.612229000	-0.489646000
6	-3.966843000	4.520414000	0.733592000
1	-4.241208000	2.500752000	1.390541000
6	-2.010921000	4.949479000	-0.606383000
1	-0.730705000	3.258901000	-0.969905000
6	-3.171509000	5.406832000	0.008883000
1	-4.878773000	4.869832000	1.208865000
1	-1.390654000	5.631955000	-1.179989000
1	-3.460123000	6.450245000	-0.079343000
6	3.467513000	-1.326542000	-0.387860000
6	4.516035000	-1.973262000	0.275954000
6	3.046432000	-1.813868000	-1.628077000
6	5.124766000	-3.090023000	-0.289188000
1	4.855091000	-1.616558000	1.244789000
6	3.658956000	-2.927179000	-2.196075000
1	2.225432000	-1.328655000	-2.146540000
6	4.695646000	-3.569539000	-1.525130000
1	5.932610000	-3.589097000	0.238060000
1	3.316255000	-3.298802000	-3.157273000
1	5.166658000	-4.445163000	-1.962052000
6	3.717131000	1.522934000	-0.067575000

6	4.980593000	1.651084000	0.520750000
6	3.313970000	2.465414000	-1.016993000
6	5.816386000	2.707815000	0.175060000
1	5.322894000	0.922291000	1.250270000
6	4.153871000	3.518795000	-1.369623000
1	2.336707000	2.374372000	-1.480164000
6	5.403618000	3.644316000	-0.770966000
1	6.791506000	2.800488000	0.644202000
1	3.826516000	4.242909000	-2.109769000
1	6.057417000	4.468515000	-1.041182000
1	0.212226000	-1.429353000	2.224187000
1	0.396781000	-1.921805000	0.153643000
6	0.111866000	-2.769731000	0.825886000
6	1.023508000	-3.940855000	0.462423000
1	0.767112000	-4.809100000	1.080286000
1	0.911525000	-4.220222000	-0.590001000
1	2.069559000	-3.677280000	0.647185000
6	-1.340895000	-3.103949000	0.516559000
6	-1.805685000	-3.065731000	-0.800097000
6	-2.211508000	-3.503651000	1.529731000
6	-3.108826000	-3.444188000	-1.103651000
1	-1.138983000	-2.726676000	-1.591594000
6	-3.521702000	-3.873401000	1.229974000
1	-1.846554000	-3.518269000	2.552243000
6	-3.971255000	-3.852292000	-0.087662000
1	-3.459409000	-3.400582000	-2.130515000
1	-4.191767000	-4.182250000	2.028155000
1	-4.993326000	-4.135557000	-0.322451000
8	0.322393000	-2.429810000	2.161510000

TS2R-3R

Coordinates (Angstroms)

	X	Y	Z
44	0.756356000	0.767487000	-0.030840000
1	1.457112000	2.135474000	-0.641640000
15	2.813664000	-0.276054000	-0.341993000
15	-1.313864000	1.774699000	-0.387348000
6	2.657496000	-0.942265000	-2.063053000
6	-1.734100000	1.148191000	-2.070094000
1	3.629123000	-1.082778000	-2.546925000
1	2.151570000	-1.913617000	-2.009965000
6	1.779770000	0.018648000	-2.859126000
1	-2.484096000	1.758953000	-2.581985000
6	-0.443276000	1.060731000	-2.876100000

1	-2.130826000	0.136316000	-1.933891000
1	1.605800000	-0.384609000	-3.866005000
7	0.498141000	0.188346000	-2.152524000
1	2.256297000	1.000091000	-2.953512000
1	0.016853000	2.047059000	-2.998527000
1	-0.648644000	0.643424000	-3.871322000
6	1.012598000	1.325254000	1.716193000
8	1.194013000	1.700517000	2.802872000
1	0.052503000	-0.742780000	-2.156256000
1	-0.066179000	-0.739883000	0.363330000
6	3.316603000	-1.698810000	0.693785000
6	3.221172000	-1.550693000	2.082358000
6	3.761800000	-2.915171000	0.171171000
6	3.559344000	-2.599264000	2.930527000
1	2.864376000	-0.613644000	2.501289000
6	4.093172000	-3.969056000	1.021070000
1	3.845527000	-3.056985000	-0.902456000
6	3.990909000	-3.813976000	2.400194000
1	3.474504000	-2.471160000	4.005516000
1	4.430803000	-4.912330000	0.601711000
1	4.246077000	-4.636765000	3.061528000
6	4.367245000	0.708119000	-0.380188000
6	5.590692000	0.090369000	-0.670225000
6	4.346458000	2.076116000	-0.105755000
6	6.766647000	0.830491000	-0.698357000
1	5.629547000	-0.979025000	-0.862670000
6	5.526819000	2.817929000	-0.129573000
1	3.398989000	2.556195000	0.119176000
6	6.735887000	2.198357000	-0.427531000
1	7.709016000	0.339639000	-0.923834000
1	5.496907000	3.882046000	0.086384000
1	7.655949000	2.775718000	-0.445437000
6	-2.787285000	1.447489000	0.641587000
6	-4.005065000	1.012738000	0.114641000
6	-2.698116000	1.730200000	2.008749000
6	-5.121787000	0.882297000	0.937985000
1	-4.096385000	0.781098000	-0.942028000
6	-3.815586000	1.612689000	2.825874000
1	-1.750482000	2.047235000	2.435312000
6	-5.031541000	1.191669000	2.291017000
1	-6.063200000	0.541205000	0.516622000
1	-3.731780000	1.834272000	3.885289000
1	-5.903458000	1.094942000	2.931692000
6	-1.422770000	3.604558000	-0.553356000

6	-2.593286000	4.200512000	-1.039666000
6	-0.353528000	4.418908000	-0.178430000
6	-2.682653000	5.581293000	-1.170301000
1	-3.447671000	3.583653000	-1.308267000
6	-0.446420000	5.804926000	-0.298549000
1	0.554617000	3.960912000	0.201142000
6	-1.605944000	6.386768000	-0.800173000
1	-3.593035000	6.030548000	-1.556609000
1	0.392272000	6.428166000	-0.001484000
1	-1.676285000	7.466191000	-0.900088000
6	-3.524736000	-1.688834000	3.351511000
6	-2.716400000	-1.277345000	4.405656000
6	-1.353629000	-1.078046000	4.188320000
6	-0.806690000	-1.309522000	2.933122000
6	-1.609294000	-1.736195000	1.870735000
6	-2.975872000	-1.910356000	2.091043000
1	-4.590252000	-1.833088000	3.504981000
1	-3.145598000	-1.102783000	5.388392000
1	-0.713751000	-0.738650000	4.998017000
1	0.251497000	-1.136309000	2.765859000
1	-3.602478000	-2.227301000	1.265324000
6	-1.021529000	-2.127768000	0.538535000
6	0.188707000	-3.043558000	0.626050000
1	0.842759000	-2.764737000	1.450346000
1	-0.165715000	-4.068571000	0.799732000
1	0.779249000	-3.026923000	-0.291963000
7	-1.891136000	-2.186469000	-0.461598000
16	-1.442217000	-3.122623000	-1.779761000
6	-3.125281000	-3.306078000	-2.531010000
6	-3.754314000	-1.940227000	-2.779741000
1	-4.715039000	-2.067900000	-3.293228000
1	-3.930315000	-1.416538000	-1.836581000
1	-3.107464000	-1.327645000	-3.416681000
6	-3.961551000	-4.150403000	-1.570498000
1	-4.119634000	-3.632779000	-0.620338000
1	-4.940834000	-4.350809000	-2.021045000
1	-3.485202000	-5.116153000	-1.363152000
6	-2.893430000	-4.045276000	-3.851333000
1	-3.855192000	-4.212633000	-4.349854000
1	-2.254449000	-3.460382000	-4.519646000
1	-2.422707000	-5.022927000	-3.692025000
8	-0.648804000	-2.272535000	-2.768437000

TS2S-3S

Coordinates (Angstroms)			
	X	Y	Z
44	-0.706262000	0.777175000	-0.037691000
1	-1.386870000	2.144131000	-0.660303000
15	-2.797043000	-0.224329000	-0.313896000
15	1.372178000	1.758291000	-0.433424000
6	-2.645451000	-0.960922000	-2.006880000
6	1.746761000	1.168481000	-2.144609000
1	-3.616352000	-1.116816000	-2.487025000
1	-2.153008000	-1.936518000	-1.911029000
6	-1.773033000	-0.034251000	-2.848517000
1	2.455551000	1.816161000	-2.669354000
6	0.436323000	1.053750000	-2.915507000
1	2.194532000	0.173971000	-2.040572000
1	-1.619437000	-0.464706000	-3.847471000
7	-0.477787000	0.166196000	-2.172340000
1	-2.245837000	0.946414000	-2.963575000
1	-0.047808000	2.030060000	-3.017593000
1	0.621101000	0.650115000	-3.920826000
6	-0.931424000	1.395894000	1.691545000
8	-1.087646000	1.821589000	2.762084000
1	-0.014148000	-0.744349000	-2.133156000
1	0.089076000	-0.760843000	0.386543000
6	-3.371917000	-1.583144000	0.765496000
6	-3.294413000	-1.385891000	2.148651000
6	-3.861338000	-2.796929000	0.277809000
6	-3.693574000	-2.386214000	3.027877000
1	-2.904381000	-0.450474000	2.541036000
6	-4.252867000	-3.802197000	1.159465000
1	-3.928055000	-2.977394000	-0.791180000
6	-4.167944000	-3.599928000	2.533514000
1	-3.621376000	-2.222817000	4.098956000
1	-4.620470000	-4.746297000	0.768337000
1	-4.468315000	-4.386552000	3.219246000
6	-4.304886000	0.822166000	-0.409365000
6	-5.521395000	0.275762000	-0.837251000
6	-4.262541000	2.161029000	-0.018093000
6	-6.667987000	1.059505000	-0.890173000
1	-5.579780000	-0.773014000	-1.118098000
6	-5.414921000	2.944505000	-0.060766000
1	-3.321885000	2.587911000	0.315073000
6	-6.615646000	2.398016000	-0.501919000
1	-7.604104000	0.625557000	-1.229236000
1	-5.369163000	3.984576000	0.248860000

1	-7.512815000	3.009373000	-0.538626000
6	2.866908000	1.383983000	0.546260000
6	4.070387000	0.960069000	-0.021304000
6	2.807518000	1.620922000	1.923620000
6	5.201260000	0.789372000	0.774746000
1	4.141461000	0.763980000	-1.086759000
6	3.940510000	1.467608000	2.712706000
1	1.870815000	1.926170000	2.381567000
6	5.140663000	1.052623000	2.139156000
1	6.130537000	0.453982000	0.323239000
1	3.879905000	1.653013000	3.780442000
1	6.024081000	0.923926000	2.757906000
6	1.496404000	3.589722000	-0.558333000
6	2.675716000	4.185445000	-1.023649000
6	0.433352000	4.405472000	-0.168919000
6	2.779593000	5.567965000	-1.118877000
1	3.525941000	3.566876000	-1.301221000
6	0.540849000	5.792964000	-0.254034000
1	-0.480919000	3.948959000	0.196387000
6	1.709090000	6.375016000	-0.734304000
1	3.697026000	6.017449000	-1.487560000
1	-0.292777000	6.417003000	0.055107000
1	1.791456000	7.455810000	-0.805353000
6	3.569302000	-1.814833000	3.274482000
6	2.832261000	-1.351927000	4.359483000
6	1.477535000	-1.066224000	4.195250000
6	0.867684000	-1.264487000	2.962771000
6	1.597209000	-1.743199000	1.870380000
6	2.957238000	-2.003427000	2.037764000
1	4.629018000	-2.026634000	3.386233000
1	3.309856000	-1.205756000	5.324476000
1	0.892843000	-0.689190000	5.029803000
1	-0.186257000	-1.034610000	2.840081000
1	3.526316000	-2.365835000	1.189285000
6	0.919958000	-2.088538000	0.560052000
6	-0.294383000	-2.992304000	0.738377000
1	-0.916939000	-2.659680000	1.568439000
1	0.066920000	-4.005583000	0.949702000
1	-0.901832000	-3.042306000	-0.163566000
7	1.764769000	-2.229824000	-0.457273000
16	1.259382000	-2.739448000	-1.955618000
6	2.933543000	-3.280695000	-2.569032000
6	3.883680000	-2.086326000	-2.583972000
1	4.856732000	-2.402526000	-2.980227000

1	4.031000000	-1.684660000	-1.578156000
1	3.510553000	-1.284834000	-3.234262000
6	3.435362000	-4.397993000	-1.659308000
1	3.643267000	-4.023396000	-0.653229000
1	4.357185000	-4.825432000	-2.072250000
1	2.687224000	-5.193614000	-1.585825000
6	2.690668000	-3.802724000	-3.986406000
1	3.634250000	-4.163788000	-4.411563000
1	2.305462000	-3.015681000	-4.646971000
1	1.974023000	-4.628978000	-3.982282000
8	0.415096000	-3.991642000	-1.987980000

3R

Coordinates (Angstroms)

	X	Y	Z
44	-0.337881000	0.354457000	-0.008993000
1	-0.684006000	1.903751000	-0.023594000
15	-2.633900000	-0.007591000	0.305081000
15	1.895906000	0.996708000	0.348518000
6	2.054518000	0.693532000	2.157247000
1	2.909496000	1.203688000	2.610290000
6	0.738965000	1.123936000	2.798942000
1	2.163627000	-0.389300000	2.296299000
7	-0.359726000	0.375104000	2.164952000
1	0.569497000	2.199643000	2.670772000
1	0.764751000	0.908254000	3.876123000
6	-0.298423000	0.365788000	-1.873685000
8	-0.275885000	0.421926000	-3.032852000
1	-0.145464000	-0.675956000	2.354088000
1	-0.001578000	-1.532960000	0.357688000
6	-3.467836000	-1.474421000	-0.397809000
6	-4.450385000	-2.183814000	0.300542000
6	-3.098253000	-1.901327000	-1.676115000
6	-5.048598000	-3.303224000	-0.270425000
1	-4.743064000	-1.878621000	1.301347000
6	-3.702863000	-3.015427000	-2.250023000
1	-2.323240000	-1.369964000	-2.220104000
6	-4.675961000	-3.719975000	-1.546177000
1	-5.802885000	-3.853368000	0.284478000
1	-3.403769000	-3.339247000	-3.242462000
1	-5.139630000	-4.596666000	-1.988698000
6	-3.805977000	1.351654000	-0.076132000
6	-5.112883000	1.332229000	0.426194000
6	-3.416125000	2.403097000	-0.908140000

6	-6.005222000	2.351286000	0.114263000
1	-5.444531000	0.512963000	1.058720000
6	-4.312550000	3.421274000	-1.226793000
1	-2.407049000	2.423857000	-1.307043000
6	-5.605081000	3.399689000	-0.713056000
1	-7.014372000	2.326145000	0.514785000
1	-3.996660000	4.231312000	-1.877631000
1	-6.303367000	4.194211000	-0.959489000
6	3.340727000	0.210384000	-0.443258000
6	4.385121000	-0.362104000	0.284366000
6	3.419765000	0.251503000	-1.839892000
6	5.499729000	-0.873253000	-0.376288000
1	4.335022000	-0.426088000	1.366578000
6	4.534761000	-0.255276000	-2.496090000
1	2.607268000	0.686545000	-2.416380000
6	5.579848000	-0.815707000	-1.763672000
1	6.301764000	-1.326982000	0.198161000
1	4.587610000	-0.214689000	-3.580138000
1	6.450427000	-1.216366000	-2.274682000
6	2.313139000	2.773504000	0.131421000
6	3.484973000	3.295105000	0.693902000
6	1.504988000	3.608317000	-0.642371000
6	3.826691000	4.629241000	0.505445000
1	4.144264000	2.653742000	1.273167000
6	1.851975000	4.943477000	-0.839516000
1	0.600675000	3.210863000	-1.091510000
6	3.008675000	5.457079000	-0.262525000
1	4.735180000	5.022897000	0.951862000
1	1.214859000	5.580485000	-1.446072000
1	3.276511000	6.498833000	-0.413465000
6	0.259365000	-2.458833000	1.078636000
8	0.234886000	-2.130562000	2.362235000
6	1.622723000	-2.912892000	0.545287000
6	1.915815000	-2.921498000	-0.819956000
6	2.572944000	-3.397130000	1.441949000
6	3.123044000	-3.431679000	-1.284373000
1	1.191827000	-2.511255000	-1.523053000
6	3.784978000	-3.910233000	0.981715000
1	2.334348000	-3.367591000	2.500943000
6	4.059788000	-3.937003000	-0.382759000
1	3.341465000	-3.422536000	-2.348695000
1	4.516122000	-4.290385000	1.691142000
1	5.005229000	-4.332197000	-0.744622000
6	-0.810461000	-3.496574000	0.684599000

1	-1.794056000	-3.166447000	1.030757000
1	-0.860807000	-3.669339000	-0.396373000
1	-0.575628000	-4.445841000	1.180901000
6	-2.723213000	-0.225881000	2.137365000
1	-3.715753000	-0.019874000	2.548629000
6	-1.667389000	0.675293000	2.769917000
1	-2.464002000	-1.269922000	2.349091000
1	-1.905005000	1.733708000	2.610444000
1	-1.630229000	0.494378000	3.853310000

3S

Coordinates (Angstroms)

	X	Y	Z
44	0.337812000	0.354360000	-0.009020000
1	0.683857000	1.903668000	-0.023519000
15	2.633867000	-0.007620000	0.305083000
15	-1.895963000	0.996603000	0.348488000
6	-2.054596000	0.693383000	2.157213000
1	-2.909542000	1.203579000	2.610272000
6	-0.739040000	1.123694000	2.798956000
1	-2.163813000	-0.389439000	2.296228000
7	0.359647000	0.374901000	2.164928000
1	-0.569551000	2.199409000	2.670879000
1	-0.764851000	0.907927000	3.876121000
6	0.298376000	0.365777000	-1.873715000
8	0.275844000	0.421951000	-3.032880000
1	0.145464000	-0.676190000	2.354015000
1	0.001732000	-1.533071000	0.357545000
6	3.468052000	-1.474261000	-0.397903000
6	4.450417000	-2.183811000	0.300541000
6	3.098867000	-1.900808000	-1.676448000
6	5.048855000	-3.303023000	-0.270581000
1	4.742752000	-1.878904000	1.301533000
6	3.703715000	-3.014698000	-2.250510000
1	2.323989000	-1.369319000	-2.220511000
6	4.676637000	-3.719402000	-1.546575000
1	5.802987000	-3.853309000	0.284393000
1	3.404953000	-3.338232000	-3.243142000
1	5.140489000	-4.595938000	-1.989213000
6	3.805836000	1.351781000	-0.075925000
6	5.112729000	1.332393000	0.426417000
6	3.415912000	2.403316000	-0.907790000
6	6.004988000	2.351577000	0.114661000
1	5.444435000	0.513053000	1.058819000

6	4.312252000	3.421620000	-1.226266000
1	2.406851000	2.424037000	-1.306731000
6	5.604776000	3.400074000	-0.712500000
1	7.014134000	2.326455000	0.515195000
1	3.996300000	4.231728000	-1.876986000
1	6.302999000	4.194695000	-0.958795000
6	-3.340783000	0.210276000	-0.443304000
6	-4.385254000	-0.362064000	0.284327000
6	-3.419772000	0.251276000	-1.839943000
6	-5.499881000	-0.873185000	-0.376319000
1	-4.335212000	-0.425958000	1.366549000
6	-4.534784000	-0.255477000	-2.496138000
1	-2.607228000	0.686204000	-2.416449000
6	-5.579946000	-0.815756000	-1.763710000
1	-6.301970000	-1.326795000	0.198146000
1	-4.587585000	-0.214985000	-3.580191000
1	-6.450536000	-1.216391000	-2.274720000
6	-2.313227000	2.773389000	0.131401000
6	-3.485048000	3.294990000	0.693907000
6	-1.505115000	3.608188000	-0.642449000
6	-3.826795000	4.629114000	0.505413000
1	-4.144310000	2.653636000	1.273214000
6	-1.852132000	4.943335000	-0.839629000
1	-0.600811000	3.210734000	-1.091606000
6	-3.008821000	5.456937000	-0.262615000
1	-4.735275000	5.022770000	0.951848000
1	-1.215048000	5.580333000	-1.446229000
1	-3.276682000	6.498680000	-0.413584000
6	-0.259095000	-2.459019000	1.078431000
8	-0.234308000	-2.130912000	2.362067000
6	-1.622596000	-2.912950000	0.545319000
6	-1.915891000	-2.921564000	-0.819885000
6	-2.572738000	-3.397058000	1.442128000
6	-3.123232000	-3.431635000	-1.284116000
1	-1.191958000	-2.511422000	-1.523099000
6	-3.784901000	-3.910033000	0.982080000
1	-2.333980000	-3.367536000	2.501085000
6	-4.059906000	-3.936826000	-0.382351000
1	-3.341794000	-3.422527000	-2.348410000
1	-4.515982000	-4.290091000	1.691623000
1	-5.005440000	-4.331932000	-0.744066000
6	0.810603000	-3.496738000	0.684022000
1	1.794277000	-3.166706000	1.030045000
1	0.860736000	-3.669341000	-0.396988000

1	0.575831000	-4.446077000	1.180217000
6	2.723103000	-0.226094000	2.137340000
1	3.715648000	-0.020211000	2.548655000
6	1.667301000	0.675076000	2.769924000
1	2.463783000	-1.270140000	2.348933000
1	1.904918000	1.733498000	2.610495000
1	1.630120000	0.494118000	3.853308000

TS3R-4R

Coordinates (Angstroms)			
	X	Y	Z
44	-0.325818000	0.358422000	-0.020642000
1	-0.641093000	1.952070000	0.230478000
15	-2.607823000	0.019789000	0.333246000
15	1.919767000	0.921471000	0.284863000
6	2.164579000	0.541444000	2.076362000
1	3.001185000	1.086843000	2.523463000
6	0.866547000	0.865628000	2.808183000
1	2.378790000	-0.531295000	2.148487000
7	-0.261689000	0.163073000	2.170644000
1	0.664074000	1.941072000	2.766247000
1	0.945975000	0.573902000	3.864727000
6	-0.394310000	0.549282000	-1.861362000
8	-0.447321000	0.695770000	-3.014861000
1	-0.117223000	-0.859980000	2.277912000
1	-0.016168000	-1.395495000	0.001975000
6	-3.519314000	-1.365186000	-0.440669000
6	-4.412165000	-2.173608000	0.268915000
6	-3.300129000	-1.621273000	-1.797526000
6	-5.066179000	-3.226579000	-0.366318000
1	-4.590828000	-2.000857000	1.326201000
6	-3.960588000	-2.666902000	-2.433870000
1	-2.594412000	-1.012002000	-2.354574000
6	-4.841049000	-3.474836000	-1.717449000
1	-5.747326000	-3.856248000	0.198678000
1	-3.777681000	-2.858133000	-3.487092000
1	-5.346755000	-4.299974000	-2.210478000
6	-3.779009000	1.411616000	0.075285000
6	-5.082362000	1.348209000	0.582563000
6	-3.393723000	2.528216000	-0.668491000
6	-5.976148000	2.390961000	0.369302000
1	-5.409639000	0.473632000	1.139327000
6	-4.293132000	3.569567000	-0.891685000
1	-2.384638000	2.579554000	-1.066243000

6	-5.581145000	3.505607000	-0.369504000
1	-6.982030000	2.332064000	0.774826000
1	-3.982951000	4.433102000	-1.473004000
1	-6.280301000	4.319275000	-0.539812000
6	3.321415000	0.134234000	-0.587148000
6	4.541935000	-0.135159000	0.036746000
6	3.191767000	-0.099213000	-1.959583000
6	5.621473000	-0.608679000	-0.704036000
1	4.660503000	0.020608000	1.105116000
6	4.272339000	-0.566679000	-2.700536000
1	2.240445000	0.085389000	-2.450078000
6	5.491288000	-0.816791000	-2.074259000
1	6.565064000	-0.815981000	-0.207627000
1	4.159797000	-0.738370000	-3.767018000
1	6.336093000	-1.180582000	-2.652087000
6	2.392435000	2.694955000	0.120686000
6	3.571216000	3.187409000	0.693307000
6	1.598343000	3.559294000	-0.635191000
6	3.934309000	4.520257000	0.533540000
1	4.221431000	2.527699000	1.261901000
6	1.967079000	4.891817000	-0.806540000
1	0.683155000	3.184551000	-1.081852000
6	3.130954000	5.376283000	-0.218248000
1	4.847413000	4.890658000	0.990631000
1	1.339316000	5.550718000	-1.399367000
1	3.414509000	6.416989000	-0.346573000
6	0.082942000	-2.776192000	0.833648000
8	-0.294428000	-2.571921000	2.019410000
6	1.567215000	-3.003611000	0.597907000
6	2.115555000	-3.176131000	-0.675365000
6	2.395424000	-3.140208000	1.712777000
6	3.458260000	-3.499589000	-0.827607000
1	1.494482000	-3.035876000	-1.555259000
6	3.746195000	-3.446229000	1.562584000
1	1.953272000	-3.023344000	2.697267000
6	4.279256000	-3.634831000	0.291190000
1	3.872897000	-3.625819000	-1.823073000
1	4.377800000	-3.551989000	2.440713000
1	5.331047000	-3.876691000	0.167422000
6	-0.842529000	-3.569516000	-0.080585000
1	-1.879404000	-3.327395000	0.153390000
1	-0.665962000	-3.389902000	-1.142632000
1	-0.680318000	-4.636300000	0.125111000
6	-2.661295000	-0.325268000	2.147833000

1	-3.631503000	-0.098990000	2.600222000
6	-1.550305000	0.475270000	2.819184000
1	-2.446168000	-1.392936000	2.271414000
1	-1.728238000	1.551469000	2.724179000
1	-1.504834000	0.225401000	3.888578000

TS3S-4S

Coordinates (Angstroms)

	X	Y	Z
44	0.325807000	0.358286000	-0.020791000
1	0.641292000	1.951882000	0.230256000
15	2.607789000	0.019473000	0.333194000
15	-1.919719000	0.921629000	0.284662000
6	-2.164580000	0.541547000	2.076138000
1	-3.001223000	1.086898000	2.523221000
6	-0.866569000	0.865707000	2.808015000
1	-2.378790000	-0.531192000	2.148211000
7	0.261614000	0.163014000	2.170537000
1	-0.664022000	1.941134000	2.766037000
1	-0.946057000	0.574025000	3.864567000
6	0.394404000	0.549119000	-1.861512000
8	0.447502000	0.695670000	-3.015000000
1	0.117012000	-0.860017000	2.277828000
1	0.015815000	-1.395558000	0.002030000
6	3.519326000	-1.365388000	-0.440865000
6	4.412179000	-2.173880000	0.268640000
6	3.300170000	-1.621318000	-1.797757000
6	5.066233000	-3.226753000	-0.366714000
1	4.590800000	-2.001271000	1.325956000
6	3.960678000	-2.666843000	-2.434222000
1	2.594436000	-1.012004000	-2.354736000
6	4.841152000	-3.474836000	-1.717884000
1	5.747374000	-3.856487000	0.198219000
1	3.777800000	-2.857942000	-3.487472000
1	5.346896000	-4.299894000	-2.211010000
6	3.778965000	1.411360000	0.075526000
6	5.082253000	1.347987000	0.582972000
6	3.393726000	2.527991000	-0.668229000
6	5.976014000	2.390798000	0.369886000
1	5.409515000	0.473401000	1.139732000
6	4.293115000	3.569393000	-0.891259000
1	2.384688000	2.579299000	-1.066100000
6	5.581063000	3.505465000	-0.368915000
1	6.981843000	2.331929000	0.775546000

1	3.982971000	4.432936000	-1.472583000
1	6.280205000	4.319173000	-0.539086000
6	-3.321352000	0.134448000	-0.587428000
6	-4.541947000	-0.134832000	0.036376000
6	-3.191551000	-0.099258000	-1.959801000
6	-5.621362000	-0.608609000	-0.704416000
1	-4.660649000	0.021163000	1.104699000
6	-4.272025000	-0.566905000	-2.700784000
1	-2.240194000	0.085338000	-2.450234000
6	-5.491013000	-0.817002000	-2.074583000
1	-6.564992000	-0.815879000	-0.208072000
1	-4.159360000	-0.738773000	-3.767225000
1	-6.335726000	-1.180994000	-2.652419000
6	-2.392151000	2.695192000	0.120585000
6	-3.570748000	3.187887000	0.693382000
6	-1.597943000	3.559417000	-0.635305000
6	-3.933559000	4.520828000	0.533732000
1	-4.221018000	2.528335000	1.262093000
6	-1.966389000	4.892035000	-0.806526000
1	-0.682900000	3.184500000	-1.082113000
6	-3.130092000	5.376726000	-0.218081000
1	-4.846534000	4.891400000	0.990940000
1	-1.338527000	5.550835000	-1.399359000
1	-3.413424000	6.417505000	-0.346304000
6	-0.083280000	-2.776198000	0.833596000
8	0.294393000	-2.571972000	2.019271000
6	-1.567647000	-3.003401000	0.598251000
6	-2.116302000	-3.176007000	-0.674877000
6	-2.395613000	-3.139801000	1.713324000
6	-3.459079000	-3.499296000	-0.826790000
1	-1.495399000	-3.035957000	-1.554922000
6	-3.746461000	-3.445654000	1.563462000
1	-1.953229000	-3.022917000	2.697710000
6	-4.279840000	-3.634291000	0.292208000
1	-3.873946000	-3.625581000	-1.822151000
1	-4.377890000	-3.551233000	2.441740000
1	-5.331694000	-3.876012000	0.168704000
6	0.841905000	-3.569602000	-0.080855000
1	1.878846000	-3.327484000	0.152834000
1	0.665060000	-3.390013000	-1.142860000
1	0.679730000	-4.636377000	0.124921000
6	2.661075000	-0.325828000	2.147723000
1	3.631329000	-0.099996000	2.600233000
6	1.550283000	0.474993000	2.819079000

1	2.445518000	-1.393433000	2.271124000
1	1.728431000	1.551154000	2.724025000
1	1.504768000	0.225171000	3.888481000

4R

Coordinates (Angstroms)

	X	Y	Z
44	0.272858000	0.647363000	0.101360000
1	0.441276000	2.163985000	-0.640900000
15	2.515195000	0.234239000	-0.320319000
15	-2.028476000	0.873854000	-0.094260000
6	-2.353141000	0.028403000	-1.706547000
1	-3.297627000	0.318178000	-2.176495000
6	-1.177928000	0.298486000	-2.639534000
1	-2.415830000	-1.040503000	-1.481430000
7	0.080600000	-0.123916000	-1.996709000
1	-1.094696000	1.369641000	-2.850668000
1	-1.316270000	-0.231462000	-3.592661000
6	0.468895000	1.318635000	1.807406000
8	0.603069000	1.747217000	2.882115000
1	0.064860000	-1.142082000	-1.919192000
1	0.071969000	-0.941489000	0.659131000
6	3.384116000	-1.126579000	0.552769000
6	4.270782000	-1.999651000	-0.084994000
6	3.140753000	-1.292535000	1.919829000
6	4.899401000	-3.018708000	0.627475000
1	4.473215000	-1.898517000	-1.147418000
6	3.774355000	-2.304431000	2.634276000
1	2.433492000	-0.638041000	2.421028000
6	4.652542000	-3.172758000	1.988872000
1	5.579920000	-3.692957000	0.115420000
1	3.573734000	-2.421575000	3.695271000
1	5.140334000	-3.968664000	2.544299000
6	3.752082000	1.594306000	-0.228197000
6	5.110557000	1.364540000	-0.480361000
6	3.333709000	2.884789000	0.102162000
6	6.028406000	2.406197000	-0.412335000
1	5.461087000	0.363710000	-0.717535000
6	4.255000000	3.928434000	0.174855000
1	2.280002000	3.065653000	0.292896000
6	5.601104000	3.692309000	-0.083808000
1	7.079318000	2.214263000	-0.609290000
1	3.915889000	4.927158000	0.434774000
1	6.320062000	4.504781000	-0.026736000

6	-3.188870000	0.055307000	1.070593000
6	-4.563790000	-0.016550000	0.819656000
6	-2.681075000	-0.522699000	2.235783000
6	-5.413129000	-0.659398000	1.714163000
1	-4.981949000	0.433037000	-0.076659000
6	-3.532269000	-1.158860000	3.137680000
1	-1.611884000	-0.485915000	2.421765000
6	-4.898161000	-1.229110000	2.878361000
1	-6.478219000	-0.711747000	1.507024000
1	-3.124587000	-1.599085000	4.043201000
1	-5.562463000	-1.724177000	3.581086000
6	-2.754473000	2.554502000	-0.262068000
6	-3.860530000	2.844879000	-1.067270000
6	-2.177335000	3.587057000	0.484021000
6	-4.381048000	4.135514000	-1.121668000
1	-4.327064000	2.067841000	-1.665960000
6	-2.703776000	4.874054000	0.440791000
1	-1.298378000	3.380414000	1.086842000
6	-3.806312000	5.151959000	-0.363669000
1	-5.236275000	4.346147000	-1.757654000
1	-2.243862000	5.663398000	1.028191000
1	-4.213357000	6.158196000	-0.405123000
6	0.350419000	-3.461346000	-0.796559000
8	1.007936000	-3.132015000	-1.775256000
6	-1.142679000	-3.484524000	-0.893200000
6	-1.960989000	-3.384613000	0.234886000
6	-1.725369000	-3.577182000	-2.162346000
6	-3.344969000	-3.369696000	0.093759000
1	-1.520419000	-3.277803000	1.220449000
6	-3.108344000	-3.585617000	-2.300620000
1	-1.078465000	-3.647218000	-3.031399000
6	-3.919289000	-3.477364000	-1.170764000
1	-3.973427000	-3.257995000	0.971435000
1	-3.555577000	-3.671200000	-3.286513000
1	-5.000254000	-3.468950000	-1.276550000
6	1.007127000	-3.852847000	0.498204000
1	2.079875000	-3.977671000	0.340817000
1	0.854946000	-3.048461000	1.226927000
1	0.572338000	-4.771948000	0.905053000
6	2.525689000	-0.298829000	-2.102216000
1	3.426321000	0.042896000	-2.621402000
6	1.272130000	0.226993000	-2.794547000
1	2.507092000	-1.392892000	-2.117218000
1	1.299187000	1.316898000	-2.879474000

1	1.195371000	-0.203820000	-3.803448000
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4S

Coordinates (Angstroms)

	X	Y	Z
44	-0.272903000	0.647264000	0.101354000
1	-0.441230000	2.163795000	-0.641138000
15	-2.515203000	0.234153000	-0.320365000
15	2.028457000	0.873958000	-0.094293000
6	2.353186000	0.028889000	-1.706784000
1	3.297462000	0.319253000	-2.176786000
6	1.177819000	0.298854000	-2.639595000
1	2.416398000	-1.040056000	-1.482005000
7	-0.080635000	-0.123875000	-1.996763000
1	1.094420000	1.370031000	-2.850519000
1	1.316155000	-0.230920000	-3.592815000
6	-0.468766000	1.318290000	1.807525000
8	-0.602683000	1.746654000	2.882353000
1	-0.064567000	-1.142024000	-1.919185000
1	-0.072356000	-0.941545000	0.659314000
6	-3.384104000	-1.126679000	0.552746000
6	-4.270871000	-1.999669000	-0.084979000
6	-3.140622000	-1.292750000	1.919778000
6	-4.899410000	-3.018796000	0.627464000
1	-4.473438000	-1.898438000	-1.147369000
6	-3.774155000	-2.304692000	2.634210000
1	-2.433307000	-0.638290000	2.420938000
6	-4.652407000	-3.172967000	1.988816000
1	-5.579986000	-3.692996000	0.115418000
1	-3.573454000	-2.421923000	3.695180000
1	-5.140135000	-3.968923000	2.544230000
6	-3.752093000	1.594197000	-0.228337000
6	-5.110403000	1.364558000	-0.481488000
6	-3.333938000	2.884458000	0.103133000
6	-6.028307000	2.406159000	-0.413380000
1	-5.460755000	0.363863000	-0.719523000
6	-4.255287000	3.928049000	0.175915000
1	-2.280340000	3.065208000	0.294576000
6	-5.601222000	3.692064000	-0.083744000
1	-7.079101000	2.214339000	-0.611078000
1	-3.916350000	4.926610000	0.436686000
1	-6.320224000	4.504494000	-0.026618000
6	3.188922000	0.055315000	1.070420000
6	4.563857000	-0.016475000	0.819529000

6	2.681097000	-0.522916000	2.235486000
6	5.413173000	-0.659455000	1.713965000
1	4.982047000	0.433253000	-0.076694000
6	3.532267000	-1.159203000	3.137314000
1	1.611898000	-0.486199000	2.421430000
6	4.898169000	-1.229372000	2.878045000
1	6.478270000	-0.711752000	1.506851000
1	3.124562000	-1.599587000	4.042748000
1	5.562444000	-1.724552000	3.580715000
6	2.754282000	2.554709000	-0.261899000
6	3.860762000	2.845167000	-1.066495000
6	2.176568000	3.587272000	0.483741000
6	4.381139000	4.135862000	-1.120717000
1	4.327735000	2.068125000	-1.664846000
6	2.702820000	4.874349000	0.440640000
1	1.297300000	3.380541000	1.086074000
6	3.805789000	5.152324000	-0.363202000
1	5.236739000	4.346542000	-1.756188000
1	2.242414000	5.663707000	1.027636000
1	4.212697000	6.158620000	-0.404559000
6	-0.350166000	-3.461131000	-0.795739000
8	-1.008120000	-3.131801000	-1.774131000
6	1.142904000	-3.484194000	-0.893024000
6	1.961752000	-3.384433000	0.234689000
6	1.724988000	-3.576731000	-2.162461000
6	3.345662000	-3.369553000	0.092888000
1	1.521648000	-3.277739000	1.220479000
6	3.107895000	-3.585198000	-2.301403000
1	1.077655000	-3.646674000	-3.031197000
6	3.919380000	-3.477105000	-1.171924000
1	3.974563000	-3.258003000	0.970267000
1	3.554655000	-3.670676000	-3.287519000
1	5.000294000	-3.468723000	-1.278215000
6	-1.006310000	-3.852933000	0.499224000
1	-2.079128000	-3.977731000	0.342245000
1	-0.853805000	-3.048688000	1.228021000
1	-0.571332000	-4.772117000	0.905681000
6	-2.525733000	-0.299071000	-2.102222000
1	-3.426410000	0.042510000	-2.621423000
6	-1.272261000	0.226824000	-2.794610000
1	-2.507008000	-1.393128000	-2.117095000
1	-1.299451000	1.316723000	-2.879535000
1	-1.195438000	-0.204012000	-3.803490000

Coordinates (Angstroms)			
	X	Y	Z
44	0.000007000	0.077277000	0.120810000
1	-0.000067000	-1.616665000	0.193989000
15	2.300663000	0.046932000	0.437973000
15	-2.300640000	0.047019000	0.438011000
6	2.452021000	-0.014532000	2.289501000
6	-2.451974000	-0.014257000	2.289549000
1	3.367598000	-0.517494000	2.616062000
1	2.486682000	1.019934000	2.652066000
6	1.227187000	-0.719924000	2.859431000
1	-3.367608000	-0.517062000	2.616193000
6	-1.227216000	-0.719731000	2.859533000
1	-2.486487000	1.020261000	2.651982000
1	1.252554000	-0.700730000	3.958458000
7	0.000015000	-0.072404000	2.359178000
1	1.197883000	-1.763556000	2.531775000
1	-1.198036000	-1.763405000	2.532001000
1	-1.252546000	-0.700400000	3.958556000
6	0.000008000	0.142454000	-1.723046000
8	0.000011000	0.170714000	-2.886678000
1	0.000093000	0.895138000	2.681189000
1	0.000032000	1.773372000	0.264988000
6	3.356367000	1.469904000	-0.035722000
6	3.042592000	2.171644000	-1.203082000
6	4.467917000	1.867238000	0.715439000
6	3.836477000	3.235466000	-1.622129000
1	2.161850000	1.893560000	-1.774179000
6	5.256126000	2.937593000	0.302252000
1	4.722762000	1.349453000	1.636267000
6	4.944514000	3.619937000	-0.870964000
1	3.582470000	3.770741000	-2.532331000
1	6.113071000	3.238441000	0.898318000
1	5.559990000	4.454401000	-1.194650000
6	3.295545000	-1.388981000	-0.143342000
6	4.633099000	-1.558871000	0.235255000
6	2.710363000	-2.327126000	-0.995944000
6	5.364488000	-2.650798000	-0.217416000
1	5.116584000	-0.831740000	0.882055000
6	3.445971000	-3.417251000	-1.457904000
1	1.670214000	-2.203892000	-1.281878000
6	4.770669000	-3.583257000	-1.067240000
1	6.400122000	-2.772182000	0.087060000

1	2.978636000	-4.138079000	-2.122557000
1	5.342493000	-4.435095000	-1.424226000
6	-3.356320000	1.469965000	-0.035833000
6	-4.468015000	1.867244000	0.715148000
6	-3.042435000	2.171675000	-1.203178000
6	-5.256254000	2.937509000	0.301793000
1	-4.722955000	1.349483000	1.635962000
6	-3.836343000	3.235418000	-1.622389000
1	-2.161569000	1.893650000	-1.774116000
6	-4.944528000	3.619821000	-0.871415000
1	-6.113319000	3.238310000	0.897710000
1	-3.582241000	3.770674000	-2.532576000
1	-5.560043000	4.454203000	-1.195241000
6	-3.295551000	-1.388920000	-0.143171000
6	-4.633010000	-1.558922000	0.235707000
6	-2.710498000	-2.326961000	-0.995976000
6	-5.364430000	-2.650858000	-0.216889000
1	-5.116401000	-0.831886000	0.882684000
6	-3.446142000	-3.417090000	-1.457867000
1	-1.670417000	-2.203648000	-1.282124000
6	-4.770743000	-3.583211000	-1.066924000
1	-6.399988000	-2.772335000	0.087811000
1	-2.978910000	-4.137833000	-2.122684000
1	-5.342594000	-4.435054000	-1.423852000

A2

Coordinates (Angstroms)

	X	Y	Z
6	1.696900000	-0.203504000	-0.000028000
8	2.209143000	-1.308052000	-0.000220000
6	2.548204000	1.046338000	0.000104000
1	3.601607000	0.761309000	0.000121000
1	2.339528000	1.659255000	-0.883981000
1	2.339516000	1.658811000	0.884548000
6	0.204063000	-0.056677000	0.000108000
6	-0.427682000	1.190943000	-0.000068000
6	-0.576277000	-1.217984000	0.000112000
6	-1.816625000	1.274598000	-0.000070000
1	0.156744000	2.106125000	-0.000113000
6	-1.962099000	-1.134479000	0.000062000
1	-0.075199000	-2.180545000	0.000194000
6	-2.584473000	0.113055000	-0.000011000
1	-2.299404000	2.247188000	-0.000211000
1	-2.559332000	-2.041549000	0.000080000

1	-3.668661000	0.180078000	-0.000125000
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A3

Coordinates (Angstroms)

	X	Y	Z
7	-1.694166000	1.162036000	0.159444000
1	-1.677779000	1.958958000	-0.468848000
1	-1.397120000	1.412785000	1.099445000
16	-0.926670000	-0.193698000	-0.507973000
6	0.843665000	0.050870000	0.032952000
6	0.920783000	0.028832000	1.555610000
1	1.969340000	0.005421000	1.873162000
1	0.467855000	0.919615000	2.006781000
1	0.418533000	-0.858466000	1.952636000
6	1.604658000	-1.137029000	-0.561285000
1	1.516605000	-1.166242000	-1.653947000
1	2.669090000	-1.054985000	-0.313801000
1	1.229896000	-2.083100000	-0.159481000
6	1.340971000	1.368513000	-0.555988000
1	2.411676000	1.481086000	-0.351901000
1	1.206480000	1.403054000	-1.644049000
1	0.829410000	2.231525000	-0.116582000
8	-1.402322000	-1.393982000	0.245040000

H₂O

Coordinates (Angstroms)

	X	Y	Z
8	0.000000000	0.000000000	0.112804000
1	0.000000000	0.789144000	-0.451214000
1	0.000000000	-0.789144000	-0.451214000

A4

Coordinates (Angstroms)

	X	Y	Z
6	3.487549000	-1.615102000	-0.532249000
6	4.527659000	-0.954094000	0.119536000
6	4.309891000	0.308852000	0.660385000
6	3.060352000	0.912204000	0.548505000
6	2.007817000	0.253347000	-0.095860000
6	2.239007000	-1.018008000	-0.636481000
1	3.652034000	-2.597689000	-0.964607000
1	5.503952000	-1.422353000	0.203479000
1	5.114667000	0.829667000	1.170672000

1	2.912509000	1.896759000	0.980181000
1	1.425996000	-1.524792000	-1.145603000
6	0.652310000	0.876126000	-0.209940000
6	0.541872000	2.356918000	0.054950000
1	0.682576000	2.547042000	1.125625000
1	1.330062000	2.894059000	-0.481603000
1	-0.434405000	2.745257000	-0.227409000
7	-0.302046000	0.073667000	-0.509344000
16	-1.915587000	0.458100000	-0.847490000
6	-2.639241000	-0.780793000	0.352460000
6	-2.202592000	-0.413853000	1.766876000
1	-2.763529000	-1.015023000	2.491660000
1	-1.136323000	-0.606938000	1.919641000
1	-2.404898000	0.642890000	1.969784000
6	-2.192595000	-2.183456000	-0.051629000
1	-1.120068000	-2.323328000	0.101657000
1	-2.728057000	-2.918456000	0.560959000
1	-2.423479000	-2.395258000	-1.102254000
6	-4.152810000	-0.618325000	0.189553000
1	-4.665275000	-1.312799000	0.864181000
1	-4.470865000	0.398644000	0.436393000
1	-4.475718000	-0.845041000	-0.833466000
8	-2.383849000	1.802398000	-0.367585000

A4C

Coordinates (Angstroms)

	X	Y	Z
6	3.172158000	-1.824322000	-0.222769000
6	4.360927000	-1.158886000	0.073936000
6	4.338810000	0.211188000	0.311361000
6	3.138832000	0.914286000	0.245769000
6	1.940385000	0.257248000	-0.053053000
6	1.974723000	-1.124750000	-0.282061000
1	3.179882000	-2.894119000	-0.411225000
1	5.298014000	-1.706080000	0.119606000
1	5.257813000	0.738702000	0.549919000
1	3.143538000	1.981122000	0.447164000
1	1.048252000	-1.640569000	-0.511275000
6	0.645624000	0.995482000	-0.103898000
6	0.650978000	2.492272000	-0.278021000
1	1.564582000	2.850959000	-0.756021000
1	-0.196541000	2.801927000	-0.899737000
1	0.546949000	2.995840000	0.691649000
7	-0.418604000	0.289569000	0.021294000

16	-1.949990000	1.018696000	0.003901000
6	-2.986132000	-0.511825000	0.060966000
6	-2.680805000	-1.296521000	1.337382000
1	-3.288915000	-2.209466000	1.366233000
1	-1.626160000	-1.585336000	1.372689000
1	-2.906912000	-0.705586000	2.231195000
6	-2.712567000	-1.365674000	-1.177689000
1	-1.658272000	-1.654389000	-1.225387000
1	-3.315655000	-2.281566000	-1.139757000
1	-2.964053000	-0.826901000	-2.097265000
6	-4.431854000	-0.007515000	0.064063000
1	-5.114934000	-0.864237000	0.094346000
1	-4.641935000	0.617875000	0.939066000
1	-4.662061000	0.569799000	-0.838603000

A4_B

Coordinates (Angstroms)

	X	Y	Z
6	-3.542202000	1.808640000	-0.223944000
6	-4.689253000	1.071080000	0.065604000
6	-4.591698000	-0.297301000	0.297285000
6	-3.354323000	-0.929699000	0.233828000
6	-2.196254000	-0.197055000	-0.050693000
6	-2.305700000	1.181431000	-0.275515000
1	-3.613837000	2.876075000	-0.409515000
1	-5.656380000	1.563004000	0.109187000
1	-5.480684000	-0.876390000	0.527853000
1	-3.298765000	-1.996647000	0.423088000
1	-1.409553000	1.750085000	-0.498521000
6	-0.859954000	-0.852983000	-0.096033000
6	-0.807651000	-2.355540000	-0.179455000
1	-0.973090000	-2.781527000	0.816843000
1	-1.590533000	-2.728710000	-0.844004000
1	0.153764000	-2.714027000	-0.545225000
7	0.155050000	-0.064040000	-0.036712000
6	2.661280000	0.901876000	0.107005000
6	2.258939000	1.578488000	1.418045000
1	2.848018000	2.494973000	1.532903000
1	1.199094000	1.848320000	1.420811000
1	2.459104000	0.932267000	2.277307000
6	2.350691000	1.784812000	-1.102062000
1	1.290450000	2.049441000	-1.144110000
1	2.930586000	2.710588000	-1.017951000
1	2.625828000	1.291000000	-2.037953000

6	4.140379000	0.500620000	0.127799000
1	4.745799000	1.407309000	0.229166000
1	4.364254000	-0.157706000	0.972132000
1	4.430972000	-0.004979000	-0.797670000
16	1.729197000	-0.662546000	-0.055537000
8	1.956990000	-1.474661000	1.140741000
8	2.022628000	-1.247872000	-1.365734000

cis-A4

Coordinates (Angstroms)			
	X	Y	Z
16	1.272442000	-0.187043000	-0.939137000
8	0.565793000	-1.488675000	-0.716814000
6	2.786360000	-0.232404000	0.154048000
6	3.558387000	1.073959000	-0.013597000
6	3.600969000	-1.417465000	-0.371498000
6	2.354797000	-0.472900000	1.596810000
1	3.003451000	1.924964000	0.387436000
1	4.512343000	0.995294000	0.521214000
1	3.783779000	1.275591000	-1.067398000
1	3.041925000	-2.353777000	-0.287902000
1	4.521081000	-1.511524000	0.215891000
1	3.887269000	-1.277109000	-1.420547000
1	1.805589000	0.384119000	1.999103000
1	1.725435000	-1.366414000	1.665851000
1	3.240328000	-0.632326000	2.222873000
6	-0.628457000	1.402031000	0.093724000
6	-1.764000000	0.429951000	0.075696000
6	-1.729135000	-0.739746000	0.839003000
6	-2.917399000	0.735859000	-0.654675000
6	-2.825999000	-1.593422000	0.860865000
1	-0.839654000	-0.980722000	1.408871000
6	-4.005348000	-0.130094000	-0.647428000
1	-2.959148000	1.643571000	-1.250254000
6	-3.963140000	-1.294055000	0.115255000
1	-2.787914000	-2.500837000	1.455978000
1	-4.887784000	0.107928000	-1.233932000
1	-4.814626000	-1.968241000	0.127574000
6	-0.980128000	2.803122000	0.528793000
1	-1.688741000	3.256318000	-0.174346000
1	-1.470470000	2.784462000	1.508150000
1	-0.082479000	3.422948000	0.574531000
7	0.600392000	1.186975000	-0.193480000

6R

Coordinates (Angstroms)			
	X	Y	Z
44	1.090175000	0.874215000	-0.012866000
1	2.023761000	2.157085000	-0.633813000
15	2.833153000	-0.594998000	-0.428160000
15	-0.840651000	2.148570000	-0.203132000
6	2.533493000	-1.096633000	-2.192513000
6	-1.354955000	1.823067000	-1.953555000
1	3.458985000	-1.376523000	-2.705243000
1	1.867796000	-1.967816000	-2.192291000
6	1.838247000	0.056100000	-2.908916000
1	-1.940439000	2.643868000	-2.379164000
6	-0.110345000	1.541230000	-2.785011000
1	-1.969302000	0.916259000	-1.939459000
1	1.569489000	-0.243768000	-3.931929000
7	0.634708000	0.439055000	-2.152877000
1	2.4944431000	0.930461000	-2.963066000
1	0.546561000	2.416041000	-2.824839000
1	-0.397711000	1.267898000	-3.810349000
6	1.473030000	1.249528000	1.753714000
8	1.716902000	1.484268000	2.869317000
1	-0.000156000	-0.367427000	-2.153651000
1	0.110643000	-0.432414000	0.382725000
6	2.926704000	-2.182526000	0.485945000
6	2.732928000	-2.146652000	1.871155000
6	3.142360000	-3.417392000	-0.132215000
6	2.746558000	-3.318613000	2.620563000
1	2.547483000	-1.195595000	2.361930000
6	3.146157000	-4.593494000	0.616006000
1	3.298014000	-3.476466000	-1.205786000
6	2.946360000	-4.546798000	1.992539000
1	2.587469000	-3.272944000	3.693986000
1	3.303167000	-5.546853000	0.119550000
1	2.944004000	-5.464296000	2.573884000
6	4.590026000	-0.049048000	-0.416968000
6	5.626950000	-0.937037000	-0.729729000
6	4.900810000	1.272984000	-0.095769000
6	6.948422000	-0.506177000	-0.734767000
1	5.405162000	-1.976183000	-0.959411000
6	6.227055000	1.703688000	-0.095355000
1	4.094449000	1.961163000	0.141692000
6	7.250198000	0.818107000	-0.417686000
1	7.743755000	-1.203742000	-0.981542000

1	6.456613000	2.735274000	0.155664000
1	8.283150000	1.154830000	-0.418726000
6	-2.335906000	1.756625000	0.778805000
6	-3.616021000	1.700685000	0.220348000
6	-2.186163000	1.527326000	2.149563000
6	-4.725229000	1.420757000	1.015274000
1	-3.760616000	1.868989000	-0.842754000
6	-3.295399000	1.269696000	2.947058000
1	-1.194930000	1.536977000	2.592782000
6	-4.566539000	1.209806000	2.381129000
1	-5.711596000	1.368310000	0.562968000
1	-3.162498000	1.093329000	4.009374000
1	-5.429655000	0.989807000	3.003026000
6	-0.784707000	3.985989000	-0.078822000
6	-1.943402000	4.760337000	-0.221150000
6	0.431422000	4.627055000	0.162553000
6	-1.883285000	6.146555000	-0.134647000
1	-2.904076000	4.279359000	-0.385190000
6	0.491274000	6.017022000	0.254237000
1	1.331000000	4.027756000	0.269183000
6	-0.663240000	6.778255000	0.104087000
1	-2.790392000	6.733808000	-0.246771000
1	1.444277000	6.502689000	0.443942000
1	-0.616327000	7.861223000	0.177907000
6	-3.725870000	-2.179691000	3.535479000
6	-2.741808000	-1.839646000	4.461392000
6	-1.428047000	-1.650803000	4.038544000
6	-1.091101000	-1.831608000	2.701583000
6	-2.071859000	-2.187101000	1.768814000
6	-3.395422000	-2.339458000	2.195080000
1	-4.753759000	-2.319989000	3.857357000
1	-2.999598000	-1.712790000	5.509203000
1	-0.660990000	-1.359528000	4.750008000
1	-0.072014000	-1.655095000	2.374495000
1	-4.156687000	-2.603225000	1.468391000
6	-1.728880000	-2.437479000	0.343088000
6	-0.415026000	-3.106934000	0.029062000
1	0.265132000	-3.106193000	0.878767000
1	-0.616524000	-4.153556000	-0.237380000
1	0.082139000	-2.623510000	-0.812698000
7	-2.640568000	-2.156981000	-0.525701000
16	-2.307415000	-2.583258000	-2.152630000
6	-3.987783000	-2.186800000	-2.817490000
6	-4.334188000	-0.726521000	-2.550025000

1	-5.327707000	-0.511930000	-2.961654000
1	-4.346003000	-0.514991000	-1.477207000
1	-3.615597000	-0.061858000	-3.039154000
6	-4.975657000	-3.139070000	-2.144156000
1	-5.058323000	-2.936132000	-1.072930000
1	-5.965349000	-3.004313000	-2.595831000
1	-4.688974000	-4.188756000	-2.281141000
6	-3.892401000	-2.464555000	-4.320075000
1	-4.862648000	-2.265082000	-4.788304000
1	-3.144580000	-1.821531000	-4.794090000
1	-3.632000000	-3.510057000	-4.524055000
8	-1.362800000	-1.567848000	-2.759795000

6S

Coordinates (Angstroms)

	X	Y	Z
44	-1.093120000	0.917278000	0.035906000
1	-2.002494000	2.137474000	-0.727996000
15	-2.816336000	-0.597285000	-0.317996000
15	0.840204000	2.182771000	-0.185583000
6	-2.427240000	-1.252447000	-2.013764000
6	1.394729000	1.780618000	-1.912906000
1	-3.320139000	-1.603731000	-2.539836000
1	-1.744438000	-2.103211000	-1.899415000
6	-1.730306000	-0.154686000	-2.809027000
1	1.939856000	2.608302000	-2.377083000
6	0.181192000	1.392967000	-2.749349000
1	2.072321000	0.922433000	-1.837370000
1	-1.421018000	-0.536594000	-3.792336000
7	-0.560422000	0.326968000	-2.052803000
1	-2.397609000	0.699190000	-2.959841000
1	-0.498720000	2.241282000	-2.871667000
1	0.500285000	1.049559000	-3.744580000
6	-1.546541000	1.451855000	1.743277000
8	-1.836345000	1.796321000	2.817291000
1	0.083528000	-0.457183000	-1.945521000
1	-0.142260000	-0.358335000	0.598815000
6	-2.934453000	-2.106903000	0.718081000
6	-2.713113000	-1.976348000	2.093163000
6	-3.188628000	-3.377888000	0.192398000
6	-2.747295000	-3.091330000	2.925009000
1	-2.487049000	-0.999693000	2.510283000
6	-3.210444000	-4.496329000	1.023093000
1	-3.352336000	-3.511329000	-0.873253000

6	-2.990295000	-4.354989000	2.390218000
1	-2.571160000	-2.973078000	3.990148000
1	-3.394376000	-5.478534000	0.597653000
1	-3.003062000	-5.227254000	3.037310000
6	-4.569006000	-0.055031000	-0.437971000
6	-5.588052000	-0.947384000	-0.793637000
6	-4.894021000	1.275723000	-0.169716000
6	-6.904308000	-0.512070000	-0.893858000
1	-5.359202000	-1.992443000	-0.985367000
6	-6.215393000	1.710557000	-0.262939000
1	-4.101576000	1.968278000	0.099198000
6	-7.219652000	0.820435000	-0.629067000
1	-7.685294000	-1.212636000	-1.175182000
1	-6.455364000	2.748712000	-0.052246000
1	-8.248629000	1.160267000	-0.706473000
6	2.319267000	1.832316000	0.834946000
6	3.619336000	1.849530000	0.319754000
6	2.133248000	1.567903000	2.194734000
6	4.713698000	1.625636000	1.151885000
1	3.792235000	2.034837000	-0.736914000
6	3.226370000	1.361266000	3.028309000
1	1.127084000	1.505996000	2.598327000
6	4.518401000	1.391039000	2.509196000
1	5.717278000	1.637064000	0.736111000
1	3.066432000	1.154866000	4.081583000
1	5.370256000	1.216886000	3.160326000
6	0.772633000	4.023380000	-0.154409000
6	1.923984000	4.803453000	-0.321910000
6	-0.454383000	4.661216000	0.035792000
6	1.845713000	6.191388000	-0.311970000
1	2.892776000	4.327829000	-0.447833000
6	-0.532317000	6.053039000	0.052134000
1	-1.348227000	4.057103000	0.159749000
6	0.615006000	6.819471000	-0.124164000
1	2.747081000	6.783171000	-0.444162000
1	-1.493529000	6.535922000	0.203141000
1	0.554038000	7.904146000	-0.111329000
6	4.068750000	-1.998410000	3.211386000
6	3.168046000	-1.890226000	4.268595000
6	1.799012000	-1.956360000	4.021457000
6	1.331514000	-2.160089000	2.727641000
6	2.231678000	-2.277315000	1.662682000
6	3.602766000	-2.177433000	1.914219000
1	5.137222000	-1.938686000	3.396886000

1	3.532587000	-1.748278000	5.282238000
1	1.089455000	-1.854421000	4.837421000
1	0.263151000	-2.206663000	2.543446000
1	4.300179000	-2.256959000	1.086754000
6	1.736254000	-2.528909000	0.279940000
6	0.444390000	-3.289959000	0.150310000
1	0.375853000	-4.072207000	0.910883000
1	0.325516000	-3.731163000	-0.837983000
1	-0.372215000	-2.581308000	0.332468000
7	2.451738000	-2.050405000	-0.674135000
16	2.028578000	-2.150504000	-2.313821000
6	3.776395000	-2.129721000	-2.949602000
6	4.417868000	-0.798521000	-2.563167000
1	5.447306000	-0.777533000	-2.940438000
1	4.441891000	-0.662789000	-1.478735000
1	3.886015000	0.048833000	-3.012400000
6	4.525716000	-3.324597000	-2.367351000
1	4.681889000	-3.210410000	-1.290867000
1	5.506417000	-3.411527000	-2.849540000
1	3.973620000	-4.252811000	-2.546257000
6	3.640085000	-2.254921000	-4.468773000
1	4.635374000	-2.223426000	-4.925547000
1	3.053161000	-1.430121000	-4.891482000
1	3.161721000	-3.198312000	-4.746818000
8	1.451758000	-3.471506000	-2.744613000

6_{B1}

Coordinates (Angstroms)

	X	Y	Z
44	0.959451000	0.935248000	0.050079000
1	1.657370000	2.125754000	-0.950504000
15	2.810670000	-0.414162000	-0.309839000
15	-1.123048000	1.952923000	-0.112040000
6	2.437709000	-1.215617000	-1.949050000
6	-1.827641000	1.145144000	-1.624218000
1	3.347319000	-1.400499000	-2.528824000
1	1.963906000	-2.184323000	-1.752819000
6	1.472732000	-0.332190000	-2.732299000
1	-2.588761000	1.762081000	-2.112476000
6	-0.686369000	0.832043000	-2.582998000
1	-2.296058000	0.209962000	-1.294939000
1	1.140312000	-0.851370000	-3.642706000
7	0.316454000	0.008795000	-1.884178000
1	1.953511000	0.606924000	-3.019708000

1	-0.190755000	1.749699000	-2.914660000
1	-1.064004000	0.298548000	-3.467201000
6	1.521621000	1.733118000	1.615445000
8	1.888479000	2.239913000	2.597550000
1	-0.150595000	-0.863708000	-1.634542000
1	0.195546000	-0.321777000	0.877559000
6	3.112744000	-1.845653000	0.801153000
6	2.810766000	-1.695146000	2.158075000
6	3.587711000	-3.081330000	0.347820000
6	2.987967000	-2.753078000	3.045046000
1	2.404870000	-0.752964000	2.513798000
6	3.754901000	-4.143947000	1.232815000
1	3.814749000	-3.231596000	-0.704538000
6	3.456730000	-3.981061000	2.583047000
1	2.748544000	-2.619571000	4.095988000
1	4.115903000	-5.100092000	0.864751000
1	3.584227000	-4.809752000	3.273510000
6	4.491039000	0.302466000	-0.518199000
6	5.596265000	-0.488650000	-0.855612000
6	4.670977000	1.673741000	-0.330298000
6	6.853152000	0.084131000	-1.012868000
1	5.481098000	-1.560590000	-0.990402000
6	5.932459000	2.247157000	-0.480456000
1	3.811845000	2.288116000	-0.079015000
6	7.023326000	1.455431000	-0.824525000
1	7.702104000	-0.539632000	-1.278024000
1	6.059150000	3.315118000	-0.329043000
1	8.005705000	1.903248000	-0.944405000
6	-2.421317000	1.712221000	1.157824000
6	-3.771583000	1.541470000	0.833930000
6	-2.047430000	1.736425000	2.504039000
6	-4.730745000	1.423592000	1.835929000
1	-4.087159000	1.492371000	-0.204638000
6	-3.006511000	1.625348000	3.505379000
1	-0.998285000	1.827538000	2.767986000
6	-4.350419000	1.474772000	3.173869000
1	-5.775315000	1.287627000	1.570005000
1	-2.700386000	1.643419000	4.547206000
1	-5.098410000	1.382842000	3.956349000
6	-1.264485000	3.756718000	-0.461329000
6	-2.503555000	4.362646000	-0.705702000
6	-0.112447000	4.545096000	-0.476492000
6	-2.585369000	5.724800000	-0.971146000
1	-3.416274000	3.773289000	-0.676496000

6	-0.194450000	5.912339000	-0.736312000
1	0.849275000	4.074372000	-0.295402000
6	-1.428342000	6.503552000	-0.986156000
1	-3.552637000	6.182274000	-1.158759000
1	0.710928000	6.512726000	-0.742990000
1	-1.493427000	7.568949000	-1.188522000
6	-3.933967000	-1.985392000	2.977090000
6	-3.076303000	-1.892502000	4.072167000
6	-1.709290000	-2.075439000	3.893172000
6	-1.200613000	-2.362225000	2.630099000
6	-2.055313000	-2.468259000	1.527506000
6	-3.427632000	-2.266219000	1.715672000
1	-5.001251000	-1.832986000	3.107536000
1	-3.473912000	-1.669501000	5.058256000
1	-1.029814000	-1.988062000	4.736043000
1	-0.129377000	-2.479408000	2.505508000
1	-4.091814000	-2.334681000	0.860551000
6	-1.516677000	-2.788336000	0.176357000
6	-0.118910000	-3.335668000	0.087472000
1	0.075904000	-4.065775000	0.878086000
1	0.062500000	-3.820915000	-0.875688000
1	0.596686000	-2.516005000	0.217861000
7	-2.288162000	-2.557782000	-0.825543000
16	-1.773238000	-2.889288000	-2.415848000
6	-3.395574000	-2.739287000	-3.286078000
6	-3.998442000	-1.349773000	-3.082140000
1	-4.958563000	-1.285264000	-3.609332000
1	-4.177739000	-1.153741000	-2.020964000
1	-3.341089000	-0.569013000	-3.478450000
6	-4.347109000	-3.818745000	-2.766427000
1	-4.525499000	-3.694312000	-1.693753000
1	-5.311311000	-3.746767000	-3.284967000
1	-3.939838000	-4.821380000	-2.933511000
6	-3.062882000	-2.971353000	-4.763059000
1	-3.984381000	-2.916096000	-5.353763000
1	-2.372635000	-2.210710000	-5.146243000
1	-2.616753000	-3.958521000	-4.929041000

6_{B2}

Coordinates (Angstroms)

	X	Y	Z
44	-0.959455000	0.935254000	0.050079000
1	-1.657386000	2.125746000	-0.950513000
15	-2.810669000	-0.414168000	-0.309820000

15	1.123045000	1.952930000	-0.112055000
6	-2.437709000	-1.215644000	-1.949021000
6	1.827634000	1.145137000	-1.624227000
1	-3.347320000	-1.400531000	-2.528792000
1	-1.963909000	-2.184348000	-1.752779000
6	-1.472734000	-0.332225000	-2.732284000
1	2.588754000	1.762067000	-2.112493000
6	0.686363000	0.832018000	-2.583002000
1	2.296051000	0.209960000	-1.294935000
1	-1.140311000	-0.851419000	-3.642682000
7	-0.316458000	0.008781000	-1.884169000
1	-1.953518000	0.606881000	-3.019710000
1	0.190749000	1.749668000	-2.914681000
1	1.064001000	0.298510000	-3.467197000
6	-1.521634000	1.733130000	1.615437000
8	-1.888518000	2.239907000	2.597542000
1	0.150590000	-0.863715000	-1.634507000
1	-0.195528000	-0.321752000	0.877571000
6	-3.112728000	-1.845648000	0.801193000
6	-2.810732000	-1.695128000	2.158109000
6	-3.587699000	-3.081330000	0.347879000
6	-2.987923000	-2.753050000	3.045093000
1	-2.404831000	-0.752942000	2.513817000
6	-3.754879000	-4.143939000	1.232887000
1	-3.814744000	-3.231608000	-0.704477000
6	-3.456692000	-3.981038000	2.583113000
1	-2.748487000	-2.619533000	4.096031000
1	-4.115885000	-5.100087000	0.864836000
1	-3.584181000	-4.809722000	3.273587000
6	-4.491040000	0.302454000	-0.518184000
6	-5.596264000	-0.488658000	-0.855614000
6	-4.670979000	1.673729000	-0.330276000
6	-6.853150000	0.084125000	-1.012872000
1	-5.481097000	-1.560596000	-0.990420000
6	-5.932461000	2.247145000	-0.480435000
1	-3.811849000	2.288102000	-0.078986000
6	-7.023325000	1.455422000	-0.824517000
1	-7.702099000	-0.539635000	-1.278042000
1	-6.059152000	3.315105000	-0.329013000
1	-8.005704000	1.903241000	-0.944398000
6	2.421323000	1.712248000	1.157804000
6	3.771588000	1.541495000	0.833903000
6	2.047447000	1.736472000	2.504022000
6	4.730757000	1.423629000	1.835896000

1	4.087157000	1.492388000	-0.204665000
6	3.006535000	1.625405000	3.505356000
1	0.998304000	1.827591000	2.767977000
6	4.350441000	1.474821000	3.173839000
1	5.775325000	1.287662000	1.569967000
1	2.700417000	1.643492000	4.547186000
1	5.098437000	1.382899000	3.956313000
6	1.264479000	3.756722000	-0.461363000
6	2.503545000	4.362644000	-0.705771000
6	0.112443000	4.545104000	-0.476505000
6	2.585357000	5.724796000	-0.971228000
1	3.416262000	3.773284000	-0.676586000
6	0.194444000	5.912344000	-0.736335000
1	-0.849275000	4.074382000	-0.295390000
6	1.428333000	6.503551000	-0.986213000
1	3.552621000	6.182265000	-1.158869000
1	-0.710932000	6.512735000	-0.742996000
1	1.493417000	7.568946000	-1.188590000
6	3.934029000	-1.985361000	2.977062000
6	3.076382000	-1.892440000	4.072149000
6	1.709366000	-2.075378000	3.893182000
6	1.200668000	-2.362196000	2.630125000
6	2.055350000	-2.468266000	1.527521000
6	3.427673000	-2.266225000	1.715660000
1	5.001315000	-1.832953000	3.107486000
1	3.474007000	-1.669407000	5.058225000
1	1.029904000	-1.987973000	4.736061000
1	0.129429000	-2.479374000	2.505553000
1	4.091841000	-2.334713000	0.860529000
6	1.516693000	-2.788361000	0.176387000
6	0.118914000	-3.335664000	0.087520000
1	-0.075931000	-4.065730000	0.878164000
1	-0.062503000	-3.820946000	-0.875621000
1	-0.596658000	-2.515972000	0.217868000
7	2.288163000	-2.557829000	-0.825529000
16	1.773196000	-2.889335000	-2.415816000
6	3.395504000	-2.739331000	-3.286098000
6	3.998401000	-1.349832000	-3.082143000
1	4.958492000	-1.285315000	-3.609386000
1	4.177761000	-1.153843000	-2.020970000
1	3.341035000	-0.569047000	-3.478386000
6	4.347045000	-3.818819000	-2.766514000
1	4.525479000	-3.694420000	-1.693843000
1	5.311228000	-3.746841000	-3.285089000

1	3.939753000	-4.821443000	-2.933611000
6	3.062753000	-2.971348000	-4.763072000
1	3.984231000	-2.916092000	-5.353808000
1	2.372505000	-2.210683000	-5.146207000
1	2.616601000	-3.958504000	-4.929066000

6C1

Coordinates (Angstroms)

	X	Y	Z
44	1.176520000	0.856030000	-0.051169000
1	2.194104000	2.054650000	-0.700642000
15	2.824057000	-0.729478000	-0.437957000
15	-0.654567000	2.266987000	-0.273774000
6	2.462546000	-1.270921000	-2.177129000
6	-1.194543000	1.954649000	-2.020631000
1	3.355095000	-1.639509000	-2.692119000
1	1.732967000	-2.088308000	-2.134707000
6	1.848486000	-0.094361000	-2.927979000
1	-1.691681000	2.823794000	-2.462490000
6	0.022257000	1.543766000	-2.842057000
1	-1.902511000	1.119015000	-1.998450000
1	1.549406000	-0.406308000	-3.938819000
7	0.683252000	0.405883000	-2.179454000
1	2.567796000	0.725899000	-3.015075000
1	0.748062000	2.360385000	-2.906401000
1	-0.286538000	1.265681000	-3.859858000
6	1.585654000	1.231089000	1.709164000
8	1.845953000	1.462385000	2.821872000
1	-0.007518000	-0.348128000	-2.138414000
1	0.092542000	-0.362513000	0.368656000
6	2.855008000	-2.286076000	0.530915000
6	2.726998000	-2.187365000	1.920898000
6	2.960301000	-3.553305000	-0.048437000
6	2.695197000	-3.330280000	2.713463000
1	2.629013000	-1.209275000	2.383315000
6	2.918793000	-4.699499000	0.743865000
1	3.063326000	-3.661822000	-1.124290000
6	2.783076000	-4.590564000	2.124570000
1	2.586639000	-3.235876000	3.789941000
1	2.989790000	-5.677921000	0.277740000
1	2.744520000	-5.484495000	2.740250000
6	4.607461000	-0.280204000	-0.474580000
6	5.579461000	-1.212867000	-0.857999000
6	5.007151000	1.005107000	-0.106135000

6	6.923870000	-0.861206000	-0.886748000
1	5.289129000	-2.225971000	-1.125868000
6	6.356651000	1.355542000	-0.127338000
1	4.253244000	1.730218000	0.186221000
6	7.314535000	0.426910000	-0.521027000
1	7.667862000	-1.592220000	-1.189940000
1	6.655479000	2.359054000	0.161984000
1	8.365592000	0.701164000	-0.540750000
6	-2.170468000	2.008449000	0.720412000
6	-3.457144000	2.064553000	0.177100000
6	-2.025097000	1.778594000	2.091682000
6	-4.576954000	1.895183000	0.988726000
1	-3.599581000	2.236647000	-0.886040000
6	-3.142614000	1.629525000	2.905047000
1	-1.031613000	1.702692000	2.522849000
6	-4.421059000	1.681584000	2.354664000
1	-5.569988000	1.933413000	0.549656000
1	-3.012214000	1.449578000	3.967084000
1	-5.292987000	1.549060000	2.988818000
6	-0.456206000	4.096155000	-0.181642000
6	-1.545575000	4.959023000	-0.358658000
6	0.804023000	4.640839000	0.069994000
6	-1.373602000	6.337013000	-0.296822000
1	-2.539250000	4.554330000	-0.531831000
6	0.975880000	6.022581000	0.137068000
1	1.647736000	3.969731000	0.202492000
6	-0.109897000	6.872173000	-0.048062000
1	-2.226545000	6.995171000	-0.436256000
1	1.961928000	6.433170000	0.334778000
1	0.024155000	7.948849000	0.006166000
6	-3.658136000	-1.730494000	3.760664000
6	-2.629848000	-1.409871000	4.644503000
6	-1.317894000	-1.330937000	4.182611000
6	-1.027717000	-1.601775000	2.850188000
6	-2.054856000	-1.934054000	1.959354000
6	-3.374065000	-1.977547000	2.423210000
1	-4.683663000	-1.787371000	4.113592000
1	-2.851081000	-1.214595000	5.690025000
1	-0.515228000	-1.055858000	4.860344000
1	-0.008101000	-1.508662000	2.492655000
1	-4.170524000	-2.226881000	1.730110000
6	-1.769368000	-2.262855000	0.538510000
6	-0.528025000	-3.046808000	0.221765000
1	0.217679000	-2.954238000	1.008984000

1	-0.804163000	-4.104230000	0.130687000
1	-0.084480000	-2.727188000	-0.721790000
7	-2.686820000	-1.934678000	-0.309621000
6	-4.239148000	-1.964099000	-2.501027000
6	-4.525528000	-0.481557000	-2.263778000
1	-5.550263000	-0.268581000	-2.588862000
1	-4.437250000	-0.223995000	-1.204955000
1	-3.847613000	0.151233000	-2.844190000
6	-5.218945000	-2.850310000	-1.729801000
1	-5.222265000	-2.607677000	-0.663577000
1	-6.227214000	-2.679906000	-2.123213000
1	-4.980581000	-3.910734000	-1.851523000
6	-4.256914000	-2.297987000	-3.996547000
1	-5.253840000	-2.076612000	-4.391842000
1	-3.529351000	-1.696437000	-4.549681000
1	-4.045193000	-3.356403000	-4.173684000
8	-1.620254000	-1.408164000	-2.586794000
16	-2.546547000	-2.342623000	-1.924200000
8	-2.304049000	-3.774622000	-2.108178000

6C2

Coordinates (Angstroms)

	X	Y	Z
44	-1.176484000	0.856018000	-0.051104000
1	-2.194037000	2.054654000	-0.700630000
15	-2.824076000	-0.729419000	-0.437934000
15	0.654646000	2.266918000	-0.273594000
6	-2.462594000	-1.270772000	-2.177152000
6	1.194752000	1.954508000	-2.020397000
1	-3.355177000	-1.639239000	-2.692171000
1	-1.733087000	-2.088225000	-2.134787000
6	-1.848444000	-0.094206000	-2.927921000
1	1.691996000	2.823598000	-2.462245000
6	-0.021992000	1.543679000	-2.841939000
1	1.902653000	1.118821000	-1.998108000
1	-1.549406000	-0.406107000	-3.938787000
7	-0.683158000	0.405883000	-2.179371000
1	-2.567687000	0.726119000	-3.014935000
1	-0.747727000	2.360356000	-2.906384000
1	0.286893000	1.265534000	-3.859693000
6	-1.585685000	1.231103000	1.709218000
8	-1.846008000	1.462407000	2.821915000
1	0.007479000	-0.348249000	-2.138292000
1	-0.092536000	-0.362530000	0.368838000

6	-2.855048000	-2.286056000	0.530877000
6	-2.727000000	-2.187384000	1.920861000
6	-2.960423000	-3.553266000	-0.048497000
6	-2.695232000	-3.330316000	2.713399000
1	-2.628948000	-1.209305000	2.383290000
6	-2.918953000	-4.699481000	0.743780000
1	-3.063486000	-3.661764000	-1.124348000
6	-2.783194000	-4.590585000	2.124482000
1	-2.586643000	-3.235942000	3.789877000
1	-2.990016000	-5.677889000	0.277632000
1	-2.744670000	-5.484531000	2.740144000
6	-4.607470000	-0.280107000	-0.474522000
6	-5.579530000	-1.212827000	-0.857659000
6	-5.007080000	1.005330000	-0.106429000
6	-6.923918000	-0.861097000	-0.886470000
1	-5.289256000	-2.226017000	-1.125264000
6	-6.356561000	1.355837000	-0.127705000
1	-4.253119000	1.730472000	0.185712000
6	-7.314502000	0.427147000	-0.521112000
1	-7.667962000	-1.592154000	-1.189435000
1	-6.655324000	2.359451000	0.161331000
1	-8.365544000	0.701455000	-0.540892000
6	2.170476000	2.008395000	0.720702000
6	3.457181000	2.064513000	0.177462000
6	2.025032000	1.778468000	2.091953000
6	4.576951000	1.895083000	0.989134000
1	3.599679000	2.236689000	-0.885656000
6	3.142505000	1.629359000	2.905367000
1	1.031525000	1.702546000	2.523063000
6	4.420982000	1.681425000	2.355052000
1	5.570005000	1.933321000	0.550110000
1	3.012053000	1.449374000	3.967392000
1	5.292871000	1.548852000	2.989250000
6	0.456280000	4.096099000	-0.181565000
6	1.545678000	4.958959000	-0.358458000
6	-0.803990000	4.640793000	0.069831000
6	1.373692000	6.336953000	-0.296733000
1	2.539380000	4.554260000	-0.531450000
6	-0.975863000	6.022537000	0.136787000
1	-1.647727000	3.969694000	0.202227000
6	0.109943000	6.872123000	-0.048213000
1	2.226656000	6.995104000	-0.436068000
1	-1.961944000	6.433143000	0.334303000
1	-0.024126000	7.948801000	0.005929000

6	3.658175000	-1.730617000	3.760473000
6	2.629896000	-1.410128000	4.644372000
6	1.317919000	-1.331249000	4.182537000
6	1.027712000	-1.602041000	2.850113000
6	2.054842000	-1.934179000	1.959215000
6	3.374075000	-1.977590000	2.423011000
1	4.683715000	-1.787444000	4.113368000
1	2.851160000	-1.214909000	5.689899000
1	0.515259000	-1.056266000	4.860316000
1	0.008085000	-1.508990000	2.492604000
1	4.170527000	-2.226803000	1.729858000
6	1.769334000	-2.262959000	0.538376000
6	0.528026000	-3.046965000	0.221605000
1	-0.217531000	-2.954805000	1.009009000
1	0.804303000	-4.104303000	0.130017000
1	0.084265000	-2.727035000	-0.721749000
7	2.686782000	-1.934746000	-0.309747000
6	4.239053000	-1.963887000	-2.501220000
6	4.525356000	-0.481346000	-2.263846000
1	5.550026000	-0.268259000	-2.589061000
1	4.437196000	-0.223910000	-1.204982000
1	3.847312000	0.151456000	-2.844099000
6	5.218937000	-2.850098000	-1.730098000
1	5.222220000	-2.607596000	-0.663843000
1	6.227188000	-2.679534000	-2.123487000
1	4.980690000	-3.910532000	-1.851956000
6	4.256767000	-2.297640000	-3.996763000
1	5.253680000	-2.076246000	-4.392086000
1	3.529190000	-1.696037000	-4.549820000
1	4.045044000	-3.356040000	-4.173995000
8	2.304094000	-3.774574000	-2.108461000
16	2.546507000	-2.342574000	-1.924340000
8	1.620118000	-1.408107000	-2.586785000

cis-6R

Coordinates (Angstroms)

	X	Y	Z
44	1.176520000	0.856030000	-0.051169000
1	2.194104000	2.054650000	-0.700642000
15	2.824057000	-0.729478000	-0.437957000
15	-0.654567000	2.266987000	-0.273774000
6	2.462546000	-1.270921000	-2.177129000
6	-1.194543000	1.954649000	-2.020631000
1	3.355095000	-1.639509000	-2.692119000

1	1.732967000	-2.088308000	-2.134707000
6	1.848486000	-0.094361000	-2.927979000
1	-1.691681000	2.823794000	-2.462490000
6	0.022257000	1.543766000	-2.842057000
1	-1.902511000	1.119015000	-1.998450000
1	1.549406000	-0.406308000	-3.938819000
7	0.683252000	0.405883000	-2.179454000
1	2.567796000	0.725899000	-3.015075000
1	0.748062000	2.360385000	-2.906401000
1	-0.286538000	1.265681000	-3.859858000
6	1.585654000	1.231089000	1.709164000
8	1.845953000	1.462385000	2.821872000
1	-0.007518000	-0.348128000	-2.138414000
1	0.092542000	-0.362513000	0.368656000
6	2.855008000	-2.286076000	0.530915000
6	2.726998000	-2.187365000	1.920898000
6	2.960301000	-3.553305000	-0.048437000
6	2.695197000	-3.330280000	2.713463000
1	2.629013000	-1.209275000	2.383315000
6	2.918793000	-4.699499000	0.743865000
1	3.063326000	-3.661822000	-1.124290000
6	2.783076000	-4.590564000	2.124570000
1	2.586639000	-3.235876000	3.789941000
1	2.989790000	-5.677921000	0.277740000
1	2.744520000	-5.484495000	2.740250000
6	4.607461000	-0.280204000	-0.474580000
6	5.579461000	-1.212867000	-0.857999000
6	5.007151000	1.005107000	-0.106135000
6	6.923870000	-0.861206000	-0.886748000
1	5.289129000	-2.225971000	-1.125868000
6	6.356651000	1.355542000	-0.127338000
1	4.253244000	1.730218000	0.186221000
6	7.314535000	0.426910000	-0.521027000
1	7.667862000	-1.592220000	-1.189940000
1	6.655479000	2.359054000	0.161984000
1	8.365592000	0.701164000	-0.540750000
6	-2.170468000	2.008449000	0.720412000
6	-3.457144000	2.064553000	0.177100000
6	-2.025097000	1.778594000	2.091682000
6	-4.576954000	1.895183000	0.988726000
1	-3.599581000	2.236647000	-0.886040000
6	-3.142614000	1.629525000	2.905047000
1	-1.031613000	1.702692000	2.522849000
6	-4.421059000	1.681584000	2.354664000

1	-5.569988000	1.933413000	0.549656000
1	-3.012214000	1.449578000	3.967084000
1	-5.292987000	1.549060000	2.988818000
6	-0.456206000	4.096155000	-0.181642000
6	-1.545575000	4.959023000	-0.358658000
6	0.804023000	4.640839000	0.069994000
6	-1.373602000	6.337013000	-0.296822000
1	-2.539250000	4.554330000	-0.531831000
6	0.975880000	6.022581000	0.137068000
1	1.647736000	3.969731000	0.202492000
6	-0.109897000	6.872173000	-0.048062000
1	-2.226545000	6.995171000	-0.436256000
1	1.961928000	6.433170000	0.334778000
1	0.024155000	7.948849000	0.006166000
6	-3.658136000	-1.730494000	3.760664000
6	-2.629848000	-1.409871000	4.644503000
6	-1.317894000	-1.330937000	4.182611000
6	-1.027717000	-1.601775000	2.850188000
6	-2.054856000	-1.934054000	1.959354000
6	-3.374065000	-1.977547000	2.423210000
1	-4.683663000	-1.787371000	4.113592000
1	-2.851081000	-1.214595000	5.690025000
1	-0.515228000	-1.055858000	4.860344000
1	-0.008101000	-1.508662000	2.492655000
1	-4.170524000	-2.226881000	1.730110000
6	-1.769368000	-2.262855000	0.538510000
6	-0.528025000	-3.046808000	0.221765000
1	0.217679000	-2.954238000	1.008984000
1	-0.804163000	-4.104230000	0.130687000
1	-0.084480000	-2.727188000	-0.721790000
7	-2.686820000	-1.934678000	-0.309621000
6	-4.239148000	-1.964099000	-2.501027000
6	-4.525528000	-0.481557000	-2.263778000
1	-5.550263000	-0.268581000	-2.588862000
1	-4.437250000	-0.223995000	-1.204955000
1	-3.847613000	0.151233000	-2.844190000
6	-5.218945000	-2.850310000	-1.729801000
1	-5.222265000	-2.607677000	-0.663577000
1	-6.227214000	-2.679906000	-2.123213000
1	-4.980581000	-3.910734000	-1.851523000
6	-4.256914000	-2.297987000	-3.996547000
1	-5.253840000	-2.076612000	-4.391842000
1	-3.529351000	-1.696437000	-4.549681000
1	-4.045193000	-3.356403000	-4.173684000

8	-1.620254000	-1.408164000	-2.586794000
16	-2.546547000	-2.342623000	-1.924200000
8	-2.304049000	-3.774622000	-2.108178000

cis-6S

Coordinates (Angstroms)

	X	Y	Z
44	1.176520000	0.856030000	-0.051169000
1	2.194104000	2.054650000	-0.700642000
15	2.824057000	-0.729478000	-0.437957000
15	-0.654567000	2.266987000	-0.273774000
6	2.462546000	-1.270921000	-2.177129000
6	-1.194543000	1.954649000	-2.020631000
1	3.355095000	-1.639509000	-2.692119000
1	1.732967000	-2.088308000	-2.134707000
6	1.848486000	-0.094361000	-2.927979000
1	-1.691681000	2.823794000	-2.462490000
6	0.022257000	1.543766000	-2.842057000
1	-1.902511000	1.119015000	-1.998450000
1	1.549406000	-0.406308000	-3.938819000
7	0.683252000	0.405883000	-2.179454000
1	2.567796000	0.725899000	-3.015075000
1	0.748062000	2.360385000	-2.906401000
1	-0.286538000	1.265681000	-3.859858000
6	1.585654000	1.231089000	1.709164000
8	1.845953000	1.462385000	2.821872000
1	-0.007518000	-0.348128000	-2.138414000
1	0.092542000	-0.362513000	0.368656000
6	2.855008000	-2.286076000	0.530915000
6	2.726998000	-2.187365000	1.920898000
6	2.960301000	-3.553305000	-0.048437000
6	2.695197000	-3.330280000	2.713463000
1	2.629013000	-1.209275000	2.383315000
6	2.918793000	-4.699499000	0.743865000
1	3.063326000	-3.661822000	-1.124290000
6	2.783076000	-4.590564000	2.124570000
1	2.586639000	-3.235876000	3.789941000
1	2.989790000	-5.677921000	0.277740000
1	2.744520000	-5.484495000	2.740250000
6	4.607461000	-0.280204000	-0.474580000
6	5.579461000	-1.212867000	-0.857999000
6	5.007151000	1.005107000	-0.106135000
6	6.923870000	-0.861206000	-0.886748000
1	5.289129000	-2.225971000	-1.125868000

6	6.356651000	1.355542000	-0.127338000
1	4.253244000	1.730218000	0.186221000
6	7.314535000	0.426910000	-0.521027000
1	7.667862000	-1.592220000	-1.189940000
1	6.655479000	2.359054000	0.161984000
1	8.365592000	0.701164000	-0.540750000
6	-2.170468000	2.008449000	0.720412000
6	-3.457144000	2.064553000	0.177100000
6	-2.025097000	1.778594000	2.091682000
6	-4.576954000	1.895183000	0.988726000
1	-3.599581000	2.236647000	-0.886040000
6	-3.142614000	1.629525000	2.905047000
1	-1.031613000	1.702692000	2.522849000
6	-4.421059000	1.681584000	2.354664000
1	-5.569988000	1.933413000	0.549656000
1	-3.012214000	1.449578000	3.967084000
1	-5.292987000	1.549060000	2.988818000
6	-0.456206000	4.096155000	-0.181642000
6	-1.545575000	4.959023000	-0.358658000
6	0.804023000	4.640839000	0.069994000
6	-1.373602000	6.337013000	-0.296822000
1	-2.539250000	4.554330000	-0.531831000
6	0.975880000	6.022581000	0.137068000
1	1.647736000	3.969731000	0.202492000
6	-0.109897000	6.872173000	-0.048062000
1	-2.226545000	6.995171000	-0.436256000
1	1.961928000	6.433170000	0.334778000
1	0.024155000	7.948849000	0.006166000
6	-3.658136000	-1.730494000	3.760664000
6	-2.629848000	-1.409871000	4.644503000
6	-1.317894000	-1.330937000	4.182611000
6	-1.027717000	-1.601775000	2.850188000
6	-2.054856000	-1.934054000	1.959354000
6	-3.374065000	-1.977547000	2.423210000
1	-4.683663000	-1.787371000	4.113592000
1	-2.851081000	-1.214595000	5.690025000
1	-0.515228000	-1.055858000	4.860344000
1	-0.008101000	-1.508662000	2.492655000
1	-4.170524000	-2.226881000	1.730110000
6	-1.769368000	-2.262855000	0.538510000
6	-0.528025000	-3.046808000	0.221765000
1	0.217679000	-2.954238000	1.008984000
1	-0.804163000	-4.104230000	0.130687000
1	-0.084480000	-2.727188000	-0.721790000

7	-2.686820000	-1.934678000	-0.309621000
6	-4.239148000	-1.964099000	-2.501027000
6	-4.525528000	-0.481557000	-2.263778000
1	-5.550263000	-0.268581000	-2.588862000
1	-4.437250000	-0.223995000	-1.204955000
1	-3.847613000	0.151233000	-2.844190000
6	-5.218945000	-2.850310000	-1.729801000
1	-5.222265000	-2.607677000	-0.663577000
1	-6.227214000	-2.679906000	-2.123213000
1	-4.980581000	-3.910734000	-1.851523000
6	-4.256914000	-2.297987000	-3.996547000
1	-5.253840000	-2.076612000	-4.391842000
1	-3.529351000	-1.696437000	-4.549681000
1	-4.045193000	-3.356403000	-4.173684000
8	-1.620254000	-1.408164000	-2.586794000
16	-2.546547000	-2.342623000	-1.924200000
8	-2.304049000	-3.774622000	-2.108178000

TS6R-7R

Coordinates (Angstroms)

	X	Y	Z
44	0.756356000	0.767487000	-0.030840000
1	1.457112000	2.135474000	-0.641640000
15	2.813664000	-0.276054000	-0.341993000
15	-1.313864000	1.774699000	-0.387348000
6	2.657496000	-0.942265000	-2.063053000
6	-1.734100000	1.148191000	-2.070094000
1	3.629123000	-1.082778000	-2.546925000
1	2.151570000	-1.913617000	-2.009965000
6	1.779770000	0.018648000	-2.859126000
1	-2.484096000	1.758953000	-2.581985000
6	-0.443276000	1.060731000	-2.876100000
1	-2.130826000	0.136316000	-1.933891000
1	1.605800000	-0.384609000	-3.866005000
7	0.498141000	0.188346000	-2.152524000
1	2.256297000	1.000091000	-2.953512000
1	0.016853000	2.047059000	-2.998527000
1	-0.648644000	0.643424000	-3.871322000
6	1.012598000	1.325254000	1.716193000
8	1.194013000	1.700517000	2.802872000
1	0.052503000	-0.742780000	-2.156256000
1	-0.066179000	-0.739883000	0.363330000
6	3.316603000	-1.698810000	0.693785000
6	3.221172000	-1.550693000	2.082358000

6	3.761800000	-2.915171000	0.171171000
6	3.559344000	-2.599264000	2.930527000
1	2.864376000	-0.613644000	2.501289000
6	4.093172000	-3.969056000	1.021070000
1	3.845527000	-3.056985000	-0.902456000
6	3.990909000	-3.813976000	2.400194000
1	3.474504000	-2.471160000	4.005516000
1	4.430803000	-4.912330000	0.601711000
1	4.246077000	-4.636765000	3.061528000
6	4.367245000	0.708119000	-0.380188000
6	5.590692000	0.090369000	-0.670225000
6	4.346458000	2.076116000	-0.105755000
6	6.766647000	0.830491000	-0.698357000
1	5.629547000	-0.979025000	-0.862670000
6	5.526819000	2.817929000	-0.129573000
1	3.398989000	2.556195000	0.119176000
6	6.735887000	2.198357000	-0.427531000
1	7.709016000	0.339639000	-0.923834000
1	5.496907000	3.882046000	0.086384000
1	7.655949000	2.775718000	-0.445437000
6	-2.787285000	1.447489000	0.641587000
6	-4.005065000	1.012738000	0.114641000
6	-2.698116000	1.730200000	2.008749000
6	-5.121787000	0.882297000	0.937985000
1	-4.096385000	0.781098000	-0.942028000
6	-3.815586000	1.612689000	2.825874000
1	-1.750482000	2.047235000	2.435312000
6	-5.031541000	1.191669000	2.291017000
1	-6.063200000	0.541205000	0.516622000
1	-3.731780000	1.834272000	3.885289000
1	-5.903458000	1.094942000	2.931692000
6	-1.422770000	3.604558000	-0.553356000
6	-2.593286000	4.200512000	-1.039666000
6	-0.353528000	4.418908000	-0.178430000
6	-2.682653000	5.581293000	-1.170301000
1	-3.447671000	3.583653000	-1.308267000
6	-0.446420000	5.804926000	-0.298549000
1	0.554617000	3.960912000	0.201142000
6	-1.605944000	6.386768000	-0.800173000
1	-3.593035000	6.030548000	-1.556609000
1	0.392272000	6.428166000	-0.001484000
1	-1.676285000	7.466191000	-0.900088000
6	-3.524736000	-1.688834000	3.351511000
6	-2.716400000	-1.277345000	4.405656000

6	-1.353629000	-1.078046000	4.188320000
6	-0.806690000	-1.309522000	2.933122000
6	-1.609294000	-1.736195000	1.870735000
6	-2.975872000	-1.910356000	2.091043000
1	-4.590252000	-1.833088000	3.504981000
1	-3.145598000	-1.102783000	5.388392000
1	-0.713751000	-0.738650000	4.998017000
1	0.251497000	-1.136309000	2.765859000
1	-3.602478000	-2.227301000	1.265324000
6	-1.021529000	-2.127768000	0.538535000
6	0.188707000	-3.043558000	0.626050000
1	0.842759000	-2.764737000	1.450346000
1	-0.165715000	-4.068571000	0.799732000
1	0.779249000	-3.026923000	-0.291963000
7	-1.891136000	-2.186469000	-0.461598000
16	-1.442217000	-3.122623000	-1.779761000
6	-3.125281000	-3.306078000	-2.531010000
6	-3.754314000	-1.940227000	-2.779741000
1	-4.715039000	-2.067900000	-3.293228000
1	-3.930315000	-1.416538000	-1.836581000
1	-3.107464000	-1.327645000	-3.416681000
6	-3.961551000	-4.150403000	-1.570498000
1	-4.119634000	-3.632779000	-0.620338000
1	-4.940834000	-4.350809000	-2.021045000
1	-3.485202000	-5.116153000	-1.363152000
6	-2.893430000	-4.045276000	-3.851333000
1	-3.855192000	-4.212633000	-4.349854000
1	-2.254449000	-3.460382000	-4.519646000
1	-2.422707000	-5.022927000	-3.692025000
8	-0.648804000	-2.272535000	-2.768437000

TS6S-7S

Coordinates (Angstroms)

	X	Y	Z
44	-0.706262000	0.777175000	-0.037691000
1	-1.386870000	2.144131000	-0.660303000
15	-2.797043000	-0.224329000	-0.313896000
15	1.372178000	1.758291000	-0.433424000
6	-2.645451000	-0.960922000	-2.006880000
6	1.746761000	1.168481000	-2.144609000
1	-3.616352000	-1.116816000	-2.487025000
1	-2.153008000	-1.936518000	-1.911029000
6	-1.773033000	-0.034251000	-2.848517000
1	2.455551000	1.816161000	-2.669354000

6	0.436323000	1.053750000	-2.915507000
1	2.194532000	0.173971000	-2.040572000
1	-1.619437000	-0.464706000	-3.847471000
7	-0.477787000	0.166196000	-2.172340000
1	-2.245837000	0.946414000	-2.963575000
1	-0.047808000	2.030060000	-3.017593000
1	0.621101000	0.650115000	-3.920826000
6	-0.931424000	1.395894000	1.691545000
8	-1.087646000	1.821589000	2.762084000
1	-0.014148000	-0.744349000	-2.133156000
1	0.089076000	-0.760843000	0.386543000
6	-3.371917000	-1.583144000	0.765496000
6	-3.294413000	-1.385891000	2.148651000
6	-3.861338000	-2.796929000	0.277809000
6	-3.693574000	-2.386214000	3.027877000
1	-2.904381000	-0.450474000	2.541036000
6	-4.252867000	-3.802197000	1.159465000
1	-3.928055000	-2.977394000	-0.791180000
6	-4.167944000	-3.599928000	2.533514000
1	-3.621376000	-2.222817000	4.098956000
1	-4.620470000	-4.746297000	0.768337000
1	-4.468315000	-4.386552000	3.219246000
6	-4.304886000	0.822166000	-0.409365000
6	-5.521395000	0.275762000	-0.837251000
6	-4.262541000	2.161029000	-0.018093000
6	-6.667987000	1.059505000	-0.890173000
1	-5.579780000	-0.773014000	-1.118098000
6	-5.414921000	2.944505000	-0.060766000
1	-3.321885000	2.587911000	0.315073000
6	-6.615646000	2.398016000	-0.501919000
1	-7.604104000	0.625557000	-1.229236000
1	-5.369163000	3.984576000	0.248860000
1	-7.512815000	3.009373000	-0.538626000
6	2.866908000	1.383983000	0.546260000
6	4.070387000	0.960069000	-0.021304000
6	2.807518000	1.620922000	1.923620000
6	5.201260000	0.789372000	0.774746000
1	4.141461000	0.763980000	-1.086759000
6	3.940510000	1.467608000	2.712706000
1	1.870815000	1.926170000	2.381567000
6	5.140663000	1.052623000	2.139156000
1	6.130537000	0.453982000	0.323239000
1	3.879905000	1.653013000	3.780442000
1	6.024081000	0.923926000	2.757906000

6	1.496404000	3.589722000	-0.558333000
6	2.675716000	4.185445000	-1.023649000
6	0.433352000	4.405472000	-0.168919000
6	2.779593000	5.567965000	-1.118877000
1	3.525941000	3.566876000	-1.301221000
6	0.540849000	5.792964000	-0.254034000
1	-0.480919000	3.948959000	0.196387000
6	1.709090000	6.375016000	-0.734304000
1	3.697026000	6.017449000	-1.487560000
1	-0.292777000	6.417003000	0.055107000
1	1.791456000	7.455810000	-0.805353000
6	3.569302000	-1.814833000	3.274482000
6	2.832261000	-1.351927000	4.359483000
6	1.477535000	-1.066224000	4.195250000
6	0.867684000	-1.264487000	2.962771000
6	1.597209000	-1.743199000	1.870380000
6	2.957238000	-2.003427000	2.037764000
1	4.629018000	-2.026634000	3.386233000
1	3.309856000	-1.205756000	5.324476000
1	0.892843000	-0.689190000	5.029803000
1	-0.186257000	-1.034610000	2.840081000
1	3.526316000	-2.365835000	1.189285000
6	0.919958000	-2.088538000	0.560052000
6	-0.294383000	-2.992304000	0.738377000
1	-0.916939000	-2.659680000	1.568439000
1	0.066920000	-4.005583000	0.949702000
1	-0.901832000	-3.042306000	-0.163566000
7	1.764769000	-2.229824000	-0.457273000
16	1.259382000	-2.739448000	-1.955618000
6	2.933543000	-3.280695000	-2.569032000
6	3.883680000	-2.086326000	-2.583972000
1	4.856732000	-2.402526000	-2.980227000
1	4.031000000	-1.684660000	-1.578156000
1	3.510553000	-1.284834000	-3.234262000
6	3.435362000	-4.397993000	-1.659308000
1	3.643267000	-4.023396000	-0.653229000
1	4.357185000	-4.825432000	-2.072250000
1	2.687224000	-5.193614000	-1.585825000
6	2.690668000	-3.802724000	-3.986406000
1	3.634250000	-4.163788000	-4.411563000
1	2.305462000	-3.015681000	-4.646971000
1	1.974023000	-4.628978000	-3.982282000
8	0.415096000	-3.991642000	-1.987980000

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Coordinates (Angstroms)			
	X	Y	Z
44	0.959451000	0.935248000	0.050079000
1	1.657370000	2.125754000	-0.950504000
15	2.810670000	-0.414162000	-0.309839000
15	-1.123048000	1.952923000	-0.112040000
6	2.437709000	-1.215617000	-1.949050000
6	-1.827641000	1.145144000	-1.624218000
1	3.347319000	-1.400499000	-2.528824000
1	1.963906000	-2.184323000	-1.752819000
6	1.472732000	-0.332190000	-2.732299000
1	-2.588761000	1.762081000	-2.112476000
6	-0.686369000	0.832043000	-2.582998000
1	-2.296058000	0.209962000	-1.294939000
1	1.140312000	-0.851370000	-3.642706000
7	0.316454000	0.008795000	-1.884178000
1	1.953511000	0.606924000	-3.019708000
1	-0.190755000	1.749699000	-2.914660000
1	-1.064004000	0.298548000	-3.467201000
6	1.521621000	1.733118000	1.615445000
8	1.888479000	2.239913000	2.597550000
1	-0.150595000	-0.863708000	-1.634542000
1	0.195546000	-0.321777000	0.877559000
6	3.112744000	-1.845653000	0.801153000
6	2.810766000	-1.695146000	2.158075000
6	3.587711000	-3.081330000	0.347820000
6	2.987967000	-2.753078000	3.045046000
1	2.404870000	-0.752964000	2.513798000
6	3.754901000	-4.143947000	1.232815000
1	3.814749000	-3.231596000	-0.704538000
6	3.456730000	-3.981061000	2.583047000
1	2.748544000	-2.619571000	4.095988000
1	4.115903000	-5.100092000	0.864751000
1	3.584227000	-4.809752000	3.273510000
6	4.491039000	0.302466000	-0.518199000
6	5.596265000	-0.488650000	-0.855612000
6	4.670977000	1.673741000	-0.330298000
6	6.853152000	0.084131000	-1.012868000
1	5.481098000	-1.560590000	-0.990402000
6	5.932459000	2.247157000	-0.480456000
1	3.811845000	2.288116000	-0.079015000
6	7.023326000	1.455431000	-0.824525000
1	7.702104000	-0.539632000	-1.278024000

1	6.059150000	3.315118000	-0.329043000
1	8.005705000	1.903248000	-0.944405000
6	-2.421317000	1.712221000	1.157824000
6	-3.771583000	1.541470000	0.833930000
6	-2.047430000	1.736425000	2.504039000
6	-4.730745000	1.423592000	1.835929000
1	-4.087159000	1.492371000	-0.204638000
6	-3.006511000	1.625348000	3.505379000
1	-0.998285000	1.827538000	2.767986000
6	-4.350419000	1.474772000	3.173869000
1	-5.775315000	1.287627000	1.570005000
1	-2.700386000	1.643419000	4.547206000
1	-5.098410000	1.382842000	3.956349000
6	-1.264485000	3.756718000	-0.461329000
6	-2.503555000	4.362646000	-0.705702000
6	-0.112447000	4.545096000	-0.476492000
6	-2.585369000	5.724800000	-0.971146000
1	-3.416274000	3.773289000	-0.676496000
6	-0.194450000	5.912339000	-0.736312000
1	0.849275000	4.074372000	-0.295402000
6	-1.428342000	6.503552000	-0.986156000
1	-3.552637000	6.182274000	-1.158759000
1	0.710928000	6.512726000	-0.742990000
1	-1.493427000	7.568949000	-1.188522000
6	-3.933967000	-1.985392000	2.977090000
6	-3.076303000	-1.892502000	4.072167000
6	-1.709290000	-2.075439000	3.893172000
6	-1.200613000	-2.362225000	2.630099000
6	-2.055313000	-2.468259000	1.527506000
6	-3.427632000	-2.266219000	1.715672000
1	-5.001251000	-1.832986000	3.107536000
1	-3.473912000	-1.669501000	5.058256000
1	-1.029814000	-1.988062000	4.736043000
1	-0.129377000	-2.479408000	2.505508000
1	-4.091814000	-2.334681000	0.860551000
6	-1.516677000	-2.788336000	0.176357000
6	-0.118910000	-3.335668000	0.087472000
1	0.075904000	-4.065775000	0.878086000
1	0.062500000	-3.820915000	-0.875688000
1	0.596686000	-2.516005000	0.217861000
7	-2.288162000	-2.557782000	-0.825543000
16	-1.773238000	-2.889288000	-2.415848000
6	-3.395574000	-2.739287000	-3.286078000
6	-3.998442000	-1.349773000	-3.082140000

1	-4.958563000	-1.285264000	-3.609332000
1	-4.177739000	-1.153741000	-2.020964000
1	-3.341089000	-0.569013000	-3.478450000
6	-4.347109000	-3.818745000	-2.766427000
1	-4.525499000	-3.694312000	-1.693753000
1	-5.311311000	-3.746767000	-3.284967000
1	-3.939838000	-4.821380000	-2.933511000
6	-3.062882000	-2.971353000	-4.763059000
1	-3.984381000	-2.916096000	-5.353763000
1	-2.372635000	-2.210710000	-5.146243000
1	-2.616753000	-3.958521000	-4.929041000

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Coordinates (Angstroms)

	X	Y	Z
44	-0.959455000	0.935254000	0.050079000
1	-1.657386000	2.125746000	-0.950513000
15	-2.810669000	-0.414168000	-0.309820000
15	1.123045000	1.952930000	-0.112055000
6	-2.437709000	-1.215644000	-1.949021000
6	1.827634000	1.145137000	-1.624227000
1	-3.347320000	-1.400531000	-2.528792000
1	-1.963909000	-2.184348000	-1.752779000
6	-1.472734000	-0.332225000	-2.732284000
1	2.588754000	1.762067000	-2.112493000
6	0.686363000	0.832018000	-2.583002000
1	2.296051000	0.209960000	-1.294935000
1	-1.140311000	-0.851419000	-3.642682000
7	-0.316458000	0.008781000	-1.884169000
1	-1.953518000	0.606881000	-3.019710000
1	0.190749000	1.749668000	-2.914681000
1	1.064001000	0.298510000	-3.467197000
6	-1.521634000	1.733130000	1.615437000
8	-1.888518000	2.239907000	2.597542000
1	0.150590000	-0.863715000	-1.634507000
1	-0.195528000	-0.321752000	0.877571000
6	-3.112728000	-1.845648000	0.801193000
6	-2.810732000	-1.695128000	2.158109000
6	-3.587699000	-3.081330000	0.347879000
6	-2.987923000	-2.753050000	3.045093000
1	-2.404831000	-0.752942000	2.513817000
6	-3.754879000	-4.143939000	1.232887000
1	-3.814744000	-3.231608000	-0.704477000
6	-3.456692000	-3.981038000	2.583113000

1	-2.748487000	-2.619533000	4.096031000
1	-4.115885000	-5.100087000	0.864836000
1	-3.584181000	-4.809722000	3.273587000
6	-4.491040000	0.302454000	-0.518184000
6	-5.596264000	-0.488658000	-0.855614000
6	-4.670979000	1.673729000	-0.330276000
6	-6.853150000	0.084125000	-1.012872000
1	-5.481097000	-1.560596000	-0.990420000
6	-5.932461000	2.247145000	-0.480435000
1	-3.811849000	2.288102000	-0.078986000
6	-7.023325000	1.455422000	-0.824517000
1	-7.702099000	-0.539635000	-1.278042000
1	-6.059152000	3.315105000	-0.329013000
1	-8.005704000	1.903241000	-0.944398000
6	2.421323000	1.712248000	1.157804000
6	3.771588000	1.541495000	0.833903000
6	2.047447000	1.736472000	2.504022000
6	4.730757000	1.423629000	1.835896000
1	4.087157000	1.492388000	-0.204665000
6	3.006535000	1.625405000	3.505356000
1	0.998304000	1.827591000	2.767977000
6	4.350441000	1.474821000	3.173839000
1	5.775325000	1.287662000	1.569967000
1	2.700417000	1.643492000	4.547186000
1	5.098437000	1.382899000	3.956313000
6	1.264479000	3.756722000	-0.461363000
6	2.503545000	4.362644000	-0.705771000
6	0.112443000	4.545104000	-0.476505000
6	2.585357000	5.724796000	-0.971228000
1	3.416262000	3.773284000	-0.676586000
6	0.194444000	5.912344000	-0.736335000
1	-0.849275000	4.074382000	-0.295390000
6	1.428333000	6.503551000	-0.986213000
1	3.552621000	6.182265000	-1.158869000
1	-0.710932000	6.512735000	-0.742996000
1	1.493417000	7.568946000	-1.188590000
6	3.934029000	-1.985361000	2.977062000
6	3.076382000	-1.892440000	4.072149000
6	1.709366000	-2.075378000	3.893182000
6	1.200668000	-2.362196000	2.630125000
6	2.055350000	-2.468266000	1.527521000
6	3.427673000	-2.266225000	1.715660000
1	5.001315000	-1.832953000	3.107486000
1	3.474007000	-1.669407000	5.058225000

1	1.029904000	-1.987973000	4.736061000
1	0.129429000	-2.479374000	2.505553000
1	4.091841000	-2.334713000	0.860529000
6	1.516693000	-2.788361000	0.176387000
6	0.118914000	-3.335664000	0.087520000
1	-0.075931000	-4.065730000	0.878164000
1	-0.062503000	-3.820946000	-0.875621000
1	-0.596658000	-2.515972000	0.217868000
7	2.288163000	-2.557829000	-0.825529000
16	1.773196000	-2.889335000	-2.415816000
6	3.395504000	-2.739331000	-3.286098000
6	3.998401000	-1.349832000	-3.082143000
1	4.958492000	-1.285315000	-3.609386000
1	4.177761000	-1.153843000	-2.020970000
1	3.341035000	-0.569047000	-3.478386000
6	4.347045000	-3.818819000	-2.766514000
1	4.525479000	-3.694420000	-1.693843000
1	5.311228000	-3.746841000	-3.285089000
1	3.939753000	-4.821443000	-2.933611000
6	3.062753000	-2.971348000	-4.763072000
1	3.984231000	-2.916092000	-5.353808000
1	2.372505000	-2.210683000	-5.146207000
1	2.616601000	-3.958504000	-4.929066000

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Coordinates (Angstroms)

	X	Y	Z
44	1.176520000	0.856030000	-0.051169000
1	2.194104000	2.054650000	-0.700642000
15	2.824057000	-0.729478000	-0.437957000
15	-0.654567000	2.266987000	-0.273774000
6	2.462546000	-1.270921000	-2.177129000
6	-1.194543000	1.954649000	-2.020631000
1	3.355095000	-1.639509000	-2.692119000
1	1.732967000	-2.088308000	-2.134707000
6	1.848486000	-0.094361000	-2.927979000
1	-1.691681000	2.823794000	-2.462490000
6	0.022257000	1.543766000	-2.842057000
1	-1.902511000	1.119015000	-1.998450000
1	1.549406000	-0.406308000	-3.938819000
7	0.683252000	0.405883000	-2.179454000
1	2.567796000	0.725899000	-3.015075000
1	0.748062000	2.360385000	-2.906401000
1	-0.286538000	1.265681000	-3.859858000

6	1.585654000	1.231089000	1.709164000
8	1.845953000	1.462385000	2.821872000
1	-0.007518000	-0.348128000	-2.138414000
1	0.092542000	-0.362513000	0.368656000
6	2.855008000	-2.286076000	0.530915000
6	2.726998000	-2.187365000	1.920898000
6	2.960301000	-3.553305000	-0.048437000
6	2.695197000	-3.330280000	2.713463000
1	2.629013000	-1.209275000	2.383315000
6	2.918793000	-4.699499000	0.743865000
1	3.063326000	-3.661822000	-1.124290000
6	2.783076000	-4.590564000	2.124570000
1	2.586639000	-3.235876000	3.789941000
1	2.989790000	-5.677921000	0.277740000
1	2.744520000	-5.484495000	2.740250000
6	4.607461000	-0.280204000	-0.474580000
6	5.579461000	-1.212867000	-0.857999000
6	5.007151000	1.005107000	-0.106135000
6	6.923870000	-0.861206000	-0.886748000
1	5.289129000	-2.225971000	-1.125868000
6	6.356651000	1.355542000	-0.127338000
1	4.253244000	1.730218000	0.186221000
6	7.314535000	0.426910000	-0.521027000
1	7.667862000	-1.592220000	-1.189940000
1	6.655479000	2.359054000	0.161984000
1	8.365592000	0.701164000	-0.540750000
6	-2.170468000	2.008449000	0.720412000
6	-3.457144000	2.064553000	0.177100000
6	-2.025097000	1.778594000	2.091682000
6	-4.576954000	1.895183000	0.988726000
1	-3.599581000	2.236647000	-0.886040000
6	-3.142614000	1.629525000	2.905047000
1	-1.031613000	1.702692000	2.522849000
6	-4.421059000	1.681584000	2.354664000
1	-5.569988000	1.933413000	0.549656000
1	-3.012214000	1.449578000	3.967084000
1	-5.292987000	1.549060000	2.988818000
6	-0.456206000	4.096155000	-0.181642000
6	-1.545575000	4.959023000	-0.358658000
6	0.804023000	4.640839000	0.069994000
6	-1.373602000	6.337013000	-0.296822000
1	-2.539250000	4.554330000	-0.531831000
6	0.975880000	6.022581000	0.137068000
1	1.647736000	3.969731000	0.202492000

6	-0.109897000	6.872173000	-0.048062000
1	-2.226545000	6.995171000	-0.436256000
1	1.961928000	6.433170000	0.334778000
1	0.024155000	7.948849000	0.006166000
6	-3.658136000	-1.730494000	3.760664000
6	-2.629848000	-1.409871000	4.644503000
6	-1.317894000	-1.330937000	4.182611000
6	-1.027717000	-1.601775000	2.850188000
6	-2.054856000	-1.934054000	1.959354000
6	-3.374065000	-1.977547000	2.423210000
1	-4.683663000	-1.787371000	4.113592000
1	-2.851081000	-1.214595000	5.690025000
1	-0.515228000	-1.055858000	4.860344000
1	-0.008101000	-1.508662000	2.492655000
1	-4.170524000	-2.226881000	1.730110000
6	-1.769368000	-2.262855000	0.538510000
6	-0.528025000	-3.046808000	0.221765000
1	0.217679000	-2.954238000	1.008984000
1	-0.804163000	-4.104230000	0.130687000
1	-0.0844480000	-2.727188000	-0.721790000
7	-2.686820000	-1.934678000	-0.309621000
6	-4.239148000	-1.964099000	-2.501027000
6	-4.525528000	-0.481557000	-2.263778000
1	-5.550263000	-0.268581000	-2.588862000
1	-4.437250000	-0.223995000	-1.204955000
1	-3.847613000	0.151233000	-2.844190000
6	-5.218945000	-2.850310000	-1.729801000
1	-5.222265000	-2.607677000	-0.663577000
1	-6.227214000	-2.679906000	-2.123213000
1	-4.980581000	-3.910734000	-1.851523000
6	-4.256914000	-2.297987000	-3.996547000
1	-5.253840000	-2.076612000	-4.391842000
1	-3.529351000	-1.696437000	-4.549681000
1	-4.045193000	-3.356403000	-4.173684000
8	-1.620254000	-1.408164000	-2.586794000
16	-2.546547000	-2.342623000	-1.924200000
8	-2.304049000	-3.774622000	-2.108178000

TS6-7_{C₂}

Coordinates (Angstroms)

	X	Y	Z
44	-1.176484000	0.856018000	-0.051104000
1	-2.194037000	2.054654000	-0.700630000
15	-2.824076000	-0.729419000	-0.437934000

15	0.654646000	2.266918000	-0.273594000
6	-2.462594000	-1.270772000	-2.177152000
6	1.194752000	1.954508000	-2.020397000
1	-3.355177000	-1.639239000	-2.692171000
1	-1.733087000	-2.088225000	-2.134787000
6	-1.848444000	-0.094206000	-2.927921000
1	1.691996000	2.823598000	-2.462245000
6	-0.021992000	1.543679000	-2.841939000
1	1.902653000	1.118821000	-1.998108000
1	-1.549406000	-0.406107000	-3.938787000
7	-0.683158000	0.405883000	-2.179371000
1	-2.567687000	0.726119000	-3.014935000
1	-0.747727000	2.360356000	-2.906384000
1	0.286893000	1.265534000	-3.859693000
6	-1.585685000	1.231103000	1.709218000
8	-1.846008000	1.462407000	2.821915000
1	0.007479000	-0.348249000	-2.138292000
1	-0.092536000	-0.362530000	0.368838000
6	-2.855048000	-2.286056000	0.530877000
6	-2.727000000	-2.187384000	1.920861000
6	-2.960423000	-3.553266000	-0.048497000
6	-2.695232000	-3.330316000	2.713399000
1	-2.628948000	-1.209305000	2.383290000
6	-2.918953000	-4.699481000	0.743780000
1	-3.063486000	-3.661764000	-1.124348000
6	-2.783194000	-4.590585000	2.124482000
1	-2.586643000	-3.235942000	3.789877000
1	-2.990016000	-5.677889000	0.277632000
1	-2.744670000	-5.484531000	2.740144000
6	-4.607470000	-0.280107000	-0.474522000
6	-5.579530000	-1.212827000	-0.857659000
6	-5.007080000	1.005330000	-0.106429000
6	-6.923918000	-0.861097000	-0.886470000
1	-5.289256000	-2.226017000	-1.125264000
6	-6.356561000	1.355837000	-0.127705000
1	-4.253119000	1.730472000	0.185712000
6	-7.314502000	0.427147000	-0.521112000
1	-7.667962000	-1.592154000	-1.189435000
1	-6.655324000	2.359451000	0.161331000
1	-8.365544000	0.701455000	-0.540892000
6	2.170476000	2.008395000	0.720702000
6	3.457181000	2.064513000	0.177462000
6	2.025032000	1.778468000	2.091953000
6	4.576951000	1.895083000	0.989134000

1	3.599679000	2.236689000	-0.885656000
6	3.142505000	1.629359000	2.905367000
1	1.031525000	1.702546000	2.523063000
6	4.420982000	1.681425000	2.355052000
1	5.570005000	1.933321000	0.550110000
1	3.012053000	1.449374000	3.967392000
1	5.292871000	1.548852000	2.989250000
6	0.456280000	4.096099000	-0.181565000
6	1.545678000	4.958959000	-0.358458000
6	-0.803990000	4.640793000	0.069831000
6	1.373692000	6.336953000	-0.296733000
1	2.539380000	4.554260000	-0.531450000
6	-0.975863000	6.022537000	0.136787000
1	-1.647727000	3.969694000	0.202227000
6	0.109943000	6.872123000	-0.048213000
1	2.226656000	6.995104000	-0.436068000
1	-1.961944000	6.433143000	0.334303000
1	-0.024126000	7.948801000	0.005929000
6	3.658175000	-1.730617000	3.760473000
6	2.629896000	-1.410128000	4.644372000
6	1.317919000	-1.331249000	4.182537000
6	1.027712000	-1.602041000	2.850113000
6	2.054842000	-1.934179000	1.959215000
6	3.374075000	-1.977590000	2.423011000
1	4.683715000	-1.787444000	4.113368000
1	2.851160000	-1.214909000	5.689899000
1	0.515259000	-1.056266000	4.860316000
1	0.008085000	-1.508990000	2.492604000
1	4.170527000	-2.226803000	1.729858000
6	1.769334000	-2.262959000	0.538376000
6	0.528026000	-3.046965000	0.221605000
1	-0.217531000	-2.954805000	1.009009000
1	0.804303000	-4.104303000	0.130017000
1	0.084265000	-2.727035000	-0.721749000
7	2.686782000	-1.934746000	-0.309747000
6	4.239053000	-1.963887000	-2.501220000
6	4.525356000	-0.481346000	-2.263846000
1	5.550026000	-0.268259000	-2.589061000
1	4.437196000	-0.223910000	-1.204982000
1	3.847312000	0.151456000	-2.844099000
6	5.218937000	-2.850098000	-1.730098000
1	5.222220000	-2.607596000	-0.663843000
1	6.227188000	-2.679534000	-2.123487000
1	4.980690000	-3.910532000	-1.851956000

6	4.256767000	-2.297640000	-3.996763000
1	5.253680000	-2.076246000	-4.392086000
1	3.529190000	-1.696037000	-4.549820000
1	4.045044000	-3.356040000	-4.173995000
8	2.304094000	-3.774574000	-2.108461000
16	2.546507000	-2.342574000	-1.924340000
8	1.620118000	-1.408107000	-2.586785000

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Coordinates (Angstroms)			
	X	Y	Z
44	1.210856000	0.782776000	0.065267000
1	2.282126000	1.707329000	-0.875039000
15	2.680240000	-1.009475000	-0.087476000
15	-0.461998000	2.336759000	-0.331256000
6	2.114666000	-1.849932000	-1.644301000
6	-1.136161000	1.806620000	-1.978427000
1	2.915609000	-2.415051000	-2.131311000
1	1.318318000	-2.551338000	-1.368895000
6	1.554376000	-0.794540000	-2.590397000
1	-1.500026000	2.662247000	-2.554832000
6	-0.054853000	1.052690000	-2.744427000
1	-1.980528000	1.133819000	-1.814086000
1	1.145264000	-1.271911000	-3.492428000
7	0.508638000	-0.018176000	-1.899895000
1	2.337028000	-0.092595000	-2.894492000
1	0.769165000	1.721009000	-3.010814000
1	-0.475883000	0.630875000	-3.669044000
6	1.785253000	1.489485000	1.673215000
8	2.153455000	1.943085000	2.679969000
1	-0.243207000	-0.665510000	-1.655659000
1	0.078522000	-0.236950000	0.802404000
6	2.667023000	-2.350511000	1.162839000
6	2.466459000	-2.001922000	2.501882000
6	2.811529000	-3.701271000	0.830257000
6	2.408611000	-2.982432000	3.487665000
1	2.325236000	-0.958784000	2.767549000
6	2.742703000	-4.684030000	1.814402000
1	2.959472000	-4.000107000	-0.204203000
6	2.540554000	-4.326159000	3.144966000
1	2.245936000	-2.696857000	4.522749000
1	2.845079000	-5.730409000	1.541139000
1	2.483118000	-5.092751000	3.912197000
6	4.481089000	-0.743107000	-0.349507000

6	5.332763000	-1.796514000	-0.704325000
6	5.019053000	0.532217000	-0.169105000
6	6.692582000	-1.575380000	-0.888071000
1	4.936242000	-2.800673000	-0.831235000
6	6.384416000	0.752607000	-0.342856000
1	4.356346000	1.351197000	0.094512000
6	7.221227000	-0.297831000	-0.706092000
1	7.342155000	-2.399631000	-1.168647000
1	6.792000000	1.748821000	-0.197471000
1	8.284343000	-0.124889000	-0.846670000
6	-1.911283000	2.462712000	0.788302000
6	-3.142394000	1.849050000	0.548058000
6	-1.731647000	3.167492000	1.985806000
6	-4.178080000	1.956866000	1.473860000
1	-3.322727000	1.262795000	-0.346309000
6	-2.764944000	3.273465000	2.909139000
1	-0.777775000	3.645293000	2.195836000
6	-3.995592000	2.671095000	2.652434000
1	-5.120694000	1.457135000	1.273211000
1	-2.607195000	3.824891000	3.831706000
1	-4.802164000	2.747166000	3.376150000
6	-0.059199000	4.113288000	-0.586715000
6	-1.074944000	5.049600000	-0.822813000
6	1.267344000	4.543764000	-0.552888000
6	-0.765301000	6.388485000	-1.031172000
1	-2.114832000	4.731651000	-0.832410000
6	1.577231000	5.887594000	-0.758756000
1	2.052014000	3.814889000	-0.371914000
6	0.564320000	6.810079000	-0.998396000
1	-1.560188000	7.106234000	-1.212849000
1	2.613964000	6.210689000	-0.727113000
1	0.805503000	7.857415000	-1.157057000
16	-2.977781000	-1.419070000	-1.829530000
8	-4.324049000	-1.110314000	-1.249495000
6	-3.247093000	-2.734781000	-3.122062000
6	-1.906058000	-3.035341000	-3.789205000
6	-4.222623000	-2.104438000	-4.119420000
6	-3.861800000	-3.969050000	-2.470041000
1	-1.193320000	-3.467471000	-3.082538000
1	-2.063020000	-3.751107000	-4.604833000
1	-1.463890000	-2.130823000	-4.224662000
1	-5.172958000	-1.852795000	-3.640328000
1	-4.421691000	-2.817378000	-4.927249000
1	-3.810014000	-1.193781000	-4.570304000

1	-3.159842000	-4.451596000	-1.783231000
1	-4.772200000	-3.704000000	-1.921968000
1	-4.133328000	-4.694816000	-3.245332000
6	-1.878043000	-2.443166000	0.394205000
6	-2.857928000	-1.928277000	1.397203000
6	-4.194389000	-2.335692000	1.382992000
6	-2.396716000	-1.110618000	2.435171000
6	-5.059097000	-1.926463000	2.392736000
1	-4.554375000	-2.973619000	0.584020000
6	-3.269574000	-0.690971000	3.432409000
1	-1.365794000	-0.768520000	2.435610000
6	-4.599646000	-1.102860000	3.417623000
1	-6.095742000	-2.250111000	2.374844000
1	-2.908972000	-0.029234000	4.213658000
1	-5.279600000	-0.778521000	4.200447000
6	-0.716515000	-3.201185000	0.973841000
1	-0.096094000	-2.528132000	1.574216000
1	-1.076163000	-3.996341000	1.636250000
1	-0.102715000	-3.633415000	0.181797000
7	-1.922700000	-2.351341000	-0.885481000

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Coordinates (Angstroms)			
	X	Y	Z
44	1.008454000	1.004589000	0.145353000
1	1.734706000	2.107117000	-0.917404000
15	-0.918016000	2.297296000	0.117804000
15	2.690440000	-0.498568000	-0.415118000
6	-1.793190000	1.692722000	-1.398019000
6	1.939862000	-1.405798000	-1.845857000
1	-2.434455000	2.457360000	-1.847572000
1	-2.417726000	0.845972000	-1.091787000
6	-0.754413000	1.189009000	-2.391338000
1	2.678169000	-1.877767000	-2.500902000
6	1.075960000	-0.422423000	-2.627298000
1	1.311402000	-2.200608000	-1.426102000
1	-1.254598000	0.741514000	-3.259955000
7	0.084428000	0.179779000	-1.719690000
1	-0.101876000	1.999978000	-2.728600000
1	1.690236000	0.384504000	-3.040437000
1	0.566055000	-0.936129000	-3.453329000
6	1.777368000	1.746242000	1.650275000
8	2.261144000	2.226897000	2.595161000
1	-0.558507000	-0.574766000	-1.464169000

1	0.193143000	-0.182535000	1.042407000
6	-2.179344000	2.159387000	1.441914000
6	-1.742074000	2.124806000	2.769749000
6	-3.550953000	2.089580000	1.180252000
6	-2.656824000	2.033315000	3.814045000
1	-0.677234000	2.148833000	2.984074000
6	-4.467627000	1.990328000	2.224768000
1	-3.917869000	2.102673000	0.158000000
6	-4.022295000	1.964286000	3.543732000
1	-2.301476000	2.005440000	4.840058000
1	-5.529894000	1.928860000	2.005881000
1	-4.737260000	1.885803000	4.357752000
6	-0.811171000	4.121730000	-0.099349000
6	-1.963158000	4.898612000	-0.275098000
6	0.434114000	4.751820000	-0.078426000
6	-1.869807000	6.275429000	-0.441860000
1	-2.943420000	4.428969000	-0.272105000
6	0.527635000	6.133894000	-0.236430000
1	1.329924000	4.151566000	0.050177000
6	-0.621179000	6.896064000	-0.422523000
1	-2.771440000	6.864904000	-0.582209000
1	1.502538000	6.612340000	-0.216385000
1	-0.546525000	7.972349000	-0.550121000
6	3.233779000	-1.829587000	0.728812000
6	3.932622000	-2.959131000	0.285844000
6	2.959290000	-1.697783000	2.092370000
6	4.359908000	-3.927550000	1.188946000
1	4.145941000	-3.092286000	-0.770773000
6	3.389539000	-2.665362000	2.998277000
1	2.392236000	-0.839269000	2.439490000
6	4.094017000	-3.778702000	2.549695000
1	4.900043000	-4.799058000	0.830257000
1	3.170424000	-2.546768000	4.055268000
1	4.430312000	-4.532373000	3.255829000
6	4.291980000	0.152110000	-1.048211000
6	5.110546000	-0.563792000	-1.928684000
6	4.717193000	1.408596000	-0.606892000
6	6.323878000	-0.036273000	-2.359832000
1	4.809578000	-1.541059000	-2.294406000
6	5.937035000	1.932172000	-1.027170000
1	4.076412000	1.985148000	0.052803000
6	6.741507000	1.212636000	-1.906466000
1	6.943219000	-0.602776000	-3.049428000
1	6.253283000	2.909136000	-0.672970000

1	7.688265000	1.625401000	-2.243238000
6	-1.428621000	-5.742197000	0.793549000
6	-0.050119000	-5.638411000	0.965795000
6	0.536490000	-4.387773000	1.141861000
6	-0.250720000	-3.239867000	1.149262000
6	-1.631225000	-3.339217000	0.954346000
6	-2.218130000	-4.596749000	0.782949000
1	-1.892383000	-6.715749000	0.665109000
1	0.565594000	-6.533378000	0.968122000
1	1.609193000	-4.298336000	1.281498000
1	0.205719000	-2.262140000	1.283391000
1	-3.293179000	-4.680482000	0.652020000
6	-2.470583000	-2.100191000	0.979285000
6	-2.475591000	-1.329850000	2.263915000
1	-1.493504000	-0.856923000	2.391232000
1	-2.637369000	-2.003361000	3.112419000
1	-3.240048000	-0.551496000	2.240569000
7	-3.174996000	-1.636315000	0.007932000
16	-3.054592000	-2.444048000	-1.519451000
8	-2.044510000	-1.655867000	-2.315267000
6	-4.726742000	-1.927815000	-2.122397000
6	-5.755563000	-2.543043000	-1.173812000
6	-4.841285000	-2.529655000	-3.525870000
6	-4.825016000	-0.407076000	-2.170476000
1	-5.684463000	-2.108037000	-0.172486000
1	-6.762932000	-2.351382000	-1.560662000
1	-5.634402000	-3.630547000	-1.094199000
1	-4.070922000	-2.129564000	-4.192971000
1	-5.820967000	-2.282615000	-3.949499000
1	-4.749474000	-3.622167000	-3.507130000
1	-4.758726000	0.024557000	-1.168315000
1	-4.025760000	0.012288000	-2.789790000
1	-5.786519000	-0.120641000	-2.612684000

7R

Coordinates (Angstroms)

	X	Y	Z
44	0.131373000	-0.927423000	0.112859000
1	0.295366000	-2.022232000	-0.987939000
15	-2.172689000	-1.244263000	-0.251458000
15	2.411836000	-0.472173000	-0.302860000
6	-2.522652000	-0.080492000	-1.637319000
6	2.269684000	0.961084000	-1.448454000
1	-3.357089000	-0.423273000	-2.256469000

1	-2.778681000	0.907141000	-1.243660000
6	-1.253251000	0.077402000	-2.461857000
1	3.182471000	1.156227000	-2.019291000
6	1.096706000	0.665475000	-2.374181000
1	2.037876000	1.841889000	-0.838341000
1	-1.416941000	0.872741000	-3.196059000
7	-0.128625000	0.457998000	-1.579667000
1	-0.991762000	-0.857766000	-2.970212000
1	1.292653000	-0.239530000	-2.962203000
1	0.946185000	1.496563000	-3.072747000
6	0.344398000	-2.236234000	1.425150000
8	0.472765000	-3.094286000	2.194206000
1	-0.360466000	1.407689000	-1.160091000
1	-2.116975000	1.716698000	0.735586000
6	-3.393034000	-0.898197000	1.065122000
6	-3.303467000	-1.651783000	2.242853000
6	-4.365875000	0.098726000	0.966665000
6	-4.170299000	-1.410128000	3.301907000
1	-2.541911000	-2.422583000	2.335115000
6	-5.230875000	0.343182000	2.032125000
1	-4.456435000	0.696776000	0.065658000
6	-5.134172000	-0.407325000	3.198978000
1	-4.088415000	-1.996852000	4.211984000
1	-5.979219000	1.125234000	1.946220000
1	-5.806406000	-0.211108000	4.028957000
6	-2.731478000	-2.882946000	-0.858950000
6	-4.075983000	-3.068302000	-1.207159000
6	-1.846729000	-3.955952000	-0.975777000
6	-4.520103000	-4.298001000	-1.677746000
1	-4.783882000	-2.250087000	-1.099742000
6	-2.293083000	-5.190423000	-1.444901000
1	-0.805734000	-3.827030000	-0.699547000
6	-3.626733000	-5.362056000	-1.799209000
1	-5.564533000	-4.428920000	-1.944652000
1	-1.593280000	-6.016511000	-1.530637000
1	-3.974364000	-6.323444000	-2.166108000
6	3.652546000	-0.021539000	0.955734000
6	4.479743000	1.098308000	0.844394000
6	3.792094000	-0.870093000	2.057622000
6	5.432687000	1.364697000	1.825646000
1	4.380816000	1.776961000	0.002151000
6	4.748169000	-0.607992000	3.031777000
1	3.139758000	-1.732798000	2.161630000
6	5.567824000	0.513367000	2.919226000

1	6.068162000	2.240769000	1.735304000
1	4.846293000	-1.274365000	3.883576000
1	6.310935000	0.722847000	3.682918000
6	3.328723000	-1.743628000	-1.262116000
6	4.507786000	-1.404306000	-1.937041000
6	2.891865000	-3.069777000	-1.291224000
6	5.217036000	-2.365170000	-2.648560000
1	4.885894000	-0.385991000	-1.898763000
6	3.607567000	-4.035447000	-1.995918000
1	1.988274000	-3.349224000	-0.759648000
6	4.765319000	-3.683678000	-2.682062000
1	6.125920000	-2.086849000	-3.173722000
1	3.255028000	-5.062605000	-2.009360000
1	5.319964000	-4.434568000	-3.237110000
6	1.861373000	1.983656000	2.897607000
6	1.505509000	0.933656000	3.746107000
6	0.257767000	0.339723000	3.612861000
6	-0.642610000	0.812230000	2.653285000
6	-0.301530000	1.872050000	1.805258000
6	0.975208000	2.437067000	1.928392000
1	2.841615000	2.441714000	2.991912000
1	2.206060000	0.579679000	4.496312000
1	-0.032728000	-0.481974000	4.261923000
1	-1.641589000	0.389444000	2.599452000
1	1.243831000	3.252432000	1.263693000
6	-1.355802000	2.501628000	0.905149000
6	-2.056891000	3.601895000	1.728146000
1	-2.456755000	3.191443000	2.663469000
1	-1.345029000	4.399440000	1.972173000
1	-2.886050000	4.044029000	1.168201000
7	-0.726936000	2.949678000	-0.334537000
16	-1.723127000	3.797861000	-1.314381000
6	-0.521584000	5.050475000	-1.993643000
6	0.638597000	4.329184000	-2.667662000
1	1.313909000	5.051327000	-3.144609000
1	1.211270000	3.748627000	-1.938110000
1	0.256396000	3.651516000	-3.438643000
6	-0.052653000	5.922112000	-0.833052000
1	0.478760000	5.323132000	-0.088678000
1	0.620819000	6.708346000	-1.198041000
1	-0.899431000	6.411268000	-0.335135000
6	-1.301543000	5.878781000	-3.016340000
1	-0.650957000	6.645054000	-3.456795000
1	-1.683510000	5.241391000	-3.819294000

1	-2.154135000	6.388744000	-2.550786000
8	-2.114283000	2.979893000	-2.546248000

7S

Coordinates (Angstroms)

	X	Y	Z
44	-0.134949000	-0.919783000	0.123213000
1	-0.297661000	-1.978921000	-1.016186000
15	-2.408996000	-0.439410000	-0.299870000
15	2.167822000	-1.256279000	-0.244254000
6	-2.247555000	1.015026000	-1.415128000
6	2.532232000	-0.084075000	-1.618883000
1	-3.157311000	1.233194000	-1.982623000
1	-2.001899000	1.881079000	-0.789128000
6	-1.078112000	0.718128000	-2.344978000
1	3.358970000	-0.436902000	-2.242689000
6	1.264406000	0.105276000	-2.438926000
1	2.807445000	0.896267000	-1.220368000
1	-0.921478000	1.554126000	-3.036164000
7	0.145602000	0.492984000	-1.552710000
1	-1.282277000	-0.179454000	-2.941574000
1	0.987241000	-0.818979000	-2.958693000
1	1.441854000	0.906107000	-3.164092000
6	-0.375639000	-2.267695000	1.388286000
8	-0.523118000	-3.149290000	2.126702000
1	0.384589000	1.438935000	-1.131694000
1	2.086604000	1.679681000	0.753507000
6	-3.666182000	-0.013214000	0.950814000
6	-4.458577000	1.134051000	0.876152000
6	-3.856516000	-0.910882000	2.005393000
6	-5.427433000	1.379612000	1.847510000
1	-4.319725000	1.850141000	0.071454000
6	-4.829409000	-0.670127000	2.968162000
1	-3.232745000	-1.797708000	2.080190000
6	-5.614339000	0.479188000	2.892759000
1	-6.034762000	2.277951000	1.786434000
1	-4.968802000	-1.375893000	3.781616000
1	-6.370501000	0.671732000	3.648100000
6	-3.322363000	-1.684915000	-1.296970000
6	-4.495327000	-1.325169000	-1.972113000
6	-2.889374000	-3.011302000	-1.356490000
6	-5.201422000	-2.265337000	-2.713759000
1	-4.871493000	-0.307306000	-1.909997000
6	-3.602307000	-3.956653000	-2.090922000

1	-1.990830000	-3.307105000	-0.825391000
6	-4.753308000	-3.583986000	-2.777305000
1	-6.105239000	-1.970874000	-3.238832000
1	-3.252756000	-4.984277000	-2.127594000
1	-5.305839000	-4.318585000	-3.355748000
6	3.391685000	-0.938521000	1.078284000
6	3.350933000	-1.769802000	2.205711000
6	4.313280000	0.110045000	1.039653000
6	4.215583000	-1.554929000	3.272173000
1	2.634323000	-2.586705000	2.250607000
6	5.174723000	0.328284000	2.113785000
1	4.368209000	0.769631000	0.179759000
6	5.126933000	-0.500264000	3.229692000
1	4.174615000	-2.206822000	4.139795000
1	5.883790000	1.149632000	2.073066000
1	5.797934000	-0.326241000	4.065609000
6	2.711208000	-2.896119000	-0.861962000
6	4.058193000	-3.097396000	-1.191749000
6	1.813109000	-3.954971000	-1.002974000
6	4.492242000	-4.329636000	-1.665092000
1	4.775237000	-2.289548000	-1.067714000
6	2.249230000	-5.191940000	-1.475169000
1	0.769839000	-3.813333000	-0.742569000
6	3.585945000	-5.379970000	-1.808803000
1	5.538782000	-4.473283000	-1.916741000
1	1.539253000	-6.007232000	-1.578819000
1	3.925906000	-6.343612000	-2.176994000
7	0.748349000	2.981746000	-0.298408000
16	1.787970000	3.816526000	-1.244186000
8	2.217518000	2.992132000	-2.459288000
6	0.616727000	5.074060000	-1.963766000
6	1.433699000	5.889800000	-2.967764000
1	1.832605000	5.244372000	-3.756005000
1	0.803607000	6.659832000	-3.430687000
1	2.277701000	6.393911000	-2.480578000
6	-0.529504000	4.358789000	-2.667678000
1	-1.134806000	3.795203000	-1.951166000
1	-1.177594000	5.083285000	-3.177609000
1	-0.129923000	3.666284000	-3.416552000
6	0.120723000	5.956449000	-0.822760000
1	0.956586000	6.436061000	-0.297844000
1	-0.529163000	6.750202000	-1.213298000
1	-0.443817000	5.366844000	-0.095625000
6	1.345497000	2.479933000	0.935910000

6	2.065679000	3.531808000	1.803306000
1	1.376018000	4.344041000	2.061921000
1	2.438137000	3.080052000	2.730848000
1	2.916771000	3.964723000	1.269207000
6	0.257573000	1.851197000	1.793925000
6	0.529558000	0.708466000	2.554486000
6	-0.980824000	2.485703000	1.965821000
6	-0.397704000	0.229565000	3.488315000
1	1.505382000	0.237666000	2.479206000
6	-1.889701000	2.023376000	2.907877000
1	-1.199332000	3.362791000	1.364284000
6	-1.600502000	0.893325000	3.677090000
1	-0.159610000	-0.655466000	4.072181000
1	-2.838236000	2.534965000	3.042482000
1	-2.318950000	0.533998000	4.407196000

TS7R-8R

Coordinates (Angstroms)			
	X	Y	Z
44	0.190240000	-0.926605000	0.114240000
1	0.378528000	-1.985225000	-1.021111000
15	-2.097837000	-1.364779000	-0.200104000
15	2.420278000	-0.328591000	-0.336870000
6	-2.546656000	-0.221957000	-1.573479000
6	2.174144000	1.135372000	-1.421010000
1	-3.342059000	-0.634504000	-2.201626000
1	-2.902717000	0.726960000	-1.165145000
6	-1.286498000	0.063013000	-2.380664000
1	3.056502000	1.398650000	-2.012842000
6	0.984959000	0.788152000	-2.310603000
1	1.915352000	1.980718000	-0.772774000
1	-1.522618000	0.864816000	-3.092168000
7	-0.196816000	0.496129000	-1.491330000
1	-0.981498000	-0.832536000	-2.942655000
1	1.239166000	-0.079519000	-2.940668000
1	0.774890000	1.623052000	-2.992173000
6	0.525680000	-2.246537000	1.395277000
8	0.737532000	-3.107820000	2.145277000
1	-0.576855000	1.653910000	-0.990988000
1	-2.112357000	1.380446000	0.824889000
6	-3.305022000	-1.074642000	1.148180000
6	-3.116047000	-1.767697000	2.350714000
6	-4.369945000	-0.175976000	1.044692000
6	-3.972467000	-1.563130000	3.426602000

1	-2.288816000	-2.467013000	2.447385000
6	-5.224017000	0.032933000	2.126074000
1	-4.542564000	0.371755000	0.123745000
6	-5.025860000	-0.656464000	3.317879000
1	-3.812144000	-2.104206000	4.354438000
1	-6.041852000	0.741446000	2.033653000
1	-5.689533000	-0.488564000	4.160904000
6	-2.593943000	-3.031314000	-0.787969000
6	-3.936091000	-3.285805000	-1.098877000
6	-1.658269000	-4.056621000	-0.932088000
6	-4.329381000	-4.537716000	-1.556228000
1	-4.680700000	-2.502986000	-0.975564000
6	-2.053222000	-5.313352000	-1.388395000
1	-0.617464000	-3.871854000	-0.688508000
6	-3.386078000	-5.554450000	-1.703257000
1	-5.372773000	-4.722215000	-1.794422000
1	-1.314408000	-6.102256000	-1.495404000
1	-3.693844000	-6.533268000	-2.059743000
6	3.662474000	0.123156000	0.922453000
6	4.414128000	1.298130000	0.865789000
6	3.885415000	-0.781714000	1.964632000
6	5.371763000	1.565684000	1.842476000
1	4.250739000	2.018303000	0.069185000
6	4.849196000	-0.520881000	2.931564000
1	3.295786000	-1.692458000	2.025776000
6	5.591315000	0.657594000	2.874600000
1	5.945695000	2.486685000	1.795325000
1	5.014086000	-1.233558000	3.734231000
1	6.339697000	0.866701000	3.633393000
6	3.397415000	-1.504358000	-1.357417000
6	4.543091000	-1.065671000	-2.032033000
6	3.050280000	-2.855273000	-1.423736000
6	5.308478000	-1.952880000	-2.779646000
1	4.851287000	-0.025646000	-1.963941000
6	3.822660000	-3.747564000	-2.164991000
1	2.173088000	-3.210527000	-0.892530000
6	4.947058000	-3.297517000	-2.849215000
1	6.191121000	-1.596745000	-3.302694000
1	3.541609000	-4.795815000	-2.207933000
1	5.545711000	-3.991625000	-3.431823000
6	1.877698000	2.400245000	2.732922000
6	1.792650000	1.287326000	3.571963000
6	0.688910000	0.450595000	3.487366000
6	-0.344629000	0.741195000	2.590213000

6	-0.272860000	1.860539000	1.754676000
6	0.865764000	2.672847000	1.823028000
1	2.745581000	3.050728000	2.787484000
1	2.593600000	1.071732000	4.271803000
1	0.614657000	-0.426775000	4.123755000
1	-1.243478000	0.130186000	2.588235000
1	0.931174000	3.533670000	1.165456000
6	-1.473564000	2.272632000	0.915438000
6	-2.284567000	3.297726000	1.722419000
1	-2.489135000	2.895547000	2.720746000
1	-1.726194000	4.234601000	1.833371000
1	-3.242454000	3.522945000	1.245980000
7	-1.003815000	2.724908000	-0.400367000
16	-2.081461000	3.642874000	-1.267716000
6	-0.943208000	4.944103000	-1.960834000
6	0.188069000	4.289601000	-2.740355000
1	0.784566000	5.052139000	-3.256887000
1	0.850600000	3.730985000	-2.072588000
1	-0.220145000	3.605789000	-3.492200000
6	-0.422378000	5.776242000	-0.792948000
1	0.182570000	5.166536000	-0.116494000
1	0.202430000	6.595866000	-1.169183000
1	-1.243293000	6.219841000	-0.216397000
6	-1.814411000	5.795614000	-2.887479000
1	-1.219526000	6.613537000	-3.311876000
1	-2.213634000	5.193150000	-3.708476000
1	-2.659557000	6.240753000	-2.348007000
8	-2.570084000	2.884909000	-2.489770000

TS7S-8S

Coordinates (Angstroms)

	X	Y	Z
44	0.607123000	0.778261000	0.104835000
1	1.185509000	1.785278000	-0.941500000
15	2.498922000	-0.528607000	-0.398246000
15	-1.387314000	1.994480000	-0.187948000
6	-2.156728000	1.180790000	-1.651974000
1	-2.721039000	1.898697000	-2.255060000
6	-1.038487000	0.532166000	-2.462393000
1	-2.855942000	0.404621000	-1.324863000
7	-0.196300000	-0.309661000	-1.598703000
1	-0.422812000	1.304014000	-2.947583000
1	-1.488142000	-0.077659000	-3.259956000
6	1.329353000	1.819560000	1.479939000

8	1.801358000	2.515393000	2.280365000
1	-0.937840000	-1.223691000	-1.117872000
1	-2.450390000	-0.659930000	0.680288000
6	3.508884000	-1.455687000	0.808868000
6	4.000884000	-0.768516000	1.922433000
6	3.832533000	-2.803656000	0.640313000
6	4.808105000	-1.417438000	2.850290000
1	3.743289000	0.276769000	2.071709000
6	4.632404000	-3.456282000	1.575647000
1	3.454330000	-3.358073000	-0.213389000
6	5.121193000	-2.764917000	2.680647000
1	5.185088000	-0.874073000	3.711645000
1	4.872228000	-4.506773000	1.438875000
1	5.745766000	-3.274656000	3.408439000
6	3.815099000	0.302196000	-1.376875000
6	4.691487000	-0.441692000	-2.175551000
6	4.000433000	1.683106000	-1.276895000
6	5.714054000	0.186252000	-2.878310000
1	4.587290000	-1.520852000	-2.247004000
6	5.032467000	2.311400000	-1.970501000
1	3.335217000	2.269765000	-0.651524000
6	5.885878000	1.565510000	-2.777467000
1	6.380677000	-0.403008000	-3.501147000
1	5.166205000	3.385308000	-1.879262000
1	6.687428000	2.055372000	-3.322681000
6	-2.660858000	2.049436000	1.128903000
6	-3.894778000	1.398260000	1.043866000
6	-2.330818000	2.733450000	2.306727000
6	-4.777626000	1.426590000	2.122736000
1	-4.175899000	0.842516000	0.154531000
6	-3.215649000	2.764589000	3.378023000
1	-1.372358000	3.240713000	2.388855000
6	-4.442208000	2.107315000	3.288184000
1	-5.729531000	0.910074000	2.044950000
1	-2.946588000	3.297808000	4.285047000
1	-5.132760000	2.124556000	4.126269000
6	-1.261931000	3.768048000	-0.640202000
6	-0.031613000	4.425458000	-0.669707000
6	-2.425811000	4.485284000	-0.947843000
6	0.038064000	5.776365000	-1.007583000
1	0.874530000	3.880664000	-0.426673000
6	-2.355727000	5.830565000	-1.288341000
1	-3.393857000	3.991692000	-0.909621000
6	-1.121222000	6.478844000	-1.318440000

1	1.001529000	6.277251000	-1.024750000
1	-3.264976000	6.375589000	-1.524441000
1	-1.066262000	7.531771000	-1.579506000
6	0.420472000	-0.764875000	3.436971000
6	1.233439000	-1.888847000	3.466328000
6	1.023959000	-2.915659000	2.542624000
6	0.004346000	-2.818109000	1.606203000
6	-0.848278000	-1.705281000	1.588515000
6	-0.621281000	-0.675431000	2.506780000
1	0.577100000	0.044048000	4.145023000
1	2.035378000	-1.967356000	4.193582000
1	1.668120000	-3.789881000	2.554060000
1	-0.1644482000	-3.613227000	0.885527000
1	-1.301788000	0.171252000	2.539524000
6	-2.094669000	-1.698606000	0.717973000
6	-3.1964440000	-2.485717000	1.432562000
1	-2.920861000	-3.540235000	1.545547000
1	-3.355290000	-2.067307000	2.433481000
1	-4.130584000	-2.405915000	0.872900000
7	-1.737196000	-2.145746000	-0.628620000
16	-2.890369000	-2.373982000	-1.782896000
6	-3.395984000	-4.204192000	-1.758018000
6	-4.620478000	-4.470940000	-0.891147000
1	-5.088263000	-5.417125000	-1.191676000
1	-4.368935000	-4.550689000	0.168577000
1	-5.355131000	-3.668144000	-1.013106000
6	-2.191443000	-5.038091000	-1.338574000
1	-1.948594000	-4.879547000	-0.284066000
1	-2.408203000	-6.103729000	-1.488514000
1	-1.300122000	-4.788790000	-1.926991000
6	-3.744934000	-4.464541000	-3.229825000
1	-4.022743000	-5.516277000	-3.370155000
1	-4.592551000	-3.847106000	-3.549709000
1	-2.897715000	-4.248033000	-3.890779000
8	-4.172214000	-1.603287000	-1.492265000
6	1.771587000	-1.774238000	-1.540071000
1	2.514692000	-2.310233000	-2.138076000
1	1.227780000	-2.499303000	-0.923982000
6	0.784866000	-1.022402000	-2.424467000
1	0.267054000	-1.736800000	-3.082931000
1	1.328886000	-0.316602000	-3.071182000

8R

Coordinates (Angstroms)

	X	Y	Z
44	-0.432794000	0.914612000	0.085297000
1	-0.821090000	2.086435000	-0.871249000
15	1.747854000	1.726426000	-0.174915000
15	-2.525864000	-0.028098000	-0.400808000
6	2.385626000	0.749572000	-1.595395000
6	-2.045320000	-1.357035000	-1.578327000
1	3.106366000	1.312457000	-2.196459000
1	2.891489000	-0.143582000	-1.221191000
6	1.190493000	0.298514000	-2.428734000
1	-2.880070000	-1.715592000	-2.189492000
6	-0.930639000	-0.754354000	-2.428642000
1	-1.648407000	-2.190631000	-0.986107000
1	1.558677000	-0.449348000	-3.150314000
7	0.152965000	-0.277614000	-1.578641000
1	0.804773000	1.150015000	-3.020737000
1	-1.356270000	0.056745000	-3.051904000
1	-0.566612000	-1.514825000	-3.137379000
6	-0.942435000	1.962399000	1.554202000
8	-1.277928000	2.662168000	2.422015000
1	1.100528000	-1.957055000	-0.878482000
1	2.252373000	-0.991094000	0.889543000
6	2.981899000	1.541535000	1.170721000
6	2.646483000	2.045095000	2.433670000
6	4.217361000	0.909843000	1.000209000
6	3.526589000	1.919145000	3.502949000
1	1.685898000	2.532305000	2.582292000
6	5.095237000	0.777165000	2.074652000
1	4.503460000	0.504400000	0.034320000
6	4.752452000	1.279621000	3.326165000
1	3.252018000	2.314981000	4.476325000
1	6.048760000	0.277974000	1.929240000
1	5.438353000	1.174433000	4.161642000
6	1.979871000	3.488768000	-0.633013000
6	3.233459000	3.942056000	-1.062262000
6	0.928153000	4.400398000	-0.528451000
6	3.425282000	5.277148000	-1.396674000
1	4.068720000	3.248768000	-1.125540000
6	1.122071000	5.741106000	-0.856884000
1	-0.044413000	4.058046000	-0.189402000
6	2.367323000	6.179936000	-1.294992000
1	4.401049000	5.615728000	-1.732811000
1	0.296758000	6.441938000	-0.770673000
1	2.517431000	7.224404000	-1.552590000

6	-3.632725000	-0.788099000	0.839276000
6	-4.164400000	-2.071006000	0.692129000
6	-3.987403000	-0.027202000	1.957590000
6	-5.040064000	-2.583869000	1.647030000
1	-3.894608000	-2.681810000	-0.164698000
6	-4.870018000	-0.534232000	2.904712000
1	-3.565168000	0.964968000	2.091205000
6	-5.396810000	-1.815794000	2.751994000
1	-5.447451000	-3.583383000	1.523638000
1	-5.140450000	0.068013000	3.767234000
1	-6.084422000	-2.213655000	3.492795000
6	-3.726364000	0.990755000	-1.352714000
6	-4.839860000	0.384072000	-1.947757000
6	-3.564200000	2.371538000	-1.475726000
6	-5.756206000	1.138941000	-2.670243000
1	-5.000383000	-0.685430000	-1.836663000
6	-4.485081000	3.130391000	-2.196163000
1	-2.712292000	2.853517000	-1.007292000
6	-5.577534000	2.515840000	-2.798901000
1	-6.612635000	0.654766000	-3.130480000
1	-4.342964000	4.203253000	-2.287562000
1	-6.291918000	3.106794000	-3.364842000
6	-1.449684000	-3.043897000	2.506838000
6	-1.654511000	-2.026764000	3.436989000
6	-0.734951000	-0.987896000	3.532718000
6	0.393790000	-0.976229000	2.713938000
6	0.613230000	-2.000497000	1.788320000
6	-0.327418000	-3.028605000	1.685007000
1	-2.174512000	-3.847891000	2.418551000
1	-2.539429000	-2.035614000	4.065417000
1	-0.893678000	-0.180703000	4.241942000
1	1.124911000	-0.176712000	2.808366000
1	-0.167334000	-3.819577000	0.959322000
6	1.914738000	-2.028072000	1.002994000
6	2.983754000	-2.766826000	1.812027000
1	3.039235000	-2.325747000	2.811896000
1	2.733642000	-3.829028000	1.913966000
1	3.975237000	-2.682472000	1.357527000
7	1.668754000	-2.626618000	-0.318303000
16	2.996243000	-3.214157000	-1.172669000
6	2.097525000	-4.446371000	-2.233534000
6	0.949981000	-3.774649000	-2.976811000
1	0.532471000	-4.467391000	-3.717248000
1	0.146146000	-3.488457000	-2.292202000

1	1.303720000	-2.883826000	-3.506636000
6	1.609746000	-5.568367000	-1.320113000
1	0.881467000	-5.200984000	-0.592045000
1	1.129570000	-6.347004000	-1.924743000
1	2.439259000	-6.033536000	-0.774325000
6	3.149624000	-4.962132000	-3.218492000
1	2.705642000	-5.737511000	-3.853278000
1	3.515121000	-4.155462000	-3.860215000
1	4.007927000	-5.405673000	-2.699340000
8	3.541664000	-2.172083000	-2.116645000

8S

Coordinates (Angstroms)

	X	Y	Z
44	0.711663000	0.822481000	0.076968000
1	1.344463000	1.839191000	-0.924383000
15	2.513976000	-0.596633000	-0.425281000
15	-1.242016000	2.089474000	-0.159471000
6	-2.094232000	1.278752000	-1.578054000
1	-2.672637000	1.995744000	-2.168908000
6	-1.022781000	0.576609000	-2.409287000
1	-2.791252000	0.534648000	-1.182983000
7	-0.162706000	-0.231014000	-1.550795000
1	-0.444417000	1.329258000	-2.976811000
1	-1.526798000	-0.057579000	-3.157341000
6	1.463877000	1.780250000	1.502543000
8	1.954777000	2.426551000	2.336663000
1	-1.285540000	-1.615195000	-0.832306000
1	-2.630985000	-0.718995000	0.863714000
6	3.472937000	-1.546899000	0.808421000
6	4.029030000	-0.855765000	1.889705000
6	3.687417000	-2.922303000	0.697464000
6	4.790329000	-1.527118000	2.840256000
1	3.858263000	0.212189000	1.995802000
6	4.440887000	-3.597047000	1.655677000
1	3.259389000	-3.480014000	-0.130099000
6	4.994097000	-2.901557000	2.727019000
1	5.218046000	-0.979444000	3.674829000
1	4.596695000	-4.667932000	1.561563000
1	5.582857000	-3.428418000	3.472355000
6	3.868125000	0.110589000	-1.447749000
6	4.700912000	-0.717660000	-2.209528000
6	4.120774000	1.484192000	-1.424537000
6	5.746182000	-0.179880000	-2.952210000

1	4.543879000	-1.792952000	-2.219148000
6	5.174193000	2.022636000	-2.160272000
1	3.489393000	2.133657000	-0.826210000
6	5.983492000	1.193425000	-2.930402000
1	6.379367000	-0.833046000	-3.545590000
1	5.358571000	3.092627000	-2.131447000
1	6.801428000	1.613589000	-3.508557000
6	-2.447339000	2.154387000	1.220747000
6	-3.733044000	1.609927000	1.160615000
6	-2.005969000	2.723197000	2.423328000
6	-4.555605000	1.623251000	2.287102000
1	-4.106108000	1.149145000	0.251204000
6	-2.830828000	2.743594000	3.541774000
1	-1.004483000	3.142006000	2.488103000
6	-4.107621000	2.186294000	3.477057000
1	-5.546570000	1.183330000	2.227556000
1	-2.472706000	3.185198000	4.467031000
1	-4.748814000	2.190336000	4.353689000
6	-1.113916000	3.859202000	-0.623518000
6	0.124027000	4.500076000	-0.684434000
6	-2.275270000	4.588631000	-0.909420000
6	0.202886000	5.847620000	-1.033635000
1	1.027618000	3.943169000	-0.457941000
6	-2.196152000	5.930525000	-1.261546000
1	-3.247847000	4.106508000	-0.845334000
6	-0.954308000	6.562278000	-1.324716000
1	1.171798000	6.336326000	-1.077131000
1	-3.103374000	6.485505000	-1.482010000
1	-0.891715000	7.612234000	-1.596061000
6	0.465244000	-0.937871000	3.344417000
6	1.197297000	-2.118749000	3.356550000
6	0.815012000	-3.174465000	2.528824000
6	-0.293067000	-3.049367000	1.699340000
6	-1.048536000	-1.871389000	1.694940000
6	-0.657529000	-0.817770000	2.522620000
1	0.761460000	-0.102145000	3.971729000
1	2.074588000	-2.215027000	3.988348000
1	1.390597000	-4.095425000	2.528165000
1	-0.589477000	-3.869029000	1.050744000
1	-1.246731000	0.095037000	2.544190000
6	-2.333022000	-1.774825000	0.891449000
6	-3.445544000	-2.530793000	1.616209000
1	-3.189290000	-3.584913000	1.759898000
1	-3.581428000	-2.080431000	2.605921000

1	-4.386079000	-2.449898000	1.069242000
7	-2.039439000	-2.245233000	-0.480502000
16	-3.249561000	-2.094776000	-1.683307000
6	-3.623327000	-3.874884000	-2.065679000
6	-4.092126000	-4.658035000	-0.848945000
1	-4.382230000	-5.669838000	-1.158349000
1	-3.295599000	-4.748841000	-0.106178000
1	-4.962478000	-4.185470000	-0.383929000
6	-2.334888000	-4.459689000	-2.644464000
1	-1.530447000	-4.450384000	-1.902472000
1	-2.511572000	-5.498092000	-2.948465000
1	-1.999002000	-3.905220000	-3.529073000
6	-4.724911000	-3.809569000	-3.127210000
1	-4.957136000	-4.822469000	-3.475598000
1	-5.638491000	-3.367060000	-2.718830000
1	-4.415606000	-3.219837000	-3.998833000
8	-4.500675000	-1.480105000	-1.106418000
6	1.687997000	-1.832002000	-1.509828000
1	2.380918000	-2.428316000	-2.111630000
1	1.124623000	-2.504914000	-0.851938000
6	0.717210000	-1.040676000	-2.381165000
1	0.128023000	-1.748293000	-2.991467000
1	1.297966000	-0.426444000	-3.097117000

A5R

Coordinates (Angstroms)			
	X	Y	Z
1	-0.123546000	0.279940000	-0.899808000
1	0.782337000	-1.956498000	-0.175317000
6	3.511910000	1.659479000	0.184267000
6	4.550542000	0.963454000	-0.430964000
6	4.369966000	-0.369934000	-0.786533000
6	3.155824000	-1.002371000	-0.530633000
6	2.112135000	-0.314135000	0.088620000
6	2.301885000	1.024454000	0.444033000
1	3.645334000	2.701270000	0.461639000
1	5.495309000	1.459556000	-0.633061000
1	5.173024000	-0.918560000	-1.270262000
1	3.016487000	-2.042514000	-0.815572000
1	1.491678000	1.568855000	0.921550000
6	0.807797000	-1.021849000	0.403183000
6	0.712526000	-1.360904000	1.891424000
1	1.554941000	-1.994342000	2.186005000
1	0.737163000	-0.444645000	2.490599000

1	-0.213112000	-1.899107000	2.119061000
7	-0.309491000	-0.133330000	0.014880000
16	-1.840040000	-0.882046000	-0.026522000
6	-2.857258000	0.677049000	-0.026546000
6	-2.454446000	1.569709000	-1.197292000
1	-3.193370000	2.370051000	-1.317644000
1	-1.481102000	2.044110000	-1.034349000
1	-2.424839000	0.996296000	-2.130263000
6	-2.659619000	1.363026000	1.322779000
1	-1.621487000	1.675445000	1.464167000
1	-3.299284000	2.251865000	1.374497000
1	-2.937702000	0.703835000	2.153517000
6	-4.300285000	0.193983000	-0.194064000
1	-4.978469000	1.054266000	-0.167565000
1	-4.434288000	-0.321656000	-1.149262000
1	-4.594749000	-0.489094000	0.611509000
8	-2.061639000	-1.535599000	-1.359862000

A5S

Coordinates (Angstroms)

	X	Y	Z
1	-0.176332000	0.373148000	-1.305650000
1	-0.678746000	-1.833283000	-0.192894000
6	-4.442967000	-0.582502000	-0.508007000
6	-4.696561000	0.762250000	-0.255213000
6	-3.656438000	1.595335000	0.152423000
6	-2.372215000	1.084247000	0.308105000
6	-2.108131000	-0.265069000	0.053620000
6	-3.154857000	-1.090943000	-0.357083000
1	-5.246993000	-1.238641000	-0.828957000
1	-5.699187000	1.161825000	-0.376744000
1	-3.846897000	2.646204000	0.350904000
1	-1.561005000	1.734742000	0.624459000
1	-2.960320000	-2.141264000	-0.560489000
6	-0.714709000	-0.831928000	0.256327000
6	-0.397098000	-0.980080000	1.742494000
1	-0.424358000	-0.009073000	2.247463000
1	-1.144497000	-1.629840000	2.210229000
1	0.586257000	-1.434724000	1.877725000
7	0.239833000	0.075512000	-0.425375000
16	1.784301000	-0.589425000	-0.867614000
6	2.900452000	0.604080000	0.015859000
6	2.660921000	0.576914000	1.517837000
1	3.395251000	1.221952000	2.014658000

1	1.661935000	0.945383000	1.765342000
1	2.776856000	-0.436022000	1.914929000
6	2.628123000	1.983485000	-0.581207000
1	1.610900000	2.318805000	-0.357109000
1	3.329406000	2.708972000	-0.153171000
1	2.768495000	1.991265000	-1.669128000
6	4.315078000	0.125027000	-0.322851000
1	5.046869000	0.813971000	0.113649000
1	4.500618000	-0.874592000	0.081633000
1	4.488039000	0.098157000	-1.405419000
8	1.947058000	-1.924958000	-0.203226000

1K

Coordinates (Angstroms)

	X	Y	Z
7	-0.443505000	1.212321000	0.396482000
1	-0.275772000	0.945344000	1.372389000
16	0.314548000	0.190519000	-0.607115000
6	2.044820000	0.023661000	0.085374000
6	1.978514000	-0.545484000	1.498885000
1	2.988925000	-0.775162000	1.857873000
1	1.539415000	0.166378000	2.207949000
1	1.390084000	-1.468925000	1.511897000
6	2.783994000	-0.939991000	-0.843588000
1	2.798356000	-0.566479000	-1.874719000
1	3.824196000	-1.056775000	-0.515277000
1	2.306031000	-1.923859000	-0.843254000
6	2.686328000	1.408570000	0.064663000
1	3.712050000	1.350096000	0.449672000
1	2.733042000	1.813075000	-0.953469000
1	2.121212000	2.114115000	0.681036000
8	-0.226107000	-1.254148000	-0.477600000
1	-2.053283000	1.625074000	0.011080000
8	-3.045918000	1.576173000	-0.175163000
1	-3.206402000	2.211999000	-0.880590000
19	-2.662727000	-0.959272000	0.226525000

2K

Coordinates (Angstroms)

	X	Y	Z
6	-0.850375000	0.412460000	0.875268000
8	-0.786622000	1.734517000	0.635956000
6	-0.740002000	0.095875000	2.378367000

1	-1.617154000	0.518614000	2.876389000
1	-0.703922000	-0.978886000	2.588137000
1	0.147678000	0.573551000	2.806747000
6	-2.159079000	-0.220770000	0.338565000
6	-3.216213000	0.615309000	-0.015535000
6	-2.331793000	-1.602952000	0.224331000
6	-4.416927000	0.088720000	-0.487781000
1	-3.071617000	1.685954000	0.088227000
6	-3.529058000	-2.134048000	-0.245425000
1	-1.514955000	-2.265170000	0.497362000
6	-4.576767000	-1.288711000	-0.607675000
1	-5.229094000	0.756946000	-0.763000000
1	-3.644881000	-3.211071000	-0.334853000
1	-5.509700000	-1.703055000	-0.980025000
7	0.240230000	-0.363155000	0.133380000
1	0.214254000	-0.062352000	-0.843902000
16	1.801017000	-0.337955000	0.726133000
6	2.526052000	-1.640266000	-0.390348000
6	2.358950000	-1.236451000	-1.853033000
1	2.972469000	-1.890261000	-2.483570000
1	1.322778000	-1.334346000	-2.192429000
1	2.691415000	-0.205209000	-2.012102000
6	4.009488000	-1.693880000	-0.014930000
1	4.149159000	-1.926425000	1.047477000
1	4.504109000	-2.479417000	-0.597078000
1	4.505357000	-0.742381000	-0.226758000
6	1.833675000	-2.964470000	-0.076873000
1	2.315678000	-3.768479000	-0.645249000
1	1.910193000	-3.216556000	0.987368000
1	0.775447000	-2.934040000	-0.348640000
8	2.546012000	0.937099000	0.351157000
1	-0.800401000	1.900795000	-0.942066000
8	-0.461034000	2.055746000	-1.887701000
1	-1.236877000	2.026316000	-2.457522000
19	1.236191000	3.094792000	-0.113746000

3K

Coordinates (Angstroms)

	X	Y	Z
6	-2.104773000	-0.238550000	-1.113541000
6	1.866219000	-0.278191000	1.167435000
8	0.716567000	-1.166707000	1.318569000
6	2.220103000	0.247170000	2.569437000
1	2.534088000	-0.569369000	3.231352000

1	3.040786000	0.967414000	2.510584000
1	1.355794000	0.746138000	3.016783000
6	3.049251000	-1.070095000	0.591082000
6	2.962000000	-2.431072000	0.301276000
6	4.243753000	-0.401711000	0.302336000
6	4.039658000	-3.111532000	-0.267211000
1	2.038555000	-2.966283000	0.499142000
6	5.320266000	-1.076557000	-0.261081000
1	4.318256000	0.663505000	0.497950000
6	5.221978000	-2.437701000	-0.550553000
1	3.947401000	-4.170830000	-0.490631000
1	6.238015000	-0.538518000	-0.481210000
1	6.061426000	-2.964015000	-0.995334000
7	1.544529000	0.722000000	0.189170000
1	1.973139000	0.213551000	-1.472200000
16	0.306067000	1.705800000	0.601175000
6	0.801551000	3.259166000	-0.283695000
6	0.925032000	2.998230000	-1.781418000
1	1.132164000	3.943418000	-2.298175000
1	1.734347000	2.300868000	-2.010596000
1	-0.009308000	2.590688000	-2.179904000
6	-0.315937000	4.268050000	-0.006552000
1	-0.436458000	4.453210000	1.067408000
1	-0.078386000	5.223449000	-0.488741000
1	-1.270603000	3.909380000	-0.402637000
6	2.123995000	3.727667000	0.318336000
1	2.407705000	4.689856000	-0.124393000
1	2.046492000	3.868652000	1.403481000
1	2.919463000	3.004919000	0.118991000
8	-0.975335000	1.280829000	-0.163903000
1	0.891057000	-1.766098000	2.058013000
8	2.048529000	-0.263338000	-2.345577000
1	2.854003000	-0.786313000	-2.246110000
7	-2.514826000	-0.483153000	1.453411000
1	-2.029890000	0.222875000	0.866585000
16	-3.403814000	-1.621417000	0.602895000
6	-4.696366000	-0.481464000	-0.095443000
6	-4.055311000	0.501620000	-1.071312000
1	-4.841848000	1.116944000	-1.523739000
1	-3.337822000	1.171626000	-0.588829000
1	-3.543031000	-0.033243000	-1.877474000
6	-5.670758000	-1.407588000	-0.831050000
1	-6.137206000	-2.128067000	-0.149051000
1	-6.468779000	-0.808375000	-1.283013000

1	-5.166640000	-1.960919000	-1.629349000
6	-5.392357000	0.227507000	1.064737000
1	-6.257070000	0.778192000	0.676421000
1	-5.760296000	-0.485342000	1.812238000
1	-4.724819000	0.933985000	1.563261000
8	-2.642217000	-2.145412000	-0.601877000
1	-1.820327000	-0.952200000	2.029265000
19	-0.331210000	-1.080797000	-1.290998000

TS3K-4K

Coordinates (Angstroms)

	X	Y	Z
6	-1.998957000	-0.053177000	-0.964373000
8	-0.236910000	-1.392273000	-1.461583000
6	-2.117931000	0.314618000	-2.420521000
1	-2.336578000	-0.557521000	-3.037220000
1	-2.954873000	1.017394000	-2.529664000
1	-1.210678000	0.792367000	-2.790864000
6	-2.921161000	-1.119125000	-0.447714000
6	-3.069093000	-2.348361000	-1.099552000
6	-3.658829000	-0.881932000	0.716643000
6	-3.931006000	-3.315176000	-0.595942000
1	-2.466077000	-2.560981000	-1.974221000
6	-4.522722000	-1.850711000	1.221199000
1	-3.561386000	0.073943000	1.220645000
6	-4.660973000	-3.070198000	0.566682000
1	-4.027186000	-4.268274000	-1.107765000
1	-5.089433000	-1.646723000	2.124967000
1	-5.335574000	-3.826754000	0.956736000
7	-1.510747000	0.718705000	-0.026372000
1	-1.196034000	0.422678000	2.016523000
16	-0.401203000	1.923045000	-0.458793000
6	-1.351107000	3.421066000	0.094823000
6	-1.697291000	3.313625000	1.575492000
1	-2.154414000	4.253143000	1.906787000
1	-2.410786000	2.506896000	1.765087000
1	-0.802545000	3.139008000	2.179492000
6	-0.410322000	4.600730000	-0.162989000
1	-0.154018000	4.689825000	-1.224983000
1	-0.902761000	5.530693000	0.142188000
1	0.516364000	4.500663000	0.410173000
6	-2.601399000	3.511372000	-0.777649000
1	-3.128906000	4.445978000	-0.555747000
1	-2.354873000	3.517710000	-1.845979000

1	-3.289190000	2.683716000	-0.578812000
8	0.730342000	1.762537000	0.546227000
1	-0.305763000	-1.714812000	-2.367353000
8	-0.463201000	0.278734000	2.641561000
1	0.208874000	0.842828000	2.213674000
7	2.223339000	-0.215577000	-1.129304000
1	2.001397000	0.510560000	-0.438372000
16	3.210623000	-1.406981000	-0.506610000
6	4.662649000	-0.352070000	-0.016341000
6	4.226770000	0.682341000	1.018849000
1	5.114250000	1.175050000	1.432823000
1	3.588576000	1.461300000	0.589945000
1	3.689140000	0.202476000	1.842915000
6	5.669439000	-1.329272000	0.596665000
1	5.968803000	-2.102495000	-0.120663000
1	6.571151000	-0.783720000	0.896783000
1	5.253653000	-1.819664000	1.481721000
6	5.228103000	0.297034000	-1.277757000
1	6.142124000	0.846518000	-1.022674000
1	5.489808000	-0.452414000	-2.033744000
1	4.515052000	0.996630000	-1.721268000
8	2.665773000	-1.950624000	0.807357000
1	1.305275000	-0.648861000	-1.423333000
19	0.038563000	-1.869350000	0.983937000

4K

Coordinates (Angstroms)

	X	Y	Z
6	-2.169730000	-0.156235000	-1.087770000
8	-1.142851000	-1.107760000	-1.500151000
6	-2.694485000	0.534218000	-2.359511000
1	-3.151513000	-0.188506000	-3.047311000
1	-3.458330000	1.269899000	-2.093601000
1	-1.879097000	1.048159000	-2.878281000
6	-3.325337000	-0.906028000	-0.413278000
6	-3.469381000	-2.288523000	-0.519793000
6	-4.286397000	-0.187158000	0.303432000
6	-4.549558000	-2.940882000	0.074546000
1	-2.728292000	-2.869537000	-1.060039000
6	-5.364588000	-0.833741000	0.895010000
1	-4.169224000	0.886610000	0.410316000
6	-5.501825000	-2.216340000	0.781920000
1	-4.642906000	-4.019523000	-0.018168000
1	-6.097778000	-0.257549000	1.452577000

1	-6.343619000	-2.722454000	1.245650000
7	-1.609141000	0.727781000	-0.103623000
1	-1.600287000	0.136689000	1.601564000
16	-0.318947000	1.578719000	-0.625956000
6	-0.592166000	3.199365000	0.234475000
6	-0.749290000	2.981152000	1.735622000
1	-0.794409000	3.950486000	2.246315000
1	-1.671852000	2.437782000	1.958617000
1	0.106911000	2.425596000	2.133023000
6	0.643137000	4.051237000	-0.062334000
1	0.783425000	4.196509000	-1.140080000
1	0.529033000	5.040204000	0.397205000
1	1.546255000	3.584230000	0.340899000
6	-1.847202000	3.821934000	-0.372399000
1	-2.019643000	4.809924000	0.070802000
1	-1.748262000	3.954142000	-1.456546000
1	-2.724391000	3.198561000	-0.178056000
8	0.957460000	1.038098000	0.071830000
1	-1.411267000	-1.512863000	-2.335431000
8	-1.391334000	-0.319458000	2.464381000
1	-1.025964000	0.383746000	3.013877000
7	2.881999000	-0.201759000	-1.600365000
1	2.200418000	0.305063000	-1.001784000
16	3.673569000	-1.483137000	-0.869386000
6	4.687445000	-0.518980000	0.356579000
6	3.779767000	0.102364000	1.415087000
1	4.401041000	0.638428000	2.142177000
1	3.060759000	0.812371000	0.995141000
1	3.230300000	-0.674266000	1.956946000
6	5.617196000	-1.558778000	0.991398000
1	6.295453000	-2.000053000	0.252009000
1	6.228302000	-1.075120000	1.761425000
1	5.048849000	-2.364844000	1.466090000
6	5.491002000	0.536246000	-0.400956000
1	6.218476000	0.987687000	0.283743000
1	6.047667000	0.097470000	-1.237391000
1	4.846781000	1.324998000	-0.796177000
8	2.730306000	-2.323774000	-0.027776000
1	2.436822000	-0.513506000	-2.458791000
19	0.350642000	-1.500935000	0.754118000

A4 (M06-L)

Coordinates (Angstroms)

X	Y	Z
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6	3.501825000	-1.601368000	-0.531150000
6	4.537908000	-0.923004000	0.111883000
6	4.305902000	0.340796000	0.646609000
6	3.048506000	0.927104000	0.537798000
6	1.996719000	0.252442000	-0.098934000
6	2.245449000	-1.022257000	-0.632260000
1	3.677822000	-2.587009000	-0.958784000
1	5.523211000	-1.378862000	0.192838000
1	5.107717000	0.875981000	1.151934000
1	2.886430000	1.914429000	0.965760000
1	1.433753000	-1.541370000	-1.137174000
6	0.645786000	0.856864000	-0.203555000
6	0.508083000	2.315902000	0.119261000
1	0.626701000	2.471447000	1.200254000
1	1.295755000	2.899046000	-0.371985000
1	-0.469041000	2.706668000	-0.163462000
7	-0.307243000	0.049024000	-0.533968000
16	-1.916455000	0.435451000	-0.886916000
6	-2.630220000	-0.783932000	0.377304000
6	-2.169080000	-0.347421000	1.754360000
1	-2.704063000	-0.914032000	2.527765000
1	-1.095803000	-0.521126000	1.894790000
1	-2.378074000	0.717716000	1.915596000
6	-2.174143000	-2.185599000	0.017897000
1	-1.097024000	-2.311726000	0.165812000
1	-2.693784000	-2.915019000	0.654186000
1	-2.408689000	-2.437486000	-1.024684000
6	-4.135693000	-0.627116000	0.226549000
1	-4.646481000	-1.283742000	0.942088000
1	-4.451317000	0.402714000	0.426083000
1	-4.478108000	-0.903563000	-0.779227000
8	-2.425161000	1.785135000	-0.453491000

5 (M06-L)

Coordinates (Angstroms)

	X	Y	Z
44	0.000000000	0.085271000	0.080757000
1	0.000010000	-1.631946000	0.164944000
15	2.294486000	0.041328000	0.410301000
15	-2.294492000	0.041303000	0.410300000
6	2.441673000	-0.021934000	2.260282000
6	-2.441710000	-0.022027000	2.260277000
1	3.365515000	-0.516972000	2.585799000
1	2.478580000	1.014731000	2.624143000

6	1.228668000	-0.729963000	2.831887000
1	-3.365539000	-0.517108000	2.585765000
6	-1.228690000	-0.730019000	2.831885000
1	-2.478661000	1.014626000	2.624168000
1	1.260680000	-0.736120000	3.933865000
7	-0.000027000	-0.074093000	2.350677000
1	1.187640000	-1.771661000	2.487820000
1	-1.187620000	-1.771712000	2.487805000
1	-1.260707000	-0.736188000	3.933863000
6	-0.000021000	0.163930000	-1.752370000
8	0.000162000	0.204670000	-2.927766000
1	-0.000050000	0.890772000	2.685278000
1	-0.000011000	1.797910000	0.237633000
6	3.361344000	1.461155000	-0.038811000
6	3.048199000	2.197897000	-1.186299000
6	4.473962000	1.836984000	0.724089000
6	3.840054000	3.275622000	-1.571631000
1	2.163438000	1.932049000	-1.764877000
6	5.260361000	2.920961000	0.343864000
1	4.725977000	1.287655000	1.631736000
6	4.946659000	3.639386000	-0.807402000
1	3.583930000	3.841233000	-2.465867000
1	6.118449000	3.206344000	0.950476000
1	5.559904000	4.488819000	-1.103669000
6	3.294340000	-1.395579000	-0.149603000
6	4.605865000	-1.590529000	0.303164000
6	2.747594000	-2.311845000	-1.052715000
6	5.349426000	-2.684322000	-0.124975000
1	5.055912000	-0.878927000	0.996280000
6	3.496758000	-3.402463000	-1.490267000
1	1.722261000	-2.169749000	-1.394240000
6	4.794492000	-3.593221000	-1.024964000
1	6.364921000	-2.826638000	0.241631000
1	3.060349000	-4.108588000	-2.194683000
1	5.376448000	-4.449712000	-1.361636000
6	-3.361363000	1.461137000	-0.038760000
6	-4.473988000	1.836921000	0.724153000
6	-3.048220000	2.197937000	-1.186213000
6	-5.260398000	2.920906000	0.343974000
1	-4.726000000	1.287548000	1.631774000
6	-3.840086000	3.275670000	-1.571498000
1	-2.163453000	1.932126000	-1.764797000
6	-4.946699000	3.639386000	-0.807258000
1	-6.118491000	3.206252000	0.950596000

1	-3.583964000	3.841326000	-2.465706000
1	-5.559952000	4.488827000	-1.103488000
6	-3.294331000	-1.395587000	-0.149675000
6	-4.605853000	-1.590579000	0.303086000
6	-2.747578000	-2.311792000	-1.052844000
6	-5.349401000	-2.684357000	-0.125114000
1	-5.055906000	-0.879022000	0.996245000
6	-3.496731000	-3.402393000	-1.490457000
1	-1.722251000	-2.169659000	-1.394370000
6	-4.794460000	-3.593195000	-1.025159000
1	-6.364894000	-2.826706000	0.241488000
1	-3.060318000	-4.108470000	-2.194919000
1	-5.376407000	-4.449672000	-1.361880000

6R (M06-L)

Coordinates (Angstroms)

	X	Y	Z
44	1.024690000	0.860428000	0.036668000
1	1.974751000	2.133659000	-0.634543000
15	2.805089000	-0.553423000	-0.400522000
15	-0.901337000	2.136421000	-0.186969000
6	2.507528000	-1.081931000	-2.153674000
6	-1.475682000	1.661496000	-1.880010000
1	3.437681000	-1.339958000	-2.675408000
1	1.882769000	-1.986787000	-2.130433000
6	1.760884000	0.019320000	-2.882500000
1	-2.142749000	2.410114000	-2.327024000
6	-0.268948000	1.401524000	-2.757728000
1	-2.039583000	0.723869000	-1.765890000
1	1.494564000	-0.304785000	-3.902516000
7	0.551330000	0.359910000	-2.119517000
1	2.374289000	0.926676000	-2.958932000
1	0.350525000	2.302390000	-2.865232000
1	-0.584798000	1.076027000	-3.763255000
6	1.402672000	1.220918000	1.797475000
8	1.647358000	1.428328000	2.931083000
1	-0.038004000	-0.481070000	-2.085910000
1	0.006220000	-0.436246000	0.457405000
6	2.998420000	-2.139382000	0.497624000
6	2.762212000	-2.150186000	1.878088000
6	3.336922000	-3.340207000	-0.137030000
6	2.860468000	-3.332340000	2.605860000
1	2.476325000	-1.223753000	2.378568000
6	3.425691000	-4.525807000	0.589535000

1	3.522436000	-3.359025000	-1.211160000
6	3.187450000	-4.524603000	1.961366000
1	2.666915000	-3.324265000	3.677720000
1	3.678875000	-5.454022000	0.079094000
1	3.252196000	-5.452276000	2.527502000
6	4.529564000	0.081028000	-0.413429000
6	5.579555000	-0.666327000	-0.963086000
6	4.807357000	1.327792000	0.152775000
6	6.877318000	-0.166631000	-0.964781000
1	5.383974000	-1.651196000	-1.391308000
6	6.109831000	1.822528000	0.162359000
1	3.985566000	1.910944000	0.568835000
6	7.143887000	1.080706000	-0.401239000
1	7.683735000	-0.751817000	-1.404287000
1	6.313826000	2.795294000	0.606997000
1	8.160400000	1.471278000	-0.400797000
6	-2.383257000	1.860072000	0.847544000
6	-3.674293000	1.801509000	0.308821000
6	-2.221920000	1.718636000	2.231040000
6	-4.779709000	1.614708000	1.135398000
1	-3.826040000	1.899671000	-0.766275000
6	-3.327364000	1.547552000	3.057223000
1	-1.218744000	1.732915000	2.658412000
6	-4.608637000	1.494309000	2.511378000
1	-5.776853000	1.563862000	0.699925000
1	-3.185389000	1.437976000	4.131094000
1	-5.472285000	1.347294000	3.158647000
6	-0.826210000	3.973515000	-0.255469000
6	-1.957191000	4.733745000	-0.582951000
6	0.376842000	4.630504000	0.014558000
6	-1.879932000	6.120090000	-0.658164000
1	-2.909775000	4.236570000	-0.774067000
6	0.452062000	6.020451000	-0.053218000
1	1.255852000	4.034381000	0.260365000
6	-0.672717000	6.766227000	-0.393311000
1	-2.764249000	6.699466000	-0.919296000
1	1.395857000	6.521159000	0.158089000
1	-0.612670000	7.852063000	-0.449828000
6	-3.676466000	-1.929704000	3.533881000
6	-2.678975000	-1.653142000	4.468443000
6	-1.344151000	-1.630886000	4.069774000
6	-1.002816000	-1.912689000	2.752012000
6	-1.997527000	-2.201212000	1.805498000
6	-3.339570000	-2.188329000	2.212261000

1	-4.722293000	-1.939824000	3.837038000
1	-2.942976000	-1.445566000	5.504583000
1	-0.560652000	-1.391248000	4.787162000
1	0.040098000	-1.864228000	2.444495000
1	-4.111001000	-2.403469000	1.475581000
6	-1.660046000	-2.531640000	0.404690000
6	-0.336764000	-3.170166000	0.100453000
1	0.321677000	-3.232640000	0.968329000
1	-0.513469000	-4.193798000	-0.262069000
1	0.188987000	-2.630535000	-0.693800000
7	-2.589547000	-2.316565000	-0.478957000
16	-2.224383000	-2.815742000	-2.092937000
6	-3.920771000	-2.440171000	-2.782250000
6	-4.240502000	-0.973377000	-2.573237000
1	-5.222881000	-0.743893000	-3.007025000
1	-4.265782000	-0.723110000	-1.506569000
1	-3.497766000	-0.337805000	-3.071127000
6	-4.899471000	-3.351763000	-2.061814000
1	-4.973287000	-3.099256000	-0.998754000
1	-5.897718000	-3.245165000	-2.506185000
1	-4.614259000	-4.409063000	-2.145924000
6	-3.821499000	-2.782156000	-4.261957000
1	-4.786562000	-2.601064000	-4.751693000
1	-3.067158000	-2.165717000	-4.764247000
1	-3.563438000	-3.837193000	-4.422575000
8	-1.280805000	-1.819085000	-2.741293000

6S (M06-L)

Coordinates (Angstroms)

	X	Y	Z
44	-1.107161000	0.928766000	0.061906000
1	-1.911425000	2.037478000	-0.984859000
15	-2.805245000	-0.603196000	-0.310803000
15	0.849115000	2.158471000	-0.120705000
6	-2.324017000	-1.401656000	-1.921478000
6	1.640796000	1.423162000	-1.628482000
1	-3.201974000	-1.703435000	-2.506124000
1	-1.761458000	-2.317359000	-1.689736000
6	-1.451244000	-0.453255000	-2.719537000
1	2.322896000	2.123405000	-2.128816000
6	0.564178000	0.946871000	-2.582641000
1	2.236269000	0.563032000	-1.284787000
1	-1.057654000	-0.952457000	-3.620690000
7	-0.346596000	0.031502000	-1.873036000

1	-2.018922000	0.430715000	-3.036274000
1	-0.042402000	1.785774000	-2.947702000
1	1.015242000	0.441691000	-3.454455000
6	-1.758520000	1.688418000	1.600984000
8	-2.192671000	2.180918000	2.577094000
1	0.205893000	-0.776221000	-1.575247000
1	-0.216184000	-0.263256000	0.913727000
6	-2.978504000	-2.047933000	0.806616000
6	-2.637658000	-1.887918000	2.155279000
6	-3.378718000	-3.313148000	0.356998000
6	-2.706678000	-2.964931000	3.034950000
1	-2.281135000	-0.916961000	2.500612000
6	-3.436487000	-4.392401000	1.234664000
1	-3.628880000	-3.467663000	-0.693175000
6	-3.102487000	-4.219620000	2.576174000
1	-2.434637000	-2.825175000	4.080636000
1	-3.738778000	-5.372182000	0.868172000
1	-3.143872000	-5.064434000	3.261694000
6	-4.541741000	-0.072238000	-0.578910000
6	-5.517054000	-0.965094000	-1.042093000
6	-4.906164000	1.250774000	-0.311273000
6	-6.825663000	-0.542163000	-1.243531000
1	-5.254358000	-2.003443000	-1.247587000
6	-6.219891000	1.672246000	-0.505760000
1	-4.144562000	1.948975000	0.036060000
6	-7.179525000	0.779559000	-0.974222000
1	-7.571934000	-1.244841000	-1.610845000
1	-6.491345000	2.704944000	-0.293084000
1	-8.205000000	1.110955000	-1.130542000
6	2.177195000	2.055351000	1.132912000
6	3.535150000	2.013740000	0.792612000
6	1.818024000	2.021531000	2.485430000
6	4.511839000	1.950630000	1.783663000
1	3.839476000	2.024448000	-0.254594000
6	2.794585000	1.968432000	3.474722000
1	0.762922000	2.007982000	2.759012000
6	4.143225000	1.936175000	3.126212000
1	5.563767000	1.912433000	1.503897000
1	2.499489000	1.936473000	4.522260000
1	4.906690000	1.883227000	3.901369000
6	0.789063000	3.962432000	-0.468564000
6	1.940674000	4.681298000	-0.815718000
6	-0.428560000	4.640509000	-0.366213000
6	1.871572000	6.046285000	-1.072227000

1	2.903336000	4.171230000	-0.878445000
6	-0.495774000	6.009863000	-0.614574000
1	-1.323584000	4.077021000	-0.101922000
6	0.650914000	6.713105000	-0.971567000
1	2.772239000	6.593715000	-1.346187000
1	-1.450322000	6.526916000	-0.529627000
1	0.597591000	7.782633000	-1.169472000
6	3.853733000	-1.622829000	3.249623000
6	2.924247000	-1.707469000	4.286256000
6	1.604668000	-2.052117000	4.004799000
6	1.218722000	-2.328291000	2.698471000
6	2.145416000	-2.249117000	1.648442000
6	3.467153000	-1.883537000	1.942958000
1	4.885347000	-1.347445000	3.463240000
1	3.228173000	-1.498565000	5.311100000
1	0.868077000	-2.105297000	4.805116000
1	0.180577000	-2.578644000	2.489509000
1	4.186536000	-1.813937000	1.128841000
6	1.734788000	-2.541128000	0.257642000
6	0.427242000	-3.245437000	0.059354000
1	0.303555000	-4.079546000	0.759698000
1	0.305424000	-3.618444000	-0.958491000
1	-0.377101000	-2.528745000	0.288910000
7	2.529177000	-2.119155000	-0.675447000
16	2.211930000	-2.279668000	-2.344157000
6	4.026091000	-2.361215000	-2.834364000
6	4.679763000	-1.049631000	-2.438497000
1	5.722393000	-1.041106000	-2.783454000
1	4.677573000	-0.906466000	-1.352324000
1	4.175086000	-0.190012000	-2.901750000
6	4.647119000	-3.564423000	-2.151001000
1	4.720938000	-3.419577000	-1.067275000
1	5.658338000	-3.736272000	-2.542162000
1	4.053464000	-4.466547000	-2.342135000
6	3.997430000	-2.537441000	-4.345133000
1	5.022986000	-2.603677000	-4.729103000
1	3.510606000	-1.690492000	-4.847540000
1	3.467854000	-3.453386000	-4.629415000
8	1.617854000	-3.596968000	-2.777000000

TS6R-7R (M06-L)

Coordinates (Angstroms)

	X	Y	Z
44	0.763274000	0.752872000	-0.021375000

1	1.506136000	2.116899000	-0.648860000
15	2.798444000	-0.311198000	-0.388564000
15	-1.293365000	1.802172000	-0.357523000
6	2.622862000	-0.927169000	-2.124198000
6	-1.747638000	1.164530000	-2.025834000
1	3.591977000	-1.061344000	-2.621503000
1	2.128545000	-1.909012000	-2.085267000
6	1.737917000	0.035623000	-2.894316000
1	-2.523155000	1.765175000	-2.518850000
6	-0.489691000	1.073535000	-2.867410000
1	-2.141744000	0.148365000	-1.873729000
1	1.559780000	-0.342529000	-3.914097000
7	0.461960000	0.187687000	-2.176864000
1	2.204391000	1.026963000	-2.973718000
1	-0.018012000	2.057766000	-2.996558000
1	-0.722116000	0.670636000	-3.866780000
6	1.057547000	1.279283000	1.719922000
8	1.268876000	1.640986000	2.818939000
1	0.011398000	-0.743412000	-2.175775000
1	-0.134923000	-0.753426000	0.342078000
6	3.336271000	-1.765919000	0.579618000
6	3.333079000	-1.647536000	1.976520000
6	3.710651000	-2.985268000	0.005687000
6	3.687299000	-2.725871000	2.779561000
1	3.038275000	-0.702064000	2.435514000
6	4.057369000	-4.067958000	0.811983000
1	3.723702000	-3.103747000	-1.077532000
6	4.043214000	-3.942101000	2.198095000
1	3.675201000	-2.619926000	3.862987000
1	4.337140000	-5.014484000	0.352003000
1	4.308464000	-4.790923000	2.825755000
6	4.345793000	0.678426000	-0.403795000
6	5.541118000	0.123151000	-0.880314000
6	4.357201000	1.979974000	0.103335000
6	6.717415000	0.864787000	-0.870415000
1	5.553594000	-0.903443000	-1.251044000
6	5.538938000	2.718190000	0.124570000
1	3.427628000	2.412286000	0.471945000
6	6.717423000	2.165392000	-0.367434000
1	7.638692000	0.425834000	-1.250218000
1	5.535188000	3.730703000	0.524926000
1	7.639555000	2.744242000	-0.355717000
6	-2.773592000	1.515190000	0.670351000
6	-3.992723000	1.074291000	0.144226000

6	-2.688775000	1.803970000	2.038697000
6	-5.108194000	0.939326000	0.968496000
1	-4.081387000	0.839424000	-0.915956000
6	-3.805405000	1.679373000	2.856439000
1	-1.738623000	2.130667000	2.463270000
6	-5.018828000	1.248285000	2.322344000
1	-6.050664000	0.592572000	0.546977000
1	-3.724219000	1.907128000	3.918043000
1	-5.892056000	1.145145000	2.964941000
6	-1.356725000	3.628573000	-0.549488000
6	-2.504329000	4.243076000	-1.069011000
6	-0.275328000	4.425473000	-0.165926000
6	-2.557878000	5.623460000	-1.225194000
1	-3.367966000	3.635636000	-1.345193000
6	-0.333874000	5.810369000	-0.311511000
1	0.616918000	3.946969000	0.237898000
6	-1.469829000	6.409735000	-0.847494000
1	-3.451631000	6.088053000	-1.639160000
1	0.515246000	6.421162000	-0.009126000
1	-1.512117000	7.491147000	-0.967617000
6	-3.403294000	-1.657330000	3.493658000
6	-2.531183000	-1.247285000	4.497729000
6	-1.175421000	-1.090006000	4.208270000
6	-0.701546000	-1.355742000	2.931059000
6	-1.568337000	-1.773330000	1.913507000
6	-2.927349000	-1.914055000	2.210533000
1	-4.465638000	-1.773184000	3.706355000
1	-2.905231000	-1.041045000	5.499932000
1	-0.484594000	-0.749161000	4.978429000
1	0.353488000	-1.206309000	2.701216000
1	-3.601627000	-2.234570000	1.418731000
6	-1.054583000	-2.147494000	0.555518000
6	0.166839000	-3.042555000	0.555671000
1	0.864191000	-2.784240000	1.355680000
1	-0.154359000	-4.084131000	0.708247000
1	0.711251000	-2.989804000	-0.393943000
7	-1.985766000	-2.201576000	-0.400326000
16	-1.573432000	-3.113517000	-1.764187000
6	-3.301816000	-3.236770000	-2.467353000
6	-3.862171000	-1.847305000	-2.692473000
1	-4.851002000	-1.913324000	-3.166327000
1	-3.968528000	-1.313834000	-1.740931000
1	-3.208974000	-1.266414000	-3.356342000
6	-4.130890000	-4.036416000	-1.477703000

1	-4.244762000	-3.499581000	-0.529413000
1	-5.132159000	-4.220767000	-1.889733000
1	-3.677936000	-5.014125000	-1.264817000
6	-3.132635000	-3.982127000	-3.783250000
1	-4.107681000	-4.108480000	-4.271330000
1	-2.477634000	-3.431498000	-4.467984000
1	-2.704740000	-4.982270000	-3.633510000
8	-0.802547000	-2.249469000	-2.765290000

TS6S-7S (M06-L)

Coordinates (Angstroms)

	X	Y	Z
44	-0.717405000	0.766480000	-0.018795000
1	-1.425210000	2.138468000	-0.667835000
15	-2.794145000	-0.242518000	-0.331230000
15	1.350635000	1.775336000	-0.411562000
6	-2.643195000	-0.933409000	-2.041647000
6	1.746887000	1.154186000	-2.104681000
1	-3.618636000	-1.076551000	-2.523631000
1	-2.166495000	-1.922336000	-1.964840000
6	-1.764889000	-0.008566000	-2.864910000
1	2.490985000	1.774750000	-2.620522000
6	0.463488000	1.049614000	-2.906142000
1	2.174638000	0.148027000	-1.975385000
1	-1.622531000	-0.411261000	-3.880388000
7	-0.466837000	0.160475000	-2.189000000
1	-2.218934000	0.987338000	-2.956198000
1	-0.023912000	2.028122000	-3.013199000
1	0.665694000	0.657441000	-3.916398000
6	-0.963247000	1.338792000	1.712481000
8	-1.136581000	1.731427000	2.806493000
1	-0.012450000	-0.758501000	-2.151116000
1	0.134756000	-0.778105000	0.384623000
6	-3.391216000	-1.630983000	0.693837000
6	-3.379847000	-1.457496000	2.084647000
6	-3.830812000	-2.849512000	0.166542000
6	-3.792458000	-2.482327000	2.928601000
1	-3.031961000	-0.513179000	2.506857000
6	-4.234131000	-3.879002000	1.014344000
1	-3.849502000	-3.011501000	-0.910823000
6	-4.213698000	-3.699257000	2.394290000
1	-3.774453000	-2.334636000	4.007013000
1	-4.563141000	-4.826821000	0.591822000
1	-4.524019000	-4.507498000	3.054145000

6	-4.297470000	0.810268000	-0.400780000
6	-5.504542000	0.292961000	-0.890129000
6	-4.266981000	2.121312000	0.080408000
6	-6.650182000	1.080727000	-0.919385000
1	-5.551776000	-0.739976000	-1.239026000
6	-5.418442000	2.906164000	0.062509000
1	-3.329173000	2.524153000	0.460760000
6	-6.608143000	2.390368000	-0.442846000
1	-7.580448000	0.670407000	-1.308771000
1	-5.382072000	3.925707000	0.442686000
1	-7.506416000	3.005165000	-0.461089000
6	2.863549000	1.460513000	0.558787000
6	4.055190000	0.995797000	-0.008294000
6	2.834757000	1.764453000	1.926427000
6	5.197787000	0.848372000	0.775722000
1	4.103002000	0.747690000	-1.067970000
6	3.978885000	1.628473000	2.702932000
1	1.907655000	2.113221000	2.383996000
6	5.164385000	1.172116000	2.128511000
1	6.117728000	0.480919000	0.322828000
1	3.940680000	1.866167000	3.764589000
1	6.058765000	1.058695000	2.739414000
6	1.435539000	3.602584000	-0.585596000
6	2.586380000	4.207054000	-1.110217000
6	0.371910000	4.410378000	-0.176102000
6	2.659724000	5.588646000	-1.246027000
1	3.437906000	3.591028000	-1.404627000
6	0.450474000	5.796249000	-0.301919000
1	-0.522027000	3.940639000	0.233437000
6	1.589027000	6.385928000	-0.842724000
1	3.556235000	6.045488000	-1.662430000
1	-0.384611000	6.415512000	0.021564000
1	1.647528000	7.468265000	-0.945500000
6	3.568695000	-1.698090000	3.323430000
6	2.799912000	-1.255528000	4.395764000
6	1.430927000	-1.054529000	4.220881000
6	0.839821000	-1.310752000	2.989374000
6	1.601873000	-1.764482000	1.905824000
6	2.975517000	-1.947504000	2.088868000
1	4.640825000	-1.849624000	3.444952000
1	3.264242000	-1.061555000	5.361993000
1	0.819222000	-0.694889000	5.047441000
1	-0.227534000	-1.134353000	2.854035000
1	3.569087000	-2.299512000	1.247572000

6	0.958086000	-2.120399000	0.591694000
6	-0.267239000	-3.006143000	0.721846000
1	-0.902254000	-2.695957000	1.555895000
1	0.060035000	-4.039746000	0.898630000
1	-0.867667000	-3.012441000	-0.191181000
7	1.830139000	-2.255276000	-0.412701000
16	1.326734000	-2.767831000	-1.923700000
6	3.038581000	-3.287597000	-2.517574000
6	3.966159000	-2.088412000	-2.492536000
1	4.947763000	-2.367887000	-2.900713000
1	4.110423000	-1.718258000	-1.471867000
1	3.581036000	-1.264826000	-3.111692000
6	3.512729000	-4.404930000	-1.608162000
1	3.698056000	-4.038699000	-0.592097000
1	4.444439000	-4.838492000	-1.995783000
1	2.760941000	-5.201542000	-1.555973000
6	2.817114000	-3.791817000	-3.935014000
1	3.763340000	-4.154452000	-4.356767000
1	2.441749000	-2.998741000	-4.596477000
1	2.096883000	-4.617231000	-3.950648000
8	0.513306000	-4.042982000	-1.982682000

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