

Supporting Information

For

Theoretical Study on Asymmetric Ketone Hydrogenation Catalyzed by Mn Complexes: From the Catalytic Mechanism to the Catalyst Design

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1. The inner mechanism of asymmetric hydrogenations of acetophenone and 1,1-dimethyl acetone catalyzed by Mn-LYB complex

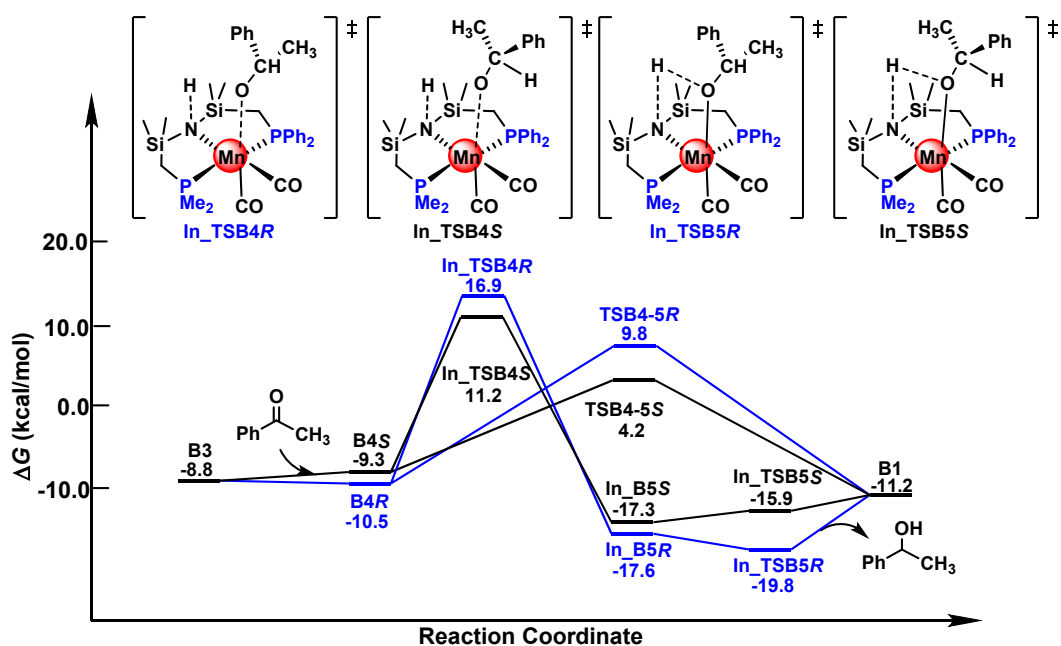


Figure S1. The inner mechanism Gibbs free energy profiles of asymmetric hydrogenations of acetophenone and 1,1-dimethyl acetone catalyzed by Mn(CO)₂-LYB complex (unit: kcal/mol).

2. The dihydrogen activation step of H₂-hydrogenation and inner mechanism of asymmetric hydrogenations of acetophenone and 1,1-dimethyl acetone catalyzed by Mn-LYC complex

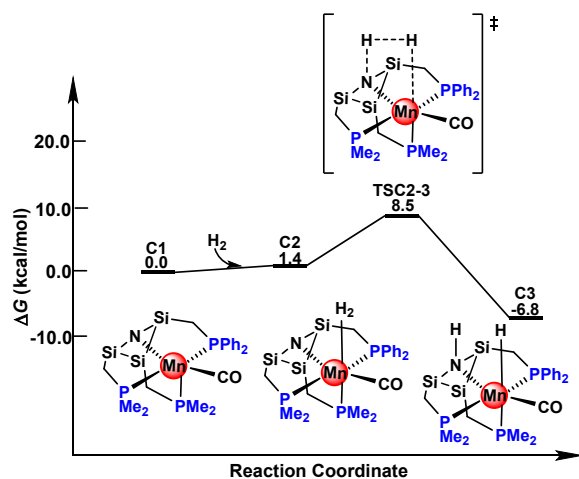


Figure S2. The Gibbs free energy profiles for the dihydrogen activation step of H₂-hydrogenation catalyzed by Mn(CO)-LYC (C) complex (unit: kcal/mol).

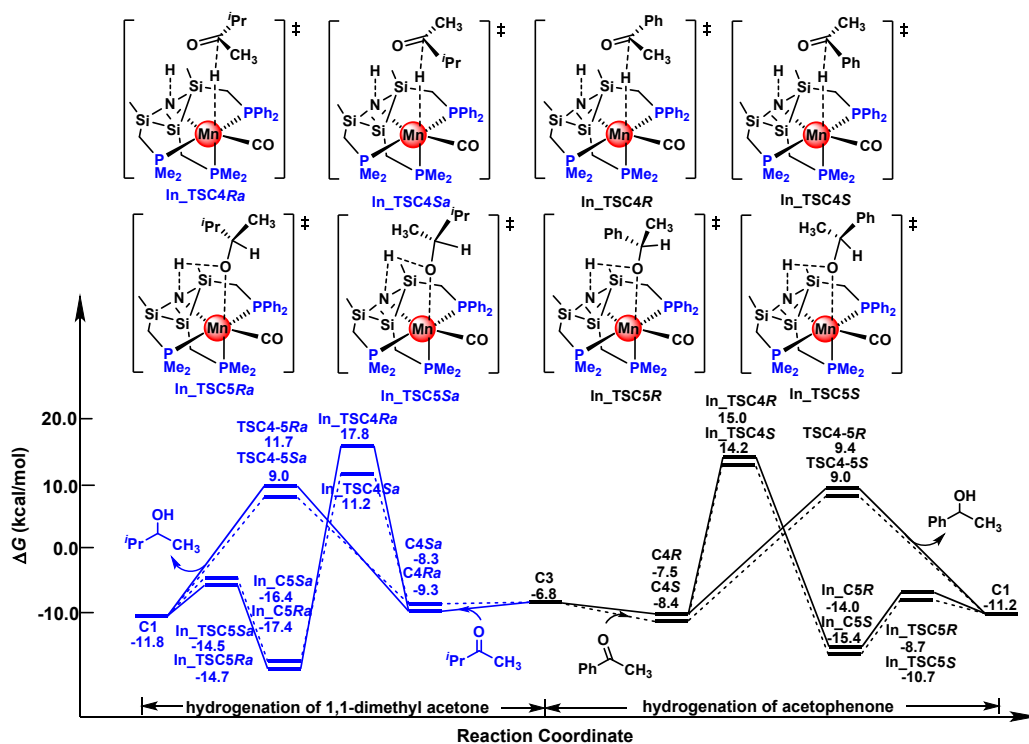


Figure S3. The inner mechanism Gibbs free energy profiles of asymmetric hydrogenations of acetophenone and 1,1-dimethyl acetone catalyzed by Mn(CO)-LYC complex (unit: kcal/mol).

3. The dihydrogen activation step of H₂-hydrogenation and inner mechanism of asymmetric hydrogenations of acetophenone and 1,1-dimethyl acetone catalyzed by Mn-LYD complex

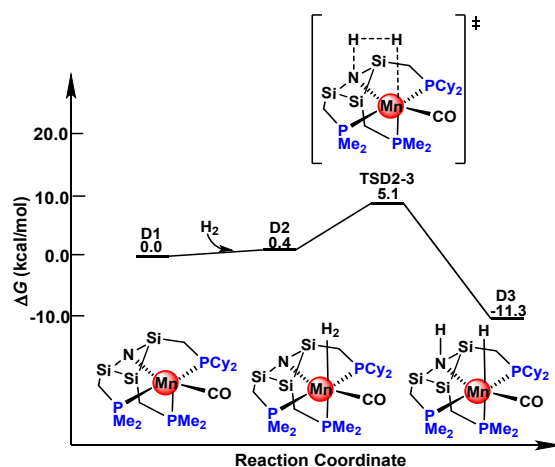


Figure S4. The Gibbs free energy profiles of the dihydrogen activation step of H₂-hydrogenation catalyzed by Mn(CO)-LYD (D) complex (unit: kcal/mol).

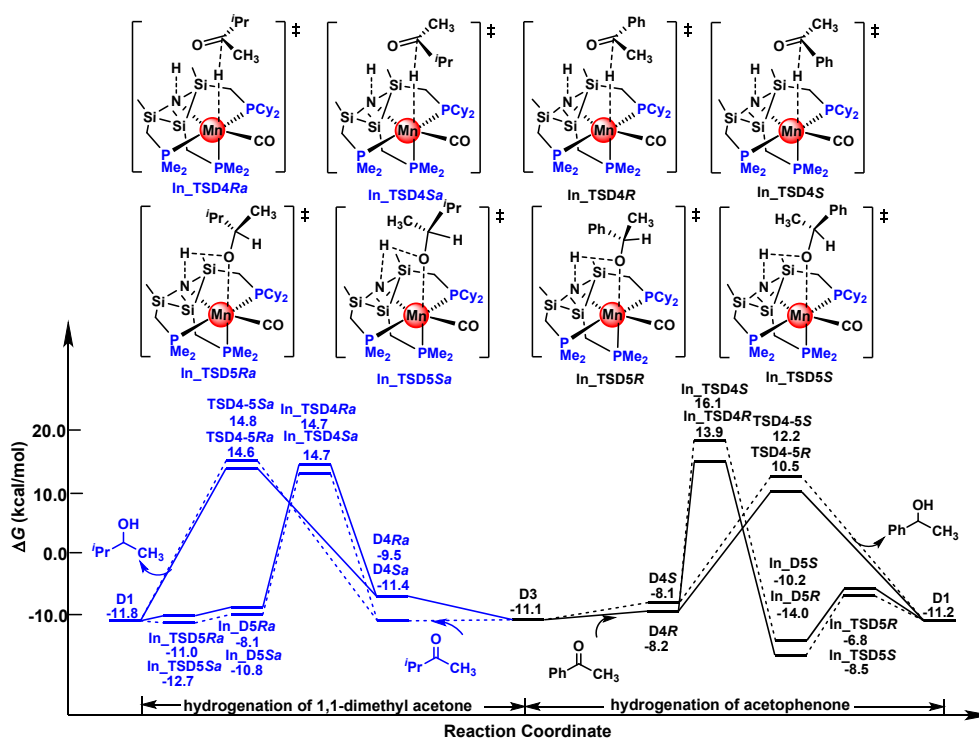


Figure S5. The inner mechanism Gibbs free energy profiles of asymmetric hydrogenations of acetophenone and 1,1-dimethyl acetone catalyzed by Mn(CO)-LYD complex (unit: kcal/mol).

4. The origin of asymmetric hydrogenation catalyzed by Mn-LYC and Mn-LYD complexes

For AKHs catalyzed by Mn-LYC (**C**) and Mn-LYD (**D**), the NCI and EDA analyses were performed to investigate the nature of the diversity of enantioselectivity as shown in Figure S3 below. For AH of acetophenone catalyzed by Mn-LYC, the difference between **TSC4-5R** and **TSC4-5S** is in that there is a π - π stacking interaction in the former and a C-H... π interaction in the latter. In spite of the fact that the interaction (E_{int}) of **TSC4-5S** is higher than that of **TSC4-5R** by 1.5 kcal/mol, the total deformation energy of the **TSC4-5S** is lower than that of **TSC4-5R** (20.7 vs 22.4 kcal/mol). The lower deformation energy and stronger interaction of **TSC4-5S** ($\Delta E_{\text{TS}}=4.9$ kcal/mol) make it more stable than those of **TSC4-5R** ($\Delta E_{\text{TS}}=5.1$ kcal/mol). For AH of 1,1-dimethyl acetone catalyzed by Mn-LYC, the transition state **TSC4-5Sa** owns a stronger interaction (-19.4 vs -16.2 kcal/mol). The total deformation energy of the **TSC4-5Sa** is higher than that of **TSC4-5Ra** (24.6 vs 23.9 kcal/mol), the effect of the interaction energy makes the deformation energy less pronounced, which makes **TSC4-5Sa** be dominant product.

For AH of acetophenone catalyzed by Mn-LYD (**D**) complex, The difference between **TSD4-5R** and **TSD4-5S** is in that **TSD4-5R** owns a lower deformation energy (27.2 vs 28.1 kcal/mol) and a stronger interactions (-16.6 vs -14.6 kcal/mol) between the catalyst and monomer compared to **TSD4-5S**. Meanwhile, there is a C-H... π interactions between the C(sp^3)-H atoms of the Cy group and the phenyl group of acetophenone. These reasons make the *R* conformation more stable (see Figure S6).

However, for AH of 1,1-dimethyl acetone catalyzed by Mn-LYD (**D**) complex, only the vdW interaction exists in **TSD4-5Ra** and **TSD4-5Sa** (see Figure S3). Although the interaction (E_{int}) of **TSD4-5Sa** is higher than that of **TSD4-5Ra** by 2.7 kcal/mol, the total deformation energy of the **TSD4-5Ra** is lower than that of **TSD4-5Sa** (29.0 vs 31.8 kcal/mol). This results **TSD4-5Ra** ($\Delta E_{\text{TS}}=14.1$ kcal/mol) being more likely to occur than **TSD4-5Sa** ($\Delta E_{\text{TS}}=14.3$ kcal/mol).

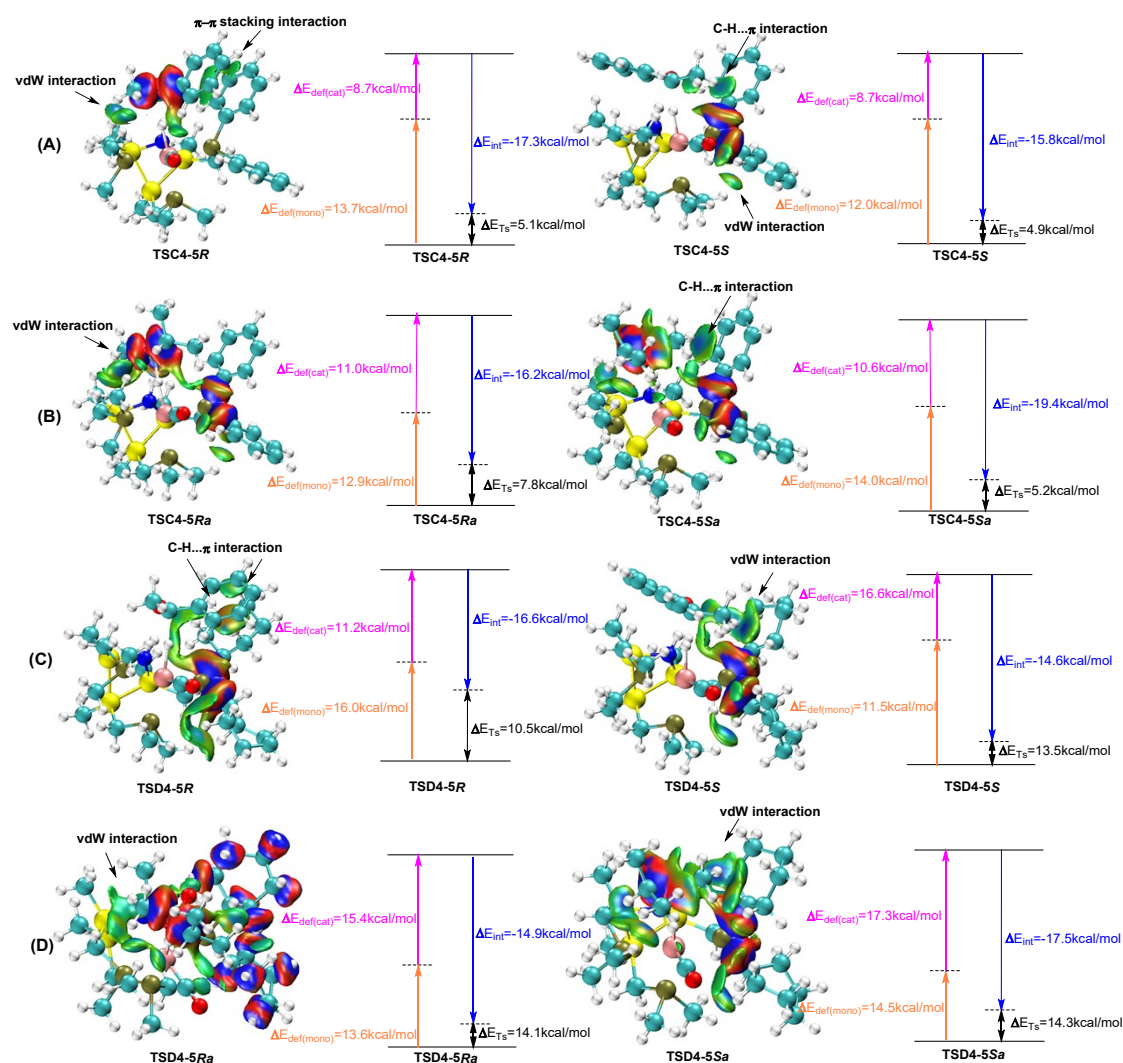


Figure S6. NCI analysis and EDA analysis (unit: kcal/mol) of transition states (A) **TSC4-5R** & **TSC4-5S**, (B) **TSC4-5Ra** & **TSC4-5Sa**, (C) **TSD4-5R** & **TSD4-5S**, and (D) **TSD4-5Ra** & **TSD4-5Sa** in AKHs catalyzed by Mn-LYC and Mn-LYD.

5. The dihydrogen activation step of H₂-hydrogenation catalyzed by Mn-LYE complex

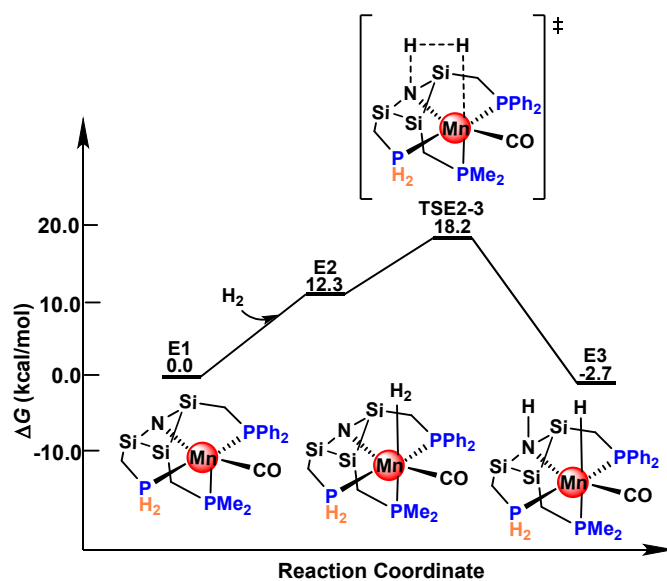


Figure S7. The Gibbs free energy profiles for the dihydrogen activation step of H₂-hydrogenation catalyzed by Mn-LYE (E) complex (unit: kcal/mol).

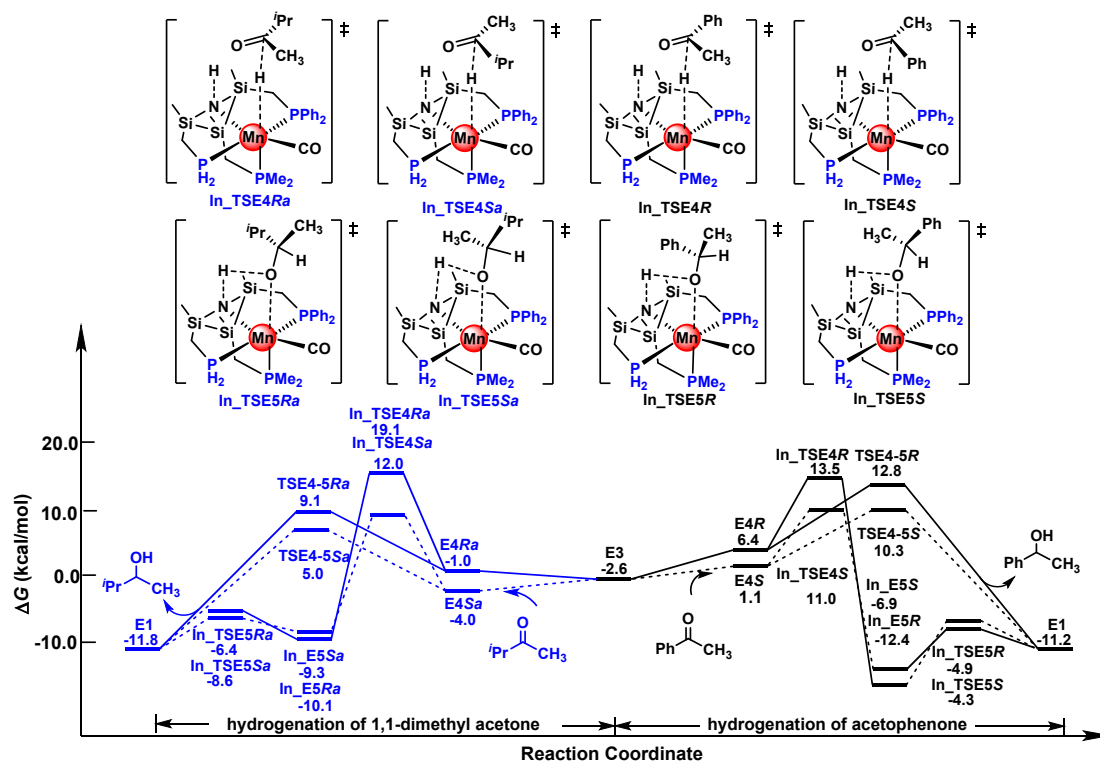


Figure S8. The inner mechanism Gibbs free energy profiles of asymmetric hydrogenations of acetophenone and 1,1-dimethyl acetone catalyzed by Mn(CO)-LYE complex (unit: kcal/mol).

6. The dihydrogen activation step of H₂-hydrogenation catalyzed by Mn-LYF complex

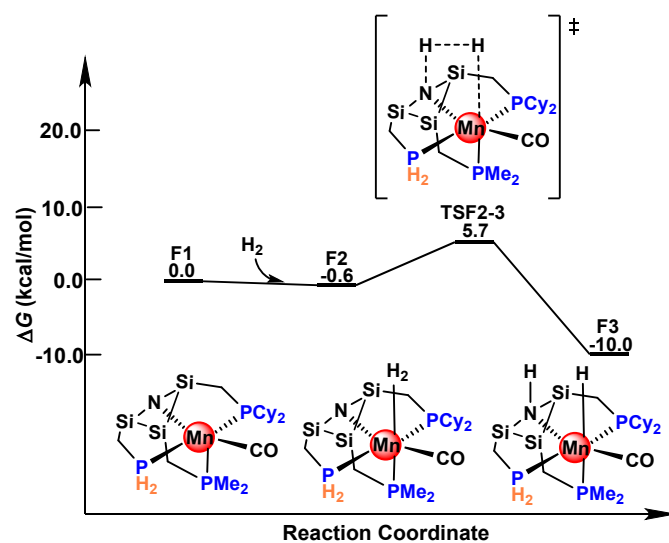


Figure S9. The Gibbs free energy profiles for the dihydrogen activation step of H₂-hydrogenation catalyzed by Mn-LYF (F) complex (unit: kcal/mol).

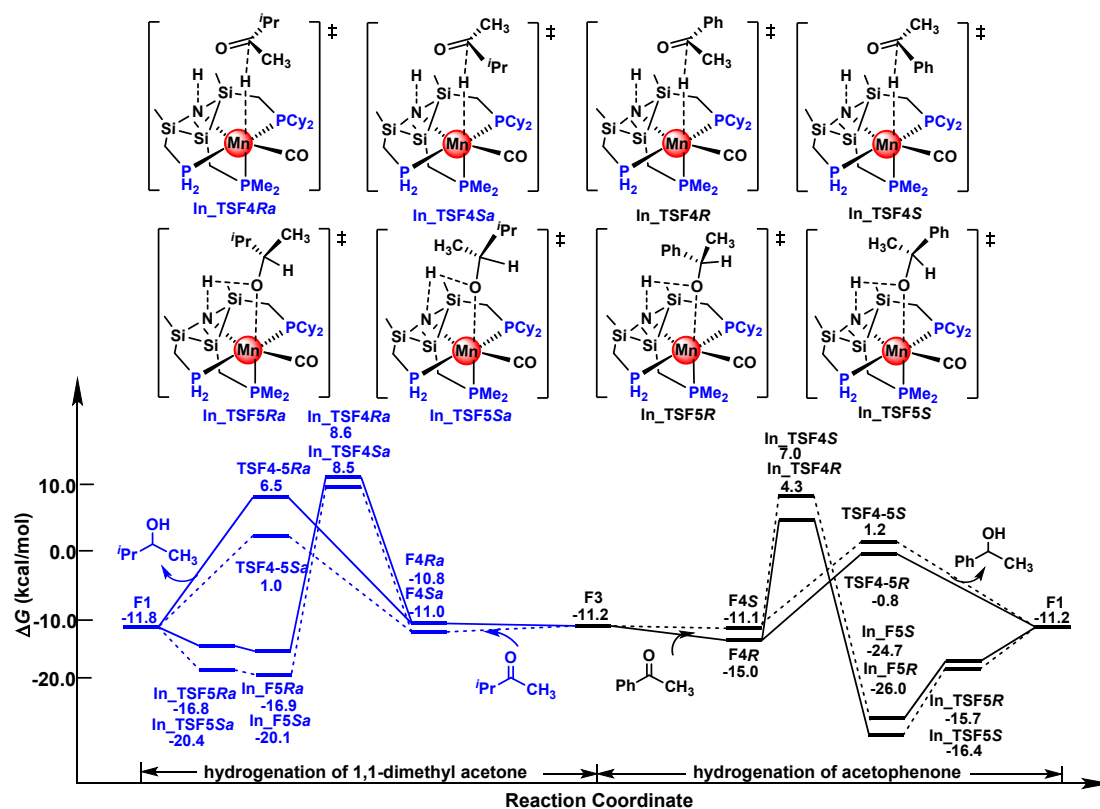


Figure S10. The inner mechanism Gibbs free energy profiles of asymmetric hydrogenations of acetophenone and 1,1-dimethyl acetone catalyzed by Mn(CO)-LYC complex (unit: kcal/mol)..

7. The theoretical ee value is calculated with the following formulas

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

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

8. Spin multiplicity and charge of the manganese complexes

Table S1. The calculated relative free energies of intermediates of Mn complexes along reaction pathways at singlet and triplet spin states at ω B97X-D/6-31G* level (the free energies of intermeidate in path A-F are relative to correspoind catalytic species **A1-F1** at singlet spin state, respectively).

Complex	<i>G</i>	<i>G</i>	ΔG
	<i>singlet</i>	<i>triplet</i>	
A1	-2811.021109	-2811.011249	6.2
A2	-2812.180527	-2812.172152	13.6
A3	-2812.196827	-2812.163040	19.3
A4	-3196.856528	-3196.821091	26.4
A5	-3196.876713	-3196.839769	14.7
A6	-3196.876713	-3196.849770	8.4
B1	-2427.781255	-2427.761208	12.6
B2	-2428.938536	-2428.922113	20.0
B3	-2428.955271	-2428.922792	19.5
B4r	-2813.619236	-2813.582338	25.7
B4s	-2813.617428	-2813.544787	49.3
C1	-3024.413970	-3024.412381	1.0
C2	-3025.569607	-3025.577284	5.9
C3	-3025.586450	-3025.584484	1.4
C4r	-3410.247221	-3410.202765	33.4
C4s	-3410.248717	-3410.203522	33.0
C4ra	-3297.174454	-3297.167480	8.1
C4sa	-3297.172948	-3297.104429	47.7
D1	-3031.542813	-3031.540955	1.1
D2	-3032.700398	-3032.710435	13.2
D3	-3032.722792	-3032.710974	2.8

D4r	-3417.377269	-3417.351359	21.1
D4s	-3417.377167	-3417.369194	9.9
D4ra	-3304.303608	-3304.298212	7.0
D4sa	-3304.306614	-3304.291419	11.2
E1	-2945.835611	-2945.835267	0.2
E2	-2946.995672	-2946.990534	11.1
E3	-2947.012513	-2947.008553	-0.1
E4r	-3331.667580	-3331.666426	7.0
E4s	-3331.675892	-3331.620354	36.0
E4ra	-3218.577184	-3218.581834	12.7
E4sa	-3218.583777	-3218.530437	45.4
F1	-2952.967176	-2952.967176	0
F2	-2954.126684	-2954.122908	10.6
F3	-2954.147253	-2954.140829	-0.6
F4r	-3338.812439	-3338.791543	11.1
F4s	-3338.806222	-3338.767452	26.2
F4ra	-3225.702554	-3225.714346	12.1
F4sa	-3225.711230	-3225.714322	12.1

9. Energies of all the structures

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

Complex	Entropy effect	E (6-31g*)	E (6-31++g**)	ΔG
A1	-2811.010720	-2811.553595	-2811.654174	0.0
H₂	-1.162299	-1.17136203	-1.17479706	/
A2	-2812.170138	-2812.727861	-2812.835810	-0.7
TSA2-3	-2812.161519	-2812.718815	-2812.828124	3.9
A3	-2812.186438	-2812.749293	-2812.855466	-9.8
PhCOCH₃	-384.659016	-384.7769242	-384.8007975	/
A4	-3196.846139	-3197.544262	-3197.672276	-8.9
TSA4-5	-3196.817584	-3197.516322	-3197.645113	8.5
B2	-3196.866604	-3197.562686	-3197.69174	-22.4
TSA5-6	-3196.862378	-3197.555086	-3197.685008	-20.3
A6	-3196.866324	-3197.562685	-3197.691738	-22.2
TSA4-6	-3196.819718	-3197.516252	-3197.644366	7.6
PhCHOHCH₃	-385.833934	-385.9748208	-386.0073452	/
A1	-2811.010720	-2811.553595	-2811.654174	-11.2
B1	-2427.770866	-2428.297222	-2428.213779	0.0
B2	-2428.928147	-2429.477746	-2429.386230	0.2
TSB2-3	-2428.918623	-2429.469192	-2429.376129	5.2
B3	-2428.944882	-2429.495673	-2429.406487	-8.8
B4r	-2813.608847	-2814.310590	-2814.199782	-10.5
TSB4-5r	-2813.576568	-2814.286420	-2814.174771	9.2
B4s	-2813.607039	-2814.312549	-2814.200890	-9.9
TSB4-5s	-2813.585553	-2814.293906	-2814.182463	3.7

C1	-3024.403581	-3024.995428	-3024.903453	0.0
C2	-3025.559218	-3026.177618	-3026.077853	1.4
TSC2-3	-3025.546684	-3026.166099	-3026.065053	8.5
C3	-3025.576061	-3026.192169	-3026.096036	-6.8
C4r	-3410.236830	-3411.006713	-3410.888238	-7.0
TSC4-5r	-3410.209943	-3410.984808	-3410.866134	9.8
C4s	-3410.238328	-3411.007708	-3410.888513	-8.4
TSC4-5s	-3410.210537	-3410.984608	-3410.865571	9.2
C4ra	-3297.164065	-3297.935082	-3297.819505	-7.7
TSC4-5ra	-3297.130601	-3297.908586	-3297.791368	12.3
C4sa	-3297.162559	-3297.936244	-3297.819841	-7.2
TSC4-5sa	-3297.132039	-3297.912660	-3297.795778	11.6
D1	-3031.532424	-3032.277272	-3032.177643	0.37
D2	-3032.690009	-3033.458158	-3033.350967	5.1
TSD2-3	-3032.681322	-3033.446388	-3033.338113	-11.3
D3	-3032.712403	-3033.476815	-3033.373366	-7.3
D4r	-3417.366880	-3418.287850	-3418.162415	11.6
TSD4-5r	-3417.336976	-3418.260826	-3418.135637	-8.3
D4s	-3417.366778	-3418.289021	-3418.161825	13.0
TSD4-5s	-3417.334301	-3418.256074	-3418.130364	0.4
D4ra	-3304.293219	-3305.212624	-3305.089246	-7.9
TSD4-5ra	-3304.254808	-3305.181306	-3305.056983	15.6
D4sa	-3304.296225	-3305.217922	-3305.094458	-9.9
TSD4-5sa	-3304.254548	-3305.182818	-3305.059216	16.2
E1	-2945.835611	-2946.355562	-2946.269858	0.0
E2	-2946.985283	-2947.541957	-2947.449444	12.3
TSE2-3	-2946.974163	-2947.528013	-2947.433737	18.2
E3	-2947.012513	-2947.555682	-2947.466462	-2.7
E4r	-3331.657191	-3332.367671	-3332.254416	6.2

TSE4-5r	-3331.645303	-3332.358936	-3332.246719	14.3
E4s	-3331.665503	-3332.374865	-3332.262463	1.5
TSE4-5s	-3331.650822	-3332.362820	-3332.250025	10.5
E4ra	-3218.586670	-3226.581909	-3226.463812	-0.7
TSE4-5ra	-3218.577184	-3219.281618	-3219.171134	10.0
E4sa	-3218.592628	-3226.584672	-3226.467300	-4.0
TSE4-5sa	-3218.583777	-3219.289084	-3219.178772	6.0
F1	-2952.956787	-2953.638001	-2953.544945	0.0
F2	-2954.116295	-2954.819507	-2954.719254	-0.6
TSF2-3	-2954.104958	-2954.809396	-2954.707856	5.7
F3	-2954.136864	-2954.840470	-2954.743932	-10.0
F4r	-3338.802050	-3339.659269	-3339.540701	-13.9
TSF4-5r	-3338.779300	-3339.639329	-3339.520692	0.3
F4s	-3338.795833	-3339.653227	-3339.533908	-10.5
TSF4-5s	-3338.776225	-3339.634614	-3339.515317	1.8
F4ra	-3225.723700	-3226.581909	-3226.463812	-12.56
TSF4-5ra	-3225.692165	-3226.55725	-3226.439055	7.1
F4sa	-3225.724800	-3226.584672	-3226.467300	-12.8
TSF4-5sa	-3225.700841	-3226.562367	-3226.445741	2.7

10. Imaginary frequencies of transition states

Table S3. Calculated imaginary frequency of transition states at ω B97X-D/BSI (LANL2DZ & 6-31G*) level.

TSA2-3	1187.13 cm^{-1}
TSA4-5	447.38 cm^{-1}
TSA5-6	1235.34 cm^{-1}
TSA4-6	502.38 cm^{-1}
TSB2-3	1123.39 cm^{-1}
TSB4-5R	448.68 cm^{-1}
TSB4-5S	550.03 cm^{-1}
TSD2-3	1251.12 cm^{-1}
TSD4-5R	381.44 cm^{-1}
TSD4-5S	619.27 cm^{-1}
TSD4-5Ra	633.11 cm^{-1}
TSD4-5Sa	615.81 cm^{-1}
TSD2-3	1276.50 cm^{-1}
TSD4-5R	514.90 cm^{-1}
TSD4-5S	627.92 cm^{-1}
TSD4-5Ra	553.39 cm^{-1}
TSD4-5Sa	549.40 cm^{-1}
TSE2-3	1291.73 cm^{-1}
TSE4-5R	335.95 cm^{-1}
TSE4-5S	444.17 cm^{-1}
TSE4-5Ra	419.07 cm^{-1}
TSE4-5Sa	534.98 cm^{-1}
TSF2-3	1253.25 cm^{-1}
TSF4-5R	434.24 cm^{-1}
TSF4-5S	345.24 cm^{-1}

TSF4-5*Ra* 449.62 cm^{-1}

TSF4-5*Sa* 601.06 cm^{-1}

11. Dartesian Doordinates of all stationary point along reaDtion pathways

A1

	Doordinates (Angstroms)		
	X	Y	Z

25	0.014055000	0.015225000	0.300962000
7	-0.073475000	1.849533000	-0.503187000
6	0.005889000	-1.738477000	0.599336000
8	0.011195000	-2.879936000	0.820193000
6	2.537460000	1.243130000	-1.539785000
1	3.596925000	1.469647000	-1.693958000
1	2.122843000	0.941880000	-2.510662000
6	-2.758927000	1.839614000	0.614698000
6	0.361588000	0.374952000	1.984683000
8	0.579157000	0.716232000	3.071915000
15	-2.261162000	0.101020000	0.447431000
15	2.216298000	-0.152975000	-0.413095000
6	2.631099000	-1.652560000	-1.388854000
6	3.877034000	-2.281417000	-1.329803000
6	1.655996000	-2.153955000	-2.259283000
6	4.142298000	-3.393222000	-2.125571000
1	4.643598000	-1.909762000	-0.656068000
6	1.924620000	-3.259373000	-3.059940000
1	0.677525000	-1.679662000	-2.310047000
6	3.168708000	-3.882953000	-2.992000000
1	5.112644000	-3.877597000	-2.066132000
1	1.159450000	-3.638033000	-3.731485000
1	3.377268000	-4.751984000	-3.609379000
6	3.496354000	-0.128509000	0.891686000
6	4.573439000	0.760236000	0.911747000
6	3.371060000	-1.063857000	1.927507000
6	5.504872000	0.716160000	1.947944000
1	4.693566000	1.500426000	0.127645000
6	4.306857000	-1.115898000	2.953084000
1	2.536826000	-1.760725000	1.929860000
6	5.376358000	-0.222302000	2.966666000
1	6.332096000	1.419934000	1.955220000
1	4.197508000	-1.851112000	3.744712000
1	6.105577000	-0.256322000	3.770768000
6	-2.973955000	-0.492959000	-1.136465000
6	-3.823281000	0.279252000	-1.932870000
6	-2.636263000	-1.783344000	-1.567856000
6	-4.315595000	-0.220348000	-3.137498000

1	-4.105033000	1.280623000	-1.625502000
6	-3.132619000	-2.284435000	-2.766033000
1	-1.990696000	-2.408476000	-0.958115000
6	-3.970707000	-1.500874000	-3.557392000
1	-4.970451000	0.396365000	-3.746192000
1	-2.864337000	-3.288828000	-3.080688000
1	-4.356374000	-1.890251000	-4.495083000
6	-3.229009000	-0.831023000	1.693414000
6	-2.599227000	-1.344954000	2.829172000
6	-4.610343000	-1.003270000	1.543465000
6	-3.336803000	-2.016537000	3.802293000
1	-1.528475000	-1.224566000	2.958649000
6	-5.345676000	-1.674312000	2.513536000
1	-5.111398000	-0.618343000	0.659004000
6	-4.709043000	-2.182912000	3.645067000
1	-2.835349000	-2.414359000	4.679519000
1	-6.416067000	-1.805866000	2.384999000
1	-5.283522000	-2.710712000	4.400877000
14	-1.484279000	2.847953000	-0.378720000
14	1.423419000	2.632687000	-0.888830000
6	-2.197266000	3.342361000	-2.057926000
1	-3.217736000	3.737190000	-1.965740000
1	-1.588767000	4.133416000	-2.512580000
1	-2.216663000	2.501197000	-2.759752000
6	-1.232301000	4.447272000	0.598418000
1	-0.564538000	5.153662000	0.090459000
1	-2.193488000	4.958369000	0.744060000
1	-0.810586000	4.242298000	1.590087000
6	1.303125000	3.936256000	-2.251524000
1	0.816445000	3.532774000	-3.147650000
1	0.745774000	4.827110000	-1.937965000
1	2.307725000	4.271472000	-2.541547000
6	2.255000000	3.427890000	0.607069000
1	3.257044000	3.803936000	0.362083000
1	1.670220000	4.278394000	0.977301000
1	2.354590000	2.715542000	1.434453000
1	-3.813714000	2.036582000	0.394607000
1	-2.599732000	2.080622000	1.674385000

A2

Doordinates (Angstroms)			

	X	Y	Z
25	-0.005128000	-0.142706000	-0.073482000
7	0.036496000	1.971506000	0.277756000

6	-0.015227000	-1.901783000	-0.333784000
8	-0.015604000	-3.046332000	-0.527682000
6	-2.539655000	1.434936000	1.384516000
1	-3.591087000	1.683779000	1.557152000
1	-2.055575000	1.317349000	2.362166000
6	2.692289000	1.698565000	-0.816315000
6	-0.256568000	0.301817000	-1.782165000
8	-0.388071000	0.677059000	-2.867258000
15	2.281095000	-0.009233000	-0.343683000
15	-2.256995000	-0.112683000	0.478402000
6	-2.851842000	-1.484911000	1.554134000
6	-3.039627000	-2.756948000	0.999958000
6	-3.063151000	-1.310643000	2.924264000
6	-3.428891000	-3.827784000	1.796695000
1	-2.886989000	-2.917162000	-0.063259000
6	-3.451282000	-2.384841000	3.723109000
1	-2.936868000	-0.334374000	3.381990000
6	-3.633903000	-3.644948000	3.162621000
1	-3.571582000	-4.806274000	1.347745000
1	-3.615089000	-2.230922000	4.785751000
1	-3.937347000	-4.480994000	3.785977000
6	-3.478854000	-0.158129000	-0.888194000
6	-4.711748000	0.497125000	-0.806464000
6	-3.190201000	-0.910524000	-2.031406000
6	-5.627246000	0.413205000	-1.850737000
1	-4.966916000	1.080251000	0.072271000
6	-4.110165000	-1.003866000	-3.072013000
1	-2.239022000	-1.428163000	-2.113283000
6	-5.328306000	-0.336763000	-2.985845000
1	-6.577460000	0.933672000	-1.775831000
1	-3.868415000	-1.590454000	-3.953373000
1	-6.044702000	-0.400032000	-3.799662000
6	3.237856000	-0.372150000	1.180827000
6	4.164189000	0.514161000	1.733876000
6	3.022116000	-1.605216000	1.811328000
6	4.857890000	0.180175000	2.896309000
1	4.347409000	1.476419000	1.268807000
6	3.719588000	-1.941801000	2.965502000
1	2.303369000	-2.307654000	1.395959000
6	4.638292000	-1.046756000	3.512925000
1	5.570304000	0.884225000	3.316268000
1	3.543762000	-2.902073000	3.441278000
1	5.178723000	-1.306250000	4.418556000
6	3.141818000	-1.069595000	-1.575171000

6	2.431276000	-1.666468000	-2.619601000
6	4.529760000	-1.246452000	-1.515147000
6	3.092134000	-2.420530000	-3.587059000
1	1.354929000	-1.549651000	-2.684886000
6	5.189213000	-2.000706000	-2.479012000
1	5.099720000	-0.798519000	-0.705812000
6	4.471124000	-2.590186000	-3.517985000
1	2.524740000	-2.879501000	-4.391298000
1	6.265425000	-2.132846000	-2.416004000
1	4.986348000	-3.182061000	-4.268948000
14	1.485228000	2.858002000	0.101714000
14	-1.469885000	2.743261000	0.503915000
6	2.240912000	3.410016000	1.746273000
1	3.246366000	3.835793000	1.628424000
1	1.612373000	4.189522000	2.196510000
1	2.300467000	2.585729000	2.466610000
6	1.359939000	4.408350000	-0.978606000
1	0.702359000	5.170404000	-0.542274000
1	2.345484000	4.873939000	-1.114555000
1	0.968199000	4.162610000	-1.973427000
6	-1.440070000	4.244997000	1.656433000
1	-0.974575000	4.000787000	2.619106000
1	-0.893149000	5.093288000	1.227199000
1	-2.461644000	4.593110000	1.858940000
6	-2.345467000	3.277767000	-1.082622000
1	-3.363066000	3.640537000	-0.886660000
1	-1.793058000	4.094114000	-1.565928000
1	-2.415694000	2.459543000	-1.808158000
1	3.758907000	1.933198000	-0.733092000
1	2.434584000	1.769203000	-1.881703000
1	0.637807000	-0.220035000	1.618078000
1	-0.120366000	-0.378853000	1.722170000

A3

Doordinates (Angstroms)			
	X	Y	Z
25	0.014758000	-0.183915000	0.272083000
7	-0.154582000	1.895591000	-0.713509000
6	0.017982000	-1.870330000	0.778553000
8	0.004758000	-2.993935000	1.080312000
6	2.408721000	1.065122000	-1.644939000
1	3.455785000	1.249413000	-1.906201000
1	1.907085000	0.721094000	-2.558727000

6	-2.671919000	1.695350000	0.792911000
6	0.285835000	0.467042000	1.906350000
8	0.463423000	0.872893000	2.985419000
15	-2.240535000	-0.036662000	0.350934000
15	2.156154000	-0.283324000	-0.417713000
6	2.774559000	-1.774906000	-1.314828000
6	1.872727000	-2.663608000	-1.907204000
6	4.146713000	-2.013476000	-1.461757000
6	2.329907000	-3.761948000	-2.631764000
1	0.807738000	-2.488300000	-1.802046000
6	4.603498000	-3.108544000	-2.187938000
1	4.868697000	-1.345843000	-1.000773000
6	3.695420000	-3.987308000	-2.774652000
1	1.613738000	-4.445232000	-3.079462000
1	5.671483000	-3.278223000	-2.291793000
1	4.052451000	-4.845951000	-3.336314000
6	3.490958000	-0.044409000	0.830467000
6	4.606823000	0.777685000	0.647502000
6	3.365866000	-0.738130000	2.040169000
6	5.565885000	0.913911000	1.649158000
1	4.740597000	1.325133000	-0.280095000
6	4.326808000	-0.612223000	3.037719000
1	2.503516000	-1.378156000	2.205883000
6	5.427675000	0.219899000	2.847083000
1	6.421619000	1.563920000	1.489696000
1	4.208713000	-1.156002000	3.970404000
1	6.174284000	0.325898000	3.628862000
6	-3.152602000	-0.356562000	-1.214543000
6	-4.107679000	0.512934000	-1.746997000
6	-2.878925000	-1.550319000	-1.895229000
6	-4.764007000	0.208211000	-2.939839000
1	-4.351809000	1.440845000	-1.240809000
6	-3.545470000	-1.864514000	-3.073437000
1	-2.131160000	-2.231313000	-1.498130000
6	-4.485859000	-0.981020000	-3.603875000
1	-5.495585000	0.902878000	-3.342760000
1	-3.325428000	-2.796971000	-3.585164000
1	-4.997964000	-1.220572000	-4.531340000
6	-3.218814000	-1.013442000	1.566525000
6	-2.620208000	-1.364896000	2.780792000
6	-4.555139000	-1.364003000	1.345805000
6	-3.343170000	-2.044531000	3.757241000
1	-1.581623000	-1.109473000	2.965386000
6	-5.276207000	-2.048336000	2.320143000

1	-5.037945000	-1.108078000	0.407200000
6	-4.672560000	-2.388217000	3.528468000
1	-2.862255000	-2.310255000	4.694026000
1	-6.312387000	-2.315817000	2.133611000
1	-5.235723000	-2.924093000	4.287231000
14	-1.526098000	2.878851000	-0.131661000
14	1.469838000	2.568111000	-1.009934000
6	-2.372675000	3.657391000	-1.618553000
1	-3.304770000	4.160268000	-1.332114000
1	-1.723145000	4.409137000	-2.083860000
1	-2.617723000	2.911816000	-2.384006000
6	-0.963083000	4.207735000	1.062709000
1	-0.373996000	4.996451000	0.581993000
1	-1.851662000	4.685176000	1.495936000
1	-0.380131000	3.791431000	1.891333000
6	1.399405000	3.907458000	-2.327500000
1	0.890566000	3.556042000	-3.233171000
1	0.871079000	4.799170000	-1.967933000
1	2.408997000	4.224743000	-2.618180000
6	2.234954000	3.258935000	0.553537000
1	3.307953000	3.417006000	0.391047000
1	1.804368000	4.227372000	0.825983000
1	2.130290000	2.583207000	1.407577000
1	-3.738152000	1.930035000	0.701392000
1	-2.425579000	1.773392000	1.859981000
1	-0.447977000	1.442473000	-1.582533000
1	-0.175426000	-0.688931000	-1.243914000

A4

Doordinates (Angstroms)			
	X	Y	Z
25	-0.936541000	0.759506000	-0.116923000
7	-0.141270000	-0.169168000	1.819843000
6	-1.345511000	1.347733000	-1.722080000
8	-1.588573000	1.718019000	-2.799815000
6	-1.856709000	-2.251671000	0.950672000
1	-2.591973000	-3.047606000	1.104913000
1	-0.948415000	-2.722150000	0.554119000
6	1.197314000	2.450105000	1.791196000
6	-2.017517000	1.892836000	0.730554000
8	-2.736353000	2.645989000	1.256954000
15	0.913591000	2.040786000	0.022978000
15	-2.348490000	-0.984183000	-0.285319000

6	-2.436716000	-1.960567000	-1.851867000
6	-1.475477000	-1.791658000	-2.851527000
6	-3.435811000	-2.924240000	-2.037802000
6	-1.504133000	-2.574052000	-4.004546000
1	-0.694414000	-1.052135000	-2.715187000
6	-3.464793000	-3.706979000	-3.187014000
1	-4.205507000	-3.060431000	-1.283064000
6	-2.496628000	-3.533892000	-4.174825000
1	-0.749190000	-2.427296000	-4.772021000
1	-4.246616000	-4.450645000	-3.313365000
1	-2.520694000	-4.141695000	-5.075041000
6	-4.139754000	-0.684341000	0.030857000
6	-4.943916000	-1.479185000	0.852396000
6	-4.719990000	0.423859000	-0.598636000
6	-6.290254000	-1.174548000	1.043852000
1	-4.528159000	-2.343508000	1.360247000
6	-6.065459000	0.724082000	-0.417763000
1	-4.108232000	1.062626000	-1.230240000
6	-6.854936000	-0.073415000	0.408327000
1	-6.896853000	-1.800933000	1.691957000
1	-6.495618000	1.589318000	-0.913757000
1	-7.903951000	0.164912000	0.558614000
6	2.498780000	1.305476000	-0.555835000
6	3.670288000	1.272066000	0.203540000
6	2.531604000	0.792000000	-1.859305000
6	4.846369000	0.733193000	-0.320464000
1	3.684053000	1.669644000	1.213011000
6	3.707468000	0.277397000	-2.391451000
1	1.624117000	0.798345000	-2.456786000
6	4.869981000	0.244020000	-1.620580000
1	5.743117000	0.699199000	0.291117000
1	3.716884000	-0.105683000	-3.408302000
1	5.784937000	-0.172780000	-2.029950000
6	0.981495000	3.700788000	-0.776674000
6	-0.213743000	4.386122000	-1.014581000
6	2.191767000	4.323675000	-1.101937000
6	-0.200972000	5.665721000	-1.563828000
1	-1.161906000	3.916516000	-0.774046000
6	2.204905000	5.601350000	-1.653131000
1	3.132275000	3.807463000	-0.931530000
6	1.007957000	6.275337000	-1.885762000
1	-1.139441000	6.181475000	-1.745523000
1	3.152251000	6.070831000	-1.902904000
1	1.018576000	7.270119000	-2.321965000

14	0.800178000	0.935944000	2.848813000
14	-1.318191000	-1.321870000	2.496307000
6	2.372458000	0.066782000	3.397131000
1	3.008685000	0.729170000	3.997773000
1	2.143872000	-0.818980000	4.001779000
1	2.951673000	-0.265522000	2.529162000
6	-0.191600000	1.515194000	4.330850000
1	-0.388964000	0.719514000	5.057662000
1	0.375171000	2.298629000	4.850785000
1	-1.148616000	1.953298000	4.026302000
6	-0.482631000	-2.486213000	3.713542000
1	0.411883000	-2.934435000	3.267204000
1	-0.180779000	-1.964302000	4.630377000
1	-1.156888000	-3.299353000	4.010645000
6	-2.764803000	-0.470052000	3.332227000
1	-3.565822000	-1.201837000	3.495528000
1	-2.493152000	-0.068253000	4.313418000
1	-3.182494000	0.344511000	2.733247000
1	2.170523000	2.909214000	1.997666000
1	0.437929000	3.210642000	2.016111000
1	0.530229000	-0.764981000	1.320444000
1	0.019387000	-0.319594000	-0.816910000
6	2.318552000	-2.645447000	-0.041966000
6	1.591625000	-2.864888000	-1.341314000
1	1.924613000	-2.133657000	-2.085325000
1	1.792817000	-3.867209000	-1.736479000
1	0.520613000	-2.739600000	-1.187811000
8	1.712746000	-2.363359000	0.983508000
6	3.806184000	-2.783509000	-0.010150000
6	4.548554000	-3.109893000	-1.148995000
6	4.471242000	-2.555637000	1.199118000
6	5.934741000	-3.207294000	-1.077964000
1	4.051988000	-3.282390000	-2.098333000
6	5.855090000	-2.645523000	1.269132000
1	3.884486000	-2.309195000	2.077660000
6	6.588972000	-2.971487000	0.128776000
1	6.504478000	-3.462864000	-1.966468000
1	6.363379000	-2.466024000	2.211786000
1	7.671303000	-3.046572000	0.182873000

A5

Doordinates (Angstroms)

	X	Y	Z
25	0.021282000	-0.759330000	-0.111313000

7	-0.027680000	0.189007000	1.989323000
6	-0.020080000	-1.282149000	-1.796637000
8	-0.076217000	-1.639356000	-2.901750000
6	2.641262000	0.826975000	1.263344000
1	3.699328000	0.971034000	1.500474000
1	2.225139000	1.792854000	0.952938000
6	-2.704272000	-1.014046000	1.869411000
6	0.210906000	-2.397042000	0.549799000
8	0.324904000	-3.443862000	1.041430000
15	-2.271514000	-0.971220000	0.085021000
15	2.314508000	-0.294387000	-0.138575000
14	-1.521542000	0.029903000	2.915530000
14	1.575128000	0.310331000	2.727194000
6	-2.202174000	1.745155000	3.268457000
1	-3.221908000	1.714118000	3.672024000
1	-1.572724000	2.255325000	4.008081000
1	-2.206574000	2.370066000	2.367181000
6	-1.237100000	-0.911285000	4.515129000
1	-0.579061000	-0.380142000	5.212317000
1	-2.196285000	-1.064114000	5.026410000
1	-0.806114000	-1.901158000	4.324453000
6	1.647350000	1.683060000	4.010481000
1	1.316563000	2.634863000	3.577052000
1	1.017619000	1.472082000	4.883241000
1	2.671864000	1.823287000	4.378567000
6	2.128875000	-1.315935000	3.476813000
1	3.204388000	-1.281738000	3.691461000
1	1.617271000	-1.522759000	4.423327000
1	1.953826000	-2.161864000	2.804174000
1	-3.766525000	-0.819454000	2.057472000
1	-2.523574000	-2.056109000	2.166233000
1	-0.119017000	0.991959000	1.317264000
6	-0.563093000	2.213486000	-1.143877000
6	-0.060839000	2.181295000	-2.590518000
1	-0.579970000	2.929010000	-3.203787000
1	1.016308000	2.375248000	-2.643291000
1	-0.245994000	1.193520000	-3.025826000
8	0.059241000	1.266522000	-0.344358000
1	-1.650327000	2.060509000	-1.184663000
6	-3.119673000	-2.477449000	-0.551295000
6	-2.412947000	-3.528969000	-1.136583000
6	-4.510443000	-2.591036000	-0.417929000
6	-3.079156000	-4.671732000	-1.577605000
1	-1.337953000	-3.464805000	-1.257375000

6	-5.174790000	-3.730796000	-0.852690000
1	-5.079676000	-1.775701000	0.021393000
6	-4.458095000	-4.776057000	-1.435166000
1	-2.514531000	-5.479446000	-2.033909000
1	-6.252604000	-3.804414000	-0.740358000
1	-4.975903000	-5.666783000	-1.778859000
6	-3.328908000	0.326093000	-0.655252000
6	-4.011009000	1.283518000	0.095210000
6	-3.387158000	0.391733000	-2.053972000
6	-4.725261000	2.300475000	-0.538678000
1	-3.986259000	1.254856000	1.179527000
6	-4.099258000	1.403113000	-2.684964000
1	-2.857168000	-0.344067000	-2.653652000
6	-4.765552000	2.366488000	-1.927264000
1	-5.247451000	3.042457000	0.058828000
1	-4.127761000	1.446776000	-3.769627000
1	-5.314327000	3.163670000	-2.419923000
6	3.037608000	0.553628000	-1.598377000
6	3.716623000	1.769724000	-1.494542000
6	2.899188000	-0.032266000	-2.860269000
6	4.222334000	2.400021000	-2.629835000
1	3.853445000	2.240983000	-0.526393000
6	3.408373000	0.591841000	-3.993518000
1	2.385954000	-0.981897000	-2.967409000
6	4.064415000	1.815780000	-3.882606000
1	4.737908000	3.350952000	-2.530995000
1	3.284492000	0.123429000	-4.965487000
1	4.455106000	2.308065000	-4.768329000
6	3.481879000	-1.701927000	0.060447000
6	4.658061000	-1.637316000	0.813841000
6	3.188513000	-2.888740000	-0.621429000
6	5.513713000	-2.732967000	0.890625000
1	4.920083000	-0.729406000	1.348325000
6	4.048515000	-3.980484000	-0.556379000
1	2.274352000	-2.964106000	-1.204616000
6	5.212489000	-3.906118000	0.203676000
1	6.421272000	-2.667003000	1.483973000
1	3.803595000	-4.892491000	-1.092939000
1	5.882634000	-4.758986000	0.261259000
6	-0.346819000	3.582149000	-0.508186000
6	-1.423331000	4.367280000	-0.095956000
6	0.948385000	4.059737000	-0.282427000
6	-1.216972000	5.595369000	0.534061000
1	-2.435963000	4.007922000	-0.267297000

6	1.161943000	5.281936000	0.345155000
1	1.792045000	3.460262000	-0.612835000
6	0.076542000	6.055623000	0.759479000
1	-2.069459000	6.191023000	0.850610000
1	2.176149000	5.637622000	0.509352000
1	0.240703000	7.010154000	1.251937000

A6

Doordinates (Angstroms)			
	X	Y	Z
25	0.021231000	-0.759376000	-0.111244000
7	-0.027726000	0.189701000	1.989133000
6	-0.020182000	-1.282767000	-1.796383000
8	-0.076400000	-1.640337000	-2.901374000
6	2.641446000	0.826869000	1.263110000
1	3.699516000	0.970763000	1.500339000
1	2.225691000	1.792750000	0.952211000
6	-2.704349000	-1.013276000	1.869594000
6	0.210699000	-2.396912000	0.550361000
8	0.324587000	-3.443628000	1.042245000
15	-2.271596000	-0.971093000	0.085215000
15	2.314537000	-0.294883000	-0.138437000
14	-1.521547000	0.030892000	2.915427000
14	1.574933000	0.311598000	2.727147000
6	-2.202072000	1.746252000	3.267950000
1	-3.221533000	1.715372000	3.672209000
1	-1.572122000	2.256832000	4.006862000
1	-2.207075000	2.370699000	2.366358000
6	-1.236952000	-0.909936000	4.515207000
1	-0.579251000	-0.378397000	5.212414000
1	-2.196136000	-1.063110000	5.026386000
1	-0.805471000	-1.899637000	4.324748000
6	1.646876000	1.685606000	4.009103000
1	1.317599000	2.637305000	3.574306000
1	1.015713000	1.476106000	4.881188000
1	2.671016000	1.825175000	4.378492000
6	2.128226000	-1.313828000	3.479014000
1	3.204393000	-1.280911000	3.690522000
1	1.618992000	-1.517001000	4.427608000
1	1.949718000	-2.161258000	2.809192000
1	-3.766582000	-0.818537000	2.057636000
1	-2.523742000	-2.055247000	2.166800000
1	-0.119072000	0.992356000	1.316716000

6	-0.562789000	2.213265000	-1.144541000
6	-0.060341000	2.180860000	-2.591112000
1	-0.579324000	2.928539000	-3.204549000
1	1.016831000	2.374719000	-2.643750000
1	-0.245508000	1.193033000	-3.026302000
8	0.059347000	1.266343000	-0.344852000
1	-1.650043000	2.060414000	-1.185443000
6	-3.119881000	-2.477428000	-0.550661000
6	-2.413293000	-3.529176000	-1.135703000
6	-4.510663000	-2.590819000	-0.417230000
6	-3.079652000	-4.671971000	-1.576411000
1	-1.338295000	-3.465174000	-1.256552000
6	-5.175160000	-3.730612000	-0.851674000
1	-5.079783000	-1.775301000	0.021899000
6	-4.458599000	-4.776102000	-1.433906000
1	-2.515141000	-5.479869000	-2.032531000
1	-6.252979000	-3.804076000	-0.739295000
1	-4.976517000	-5.666859000	-1.777352000
6	-3.328804000	0.326100000	-0.655525000
6	-4.010968000	1.283743000	0.094608000
6	-3.386878000	0.391406000	-2.054267000
6	-4.725077000	2.300589000	-0.539618000
1	-3.986411000	1.255327000	1.178933000
6	-4.098853000	1.402662000	-2.685596000
1	-2.856844000	-0.344563000	-2.653702000
6	-4.765186000	2.366268000	-1.928225000
1	-5.247304000	3.042743000	0.057643000
1	-4.127218000	1.446051000	-3.770274000
1	-5.313851000	3.163362000	-2.421150000
6	3.037716000	0.552748000	-1.598457000
6	3.716974000	1.768731000	-1.494857000
6	2.899012000	-0.033240000	-2.860273000
6	4.222637000	2.398823000	-2.630285000
1	3.854024000	2.240077000	-0.526786000
6	3.408155000	0.590655000	-3.993659000
1	2.385579000	-0.982781000	-2.967256000
6	4.064432000	1.814487000	-3.882973000
1	4.738389000	3.349675000	-2.531610000
1	3.284046000	0.122167000	-4.965563000
1	4.455069000	2.306623000	-4.768803000
6	3.481713000	-1.702526000	0.060857000
6	4.657980000	-1.637873000	0.814113000
6	3.188206000	-2.889420000	-0.620814000
6	5.513595000	-2.733550000	0.890937000

1	4.920122000	-0.729903000	1.348434000
6	4.048163000	-3.981195000	-0.555719000
1	2.273983000	-2.964813000	-1.203901000
6	5.212244000	-3.906774000	0.204170000
1	6.421237000	-2.667534000	1.484153000
1	3.803139000	-4.893261000	-1.092129000
1	5.882369000	-4.759657000	0.261764000
6	-0.346417000	3.581954000	-0.508931000
6	-1.422849000	4.367296000	-0.096914000
6	0.948844000	4.059298000	-0.282953000
6	-1.216361000	5.595356000	0.533122000
1	-2.435523000	4.008129000	-0.268408000
6	1.162530000	5.281460000	0.344652000
1	1.792436000	3.459637000	-0.613205000
6	0.077200000	6.055360000	0.758770000
1	-2.068787000	6.191181000	0.849514000
1	2.176778000	5.636942000	0.509030000
1	0.241450000	7.009861000	1.251255000

TSA2-3

Doordinates (Angstroms)			
	X	Y	Z
25	0.015622000	-0.162794000	0.115683000
7	-0.074143000	1.981873000	-0.423308000
6	0.040440000	-1.933152000	0.163474000
8	0.070323000	-3.093663000	0.178348000
6	2.576676000	1.441102000	-1.322752000
1	3.640096000	1.684837000	-1.415286000
1	2.203092000	1.262429000	-2.340327000
6	-2.676613000	1.663743000	0.816265000
6	0.294939000	0.072941000	1.864456000
8	0.457007000	0.291625000	2.989420000
15	-2.254549000	-0.054462000	0.367740000
15	2.252425000	-0.116282000	-0.422219000
6	2.905000000	-1.418629000	-1.545399000
6	2.057545000	-1.949442000	-2.524039000
6	4.233728000	-1.852553000	-1.492256000
6	2.530297000	-2.890326000	-3.434164000
1	1.021334000	-1.627257000	-2.573110000
6	4.703715000	-2.798759000	-2.399047000
1	4.907922000	-1.456770000	-0.738206000
6	3.853717000	-3.318690000	-3.372106000
1	1.859337000	-3.293956000	-4.187016000

1	5.736729000	-3.130007000	-2.342970000
1	4.220772000	-4.058277000	-4.077882000
6	3.429710000	-0.170358000	0.978877000
6	4.413007000	0.796592000	1.196192000
6	3.323608000	-1.240036000	1.877583000
6	5.270069000	0.702087000	2.291198000
1	4.514113000	1.638317000	0.519932000
6	4.184751000	-1.340559000	2.963667000
1	2.560568000	-1.999475000	1.725382000
6	5.159444000	-0.366169000	3.174711000
1	6.024744000	1.466923000	2.449589000
1	4.090399000	-2.175103000	3.652047000
1	5.828388000	-0.439559000	4.027142000
6	-3.215094000	-0.429302000	-1.151860000
6	-4.219050000	0.404415000	-1.649089000
6	-2.926695000	-1.617376000	-1.835609000
6	-4.915916000	0.065264000	-2.807967000
1	-4.460098000	1.334584000	-1.145768000
6	-3.629001000	-1.962415000	-2.984616000
1	-2.146427000	-2.277657000	-1.467276000
6	-4.623778000	-1.118343000	-3.476849000
1	-5.686072000	0.731815000	-3.185254000
1	-3.396206000	-2.889425000	-3.500524000
1	-5.166247000	-1.382753000	-4.379914000
6	-3.127003000	-1.078722000	1.619210000
6	-2.414914000	-1.900832000	2.494116000
6	-4.521836000	-1.017376000	1.730796000
6	-3.081544000	-2.645489000	3.465880000
1	-1.335046000	-1.967781000	2.420433000
6	-5.187134000	-1.757165000	2.700992000
1	-5.094227000	-0.392338000	1.049938000
6	-4.466076000	-2.573686000	3.572030000
1	-2.513092000	-3.281970000	4.137516000
1	-6.269007000	-1.698783000	2.777934000
1	-4.985787000	-3.153520000	4.329338000
14	-1.556358000	2.837849000	-0.173754000
14	1.453658000	2.776113000	-0.577125000
6	-2.362703000	3.322170000	-1.808295000
1	-3.368702000	3.740808000	-1.675438000
1	-1.755672000	4.087963000	-2.308697000
1	-2.436877000	2.468598000	-2.491988000
6	-1.372309000	4.399693000	0.869397000
1	-0.747522000	5.160656000	0.386904000
1	-2.357094000	4.854128000	1.041435000

1	-0.934909000	4.175708000	1.849495000
6	1.435469000	4.233953000	-1.777245000
1	1.070778000	3.930127000	-2.765915000
1	0.799942000	5.055255000	-1.424387000
1	2.445827000	4.643777000	-1.906489000
6	2.139241000	3.380887000	1.070831000
1	3.166898000	3.753997000	0.973339000
1	1.530967000	4.207255000	1.458068000
1	2.138645000	2.588632000	1.827783000
1	-3.748390000	1.887076000	0.779295000
1	-2.368779000	1.761238000	1.866370000
1	-0.220770000	0.834381000	-1.307905000
1	-0.260295000	-0.085943000	-1.589424000

TSA4-5

Doordinates (Angstroms)			
	X	Y	Z
25	0.337883000	-0.349704000	-0.172884000
7	0.337035000	-0.708154000	2.052043000
6	0.148868000	0.206517000	-1.830904000
8	-0.025581000	0.603214000	-2.912785000
6	2.991926000	0.449249000	1.786120000
1	4.066306000	0.343045000	1.967051000
1	2.709768000	1.435837000	2.167157000
6	-1.930575000	-2.377076000	1.204755000
6	0.913191000	-1.992060000	-0.554901000
8	1.284386000	-3.067339000	-0.790553000
15	-1.809967000	-1.190066000	-0.189201000
15	2.517562000	0.404451000	0.015138000
14	-0.944212000	-1.782276000	2.694993000
14	1.979214000	-0.826133000	2.730543000
6	-1.965428000	-0.808692000	3.927083000
1	-2.840370000	-1.376576000	4.267316000
1	-1.359206000	-0.573045000	4.811266000
1	-2.291726000	0.144451000	3.500241000
6	-0.296507000	-3.336414000	3.530729000
1	0.312487000	-3.138258000	4.419511000
1	-1.168504000	-3.916988000	3.861319000
1	0.275681000	-3.974627000	2.849222000
6	1.962361000	-0.353664000	4.549096000
1	1.465716000	0.613328000	4.693803000
1	1.435420000	-1.094740000	5.161938000
1	2.981577000	-0.267714000	4.946616000
6	2.766825000	-2.513146000	2.497623000

1	3.848259000	-2.412068000	2.655423000
1	2.409248000	-3.250720000	3.221566000
1	2.621089000	-2.920029000	1.491938000
1	-2.961307000	-2.667841000	1.435267000
1	-1.423768000	-3.282443000	0.845904000
1	-0.019388000	0.249662000	2.267590000
1	-0.146949000	1.214564000	0.259722000
6	0.585418000	3.240963000	1.274213000
6	-0.651137000	2.349481000	1.300355000
8	-0.926599000	1.763712000	2.377498000
1	0.302953000	4.181298000	1.765955000
1	1.390924000	2.793156000	1.855854000
1	0.938968000	3.475122000	0.270115000
6	-2.314276000	-2.263858000	-1.609911000
6	-1.467469000	-2.525149000	-2.687653000
6	-3.578033000	-2.871513000	-1.589459000
6	-1.868227000	-3.374021000	-3.719224000
1	-0.487023000	-2.068173000	-2.737090000
6	-3.977392000	-3.720957000	-2.613146000
1	-4.263305000	-2.668722000	-0.770579000
6	-3.120372000	-3.975485000	-3.683624000
1	-1.193309000	-3.562679000	-4.548991000
1	-4.959456000	-4.183650000	-2.578031000
1	-3.431801000	-4.638646000	-4.485581000
6	-3.339124000	-0.181739000	-0.068447000
6	-4.159038000	-0.168226000	1.060404000
6	-3.748667000	0.518442000	-1.209729000
6	-5.381386000	0.502743000	1.039627000
1	-3.863368000	-0.689850000	1.963826000
6	-4.970363000	1.176938000	-1.234076000
1	-3.119501000	0.526109000	-2.095607000
6	-5.796290000	1.162193000	-0.110884000
1	-6.010608000	0.498005000	1.925210000
1	-5.276018000	1.707383000	-2.130491000
1	-6.753954000	1.674255000	-0.132002000
6	3.101116000	2.030794000	-0.631490000
6	2.493836000	2.616954000	-1.745367000
6	4.185823000	2.684136000	-0.037533000
6	2.953674000	3.832168000	-2.247630000
1	1.650662000	2.135582000	-2.225504000
6	4.642869000	3.900443000	-0.535034000
1	4.683026000	2.247380000	0.823307000
6	4.026071000	4.479454000	-1.641144000
1	2.466559000	4.274546000	-3.111739000

1	5.483988000	4.394881000	-0.057542000
1	4.382021000	5.429341000	-2.029339000
6	3.743187000	-0.697424000	-0.807666000
6	4.812891000	-1.318520000	-0.162670000
6	3.562765000	-0.923277000	-2.178624000
6	5.680566000	-2.150905000	-0.869280000
1	4.981808000	-1.170210000	0.898449000
6	4.432213000	-1.743369000	-2.885826000
1	2.726702000	-0.460749000	-2.697066000
6	5.494529000	-2.363987000	-2.230355000
1	6.504423000	-2.632010000	-0.349888000
1	4.275475000	-1.905204000	-3.948194000
1	6.170482000	-3.012341000	-2.780048000
6	-1.764313000	2.913743000	0.437809000
6	-1.562947000	3.274618000	-0.896663000
6	-2.969137000	3.239259000	1.057267000
6	-2.545567000	3.966320000	-1.595197000
1	-0.632750000	3.005743000	-1.389455000
6	-3.948630000	3.945687000	0.363540000
1	-3.119568000	2.947463000	2.091721000
6	-3.737468000	4.315989000	-0.961069000
1	-2.380497000	4.235737000	-2.634797000
1	-4.881507000	4.199897000	0.858792000
1	-4.502308000	4.865791000	-1.502857000

TSA4-6

Doordinates (Angstroms)			
	X	Y	Z
25	-0.315511000	0.335547000	-0.124981000
7	-0.229729000	-0.210000000	2.043590000
6	-0.186295000	0.387279000	-1.882829000
8	-0.035118000	0.365535000	-3.037495000
6	-2.810271000	-1.281967000	1.454970000
1	-3.860046000	-1.457075000	1.708274000
1	-2.307912000	-2.255126000	1.372208000
6	2.067820000	1.634295000	1.829478000
6	-0.892088000	1.991804000	0.190472000
8	-1.237421000	3.071576000	0.442726000
15	1.800534000	1.221038000	0.058633000
15	-2.520542000	-0.437685000	-0.135916000
6	-3.226886000	-1.573092000	-1.407863000
6	-2.941235000	-1.364075000	-2.760054000
6	-4.083950000	-2.620689000	-1.057379000

6	-3.486361000	-2.192249000	-3.736949000
1	-2.283455000	-0.557347000	-3.061706000
6	-4.625229000	-3.452977000	-2.033189000
1	-4.323645000	-2.807166000	-0.015321000
6	-4.325508000	-3.242876000	-3.376134000
1	-3.248327000	-2.017764000	-4.782231000
1	-5.281987000	-4.267251000	-1.740698000
1	-4.743195000	-3.895125000	-4.137503000
6	-3.795992000	0.889375000	-0.241217000
6	-4.903103000	0.964568000	0.606138000
6	-3.664890000	1.841010000	-1.259656000
6	-5.851325000	1.973280000	0.449030000
1	-5.038555000	0.238534000	1.400911000
6	-4.616157000	2.841056000	-1.426072000
1	-2.803527000	1.807346000	-1.922429000
6	-5.710921000	2.912690000	-0.567319000
1	-6.700896000	2.021235000	1.124234000
1	-4.496633000	3.572680000	-2.219808000
1	-6.450826000	3.698286000	-0.689779000
6	3.367766000	0.414888000	-0.470821000
6	4.237324000	-0.206792000	0.426693000
6	3.745690000	0.516223000	-1.815530000
6	5.475996000	-0.679054000	-0.001860000
1	3.966451000	-0.315676000	1.471735000
6	4.983275000	0.049055000	-2.241396000
1	3.083990000	0.996788000	-2.530921000
6	5.858708000	-0.539020000	-1.331392000
1	6.141878000	-1.156987000	0.710557000
1	5.266253000	0.153989000	-3.284912000
1	6.829503000	-0.898316000	-1.660875000
6	2.089776000	2.859260000	-0.755339000
6	1.216507000	3.381110000	-1.710291000
6	3.236736000	3.594617000	-0.424839000
6	1.475709000	4.608914000	-2.318148000
1	0.322858000	2.835786000	-1.988840000
6	3.494338000	4.821086000	-1.024414000
1	3.944111000	3.198520000	0.299116000
6	2.611769000	5.332308000	-1.975744000
1	0.782405000	4.995848000	-3.059290000
1	4.388034000	5.376778000	-0.755011000
1	2.812548000	6.289362000	-2.448550000
14	1.149584000	0.441562000	2.965250000
14	-1.835727000	-0.386043000	2.793300000
6	2.214374000	-1.008582000	3.490041000

1	3.133084000	-0.676495000	3.989192000
1	1.665425000	-1.649489000	4.190910000
1	2.489370000	-1.633662000	2.633926000
6	0.641697000	1.449703000	4.468247000
1	0.084575000	0.875507000	5.216286000
1	1.552225000	1.820025000	4.957657000
1	0.046165000	2.326677000	4.191140000
6	-1.755690000	-1.515236000	4.293211000
1	-1.275367000	-2.463710000	4.026998000
1	-1.199937000	-1.074561000	5.128922000
1	-2.764748000	-1.743603000	4.659480000
6	-2.612563000	1.256401000	3.255230000
1	-3.680805000	1.104388000	3.454467000
1	-2.173475000	1.669187000	4.169384000
1	-2.531698000	2.009933000	2.466304000
1	3.125124000	1.757602000	2.088510000
1	1.593219000	2.614694000	1.968047000
1	0.027070000	-1.203059000	1.845270000
1	0.227773000	-1.271138000	-0.306956000
6	0.410404000	-2.810518000	0.180990000
6	-0.527226000	-3.432143000	-0.845730000
1	-0.418546000	-3.005590000	-1.844986000
1	-0.291594000	-4.503390000	-0.899077000
1	-1.562233000	-3.329319000	-0.524024000
8	0.089272000	-2.860213000	1.398323000
6	1.872223000	-2.983766000	-0.180991000
6	2.369747000	-2.710434000	-1.456827000
6	2.699185000	-3.611053000	0.751112000
6	3.660116000	-3.089556000	-1.802487000
1	1.744627000	-2.188985000	-2.176503000
6	3.998495000	-3.980411000	0.410029000
1	2.293866000	-3.832429000	1.733594000
6	4.476466000	-3.732524000	-0.872305000
1	4.037686000	-2.871806000	-2.796844000
1	4.629961000	-4.476794000	1.142101000
1	5.486771000	-4.024159000	-1.145643000

TSA5-6

Doordinates (Angstroms)			
	X	Y	Z
25	0.005159000	-0.800511000	-0.065620000
7	-0.025552000	0.339180000	1.842604000
6	-0.068079000	-1.416116000	-1.722809000

8	-0.155175000	-1.828445000	-2.806776000
6	2.697847000	0.814482000	1.151685000
1	3.758474000	0.895111000	1.406751000
1	2.374315000	1.782036000	0.753587000
6	-2.711290000	-0.803158000	1.918302000
6	0.182363000	-2.395222000	0.691637000
8	0.290699000	-3.406969000	1.248552000
15	-2.292048000	-0.954827000	0.145969000
15	2.313170000	-0.402536000	-0.148400000
14	-1.490835000	0.366385000	2.784700000
14	1.532640000	0.512287000	2.609116000
6	-2.158343000	2.123500000	2.891587000
1	-3.149730000	2.171491000	3.360024000
1	-1.480932000	2.741343000	3.494960000
1	-2.220319000	2.595657000	1.904473000
6	-1.299489000	-0.316531000	4.531763000
1	-0.656274000	0.300289000	5.170221000
1	-2.282647000	-0.369196000	5.017961000
1	-0.888812000	-1.333080000	4.516733000
6	1.627480000	2.039271000	3.712366000
1	1.376830000	2.940861000	3.139502000
1	0.938418000	1.983308000	4.563574000
1	2.637275000	2.172323000	4.121873000
6	2.077297000	-1.005288000	3.578233000
1	3.145133000	-0.943720000	3.824334000
1	1.530859000	-1.099743000	4.523669000
1	1.922128000	-1.928063000	3.008875000
1	-3.771812000	-0.596448000	2.101879000
1	-2.510709000	-1.800167000	2.334574000
1	-0.070347000	1.140160000	0.831381000
6	-0.566785000	2.284129000	-1.104095000
6	-0.163945000	2.160632000	-2.569959000
1	-0.668036000	2.920870000	-3.177760000
1	0.919114000	2.276724000	-2.687267000
1	-0.441949000	1.172575000	-2.950561000
8	0.081420000	1.284258000	-0.360282000
1	-1.655084000	2.174319000	-1.038696000
6	-3.183272000	-2.478512000	-0.375014000
6	-2.506921000	-3.587815000	-0.884903000
6	-4.575848000	-2.543811000	-0.231173000
6	-3.204894000	-4.742018000	-1.238207000
1	-1.431078000	-3.560886000	-1.013794000
6	-5.271958000	-3.694408000	-0.579500000
1	-5.121209000	-1.684019000	0.149821000

6	-4.585494000	-4.798475000	-1.084475000
1	-2.664260000	-5.596145000	-1.635152000
1	-6.350883000	-3.730814000	-0.459679000
1	-5.128280000	-5.698739000	-1.357875000
6	-3.280704000	0.320141000	-0.720186000
6	-4.011619000	1.309488000	-0.060632000
6	-3.231759000	0.333171000	-2.120279000
6	-4.659284000	2.310922000	-0.784307000
1	-4.072600000	1.320664000	1.022233000
6	-3.879465000	1.328177000	-2.841297000
1	-2.670649000	-0.432477000	-2.649711000
6	-4.586510000	2.327972000	-2.173441000
1	-5.217331000	3.079374000	-0.256887000
1	-3.822379000	1.330941000	-3.925731000
1	-5.083307000	3.112999000	-2.735875000
6	3.399220000	-1.851730000	0.159521000
6	3.102936000	-3.039769000	-0.520291000
6	4.490066000	-1.836051000	1.032855000
6	3.879928000	-4.178445000	-0.338664000
1	2.245688000	-3.082679000	-1.187568000
6	5.259763000	-2.980413000	1.228295000
1	4.744974000	-0.934180000	1.579547000
6	4.959371000	-4.152597000	0.540985000
1	3.633410000	-5.090532000	-0.874320000
1	6.095575000	-2.953615000	1.921599000
1	5.558049000	-5.045477000	0.695676000
6	3.032644000	0.304821000	-1.687747000
6	3.738467000	1.510973000	-1.686724000
6	2.855677000	-0.364518000	-2.903232000
6	4.231412000	2.049342000	-2.873527000
1	3.911645000	2.042281000	-0.756514000
6	3.352003000	0.168232000	-4.088183000
1	2.324791000	-1.309703000	-2.934294000
6	4.034171000	1.382722000	-4.078653000
1	4.769587000	2.992650000	-2.852202000
1	3.198166000	-0.364087000	-5.022271000
1	4.414557000	1.803967000	-5.004597000
6	-0.214936000	3.642644000	-0.522085000
6	-1.212014000	4.514906000	-0.087669000
6	1.121407000	4.030837000	-0.386434000
6	-0.886251000	5.744762000	0.483785000
1	-2.255159000	4.224629000	-0.195655000
6	1.452735000	5.253384000	0.186959000
1	1.901745000	3.363434000	-0.741535000

6	0.447431000	6.114472000	0.628327000
1	-1.675514000	6.410949000	0.821363000
1	2.496425000	5.538580000	0.289657000
1	0.704221000	7.068431000	1.080134000

B1

Doordinates (Angstroms)			
	X	Y	Z
25	-0.604777000	-0.827538000	0.305568000
7	-1.562315000	0.730258000	-0.453725000
6	-0.232559000	-2.272551000	-0.633655000
8	-0.024075000	-3.195043000	-1.306374000
6	0.970657000	1.219813000	-1.774932000
1	1.742257000	1.962718000	-2.004125000
1	0.832765000	0.564491000	-2.644664000
6	-3.830949000	-0.305037000	1.018201000
6	0.143980000	-1.528611000	1.749163000
8	0.601522000	-1.966956000	2.724527000
15	-2.636783000	-1.678887000	0.955791000
15	1.355896000	0.167337000	-0.342910000
14	-3.296627000	0.847665000	-0.388013000
14	-0.730530000	1.956459000	-1.367221000
6	-4.146577000	0.284083000	-1.981464000
1	-5.184072000	-0.021220000	-1.793558000
1	-4.174516000	1.089137000	-2.724969000
1	-3.624520000	-0.562187000	-2.442764000
6	-3.938770000	2.578765000	0.010732000
1	-3.766276000	3.289920000	-0.806182000
1	-5.022187000	2.547615000	0.186642000
1	-3.466937000	2.983947000	0.913960000
6	-1.542095000	2.374782000	-3.022486000
1	-1.726237000	1.472797000	-3.618311000
1	-2.497770000	2.899624000	-2.904694000
1	-0.883863000	3.030227000	-3.608213000
6	-0.494964000	3.584478000	-0.442709000
1	0.177143000	4.249433000	-1.000923000
1	-1.447861000	4.112538000	-0.319240000
1	-0.063262000	3.437093000	0.552954000
1	-4.873504000	-0.641182000	0.975730000
1	-3.678028000	0.223804000	1.968456000
6	-2.806991000	-2.551577000	2.561034000
1	-3.849701000	-2.833279000	2.744138000
1	-2.188766000	-3.455606000	2.569339000
1	-2.469984000	-1.901587000	3.374593000

6	-3.393198000	-2.888255000	-0.198514000
1	-2.821018000	-3.821498000	-0.171884000
1	-4.433700000	-3.105180000	0.067548000
1	-3.358796000	-2.505469000	-1.222171000
6	2.082509000	1.338879000	0.870862000
6	3.307344000	1.970336000	0.627548000
6	1.388210000	1.634699000	2.046416000
6	3.821771000	2.886267000	1.538687000
1	3.866142000	1.739830000	-0.276287000
6	1.902829000	2.552097000	2.960230000
1	0.431614000	1.157747000	2.240742000
6	3.118837000	3.179124000	2.706723000
1	4.773214000	3.371196000	1.340242000
1	1.352646000	2.774298000	3.869950000
1	3.521121000	3.893967000	3.418798000
6	2.797802000	-0.863738000	-0.811588000
6	3.469147000	-0.688306000	-2.024050000
6	3.236651000	-1.860063000	0.069019000
6	4.560607000	-1.490681000	-2.350902000
1	3.143421000	0.076301000	-2.722807000
6	4.329441000	-2.656432000	-0.255040000
1	2.725160000	-2.015437000	1.014679000
6	4.993081000	-2.474196000	-1.467077000
1	5.070952000	-1.344950000	-3.298610000
1	4.660263000	-3.424011000	0.438393000
1	5.843300000	-3.100190000	-1.722239000

B2

Doordinates (Angstroms)			
	X	Y	Z
25	-0.567987000	-0.746012000	0.492938000
7	-1.674184000	0.856836000	-0.393384000
6	0.315230000	-2.029762000	1.348401000
8	0.859607000	-2.885645000	1.912953000
6	-3.824728000	-0.280343000	1.158891000
1	-4.849694000	-0.670176000	1.153575000
1	-3.690011000	0.302630000	2.080287000
6	0.836718000	1.287976000	-1.707630000
6	-0.653900000	-1.666154000	-1.029679000
8	-0.738033000	-2.226895000	-2.036454000
15	1.347679000	0.234838000	-0.318916000
15	-2.578941000	-1.606131000	1.175402000
14	-0.794889000	2.103833000	-1.153909000

14	-3.377062000	0.863472000	-0.300736000
6	-0.382014000	3.569746000	-0.031518000
1	0.320964000	4.267509000	-0.505240000
1	-1.293643000	4.132256000	0.209732000
1	0.062145000	3.244495000	0.917156000
6	-1.573342000	2.815022000	-2.726312000
1	-2.501436000	3.363436000	-2.523603000
1	-0.884989000	3.518305000	-3.213658000
1	-1.806246000	2.022697000	-3.448310000
6	-4.155121000	2.543954000	0.098001000
1	-3.724629000	2.976357000	1.009880000
1	-4.021377000	3.273672000	-0.710143000
1	-5.236406000	2.439546000	0.260536000
6	-4.245853000	0.222536000	-1.857002000
1	-5.307143000	0.000776000	-1.683511000
1	-4.195755000	0.973924000	-2.655730000
1	-3.766330000	-0.684770000	-2.244035000
1	1.610488000	1.965471000	-2.081078000
1	0.547585000	0.618971000	-2.527688000
6	-3.311816000	-2.931483000	0.142050000
1	-2.619950000	-3.777808000	0.081299000
1	-4.261853000	-3.278659000	0.562628000
1	-3.491142000	-2.564009000	-0.872150000
6	-2.666323000	-2.361058000	2.847377000
1	-3.696291000	-2.630434000	3.105944000
1	-2.044625000	-3.261825000	2.888605000
1	-2.288176000	-1.652920000	3.592383000
1	-0.324190000	0.523840000	1.734357000
1	-0.884845000	0.072323000	2.055980000
6	2.336449000	1.314088000	0.793028000
6	3.167616000	2.321897000	0.291127000
6	2.302211000	1.098284000	2.173971000
6	3.922455000	3.112034000	1.151431000
1	3.234028000	2.495482000	-0.778438000
6	3.064661000	1.882885000	3.036475000
1	1.680157000	0.307348000	2.583185000
6	3.869805000	2.896588000	2.527097000
1	4.555900000	3.896009000	0.746870000
1	3.024523000	1.701753000	4.106600000
1	4.459178000	3.514905000	3.197743000
6	2.640124000	-0.915080000	-0.941569000
6	2.853643000	-1.120690000	-2.305986000
6	3.397477000	-1.648764000	-0.020412000
6	3.801378000	-2.044756000	-2.742125000

1	2.285822000	-0.559841000	-3.041505000
6	4.344106000	-2.568709000	-0.455539000
1	3.252106000	-1.498849000	1.045802000
6	4.546925000	-2.771122000	-1.819515000
1	3.955708000	-2.193826000	-3.806850000
1	4.923803000	-3.129490000	0.271844000
1	5.284726000	-3.491736000	-2.159844000

B3

Doordinates (Angstroms)			
	X	Y	Z
25	-0.567546000	-0.933172000	0.397692000
7	-1.503787000	1.073358000	-0.247702000
6	0.247941000	-2.309122000	1.133253000
8	0.785163000	-3.201263000	1.650267000
6	-3.620320000	-0.043377000	1.348754000
1	-4.677583000	-0.301178000	1.486877000
1	-3.307910000	0.557288000	2.213629000
6	1.016344000	0.950286000	-1.782356000
6	-0.808772000	-1.737924000	-1.162458000
8	-0.997757000	-2.308987000	-2.164834000
15	1.370491000	0.075013000	-0.201258000
15	-2.527160000	-1.522279000	1.286301000
14	-0.595733000	1.904914000	-1.544616000
14	-3.282282000	0.953786000	-0.212935000
6	-0.249658000	3.660103000	-0.972188000
1	0.374566000	4.200168000	-1.694460000
1	-1.182582000	4.224322000	-0.849714000
1	0.278028000	3.671841000	-0.010874000
6	-1.541684000	1.908259000	-3.162937000
1	-2.473014000	2.483687000	-3.117739000
1	-0.911021000	2.370347000	-3.933440000
1	-1.776584000	0.893328000	-3.501201000
6	-4.052594000	2.665681000	-0.088777000
1	-3.648062000	3.222414000	0.765375000
1	-3.868117000	3.259299000	-0.992717000
1	-5.139848000	2.602052000	0.043894000
6	-3.934166000	0.063172000	-1.731199000
1	-4.902901000	-0.395614000	-1.496500000
1	-4.097768000	0.751155000	-2.567081000
1	-3.262616000	-0.730616000	-2.073383000
1	1.836153000	1.587768000	-2.131280000
1	0.852694000	0.178130000	-2.543990000

1	-1.213350000	1.483847000	0.642451000
1	-0.520756000	-0.236329000	1.856802000
6	-3.580829000	-2.789376000	0.467771000
1	-3.036026000	-3.740067000	0.458263000
1	-4.536584000	-2.934861000	0.984326000
1	-3.776842000	-2.515060000	-0.572390000
6	-2.529743000	-2.158846000	3.007406000
1	-3.548009000	-2.301023000	3.386337000
1	-2.002872000	-3.118418000	3.043551000
1	-1.992148000	-1.456844000	3.650750000
6	2.101550000	1.442854000	0.798319000
6	3.092221000	2.282266000	0.267106000
6	1.644218000	1.686317000	2.094446000
6	3.594986000	3.345689000	1.007907000
1	3.487039000	2.099136000	-0.728637000
6	2.147477000	2.752454000	2.839430000
1	0.881385000	1.034083000	2.509148000
6	3.118047000	3.587165000	2.296276000
1	4.359806000	3.988183000	0.581150000
1	1.777182000	2.927073000	3.845632000
1	3.508037000	4.420791000	2.873251000
6	2.821946000	-0.988927000	-0.577491000
6	2.676629000	-1.972899000	-1.563671000
6	4.027544000	-0.911598000	0.123917000
6	3.722014000	-2.839991000	-1.859128000
1	1.735257000	-2.073924000	-2.096281000
6	5.072826000	-1.786709000	-0.167443000
1	4.157326000	-0.169378000	0.905270000
6	4.925337000	-2.748290000	-1.161704000
1	3.593431000	-3.595752000	-2.628632000
1	6.004062000	-1.713972000	0.387117000
1	5.739918000	-3.430021000	-1.388681000

B4r

Doordinates (Angstroms)			
	X	Y	Z
25	-1.739919000	-0.469672000	-0.609186000
7	-0.312595000	-1.551787000	0.819320000
6	-2.569999000	0.403674000	-1.885630000
8	-3.080318000	0.964836000	-2.771095000
6	-0.575457000	-3.537166000	-1.214420000
1	-0.765666000	-4.566504000	-1.541148000
1	0.389380000	-3.218453000	-1.630194000
6	-0.698454000	1.028093000	2.193770000

6	-3.191635000	-0.732147000	0.382465000
8	-4.180646000	-0.913200000	0.977845000
15	-1.016183000	1.394166000	0.418536000
15	-1.849592000	-2.354419000	-1.810225000
14	-0.139168000	-0.766102000	2.404554000
14	-0.479133000	-3.317547000	0.651770000
6	1.651143000	-0.853360000	2.972592000
1	1.801145000	-0.279511000	3.895757000
1	1.948735000	-1.889622000	3.172360000
1	2.333952000	-0.462755000	2.210851000
6	-1.259468000	-1.569238000	3.676323000
1	-0.931181000	-2.573625000	3.965473000
1	-1.264599000	-0.956180000	4.587096000
1	-2.293401000	-1.633284000	3.318939000
6	1.019512000	-4.206702000	1.357618000
1	1.945313000	-3.789633000	0.946506000
1	1.063327000	-4.119614000	2.450414000
1	0.991158000	-5.277604000	1.118848000
6	-2.036418000	-3.964480000	1.481418000
1	-2.333160000	-4.908595000	1.007049000
1	-1.876307000	-4.174142000	2.544019000
1	-2.876846000	-3.268817000	1.400821000
1	-0.056719000	1.767488000	2.686563000
1	-1.686698000	1.105407000	2.666163000
1	0.528696000	-1.327135000	0.273495000
1	-0.441945000	-0.332112000	-1.544517000
6	-3.390915000	-3.361067000	-1.816852000
1	-4.196401000	-2.763973000	-2.258796000
1	-3.280429000	-4.287501000	-2.392291000
1	-3.688426000	-3.610266000	-0.794754000
6	-1.535566000	-2.237932000	-3.615645000
1	-1.541928000	-3.225813000	-4.089556000
1	-2.304167000	-1.615330000	-4.085348000
1	-0.566696000	-1.759224000	-3.782691000
6	6.989921000	0.490414000	0.378274000
6	6.516033000	0.937137000	-0.853553000
6	5.266330000	0.528189000	-1.307483000
6	4.480985000	-0.331136000	-0.531856000
6	4.968613000	-0.781785000	0.699818000
6	6.215282000	-0.370954000	1.154385000
1	7.963960000	0.813788000	0.734197000
1	7.119617000	1.605652000	-1.459961000
1	4.900683000	0.893794000	-2.261579000
1	4.353717000	-1.452132000	1.291832000

1	6.586294000	-0.722767000	2.112443000
6	3.114912000	-0.761977000	-0.961127000
8	2.458783000	-1.499463000	-0.236636000
6	2.572746000	-0.284203000	-2.278784000
1	2.568555000	0.809575000	-2.321611000
1	3.197871000	-0.650863000	-3.101986000
1	1.547639000	-0.639003000	-2.395978000
6	0.552458000	2.142743000	-0.187586000
6	1.750546000	2.116932000	0.528267000
6	0.535444000	2.763535000	-1.443891000
6	2.905910000	2.702604000	0.008234000
1	1.800654000	1.644961000	1.504001000
6	1.679379000	3.363641000	-1.955735000
1	-0.384804000	2.780880000	-2.022044000
6	2.871728000	3.334285000	-1.229708000
1	3.831060000	2.662041000	0.575666000
1	1.642602000	3.851972000	-2.925312000
1	3.768500000	3.797511000	-1.631347000
6	-2.077527000	2.897058000	0.534933000
6	-3.452112000	2.788220000	0.312574000
6	-1.550425000	4.139120000	0.910667000
6	-4.285001000	3.895848000	0.460105000
1	-3.876655000	1.833617000	0.020507000
6	-2.380368000	5.245626000	1.055539000
1	-0.482970000	4.245853000	1.084151000
6	-3.751045000	5.125998000	0.829937000
1	-5.351179000	3.793365000	0.280129000
1	-1.956732000	6.203495000	1.343957000
1	-4.398858000	5.991039000	0.940270000

B4s

Doordinates (Angstroms)			
	X	Y	Z
25	-0.228929000	-0.727231000	-0.915074000
7	0.487937000	-1.411971000	1.159638000
6	-0.560128000	0.108736000	-2.421826000
8	-0.729302000	0.705905000	-3.408881000
6	2.887469000	-1.840997000	-0.332232000
1	3.715723000	-2.477705000	-0.665855000
1	3.312011000	-0.921976000	0.090167000
6	-2.395812000	-0.920270000	1.596299000
6	-1.057900000	-2.240077000	-1.335513000
8	-1.600517000	-3.226028000	-1.647815000

15	-2.013799000	0.138301000	0.143098000
15	1.775524000	-1.358513000	-1.709845000
14	-0.797106000	-1.550094000	2.383057000
14	1.811410000	-2.601240000	1.010065000
6	-0.307864000	-0.508902000	3.866965000
1	-1.086113000	-0.521531000	4.640116000
1	0.619315000	-0.883035000	4.317051000
1	-0.134537000	0.534906000	3.582350000
6	-1.081117000	-3.332989000	2.894284000
1	-0.209962000	-3.785385000	3.381272000
1	-1.909145000	-3.366319000	3.614288000
1	-1.365353000	-3.960227000	2.041988000
6	2.774086000	-2.759323000	2.617001000
1	3.166849000	-1.786021000	2.929395000
1	2.153684000	-3.156520000	3.429773000
1	3.622834000	-3.444291000	2.493076000
6	1.172677000	-4.294408000	0.504824000
1	1.995122000	-4.865186000	0.054167000
1	0.818557000	-4.869424000	1.366823000
1	0.360430000	-4.248123000	-0.226476000
1	-3.103203000	-0.475915000	2.306037000
1	-2.899385000	-1.795481000	1.164039000
1	0.957825000	-0.516885000	1.323094000
1	0.590470000	0.613446000	-0.531597000
6	1.845900000	-2.819141000	-2.826628000
1	1.221294000	-2.622304000	-3.704963000
1	2.867554000	-3.036655000	-3.159242000
1	1.441342000	-3.702220000	-2.323472000
6	2.743008000	-0.143731000	-2.684664000
1	3.766093000	-0.492793000	-2.861274000
1	2.253408000	0.022548000	-3.650412000
1	2.763907000	0.807023000	-2.147720000
6	4.964257000	2.818389000	-1.943994000
6	3.735510000	3.438737000	-1.726392000
6	2.970141000	3.097524000	-0.615644000
6	3.423164000	2.118293000	0.274105000
6	4.654637000	1.495985000	0.046193000
6	5.426109000	1.849666000	-1.054071000
1	5.561564000	3.088971000	-2.809933000
1	3.370413000	4.184561000	-2.425732000
1	2.005348000	3.571258000	-0.462569000
1	4.998538000	0.741079000	0.746399000
1	6.384987000	1.368213000	-1.221225000
6	2.609304000	1.696175000	1.453231000

8	2.820121000	0.620561000	1.997593000
6	1.523707000	2.610398000	1.950346000
1	1.829634000	3.660449000	1.941340000
1	0.653634000	2.506286000	1.292381000
1	1.239062000	2.316039000	2.961924000
6	-1.878265000	1.850063000	0.802183000
6	-2.085432000	2.202390000	2.136567000
6	-1.535219000	2.855306000	-0.113391000
6	-1.941207000	3.527106000	2.553797000
1	-2.353284000	1.449081000	2.870498000
6	-1.409866000	4.176939000	0.296566000
1	-1.352567000	2.594653000	-1.152412000
6	-1.605480000	4.515912000	1.636498000
1	-2.095555000	3.780278000	3.598884000
1	-1.148938000	4.943108000	-0.427897000
1	-1.495623000	5.547063000	1.959778000
6	-3.656497000	0.247542000	-0.689609000
6	-4.733672000	0.891563000	-0.067313000
6	-3.860068000	-0.353629000	-1.933267000
6	-5.983956000	0.929411000	-0.673477000
1	-4.593072000	1.376321000	0.895517000
6	-5.113067000	-0.315276000	-2.543099000
1	-3.038213000	-0.854959000	-2.432446000
6	-6.176178000	0.324763000	-1.915286000
1	-6.809831000	1.433262000	-0.179147000
1	-5.253186000	-0.786871000	-3.511478000
1	-7.151952000	0.357257000	-2.391514000

TSB2-3

Doordinates (Angstroms)			
	X	Y	Z
25	-0.571384000	-0.812197000	0.438650000
7	-1.652061000	0.991363000	-0.283749000
6	0.304223000	-2.001279000	1.414254000
8	0.857359000	-2.767145000	2.088334000
6	-3.802695000	-0.251720000	1.147216000
1	-4.835557000	-0.619837000	1.152989000
1	-3.648133000	0.328196000	2.067173000
6	0.849305000	1.235659000	-1.721921000
6	-0.595583000	-1.832268000	-1.022703000
8	-0.631051000	-2.487868000	-1.977551000
15	1.339569000	0.192152000	-0.310572000
15	-2.583979000	-1.613303000	1.153039000
14	-0.741040000	2.137855000	-1.200063000

14	-3.374016000	0.875489000	-0.318858000
6	-0.297881000	3.668399000	-0.193356000
1	0.399320000	4.325775000	-0.728311000
1	-1.200713000	4.251467000	0.030914000
1	0.165726000	3.399626000	0.763113000
6	-1.591550000	2.682035000	-2.794349000
1	-2.508220000	3.254733000	-2.610868000
1	-0.922247000	3.323909000	-3.382140000
1	-1.852673000	1.819168000	-3.419062000
6	-4.258045000	2.521542000	-0.046773000
1	-3.925753000	2.997171000	0.884141000
1	-4.080733000	3.231452000	-0.863591000
1	-5.343671000	2.373854000	0.023523000
6	-4.020194000	0.109981000	-1.921184000
1	-5.016774000	-0.332450000	-1.794695000
1	-4.098671000	0.866501000	-2.711578000
1	-3.344173000	-0.671717000	-2.288048000
1	1.643998000	1.884491000	-2.104917000
1	0.545769000	0.556622000	-2.529166000
6	-3.396807000	-2.931404000	0.169872000
1	-2.752040000	-3.815770000	0.134515000
1	-4.360881000	-3.214114000	0.606969000
1	-3.561816000	-2.591350000	-0.856553000
6	-2.664207000	-2.316923000	2.845830000
1	-3.695843000	-2.550905000	3.130795000
1	-2.065886000	-3.232546000	2.901018000
1	-2.250535000	-1.596985000	3.559307000
1	-1.101759000	0.741145000	1.050497000
1	-0.685564000	0.279893000	1.776299000
6	2.255673000	1.320556000	0.811684000
6	3.177971000	2.250331000	0.316411000
6	2.061200000	1.232047000	2.192031000
6	3.870050000	3.089679000	1.182024000
1	3.363410000	2.320544000	-0.751717000
6	2.761294000	2.066658000	3.061334000
1	1.354075000	0.509543000	2.587224000
6	3.660683000	3.000669000	2.557575000
1	4.576894000	3.812329000	0.784693000
1	2.598991000	1.985908000	4.132200000
1	4.202491000	3.656007000	3.233387000
6	2.686587000	-0.908619000	-0.895529000
6	2.927970000	-1.135283000	-2.251723000
6	3.455548000	-1.592851000	0.053872000
6	3.917111000	-2.031252000	-2.653202000

1	2.348817000	-0.614249000	-3.007746000
6	4.443037000	-2.485032000	-0.347165000
1	3.285337000	-1.425563000	1.114165000
6	4.675160000	-2.708097000	-1.703314000
1	4.093189000	-2.197818000	-3.712003000
1	5.031441000	-3.008555000	0.400756000
1	5.444565000	-3.407509000	-2.016970000

TSB4-5R

Doordinates (Angstroms)			
	X	Y	Z
25	-0.903456000	0.316471000	-0.832292000
7	-1.835998000	-0.239031000	1.140958000
6	-0.065469000	0.343179000	-2.382224000
8	0.473613000	0.286974000	-3.411788000
6	-3.885178000	-1.289756000	-0.649024000
1	-4.939463000	-1.273101000	-0.951720000
1	-3.581537000	-2.339537000	-0.587917000
6	0.207341000	1.710322000	1.963673000
6	-1.526110000	1.977103000	-0.884165000
8	-1.951031000	3.059748000	-0.936808000
15	0.891576000	1.132423000	0.359278000
15	-2.811617000	-0.419629000	-1.856429000
14	-1.147943000	0.557437000	2.586359000
14	-3.597566000	-0.479236000	1.028763000
6	-0.524214000	-0.772562000	3.750251000
1	0.028454000	-0.346064000	4.596416000
1	-1.373768000	-1.332756000	4.161160000
1	0.111709000	-1.491998000	3.225234000
6	-2.371285000	1.647195000	3.508279000
1	-3.214261000	1.095307000	3.938599000
1	-1.834530000	2.114867000	4.344826000
1	-2.768086000	2.457366000	2.887712000
6	-4.199010000	-1.626794000	2.389794000
1	-3.629832000	-2.564154000	2.389202000
1	-4.098671000	-1.175457000	3.384235000
1	-5.258115000	-1.877362000	2.249960000
6	-4.529487000	1.154390000	1.077195000
1	-5.462270000	1.055951000	0.507852000
1	-4.805491000	1.437933000	2.097603000
1	-3.959054000	1.980935000	0.640676000
1	0.977029000	1.935575000	2.709881000
1	-0.288150000	2.661709000	1.729655000

1	-1.402853000	-1.188021000	1.149250000
1	-0.360431000	-1.294688000	-0.807052000
6	-3.937648000	0.876765000	-2.518600000
1	-3.414773000	1.448069000	-3.293120000
1	-4.837078000	0.432191000	-2.959239000
1	-4.238057000	1.575273000	-1.733710000
6	-2.739477000	-1.513593000	-3.329624000
1	-3.745956000	-1.813516000	-3.642109000
1	-2.260233000	-0.976343000	-4.155072000
1	-2.150692000	-2.408171000	-3.122388000
6	-0.058680000	-2.743696000	-0.088399000
8	-0.391437000	-2.627763000	1.115525000
6	2.413883000	0.215004000	0.827200000
6	2.696803000	-0.183938000	2.134293000
6	3.379988000	0.009944000	-0.165167000
6	3.932550000	-0.746664000	2.451643000
1	1.964171000	-0.051202000	2.922595000
6	4.615517000	-0.536753000	0.153554000
1	3.171599000	0.300605000	-1.191562000
6	4.898952000	-0.909565000	1.466780000
1	4.137737000	-1.045726000	3.475689000
1	5.357028000	-0.679777000	-0.626430000
1	5.866233000	-1.336995000	1.714985000
6	1.708054000	2.672128000	-0.261801000
6	2.641552000	3.328493000	0.552991000
6	1.420441000	3.213938000	-1.514764000
6	3.258665000	4.498777000	0.130557000
1	2.898738000	2.912214000	1.523625000
6	2.044212000	4.385272000	-1.944388000
1	0.707015000	2.727949000	-2.169438000
6	2.960485000	5.031591000	-1.123484000
1	3.977050000	4.994177000	0.777500000
1	1.808052000	4.789870000	-2.924267000
1	3.444305000	5.944847000	-1.457683000
6	1.405511000	-2.869579000	-0.463001000
6	1.860849000	-2.680149000	-1.770455000
6	2.283093000	-3.374429000	0.495374000
6	3.163558000	-3.015580000	-2.120009000
1	1.192246000	-2.259842000	-2.516335000
6	3.585461000	-3.720487000	0.144132000
1	1.924749000	-3.511442000	1.510691000
6	4.026084000	-3.552536000	-1.165215000
1	3.505295000	-2.860399000	-3.139746000
1	4.258951000	-4.118854000	0.897772000

1	5.042123000	-3.824167000	-1.438312000
6	-0.943347000	-3.591325000	-0.996307000
1	-0.722022000	-3.456166000	-2.055920000
1	-0.741030000	-4.640364000	-0.742930000
1	-1.997744000	-3.395878000	-0.803983000

TSB4-5S

Doordinates (Angstroms)			
	X	Y	Z
25	0.152512000	-0.360402000	-0.809162000
7	0.701289000	-1.558766000	1.001259000
6	-0.060751000	0.889961000	-2.035171000
8	-0.150133000	1.747038000	-2.816713000
6	3.264562000	-1.548512000	-0.302897000
1	4.158076000	-2.065750000	-0.672225000
1	3.575035000	-0.714648000	0.339541000
6	-2.247400000	-1.527633000	1.163988000
6	-0.510583000	-1.710049000	-1.747945000
8	-0.933375000	-2.602345000	-2.364495000
15	-1.932205000	-0.075516000	0.086914000
15	2.246811000	-0.839168000	-1.643490000
14	-0.658210000	-2.071458000	2.030225000
14	2.125580000	-2.607272000	0.758436000
6	-0.437150000	-1.267404000	3.710795000
1	0.460911000	-1.668389000	4.197026000
1	-0.299177000	-0.183963000	3.636786000
1	-1.289146000	-1.465764000	4.372628000
6	-0.774241000	-3.935381000	2.231744000
1	0.102246000	-4.372786000	2.722267000
1	-1.645455000	-4.166836000	2.858681000
1	-0.921535000	-4.443874000	1.272713000
6	2.956333000	-2.956199000	2.407136000
1	3.158486000	-2.011927000	2.925755000
1	2.339973000	-3.583256000	3.062646000
1	3.913889000	-3.473186000	2.265936000
6	1.662376000	-4.213883000	-0.103621000
1	2.522713000	-4.594256000	-0.668437000
1	1.380863000	-4.989079000	0.616911000
1	0.830953000	-4.091678000	-0.805743000
1	-3.103069000	-1.408107000	1.837798000
1	-2.510210000	-2.335791000	0.468246000
1	1.133184000	-0.745763000	1.492818000
1	0.848012000	0.903653000	0.131330000

6	2.318365000	-2.130027000	-2.954398000
1	1.812341000	-1.760068000	-3.852655000
1	3.357343000	-2.365792000	-3.211232000
1	1.816560000	-3.048496000	-2.642198000
6	3.300260000	0.433494000	-2.438816000
1	4.208055000	-0.024641000	-2.846826000
1	2.750938000	0.916821000	-3.253148000
1	3.587938000	1.196834000	-1.717313000
6	4.560262000	3.779596000	-1.019762000
6	3.191680000	3.936874000	-1.243106000
6	2.274597000	3.197799000	-0.505470000
6	2.712407000	2.286595000	0.459316000
6	4.080954000	2.137603000	0.682333000
6	5.002890000	2.879996000	-0.053930000
1	5.275896000	4.356447000	-1.598709000
1	2.840476000	4.630928000	-2.001306000
1	1.212008000	3.302600000	-0.704293000
1	4.408650000	1.433459000	1.440622000
1	6.066709000	2.753644000	0.127101000
6	1.751747000	1.501313000	1.332726000
8	2.198980000	0.526687000	1.994851000
6	0.673608000	2.355151000	1.978500000
1	1.169699000	2.965026000	2.745322000
1	0.164989000	3.022563000	1.282792000
1	-0.065897000	1.722514000	2.467950000
6	-2.373294000	1.392785000	1.093708000
6	-2.684965000	1.340763000	2.452693000
6	-2.378821000	2.634061000	0.445480000
6	-2.977717000	2.508531000	3.156898000
1	-2.686471000	0.394092000	2.983309000
6	-2.683008000	3.796154000	1.143203000
1	-2.136895000	2.692467000	-0.613134000
6	-2.975368000	3.736887000	2.505815000
1	-3.205793000	2.452577000	4.217456000
1	-2.682974000	4.751531000	0.626653000
1	-3.202553000	4.646368000	3.054233000
6	-3.399946000	-0.085995000	-1.034076000
6	-4.687147000	-0.080970000	-0.479591000
6	-3.268981000	-0.095517000	-2.423115000
6	-5.812578000	-0.098475000	-1.293992000
1	-4.812087000	-0.049065000	0.599818000
6	-4.397522000	-0.108027000	-3.242780000
1	-2.285800000	-0.090890000	-2.878564000
6	-5.669072000	-0.112997000	-2.681247000

1	-6.802410000	-0.095333000	-0.846924000
1	-4.275479000	-0.114464000	-4.321934000
1	-6.547865000	-0.123822000	-3.319717000

D1

Doordinates (Angstroms)			
	X	Y	Z

25	-0.332750000	-0.320230000	0.909078000
7	-1.306308000	1.142967000	-0.160357000
6	0.976083000	0.626003000	-2.033394000
1	1.645537000	1.319721000	-2.554178000
1	0.942616000	-0.313246000	-2.599626000
6	-3.680951000	0.044390000	1.271505000
6	0.530150000	-1.193509000	2.165265000
8	1.049728000	-1.773702000	3.043471000
15	-2.160025000	-0.196587000	2.261237000
15	1.517573000	0.230925000	-0.326894000
14	-3.031195000	0.869030000	-0.321000000
14	-0.809722000	1.273132000	-1.835414000
6	-4.106292000	2.403116000	-0.596730000
1	-3.894446000	2.909505000	-1.545216000
1	-5.171393000	2.136514000	-0.598297000
1	-3.948373000	3.131242000	0.210606000
6	-0.852141000	3.006969000	-2.583256000
1	-0.603413000	2.991187000	-3.651938000
1	-1.831935000	3.484822000	-2.473991000
1	-0.114435000	3.643755000	-2.076832000
1	-4.123662000	-0.933947000	1.051892000
1	-4.437926000	0.641212000	1.795765000
6	-2.032166000	1.382071000	3.196234000
1	-2.920489000	1.569621000	3.810639000
1	-1.149524000	1.353653000	3.844768000
1	-1.903315000	2.203387000	2.484814000
6	-2.611730000	-1.369172000	3.600892000
1	-1.776405000	-1.464211000	4.302729000
1	-3.495915000	-1.020884000	4.146180000
1	-2.821347000	-2.359087000	3.186347000
15	-0.839239000	-2.194148000	-0.221525000
6	-1.655008000	-1.979168000	-1.884073000
1	-0.880750000	-2.133083000	-2.649193000
1	-2.373631000	-2.798386000	-2.025483000
14	-2.502595000	-0.298744000	-2.282108000
6	0.514891000	-3.370083000	-0.644987000

1	1.257612000	-2.880415000	-1.281702000
1	1.024465000	-3.690337000	0.269774000
1	0.130003000	-4.253696000	-1.167128000
6	-1.999863000	-3.373952000	0.591853000
1	-2.981772000	-2.911448000	0.733386000
1	-2.129453000	-4.286975000	-0.000421000
1	-1.598526000	-3.646513000	1.573652000
6	-3.554621000	-0.561339000	-3.837020000
1	-2.943315000	-0.917656000	-4.675410000
1	-4.343459000	-1.304178000	-3.663572000
1	-4.038977000	0.370500000	-4.150448000
6	2.266589000	1.820006000	0.237645000
6	3.631419000	2.099787000	0.113278000
6	1.424176000	2.790740000	0.794350000
6	4.143267000	3.323394000	0.537598000
1	4.304183000	1.360121000	-0.310789000
6	1.937469000	4.016665000	1.210614000
1	0.360006000	2.583714000	0.881191000
6	3.298092000	4.284823000	1.086358000
1	5.206121000	3.524639000	0.437145000
1	1.270188000	4.761587000	1.635164000
1	3.700088000	5.238024000	1.418109000
6	2.990063000	-0.850125000	-0.514017000
6	3.596522000	-1.090322000	-1.751045000
6	3.520056000	-1.465666000	0.626383000
6	4.697337000	-1.939692000	-1.848355000
1	3.214060000	-0.614620000	-2.649088000
6	4.623548000	-2.306868000	0.530643000
1	3.064702000	-1.292573000	1.595728000
6	5.212577000	-2.549693000	-0.708646000
1	5.155297000	-2.118573000	-2.817047000
1	5.021103000	-2.776700000	1.425524000
1	6.069336000	-3.213046000	-0.784777000

D2

Doordinates (Angstroms)			
	X	Y	Z
25	-0.300590000	-0.512888000	0.948631000
7	-1.320887000	1.200349000	0.093418000
6	0.936604000	0.947842000	-1.835927000
1	1.634491000	1.644733000	-2.311556000
1	0.818900000	0.099794000	-2.522258000
6	-3.696731000	-0.257821000	1.138437000

6	0.435255000	-1.866432000	1.797777000
8	0.860070000	-2.783492000	2.390367000
15	-2.242425000	-0.662884000	2.173988000
15	1.533574000	0.239296000	-0.258869000
14	-3.042390000	1.041279000	-0.100121000
14	-0.794920000	1.683677000	-1.485671000
6	-4.060805000	2.611718000	0.173846000
1	-3.739450000	3.425370000	-0.487026000
1	-5.129348000	2.436298000	-0.006841000
1	-3.949081000	2.964427000	1.208128000
6	-0.721978000	3.543476000	-1.824865000
1	-0.237803000	3.766182000	-2.784568000
1	-1.726885000	3.981217000	-1.854357000
1	-0.166795000	4.060353000	-1.031427000
1	-4.016851000	-1.160533000	0.606229000
1	-4.546687000	0.092469000	1.737336000
6	-2.323860000	0.652361000	3.458053000
1	-3.304590000	0.683777000	3.945881000
1	-1.556105000	0.477377000	4.219198000
1	-2.123047000	1.621899000	2.990756000
6	-2.733783000	-2.132077000	3.163716000
1	-1.963647000	-2.343105000	3.913589000
1	-3.688387000	-1.965599000	3.675344000
1	-2.827756000	-3.013810000	2.524126000
15	-0.975196000	-1.957590000	-0.735886000
6	-1.899725000	-1.371921000	-2.248758000
1	-1.221280000	-1.485079000	-3.106263000
1	-2.720698000	-2.078719000	-2.432990000
14	-2.589923000	0.424396000	-2.309286000
6	0.372202000	-2.942334000	-1.520355000
1	1.074292000	-2.291643000	-2.049736000
1	0.933782000	-3.477718000	-0.748315000
1	-0.034880000	-3.669039000	-2.232765000
6	-2.040160000	-3.363007000	-0.194562000
1	-3.015113000	-3.003225000	0.146062000
1	-2.202017000	-4.077373000	-1.009680000
1	-1.554068000	-3.883789000	0.637091000
1	0.307428000	0.390217000	2.386641000
6	-3.620037000	0.537675000	-3.898802000
1	-3.004948000	0.333182000	-4.784304000
1	-4.440081000	-0.191474000	-3.890761000
1	-4.060403000	1.533792000	-4.021634000
1	0.041077000	0.962504000	1.922704000
6	2.404512000	1.627465000	0.584037000

6	2.502237000	2.916367000	0.058137000
6	2.985469000	1.366135000	1.831967000
6	3.162811000	3.923255000	0.761817000
1	2.060478000	3.155929000	-0.903218000
6	3.653466000	2.365304000	2.529358000
1	2.908729000	0.370517000	2.264177000
6	3.742049000	3.651005000	1.995769000
1	3.224105000	4.921226000	0.337237000
1	4.103117000	2.143061000	3.492884000
1	4.258762000	4.434816000	2.542034000
6	2.987747000	-0.789986000	-0.738251000
6	3.747621000	-0.491283000	-1.874511000
6	3.365916000	-1.876916000	0.055089000
6	4.851935000	-1.266754000	-2.215070000
1	3.479686000	0.353681000	-2.502319000
6	4.474824000	-2.650197000	-0.280599000
1	2.786719000	-2.132162000	0.935634000
6	5.217910000	-2.349438000	-1.418519000
1	5.428114000	-1.023367000	-3.103409000
1	4.752330000	-3.493002000	0.346165000
1	6.079426000	-2.955353000	-1.684553000

D3

	Doordinates (Angstroms)		
	X	Y	Z
25	-0.311187000	-0.652537000	0.826563000
7	-1.272302000	1.349398000	0.191645000
6	0.974445000	0.988494000	-1.799134000
1	1.684696000	1.701018000	-2.232774000
1	0.868973000	0.168750000	-2.520873000
6	-3.636804000	-0.180112000	1.324009000
6	0.416927000	-2.023811000	1.608436000
8	0.870129000	-2.929123000	2.208030000
15	-2.102601000	-0.758975000	2.180349000
15	1.511038000	0.190756000	-0.222601000
14	-3.040975000	1.051268000	0.018991000
14	-0.740731000	1.727667000	-1.482080000
6	-4.031491000	2.649054000	0.182173000
1	-3.716222000	3.411903000	-0.538664000
1	-5.101163000	2.462457000	0.024601000
1	-3.915921000	3.074729000	1.187653000
6	-0.724151000	3.583297000	-1.813500000

1	-0.317405000	3.801178000	-2.808630000
1	-1.728234000	4.018872000	-1.760595000
1	-0.099936000	4.104345000	-1.076680000
1	-4.104623000	-1.038975000	0.828221000
1	-4.377097000	0.247520000	2.012589000
6	-2.064533000	0.415130000	3.600225000
1	-3.001293000	0.408409000	4.170913000
1	-1.232947000	0.147279000	4.259117000
1	-1.874086000	1.429486000	3.233785000
6	-2.643652000	-2.280989000	3.064209000
1	-1.828328000	-2.628520000	3.707762000
1	-3.527761000	-2.092162000	3.683713000
1	-2.873693000	-3.079120000	2.353528000
15	-1.055178000	-1.955377000	-0.875030000
6	-1.940223000	-1.319994000	-2.408739000
1	-1.225512000	-1.319900000	-3.243267000
1	-2.741669000	-2.013683000	-2.693781000
14	-2.570002000	0.453736000	-2.195499000
6	0.226240000	-3.007969000	-1.689659000
1	0.998971000	-2.382410000	-2.147792000
1	0.713509000	-3.631378000	-0.932995000
1	-0.207722000	-3.658647000	-2.458198000
6	-2.230397000	-3.304114000	-0.407464000
1	-3.188967000	-2.878375000	-0.093293000
1	-2.412916000	-3.997631000	-1.236900000
1	-1.809069000	-3.863651000	0.433994000
1	0.235157000	0.196638000	2.059000000
1	-0.921322000	1.917018000	0.960461000
6	-3.699786000	1.024974000	-3.596841000
1	-3.208845000	0.915925000	-4.570954000
1	-4.628016000	0.442049000	-3.625479000
1	-3.971251000	2.079734000	-3.473963000
6	2.350165000	1.577391000	0.670758000
6	2.512179000	2.865593000	0.157968000
6	2.849893000	1.301483000	1.950758000
6	3.149064000	3.858835000	0.905049000
1	2.145897000	3.119592000	-0.831663000
6	3.501984000	2.281710000	2.687307000
1	2.704785000	0.311710000	2.375630000
6	3.648697000	3.569185000	2.168359000
1	3.256242000	4.857000000	0.489194000
1	3.887747000	2.045643000	3.675040000
1	4.148759000	4.339083000	2.749195000
6	3.012057000	-0.752990000	-0.746294000

6	3.935699000	-0.214839000	-1.651129000
6	3.259911000	-2.017934000	-0.209539000
6	5.069830000	-0.930254000	-2.019665000
1	3.775802000	0.776456000	-2.067189000
6	4.399613000	-2.734146000	-0.571853000
1	2.560649000	-2.448514000	0.497363000
6	5.304233000	-2.194479000	-1.480080000
1	5.775564000	-0.499869000	-2.724826000
1	4.575579000	-3.715695000	-0.141012000
1	6.192064000	-2.752194000	-1.764755000

D4R

Doordinates (Angstroms)			
	X	Y	Z
25	1.371808000	-0.112352000	0.933285000
7	-0.029160000	-1.299475000	-0.531874000
6	0.767057000	1.023124000	-2.168210000
1	0.026573000	1.509973000	-2.814438000
1	1.748706000	1.322135000	-2.545809000
6	0.492374000	-3.342345000	1.498107000
6	1.997747000	0.863888000	2.231475000
8	2.330308000	1.498472000	3.163110000
15	1.404602000	-1.925262000	2.262408000
15	0.693767000	1.570614000	-0.397564000
14	0.392716000	-3.022323000	-0.353153000
14	0.573370000	-0.863100000	-2.151189000
6	-0.890186000	-4.203406000	-1.075578000
1	-0.996953000	-4.107505000	-2.161336000
1	-0.623453000	-5.245825000	-0.858677000
1	-1.871482000	-4.006781000	-0.627566000
6	-0.610161000	-1.298290000	-3.560992000
1	-0.220116000	-0.919919000	-4.515118000
1	-0.770798000	-2.375687000	-3.674470000
1	-1.593246000	-0.836368000	-3.401161000
1	0.922118000	-4.312147000	1.774017000
1	-0.544608000	-3.332580000	1.862983000
6	0.568823000	-1.742785000	3.893634000
1	0.545927000	-2.686031000	4.452089000
1	1.093841000	-0.986866000	4.487624000
1	-0.452097000	-1.385139000	3.733457000
6	2.936750000	-2.782834000	2.846461000
1	3.526269000	-2.102149000	3.469863000
1	2.693425000	-3.668844000	3.444919000

1	3.555631000	-3.096622000	2.000280000
15	3.410612000	-0.426638000	-0.032300000
6	3.762061000	-2.046063000	-0.877658000
1	4.634867000	-1.971479000	-1.539870000
1	3.994692000	-2.809915000	-0.126034000
14	2.189726000	-2.563482000	-1.801318000
6	4.095259000	0.664898000	-1.369984000
1	3.632460000	0.429894000	-2.333479000
1	3.912302000	1.720527000	-1.149312000
1	5.176008000	0.512743000	-1.475512000
6	4.842962000	-0.278749000	1.125605000
1	4.673600000	-0.862000000	2.032800000
1	5.777118000	-0.608301000	0.655812000
1	4.953577000	0.770309000	1.421761000
6	2.563338000	-3.755918000	-3.219871000
1	3.220411000	-3.291664000	-3.964927000
1	3.066059000	-4.658616000	-2.852503000
1	1.646491000	-4.069942000	-3.731362000
1	-0.005649000	0.099793000	1.707576000
1	-0.981140000	-1.050188000	-0.257785000
6	-3.666346000	-0.878430000	0.648593000
8	-3.008179000	-1.547384000	-0.136559000
6	-1.066328000	2.092558000	-0.195408000
6	-2.102265000	1.692625000	-1.041357000
6	-1.377766000	2.910305000	0.899042000
6	-3.412667000	2.119668000	-0.819349000
1	-1.905627000	1.043097000	-1.889109000
6	-2.679030000	3.346936000	1.116118000
1	-0.590085000	3.208472000	1.586767000
6	-3.703803000	2.954732000	0.253186000
1	-4.204059000	1.793216000	-1.487749000
1	-2.896288000	3.991689000	1.963226000
1	-4.723122000	3.289861000	0.422125000
6	1.477933000	3.238792000	-0.504094000
6	0.986725000	4.202576000	-1.394278000
6	2.590893000	3.552184000	0.277762000
6	1.602139000	5.443281000	-1.508585000
1	0.108810000	3.981800000	-1.996484000
6	3.209121000	4.797943000	0.167033000
1	2.973725000	2.820419000	0.981113000
6	2.718893000	5.742878000	-0.727925000
1	1.211149000	6.179505000	-2.205378000
1	4.073571000	5.027084000	0.783904000
1	3.200514000	6.712580000	-0.816554000

6	-5.115015000	-0.622692000	0.369447000
6	-5.910009000	0.158049000	1.214411000
6	-5.675145000	-1.162181000	-0.793621000
6	-7.244322000	0.395972000	0.899633000
1	-5.490430000	0.590559000	2.117057000
6	-7.007042000	-0.924870000	-1.107803000
1	-5.046421000	-1.764460000	-1.441504000
6	-7.793352000	-0.143790000	-0.261359000
1	-7.855429000	1.005133000	1.558871000
1	-7.435031000	-1.347341000	-2.012115000
1	-8.834832000	0.043797000	-0.506361000
6	-3.047311000	-0.311254000	1.896144000
1	-3.492996000	-0.778885000	2.783168000
1	-1.968438000	-0.485104000	1.885884000
1	-3.217700000	0.767330000	1.965491000

D4S

Doordinates (Angstroms)			
	X	Y	Z
25	-0.487398000	-0.516845000	-0.902499000
7	0.634517000	-0.326818000	1.134531000
6	-2.183161000	-0.023664000	1.960874000
1	-2.459261000	0.709710000	2.727282000
1	-3.007452000	-0.739822000	1.910016000
6	2.743298000	-1.478518000	-0.539386000
6	-1.131182000	-0.227014000	-2.494669000
8	-1.481945000	0.028865000	-3.586585000
15	1.411187000	-1.316995000	-1.811937000
15	-2.001641000	0.690996000	0.257887000
14	1.903875000	-1.581338000	1.139823000
14	-0.542001000	-0.890233000	2.348242000
6	3.195780000	-1.325420000	2.497420000
1	2.923978000	-1.806464000	3.443562000
1	4.170847000	-1.723359000	2.190365000
1	3.307924000	-0.250824000	2.682959000
6	-0.053569000	-0.445540000	4.119110000
1	-0.831759000	-0.750047000	4.830518000
1	0.882873000	-0.923778000	4.427113000
1	0.086460000	0.638223000	4.223237000
1	3.433189000	-2.301768000	-0.759011000
1	3.338172000	-0.555618000	-0.532753000
6	2.188647000	-0.256347000	-3.100340000
1	3.173804000	-0.630111000	-3.402131000

1	1.534794000	-0.216588000	-3.978660000
1	2.282796000	0.759271000	-2.710111000
6	1.591043000	-2.941034000	-2.682333000
1	0.957161000	-2.961029000	-3.575280000
1	2.628250000	-3.100268000	-3.000189000
1	1.300212000	-3.773342000	-2.034177000
15	-1.541815000	-2.525051000	-0.674223000
6	-0.680831000	-3.871888000	0.276772000
1	-1.383080000	-4.660701000	0.577189000
1	0.077726000	-4.342855000	-0.358860000
14	0.183935000	-3.067573000	1.758375000
6	-3.209182000	-2.740194000	0.115272000
1	-3.126583000	-2.697505000	1.205699000
1	-3.903510000	-1.959878000	-0.209070000
1	-3.634755000	-3.715988000	-0.147258000
6	-1.942565000	-3.371353000	-2.266402000
1	-1.077428000	-3.381750000	-2.932307000
1	-2.279254000	-4.401587000	-2.101363000
1	-2.743385000	-2.819713000	-2.771281000
6	0.498333000	-4.308297000	3.150284000
1	-0.439632000	-4.758196000	3.497194000
1	1.152578000	-5.122689000	2.816845000
1	0.975386000	-3.828714000	4.012649000
1	0.295188000	0.860177000	-1.150758000
1	0.937256000	0.646795000	1.140424000
6	2.952010000	2.420480000	0.498553000
6	2.026125000	3.341798000	-0.246324000
1	1.441158000	2.748869000	-0.962394000
1	1.328915000	3.789545000	0.462675000
1	2.561686000	4.125445000	-0.790634000
8	2.668015000	2.021298000	1.619912000
6	4.210819000	1.949223000	-0.161573000
6	4.454345000	2.148762000	-1.523951000
6	5.139396000	1.231739000	0.601462000
6	5.596786000	1.618657000	-2.117271000
1	3.746872000	2.701380000	-2.133840000
6	6.284202000	0.712281000	0.012403000
1	4.944203000	1.083285000	1.657807000
6	6.510563000	0.899779000	-1.351133000
1	5.770823000	1.766247000	-3.178728000
1	6.998709000	0.157198000	0.612942000
1	7.401317000	0.486374000	-1.815309000
6	-1.564388000	2.454673000	0.582547000
6	-1.159330000	2.953691000	1.820787000

6	-1.640637000	3.339362000	-0.502412000
6	-0.866055000	4.309436000	1.983175000
1	-1.070638000	2.297362000	2.681082000
6	-1.359339000	4.689499000	-0.341769000
1	-1.927426000	2.960796000	-1.480707000
6	-0.975620000	5.182139000	0.907132000
1	-0.552384000	4.677486000	2.956006000
1	-1.436674000	5.361645000	-1.191693000
1	-0.756983000	6.238405000	1.034848000
6	-3.766910000	0.933423000	-0.229507000
6	-4.637424000	1.669124000	0.584984000
6	-4.263049000	0.374180000	-1.408294000
6	-5.972568000	1.830117000	0.234723000
1	-4.263404000	2.128989000	1.496439000
6	-5.602241000	0.536502000	-1.763932000
1	-3.599435000	-0.189830000	-2.054682000
6	-6.458856000	1.261980000	-0.942926000
1	-6.634524000	2.404529000	0.876646000
1	-5.971942000	0.096203000	-2.685689000
1	-7.501899000	1.390346000	-1.218200000

TSD2-3

Doordinates (Angstroms)			
	X	Y	Z
25	-0.314692000	-0.474931000	0.906876000
7	-1.348080000	1.345231000	0.084379000
6	0.930442000	0.965431000	-1.860801000
1	1.621312000	1.674243000	-2.329310000
1	0.829548000	0.119132000	-2.552190000
6	-3.690659000	-0.164235000	1.249102000
6	0.502515000	-1.636547000	1.928020000
8	0.999943000	-2.401467000	2.664307000
15	-2.195799000	-0.633801000	2.207086000
15	1.515853000	0.249732000	-0.278865000
14	-3.066514000	1.016395000	-0.108916000
14	-0.810455000	1.685782000	-1.550949000
6	-4.164345000	2.553681000	-0.060922000
1	-3.881438000	3.284219000	-0.827741000
1	-5.220231000	2.298400000	-0.217879000
1	-4.080274000	3.051373000	0.914429000
6	-0.773988000	3.514699000	-2.013536000
1	-0.409005000	3.665818000	-3.037353000
1	-1.767266000	3.972493000	-1.941113000

1	-0.112010000	4.065701000	-1.332932000
1	-4.123087000	-1.063127000	0.795050000
1	-4.464263000	0.285076000	1.884958000
6	-2.211070000	0.628342000	3.543761000
1	-3.144604000	0.603174000	4.117856000
1	-1.366630000	0.453021000	4.217528000
1	-2.085437000	1.622674000	3.102899000
6	-2.680535000	-2.127328000	3.162865000
1	-1.870117000	-2.399684000	3.847297000
1	-3.588553000	-1.941008000	3.747238000
1	-2.860957000	-2.975121000	2.497726000
15	-0.930400000	-2.028584000	-0.669234000
6	-1.739097000	-1.466416000	-2.255024000
1	-0.964347000	-1.462591000	-3.034592000
1	-2.467368000	-2.227677000	-2.566620000
14	-2.543146000	0.273577000	-2.265980000
6	0.397177000	-3.117281000	-1.340503000
1	1.156027000	-2.526762000	-1.862033000
1	0.893958000	-3.639011000	-0.515640000
1	-0.010670000	-3.857522000	-2.038984000
6	-2.108256000	-3.349783000	-0.149908000
1	-3.079988000	-2.919337000	0.108941000
1	-2.258591000	-4.087890000	-0.946122000
1	-1.706763000	-3.861436000	0.730877000
1	0.040837000	0.854134000	1.930426000
1	-0.532310000	1.250185000	1.235949000
6	-3.626416000	0.414806000	-3.812251000
1	-3.039864000	0.248951000	-4.724186000
1	-4.432487000	-0.329064000	-3.797668000
1	-4.087564000	1.406028000	-3.888320000
6	2.394641000	1.635007000	0.561150000
6	2.588855000	2.894799000	-0.006173000
6	2.878119000	1.398701000	1.854527000
6	3.250230000	3.898972000	0.701405000
1	2.222964000	3.116077000	-1.003593000
6	3.550760000	2.392661000	2.554204000
1	2.712123000	0.431166000	2.321472000
6	3.736176000	3.650060000	1.979385000
1	3.384492000	4.875985000	0.245806000
1	3.922423000	2.190292000	3.554637000
1	4.253398000	4.431192000	2.529168000
6	2.954960000	-0.797724000	-0.761600000
6	3.671001000	-0.558914000	-1.939313000
6	3.361471000	-1.845066000	0.071117000

6	4.761774000	-1.353280000	-2.281736000
1	3.378475000	0.251322000	-2.600739000
6	4.457433000	-2.635121000	-0.266252000
1	2.814938000	-2.056378000	0.983657000
6	5.157828000	-2.393812000	-1.445130000
1	5.302952000	-1.157094000	-3.203109000
1	4.758684000	-3.445074000	0.391949000
1	6.008720000	-3.014160000	-1.712054000

TSD4-5r

Doordinates (Angstroms)			

	X	Y	Z
25	-0.691835000	0.060657000	-0.861895000
7	-1.238993000	-1.037088000	1.069271000
6	0.085620000	1.412361000	2.113500000
1	0.749634000	1.365871000	2.983546000
1	-0.261086000	2.443586000	2.025754000
6	-2.914911000	-2.430633000	-0.835189000
6	-0.030290000	0.537028000	-2.401858000
8	0.407153000	0.759512000	-3.469036000
15	-2.366618000	-1.084980000	-1.953091000
15	0.967418000	0.946509000	0.542747000
14	-2.905968000	-1.632106000	0.869961000
14	-1.378707000	0.230456000	2.313798000
6	-3.418093000	-2.941710000	2.127612000
1	-3.530951000	-2.548242000	3.143623000
1	-4.375486000	-3.394848000	1.841232000
1	-2.667357000	-3.741471000	2.156582000
6	-1.342335000	-0.409020000	4.090586000
1	-1.483457000	0.419047000	4.797223000
1	-2.118472000	-1.154640000	4.293299000
1	-0.372451000	-0.869624000	4.317121000
1	-3.852675000	-2.902974000	-1.147488000
1	-2.140818000	-3.202604000	-0.760348000
6	-1.930329000	-1.837666000	-3.575866000
1	-2.565542000	-2.701379000	-3.801768000
1	-2.077226000	-1.083568000	-4.357695000
1	-0.883636000	-2.137629000	-3.596157000
6	-4.062048000	-0.494478000	-2.431039000
1	-4.039042000	0.439444000	-2.997922000
1	-4.548054000	-1.256299000	-3.051893000
1	-4.681731000	-0.348099000	-1.542298000
15	-1.972443000	1.982331000	-0.740313000

6	-3.648403000	1.824059000	0.053317000
1	-3.988389000	2.800094000	0.424481000
1	-4.385306000	1.505035000	-0.689727000
14	-3.562182000	0.559957000	1.470580000
6	-1.490450000	3.593312000	0.046039000
1	-1.627562000	3.563481000	1.130490000
1	-0.448862000	3.844087000	-0.172129000
1	-2.130259000	4.393838000	-0.343185000
6	-2.340035000	2.686889000	-2.408175000
1	-2.562587000	1.906051000	-3.137971000
1	-3.170901000	3.400915000	-2.372908000
1	-1.443835000	3.212699000	-2.756112000
6	-5.003595000	0.782677000	2.672795000
1	-4.981986000	1.774548000	3.139357000
1	-5.967847000	0.676929000	2.161474000
1	-4.969002000	0.035612000	3.473865000
1	0.141747000	-1.389357000	-1.114752000
1	-0.498881000	-1.756498000	1.051761000
6	0.930899000	-2.863508000	-0.687673000
8	0.517727000	-3.162042000	0.452301000
6	2.380004000	0.034326000	1.331135000
6	2.109795000	-0.968977000	2.270116000
6	3.713605000	0.382767000	1.103430000
6	3.132979000	-1.566836000	2.996277000
1	1.093248000	-1.303539000	2.441849000
6	4.741204000	-0.220643000	1.825754000
1	3.963433000	1.138285000	0.366096000
6	4.455450000	-1.184545000	2.786288000
1	2.892860000	-2.336434000	3.724456000
1	5.770211000	0.068372000	1.631616000
1	5.257424000	-1.646441000	3.355193000
6	1.831819000	2.506069000	0.077332000
6	2.214820000	3.450252000	1.038195000
6	2.144169000	2.750553000	-1.262456000
6	2.873668000	4.617224000	0.666298000
1	2.005148000	3.272349000	2.088850000
6	2.809929000	3.917094000	-1.636233000
1	1.869148000	2.029282000	-2.022388000
6	3.170183000	4.855617000	-0.674741000
1	3.160056000	5.340434000	1.424514000
1	3.041257000	4.090074000	-2.683370000
1	3.683662000	5.767629000	-0.965439000
6	2.363285000	-2.397401000	-0.892585000
6	2.749396000	-1.531145000	-1.917121000

6	3.347318000	-3.009208000	-0.116762000
6	4.094809000	-1.271702000	-2.153341000
1	1.988199000	-1.047198000	-2.518811000
6	4.695978000	-2.764476000	-0.363240000
1	3.043805000	-3.676781000	0.683381000
6	5.074619000	-1.894884000	-1.381578000
1	4.379290000	-0.582602000	-2.944110000
1	5.451240000	-3.246978000	0.250894000
1	6.126569000	-1.697663000	-1.569086000
6	0.446137000	-3.673219000	-1.885626000
1	0.952384000	-4.646222000	-1.823900000
1	-0.629416000	-3.851634000	-1.854960000
1	0.722723000	-3.216774000	-2.837926000

TSD4-5S

Doordinates (Angstroms)			
	X	Y	Z
25	0.030682000	-0.327376000	-0.775125000
7	0.973048000	-0.308887000	1.288062000
6	-1.907648000	-0.448353000	1.970298000
1	-2.235664000	0.196079000	2.794211000
1	-2.651184000	-1.246534000	1.892957000
6	3.302572000	-1.018780000	-0.394461000
6	-0.486408000	0.160718000	-2.370873000
8	-0.744491000	0.558746000	-3.443195000
15	2.008555000	-1.081660000	-1.692365000
15	-1.860010000	0.467173000	0.349712000
14	2.392969000	-1.382999000	1.216326000
14	-0.185110000	-1.155825000	2.336566000
6	3.613155000	-1.159175000	2.638794000
1	3.140242000	-1.235047000	3.623621000
1	4.404150000	-1.918370000	2.590227000
1	4.096643000	-0.176681000	2.572384000
6	0.110427000	-0.914513000	4.188213000
1	-0.714327000	-1.351906000	4.765690000
1	1.037481000	-1.381215000	4.538653000
1	0.159312000	0.153150000	4.438782000
1	4.150316000	-1.680884000	-0.605345000
1	3.688825000	0.002721000	-0.311283000
6	2.612590000	-0.086412000	-3.113374000
1	3.693995000	-0.191399000	-3.250975000
1	2.104340000	-0.432055000	-4.020689000
1	2.364117000	0.963174000	-2.963217000

6	2.417920000	-2.753317000	-2.389438000
1	1.655285000	-3.122804000	-3.080051000
1	3.366848000	-2.687269000	-2.934722000
1	2.552372000	-3.487939000	-1.591410000
15	-0.912810000	-2.456564000	-0.875060000
6	0.094752000	-3.805271000	-0.088079000
1	-0.534096000	-4.684593000	0.101960000
1	0.891773000	-4.133009000	-0.759068000
14	0.834591000	-3.134708000	1.530281000
6	-2.534913000	-3.041645000	-0.182477000
1	-2.485829000	-3.111076000	0.908422000
1	-3.364901000	-2.389185000	-0.455956000
1	-2.743618000	-4.045397000	-0.570664000
6	-1.198144000	-3.024582000	-2.607881000
1	-0.405788000	-2.679091000	-3.274859000
1	-1.284769000	-4.115032000	-2.675810000
1	-2.136690000	-2.579135000	-2.957219000
6	1.226600000	-4.532448000	2.740550000
1	0.322174000	-5.091076000	3.009943000
1	1.940972000	-5.244963000	2.311005000
1	1.664548000	-4.139374000	3.665415000
1	0.934897000	1.155400000	-0.762266000
1	1.100766000	0.715616000	1.395427000
6	1.383604000	2.553632000	-0.042203000
6	0.516921000	3.422607000	-0.941174000
1	0.655365000	3.208627000	-2.003279000
1	-0.530654000	3.271535000	-0.691215000
1	0.770036000	4.475287000	-0.754689000
8	1.098203000	2.449085000	1.177829000
6	2.872374000	2.527556000	-0.376743000
6	3.398153000	2.838027000	-1.632690000
6	3.763332000	2.255832000	0.666280000
6	4.773772000	2.824594000	-1.852839000
1	2.737079000	3.096223000	-2.453698000
6	5.137725000	2.243839000	0.453538000
1	3.347458000	2.061856000	1.649538000
6	5.648857000	2.518221000	-0.813761000
1	5.162225000	3.060030000	-2.839877000
1	5.811892000	2.024322000	1.277164000
1	6.721329000	2.509284000	-0.986777000
6	-2.195113000	2.207583000	0.878096000
6	-1.657995000	2.734640000	2.054563000
6	-2.954371000	3.048533000	0.055299000
6	-1.885637000	4.061294000	2.408009000

1	-1.035872000	2.120858000	2.695948000
6	-3.175882000	4.377461000	0.402632000
1	-3.379453000	2.667269000	-0.868616000
6	-2.643293000	4.887791000	1.583606000
1	-1.455948000	4.452682000	3.325699000
1	-3.769129000	5.011768000	-0.249881000
1	-2.815592000	5.924834000	1.857513000
6	-3.535982000	0.119689000	-0.354720000
6	-4.661021000	0.084343000	0.478966000
6	-3.716001000	-0.076573000	-1.725532000
6	-5.925917000	-0.167314000	-0.040414000
1	-4.549435000	0.261403000	1.545377000
6	-4.984668000	-0.321640000	-2.250508000
1	-2.864516000	-0.043421000	-2.394017000
6	-6.091062000	-0.374467000	-1.409241000
1	-6.785348000	-0.195516000	0.623468000
1	-5.103332000	-0.472413000	-3.319668000
1	-7.078897000	-0.568784000	-1.816930000

D4Ra

Doordinates (Angstroms)			
	X	Y	Z
25	0.906602000	0.240726000	0.957502000
7	0.544020000	-1.574214000	-0.430039000
6	-0.550871000	0.626407000	-2.058419000
1	-1.516390000	0.324172000	-2.480272000
1	-0.159743000	1.420613000	-2.701472000
6	2.558089000	-2.752097000	1.409511000
6	0.895669000	1.370103000	2.278062000
8	0.867684000	2.049811000	3.238664000
15	2.148534000	-1.136860000	2.231058000
15	-0.688811000	1.240371000	-0.308332000
14	1.970170000	-2.639204000	-0.376801000
14	0.585540000	-0.888549000	-2.070644000
6	1.617409000	-4.387820000	-0.994761000
1	0.841330000	-4.858185000	-0.377116000
1	1.269607000	-4.409456000	-2.032891000
1	2.516825000	-5.013072000	-0.928778000
6	-0.106693000	-2.033783000	-3.408001000
1	-0.237939000	-1.489209000	-4.352195000
1	0.534829000	-2.896970000	-3.616801000
1	-1.088783000	-2.410801000	-3.095938000
1	3.631035000	-2.965747000	1.483339000

1	2.036359000	-3.575549000	1.915127000
6	1.333452000	-1.688772000	3.787692000
1	1.975584000	-2.343769000	4.388610000
1	1.063510000	-0.807331000	4.379207000
1	0.406981000	-2.213235000	3.537049000
6	3.792398000	-0.659991000	2.929918000
1	3.679392000	0.246282000	3.534693000
1	4.205168000	-1.452052000	3.565618000
1	4.507864000	-0.451059000	2.127982000
15	2.641873000	1.274667000	-0.112894000
6	3.887431000	0.205332000	-0.981119000
1	4.538763000	0.797069000	-1.637772000
1	4.530408000	-0.275842000	-0.233052000
14	2.934848000	-1.145307000	-1.914318000
6	2.411341000	2.511813000	-1.475892000
1	1.947183000	2.050888000	-2.353051000
1	1.770589000	3.332214000	-1.143610000
1	3.377998000	2.928675000	-1.782497000
6	3.712548000	2.334066000	0.955491000
1	4.060860000	1.785838000	1.833168000
1	4.580890000	2.714520000	0.404856000
1	3.122262000	3.185959000	1.310231000
6	3.888700000	-1.787536000	-3.414050000
1	4.070753000	-0.988313000	-4.142449000
1	4.863871000	-2.191159000	-3.116290000
1	3.339177000	-2.586813000	-3.924393000
1	-0.264978000	-0.489118000	1.761248000
1	-0.356629000	-1.950980000	-0.128252000
6	-3.033224000	-2.558653000	0.333030000
8	-2.174798000	-2.637859000	-0.531241000
6	-2.484070000	1.025408000	0.116275000
6	-3.515143000	1.163489000	-0.819787000
6	-2.823867000	0.867021000	1.462629000
6	-4.849167000	1.142443000	-0.422804000
1	-3.287466000	1.309446000	-1.871956000
6	-4.158243000	0.859279000	1.865723000
1	-2.029604000	0.744993000	2.193303000
6	-5.174973000	0.997672000	0.924617000
1	-5.634058000	1.246255000	-1.166867000
1	-4.399705000	0.743027000	2.918754000
1	-6.215819000	0.991384000	1.236413000
6	-0.768696000	3.081436000	-0.537136000
6	-1.275430000	3.672752000	-1.699688000
6	-0.350992000	3.915624000	0.504154000

6	-1.343297000	5.056840000	-1.827520000
1	-1.625602000	3.052829000	-2.520235000
6	-0.422114000	5.301757000	0.381113000
1	0.040512000	3.482790000	1.417592000
6	-0.913457000	5.877057000	-0.786954000
1	-1.736737000	5.495355000	-2.740484000
1	-0.088723000	5.931160000	1.201522000
1	-0.965411000	6.957529000	-0.886400000
6	-2.645387000	-2.539001000	1.791949000
1	-3.458204000	-2.208006000	2.443244000
1	-2.350662000	-3.553289000	2.090250000
1	-1.777741000	-1.880142000	1.919217000
6	-4.508414000	-2.518395000	-0.018839000
1	-4.912396000	-1.633023000	0.490093000
6	-5.210456000	-3.758272000	0.560193000
1	-6.283911000	-3.712674000	0.348952000
1	-4.817250000	-4.675973000	0.106813000
1	-5.087086000	-3.834167000	1.645546000
6	-4.735420000	-2.385168000	-1.519609000
1	-5.804685000	-2.274633000	-1.731164000
1	-4.214792000	-1.510500000	-1.919533000
1	-4.368197000	-3.268102000	-2.053491000

D4Sa

Doordinates (Angstroms)			
	X	Y	Z
25	-0.316800000	-0.475043000	-0.910657000
7	0.925327000	-0.464730000	1.079707000
6	-1.839604000	0.063095000	2.030397000
1	-2.023810000	0.794851000	2.825983000
1	-2.720050000	-0.583967000	1.997017000
6	2.801818000	-1.854731000	-0.731687000
6	-1.000863000	-0.084230000	-2.462481000
8	-1.373443000	0.233675000	-3.530823000
15	1.475817000	-1.365261000	-1.928829000
15	-1.672206000	0.814257000	0.345061000
14	2.062847000	-1.838110000	0.996201000
14	-0.260286000	-0.946539000	2.319903000
6	3.485257000	-1.749804000	2.232484000
1	3.158236000	-1.801833000	3.276649000
1	4.188525000	-2.575528000	2.063626000
1	4.029885000	-0.808965000	2.090325000
6	0.295061000	-0.604465000	4.095909000

1	-0.483884000	-0.912110000	4.805532000
1	1.214566000	-1.135616000	4.365209000
1	0.477765000	0.466593000	4.253932000
1	3.272819000	-2.805310000	-1.007262000
1	3.585028000	-1.087033000	-0.727304000
6	2.376724000	-0.236531000	-3.074129000
1	3.270186000	-0.704160000	-3.504326000
1	1.703956000	0.065256000	-3.884327000
1	2.659147000	0.668464000	-2.529256000
6	1.415416000	-2.858436000	-3.019083000
1	0.750871000	-2.665424000	-3.868466000
1	2.408265000	-3.108527000	-3.410682000
1	1.029666000	-3.724984000	-2.472602000
15	-1.503798000	-2.405558000	-0.688488000
6	-0.700036000	-3.845756000	0.168686000
1	-1.437649000	-4.611317000	0.443864000
1	0.020456000	-4.317775000	-0.510697000
14	0.247053000	-3.168737000	1.668831000
6	-3.135909000	-2.527163000	0.191329000
1	-2.988692000	-2.517846000	1.275743000
1	-3.793496000	-1.694859000	-0.075953000
1	-3.641069000	-3.465295000	-0.067402000
6	-2.065069000	-3.158444000	-2.280142000
1	-1.254117000	-3.190857000	-3.009919000
1	-2.455727000	-4.172080000	-2.130992000
1	-2.863591000	-2.537562000	-2.701434000
6	0.472522000	-4.476399000	3.015987000
1	-0.495491000	-4.840254000	3.381258000
1	1.029006000	-5.342069000	2.637477000
1	1.022236000	-4.073379000	3.874175000
1	0.532802000	0.852410000	-1.150549000
1	1.341476000	0.466671000	1.037903000
6	3.534311000	2.107515000	-0.262673000
6	2.435113000	3.098137000	-0.531243000
1	1.585485000	2.541373000	-0.950119000
1	2.090198000	3.536151000	0.409871000
1	2.727247000	3.891365000	-1.224107000
8	3.383015000	1.220007000	0.561631000
6	-1.052024000	2.512301000	0.717006000
6	-0.441140000	2.868604000	1.920380000
6	-1.160982000	3.482195000	-0.288791000
6	0.025667000	4.167856000	2.128648000
1	-0.325153000	2.141002000	2.718118000
6	-0.704503000	4.777755000	-0.081826000

1	-1.608723000	3.215609000	-1.243202000
6	-0.113412000	5.128100000	1.133126000
1	0.494608000	4.424046000	3.074692000
1	-0.808081000	5.518260000	-0.869932000
1	0.241883000	6.141583000	1.296213000
6	-3.425261000	1.220336000	-0.065886000
6	-4.197584000	2.030512000	0.776567000
6	-4.013976000	0.695970000	-1.217716000
6	-5.528134000	2.300096000	0.477634000
1	-3.750685000	2.460530000	1.669660000
6	-5.348142000	0.965956000	-1.521031000
1	-3.424097000	0.075032000	-1.883056000
6	-6.107234000	1.765784000	-0.673765000
1	-6.115444000	2.930023000	1.139888000
1	-5.789911000	0.550691000	-2.422439000
1	-7.146858000	1.976825000	-0.907919000
6	4.837604000	2.266219000	-1.033783000
1	4.569220000	2.502599000	-2.072813000
6	5.588026000	3.478506000	-0.452664000
1	6.510532000	3.655384000	-1.015302000
1	4.988844000	4.394572000	-0.494055000
1	5.859287000	3.296122000	0.593613000
6	5.696788000	1.007924000	-1.000588000
1	5.195599000	0.170680000	-1.497271000
1	6.647474000	1.182474000	-1.516144000
1	5.912997000	0.708334000	0.029560000

TSD4-5Ra

Doordinates (Angstroms)			
	X	Y	Z
25	0.454365000	0.014556000	-0.841451000
7	1.258678000	0.759619000	1.153374000
6	-0.867511000	-1.108986000	2.082222000
1	-1.509822000	-0.754416000	2.896172000
1	-0.915958000	-2.200728000	2.104149000
6	3.618000000	1.280889000	-0.678417000
6	-0.291349000	-0.100206000	-2.419235000
8	-0.753121000	-0.080450000	-3.497077000
15	2.394226000	0.617184000	-1.901598000
15	-1.486646000	-0.515053000	0.427294000
14	3.042687000	0.773844000	1.051698000
14	0.909159000	-0.515030000	2.348614000
6	3.870614000	1.920011000	2.300164000

1	3.617692000	1.672259000	3.336613000
1	4.962326000	1.867443000	2.201500000
1	3.575323000	2.962788000	2.128021000
6	1.021868000	0.070403000	4.140830000
1	0.726244000	-0.734003000	4.826713000
1	2.029497000	0.391603000	4.426811000
1	0.342079000	0.915080000	4.312780000
1	4.621178000	0.887511000	-0.885798000
1	3.686607000	2.371656000	-0.753289000
6	2.198828000	1.913617000	-3.199609000
1	3.142782000	2.430865000	-3.404969000
1	1.864102000	1.423390000	-4.120167000
1	1.432179000	2.634622000	-2.920777000
6	3.496448000	-0.471083000	-2.922026000
1	2.957192000	-0.818188000	-3.809066000
1	4.364581000	0.105575000	-3.262317000
1	3.859213000	-1.346193000	-2.378808000
15	1.112878000	-2.234603000	-0.745222000
6	2.775575000	-2.534310000	0.027028000
1	2.917528000	-3.605275000	0.221616000
1	3.576864000	-2.229174000	-0.652443000
14	2.922114000	-1.504490000	1.620252000
6	0.277824000	-3.660155000	0.104951000
1	0.352212000	-3.566339000	1.192019000
1	-0.774337000	-3.746766000	-0.168707000
1	0.785025000	-4.588318000	-0.183022000
6	1.228558000	-3.035232000	-2.403144000
1	1.667747000	-2.367411000	-3.144339000
1	1.807561000	-3.965083000	-2.364081000
1	0.210581000	-3.271858000	-2.733103000
6	4.110833000	-2.292750000	2.857774000
1	3.758080000	-3.283409000	3.168698000
1	5.110153000	-2.417463000	2.424196000
1	4.209805000	-1.676300000	3.758444000
1	0.199184000	1.728753000	-0.929010000
1	0.710026000	1.637040000	1.214124000
6	-0.083130000	3.183321000	-0.305601000
8	-0.507095000	2.998968000	0.862848000
6	-2.867382000	0.595976000	0.961552000
6	-2.682877000	1.509218000	2.002742000
6	-4.106661000	0.564513000	0.312908000
6	-3.711165000	2.362045000	2.391487000
1	-1.723902000	1.583861000	2.501906000
6	-5.135135000	1.419605000	0.697544000

1	-4.279125000	-0.130059000	-0.503233000
6	-4.940822000	2.321973000	1.739512000
1	-3.544099000	3.069716000	3.198466000
1	-6.089490000	1.377537000	0.180311000
1	-5.741636000	2.991203000	2.041341000
6	-2.523725000	-1.937218000	-0.139947000
6	-3.255541000	-2.704684000	0.774991000
6	-2.622765000	-2.246306000	-1.498179000
6	-4.036619000	-3.772314000	0.346865000
1	-3.218949000	-2.465951000	1.834368000
6	-3.412003000	-3.311362000	-1.931595000
1	-2.081105000	-1.657437000	-2.227774000
6	-4.113156000	-4.082298000	-1.010465000
1	-4.591673000	-4.360510000	1.072177000
1	-3.475277000	-3.534737000	-2.992820000
1	-4.723474000	-4.915866000	-1.345975000
6	1.307660000	3.821734000	-0.390476000
1	1.211417000	4.844732000	-0.006525000
1	1.996792000	3.304955000	0.277894000
1	1.735397000	3.875513000	-1.393398000
6	-1.041155000	3.629707000	-1.429457000
1	-0.534792000	3.459227000	-2.388326000
6	-2.347712000	2.855230000	-1.419743000
1	-2.872878000	3.004444000	-0.472604000
1	-3.002093000	3.184079000	-2.236379000
1	-2.154925000	1.786189000	-1.542837000
6	-1.310621000	5.136225000	-1.280326000
1	-0.402845000	5.737073000	-1.403977000
1	-2.031652000	5.470274000	-2.035464000
1	-1.733077000	5.349860000	-0.291745000

TSD4-5Sa

Doordinates (Angstroms)			

	X	Y	Z
25	0.348968000	-0.098010000	-0.787196000
7	1.111660000	0.313815000	1.325749000
6	-1.313295000	-1.315148000	1.878622000
1	-1.984091000	-1.077169000	2.711801000
1	-1.469533000	-2.368825000	1.638173000
6	3.458410000	0.962628000	-0.252844000
6	-0.291649000	0.089245000	-2.400833000
8	-0.674301000	0.306530000	-3.488053000
15	2.523657000	0.150979000	-1.597643000

15	-1.685926000	-0.306009000	0.366390000
14	2.872630000	0.044171000	1.283799000
14	0.499589000	-1.016735000	2.335555000
6	3.805599000	0.741253000	2.766143000
1	3.519230000	0.278685000	3.716666000
1	4.886452000	0.598930000	2.640664000
1	3.618201000	1.819115000	2.846822000
6	0.574666000	-0.720089000	4.200389000
1	0.151418000	-1.582799000	4.731373000
1	1.598300000	-0.580912000	4.564298000
1	-0.003557000	0.163655000	4.498581000
1	4.540492000	0.998840000	-0.419390000
1	3.075617000	1.974434000	-0.069179000
6	2.743111000	1.096987000	-3.163032000
1	3.734364000	1.560536000	-3.215313000
1	2.645673000	0.392971000	-3.997882000
1	1.976129000	1.858457000	-3.286968000
6	3.792697000	-1.152702000	-1.982520000
1	3.431252000	-1.910474000	-2.682207000
1	4.665125000	-0.667543000	-2.436127000
1	4.131589000	-1.649137000	-1.069931000
15	0.529144000	-2.391554000	-1.001792000
6	1.934900000	-3.204981000	-0.087275000
1	1.676158000	-4.245686000	0.149475000
1	2.821282000	-3.252382000	-0.727068000
14	2.330044000	-2.251960000	1.511187000
6	-0.774292000	-3.658048000	-0.629222000
1	-0.899128000	-3.810176000	0.445799000
1	-1.737447000	-3.364544000	-1.053920000
1	-0.478785000	-4.618888000	-1.066292000
6	0.781406000	-2.902542000	-2.760054000
1	1.436431000	-2.210780000	-3.292960000
1	1.184809000	-3.918841000	-2.837497000
1	-0.192999000	-2.875537000	-3.260476000
6	3.348770000	-3.328773000	2.685006000
1	2.802687000	-4.237163000	2.966522000
1	4.289234000	-3.640912000	2.215007000
1	3.601046000	-2.791688000	3.606335000
1	0.388230000	1.645780000	-0.803321000
1	0.843750000	1.311570000	1.409358000
6	0.531610000	3.137377000	-0.225297000
6	-0.942279000	3.533892000	-0.247602000
1	-1.495833000	3.076869000	-1.070722000
1	-1.401552000	3.266898000	0.699453000

1	-1.005777000	4.626133000	-0.352492000
8	1.107722000	3.036660000	0.893434000
6	-2.598820000	1.091709000	1.158861000
6	-2.159367000	1.621523000	2.376767000
6	-3.698714000	1.686126000	0.533003000
6	-2.799172000	2.712658000	2.956422000
1	-1.293113000	1.204334000	2.879512000
6	-4.336919000	2.781589000	1.107964000
1	-4.063233000	1.296784000	-0.413176000
6	-3.889955000	3.299051000	2.321189000
1	-2.433323000	3.111366000	3.898153000
1	-5.188509000	3.231398000	0.605475000
1	-4.386615000	4.155513000	2.767649000
6	-3.111414000	-1.192950000	-0.396125000
6	-4.000952000	-1.951260000	0.374357000
6	-3.332786000	-1.094417000	-1.772458000
6	-5.070055000	-2.613117000	-0.220539000
1	-3.861141000	-2.029144000	1.448507000
6	-4.409730000	-1.748652000	-2.368705000
1	-2.663933000	-0.504226000	-2.387664000
6	-5.275597000	-2.515721000	-1.595554000
1	-5.745564000	-3.204388000	0.391240000
1	-4.565996000	-1.658284000	-3.439790000
1	-6.111213000	-3.031428000	-2.059991000
6	1.345750000	3.746918000	-1.390504000
1	2.235652000	3.128458000	-1.528643000
6	1.837842000	5.135054000	-0.958959000
1	2.477841000	5.574184000	-1.733872000
1	1.002301000	5.825790000	-0.789777000
1	2.410744000	5.063467000	-0.030138000
6	0.580077000	3.823244000	-2.710435000
1	1.251955000	4.101813000	-3.531491000
1	0.108030000	2.867432000	-2.961510000
1	-0.209691000	4.582508000	-2.668945000

D1

Doordinates (Angstroms)			
	X	Y	Z
25	-0.403861000	0.189816000	0.860912000
7	-1.494648000	0.840127000	-0.761040000
6	0.781324000	-0.326619000	-2.290797000
1	1.336064000	0.240147000	-3.049180000
1	0.931203000	-1.390901000	-2.511817000

6	-3.734733000	0.728623000	1.174177000
6	0.578666000	0.207195000	2.315275000
8	1.186369000	0.251322000	3.319647000
15	-2.147917000	1.075204000	2.023626000
15	1.390268000	-0.000638000	-0.580506000
14	-3.195273000	0.443223000	-0.633299000
14	-1.074969000	0.083689000	-2.279580000
6	-4.404673000	1.461664000	-1.680622000
1	-4.294379000	1.290101000	-2.756793000
1	-5.442273000	1.218447000	-1.415781000
1	-4.257471000	2.534657000	-1.497372000
6	-1.395152000	1.083995000	-3.856195000
1	-1.070064000	0.523022000	-4.742296000
1	-2.449359000	1.343328000	-3.997847000
1	-0.824752000	2.022764000	-3.833825000
1	-4.194745000	-0.163017000	1.613650000
1	-4.454211000	1.551138000	1.274652000
6	-2.000720000	2.903461000	1.899396000
1	-2.867117000	3.419469000	2.329737000
1	-1.096307000	3.230711000	2.424566000
1	-1.901514000	3.170233000	0.842928000
6	-2.489808000	0.859736000	3.815827000
1	-1.598784000	1.123544000	4.395499000
1	-3.324997000	1.491482000	4.138632000
1	-2.737031000	-0.183637000	4.031886000
15	-0.926768000	-1.987802000	1.045404000
6	-1.612594000	-2.750502000	-0.497758000
1	-0.762082000	-3.135269000	-1.077396000
1	-2.214399000	-3.628498000	-0.224572000
14	-2.615865000	-1.594136000	-1.662062000
6	0.358049000	-3.224317000	1.514208000
1	1.174404000	-3.214132000	0.788392000
1	0.770788000	-2.973119000	2.496945000
1	-0.059121000	-4.237315000	1.553188000
6	-2.210686000	-2.484333000	2.274206000
1	-3.164494000	-1.992864000	2.063226000
1	-2.373645000	-3.568331000	2.262743000
1	-1.882318000	-2.192812000	3.277229000
6	-3.696742000	-2.704217000	-2.757829000
1	-3.084388000	-3.370317000	-3.378364000
1	-4.362445000	-3.332945000	-2.153196000
1	-4.322263000	-2.105147000	-3.429562000
6	2.776384000	-1.239413000	-0.436346000
6	3.898119000	-1.084846000	-1.488210000

6	3.380080000	-1.405942000	0.964422000
6	5.165498000	-1.872291000	-1.091658000
1	3.527446000	-1.434609000	-2.459062000
6	4.151140000	-2.738590000	1.054862000
1	4.061216000	-0.573292000	1.168034000
6	4.809654000	-3.123114000	-0.286489000
1	5.736740000	-2.133939000	-1.989382000
1	3.471068000	-3.538681000	1.372507000
1	4.125650000	-3.744460000	-0.880158000
1	2.246272000	-2.177001000	-0.661334000
1	2.606573000	-1.364326000	1.734525000
1	4.916800000	-2.654320000	1.835015000
1	5.701757000	-3.733660000	-0.108199000
1	5.819962000	-1.235821000	-0.481735000
1	4.163477000	-0.030250000	-1.619566000
6	2.221956000	1.661271000	-0.737136000
6	1.192548000	2.792456000	-0.871526000
6	3.156905000	1.949140000	0.462895000
6	1.885305000	4.120173000	-1.229544000
1	0.424696000	2.558311000	-1.613392000
6	3.328567000	3.457329000	0.729123000
1	2.769759000	1.471353000	1.369542000
6	3.275952000	4.250956000	-0.575937000
1	1.982316000	4.202737000	-2.319106000
1	4.273395000	3.631956000	1.255914000
1	4.048141000	3.864588000	-1.254748000
1	3.516802000	5.305458000	-0.401839000
1	2.531850000	3.811003000	1.396685000
1	4.137586000	1.500487000	0.264421000
1	2.817071000	1.641391000	-1.660549000
1	0.654278000	2.884409000	0.081148000
1	1.242462000	4.949821000	-0.911414000

D2

Doordinates (Angstroms)			
	X	Y	Z
25	-0.372332000	0.122075000	1.022894000
7	-1.497524000	1.047900000	-0.640949000
6	0.842157000	0.015713000	-2.206898000
1	1.475563000	0.592743000	-2.892054000
1	0.907982000	-1.033035000	-2.523473000
6	-3.786065000	0.464450000	1.157007000
6	0.441714000	-0.436314000	2.478424000

8	0.914794000	-0.809709000	3.482794000
15	-2.277427000	0.716954000	2.169601000
15	1.444441000	0.109388000	-0.468480000
14	-3.168494000	0.562132000	-0.648341000
14	-0.985069000	0.555636000	-2.224484000
6	-4.396999000	1.718909000	-1.516020000
1	-4.209708000	1.814731000	-2.591546000
1	-5.425707000	1.354379000	-1.392958000
1	-4.344461000	2.725981000	-1.080014000
6	-1.179588000	1.802542000	-3.636377000
1	-0.848532000	1.367706000	-4.588676000
1	-2.219481000	2.123947000	-3.762294000
1	-0.580408000	2.704822000	-3.456195000
1	-4.239060000	-0.501980000	1.396295000
1	-4.540881000	1.231268000	1.373268000
6	-2.325163000	2.537324000	2.438236000
1	-3.272557000	2.856494000	2.887345000
1	-1.503992000	2.839451000	3.096968000
1	-2.196453000	3.038540000	1.473332000
6	-2.717992000	0.125415000	3.854466000
1	-1.913087000	0.377698000	4.553182000
1	-3.647318000	0.589060000	4.204064000
1	-2.845624000	-0.960586000	3.865280000
15	-0.999138000	-2.063069000	0.598699000
6	-1.497789000	-2.546563000	-1.110873000
1	-0.581935000	-2.734177000	-1.688481000
1	-2.035475000	-3.503970000	-1.068768000
14	-2.527822000	-1.218622000	-2.051609000
6	0.233618000	-3.367806000	1.030643000
1	1.150237000	-3.254829000	0.450242000
1	0.494557000	-3.286759000	2.091004000
1	-0.173362000	-4.368084000	0.844184000
6	-2.407227000	-2.775809000	1.556770000
1	-3.350244000	-2.288754000	1.300879000
1	-2.512193000	-3.846991000	1.350457000
1	-2.222488000	-2.648013000	2.627587000
6	-3.541410000	-2.134389000	-3.370230000
1	-2.891821000	-2.731781000	-4.022587000
1	-4.268515000	-2.817676000	-2.913089000
1	-4.097122000	-1.433206000	-4.003301000
6	2.755338000	-1.218969000	-0.472826000
6	3.831901000	-1.102351000	-1.573927000
6	3.415558000	-1.481045000	0.886231000
6	5.035934000	-2.031101000	-1.298494000

1	3.381151000	-1.350524000	-2.541535000
6	4.108258000	-2.861172000	0.895116000
1	4.153685000	-0.693611000	1.080016000
6	4.615532000	-3.266859000	-0.502262000
1	5.507674000	-2.317371000	-2.245014000
1	3.411046000	-3.621620000	1.267128000
1	3.824335000	-3.793992000	-1.052711000
1	2.150878000	-2.103486000	-0.715138000
1	2.684856000	-1.427192000	1.696483000
1	4.945504000	-2.836408000	1.602622000
1	5.448200000	-3.973397000	-0.413326000
1	5.798728000	-1.488426000	-0.724885000
1	4.197816000	-0.073384000	-1.658512000
6	2.414192000	1.706296000	-0.452200000
6	1.598699000	2.913109000	-0.945150000
6	3.038817000	1.968422000	0.945802000
6	2.478570000	4.171825000	-1.056463000
1	1.156481000	2.701122000	-1.922744000
6	3.073394000	3.461310000	1.302267000
1	2.499330000	1.419797000	1.726853000
6	3.506981000	4.286301000	0.090582000
1	3.002802000	4.167383000	-2.019695000
1	3.754725000	3.621122000	2.145605000
1	4.484741000	3.914993000	-0.245540000
1	3.654830000	5.336269000	0.365920000
1	2.080181000	3.791279000	1.636123000
1	4.064235000	1.579660000	0.951424000
1	3.226969000	1.581171000	-1.178454000
1	0.756492000	3.107028000	-0.275236000
1	1.824084000	5.051406000	-1.065433000
1	0.253810000	1.683250000	1.630122000
1	-0.107200000	1.875898000	0.959066000

D3

Doordinates (Angstroms)			
	X	Y	Z
25	-0.356868000	0.013774000	0.992594000
7	-1.536280000	1.163631000	-0.677469000
6	0.837634000	0.093572000	-2.213111000
1	1.445528000	0.734727000	-2.864242000
1	0.955276000	-0.934617000	-2.579234000
6	-3.713619000	0.512922000	1.284832000
6	0.509734000	-0.493115000	2.413535000

8	1.060943000	-0.764392000	3.416451000
15	-2.122346000	0.673777000	2.220696000
15	1.413297000	0.129003000	-0.442962000
14	-3.232990000	0.591236000	-0.541446000
14	-0.994391000	0.535731000	-2.265095000
6	-4.466262000	1.726078000	-1.416744000
1	-4.289056000	1.807896000	-2.494835000
1	-5.488310000	1.350274000	-1.278235000
1	-4.429760000	2.739108000	-0.994754000
6	-1.296292000	1.764429000	-3.665278000
1	-1.004116000	1.333331000	-4.630917000
1	-2.345985000	2.068585000	-3.738329000
1	-0.698316000	2.673341000	-3.518203000
1	-4.172112000	-0.453744000	1.519154000
1	-4.441935000	1.287780000	1.556679000
6	-2.157848000	2.475471000	2.610608000
1	-3.078902000	2.776361000	3.124979000
1	-1.294370000	2.716878000	3.237912000
1	-2.059432000	3.053467000	1.685446000
6	-2.539566000	0.004124000	3.884755000
1	-1.697703000	0.177771000	4.563404000
1	-3.432951000	0.485153000	4.299200000
1	-2.713359000	-1.073840000	3.832349000
15	-1.003581000	-2.111318000	0.559984000
6	-1.683034000	-2.629845000	-1.101697000
1	-0.837162000	-2.918971000	-1.740952000
1	-2.322531000	-3.517244000	-1.006805000
14	-2.567071000	-1.177285000	-1.938657000
6	0.258284000	-3.441898000	0.812360000
1	1.076346000	-3.341438000	0.095770000
1	0.677146000	-3.358632000	1.820554000
1	-0.183251000	-4.438539000	0.692187000
6	-2.303556000	-2.869289000	1.641590000
1	-3.262011000	-2.352848000	1.538983000
1	-2.458559000	-3.929015000	1.406221000
1	-1.979237000	-2.793713000	2.684489000
6	-3.725324000	-1.727906000	-3.326291000
1	-3.178419000	-2.256381000	-4.116151000
1	-4.498291000	-2.407707000	-2.948476000
1	-4.229835000	-0.869998000	-3.785447000
6	2.758011000	-1.172987000	-0.543102000
6	3.871222000	-0.935910000	-1.585475000
6	3.382455000	-1.574290000	0.798803000
6	5.062902000	-1.901007000	-1.384488000

1	3.454807000	-1.058496000	-2.592661000
6	4.070265000	-2.952420000	0.679860000
1	4.116869000	-0.814778000	1.092442000
6	4.615802000	-3.212138000	-0.738069000
1	5.558838000	-2.085624000	-2.344173000
1	3.360424000	-3.743460000	0.950439000
1	3.840070000	-3.673878000	-1.364076000
1	2.171673000	-2.036016000	-0.888361000
1	2.633826000	-1.599448000	1.592436000
1	4.888531000	-3.007655000	1.407825000
1	5.443959000	-3.928773000	-0.701076000
1	5.812666000	-1.431017000	-0.734504000
1	4.245564000	0.091506000	-1.525343000
6	2.362837000	1.735796000	-0.420081000
6	1.482951000	2.953329000	-0.733450000
6	3.089806000	1.918547000	0.934396000
6	2.333199000	4.230336000	-0.881679000
1	0.910300000	2.796689000	-1.656279000
6	3.245607000	3.398313000	1.321562000
1	2.543256000	1.396023000	1.726858000
6	3.536917000	4.247354000	0.084274000
1	2.690730000	4.322462000	-1.914858000
1	4.043194000	3.503669000	2.065821000
1	4.425485000	3.839892000	-0.416510000
1	3.783555000	5.278369000	0.362080000
1	2.323454000	3.754236000	1.799005000
1	4.082401000	1.455884000	0.864743000
1	3.110030000	1.677450000	-1.221973000
1	0.755993000	3.070962000	0.076978000
1	1.694414000	5.102279000	-0.695153000
1	-1.283693000	2.110873000	-0.406824000
1	0.142098000	1.481980000	1.382559000

D4R

Doordinates (Angstroms)			
	X	Y	Z
25	1.288037000	-0.451723000	0.883809000
7	-0.458082000	-1.281916000	-0.400453000
6	0.753956000	0.906160000	-2.126602000
1	0.226293000	1.654148000	-2.730975000
1	1.742026000	0.762351000	-2.583052000
6	0.319687000	-3.683358000	1.270445000
6	2.377735000	0.245882000	2.043285000

8	3.083051000	0.706422000	2.866467000
15	0.776673000	-2.171158000	2.241720000
15	1.062042000	1.415431000	-0.368764000
14	-0.287679000	-3.067462000	-0.414260000
14	-0.110772000	-0.778660000	-2.084273000
6	-1.908323000	-3.932451000	-0.845460000
1	-2.287203000	-3.641467000	-1.832173000
1	-1.781439000	-5.022521000	-0.846499000
1	-2.677203000	-3.681526000	-0.105324000
6	-1.635583000	-0.709647000	-3.201111000
1	-1.327234000	-0.527647000	-4.238928000
1	-2.207798000	-1.644551000	-3.188576000
1	-2.306419000	0.107651000	-2.911993000
1	1.225318000	-4.286005000	1.126321000
1	-0.417837000	-4.313567000	1.784490000
6	-0.740942000	-1.941064000	3.256514000
1	-0.974290000	-2.826361000	3.861936000
1	-0.593899000	-1.076802000	3.912200000
1	-1.582169000	-1.721967000	2.593236000
6	1.890211000	-2.828588000	3.558344000
1	2.137004000	-2.015137000	4.249599000
1	1.406025000	-3.634221000	4.122725000
1	2.825577000	-3.208012000	3.141597000
15	3.049873000	-1.402913000	-0.197612000
6	2.935460000	-2.431491000	-1.771081000
1	3.431685000	-1.895408000	-2.591119000
1	3.486766000	-3.371960000	-1.642634000
14	1.136504000	-2.756621000	-2.249135000
6	4.440966000	-0.290569000	-0.712899000
1	4.133354000	0.344082000	-1.550112000
1	4.726821000	0.355324000	0.124402000
1	5.318169000	-0.867555000	-1.029622000
6	4.069320000	-2.577090000	0.808667000
1	3.496349000	-3.484088000	1.026169000
1	4.986926000	-2.868289000	0.283680000
1	4.340493000	-2.100931000	1.756496000
6	0.976142000	-3.877399000	-3.763607000
1	1.445107000	-3.427312000	-4.646694000
1	1.457004000	-4.847982000	-3.592056000
1	-0.077098000	-4.065214000	-4.002617000
6	2.445347000	2.659364000	-0.558466000
6	2.354593000	3.569478000	-1.804534000
6	2.686154000	3.511212000	0.696642000
6	3.212470000	4.842840000	-1.655244000

1	2.689809000	3.006612000	-2.684188000
6	4.073325000	4.180497000	0.622897000
1	1.904664000	4.277998000	0.768066000
6	4.462475000	4.555146000	-0.822201000
1	3.480484000	5.230308000	-2.644880000
1	4.826020000	3.502239000	1.042518000
1	5.013407000	3.727765000	-1.289836000
1	3.328628000	2.023767000	-0.666848000
1	2.618776000	2.909256000	1.605954000
1	4.073138000	5.076892000	1.254873000
1	5.140406000	5.416077000	-0.823606000
1	2.630487000	5.631980000	-1.161183000
1	1.314966000	3.857341000	-2.004199000
6	-0.378603000	2.562696000	-0.009831000
6	-1.729935000	2.034168000	-0.514511000
6	-0.454159000	2.942442000	1.500167000
6	-2.852447000	3.005283000	-0.138578000
1	-1.710610000	1.915558000	-1.602646000
6	-1.790958000	2.556025000	2.137202000
1	0.345836000	2.451389000	2.061810000
6	-2.978679000	3.177667000	1.393919000
1	-2.633079000	3.973734000	-0.607114000
1	-1.799990000	2.866374000	3.189234000
1	-3.044397000	4.244191000	1.642785000
1	-3.913143000	2.724984000	1.747752000
1	-1.868094000	1.461460000	2.138025000
1	-0.308609000	4.025299000	1.608891000
1	-0.183134000	3.479730000	-0.582362000
1	-1.939691000	1.046281000	-0.089084000
1	-3.799107000	2.662357000	-0.569038000
1	-1.253508000	-0.898896000	0.106815000
1	0.089702000	0.206883000	1.700313000
6	-4.085785000	-0.553984000	1.354885000
8	-3.172727000	-1.316806000	1.073992000
6	-4.858114000	0.109712000	0.263018000
6	-5.876405000	1.033982000	0.514898000
6	-4.516070000	-0.194131000	-1.058852000
6	-6.532667000	1.655486000	-0.543412000
1	-6.154051000	1.281890000	1.534753000
6	-5.171878000	0.423461000	-2.114586000
1	-3.725313000	-0.915487000	-1.237062000
6	-6.179608000	1.353399000	-1.857060000
1	-7.316214000	2.379624000	-0.342796000
1	-4.897106000	0.183824000	-3.137717000

1	-6.690217000	1.842137000	-2.681676000
6	-4.433479000	-0.264952000	2.793075000
1	-5.486017000	-0.491262000	2.996436000
1	-3.797132000	-0.864939000	3.445809000
1	-4.272989000	0.796090000	3.015652000

D4S

Doordinates (Angstroms)			
	X	Y	Z
25	0.648634000	-0.380993000	1.022145000
7	-0.900739000	-0.819049000	-0.721996000
6	1.553098000	0.096898000	-2.244316000
1	1.495851000	0.866385000	-3.024693000
1	2.436091000	-0.515878000	-2.468615000
6	-1.908039000	-2.589549000	1.490111000
6	1.488864000	0.192640000	2.431808000
8	1.969568000	0.607946000	3.421994000
15	-1.046697000	-1.155594000	2.288772000
15	1.786765000	0.822610000	-0.547774000
14	-1.527532000	-2.462166000	-0.355394000
14	0.047904000	-1.038682000	-2.224794000
6	-3.086373000	-2.930463000	-1.315339000
1	-2.971381000	-2.804739000	-2.397875000
1	-3.314538000	-3.989552000	-1.134088000
1	-3.965896000	-2.356490000	-1.000783000
6	-0.941706000	-0.752676000	-3.808087000
1	-0.309853000	-0.972020000	-4.678630000
1	-1.830570000	-1.388951000	-3.879217000
1	-1.264933000	0.292347000	-3.901081000
1	-1.508234000	-3.525104000	1.897337000
1	-2.987917000	-2.589182000	1.687580000
6	-2.450438000	0.017764000	2.477672000
1	-3.293941000	-0.420400000	3.024199000
1	-2.093568000	0.908778000	3.002104000
1	-2.791371000	0.337343000	1.489063000
6	-0.867479000	-1.684182000	4.044389000
1	-0.440995000	-0.856554000	4.621226000
1	-1.834226000	-1.959048000	4.481193000
1	-0.189781000	-2.537285000	4.128213000
15	1.905680000	-2.266465000	0.954938000
6	1.993050000	-3.338934000	-0.569221000
1	2.779363000	-2.942518000	-1.226346000
1	2.281897000	-4.367347000	-0.314932000

14	0.353416000	-3.254752000	-1.516561000
6	3.709211000	-2.092976000	1.333587000
1	4.215072000	-1.501337000	0.568090000
1	3.829180000	-1.578069000	2.292550000
1	4.201812000	-3.070740000	1.394718000
6	1.573706000	-3.597968000	2.200104000
1	0.570473000	-4.016817000	2.079752000
1	2.299852000	-4.415309000	2.115178000
1	1.655032000	-3.170535000	3.204433000
6	0.117187000	-4.697893000	-2.713403000
1	0.913023000	-4.728492000	-3.466508000
1	0.124023000	-5.657064000	-2.182316000
1	-0.840537000	-4.614853000	-3.240323000
6	3.650871000	1.013622000	-0.553595000
6	4.255822000	1.832557000	-1.713244000
6	4.258213000	1.471073000	0.778243000
6	5.740458000	2.182080000	-1.459457000
1	4.159217000	1.265008000	-2.646609000
6	5.763487000	1.128424000	0.830398000
1	4.118753000	2.553950000	0.880872000
6	6.414398000	1.140208000	-0.566360000
1	6.268263000	2.280245000	-2.414889000
1	5.902480000	0.143300000	1.291903000
1	6.321018000	0.151847000	-1.036841000
1	3.958191000	-0.030861000	-0.700452000
1	3.743061000	1.013701000	1.625094000
1	6.272219000	1.849523000	1.481301000
1	7.488730000	1.338684000	-0.481888000
1	5.810301000	3.160231000	-0.965966000
1	3.701923000	2.765997000	-1.859384000
6	1.171896000	2.561615000	-0.832541000
6	-0.305097000	2.603121000	-1.245454000
6	1.413592000	3.439910000	0.420571000
6	-0.721717000	4.027650000	-1.649156000
1	-0.501503000	1.921933000	-2.084117000
6	0.321497000	4.502410000	0.615327000
1	1.457043000	2.811356000	1.316405000
6	-0.101705000	5.102210000	-0.726263000
1	-0.423595000	4.217449000	-2.687617000
1	0.684487000	5.285409000	1.290800000
1	0.785400000	5.537152000	-1.205662000
1	-0.806684000	5.928324000	-0.578518000
1	-0.545047000	4.043996000	1.108976000
1	2.387871000	3.934755000	0.322543000

1	1.742765000	2.972175000	-1.675367000
1	-0.905958000	2.250903000	-0.400978000
1	-1.816671000	4.100641000	-1.629492000
1	-1.461259000	0.015944000	-0.568549000
1	-0.198273000	0.970241000	1.157535000
6	-5.090421000	0.193533000	-1.300331000
8	-5.984787000	-0.622422000	-1.158387000
6	-4.821226000	1.219893000	-0.244332000
6	-3.812909000	2.180374000	-0.378128000
6	-5.590891000	1.193372000	0.924108000
6	-3.578391000	3.098825000	0.640120000
1	-3.202402000	2.219744000	-1.275070000
6	-5.356602000	2.110340000	1.940255000
1	-6.366533000	0.440147000	1.017379000
6	-4.348620000	3.064165000	1.799255000
1	-2.790094000	3.837135000	0.530968000
1	-5.954005000	2.081106000	2.846538000
1	-4.160369000	3.778521000	2.595175000
6	-4.208588000	0.174507000	-2.527337000
1	-3.166553000	-0.004205000	-2.240331000
1	-4.538250000	-0.623806000	-3.194072000
1	-4.247526000	1.131678000	-3.059327000

TSD2-3

Doordinates (Angstroms)			
	X	Y	Z
25	-0.504954000	-0.478190000	0.894042000
7	-1.434193000	1.374969000	-0.005476000
6	0.800875000	0.808421000	-1.966021000
1	1.513332000	1.497507000	-2.432935000
1	0.682644000	-0.044280000	-2.647129000
6	-3.843079000	0.090331000	1.288712000
6	0.275768000	-1.642610000	1.947946000
8	0.740396000	-2.407009000	2.703586000
15	-2.359725000	-0.436613000	2.236651000
15	1.370113000	0.147755000	-0.348004000
14	-3.168284000	1.120870000	-0.164096000
14	-0.909182000	1.592366000	-1.670350000
6	-4.192683000	2.710400000	-0.222415000
1	-3.875179000	3.385500000	-1.025564000
1	-5.257907000	2.491957000	-0.373235000
1	-4.094820000	3.256910000	0.725263000
6	-0.826589000	3.393304000	-2.233672000

1	-0.485853000	3.476684000	-3.273348000
1	-1.799916000	3.891885000	-2.158779000
1	-0.123085000	3.955727000	-1.604997000
1	-4.366178000	-0.794442000	0.909708000
1	-4.553828000	0.646067000	1.913789000
6	-2.251320000	0.903015000	3.494345000
1	-3.162821000	0.971312000	4.099784000
1	-1.395024000	0.716190000	4.149969000
1	-2.084301000	1.860702000	2.990312000
6	-2.930554000	-1.822260000	3.302447000
1	-2.126654000	-2.104167000	3.990732000
1	-3.810116000	-1.531628000	3.888069000
1	-3.186430000	-2.699587000	2.703235000
15	-1.264231000	-2.079780000	-0.559650000
6	-1.966529000	-1.548329000	-2.200403000
1	-1.147551000	-1.579003000	-2.933076000
1	-2.696879000	-2.296685000	-2.537565000
14	-2.711516000	0.217509000	-2.278853000
6	-0.085171000	-3.392223000	-1.104035000
1	0.759365000	-2.953393000	-1.640857000
1	0.306380000	-3.917879000	-0.226830000
1	-0.572623000	-4.119360000	-1.763799000
6	-2.606420000	-3.212589000	0.012611000
1	-3.525471000	-2.662714000	0.232838000
1	-2.835288000	-3.969673000	-0.746434000
1	-2.278189000	-3.723627000	0.923465000
1	-0.063221000	0.870522000	1.861042000
1	-0.623054000	1.258631000	1.155818000
6	-3.817962000	0.327818000	-3.812196000
1	-3.251355000	0.111870000	-4.726350000
1	-4.642048000	-0.394241000	-3.756038000
1	-4.255367000	1.327074000	-3.918651000
6	2.150497000	1.659365000	0.429447000
6	2.921598000	1.310066000	1.709882000
6	2.972259000	2.607395000	-0.478890000
6	3.164047000	2.572097000	2.559003000
1	2.366044000	0.573070000	2.299952000
6	3.986218000	3.436919000	0.329605000
1	3.500980000	2.066318000	-1.266075000
6	3.407158000	3.825102000	1.690296000
1	2.297355000	2.739817000	3.209180000
1	4.271824000	4.327657000	-0.241638000
1	2.460293000	4.357302000	1.528320000
6	2.737391000	-1.032032000	-0.812726000

6	3.973782000	-0.450260000	-1.509805000
6	3.148664000	-1.943193000	0.370284000
6	4.827550000	-1.574727000	-2.132688000
1	3.683118000	0.253721000	-2.296218000
6	4.550075000	-2.548614000	0.178578000
1	3.116169000	-1.399347000	1.318295000
6	4.800542000	-2.869253000	-1.294219000
1	4.467921000	-1.786250000	-3.146960000
1	4.649839000	-3.446519000	0.798302000
1	3.999599000	-3.531942000	-1.649685000
1	4.070407000	4.525247000	2.210101000
1	4.907489000	2.858841000	0.483188000
1	2.277806000	3.286924000	-0.988196000
1	3.880058000	0.846328000	1.442519000
1	1.260657000	2.215628000	0.750432000
1	4.022519000	2.398928000	3.218844000
1	2.240799000	-1.662850000	-1.562113000
1	2.411527000	-2.747230000	0.461898000
1	4.569908000	0.116082000	-0.783994000
1	5.316823000	-1.844081000	0.528076000
1	5.737938000	-3.421666000	-1.421950000
1	5.859056000	-1.217530000	-2.237388000

TSD4-5R

Doordinates (Angstroms)			
	X	Y	Z
25	-0.702573000	-0.064599000	-0.844198000
7	-1.156464000	-1.042510000	1.171643000
6	-0.119501000	1.646243000	1.978601000
1	0.504272000	1.780565000	2.871336000
1	-0.586889000	2.612464000	1.785264000
6	-2.714730000	-2.732061000	-0.614775000
6	-0.030123000	0.354321000	-2.404660000
8	0.447632000	0.530743000	-3.460471000
15	-2.288048000	-1.430503000	-1.838217000
15	0.899159000	1.150789000	0.498313000
14	-2.750833000	-1.827553000	1.036139000
14	-1.439164000	0.325358000	2.280258000
6	-3.098685000	-3.099616000	2.384109000
1	-3.128185000	-2.664712000	3.388767000
1	-4.060531000	-3.598890000	2.211102000
1	-2.317609000	-3.870101000	2.375685000
6	-1.427448000	-0.111032000	4.121512000

1	-1.609401000	0.793993000	4.716219000
1	-2.206856000	-0.835425000	4.381983000
1	-0.468061000	-0.530908000	4.446849000
1	-3.613395000	-3.302038000	-0.875699000
1	-1.884477000	-3.430145000	-0.476536000
6	-1.759475000	-2.217431000	-3.419301000
1	-2.240054000	-3.188944000	-3.577702000
1	-2.051065000	-1.550387000	-4.238916000
1	-0.677363000	-2.329893000	-3.455039000
6	-4.034668000	-1.072198000	-2.374652000
1	-4.116237000	-0.161433000	-2.973955000
1	-4.395445000	-1.910243000	-2.982766000
1	-4.700733000	-0.986542000	-1.511932000
15	-2.218681000	1.718804000	-0.857645000
6	-3.884887000	1.389178000	-0.098895000
1	-4.373501000	2.338332000	0.156975000
1	-4.538873000	0.890783000	-0.817329000
14	-3.649157000	0.315128000	1.449100000
6	-2.049577000	3.429938000	-0.147035000
1	-2.215520000	3.420684000	0.933889000
1	-1.072121000	3.870418000	-0.347608000
1	-2.812028000	4.080966000	-0.590684000
6	-2.626397000	2.252993000	-2.580424000
1	-2.652931000	1.402865000	-3.265304000
1	-3.583270000	2.786246000	-2.622357000
1	-1.839548000	2.929021000	-2.934021000
6	-5.100562000	0.500836000	2.645818000
1	-5.258400000	1.552569000	2.913150000
1	-6.032449000	0.129332000	2.203123000
1	-4.926477000	-0.056837000	3.573058000
1	0.217056000	-1.536535000	-1.038161000
1	-0.348642000	-1.678419000	1.225335000
6	0.970289000	-3.029062000	-0.579706000
8	0.616071000	-3.226195000	0.602458000
6	2.402689000	-2.637660000	-0.902811000
6	2.752914000	-1.886415000	-2.027452000
6	3.410516000	-3.215002000	-0.131362000
6	4.089160000	-1.693915000	-2.357837000
1	1.971817000	-1.425227000	-2.622933000
6	4.751591000	-3.032604000	-0.467475000
1	3.131974000	-3.804850000	0.737326000
6	5.094629000	-2.267706000	-1.578133000
1	4.348184000	-1.090012000	-3.223201000
1	5.527957000	-3.484507000	0.143941000

1	6.139180000	-2.117275000	-1.835962000
6	0.446131000	-3.955006000	-1.677364000
1	0.947135000	-4.918333000	-1.511243000
1	-0.627526000	-4.126840000	-1.624928000
1	0.716558000	-3.617477000	-2.678790000
6	1.673172000	2.760913000	-0.120627000
6	1.232793000	3.180630000	-1.541005000
6	1.604485000	3.941836000	0.859027000
6	1.407930000	4.688888000	-1.782952000
1	1.828894000	2.620527000	-2.269065000
6	2.573956000	5.062136000	0.431421000
1	0.582602000	4.336524000	0.901440000
6	2.677807000	5.201429000	-1.102950000
1	1.434570000	4.887614000	-2.860398000
1	3.568018000	4.863810000	0.849927000
1	3.531046000	4.619500000	-1.475781000
6	2.395700000	0.554203000	1.479705000
6	2.084684000	-0.638443000	2.394223000
6	3.671430000	0.252331000	0.684397000
6	3.239569000	-0.888678000	3.370776000
1	1.174854000	-0.459943000	2.975315000
6	4.851178000	0.005349000	1.633345000
1	3.506625000	-0.629805000	0.067946000
6	4.562518000	-1.114292000	2.637022000
1	3.334147000	-0.021062000	4.040909000
1	5.073208000	0.934731000	2.179061000
1	5.386374000	-1.199615000	3.356525000
1	2.735025000	2.507298000	-0.193053000
1	0.198220000	2.892163000	-1.734156000
1	0.542425000	5.239985000	-1.388192000
1	2.873196000	6.244571000	-1.375089000
1	2.235166000	6.007875000	0.871428000
1	1.847291000	3.619482000	1.877394000
1	3.934819000	1.066772000	0.001279000
1	2.615054000	1.419592000	2.128170000
1	1.900673000	-1.533513000	1.787270000
1	5.745317000	-0.239775000	1.046897000
1	4.507431000	-2.067428000	2.099188000
1	3.007659000	-1.753434000	4.004639000

TSD4-5S

Doordinates (Angstroms)
X Y Z

25	0.208483000	-0.377304000	-0.699816000
7	0.799294000	-0.504412000	1.476410000
6	-2.156971000	-0.962124000	1.576335000
1	-2.793103000	-0.602383000	2.394944000
1	-2.685177000	-1.803436000	1.125550000
6	3.380702000	-0.918062000	0.139164000
6	-0.152254000	0.197290000	-2.312849000
8	-0.321533000	0.651001000	-3.380532000
15	2.327749000	-1.044742000	-1.355609000
15	-1.893116000	0.344946000	0.275663000
14	2.275398000	-1.498423000	1.548002000
14	-0.463530000	-1.515125000	2.226411000
6	3.233253000	-1.330680000	3.164144000
1	2.684343000	-1.709491000	4.032913000
1	4.184473000	-1.875059000	3.109601000
1	3.464581000	-0.274387000	3.351846000
6	-0.515978000	-1.439111000	4.115782000
1	-1.315406000	-2.088488000	4.496346000
1	0.421765000	-1.772077000	4.573955000
1	-0.716057000	-0.423684000	4.479551000
1	4.337438000	-1.443774000	0.041159000
1	3.592097000	0.136864000	0.339724000
6	3.081768000	-0.001588000	-2.666662000
1	4.172963000	0.032451000	-2.577309000
1	2.818933000	-0.423183000	-3.643761000
1	2.684190000	1.009539000	-2.611839000
6	2.979290000	-2.676990000	-1.968246000
1	2.360198000	-3.112352000	-2.757331000
1	3.985974000	-2.524816000	-2.375187000
1	3.062926000	-3.396833000	-1.149315000
15	-0.608242000	-2.532903000	-1.127022000
6	0.337196000	-3.903036000	-0.294785000
1	-0.271840000	-4.815853000	-0.259479000
1	1.229070000	-4.153710000	-0.872816000
14	0.813606000	-3.350242000	1.460749000
6	-2.281699000	-3.314943000	-0.856643000
1	-2.434109000	-3.554886000	0.199560000
1	-3.112381000	-2.690240000	-1.193250000
1	-2.324519000	-4.256913000	-1.415931000
6	-0.500022000	-2.937198000	-2.927563000
1	0.390337000	-2.498385000	-3.382109000
1	-0.503487000	-4.019232000	-3.103303000
1	-1.370287000	-2.500190000	-3.430597000
6	1.117659000	-4.843053000	2.579253000

1	0.226743000	-5.479640000	2.640783000
1	1.939627000	-5.460532000	2.197772000
1	1.378144000	-4.534651000	3.598107000
1	1.160331000	1.069132000	-0.546323000
1	0.916249000	0.504437000	1.665593000
6	1.663949000	2.458980000	0.240470000
6	0.531751000	3.290100000	-0.342101000
1	0.398156000	3.147955000	-1.415944000
1	-0.387134000	3.001644000	0.151619000
1	0.729751000	4.352137000	-0.140449000
8	1.663942000	2.185368000	1.466274000
6	3.017018000	2.681781000	-0.420109000
6	3.158443000	3.202072000	-1.710164000
6	4.171352000	2.452855000	0.333098000
6	4.419474000	3.443266000	-2.247959000
1	2.281820000	3.410815000	-2.314948000
6	5.434451000	2.682202000	-0.203215000
1	4.054800000	2.107899000	1.355623000
6	5.563494000	3.172911000	-1.500714000
1	4.507653000	3.841922000	-3.254744000
1	6.319986000	2.488968000	0.396200000
1	6.547714000	3.356414000	-1.922436000
6	-2.464435000	1.805124000	1.323873000
6	-1.511765000	2.093541000	2.495394000
6	-2.832646000	3.099857000	0.550954000
6	-2.150770000	3.061920000	3.508967000
1	-1.257667000	1.165449000	3.017180000
6	-2.577826000	4.365901000	1.382956000
1	-2.305601000	3.174696000	-0.404490000
6	-3.014602000	4.147462000	2.830996000
1	-2.766073000	2.497868000	4.221260000
1	-3.114808000	5.210115000	0.935450000
1	-4.070688000	3.843984000	2.833179000
6	-3.314898000	0.106769000	-0.908634000
6	-4.701027000	-0.160314000	-0.290469000
6	-3.440198000	1.173555000	-2.008368000
6	-5.824344000	-0.027270000	-1.343375000
1	-4.717848000	-1.167418000	0.143858000
6	-4.213054000	0.576575000	-3.200536000
1	-3.981740000	2.040600000	-1.618321000
6	-5.318043000	-0.399675000	-2.739188000
1	-6.677937000	-0.653186000	-1.059434000
1	-3.512703000	0.055433000	-3.864208000
1	-4.927178000	-1.426152000	-2.711382000

1	-2.991962000	-0.798488000	-1.431226000
1	-2.462399000	1.533297000	-2.338990000
1	-4.654129000	1.391352000	-3.786945000
1	-6.143043000	-0.407671000	-3.459824000
1	-6.193880000	1.005996000	-1.366481000
1	-4.895956000	0.536272000	0.534078000
1	-3.393826000	1.433027000	1.776088000
1	-3.900097000	3.056177000	0.303244000
1	-1.511903000	4.625766000	1.360388000
1	-2.962120000	5.084061000	3.397034000
1	-1.349727000	3.530815000	4.092225000
1	-0.559992000	2.489384000	2.131565000

D4Ra

Doordinates (Angstroms)			
	X	Y	Z
25	0.775165000	-0.624418000	0.917088000
7	-0.854734000	-1.107694000	-0.673996000
6	0.975411000	0.725482000	-2.131651000
1	0.561833000	1.465692000	-2.828442000
1	2.018169000	0.570802000	-2.419313000
6	-1.330093000	-3.235730000	1.287226000
6	1.672041000	0.016027000	2.261249000
8	2.199440000	0.468325000	3.210737000
15	0.049195000	-2.350499000	2.151542000
15	0.922480000	1.265101000	-0.353779000
14	-1.166188000	-2.853910000	-0.550613000
14	0.009195000	-0.903647000	-2.218625000
6	-2.771877000	-3.389066000	-1.391592000
1	-3.623427000	-2.840534000	-0.969133000
1	-2.769113000	-3.208601000	-2.471960000
1	-2.956314000	-4.459373000	-1.233117000
6	-1.149422000	-0.778857000	-3.708686000
1	-0.581607000	-0.592470000	-4.629430000
1	-1.743123000	-1.685877000	-3.865455000
1	-1.849952000	0.055987000	-3.577485000
1	-1.363679000	-4.303771000	1.532277000
1	-2.286464000	-2.800981000	1.609776000
6	-0.692688000	-1.921875000	3.784638000
1	-1.107995000	-2.799660000	4.293847000
1	0.078458000	-1.472882000	4.420298000
1	-1.476683000	-1.172689000	3.644381000
6	1.056791000	-3.797098000	2.725623000

1	1.834786000	-3.454244000	3.416197000
1	0.432353000	-4.525866000	3.255965000
1	1.542595000	-4.304582000	1.887025000
15	2.596057000	-1.677515000	0.048543000
6	2.337489000	-3.298460000	-0.830970000
1	3.214084000	-3.575854000	-1.431796000
1	2.189579000	-4.098156000	-0.096320000
14	0.763926000	-3.125439000	-1.871490000
6	3.780418000	-0.971319000	-1.205194000
1	3.349742000	-1.016722000	-2.210209000
1	4.030917000	0.069779000	-0.982922000
1	4.710937000	-1.551558000	-1.217081000
6	3.875061000	-2.123922000	1.306665000
1	3.415713000	-2.587877000	2.181757000
1	4.629149000	-2.805634000	0.895547000
1	4.374136000	-1.208156000	1.642613000
6	0.733044000	-4.335443000	-3.324741000
1	1.555774000	-4.136782000	-4.022021000
1	0.833964000	-5.371325000	-2.979426000
1	-0.206088000	-4.259834000	-3.884522000
1	-0.486749000	0.023162000	1.644222000
1	-1.636918000	-0.485576000	-0.458723000
6	-4.135327000	0.484528000	0.475116000
8	-3.492664000	0.342184000	-0.552978000
6	-0.573859000	2.385943000	-0.408836000
6	-0.442111000	3.672391000	-1.237429000
6	-1.152583000	2.699685000	0.994790000
6	-1.827739000	4.293368000	-1.502373000
1	0.184272000	4.389522000	-0.694287000
6	-1.999579000	3.983694000	0.998600000
1	-1.769113000	1.852405000	1.299972000
6	-2.784564000	4.100751000	-0.308143000
1	-1.704376000	5.361743000	-1.717743000
1	-2.676559000	3.974977000	1.861339000
1	-3.513010000	4.918391000	-0.265349000
6	2.423228000	2.364805000	-0.151094000
6	2.924318000	3.173637000	-1.356174000
6	2.328563000	3.294969000	1.080185000
6	4.394182000	3.590549000	-1.130599000
1	2.840998000	2.612167000	-2.291805000
6	3.464017000	4.344427000	1.092669000
1	1.370982000	3.824185000	1.086232000
6	4.706406000	3.837874000	0.359802000
1	5.064386000	2.814133000	-1.519846000

1	3.122283000	5.267299000	0.604944000
1	5.045478000	2.907883000	0.834524000
6	-3.634362000	-0.075848000	1.783662000
1	-3.846266000	0.597085000	2.621310000
1	-4.148575000	-1.023686000	1.989028000
1	-2.556370000	-0.256295000	1.720877000
6	-5.459221000	1.236769000	0.474887000
1	-5.257754000	2.161230000	1.039291000
6	-6.548454000	0.458262000	1.228224000
1	-7.484453000	1.026134000	1.222112000
1	-6.741842000	-0.507929000	0.747176000
1	-6.281961000	0.272373000	2.273168000
6	-5.904933000	1.601999000	-0.938146000
1	-6.822778000	2.198460000	-0.902046000
1	-5.142283000	2.177386000	-1.469162000
1	-6.108107000	0.699962000	-1.525959000
1	3.192749000	1.616114000	0.078494000
1	2.358286000	2.690086000	1.991411000
1	3.706588000	4.613161000	2.126650000
1	5.531063000	4.552660000	0.459214000
1	4.601340000	4.498971000	-1.709510000
1	2.301114000	4.066514000	-1.476854000
1	-1.313348000	1.755664000	-0.924935000
1	-0.364008000	2.762142000	1.750760000
1	-1.359831000	4.868795000	1.118928000
1	-3.357736000	3.175352000	-0.446517000
1	-2.267758000	3.841150000	-2.399727000
1	0.064349000	3.486188000	-2.190199000

D4Sa

Doordinates (Angstroms)			
	X	Y	Z
25	-0.292968000	-0.486419000	-0.906630000
7	1.069312000	-0.499659000	1.013771000
6	-1.632391000	-0.089222000	2.183100000
1	-1.668109000	0.674589000	2.971082000
1	-2.505269000	-0.733426000	2.335508000
6	2.917759000	-1.679690000	-0.938068000
6	-1.073804000	-0.084414000	-2.411616000
8	-1.500278000	0.234671000	-3.459243000
15	1.497425000	-1.232118000	-2.044403000
15	-1.719285000	0.647045000	0.474485000
14	2.269111000	-1.801532000	0.826039000

14	-0.019609000	-1.071040000	2.299148000
6	3.744094000	-1.671387000	1.997646000
1	3.493327000	-1.889667000	3.041263000
1	4.538831000	-2.366398000	1.697076000
1	4.148606000	-0.653350000	1.951755000
6	0.652204000	-0.795751000	4.047719000
1	-0.071051000	-1.145686000	4.795840000
1	1.598207000	-1.315860000	4.233078000
1	0.823565000	0.273277000	4.231295000
1	3.439672000	-2.578468000	-1.287145000
1	3.647453000	-0.859373000	-0.947587000
6	2.272792000	-0.031104000	-3.208490000
1	3.159782000	-0.445160000	-3.702890000
1	1.538791000	0.256484000	-3.968828000
1	2.547366000	0.873551000	-2.661141000
6	1.489320000	-2.696777000	-3.176341000
1	0.769915000	-2.533656000	-3.986156000
1	2.477562000	-2.855025000	-3.624072000
1	1.205230000	-3.606404000	-2.637911000
15	-1.337680000	-2.504862000	-0.750089000
6	-0.418866000	-3.913887000	0.043236000
1	-1.095473000	-4.734687000	0.315260000
1	0.303200000	-4.319576000	-0.677128000
14	0.547270000	-3.240538000	1.530467000
6	-2.955770000	-2.768035000	0.122906000
1	-2.889190000	-2.500346000	1.181421000
1	-3.734177000	-2.158793000	-0.345564000
1	-3.264955000	-3.817865000	0.055676000
6	-1.875898000	-3.261550000	-2.349169000
1	-1.047032000	-3.339411000	-3.054055000
1	-2.305411000	-4.259000000	-2.196767000
1	-2.636605000	-2.618348000	-2.804964000
6	0.882768000	-4.585387000	2.817262000
1	-0.055836000	-5.002383000	3.202091000
1	1.460558000	-5.412885000	2.388900000
1	1.444780000	-4.189521000	3.670697000
1	0.463190000	0.921053000	-1.101629000
1	1.430131000	0.452569000	0.987103000
6	3.761904000	2.124440000	-0.283066000
6	2.865356000	3.063276000	-1.055909000
1	1.891361000	2.584368000	-1.203978000
1	2.710796000	3.973079000	-0.462836000
1	3.287363000	3.353898000	-2.021944000
8	3.331288000	1.491018000	0.665397000

6	-1.353786000	2.444333000	0.829501000
6	0.026098000	2.672919000	1.454301000
6	-1.497548000	3.295314000	-0.452595000
6	0.179847000	4.130499000	1.934484000
1	0.200992000	1.998556000	2.300904000
6	-0.701850000	4.613824000	-0.379979000
1	-1.151129000	2.711905000	-1.313806000
6	-0.611303000	5.121918000	1.058459000
1	-0.153306000	4.218569000	2.975862000
1	0.312508000	4.455878000	-0.767672000
1	-1.628366000	5.242555000	1.455186000
6	-3.571726000	0.682427000	0.216330000
6	-4.370249000	1.610607000	1.140963000
6	-3.974011000	0.903818000	-1.259702000
6	-5.869690000	1.250638000	1.093836000
1	-4.007970000	1.543410000	2.173416000
6	-5.431121000	1.384940000	-1.391402000
1	-3.307895000	1.620229000	-1.748699000
6	-6.308474000	0.763990000	-0.303712000
1	-6.083771000	0.472378000	1.836689000
1	-5.475141000	2.478811000	-1.302583000
1	-7.365677000	0.997483000	-0.471799000
6	5.217220000	2.023331000	-0.717017000
1	5.197140000	1.765489000	-1.786678000
6	5.890500000	3.400373000	-0.581090000
1	6.924277000	3.347161000	-0.937595000
1	5.376867000	4.173396000	-1.161653000
1	5.912105000	3.718467000	0.467786000
6	5.979926000	0.950881000	0.052415000
1	5.519395000	-0.034993000	-0.062040000
1	7.011388000	0.887315000	-0.310854000
1	6.008604000	1.181438000	1.122382000
1	0.789473000	2.439471000	0.707467000
1	-2.100395000	2.772466000	1.564583000
1	-2.559015000	3.518016000	-0.616332000
1	-1.166243000	5.363902000	-1.030180000
1	-0.146161000	6.113613000	1.095631000
1	1.245498000	4.392652000	1.928064000
1	-3.866431000	-0.336968000	0.487339000
1	-4.229011000	2.652611000	0.828512000
1	-6.457575000	2.129477000	1.385204000
1	-6.220931000	-0.329409000	-0.365313000
1	-5.813566000	1.141559000	-2.388840000
1	-3.842793000	-0.039825000	-1.801360000

TSD4-5Ra

Doordinates (Angstroms)

	X	Y	Z
25	0.564149000	-0.072397000	-0.834149000
7	1.294675000	0.782200000	1.140958000
6	-0.694210000	-1.299639000	2.024799000
1	-1.368584000	-1.218479000	2.883592000
1	-0.555609000	-2.365295000	1.846793000
6	3.651311000	1.337958000	-0.686368000
6	-0.219152000	-0.419892000	-2.361456000
8	-0.736199000	-0.610192000	-3.395601000
15	2.514073000	0.525370000	-1.904163000
15	-1.409098000	-0.534515000	0.485879000
14	3.079918000	0.883898000	1.056813000
14	0.979441000	-0.489343000	2.366109000
6	3.823856000	2.120713000	2.270653000
1	3.548156000	1.905126000	3.308765000
1	4.919457000	2.108459000	2.207805000
1	3.493374000	3.142286000	2.043639000
6	0.995970000	0.164422000	4.136821000
1	0.741054000	-0.636664000	4.842287000
1	1.973784000	0.562598000	4.430352000
1	0.258365000	0.965702000	4.265397000
1	4.691894000	1.030145000	-0.850043000
1	3.621314000	2.425757000	-0.813745000
6	2.365836000	1.736266000	-3.285181000
1	3.351743000	2.007430000	-3.679786000
1	1.776124000	1.278744000	-4.087021000
1	1.849313000	2.640493000	-2.972069000
6	3.705102000	-0.572766000	-2.815201000
1	3.245384000	-0.912338000	-3.749231000
1	4.602825000	-0.000863000	-3.076881000
1	4.013615000	-1.455348000	-2.252653000
15	1.350589000	-2.290414000	-0.627297000
6	3.011073000	-2.481629000	0.194886000
1	3.192297000	-3.535169000	0.443454000
1	3.816309000	-2.177116000	-0.479816000
14	3.073234000	-1.363278000	1.732511000
6	0.600042000	-3.785196000	0.198157000
1	0.728073000	-3.750800000	1.283687000
1	-0.462230000	-3.901446000	-0.027495000
1	1.118336000	-4.681008000	-0.162949000

6	1.553762000	-3.100895000	-2.277088000
1	1.861978000	-2.390476000	-3.043242000
1	2.275234000	-3.924949000	-2.235882000
1	0.580955000	-3.505785000	-2.578376000
6	4.288522000	-1.996517000	3.032694000
1	3.975754000	-2.969472000	3.429679000
1	5.293466000	-2.117120000	2.611006000
1	4.360884000	-1.299020000	3.874881000
1	0.279570000	1.630469000	-1.062723000
1	0.705034000	1.620584000	1.124821000
6	-0.156449000	3.124136000	-0.704609000
8	-0.868298000	3.079547000	0.326613000
6	-2.723490000	0.517956000	1.319850000
6	-2.162003000	1.347211000	2.506247000
6	-3.526965000	1.449399000	0.407129000
6	-3.053534000	2.556622000	2.842927000
1	-2.079673000	0.708587000	3.393036000
6	-4.795707000	1.934666000	1.128908000
1	-2.873349000	2.287844000	0.164216000
6	-4.529615000	2.225101000	2.621411000
1	-2.874769000	2.864368000	3.880045000
1	-5.159145000	2.841598000	0.629841000
1	-4.788672000	1.346378000	3.228329000
6	-2.424311000	-1.923047000	-0.252242000
6	-3.118585000	-2.870255000	0.750935000
6	-3.436913000	-1.467521000	-1.313823000
6	-4.246714000	-3.686688000	0.086157000
1	-2.376723000	-3.557093000	1.175869000
6	-3.843766000	-2.667337000	-2.190767000
1	-4.322454000	-1.057248000	-0.814415000
6	-3.916691000	-3.978112000	-1.378856000
1	-4.409232000	-4.617343000	0.641532000
1	-4.814785000	-2.458777000	-2.655280000
1	-4.657151000	-4.657420000	-1.815404000
6	1.216591000	3.782788000	-0.508276000
1	1.034310000	4.834941000	-0.258345000
1	1.730667000	3.343515000	0.348691000
1	1.872323000	3.754255000	-1.380582000
6	-0.784371000	3.411026000	-2.087984000
1	-0.049354000	3.127145000	-2.847210000
6	-2.058824000	2.622697000	-2.357009000
1	-2.911020000	3.044962000	-1.816408000
1	-2.298186000	2.642959000	-3.427117000
1	-1.936586000	1.580887000	-2.050359000

6	-1.053408000	4.918989000	-2.215000000
1	-0.131318000	5.510837000	-2.196887000
1	-1.565182000	5.136300000	-3.159987000
1	-1.696317000	5.261158000	-1.395623000
1	-1.163980000	1.724126000	2.267411000
1	-2.766836000	3.401115000	2.206331000
1	-3.419032000	-0.227497000	1.735060000
1	-3.801923000	0.976606000	-0.537259000
1	-5.592619000	1.184901000	1.034274000
1	-5.170600000	3.041124000	2.974094000
1	-1.663584000	-2.492187000	-0.799235000
1	-3.532312000	-2.306700000	1.595524000
1	-5.191325000	-3.129615000	0.133658000
1	-2.953068000	-4.503711000	-1.425434000
1	-3.121278000	-2.778015000	-3.007868000
1	-3.029093000	-0.671981000	-1.944417000

TSD4-5Sa

Doordinates (Angstroms)			
	X	Y	Z
25	0.432430000	-0.169569000	-0.775867000
7	1.226347000	0.294823000	1.316563000
6	-1.239868000	-1.287022000	1.931194000
1	-1.913903000	-1.050003000	2.763774000
1	-1.382253000	-2.348963000	1.708727000
6	3.600311000	0.809597000	-0.263628000
6	-0.236530000	-0.001433000	-2.387254000
8	-0.638079000	0.215913000	-3.465565000
15	2.644179000	-0.032348000	-1.577831000
15	-1.636501000	-0.306112000	0.401798000
14	2.980401000	-0.017114000	1.310631000
14	0.566057000	-0.966749000	2.386280000
6	3.916598000	0.736709000	2.762990000
1	3.604540000	0.337577000	3.733861000
1	4.994640000	0.558681000	2.660674000
1	3.757436000	1.822067000	2.778387000
6	0.651029000	-0.562398000	4.230644000
1	0.155031000	-1.348710000	4.814290000
1	1.678861000	-0.478518000	4.599708000
1	0.144178000	0.384977000	4.452869000
1	4.683361000	0.796197000	-0.427046000
1	3.262553000	1.841687000	-0.117776000
6	2.898311000	0.814815000	-3.195302000

1	3.887769000	1.280743000	-3.259906000
1	2.822841000	0.056451000	-3.983833000
1	2.128320000	1.559121000	-3.385051000
6	3.902783000	-1.374112000	-1.877658000
1	3.553861000	-2.156392000	-2.555487000
1	4.791419000	-0.915685000	-2.327771000
1	4.214205000	-1.836342000	-0.937718000
15	0.611912000	-2.484772000	-0.942432000
6	1.975473000	-3.276603000	0.060795000
1	1.681868000	-4.295504000	0.345973000
1	2.875635000	-3.386751000	-0.550825000
14	2.373078000	-2.278882000	1.630813000
6	-0.660928000	-3.812501000	-0.662826000
1	-0.998051000	-3.861920000	0.376119000
1	-1.528134000	-3.661347000	-1.311393000
1	-0.221918000	-4.783792000	-0.919062000
6	0.960142000	-3.000458000	-2.687474000
1	1.589810000	-2.279834000	-3.210557000
1	1.418865000	-3.994529000	-2.741741000
1	0.004258000	-3.033673000	-3.222028000
6	3.361017000	-3.349656000	2.836826000
1	2.793029000	-4.238569000	3.137112000
1	4.296752000	-3.694727000	2.380442000
1	3.620559000	-2.796167000	3.746392000
1	0.522746000	1.599111000	-0.874277000
1	0.987039000	1.298041000	1.354102000
6	0.834406000	3.139313000	-0.386985000
6	-0.575518000	3.702641000	-0.515789000
1	-1.091434000	3.364523000	-1.415713000
1	-1.160596000	3.444073000	0.359249000
1	-0.499982000	4.798862000	-0.551101000
8	1.335136000	3.037198000	0.765502000
6	-2.619454000	1.075116000	1.196617000
6	-1.795783000	1.870475000	2.225729000
6	-3.353336000	1.934063000	0.145537000
6	-2.581322000	3.061661000	2.838426000
1	-1.506698000	1.186927000	3.030790000
6	-3.900156000	3.263081000	0.712872000
1	-2.702177000	2.128004000	-0.711234000
6	-3.980720000	3.238201000	2.238615000
1	-2.658672000	2.943744000	3.925153000
1	-3.247897000	4.094935000	0.418181000
1	-4.424542000	4.168702000	2.611420000
6	-3.013675000	-1.332620000	-0.337282000

6	-4.291265000	-1.475016000	0.502560000
6	-3.340104000	-0.937480000	-1.799047000
6	-5.167380000	-2.618036000	-0.046280000
1	-4.048301000	-1.672950000	1.552956000
6	-4.771051000	-1.334666000	-2.194392000
1	-3.194154000	0.133503000	-1.968363000
6	-5.135754000	-2.691342000	-1.589380000
1	-4.827893000	-3.572867000	0.373686000
1	-5.485262000	-0.577506000	-1.843652000
1	-6.099401000	-3.044503000	-1.973237000
6	1.758432000	3.595606000	-1.541559000
1	2.563595000	2.866390000	-1.633262000
6	2.409300000	4.925450000	-1.136718000
1	3.119313000	5.254566000	-1.904920000
1	1.661219000	5.719123000	-1.016093000
1	2.943613000	4.818536000	-0.188645000
6	1.054981000	3.723144000	-2.892411000
1	1.787532000	3.874695000	-3.694353000
1	0.467908000	2.828755000	-3.128929000
1	0.374436000	4.582500000	-2.910722000
1	-3.392543000	0.553238000	1.774686000
1	-0.859985000	2.228687000	1.790386000
1	-2.019103000	3.988539000	2.668685000
1	-4.643872000	2.425366000	2.565359000
1	-4.883219000	3.474325000	0.277561000
1	-4.190804000	1.344854000	-0.242978000
1	-2.572198000	-2.330055000	-0.361311000
1	-2.627967000	-1.439826000	-2.463033000
1	-4.861905000	-0.539862000	0.486765000
1	-6.196772000	-2.473840000	0.302614000
1	-4.387464000	-3.427359000	-1.914407000
1	-4.858699000	-1.358980000	-3.286352000

E1

Doordinates (Angstroms)			
	X	Y	Z
25	-0.336611000	-0.308511000	1.130666000
7	-1.394868000	1.151907000	0.183287000
6	0.633728000	0.597107000	-1.951295000
1	1.239658000	1.272349000	-2.565672000
1	0.517640000	-0.347199000	-2.497463000
6	-3.633244000	0.124435000	1.875134000
6	0.671633000	-1.183347000	2.279386000

8	1.287654000	-1.761280000	3.092205000
15	-2.017779000	-0.263797000	2.659685000
15	1.357297000	0.206705000	-0.319655000
14	-3.134963000	0.931554000	0.219631000
14	-1.099929000	1.281573000	-1.539849000
6	-4.196551000	2.488969000	0.052654000
1	-4.089058000	2.976792000	-0.922561000
1	-5.260057000	2.252990000	0.188337000
1	-3.915797000	3.220887000	0.821801000
6	-1.189625000	3.012842000	-2.285324000
1	-1.008441000	2.990905000	-3.367490000
1	-2.157419000	3.497357000	-2.117389000
1	-0.417003000	3.645378000	-1.828067000
1	-4.180713000	-0.808685000	1.704778000
1	-4.261770000	0.766713000	2.500645000
15	-1.002265000	-2.183733000	0.089778000
6	-1.988391000	-1.958549000	-1.472099000
1	-1.300341000	-2.114730000	-2.314952000
1	-2.723591000	-2.772496000	-1.536300000
14	-2.857555000	-0.266393000	-1.776603000
6	0.278126000	-3.392439000	-0.447363000
1	0.980961000	-2.919181000	-1.140331000
1	0.849888000	-3.726328000	0.425046000
1	-0.167452000	-4.265340000	-0.938299000
6	-2.100382000	-3.303700000	1.057491000
1	-3.049779000	-2.805846000	1.280081000
1	-2.317649000	-4.232443000	0.517823000
1	-1.613376000	-3.551930000	2.006732000
6	-4.091717000	-0.524143000	-3.193055000
1	-3.592534000	-0.900397000	-4.094536000
1	-4.866502000	-1.249725000	-2.915661000
1	-4.593262000	0.414169000	-3.456130000
6	2.146344000	1.783284000	0.199377000
6	2.996674000	2.509881000	-0.640555000
6	1.885377000	2.267348000	1.483561000
6	3.562248000	3.704748000	-0.208218000
1	3.226790000	2.136947000	-1.635751000
6	2.454781000	3.461096000	1.920209000
1	1.231406000	1.704260000	2.146370000
6	3.290192000	4.182909000	1.073030000
1	4.218566000	4.263652000	-0.869153000
1	2.242908000	3.826917000	2.920690000
1	3.732706000	5.115797000	1.410381000
6	2.819537000	-0.850972000	-0.668162000

6	3.275816000	-1.102290000	-1.965508000
6	3.496325000	-1.435336000	0.409127000
6	4.377336000	-1.928219000	-2.182765000
1	2.774837000	-0.654783000	-2.818830000
6	4.597956000	-2.256006000	0.192616000
1	3.158543000	-1.253069000	1.424272000
6	5.038703000	-2.508871000	-1.105002000
1	4.717063000	-2.115921000	-3.197451000
1	5.108260000	-2.704252000	1.040159000
1	5.895199000	-3.154985000	-1.274632000
1	-1.908687000	0.767209000	3.619917000
1	-2.306620000	-1.309736000	3.565276000

E2

Doordinates (Angstroms)			
	X	Y	Z
25	-0.270637000	-0.511738000	1.230016000
7	-1.424091000	1.106535000	0.345343000
6	0.625529000	0.707383000	-1.783098000
1	1.248303000	1.389804000	-2.372567000
1	0.478325000	-0.210294000	-2.366003000
6	-3.660485000	-0.297319000	1.759284000
6	0.629639000	-1.803002000	2.028615000
8	1.172528000	-2.685807000	2.567894000
15	-2.091493000	-0.772711000	2.588878000
15	1.394382000	0.246033000	-0.185025000
14	-3.149686000	0.904450000	0.360316000
14	-1.090183000	1.428026000	-1.333211000
6	-4.181657000	2.470297000	0.599639000
1	-3.983841000	3.215197000	-0.180050000
1	-5.257005000	2.249828000	0.583863000
1	-3.949939000	2.935917000	1.567088000
6	-1.086705000	3.238175000	-1.876281000
1	-0.916530000	3.328154000	-2.957062000
1	-2.037376000	3.733874000	-1.647218000
1	-0.288148000	3.792684000	-1.366471000
1	-4.109203000	-1.198991000	1.327516000
1	-4.386698000	0.124063000	2.462456000
15	-1.048281000	-2.101584000	-0.267726000
6	-2.201974000	-1.700887000	-1.678085000
1	-1.660694000	-1.899039000	-2.613719000
1	-3.021193000	-2.432381000	-1.656111000
14	-2.934623000	0.072759000	-1.816547000

6	0.256200000	-3.075540000	-1.131386000
1	0.837331000	-2.438199000	-1.803789000
1	0.949332000	-3.494907000	-0.395036000
1	-0.182368000	-3.892258000	-1.715760000
6	-1.949533000	-3.498707000	0.533829000
1	-2.908635000	-3.163878000	0.941696000
1	-2.147094000	-4.305035000	-0.181416000
1	-1.349253000	-3.898165000	1.357793000
6	-4.136002000	0.041598000	-3.284186000
1	-3.622468000	-0.244284000	-4.210814000
1	-4.947734000	-0.678372000	-3.119790000
1	-4.591074000	1.025629000	-3.444873000
6	2.183116000	1.840850000	0.316778000
6	3.544958000	2.099773000	0.134183000
6	1.373304000	2.845014000	0.865381000
6	4.086665000	3.332288000	0.494171000
1	4.195471000	1.339885000	-0.287586000
6	1.914602000	4.079347000	1.212183000
1	0.310872000	2.657225000	1.005660000
6	3.273816000	4.325574000	1.031784000
1	5.147998000	3.514004000	0.350489000
1	1.269946000	4.848400000	1.628603000
1	3.697654000	5.286369000	1.309840000
6	2.854656000	-0.783995000	-0.600850000
6	3.313310000	-0.953868000	-1.910183000
6	3.539282000	-1.420083000	0.441275000
6	4.423686000	-1.753017000	-2.174812000
1	2.806802000	-0.459624000	-2.733958000
6	4.652971000	-2.211491000	0.179106000
1	3.202246000	-1.293212000	1.465665000
6	5.094249000	-2.384677000	-1.131133000
1	4.765431000	-1.878917000	-3.198239000
1	5.171507000	-2.698583000	0.999754000
1	5.959870000	-3.007522000	-1.337555000
1	-2.122707000	0.044375000	3.740482000
1	-2.406589000	-1.987228000	3.240729000
1	0.607712000	0.511610000	2.415800000
1	-0.079921000	0.882394000	2.332628000

E3

Doordinates (Angstroms)			
	X	Y	Z
25	-0.304216000	-0.601998000	1.130422000

7	-1.360883000	1.310444000	0.353747000
6	0.650713000	0.718591000	-1.800428000
1	1.294636000	1.366729000	-2.405180000
1	0.500006000	-0.202677000	-2.376568000
6	-3.542406000	0.066091000	2.029377000
6	0.576956000	-1.826001000	2.005449000
8	1.138805000	-2.613044000	2.671453000
15	-1.972506000	-0.751983000	2.597853000
15	1.374794000	0.172706000	-0.192009000
14	-3.125320000	0.996424000	0.439715000
14	-1.045618000	1.465922000	-1.407033000
6	-4.143018000	2.586966000	0.405873000
1	-3.996211000	3.165833000	-0.512842000
1	-5.214035000	2.362127000	0.488424000
1	-3.877240000	3.233915000	1.252188000
6	-1.129924000	3.256501000	-1.990262000
1	-0.805100000	3.350559000	-3.033686000
1	-2.144767000	3.663386000	-1.919280000
1	-0.478459000	3.892953000	-1.378254000
1	-4.307152000	-0.695381000	1.839759000
1	-3.947461000	0.742024000	2.791170000
15	-1.168407000	-2.138575000	-0.303328000
6	-2.225219000	-1.702019000	-1.789988000
1	-1.597476000	-1.766796000	-2.689632000
1	-3.021244000	-2.446829000	-1.919981000
14	-2.902395000	0.064071000	-1.700620000
6	0.017179000	-3.305494000	-1.106241000
1	0.751012000	-2.758223000	-1.706299000
1	0.563818000	-3.855626000	-0.333079000
1	-0.500330000	-4.026653000	-1.749923000
6	-2.284468000	-3.391800000	0.473769000
1	-3.222599000	-2.921706000	0.790099000
1	-2.523066000	-4.206572000	-0.219553000
1	-1.800166000	-3.814428000	1.360317000
1	0.282127000	0.419671000	2.213643000
1	-0.927621000	1.964027000	1.002966000
6	-4.228181000	0.407761000	-3.000609000
1	-3.836456000	0.268584000	-4.014901000
1	-5.082163000	-0.268783000	-2.877933000
1	-4.601895000	1.435068000	-2.921648000
6	2.208804000	1.701365000	0.426021000
6	2.238954000	2.919665000	-0.255352000
6	2.842451000	1.617159000	1.673017000
6	2.874130000	4.032766000	0.299657000

1	1.767574000	3.024735000	-1.227390000
6	3.493845000	2.716127000	2.216611000
1	2.803125000	0.682524000	2.225979000
6	3.504951000	3.933087000	1.533533000
1	2.875709000	4.975671000	-0.240433000
1	3.983419000	2.628107000	3.182247000
1	4.001093000	4.797477000	1.965592000
6	2.862052000	-0.776063000	-0.737633000
6	3.741345000	-0.258726000	-1.697873000
6	3.135586000	-2.027007000	-0.183077000
6	4.855452000	-0.984352000	-2.103842000
1	3.562183000	0.724675000	-2.125457000
6	4.254816000	-2.754889000	-0.584875000
1	2.474487000	-2.434801000	0.571809000
6	5.113428000	-2.237797000	-1.548560000
1	5.528125000	-0.571370000	-2.850381000
1	4.451398000	-3.725969000	-0.139713000
1	5.985445000	-2.803717000	-1.864033000
1	-1.828907000	-0.177359000	3.879484000
1	-2.476896000	-1.993627000	3.060081000

E4R

Doordinates (Angstroms)			
	X	Y	Z
25	-0.754035000	0.042526000	-1.071125000
7	-0.969533000	-1.457167000	0.689389000
6	-0.856166000	1.182917000	2.076885000
1	-0.262887000	1.284306000	2.993115000
1	-1.585485000	1.998391000	2.078969000
6	-2.082026000	-3.096581000	-1.557823000
6	-0.129144000	0.919121000	-2.441544000
8	0.367048000	1.412178000	-3.384607000
15	-1.487667000	-1.563976000	-2.422716000
15	0.156536000	1.352879000	0.529602000
14	-2.226151000	-2.657493000	0.271389000
14	-1.732520000	-0.491125000	1.989262000
6	-2.101380000	-4.242569000	1.283044000
1	-2.256569000	-4.072643000	2.353767000
1	-2.845127000	-4.977087000	0.949730000
1	-1.108827000	-4.694105000	1.159563000
6	-1.606417000	-1.287295000	3.699802000
1	-2.006189000	-0.609122000	4.464858000
1	-2.158119000	-2.230897000	3.775140000

1	-0.560306000	-1.495800000	3.959627000
1	-3.034490000	-3.441136000	-1.974809000
1	-1.366070000	-3.914503000	-1.693441000
15	-2.798101000	1.052038000	-1.066813000
6	-4.264437000	0.029901000	-0.549831000
1	-5.139908000	0.662638000	-0.351863000
1	-4.535156000	-0.641978000	-1.375072000
14	-3.779457000	-1.031511000	0.949486000
6	-3.227959000	2.580634000	-0.111840000
1	-3.362721000	2.345151000	0.948631000
1	-2.441156000	3.334985000	-0.198173000
1	-4.166646000	3.012341000	-0.478974000
6	-3.327251000	1.634289000	-2.737204000
1	-3.238789000	0.827769000	-3.471621000
1	-4.361959000	1.996330000	-2.733329000
1	-2.669627000	2.448882000	-3.059059000
6	-5.263596000	-1.491127000	2.023653000
1	-5.734809000	-0.598146000	2.451130000
1	-6.026261000	-2.020371000	1.440274000
1	-4.965659000	-2.142199000	2.853474000
1	0.659387000	-0.692158000	-1.184042000
1	-0.003619000	-1.780330000	0.766650000
6	2.335312000	-2.776494000	-0.414718000
8	1.883639000	-2.967159000	0.703220000
6	1.844624000	0.954047000	1.154546000
6	2.050413000	0.018762000	2.171725000
6	2.960120000	1.573452000	0.581455000
6	3.332795000	-0.261465000	2.634380000
1	1.211541000	-0.501712000	2.623986000
6	4.242053000	1.295464000	1.042716000
1	2.827028000	2.293509000	-0.221585000
6	4.431668000	0.384081000	2.078250000
1	3.469344000	-0.993119000	3.425529000
1	5.096155000	1.788814000	0.588321000
1	5.433248000	0.168070000	2.437921000
6	0.319655000	3.187423000	0.388915000
6	0.664138000	3.958879000	1.506844000
6	0.103567000	3.834017000	-0.829204000
6	0.778965000	5.340657000	1.409584000
1	0.853293000	3.472745000	2.460390000
6	0.222995000	5.220247000	-0.930969000
1	-0.157276000	3.254874000	-1.707545000
6	0.557410000	5.975662000	0.187636000
1	1.045288000	5.923935000	2.286662000

1	0.054735000	5.705574000	-1.888132000
1	0.651163000	7.055110000	0.109206000
6	3.646196000	-2.081698000	-0.621212000
6	3.830691000	-1.158799000	-1.654903000
6	4.719952000	-2.416107000	0.206598000
6	5.080433000	-0.582206000	-1.856883000
1	2.988350000	-0.861083000	-2.272893000
6	5.976191000	-1.863495000	-0.018735000
1	4.564593000	-3.123423000	1.015856000
6	6.157448000	-0.944891000	-1.050433000
1	5.211931000	0.152264000	-2.646020000
1	6.812092000	-2.143332000	0.616136000
1	7.136099000	-0.505075000	-1.221236000
6	1.684359000	-3.353897000	-1.645352000
1	2.345721000	-4.124042000	-2.062853000
1	0.728740000	-3.806483000	-1.379597000
1	1.536043000	-2.592427000	-2.414565000
1	-0.634732000	-2.114178000	-3.408824000
1	-2.581637000	-1.363363000	-3.307125000

E4S

Doordinates (Angstroms)			
	X	Y	Z
25	-0.293558000	-0.473210000	-1.004744000
7	0.854783000	-0.364871000	1.004943000
6	-1.980673000	-0.312274000	1.882620000
1	-2.317955000	0.336816000	2.699249000
1	-2.736231000	-1.096622000	1.780309000
6	2.966171000	-1.492970000	-0.767059000
6	-0.972603000	-0.090055000	-2.565881000
8	-1.344705000	0.247253000	-3.626061000
15	1.571500000	-1.239977000	-1.955851000
15	-1.885578000	0.536622000	0.237210000
14	2.211893000	-1.531304000	0.959301000
14	-0.271740000	-1.062629000	2.205445000
6	3.545528000	-1.118030000	2.224681000
1	3.292014000	-1.443456000	3.239524000
1	4.503867000	-1.577013000	1.953085000
1	3.680804000	-0.029446000	2.246666000
6	0.211302000	-0.667518000	3.989203000
1	-0.552684000	-1.028194000	4.689757000
1	1.164700000	-1.124301000	4.277220000
1	0.312340000	0.415646000	4.136257000

1	3.549890000	-2.388804000	-1.003530000
1	3.648601000	-0.639144000	-0.823916000
15	-1.166158000	-2.575889000	-0.908627000
6	-0.142714000	-3.879872000	-0.066145000
1	-0.729640000	-4.788960000	0.120107000
1	0.681841000	-4.161711000	-0.734186000
14	0.598838000	-3.150015000	1.523388000
6	-2.800868000	-3.028106000	-0.159143000
1	-2.729451000	-3.052787000	0.932988000
1	-3.572901000	-2.305737000	-0.439185000
1	-3.115152000	-4.023483000	-0.494720000
6	-1.429438000	-3.335983000	-2.570435000
1	-0.537171000	-3.214543000	-3.191466000
1	-1.667157000	-4.403400000	-2.493600000
1	-2.257545000	-2.826568000	-3.074907000
6	0.945662000	-4.468635000	2.830538000
1	0.023624000	-4.982379000	3.127470000
1	1.641702000	-5.226994000	2.453101000
1	1.388218000	-4.028615000	3.731463000
1	0.422267000	0.952896000	-1.194149000
1	1.083567000	0.626449000	1.049625000
6	2.842795000	2.600404000	0.439853000
6	1.797142000	3.527084000	-0.114716000
1	1.047554000	2.927292000	-0.648680000
1	1.302621000	4.047283000	0.706020000
1	2.221145000	4.248295000	-0.820571000
8	2.859505000	2.297190000	1.624638000
6	3.860727000	2.026734000	-0.495600000
6	3.631037000	1.954233000	-1.872838000
6	5.049632000	1.512426000	0.033634000
6	4.575194000	1.362122000	-2.707446000
1	2.700438000	2.323744000	-2.291833000
6	5.998452000	0.936984000	-0.802589000
1	5.217658000	1.573864000	1.104008000
6	5.758795000	0.856123000	-2.174555000
1	4.382650000	1.290386000	-3.773623000
1	6.921842000	0.545139000	-0.386422000
1	6.495390000	0.398360000	-2.828529000
6	-1.607469000	2.302169000	0.694254000
6	-1.166047000	2.726226000	1.948653000
6	-1.830105000	3.267506000	-0.297499000
6	-0.983577000	4.083416000	2.219698000
1	-0.963859000	2.008582000	2.738012000
6	-1.654284000	4.618673000	-0.028709000

1	-2.147763000	2.953740000	-1.289217000
6	-1.236204000	5.033170000	1.236945000
1	-0.641454000	4.392120000	3.203514000
1	-1.842763000	5.352118000	-0.807498000
1	-1.099845000	6.089773000	1.448569000
6	-3.670743000	0.635858000	-0.221730000
6	-4.598150000	1.212557000	0.655789000
6	-4.127431000	0.111425000	-1.431966000
6	-5.949676000	1.251785000	0.334922000
1	-4.257056000	1.642260000	1.594465000
6	-5.483178000	0.153300000	-1.758345000
1	-3.420454000	-0.329385000	-2.126402000
6	-6.395883000	0.719568000	-0.875015000
1	-6.657190000	1.700169000	1.026737000
1	-5.821948000	-0.257133000	-2.705386000
1	-7.452133000	0.752422000	-1.126921000
1	2.199744000	-0.512983000	-2.991613000
1	1.612251000	-2.492871000	-2.627975000

TSE2-3

Doordinates (Angstroms)			
	X	Y	Z
25	-0.315010000	-0.476362000	0.906506000
7	-1.347496000	1.345217000	0.086414000
6	0.930758000	0.967330000	-1.859339000
1	1.622001000	1.676292000	-2.327070000
1	0.829411000	0.121898000	-2.551710000
6	-3.690943000	-0.164636000	1.248679000
6	0.502208000	-1.638783000	1.926770000
8	0.999891000	-2.403651000	2.662931000
15	-2.196561000	-0.637450000	2.205867000
15	1.515908000	0.249638000	-0.278225000
14	-3.066023000	1.017597000	-0.107529000
14	-0.809627000	1.688449000	-1.548278000
6	-4.162990000	2.555439000	-0.057471000
1	-3.879623000	3.286801000	-0.823342000
1	-5.219044000	2.301049000	-0.214734000
1	-4.078551000	3.051847000	0.918509000
6	-0.771654000	3.518300000	-2.007078000
1	-0.406560000	3.671328000	-3.030562000
1	-1.764502000	3.976840000	-1.933550000
1	-0.109132000	4.067153000	-1.325265000
1	-4.124315000	-1.062327000	0.793149000

1	-4.464055000	0.284361000	1.885352000
6	-2.211346000	0.620885000	3.546123000
1	-3.145086000	0.594690000	4.119833000
1	-1.367261000	0.442836000	4.219639000
1	-2.084845000	1.616400000	3.108218000
6	-2.682840000	-2.133183000	3.157503000
1	-1.872947000	-2.408078000	3.841515000
1	-3.590933000	-1.947596000	3.741981000
1	-2.863818000	-2.979028000	2.490043000
15	-0.931149000	-2.027327000	-0.672582000
6	-1.738513000	-1.461632000	-2.257836000
1	-0.963073000	-1.455998000	-3.036714000
1	-2.466367000	-2.222302000	-2.571833000
14	-2.542858000	0.278243000	-2.265816000
6	0.395920000	-3.115770000	-1.345222000
1	1.155261000	-2.524769000	-1.865499000
1	0.892180000	-3.639147000	-0.521109000
1	-0.012098000	-3.854591000	-2.045101000
6	-2.110723000	-3.348378000	-0.156730000
1	-3.082087000	-2.917323000	0.102523000
1	-2.261505000	-4.084480000	-0.954706000
1	-1.710349000	-3.862479000	0.723098000
1	0.040607000	0.850974000	1.932240000
1	-0.532129000	1.248250000	1.238263000
6	-3.626000000	0.422412000	-3.811895000
1	-3.039441000	0.258347000	-4.724147000
1	-4.432207000	-0.321320000	-3.798809000
1	-4.086953000	1.413881000	-3.886013000
6	2.395080000	1.633864000	0.563151000
6	2.590518000	2.893894000	-0.003277000
6	2.877905000	1.396321000	1.856537000
6	3.252399000	3.897086000	0.705210000
1	2.225265000	3.116143000	-1.000700000
6	3.551031000	2.389305000	2.557136000
1	2.711083000	0.428555000	2.322720000
6	3.737624000	3.646944000	1.983228000
1	3.387615000	4.874301000	0.250337000
1	3.922117000	2.185932000	3.557587000
1	4.255241000	4.427255000	2.533807000
6	2.954783000	-0.797648000	-0.762062000
6	3.671908000	-0.556762000	-1.938698000
6	3.359963000	-1.847038000	0.068707000
6	4.762370000	-1.351163000	-2.282015000
1	3.380484000	0.255187000	-2.598521000

6	4.455559000	-2.637210000	-0.269582000
1	2.812652000	-2.059866000	0.980415000
6	5.156988000	-2.393866000	-1.447417000
1	5.304447000	-1.153322000	-3.202504000
1	4.755668000	-3.448881000	0.387028000
1	6.007575000	-3.014308000	-1.715092000

TSE4-5R

Doordinates (Angstroms)			
	X	Y	Z
25	-0.654400000	0.038963000	-1.039511000
7	-1.376352000	-1.238490000	0.709585000
6	-0.365595000	1.211260000	2.085369000
1	0.208069000	1.115010000	3.013997000
1	-0.774231000	2.224677000	2.063761000
6	-2.951776000	-2.472042000	-1.482321000
6	0.154603000	0.652269000	-2.455682000
8	0.695775000	0.960609000	-3.450868000
15	-2.031750000	-1.139915000	-2.368826000
15	0.697931000	0.982487000	0.577412000
14	-2.973417000	-1.946151000	0.327589000
14	-1.751251000	-0.072452000	2.013586000
6	-3.401405000	-3.456358000	1.368103000
1	-3.555655000	-3.226650000	2.427429000
1	-4.317367000	-3.931844000	0.995223000
1	-2.593189000	-4.195577000	1.300047000
6	-1.884155000	-0.846230000	3.731919000
1	-2.118052000	-0.073700000	4.475797000
1	-2.663949000	-1.612294000	3.797291000
1	-0.936223000	-1.311470000	4.030757000
1	-3.943798000	-2.648009000	-1.909824000
1	-2.395118000	-3.414154000	-1.546292000
15	-2.181562000	1.758303000	-1.016234000
6	-3.912342000	1.315290000	-0.505458000
1	-4.495816000	2.220215000	-0.290241000
1	-4.411622000	0.809903000	-1.342147000
14	-3.864252000	0.129525000	0.982620000
6	-2.027778000	3.340663000	-0.068388000
1	-2.227798000	3.178704000	0.994570000
1	-1.025769000	3.765909000	-0.174648000
1	-2.757745000	4.070659000	-0.436708000
6	-2.445631000	2.496420000	-2.686349000
1	-2.629448000	1.718152000	-3.432807000

1	-3.287375000	3.198257000	-2.690152000
1	-1.538080000	3.033817000	-2.981715000
6	-5.427287000	0.238738000	2.035583000
1	-5.540912000	1.233927000	2.481492000
1	-6.322954000	0.039384000	1.435573000
1	-5.402525000	-0.493441000	2.850583000
1	0.381599000	-1.238977000	-1.182023000
1	-0.585702000	-1.900875000	0.746931000
6	1.099968000	-2.755951000	-0.912880000
8	0.630620000	-3.187006000	0.159901000
6	2.120509000	0.104537000	1.370490000
6	1.879454000	-0.953536000	2.254109000
6	3.441825000	0.512872000	1.168858000
6	2.920511000	-1.548187000	2.959217000
1	0.873300000	-1.330531000	2.404516000
6	4.485440000	-0.085580000	1.869581000
1	3.664564000	1.314574000	0.472021000
6	4.227634000	-1.105125000	2.780352000
1	2.705584000	-2.360539000	3.647705000
1	5.504352000	0.249860000	1.699283000
1	5.042660000	-1.564340000	3.332588000
6	1.433404000	2.660700000	0.369776000
6	1.776851000	3.437423000	1.484404000
6	1.659848000	3.183494000	-0.905104000
6	2.318755000	4.707768000	1.326455000
1	1.626814000	3.043644000	2.485969000
6	2.207215000	4.456255000	-1.065763000
1	1.409062000	2.598639000	-1.781870000
6	2.533571000	5.222280000	0.048354000
1	2.576758000	5.296746000	2.202136000
1	2.374730000	4.846186000	-2.065638000
1	2.957937000	6.214480000	-0.075770000
6	2.542028000	-2.284431000	-0.978237000
6	3.001339000	-1.364764000	-1.924253000
6	3.464555000	-2.919104000	-0.147830000
6	4.358485000	-1.085081000	-2.035135000
1	2.290006000	-0.851841000	-2.562582000
6	4.826181000	-2.651560000	-0.268329000
1	3.101180000	-3.624021000	0.592940000
6	5.278004000	-1.734784000	-1.212294000
1	4.699383000	-0.358332000	-2.767570000
1	5.533158000	-3.154364000	0.385981000
1	6.339622000	-1.522155000	-1.304769000
6	0.629122000	-3.358330000	-2.231896000

1	1.201521000	-4.282111000	-2.392028000
1	-0.426835000	-3.625840000	-2.174224000
1	0.803807000	-2.698216000	-3.084803000
1	-1.528908000	-1.807850000	-3.507026000
1	-3.116131000	-0.518524000	-3.039657000

TSE4-5S

Doordinates (Angstroms)			
	X	Y	Z
25	0.226452000	-0.070827000	-0.744851000
7	0.841570000	-0.864522000	1.294416000
6	-2.127730000	-1.177525000	1.376834000
1	-2.689578000	-0.911974000	2.279788000
1	-2.755394000	-1.871010000	0.811223000
6	3.411695000	-1.176428000	-0.147660000
6	-0.051177000	0.951905000	-2.133710000
8	-0.155875000	1.693724000	-3.035463000
15	2.319442000	-0.536618000	-1.481724000
15	-1.794578000	0.285894000	0.286375000
14	2.265077000	-1.937346000	1.133955000
14	-0.461671000	-1.975048000	1.797835000
6	3.233093000	-2.161474000	2.732584000
1	2.672256000	-2.688259000	3.511753000
1	4.155388000	-2.726122000	2.547042000
1	3.518494000	-1.178670000	3.127425000
6	-0.479147000	-2.355295000	3.648870000
1	-1.329734000	-3.003054000	3.897867000
1	0.430349000	-2.860662000	3.990651000
1	-0.583835000	-1.434537000	4.237154000
1	4.196629000	-1.841559000	-0.520134000
1	3.891481000	-0.316696000	0.332418000
15	-0.500324000	-1.998736000	-1.782252000
6	0.402632000	-3.555589000	-1.323107000
1	-0.153859000	-4.436938000	-1.668337000
1	1.372062000	-3.574627000	-1.836534000
14	0.713857000	-3.606720000	0.556013000
6	-2.214700000	-2.698091000	-1.733341000
1	-2.410742000	-3.173853000	-0.767979000
1	-2.968181000	-1.924596000	-1.901656000
1	-2.324281000	-3.464812000	-2.508888000
6	-0.304665000	-1.946779000	-3.615871000
1	0.689946000	-1.586377000	-3.893711000
1	-0.463347000	-2.932854000	-4.067394000

1	-1.039699000	-1.247925000	-4.029979000
6	0.855535000	-5.378712000	1.191884000
1	-0.071485000	-5.936934000	1.015392000
1	1.668258000	-5.916195000	0.689174000
1	1.057547000	-5.398529000	2.268810000
1	0.926294000	1.307511000	-0.074939000
1	1.049662000	0.034719000	1.757546000
6	1.892273000	2.203343000	0.886640000
6	0.904227000	3.346083000	1.079783000
1	0.373227000	3.618103000	0.165482000
1	0.185995000	3.075508000	1.850578000
1	1.471880000	4.220759000	1.426236000
8	2.198372000	1.494580000	1.876748000
6	2.960384000	2.486982000	-0.159047000
6	2.665721000	3.065133000	-1.397157000
6	4.289660000	2.204791000	0.153150000
6	3.677111000	3.327827000	-2.313776000
1	1.633462000	3.268969000	-1.663431000
6	5.306689000	2.464657000	-0.763907000
1	4.510038000	1.778497000	1.127286000
6	5.003086000	3.023482000	-2.001881000
1	3.430630000	3.763716000	-3.277981000
1	6.337797000	2.235489000	-0.508276000
1	5.792681000	3.225464000	-2.720320000
6	-2.020252000	1.678419000	1.471845000
6	-1.651841000	1.563300000	2.815246000
6	-2.508009000	2.907343000	1.014288000
6	-1.777539000	2.644408000	3.684677000
1	-1.249464000	0.631145000	3.200554000
6	-2.629968000	3.989363000	1.879826000
1	-2.794610000	3.023219000	-0.027482000
6	-2.267615000	3.860867000	3.219071000
1	-1.485224000	2.534083000	4.724833000
1	-3.011558000	4.935295000	1.506276000
1	-2.363998000	4.704942000	3.895610000
6	-3.377016000	0.442007000	-0.651058000
6	-4.606612000	0.273853000	-0.001283000
6	-3.375628000	0.730616000	-2.017278000
6	-5.801812000	0.374693000	-0.703714000
1	-4.631224000	0.066828000	1.065382000
6	-4.573772000	0.839500000	-2.722775000
1	-2.435978000	0.869634000	-2.538164000
6	-5.787698000	0.656477000	-2.069605000
1	-6.746758000	0.237083000	-0.185863000

1	-4.552300000	1.064682000	-3.785246000
1	-6.721856000	0.737280000	-2.618011000
1	3.113456000	0.448023000	-2.103628000
1	2.521980000	-1.540300000	-2.462833000

E4Ra

Doordinates (Angstroms)			
	X	Y	Z
25	0.352228000	-0.351354000	-1.084135000
7	1.417375000	0.593033000	0.743831000
6	-0.659239000	-1.136532000	2.010642000
1	-1.222223000	-0.751044000	2.868641000
1	-0.727476000	-2.227705000	2.052601000
6	3.564490000	0.860549000	-1.339133000
6	-0.576847000	-0.568179000	-2.542400000
8	-1.176236000	-0.603506000	-3.550981000
15	2.118606000	0.209681000	-2.308224000
15	-1.372507000	-0.598926000	0.378962000
14	3.183914000	0.532561000	0.480144000
14	1.147141000	-0.581411000	2.063224000
6	4.140763000	1.768060000	1.534657000
1	4.004851000	1.595839000	2.607621000
1	5.215466000	1.713220000	1.320636000
1	3.811026000	2.792717000	1.321453000
6	1.457658000	0.126735000	3.788678000
1	1.241474000	-0.629886000	4.554000000
1	2.489611000	0.462292000	3.938405000
1	0.799908000	0.984240000	3.982506000
1	4.492794000	0.370270000	-1.651908000
1	3.697754000	1.932244000	-1.517110000
15	1.054956000	-2.520795000	-0.946453000
6	2.765118000	-2.813815000	-0.277088000
1	2.926150000	-3.875666000	-0.047647000
1	3.492966000	-2.541759000	-1.053103000
14	3.054992000	-1.690109000	1.228659000
6	0.199257000	-3.878726000	-0.019991000
1	0.331814000	-3.751502000	1.059025000
1	-0.872325000	-3.884522000	-0.236475000
1	0.617988000	-4.853490000	-0.296220000
6	1.158993000	-3.360659000	-2.586685000
1	1.720864000	-2.746502000	-3.296667000
1	1.641933000	-4.341593000	-2.508117000
1	0.149025000	-3.494756000	-2.988595000

6	4.324247000	-2.404817000	2.431164000
1	3.984811000	-3.363477000	2.840991000
1	5.286721000	-2.577544000	1.935369000
1	4.498638000	-1.724320000	3.272437000
1	-0.037282000	1.185860000	-1.302859000
1	0.960210000	1.507444000	0.739103000
6	0.579612000	3.997904000	-0.616200000
8	0.458923000	3.563429000	0.515444000
6	-2.408188000	0.836029000	0.914611000
6	-1.967377000	1.718177000	1.904858000
6	-3.654931000	1.068344000	0.323571000
6	-2.768213000	2.775996000	2.327815000
1	-0.990432000	1.591261000	2.362076000
6	-4.454520000	2.128946000	0.738858000
1	-4.015319000	0.404850000	-0.457519000
6	-4.019448000	2.979274000	1.752796000
1	-2.407808000	3.445263000	3.103790000
1	-5.423071000	2.285196000	0.272324000
1	-4.647611000	3.801048000	2.084787000
6	-2.716673000	-1.845962000	0.142480000
6	-3.532717000	-2.223948000	1.217015000
6	-2.938936000	-2.433180000	-1.104478000
6	-4.531764000	-3.176267000	1.052133000
1	-3.390518000	-1.763493000	2.191173000
6	-3.944337000	-3.385543000	-1.274125000
1	-2.323642000	-2.150432000	-1.950716000
6	-4.738078000	-3.762683000	-0.196274000
1	-5.152622000	-3.460611000	1.897149000
1	-4.101002000	-3.833112000	-2.251448000
1	-5.517519000	-4.508268000	-0.325492000
6	1.924004000	4.076690000	-1.296554000
1	2.071976000	5.058218000	-1.761238000
1	2.731339000	3.875818000	-0.589025000
1	1.942313000	3.334786000	-2.103696000
6	-0.597320000	4.540239000	-1.414639000
1	-0.341641000	4.450962000	-2.478335000
6	-1.884018000	3.774206000	-1.133810000
1	-2.163825000	3.865606000	-0.081807000
1	-2.702071000	4.171546000	-1.745566000
1	-1.760256000	2.711044000	-1.359131000
6	-0.744664000	6.035399000	-1.080443000
1	0.168907000	6.601582000	-1.297446000
1	-1.557916000	6.473279000	-1.668910000
1	-0.983912000	6.167335000	-0.019191000

1	2.800363000	-0.723741000	-3.135883000
1	1.989013000	1.193357000	-3.316531000

E4Sa

Doordinates (Angstroms)			
	X	Y	Z
25	0.030031000	-0.331790000	-0.993468000
7	1.258220000	-0.438784000	0.985835000
6	-1.546632000	-0.843028000	1.905583000
1	-1.919952000	-0.387011000	2.830198000
1	-2.216792000	-1.677341000	1.678858000
6	3.392857000	-0.949263000	-1.009699000
6	-0.743408000	0.251626000	-2.443661000
8	-1.189843000	0.735495000	-3.414791000
15	1.927008000	-0.692334000	-2.104961000
15	-1.600543000	0.278719000	0.433354000
14	2.714151000	-1.433085000	0.679826000
14	0.244505000	-1.448732000	2.054971000
6	4.073410000	-1.205234000	1.964446000
1	3.763340000	-1.498230000	2.973387000
1	4.957981000	-1.799115000	1.701843000
1	4.372906000	-0.150998000	1.990984000
6	0.718527000	-1.344477000	3.882934000
1	0.048157000	-1.968466000	4.488255000
1	1.743116000	-1.681347000	4.075198000
1	0.635829000	-0.315777000	4.257926000
1	4.113266000	-1.658318000	-1.429697000
1	3.900857000	0.010614000	-0.858504000
15	-0.620770000	-2.499218000	-1.259355000
6	0.538772000	-3.825365000	-0.665531000
1	0.031706000	-4.797235000	-0.599595000
1	1.351831000	-3.936370000	-1.394937000
14	1.291793000	-3.281711000	0.990753000
6	-2.185093000	-3.232446000	-0.587647000
1	-2.086924000	-3.421421000	0.486118000
1	-3.033729000	-2.559649000	-0.741313000
1	-2.403602000	-4.190431000	-1.074050000
6	-0.851572000	-2.970822000	-3.028762000
1	0.017353000	-2.666034000	-3.620229000
1	-1.002962000	-4.049825000	-3.149247000
1	-1.726443000	-2.446467000	-3.428117000
6	1.836510000	-4.746487000	2.053150000
1	0.984808000	-5.385058000	2.316452000

1	2.566925000	-5.370275000	1.524359000
1	2.301098000	-4.406528000	2.985746000
1	0.569679000	1.169444000	-0.927567000
1	1.393696000	0.556678000	1.152937000
6	2.910826000	2.751179000	-0.154589000
6	1.877886000	3.606741000	0.526474000
1	0.886288000	3.294642000	0.178926000
1	1.936232000	3.470085000	1.607546000
1	1.996484000	4.666843000	0.277388000
8	3.510286000	1.881959000	0.458761000
6	-1.441406000	1.958529000	1.175953000
6	-0.940220000	2.201731000	2.455513000
6	-1.790018000	3.054608000	0.374097000
6	-0.802210000	3.506821000	2.931643000
1	-0.653801000	1.379504000	3.104743000
6	-1.663759000	4.353531000	0.850160000
1	-2.159330000	2.884548000	-0.634595000
6	-1.168187000	4.584768000	2.134238000
1	-0.407927000	3.674625000	3.930045000
1	-1.946831000	5.188916000	0.216039000
1	-1.065413000	5.599949000	2.506536000
6	-3.400460000	0.302867000	0.030196000
6	-4.344684000	0.695428000	0.987678000
6	-3.847300000	-0.089385000	-1.232705000
6	-5.702474000	0.685739000	0.690703000
1	-4.013173000	1.020984000	1.970828000
6	-5.209152000	-0.098980000	-1.533705000
1	-3.126609000	-0.385628000	-1.987130000
6	-6.137987000	0.286407000	-0.573149000
1	-6.422964000	0.994358000	1.442778000
1	-5.539531000	-0.403991000	-2.522644000
1	-7.199031000	0.281429000	-0.806322000
6	3.234498000	3.030038000	-1.616855000
1	3.650768000	2.097678000	-2.016009000
6	4.336529000	4.101853000	-1.666036000
1	4.630404000	4.287697000	-2.704728000
1	3.985150000	5.051586000	-1.244598000
1	5.225571000	3.786894000	-1.109571000
6	2.021573000	3.439090000	-2.454799000
1	2.315973000	3.546849000	-3.504884000
1	1.225977000	2.690180000	-2.393803000
1	1.611585000	4.401909000	-2.127599000
1	2.095166000	-1.799546000	-2.981024000
1	2.398336000	0.275334000	-3.023861000

TSE4-5Ra

Doordinates (Angstroms)

	X	Y	Z
25	0.426257000	-0.003897000	-1.029055000
7	1.452448000	0.886764000	0.794578000
6	-0.449818000	-1.071881000	2.051416000
1	-1.023513000	-0.776384000	2.936748000
1	-0.386061000	-2.162988000	2.062673000
6	3.632925000	1.260237000	-1.290806000
6	-0.483168000	-0.211926000	-2.508874000
8	-1.049559000	-0.240070000	-3.533959000
15	2.217752000	0.563070000	-2.263765000
15	-1.293365000	-0.539558000	0.482829000
14	3.226581000	0.946237000	0.530820000
14	1.289813000	-0.336525000	2.091036000
6	4.085573000	2.250734000	1.582199000
1	3.974152000	2.066730000	2.655932000
1	5.158608000	2.289385000	1.357880000
1	3.665315000	3.242637000	1.372083000
6	1.559173000	0.364740000	3.822917000
1	1.426425000	-0.419024000	4.579727000
1	2.556699000	0.795050000	3.964239000
1	0.825827000	1.153800000	4.034711000
1	4.571227000	0.767861000	-1.569060000
1	3.759903000	2.326111000	-1.502710000
15	1.228742000	-2.178209000	-0.978255000
6	2.973010000	-2.357660000	-0.362636000
1	3.206992000	-3.415376000	-0.183151000
1	3.665203000	-2.011263000	-1.141533000
14	3.243653000	-1.301386000	1.203629000
6	0.519421000	-3.645824000	-0.097225000
1	0.651672000	-3.561431000	0.985093000
1	-0.545186000	-3.762336000	-0.310702000
1	1.039826000	-4.552739000	-0.425918000
6	1.305809000	-2.943168000	-2.655479000
1	1.742166000	-2.258627000	-3.387496000
1	1.884913000	-3.873673000	-2.647946000
1	0.284125000	-3.168231000	-2.980298000
6	4.571957000	-2.025240000	2.331832000
1	4.289011000	-3.023199000	2.686850000
1	5.531004000	-2.118373000	1.809295000
1	4.728956000	-1.389979000	3.210812000

1	0.035161000	1.625774000	-1.207839000
1	0.908629000	1.767811000	0.846928000
6	-0.129645000	3.158504000	-0.801272000
8	-0.296078000	3.191189000	0.441814000
6	-2.547680000	0.615830000	1.193854000
6	-2.132817000	1.619222000	2.073638000
6	-3.903276000	0.534652000	0.861105000
6	-3.049395000	2.515655000	2.612641000
1	-1.083235000	1.731930000	2.321444000
6	-4.821619000	1.433884000	1.396488000
1	-4.252293000	-0.229500000	0.173698000
6	-4.397505000	2.426630000	2.275360000
1	-2.704666000	3.292915000	3.288319000
1	-5.870671000	1.354726000	1.125509000
1	-5.113007000	3.129952000	2.692139000
6	-2.391897000	-1.973879000	0.105702000
6	-2.919911000	-2.773363000	1.127096000
6	-2.730396000	-2.270733000	-1.216862000
6	-3.734067000	-3.861564000	0.831101000
1	-2.696135000	-2.546900000	2.165720000
6	-3.553468000	-3.355749000	-1.515432000
1	-2.349332000	-1.658532000	-2.025276000
6	-4.048506000	-4.159759000	-0.493787000
1	-4.126107000	-4.476676000	1.636131000
1	-3.800800000	-3.571300000	-2.550881000
1	-4.681650000	-5.011237000	-0.726319000
6	1.208139000	3.692577000	-1.317656000
1	1.198513000	4.783718000	-1.204217000
1	2.020488000	3.321800000	-0.691602000
1	1.400332000	3.459348000	-2.368883000
6	-1.301398000	3.426033000	-1.770110000
1	-0.978513000	3.104150000	-2.768861000
6	-2.565056000	2.670986000	-1.395025000
1	-2.892526000	2.941634000	-0.387243000
1	-3.375491000	2.900782000	-2.097681000
1	-2.384662000	1.593438000	-1.422477000
6	-1.575302000	4.938801000	-1.804501000
1	-0.718702000	5.511321000	-2.177009000
1	-2.425414000	5.156609000	-2.461420000
1	-1.820049000	5.303840000	-0.800437000
1	2.909320000	-0.397850000	-3.041917000
1	2.070998000	1.502890000	-3.306586000

TSE4-5Sa

Doordinates (Angstroms)			
	X	Y	Z

25	0.318714000	-0.066230000	-0.949480000
7	1.427021000	0.199238000	1.011306000
6	-1.034670000	-1.226307000	1.902908000
1	-1.553576000	-0.911508000	2.815287000
1	-1.333730000	-2.260225000	1.712531000
6	3.691532000	0.486825000	-0.874494000
6	-0.551609000	0.187263000	-2.444612000
8	-1.091506000	0.432530000	-3.455313000
15	2.301721000	0.106611000	-2.020331000
15	-1.528861000	-0.215963000	0.427115000
14	3.158594000	-0.191523000	0.800382000
14	0.843693000	-1.092806000	2.093138000
6	4.274008000	0.563538000	2.114313000
1	4.089211000	0.166340000	3.117921000
1	5.330138000	0.385381000	1.876466000
1	4.114355000	1.648257000	2.144779000
6	1.197785000	-0.801561000	3.926388000
1	0.771072000	-1.615802000	4.526401000
1	2.268512000	-0.751538000	4.151519000
1	0.744142000	0.135460000	4.274450000
1	4.656792000	0.121689000	-1.238116000
1	3.764019000	1.572647000	-0.741054000
15	0.447512000	-2.357218000	-1.223806000
6	2.005146000	-3.161743000	-0.609722000
1	1.875332000	-4.250911000	-0.560204000
1	2.815145000	-2.973667000	-1.325582000
14	2.501785000	-2.432661000	1.077580000
6	-0.742512000	-3.619627000	-0.575929000
1	-0.597472000	-3.772747000	0.497456000
1	-1.779359000	-3.321910000	-0.750538000
1	-0.570009000	-4.581176000	-1.073057000
6	0.415437000	-2.868399000	-2.996257000
1	1.102039000	-2.260657000	-3.592633000
1	0.682249000	-3.924788000	-3.114576000
1	-0.593639000	-2.715909000	-3.394082000
6	3.511640000	-3.651859000	2.106314000
1	2.933157000	-4.553887000	2.338474000
1	4.417366000	-3.965123000	1.573864000
1	3.821179000	-3.199791000	3.055521000
1	0.429684000	1.638120000	-0.884072000
1	1.247321000	1.210489000	1.156592000
6	0.888368000	3.082940000	-0.382977000

6	-0.505046000	3.698006000	-0.293679000
1	-1.172544000	3.362389000	-1.090371000
1	-0.941854000	3.463854000	0.674271000
1	-0.406359000	4.790659000	-0.361429000
8	1.539055000	2.910621000	0.683800000
6	-2.251136000	1.270247000	1.241975000
6	-1.719438000	1.787258000	2.427115000
6	-3.315760000	1.944087000	0.634677000
6	-2.246223000	2.943602000	2.997842000
1	-0.875473000	1.304956000	2.911634000
6	-3.840519000	3.100590000	1.201283000
1	-3.741452000	1.562871000	-0.289405000
6	-3.308544000	3.603286000	2.386758000
1	-1.816884000	3.333603000	3.916119000
1	-4.668731000	3.608823000	0.715792000
1	-3.718822000	4.506006000	2.829878000
6	-3.093905000	-1.045204000	-0.095715000
6	-4.024900000	-1.465173000	0.863611000
6	-3.378832000	-1.264512000	-1.444711000
6	-5.200092000	-2.102761000	0.483641000
1	-3.832798000	-1.287879000	1.918444000
6	-4.560482000	-1.898481000	-1.828805000
1	-2.677606000	-0.942337000	-2.204633000
6	-5.470029000	-2.323342000	-0.866693000
1	-5.909036000	-2.425511000	1.240659000
1	-4.764134000	-2.059982000	-2.883452000
1	-6.388490000	-2.820998000	-1.164321000
6	1.690350000	3.517387000	-1.630754000
1	2.508048000	2.802196000	-1.741990000
6	2.338746000	4.878082000	-1.339336000
1	3.009812000	5.166627000	-2.157248000
1	1.586670000	5.669931000	-1.236173000
1	2.917113000	4.834030000	-0.411736000
6	0.890182000	3.554481000	-2.929544000
1	1.553655000	3.741201000	-3.782997000
1	0.367217000	2.609854000	-3.104395000
1	0.141672000	4.355685000	-2.916691000
1	2.859868000	-1.001860000	-2.704421000
1	2.479240000	1.027684000	-3.076559000

F1

Doordinates (Angstroms)
X Y Z

25	-1.008057000	0.618035000	0.481895000
1	0.360712000	-0.314682000	0.810231000
7	-0.749457000	-0.128205000	-1.536243000
1	0.025801000	-0.781700000	-1.459277000
6	-1.152087000	1.112708000	2.135852000
8	-1.238121000	1.438720000	3.277975000
6	0.776862000	1.721027000	-1.959118000
6	-1.943444000	-0.894392000	-1.879306000
6	-0.381076000	0.900178000	-2.508970000
1	1.058700000	2.500568000	-2.671179000
1	1.641717000	1.072544000	-1.785482000
1	-0.084499000	0.462074000	-3.473542000
1	-1.254998000	1.536725000	-2.680731000
1	-1.787911000	-1.567522000	-2.732720000
1	-2.732492000	-0.181651000	-2.144369000
6	-2.391404000	-1.673568000	-0.670416000
6	-3.074123000	-2.882326000	-0.785729000
1	-3.254427000	-3.301078000	-1.771012000
6	-2.534984000	-1.753533000	1.629969000
1	-2.289181000	-1.276306000	2.572704000
6	-3.508398000	-3.535378000	0.362166000
1	-4.041487000	-4.478659000	0.294721000
6	-3.235064000	-2.952005000	1.597198000
1	-3.549818000	-3.416055000	2.525804000
7	-2.109853000	-1.115106000	0.526020000
16	0.264456000	2.462671000	-0.367268000
6	1.899749000	2.901488000	0.409637000
6	1.524402000	3.715798000	1.652324000
6	2.709736000	3.764947000	-0.561065000
1	0.885630000	3.134084000	2.324746000
1	2.435572000	3.988316000	2.197922000
1	0.998658000	4.639141000	1.385592000
1	3.046119000	3.192314000	-1.431593000
1	2.130943000	4.625168000	-0.914487000
1	3.603359000	4.143804000	-0.050446000
6	2.700315000	1.668201000	0.823030000
1	3.677177000	1.986126000	1.209357000
1	2.179857000	1.110354000	1.604105000
1	2.875477000	0.986125000	-0.014439000
6	1.279257000	-2.870258000	-0.397020000
8	0.761087000	-2.847185000	-1.508527000
6	2.626004000	-2.245817000	-0.189326000
6	3.224637000	-2.176849000	1.073687000
6	3.295622000	-1.706551000	-1.294695000

6	4.472317000	-1.576912000	1.227728000
1	2.717292000	-2.575941000	1.945764000
6	4.544496000	-1.113032000	-1.142185000
1	2.823801000	-1.756456000	-2.270871000
6	5.134896000	-1.046612000	0.121021000
1	4.924952000	-1.518300000	2.212857000
1	5.054393000	-0.695163000	-2.005123000
1	6.105963000	-0.575835000	0.243850000
6	0.587062000	-3.539019000	0.759132000
1	-0.376559000	-3.927308000	0.424787000
1	1.200665000	-4.359097000	1.148431000
1	0.429487000	-2.821055000	1.569330000
6	-2.671499000	1.627608000	-0.155155000
6	-3.691724000	2.235649000	-0.506940000
6	-4.904519000	2.955252000	-0.934972000
1	-4.699953000	4.012265000	-1.147121000
1	-5.337741000	2.524494000	-1.846909000
1	-5.687831000	2.930360000	-0.167067000

F2

Doordinates (Angstroms)			
	X	Y	Z
25	-0.343839000	-0.021524000	1.264401000
7	-1.592711000	1.233223000	-0.042048000
6	0.471808000	0.431368000	-2.050671000
1	1.060344000	1.083121000	-2.707917000
1	0.427420000	-0.551078000	-2.537938000
6	-3.715451000	0.451721000	1.875958000
6	0.631292000	-0.873786000	2.457211000
8	1.219935000	-1.434379000	3.298098000
15	-2.099906000	0.185854000	2.721119000
15	1.282185000	0.197364000	-0.415126000
14	-3.283024000	0.856436000	0.058685000
14	-1.304486000	1.047960000	-1.742217000
6	-4.519392000	2.213585000	-0.421482000
1	-4.488609000	2.461782000	-1.488658000
1	-5.546864000	1.903894000	-0.187490000
1	-4.312658000	3.135417000	0.139166000
6	-1.577532000	2.555419000	-2.854419000
1	-1.363802000	2.311614000	-3.903461000
1	-2.609361000	2.920484000	-2.803141000
1	-0.924537000	3.389371000	-2.566012000
1	-4.347637000	-0.434422000	1.984218000

1	-4.257108000	1.284866000	2.337161000
15	-1.147438000	-2.056895000	0.499281000
6	-1.892569000	-2.178564000	-1.182475000
1	-1.075432000	-2.297363000	-1.907289000
1	-2.487106000	-3.100997000	-1.238380000
14	-2.937970000	-0.652118000	-1.720293000
6	0.024968000	-3.483279000	0.518763000
1	0.846506000	-3.334675000	-0.184578000
1	0.453276000	-3.595309000	1.520213000
1	-0.488940000	-4.412980000	0.249316000
6	-2.488416000	-2.854195000	1.488557000
1	-3.413502000	-2.273248000	1.444755000
1	-2.702067000	-3.855375000	1.098174000
1	-2.182044000	-2.951426000	2.535133000
6	-4.149288000	-1.255407000	-3.051886000
1	-3.615907000	-1.733731000	-3.883195000
1	-4.858597000	-1.988867000	-2.647777000
1	-4.730425000	-0.423005000	-3.464853000
6	2.509547000	-1.150301000	-0.810360000
6	3.415457000	-0.886273000	-2.034306000
6	3.351587000	-1.629738000	0.377813000
6	4.628814000	-1.840725000	-2.064843000
1	2.825625000	-1.008801000	-2.949575000
6	3.977056000	-3.007214000	0.074787000
1	4.142801000	-0.895266000	0.569753000
6	4.288779000	-3.186817000	-1.424359000
1	4.968669000	-1.973823000	-3.097911000
1	3.297167000	-3.801019000	0.407085000
1	3.420634000	-3.617685000	-1.941535000
1	1.838193000	-1.974417000	-1.083597000
1	2.754399000	-1.687364000	1.290433000
1	4.896265000	-3.119059000	0.661560000
1	5.109426000	-3.900039000	-1.557850000
1	5.468694000	-1.392584000	-1.517995000
1	3.780395000	0.146486000	-2.037992000
6	2.332795000	1.731677000	-0.233352000
6	1.515591000	3.023159000	-0.403895000
6	3.113976000	1.718224000	1.111492000
6	2.415795000	4.270777000	-0.353838000
1	0.987568000	3.009190000	-1.361478000
6	3.199147000	3.106436000	1.759535000
1	2.664762000	1.015693000	1.823524000
6	3.532346000	4.165097000	0.709505000
1	2.865282000	4.434819000	-1.340698000

1	3.957270000	3.093048000	2.550673000
1	4.480234000	3.886299000	0.230014000
1	3.701062000	5.138748000	1.182346000
1	2.245662000	3.353689000	2.245369000
1	4.131146000	1.353867000	0.924514000
1	3.057539000	1.718409000	-1.056791000
1	0.736807000	3.086413000	0.362523000
1	1.784601000	5.144023000	-0.152778000
1	-2.068707000	1.266439000	3.629700000
1	-2.385694000	-0.809886000	3.681643000
1	0.484778000	1.501255000	1.589493000
1	-0.105820000	1.520365000	2.109695000

F3

Doordinates (Angstroms)			
	X	Y	Z
25	-0.359794000	-0.154501000	1.212585000
7	-1.627065000	1.367053000	-0.045914000
6	0.507324000	0.548809000	-2.018360000
1	1.083882000	1.278410000	-2.600941000
1	0.522257000	-0.393666000	-2.580882000
6	-3.644781000	0.459592000	1.971941000
6	0.625991000	-0.972706000	2.396332000
8	1.248112000	-1.464308000	3.262227000
15	-1.979276000	0.105424000	2.722723000
15	1.264023000	0.216588000	-0.351511000
14	-3.334791000	0.861553000	0.151050000
14	-1.288727000	1.069086000	-1.779324000
6	-4.573851000	2.198313000	-0.351862000
1	-4.534712000	2.441299000	-1.419541000
1	-5.597343000	1.871952000	-0.126726000
1	-4.396060000	3.126078000	0.207651000
6	-1.652687000	2.567927000	-2.866253000
1	-1.480500000	2.329990000	-3.923441000
1	-2.684943000	2.920474000	-2.766917000
1	-0.990131000	3.404909000	-2.609564000
1	-4.290051000	-0.418932000	2.076898000
1	-4.152860000	1.288343000	2.478615000
15	-1.165656000	-2.118429000	0.416303000
6	-2.036150000	-2.239751000	-1.227523000
1	-1.276349000	-2.405642000	-2.003949000
1	-2.709501000	-3.106785000	-1.256763000
14	-2.920834000	-0.613327000	-1.634273000

6	0.024779000	-3.523504000	0.258501000
1	0.796252000	-3.291921000	-0.479044000
1	0.515500000	-3.692680000	1.222589000
1	-0.483050000	-4.445484000	-0.048639000
6	-2.416940000	-2.999101000	1.461126000
1	-3.359681000	-2.442865000	1.497426000
1	-2.627403000	-4.002571000	1.073118000
1	-2.035322000	-3.095405000	2.483367000
6	-4.240093000	-0.826659000	-2.969709000
1	-3.805746000	-1.223199000	-3.895040000
1	-5.020262000	-1.525250000	-2.644831000
1	-4.723277000	0.127620000	-3.208002000
6	2.526669000	-1.077106000	-0.844324000
6	3.560387000	-0.654227000	-1.909483000
6	3.241048000	-1.773661000	0.320476000
6	4.714923000	-1.675895000	-2.029558000
1	3.057636000	-0.539321000	-2.877190000
6	3.846737000	-3.114590000	-0.148389000
1	4.033557000	-1.116568000	0.697778000
6	4.262777000	-3.081261000	-1.632377000
1	5.116086000	-1.667705000	-3.049336000
1	3.121347000	-3.922108000	0.010026000
1	3.418696000	-3.378882000	-2.269366000
1	1.871804000	-1.828671000	-1.307178000
1	2.560575000	-1.944922000	1.156195000
1	4.716717000	-3.352255000	0.475299000
1	5.058521000	-3.811044000	-1.819273000
1	5.540919000	-1.376748000	-1.371048000
1	3.989660000	0.322682000	-1.663574000
6	2.282973000	1.761500000	-0.125503000
6	1.433923000	3.036175000	-0.044760000
6	3.197096000	1.641228000	1.116603000
6	2.326108000	4.292461000	-0.080302000
1	0.712847000	3.085781000	-0.870211000
6	3.521632000	3.010570000	1.739184000
1	2.719193000	1.006289000	1.870939000
6	3.667776000	4.074582000	0.651018000
1	2.518658000	4.581906000	-1.120898000
1	4.436741000	2.937044000	2.337651000
1	4.433258000	3.741655000	-0.063089000
1	4.028579000	5.019823000	1.071805000
1	2.719979000	3.303052000	2.429448000
1	4.130458000	1.146092000	0.820639000
1	2.907527000	1.858996000	-1.022996000

1	0.854175000	3.005522000	0.883610000
1	1.782088000	5.126323000	0.379777000
1	-1.286407000	2.215964000	0.398887000
1	0.214575000	1.190934000	1.868533000
1	-1.906159000	1.149866000	3.671837000
1	-2.321620000	-0.903025000	3.657580000

F4R

Doordinates (Angstroms)			
	X	Y	Z
25	-0.834805000	-0.310378000	-1.070565000
7	0.114697000	-1.542111000	0.671368000
6	-1.366879000	0.640091000	2.082690000
1	-0.878690000	1.124446000	2.938768000
1	-2.442512000	0.787136000	2.214157000
6	0.278457000	-3.526707000	-1.503766000
6	-1.036086000	0.717747000	-2.466402000
8	-1.043776000	1.391266000	-3.427039000
15	-0.478361000	-2.079177000	-2.374516000
15	-0.858887000	1.375477000	0.450408000
14	-0.073048000	-3.282801000	0.331888000
14	-0.979348000	-1.213464000	2.036974000
6	1.083029000	-4.390447000	1.325038000
1	0.941458000	-4.282749000	2.406045000
1	0.922833000	-5.446525000	1.073734000
1	2.124961000	-4.141550000	1.091427000
6	-0.251392000	-1.662910000	3.725979000
1	-0.936918000	-1.364807000	4.529845000
1	-0.059365000	-2.735701000	3.838741000
1	0.698726000	-1.138706000	3.893050000
1	-0.051572000	-4.485904000	-1.914543000
1	1.369131000	-3.471327000	-1.597768000
15	-3.038658000	-0.865900000	-0.845227000
6	-3.416439000	-2.592963000	-0.275113000
1	-4.476760000	-2.706352000	-0.013768000
1	-3.212068000	-3.289920000	-1.098090000
14	-2.252284000	-3.014801000	1.165783000
6	-4.279054000	-0.013759000	0.244258000
1	-4.087647000	-0.246691000	1.296600000
1	-4.240743000	1.070558000	0.119651000
1	-5.295084000	-0.349398000	0.004800000
6	-3.983739000	-0.782667000	-2.428996000
1	-3.451143000	-1.328033000	-3.214459000

1	-4.991530000	-1.202404000	-2.326921000
1	-4.066640000	0.261582000	-2.749472000
6	-3.011266000	-4.271662000	2.355783000
1	-3.915412000	-3.871983000	2.830374000
1	-3.292201000	-5.193055000	1.832070000
1	-2.307195000	-4.540522000	3.151335000
1	0.725409000	-0.001370000	-1.323031000
1	1.052720000	-1.155707000	0.612528000
6	3.666352000	-1.326693000	-1.129686000
8	3.084763000	-2.068765000	-0.352130000
6	4.770939000	-0.444828000	-0.634255000
6	5.469716000	0.428279000	-1.475099000
6	5.116268000	-0.511692000	0.719982000
6	6.500163000	1.215202000	-0.969880000
1	5.210842000	0.508136000	-2.525748000
6	6.144563000	0.273968000	1.224031000
1	4.562495000	-1.186764000	1.364267000
6	6.839684000	1.137826000	0.378621000
1	7.035714000	1.891700000	-1.628830000
1	6.403978000	0.215504000	2.276916000
1	7.643078000	1.753890000	0.771856000
6	3.298165000	-1.277291000	-2.590001000
1	4.180518000	-1.346826000	-3.234258000
1	2.617577000	-2.096128000	-2.823474000
1	2.784943000	-0.332148000	-2.801918000
6	-1.894249000	2.956151000	0.285413000
6	-2.731249000	3.019571000	-1.014367000
6	-2.748009000	3.317507000	1.509365000
6	-3.946695000	3.952211000	-0.883642000
1	-2.085667000	3.369096000	-1.827337000
6	-3.264372000	4.767330000	1.408385000
1	-3.597436000	2.627339000	1.587070000
6	-3.592312000	5.178206000	-0.042348000
1	-4.293305000	4.247851000	-1.880326000
1	-2.513363000	5.451631000	1.821503000
1	-2.723102000	5.671059000	-0.497682000
6	0.744093000	2.217993000	0.915511000
6	1.797262000	1.312058000	1.563694000
6	1.373308000	2.919987000	-0.297652000
6	3.005032000	2.138484000	2.020593000
1	1.381563000	0.765944000	2.419179000
6	2.587475000	3.756237000	0.120054000
1	1.673751000	2.149058000	-1.019001000
6	3.627249000	2.902524000	0.850015000

1	2.681327000	2.849071000	2.795299000
1	2.254255000	4.572231000	0.778054000
1	4.459208000	3.525860000	1.199769000
1	-1.138096000	3.746969000	0.215057000
1	-3.059208000	2.022406000	-1.318086000
1	-4.784640000	3.421632000	-0.409340000
1	-4.405403000	5.912503000	-0.054033000
1	-4.156926000	4.868655000	2.037505000
1	-2.174075000	3.202263000	2.434947000
1	0.646577000	3.558509000	-0.814621000
1	0.464762000	2.983884000	1.658235000
1	2.133305000	0.569797000	0.826861000
1	3.038887000	4.225387000	-0.762750000
1	4.048665000	2.178532000	0.142301000
1	3.753839000	1.483769000	2.481464000
1	0.333239000	-1.972331000	-3.529030000
1	-1.543695000	-2.754873000	-3.035277000

F4S

Doordinates (Angstroms)			
	X	Y	Z
25	0.299859000	0.375809000	-0.951985000
7	-0.898778000	0.432748000	1.039749000
6	1.928327000	0.390162000	2.017127000
1	2.157659000	-0.284499000	2.852199000
1	2.701628000	1.166802000	2.018660000
6	-2.961440000	1.517554000	-0.822526000
6	0.969763000	-0.091074000	-2.491222000
8	1.320115000	-0.475085000	-3.544541000
15	-1.603352000	0.950267000	-1.956562000
15	1.970382000	-0.478923000	0.371691000
14	-2.229566000	1.620129000	0.913322000
14	0.221228000	1.171560000	2.220737000
6	-3.582161000	1.310924000	2.192820000
1	-3.353501000	1.753321000	3.168445000
1	-4.544585000	1.717014000	1.859138000
1	-3.696504000	0.229369000	2.332587000
6	-0.316546000	0.901728000	4.014310000
1	0.425886000	1.317057000	4.708194000
1	-1.282385000	1.363772000	4.246630000
1	-0.405316000	-0.171129000	4.230859000
1	-3.370244000	2.477794000	-1.155589000
1	-3.786706000	0.798911000	-0.837553000

15	1.092688000	2.507333000	-1.063107000
6	0.132107000	3.865127000	-0.224221000
1	0.744571000	4.766992000	-0.094660000
1	-0.707907000	4.143205000	-0.875367000
14	-0.595392000	3.232726000	1.410519000
6	2.786406000	3.016270000	-0.511942000
1	2.931001000	2.824781000	0.555965000
1	3.539468000	2.454323000	-1.072676000
1	2.953870000	4.084266000	-0.695144000
6	1.212858000	3.178026000	-2.781285000
1	0.253374000	3.087827000	-3.299559000
1	1.516986000	4.231363000	-2.785083000
1	1.948861000	2.594732000	-3.344772000
6	-0.934886000	4.629540000	2.637386000
1	-0.009776000	5.152616000	2.907553000
1	-1.624772000	5.371001000	2.217365000
1	-1.381483000	4.243548000	3.561042000
1	-0.309115000	-1.114694000	-0.995750000
1	-1.155384000	-0.548435000	1.122986000
6	-3.219336000	-2.512339000	0.241633000
6	-2.409094000	-3.540564000	-0.504965000
1	-1.675670000	-3.019599000	-1.135065000
1	-1.869215000	-4.161332000	0.212031000
1	-3.033130000	-4.171046000	-1.145494000
8	-2.974608000	-2.233291000	1.406084000
6	-4.333061000	-1.820199000	-0.479141000
6	-4.383835000	-1.765256000	-1.875490000
6	-5.325132000	-1.178517000	0.270281000
6	-5.398386000	-1.055160000	-2.511344000
1	-3.617148000	-2.251659000	-2.470788000
6	-6.349511000	-0.488200000	-0.365080000
1	-5.281526000	-1.232206000	1.352901000
6	-6.381854000	-0.418296000	-1.757914000
1	-5.419696000	-0.998232000	-3.595388000
1	-7.120228000	0.000837000	0.223258000
1	-7.176916000	0.129143000	-2.255808000
6	1.826608000	-2.260671000	0.897392000
6	0.486089000	-2.581688000	1.563041000
6	2.071857000	-3.196209000	-0.309106000
6	0.482980000	-4.005904000	2.148381000
1	0.258422000	-1.870466000	2.365960000
6	1.360975000	-4.553536000	-0.160052000
1	1.728981000	-2.710642000	-1.229931000
6	1.318049000	-4.990803000	1.304140000

1	0.872118000	-3.984980000	3.173843000
1	1.866973000	-5.305779000	-0.775900000
1	2.346487000	-5.032554000	1.687986000
6	3.792066000	-0.302651000	-0.040113000
6	4.778918000	-0.979216000	0.934467000
6	4.174532000	-0.637080000	-1.486849000
6	6.215929000	-1.015672000	0.364237000
1	4.765061000	-0.442922000	1.891269000
6	5.536507000	0.001312000	-1.841116000
1	4.229798000	-1.725587000	-1.607418000
6	6.461984000	0.131508000	-0.615611000
1	6.944414000	-0.992905000	1.182702000
1	5.377052000	0.991696000	-2.285450000
1	6.279834000	1.086011000	-0.103226000
1	3.927418000	0.778422000	0.071039000
1	3.412321000	-0.288475000	-2.185241000
1	6.026456000	-0.605914000	-2.611693000
1	7.510749000	0.150129000	-0.933131000
1	6.375580000	-1.964610000	-0.164239000
1	4.471187000	-2.007539000	1.149356000
1	2.605696000	-2.432233000	1.651460000
1	3.151468000	-3.359703000	-0.415007000
1	0.336743000	-4.476253000	-0.544836000
1	0.913600000	-6.005240000	1.397275000
1	-0.555561000	-4.350932000	2.221158000
1	-0.302454000	-2.474190000	0.813756000
1	-2.295284000	0.008523000	-2.752073000
1	-1.656031000	1.986185000	-2.927595000

TSF2-3

Doordinates (Angstroms)			
	X	Y	Z
25	-0.510968000	-0.439429000	1.170711000
7	-1.559353000	1.354048000	0.266872000
6	0.459796000	0.692611000	-1.878231000
1	1.106453000	1.358649000	-2.460016000
1	0.294793000	-0.207849000	-2.484155000
6	-3.786765000	0.223775000	1.945152000
6	0.432598000	-1.503491000	2.202659000
8	1.012638000	-2.188267000	2.951638000
15	-2.234410000	-0.499320000	2.639513000
15	1.206467000	0.150537000	-0.289802000
14	-3.291455000	1.074379000	0.315520000
14	-1.230664000	1.458368000	-1.457024000
6	-4.363440000	2.628930000	0.188117000
1	-4.247853000	3.141635000	-0.773949000
1	-5.427256000	2.384921000	0.306407000
1	-4.094342000	3.342841000	0.977956000
6	-1.262883000	3.209434000	-2.163118000
1	-1.057172000	3.207876000	-3.241121000
1	-2.229640000	3.701759000	-2.008245000
1	-0.497366000	3.828958000	-1.676933000
1	-4.519636000	-0.570208000	1.765542000
1	-4.245179000	0.929972000	2.646356000
15	-1.374156000	-2.148586000	-0.089258000
6	-2.252856000	-1.741023000	-1.674501000
1	-1.514117000	-1.792206000	-2.486649000
1	-2.993025000	-2.523953000	-1.890708000
14	-3.051145000	0.000962000	-1.760721000
6	-0.255553000	-3.510248000	-0.633894000
1	0.540630000	-3.124638000	-1.276051000
1	0.208433000	-3.973541000	0.243335000
1	-0.804718000	-4.279383000	-1.189655000
6	-2.660434000	-3.194097000	0.724051000
1	-3.559828000	-2.607562000	0.938310000
1	-2.947827000	-4.038132000	0.086665000
1	-2.271545000	-3.587726000	1.669336000
1	-0.044231000	0.966108000	2.050613000
1	-0.660759000	1.310145000	1.373967000
6	-4.319076000	0.001493000	-3.166480000
1	-3.852800000	-0.284025000	-4.117434000

1	-5.132976000	-0.707404000	-2.969964000
1	-4.765808000	0.993712000	-3.298117000
6	2.029087000	1.713580000	0.315774000
6	2.955061000	1.443571000	1.509568000
6	2.713340000	2.626363000	-0.730325000
6	3.273891000	2.751021000	2.260629000
1	2.489263000	0.729425000	2.197413000
6	3.776872000	3.536670000	-0.087695000
1	3.176249000	2.051739000	-1.535591000
6	3.346941000	3.967849000	1.314793000
1	2.506725000	2.925455000	3.024157000
1	3.952360000	4.408094000	-0.728847000
1	2.363287000	4.451259000	1.247168000
6	2.530146000	-1.045577000	-0.831544000
6	3.668125000	-0.494384000	-1.700271000
6	3.090579000	-1.881073000	0.344658000
6	4.459153000	-1.646453000	-2.355420000
1	3.279655000	0.163925000	-2.484079000
6	4.462656000	-2.496765000	0.019550000
1	3.172183000	-1.278321000	1.253207000
6	4.537004000	-2.895630000	-1.453666000
1	3.992540000	-1.912076000	-3.311649000
1	4.641646000	-3.359301000	0.670774000
1	3.702629000	-3.574512000	-1.676445000
1	4.034169000	4.720253000	1.717320000
1	4.734929000	3.003686000	-0.020085000
1	1.943684000	3.249717000	-1.201645000
1	3.882597000	0.980084000	1.149176000
1	1.167663000	2.266112000	0.711749000
1	4.225690000	2.633035000	2.792208000
1	1.956332000	-1.724178000	-1.478291000
1	2.375788000	-2.676983000	0.575767000
1	4.335543000	0.115091000	-1.078735000
1	5.260942000	-1.774185000	0.236156000
1	5.454851000	-3.456143000	-1.662871000
1	5.469798000	-1.291858000	-2.590360000
1	-2.079482000	0.249719000	3.825562000
1	-2.682966000	-1.687193000	3.258979000

TSF4-5R

Doordinates (Angstroms)			
	X	Y	Z
25	-0.633803000	-0.113561000	-1.025469000

7	-1.243390000	-1.348737000	0.778042000
6	-0.605816000	1.338163000	1.974618000
1	-0.090535000	1.445349000	2.937290000
1	-1.180556000	2.254209000	1.828809000
6	-2.756932000	-2.817724000	-1.359516000
6	0.156570000	0.533770000	-2.447684000
8	0.713893000	0.863644000	-3.423979000
15	-1.893050000	-1.477535000	-2.303605000
15	0.588496000	1.147051000	0.559465000
14	-2.734355000	-2.283953000	0.451202000
14	-1.773975000	-0.145869000	1.991863000
6	-2.903604000	-3.808656000	1.539240000
1	-2.916255000	-3.568507000	2.607700000
1	-3.824081000	-4.358478000	1.307117000
1	-2.056123000	-4.481702000	1.358758000
6	-1.871152000	-0.806751000	3.761836000
1	-2.165477000	0.000940000	4.444792000
1	-2.609092000	-1.609499000	3.871060000
1	-0.907507000	-1.197576000	4.110936000
1	-3.771092000	-2.983045000	-1.738235000
1	-2.219496000	-3.765719000	-1.463554000
15	-2.414783000	1.391692000	-1.098342000
6	-4.068367000	0.683171000	-0.635000000
1	-4.814937000	1.483050000	-0.544276000
1	-4.418354000	0.017693000	-1.433762000
14	-3.894600000	-0.313285000	0.981067000
6	-2.625156000	2.999919000	-0.191453000
1	-2.880649000	2.822170000	0.857313000
1	-1.721846000	3.611765000	-0.231004000
1	-3.445213000	3.571201000	-0.641333000
6	-2.722804000	2.035790000	-2.801388000
1	-2.698120000	1.227698000	-3.537428000
1	-3.690611000	2.545685000	-2.868981000
1	-1.934076000	2.748171000	-3.066287000
6	-5.469078000	-0.277510000	2.022176000
1	-5.746414000	0.752640000	2.275973000
1	-6.313983000	-0.727664000	1.488506000
1	-5.333376000	-0.827237000	2.960369000
1	0.503489000	-1.360595000	-1.134677000
1	-0.383910000	-1.907512000	0.875540000
6	1.251705000	-2.870175000	-0.847529000
8	0.872418000	-3.233108000	0.286501000
6	2.678175000	-2.393868000	-1.052989000
6	3.054667000	-1.555982000	-2.105985000

6	3.663326000	-2.927713000	-0.223790000
6	4.392276000	-1.237708000	-2.308612000
1	2.291050000	-1.122134000	-2.742848000
6	5.006706000	-2.618670000	-0.432333000
1	3.363588000	-3.582389000	0.589023000
6	5.374169000	-1.768521000	-1.470677000
1	4.670178000	-0.567166000	-3.116999000
1	5.765223000	-3.037598000	0.223414000
1	6.420039000	-1.521223000	-1.629706000
6	0.732461000	-3.604786000	-2.077014000
1	1.343879000	-4.510870000	-2.185706000
1	-0.300765000	-3.919493000	-1.933749000
1	0.828808000	-3.022602000	-2.995994000
6	1.184230000	2.903566000	0.195125000
6	0.815802000	3.431202000	-1.210561000
6	0.857497000	3.941274000	1.279899000
6	0.799294000	4.967413000	-1.269287000
1	1.546102000	3.046199000	-1.930158000
6	1.694383000	5.220849000	1.081508000
1	-0.209941000	4.190753000	1.247026000
6	1.920932000	5.550432000	-0.409159000
1	0.893715000	5.296390000	-2.310104000
1	2.663109000	5.103990000	1.581927000
1	2.874551000	5.123561000	-0.747152000
6	2.072222000	0.614050000	1.583192000
6	1.847519000	-0.692726000	2.355483000
6	3.412337000	0.530178000	0.841146000
6	2.966697000	-0.907733000	3.381199000
1	0.890031000	-0.678136000	2.886011000
6	4.560006000	0.323154000	1.838353000
1	3.380879000	-0.300294000	0.134728000
6	4.346149000	-0.910905000	2.719720000
1	2.921369000	-0.105565000	4.132795000
1	4.644035000	1.215818000	2.476370000
1	5.132688000	-0.970508000	3.482384000
1	2.273866000	2.799073000	0.210996000
1	-0.148711000	3.038665000	-1.539153000
1	-0.165729000	5.351664000	-0.909249000
1	2.000561000	6.633800000	-0.551050000
1	1.186467000	6.056475000	1.578084000
1	1.044631000	3.534800000	2.279618000
1	3.613085000	1.432947000	0.253838000
1	2.159212000	1.425439000	2.326220000
1	1.808659000	-1.535651000	1.655051000

1	5.507549000	0.231947000	1.293723000
1	4.435135000	-1.808325000	2.097997000
1	2.804567000	-1.851957000	3.915287000
1	-1.323585000	-2.184181000	-3.384196000
1	-2.991953000	-0.976220000	-3.046528000

TSF4-5S

Doordinates (Angstroms)			
	X	Y	Z
25	-0.270983000	0.211357000	-0.794051000
7	-0.977992000	0.668192000	1.317423000
6	1.968468000	1.255994000	1.425271000
1	2.586508000	1.024146000	2.302234000
1	2.485065000	2.051699000	0.883811000
6	-3.532671000	0.969684000	-0.159118000
6	0.139570000	-0.556394000	-2.309059000
8	0.327370000	-1.135289000	-3.311502000
15	-2.352013000	0.668602000	-1.539414000
15	1.779626000	-0.208652000	0.292136000
14	-2.487452000	1.626264000	1.260918000
14	0.236911000	1.823738000	1.940313000
6	-3.495079000	1.535971000	2.848146000
1	-2.973651000	1.960486000	3.712648000
1	-4.446865000	2.069883000	2.735577000
1	-3.725757000	0.487759000	3.076514000
6	0.229920000	2.040128000	3.819711000
1	0.975206000	2.793228000	4.107670000
1	-0.740512000	2.377871000	4.200920000
1	0.484034000	1.110989000	4.344841000
1	-4.367035000	1.616140000	-0.448474000
1	-3.946797000	0.004476000	0.151399000
15	0.335645000	2.341365000	-1.527149000
6	-0.763859000	3.718402000	-0.929226000
1	-0.307287000	4.693386000	-1.144057000
1	-1.716121000	3.690799000	-1.471537000
14	-1.092258000	3.488986000	0.931740000
6	1.931475000	3.282056000	-1.353320000
1	2.063578000	3.649097000	-0.331150000
1	2.804206000	2.681237000	-1.621675000
1	1.909335000	4.153994000	-2.017097000
6	0.197373000	2.486584000	-3.362603000
1	-0.727609000	2.029965000	-3.724599000
1	0.228356000	3.532987000	-3.687154000

1	1.034119000	1.951231000	-3.824728000
6	-1.403073000	5.126555000	1.820108000
1	-0.543100000	5.800942000	1.731880000
1	-2.275278000	5.644112000	1.403570000
1	-1.591082000	4.961891000	2.887316000
1	-0.996292000	-1.253503000	-0.438154000
1	-1.082221000	-0.298699000	1.652537000
6	-1.839069000	-2.450988000	0.402730000
6	-0.774635000	-3.504769000	0.140482000
1	-0.484628000	-3.575100000	-0.909385000
1	0.104614000	-3.280000000	0.733526000
1	-1.177584000	-4.475740000	0.460418000
8	-2.004512000	-2.016167000	1.562923000
6	-3.043642000	-2.556379000	-0.516422000
6	-2.930565000	-2.808930000	-1.886766000
6	-4.315336000	-2.481041000	0.053512000
6	-4.067878000	-2.970814000	-2.671290000
1	-1.949431000	-2.836810000	-2.351612000
6	-5.456217000	-2.640943000	-0.729747000
1	-4.392358000	-2.299383000	1.121291000
6	-5.335034000	-2.885876000	-2.094965000
1	-3.964494000	-3.154610000	-3.737026000
1	-6.439378000	-2.579385000	-0.271368000
1	-6.222998000	-3.013241000	-2.707785000
6	2.268973000	-1.524539000	1.539541000
6	1.251474000	-1.660381000	2.683117000
6	2.636513000	-2.902270000	0.938213000
6	1.824171000	-2.505430000	3.841398000
1	0.981982000	-0.675705000	3.077135000
6	2.452425000	-4.049811000	1.948031000
1	2.066606000	-3.107791000	0.025868000
6	2.812453000	-3.584935000	3.357971000
1	2.326492000	-1.851659000	4.564951000
1	3.070362000	-4.903272000	1.646426000
1	3.834629000	-3.182299000	3.346860000
6	3.277509000	-0.089193000	-0.814235000
6	4.620636000	0.228132000	-0.125602000
6	3.464967000	-1.252376000	-1.800964000
6	5.816975000	-0.027789000	-1.068733000
1	4.622628000	1.276188000	0.197816000
6	4.340042000	-0.783358000	-2.979912000
1	3.955989000	-2.088464000	-1.293787000
6	5.428974000	0.215164000	-2.528993000
1	6.661769000	0.607445000	-0.779276000

1	3.704854000	-0.317349000	-3.742830000
1	5.061081000	1.245362000	-2.631095000
1	3.000245000	0.770748000	-1.433579000
1	2.509500000	-1.628428000	-2.173064000
1	4.804677000	-1.657878000	-3.450421000
1	6.307108000	0.139664000	-3.179495000
1	6.160286000	-1.064918000	-0.961817000
1	4.744721000	-0.375756000	0.781082000
1	3.182639000	-1.118493000	1.994853000
1	3.690594000	-2.871916000	0.640266000
1	1.413711000	-4.403909000	1.945581000
1	2.820848000	-4.427989000	4.057489000
1	0.990509000	-2.978263000	4.373693000
1	0.316777000	-2.093318000	2.316382000
1	-3.035486000	-0.261190000	-2.346688000
1	-2.638267000	1.799440000	-2.347606000

F4Ra

Doordinates (Angstroms)			
	X	Y	Z
25	0.241942000	0.351504000	-0.954479000
7	-0.323801000	1.565118000	0.973125000
6	1.610709000	-0.410915000	2.040520000
1	1.318415000	-0.873765000	2.992493000
1	2.698057000	-0.524634000	1.962118000
6	-1.282929000	3.419217000	-1.115387000
6	0.164756000	-0.687397000	-2.354633000
8	-0.017916000	-1.352748000	-3.303671000
15	-0.662293000	2.002856000	-2.139183000
15	0.825266000	-1.250645000	0.573559000
14	-0.402317000	3.296678000	0.551295000
14	1.116547000	1.412959000	2.016768000
6	-1.384026000	4.320355000	1.795401000
1	-0.907703000	4.370362000	2.780218000
1	-1.513669000	5.348643000	1.435395000
1	-2.386015000	3.891134000	1.930275000
6	0.804600000	1.918454000	3.813429000
1	1.692196000	1.708790000	4.424648000
1	0.568405000	2.981400000	3.933727000
1	-0.027348000	1.342306000	4.239658000
1	-1.153915000	4.382650000	-1.619158000
1	-2.358094000	3.293264000	-0.934263000
15	2.340573000	1.109261000	-1.390350000

6	2.727071000	2.864427000	-0.909372000
1	3.808038000	3.056095000	-0.921059000
1	2.279125000	3.533373000	-1.656336000
14	1.941846000	3.251690000	0.773532000
6	3.908103000	0.324978000	-0.791370000
1	3.944108000	0.293173000	0.302166000
1	3.978122000	-0.697962000	-1.173660000
1	4.784224000	0.879219000	-1.148428000
6	2.767638000	1.129869000	-3.186593000
1	1.999148000	1.658987000	-3.758178000
1	3.736611000	1.609179000	-3.368630000
1	2.806446000	0.099925000	-3.557471000
6	2.844788000	4.640850000	1.680410000
1	3.885559000	4.365424000	1.888965000
1	2.860483000	5.559972000	1.082565000
1	2.362848000	4.872510000	2.636960000
1	-1.282453000	-0.126714000	-0.770294000
1	-1.175839000	1.067271000	1.210311000
6	-4.609180000	-0.106435000	-0.016744000
8	-5.232371000	-0.865503000	0.701331000
6	-0.561353000	-2.214691000	1.364090000
6	-1.640323000	-1.330900000	1.998174000
6	-1.195930000	-3.162631000	0.318861000
6	-2.671381000	-2.169916000	2.779876000
1	-1.198288000	-0.588176000	2.674726000
6	-2.666004000	-3.486939000	0.637186000
1	-1.134012000	-2.708090000	-0.677067000
6	-2.890304000	-3.557608000	2.146371000
1	-2.346869000	-2.285847000	3.821350000
1	-3.319794000	-2.708895000	0.226667000
1	-2.189971000	-4.286705000	2.577442000
6	2.120762000	-2.563051000	0.231244000
6	2.347271000	-3.598557000	1.352371000
6	1.995893000	-3.275228000	-1.120948000
6	3.214115000	-4.786286000	0.873688000
1	2.823155000	-3.104805000	2.208635000
6	3.336163000	-3.944765000	-1.499847000
1	1.203755000	-4.030823000	-1.063326000
6	4.149202000	-4.376329000	-0.263733000
1	3.779776000	-5.198539000	1.716692000
1	3.132420000	-4.817707000	-2.131327000
1	4.824954000	-5.198546000	-0.524517000
6	-3.980472000	1.154334000	0.542051000
1	-4.603731000	2.022618000	0.293731000

1	-3.904494000	1.081206000	1.629790000
1	-2.993349000	1.306964000	0.094211000
6	-4.396711000	-0.380384000	-1.499436000
1	-3.318287000	-0.587779000	-1.590012000
6	-5.190291000	-1.594244000	-1.970812000
1	-6.268323000	-1.419134000	-1.878680000
1	-4.966722000	-1.806023000	-3.022034000
1	-4.949161000	-2.484983000	-1.384741000
6	-4.696603000	0.860386000	-2.354115000
1	-4.071326000	1.715924000	-2.077804000
1	-4.502281000	0.641569000	-3.409162000
1	-5.747889000	1.160784000	-2.262389000
1	-2.139409000	-0.782961000	1.191714000
1	-3.621705000	-1.624728000	2.797190000
1	-0.120240000	-2.809052000	2.174300000
1	-0.615328000	-4.092767000	0.286485000
1	-2.951695000	-4.426168000	0.150295000
1	-3.898827000	-3.918711000	2.374207000
1	3.027325000	-1.950130000	0.173172000
1	1.393715000	-3.996360000	1.713185000
1	2.562579000	-5.593852000	0.514802000
1	4.788806000	-3.550707000	0.076739000
1	3.935861000	-3.256700000	-2.108666000
1	1.697849000	-2.577020000	-1.904342000
1	0.071637000	2.741091000	-3.108231000
1	-1.768187000	1.746812000	-2.983068000

F4Sa

Doordinates (Angstroms)			
	X	Y	Z
25	0.113510000	-0.307342000	-0.930739000
7	1.281943000	-0.658973000	1.078327000
6	-1.564149000	-0.838930000	1.951569000
1	-1.803361000	-0.313150000	2.885476000
1	-2.335735000	-1.606704000	1.822131000
6	3.427871000	-1.186153000	-0.856909000
6	-0.545872000	0.413757000	-2.377426000
8	-0.888582000	0.974915000	-3.348960000
15	2.025976000	-0.768456000	-1.985115000
15	-1.589052000	0.289494000	0.471180000
14	2.655546000	-1.753995000	0.762990000
14	0.150709000	-1.627636000	2.058270000
6	3.993560000	-1.712566000	2.087976000

1	3.631066000	-2.020264000	3.074734000
1	4.824550000	-2.376505000	1.817606000
1	4.395217000	-0.695581000	2.175360000
6	0.601914000	-1.703446000	3.895065000
1	-0.178379000	-2.234058000	4.456310000
1	1.551053000	-2.216137000	4.086090000
1	0.681207000	-0.693526000	4.319022000
1	4.143781000	-1.882840000	-1.303885000
1	3.961709000	-0.265026000	-0.592793000
15	-0.665563000	-2.396080000	-1.394678000
6	0.362234000	-3.837666000	-0.823642000
1	-0.207853000	-4.775202000	-0.860000000
1	1.207798000	-3.955117000	-1.514371000
14	1.063172000	-3.479532000	0.904078000
6	-2.325430000	-3.072473000	-0.920304000
1	-2.446486000	-3.115451000	0.166479000
1	-3.118792000	-2.444703000	-1.336607000
1	-2.454871000	-4.085575000	-1.319334000
6	-0.802990000	-2.746602000	-3.203496000
1	0.130254000	-2.500334000	-3.718099000
1	-1.043670000	-3.798773000	-3.396004000
1	-1.591315000	-2.117973000	-3.631615000
6	1.427659000	-5.067124000	1.862814000
1	0.508232000	-5.636636000	2.043912000
1	2.113870000	-5.715567000	1.305313000
1	1.885380000	-4.852307000	2.834998000
1	0.750332000	1.165419000	-0.734999000
1	1.489141000	0.314310000	1.287765000
6	3.371691000	2.615362000	-0.092687000
6	2.526661000	3.799590000	0.301349000
1	1.545002000	3.683608000	-0.172144000
1	2.403853000	3.836192000	1.385524000
1	2.956539000	4.740511000	-0.059197000
8	3.645061000	1.735170000	0.705659000
6	-1.542097000	1.962520000	1.294428000
6	-0.255641000	2.201415000	2.090888000
6	-1.729853000	3.094978000	0.262873000
6	-0.359027000	3.489196000	2.936973000
1	-0.030918000	1.357113000	2.753527000
6	-1.260554000	4.467145000	0.795753000
1	-1.174202000	2.843314000	-0.648981000
6	-1.322178000	4.520732000	2.321606000
1	-0.691953000	3.242679000	3.952494000
1	-0.227655000	4.660393000	0.482594000

1	-1.080151000	5.525645000	2.685910000
6	-3.387159000	0.154009000	-0.026074000
6	-4.409243000	0.724974000	0.965937000
6	-3.661776000	0.676519000	-1.453803000
6	-5.824174000	0.208093000	0.632898000
1	-4.153572000	0.456066000	1.997559000
6	-5.154531000	0.983943000	-1.678781000
1	-3.070722000	1.571441000	-1.667455000
6	-6.036653000	0.020457000	-0.884325000
1	-5.997312000	-0.745604000	1.146296000
1	-5.376389000	2.012396000	-1.363399000
1	-7.093659000	0.160232000	-1.136929000
6	3.905910000	2.585944000	-1.518763000
1	4.168736000	1.543723000	-1.725727000
6	5.196779000	3.419451000	-1.573833000
1	5.640201000	3.358124000	-2.573578000
1	5.000020000	4.477000000	-1.361319000
1	5.935921000	3.056339000	-0.851822000
6	2.881494000	3.061195000	-2.552781000
1	3.267923000	2.891832000	-3.563961000
1	1.933185000	2.522460000	-2.450822000
1	2.678991000	4.134186000	-2.454053000
1	-2.378497000	1.980439000	2.005395000
1	0.571333000	2.270681000	1.376521000
1	0.639328000	3.932767000	3.038700000
1	-2.350960000	4.314029000	2.645540000
1	-1.868290000	5.264987000	0.354600000
1	-2.788929000	3.156587000	-0.013129000
1	-3.548547000	-0.929414000	-0.034546000
1	-3.323651000	-0.078554000	-2.172114000
1	-4.395754000	1.820633000	0.916842000
1	-6.564108000	0.914142000	1.028765000
1	-5.784656000	-1.008942000	-1.174039000
1	-5.384936000	0.933627000	-2.748794000
1	2.143048000	-1.860417000	-2.888576000
1	2.615426000	0.175153000	-2.859942000

TSF4-5Ra

Doordinates (Angstroms)			
	X	Y	Z
25	0.479211000	0.004449000	-0.982342000
7	1.580535000	0.785301000	0.850312000

6	-0.245775000	-1.342598000	1.970695000
1	-0.772548000	-1.279306000	2.929527000
1	-0.134954000	-2.405608000	1.750916000
6	3.631310000	1.378365000	-1.286166000
6	-0.514840000	-0.311202000	-2.393185000
8	-1.156126000	-0.491006000	-3.355167000
15	2.205156000	0.686491000	-2.253970000
15	-1.199945000	-0.560011000	0.578041000
14	3.340616000	0.924494000	0.526497000
14	1.466040000	-0.546068000	2.051618000
6	4.195162000	2.185127000	1.632330000
1	4.050013000	1.970887000	2.696555000
1	5.274374000	2.207890000	1.437561000
1	3.803425000	3.192168000	1.440315000
6	1.790160000	0.034549000	3.818226000
1	1.675288000	-0.797321000	4.524759000
1	2.797791000	0.443846000	3.952767000
1	1.075165000	0.814651000	4.106796000
1	4.581343000	0.973487000	-1.651764000
1	3.681139000	2.464756000	-1.408412000
15	1.372345000	-2.158765000	-1.077301000
6	3.158901000	-2.291157000	-0.588192000
1	3.460266000	-3.344389000	-0.516902000
1	3.781450000	-1.837332000	-1.369761000
14	3.440848000	-1.356173000	1.049328000
6	0.818642000	-3.723711000	-0.237408000
1	1.078890000	-3.717948000	0.825099000
1	-0.257596000	-3.887897000	-0.332081000
1	1.330054000	-4.577169000	-0.696804000
6	1.375742000	-2.829085000	-2.797792000
1	1.756879000	-2.093851000	-3.511250000
1	1.981683000	-3.739322000	-2.871142000
1	0.346783000	-3.068364000	-3.087099000
6	4.817637000	-2.118590000	2.089032000
1	4.586032000	-3.160089000	2.342086000
1	5.772151000	-2.113199000	1.550225000
1	4.957670000	-1.569784000	3.026956000
1	0.057295000	1.661649000	-1.066996000
1	1.021821000	1.630955000	0.975205000
6	-0.242440000	3.138613000	-0.926586000
8	-0.860597000	3.327706000	0.151585000
6	-2.338764000	0.526322000	1.591307000
6	-1.554701000	1.406334000	2.597691000
6	-3.284555000	1.431534000	0.794640000

6	-2.378331000	2.618511000	3.075432000
1	-1.257398000	0.801151000	3.461912000
6	-4.396744000	1.968040000	1.714316000
1	-2.681140000	2.252703000	0.401499000
6	-3.869279000	2.283982000	3.129634000
1	-2.014981000	2.946525000	4.056757000
1	-4.818727000	2.873974000	1.262132000
1	-4.016943000	1.418429000	3.790352000
6	-2.319952000	-1.944231000	0.008242000
6	-2.845170000	-2.888242000	1.112637000
6	-3.485536000	-1.500643000	-0.888830000
6	-4.057458000	-3.714902000	0.636031000
1	-2.041808000	-3.569832000	1.416833000
6	-4.021688000	-2.709447000	-1.680469000
1	-4.283472000	-1.085856000	-0.261921000
6	-3.953211000	-4.014667000	-0.860324000
1	-4.125894000	-4.642216000	1.216137000
1	-5.058012000	-2.508781000	-1.976720000
1	-4.743703000	-4.704466000	-1.175341000
6	1.180782000	3.716258000	-0.975585000
1	1.097507000	4.802018000	-0.847453000
1	1.777113000	3.345703000	-0.138367000
1	1.702313000	3.526562000	-1.918425000
6	-0.979746000	3.260427000	-2.284803000
1	-0.363822000	2.753180000	-3.038895000
6	-2.353360000	2.606762000	-2.256986000
1	-3.035800000	3.167335000	-1.609624000
1	-2.786565000	2.571202000	-3.263681000
1	-2.285454000	1.585244000	-1.875307000
6	-1.106017000	4.742008000	-2.669991000
1	-0.131912000	5.214190000	-2.839268000
1	-1.688319000	4.848858000	-3.593027000
1	-1.621230000	5.298642000	-1.878298000
1	-0.647063000	1.792728000	2.125655000
1	-2.215924000	3.448937000	2.379829000
1	-2.947429000	-0.187044000	2.168194000
1	-3.733193000	0.924266000	-0.060776000
1	-5.215653000	1.239304000	1.779904000
1	-4.436113000	3.109669000	3.574573000
1	-1.651066000	-2.516424000	-0.644215000
1	-3.123838000	-2.321037000	2.008888000
1	-4.987179000	-3.162865000	0.824478000
1	-3.001962000	-4.530822000	-1.050967000
1	-3.447202000	-2.822717000	-2.607298000

1	-3.182682000	-0.712008000	-1.583774000
1	2.909674000	-0.191009000	-3.116180000
1	1.990230000	1.686415000	-3.228263000

TSF4-5Sa

Doordinates (Angstroms)			
	X	Y	Z
25	0.412235000	-0.135335000	-0.943368000
7	1.542269000	0.172574000	1.003951000
6	-0.958271000	-1.207160000	1.951851000
1	-1.481320000	-0.890707000	2.862434000
1	-1.228882000	-2.254126000	1.784513000
6	3.844473000	0.248505000	-0.871605000
6	-0.462965000	0.098874000	-2.444901000
8	-0.989279000	0.349539000	-3.459781000
15	2.418847000	-0.069856000	-2.002895000
15	-1.478180000	-0.222683000	0.463535000
14	3.266401000	-0.274125000	0.844092000
14	0.913101000	-1.050529000	2.145306000
6	4.380498000	0.555315000	2.113574000
1	4.165450000	0.251616000	3.143282000
1	5.435757000	0.333709000	1.911358000
1	4.248363000	1.642662000	2.050814000
6	1.279830000	-0.668722000	3.959272000
1	0.813829000	-1.420247000	4.609553000
1	2.351464000	-0.656306000	4.185748000
1	0.872809000	0.310872000	4.240486000
1	4.756733000	-0.254097000	-1.207888000
1	4.056074000	1.322551000	-0.826129000
15	0.535441000	-2.449384000	-1.173896000
6	2.073174000	-3.229793000	-0.475741000
1	1.950293000	-4.318433000	-0.407212000
1	2.903784000	-3.054564000	-1.171420000
14	2.543383000	-2.475890000	1.210513000
6	-0.666645000	-3.753300000	-0.626330000
1	-0.831838000	-3.740629000	0.454290000
1	-1.627371000	-3.624061000	-1.132710000
1	-0.280106000	-4.742516000	-0.896812000
6	0.598114000	-2.992334000	-2.940063000
1	1.331812000	-2.421490000	-3.514448000
1	0.842697000	-4.057751000	-3.020211000
1	-0.382566000	-2.823001000	-3.397665000
6	3.507625000	-3.700215000	2.276845000

1	2.903087000	-4.582427000	2.518704000
1	4.411574000	-4.046521000	1.762306000
1	3.816958000	-3.238080000	3.221188000
1	0.555725000	1.583358000	-0.966288000
1	1.383271000	1.188426000	1.102760000
6	1.098236000	3.073888000	-0.552447000
6	-0.243485000	3.788980000	-0.679330000
1	-0.816902000	3.465273000	-1.550643000
1	-0.830359000	3.636425000	0.221577000
1	-0.052658000	4.867278000	-0.771225000
8	1.616369000	2.950711000	0.587915000
6	-2.277293000	1.228617000	1.327816000
6	-1.273742000	1.998140000	2.203631000
6	-3.070480000	2.112657000	0.345726000
6	-1.890736000	3.259857000	2.863103000
1	-0.917476000	1.323905000	2.990554000
6	-3.514529000	3.462763000	0.959346000
1	-2.485408000	2.283889000	-0.563164000
6	-3.356523000	3.484567000	2.480174000
1	-1.797340000	3.201071000	3.953397000
1	-2.912521000	4.280031000	0.542184000
1	-3.700777000	4.445207000	2.881270000
6	-2.973721000	-1.196628000	-0.093162000
6	-4.147267000	-1.266413000	0.894315000
6	-3.459413000	-0.811821000	-1.511534000
6	-5.121534000	-2.389183000	0.485657000
1	-3.791227000	-1.445755000	1.915307000
6	-4.930550000	-1.198872000	-1.740787000
1	-3.327761000	0.256726000	-1.704991000
6	-5.251825000	-2.523442000	-1.047471000
1	-4.779360000	-3.341514000	0.909250000
1	-5.593888000	-0.416247000	-1.348524000
1	-6.256423000	-2.870466000	-1.313091000
6	2.045224000	3.338972000	-1.741740000
1	2.818273000	2.571101000	-1.704371000
6	2.754598000	4.680126000	-1.503624000
1	3.505099000	4.858989000	-2.282973000
1	2.049471000	5.519790000	-1.528138000
1	3.255373000	4.682930000	-0.531115000
6	1.377103000	3.307547000	-3.114036000
1	2.132999000	3.335899000	-3.908306000
1	0.774181000	2.404138000	-3.246980000
1	0.721317000	4.174162000	-3.260008000
1	-3.003906000	0.773590000	2.013489000

1	-0.389536000	2.279083000	1.626703000
1	-1.317188000	4.143144000	2.554238000
1	-3.993393000	2.712875000	2.934085000
1	-4.553141000	3.674880000	0.681395000
1	-3.959157000	1.555586000	0.030765000
1	-2.577553000	-2.213275000	-0.151249000
1	-2.828414000	-1.325369000	-2.244865000
1	-4.678656000	-0.308039000	0.914577000
1	-6.103080000	-2.187038000	0.930474000
1	-4.554439000	-3.287687000	-1.417533000
1	-5.130704000	-1.263159000	-2.816128000
1	2.929341000	-1.210786000	-2.669264000
1	2.657765000	0.819348000	-3.073035000

H₂

Doordinates (Angstroms)			
	X	Y	Z
1	0.000000000	0.000000000	0.370782000
1	0.000000000	0.000000000	-0.370782000

PhCOCH₃

Doordinates (Angstroms)			
	X	Y	Z
6	-2.584452000	0.113024000	-0.000022000
6	-1.816626000	1.274601000	-0.000017000
6	-0.427706000	1.190972000	-0.000002000
6	0.204096000	-0.056645000	0.000006000
6	-0.576234000	-1.217968000	0.000000000
6	-1.962060000	-1.134489000	-0.000014000
1	-3.668633000	0.179997000	-0.000034000
1	-2.299404000	2.247176000	-0.000023000
1	0.156699000	2.106157000	0.000002000
1	-0.075136000	-2.180496000	0.000008000
1	-2.559265000	-2.041567000	-0.000018000
6	1.696846000	-0.203514000	0.000022000
8	2.209075000	-1.308038000	0.000019000
6	2.548195000	1.046311000	0.000009000
1	2.339607000	1.659079000	-0.884240000
1	2.339614000	1.659093000	0.884250000
1	3.601565000	0.761117000	0.000007000

PhCHOHCH₃

----- Doordinates (Angstroms)			
	X	Y	Z

6	-2.618879000	0.153033000	0.134913000
6	-1.777231000	1.244984000	0.333013000
6	-0.400235000	1.103413000	0.185640000
6	0.151813000	-0.130314000	-0.163605000
6	-0.698571000	-1.218770000	-0.365229000
6	-2.075497000	-1.081089000	-0.214058000
1	-3.693138000	0.264266000	0.249779000
1	-2.194872000	2.210795000	0.603381000
1	0.259252000	1.953131000	0.337144000
1	-0.278382000	-2.182632000	-0.645404000
1	-2.725457000	-1.936270000	-0.376634000
6	1.657557000	-0.297424000	-0.284641000
8	2.296495000	0.887648000	-0.734012000
6	2.290086000	-0.646573000	1.056190000
1	2.102855000	0.152729000	1.780914000
1	1.868938000	-1.576849000	1.450026000
1	3.371547000	-0.769892000	0.941534000
1	1.886337000	1.139641000	-1.571913000
1	1.856699000	-1.119662000	-0.990062000

iPrCOCH₃

----- Doordinates (Angstroms)			
	X	Y	Z

6	0.824106000	-0.134531000	-0.164309000
6	1.317054000	0.896987000	0.828331000
1	1.234888000	1.897428000	0.386223000
1	0.718973000	0.900173000	1.745788000
1	2.364617000	0.705368000	1.068482000
6	-0.680823000	-0.251790000	-0.387242000
1	-0.794491000	-0.841660000	-1.302971000
6	-1.357319000	1.109301000	-0.574802000
1	-0.900712000	1.677458000	-1.392764000
1	-2.416891000	0.971024000	-0.815151000
1	-1.302860000	1.716345000	0.336136000
6	-1.313269000	-1.034569000	0.773809000
1	-2.376905000	-1.205245000	0.575949000
1	-0.833763000	-2.010445000	0.904203000
1	-1.235751000	-0.485493000	1.719583000
8	1.600550000	-0.854668000	-0.760025000

iPrCHOHCH₃

Doordinates (Angstroms)			
	X	Y	Z
6	0.727645000	-0.284198000	-0.401051000
6	1.116079000	-1.097075000	0.823337000
1	1.102488000	-0.477785000	1.726027000
1	0.437623000	-1.943514000	0.967824000
1	2.129893000	-1.490361000	0.700398000
6	-0.708279000	0.278271000	-0.373130000
1	-0.807854000	0.878036000	-1.292180000
6	-0.956597000	1.206958000	0.815876000
1	-0.166115000	1.959810000	0.895128000
1	-1.915545000	1.726093000	0.707585000
1	-0.990898000	0.649617000	1.759463000
6	-1.756558000	-0.833708000	-0.444655000
1	-1.558597000	-1.523249000	-1.274149000
1	-1.782318000	-1.419647000	0.481697000
1	-2.757254000	-0.412436000	-0.591253000
8	1.688041000	0.761190000	-0.503747000
1	0.803199000	-0.939245000	-1.285842000
1	1.467307000	1.281671000	-1.286984000

In_B5r

Doordinates (Angstroms)			
	X	Y	Z
25	-0.248575000	-0.758404000	-0.871905000
7	0.717829000	-1.343962000	1.136835000
6	-0.851905000	-0.169844000	-2.424489000
8	-1.232606000	0.177058000	-3.465703000
6	2.935578000	-1.863480000	-0.613397000
1	3.721118000	-2.539768000	-0.971404000
1	3.393786000	-0.890870000	-0.395814000
6	-2.014568000	-0.667070000	2.004883000
6	-1.123129000	-2.290094000	-1.012636000
8	-1.667440000	-3.317088000	-1.077890000
15	-1.931161000	0.196172000	0.382305000
15	1.654251000	-1.565716000	-1.889335000
14	-0.334348000	-1.347276000	2.555095000
14	2.080471000	-2.463397000	0.950659000
6	0.447640000	-0.318383000	3.924210000
1	-0.262642000	-0.099530000	4.731299000
1	1.289098000	-0.863160000	4.369931000

1	0.842771000	0.634102000	3.552071000
6	-0.623492000	-3.095158000	3.176809000
1	0.277774000	-3.551889000	3.601316000
1	-1.382909000	-3.076106000	3.969085000
1	-0.997668000	-3.749524000	2.381106000
6	3.263827000	-2.350118000	2.409297000
1	3.588048000	-1.315546000	2.574319000
1	2.807161000	-2.712414000	3.338501000
1	4.163357000	-2.952921000	2.231839000
6	1.486886000	-4.235283000	0.747190000
1	2.251807000	-4.823806000	0.224560000
1	1.308122000	-4.724523000	1.710606000
1	0.561675000	-4.296936000	0.164590000
1	-2.534567000	-0.077927000	2.769481000
1	-2.640751000	-1.548372000	1.809999000
1	1.074807000	-0.377329000	0.947579000
6	1.539798000	-3.162886000	-2.788652000
1	0.820817000	-3.058017000	-3.608919000
1	2.504417000	-3.476051000	-3.203594000
1	1.170053000	-3.948239000	-2.122923000
6	2.514575000	-0.513046000	-3.115406000
1	3.414651000	-1.013673000	-3.488981000
1	1.855271000	-0.287355000	-3.959816000
1	2.805045000	0.421666000	-2.630737000
6	5.591294000	2.623959000	0.172003000
6	5.007324000	3.223042000	-0.937929000
6	3.643991000	3.060146000	-1.193004000
6	2.838217000	2.292302000	-0.350280000
6	3.443651000	1.696040000	0.764506000
6	4.798405000	1.857971000	1.027562000
1	6.651670000	2.751177000	0.371353000
1	5.612109000	3.821969000	-1.613932000
1	3.215970000	3.537921000	-2.069098000
1	2.832452000	1.089100000	1.426745000
1	5.240609000	1.386497000	1.901791000
6	1.337418000	2.054461000	-0.573157000
8	1.077429000	0.712583000	-0.356275000
6	0.847663000	2.565513000	-1.928235000
1	0.974141000	3.650898000	-2.020349000
1	1.363356000	2.080830000	-2.764476000
1	-0.218448000	2.353416000	-2.024465000
6	-1.747391000	1.967724000	0.801162000
6	-1.244481000	2.404248000	2.027768000
6	-2.055085000	2.918291000	-0.178680000

6	-1.028688000	3.760525000	2.263583000
1	-1.013994000	1.690783000	2.811503000
6	-1.843560000	4.271576000	0.056010000
1	-2.462672000	2.597099000	-1.134212000
6	-1.321221000	4.696529000	1.276742000
1	-0.629914000	4.083339000	3.221010000
1	-2.083077000	4.995758000	-0.716964000
1	-1.148741000	5.753247000	1.458193000
6	-3.684981000	0.146494000	-0.170193000
6	-4.057896000	-0.568596000	-1.309431000
6	-4.677701000	0.797357000	0.575035000
6	-5.395637000	-0.636492000	-1.697098000
1	-3.306740000	-1.075761000	-1.904372000
6	-6.011042000	0.730394000	0.189787000
1	-4.402987000	1.369029000	1.457931000
6	-6.372650000	0.010895000	-0.949238000
1	-5.668560000	-1.195072000	-2.587619000
1	-6.769436000	1.241644000	0.775737000
1	-7.414707000	-0.041446000	-1.251386000
1	0.819132000	2.675627000	0.183812000

In_B5s

Doordinates (Angstroms)			
	X	Y	Z
25	0.385335000	1.027891000	-0.777164000
7	-0.988101000	1.301208000	1.061792000
6	1.286269000	0.635786000	-2.244566000
8	1.873594000	0.393892000	-3.217150000
6	-2.661011000	2.432848000	-0.974341000
1	-3.315271000	3.240621000	-1.324489000
1	-3.205527000	1.486050000	-1.093577000
6	1.290194000	-0.129744000	2.307962000
6	1.388002000	2.438997000	-0.399365000
8	2.013370000	3.380371000	-0.123327000
15	1.662041000	-0.385898000	0.517064000
15	-1.119664000	2.303490000	-1.955982000
14	-0.344575000	0.779233000	2.619160000
14	-2.182473000	2.581765000	0.850077000
6	-1.563860000	-0.363986000	3.481163000
1	-1.138848000	-0.776544000	4.404924000
1	-2.485917000	0.165578000	3.750412000
1	-1.848234000	-1.207575000	2.840861000
6	0.018282000	2.272562000	3.697680000
1	-0.892166000	2.799978000	4.005583000

1	0.535076000	1.958030000	4.613173000
1	0.667887000	2.987953000	3.179486000
6	-3.711340000	2.315445000	1.914716000
1	-4.160873000	1.329549000	1.744559000
1	-3.481964000	2.400083000	2.984217000
1	-4.477024000	3.068689000	1.688524000
6	-1.446420000	4.264717000	1.245212000
1	-2.011402000	5.060939000	0.744150000
1	-1.482353000	4.471448000	2.320773000
1	-0.400435000	4.342503000	0.931587000
1	1.365467000	-1.066676000	2.872248000
1	2.086874000	0.527056000	2.680817000
1	-1.325382000	0.447261000	0.544373000
6	-0.676171000	4.053776000	-2.291697000
1	0.205404000	4.083233000	-2.941319000
1	-1.496139000	4.585023000	-2.788058000
1	-0.425698000	4.579001000	-1.366684000
6	-1.646917000	1.783720000	-3.636320000
1	-2.410940000	2.461447000	-4.033670000
1	-0.782338000	1.795276000	-4.308782000
1	-2.048955000	0.768236000	-3.619577000
6	-4.361159000	-3.762317000	0.809573000
6	-3.749561000	-4.275294000	-0.329222000
6	-2.922822000	-3.467830000	-1.112407000
6	-2.689430000	-2.133826000	-0.775907000
6	-3.322049000	-1.631373000	0.367233000
6	-4.145327000	-2.428204000	1.154096000
1	-5.000915000	-4.391656000	1.421881000
1	-3.907047000	-5.313511000	-0.609843000
1	-2.443283000	-3.900816000	-1.984500000
1	-3.154010000	-0.597214000	0.652910000
1	-4.617050000	-2.008138000	2.038939000
6	-1.786288000	-1.191568000	-1.583547000
8	-0.956835000	-0.514819000	-0.712511000
6	-1.006066000	-1.900850000	-2.689087000
1	-0.346866000	-2.668042000	-2.268551000
1	-1.667022000	-2.363531000	-3.432698000
1	-0.381063000	-1.170486000	-3.211050000
6	1.367720000	-2.165844000	0.217167000
6	0.318405000	-2.839602000	0.844691000
6	2.135353000	-2.843732000	-0.734732000
6	0.050511000	-4.170572000	0.541696000
1	-0.311165000	-2.325739000	1.562935000
6	1.866234000	-4.175014000	-1.040822000

1	2.951436000	-2.334359000	-1.240260000
6	0.822932000	-4.841986000	-0.402490000
1	-0.778398000	-4.673531000	1.030370000
1	2.473123000	-4.690237000	-1.779958000
1	0.611578000	-5.880465000	-0.641174000
6	3.498479000	-0.312670000	0.489218000
6	4.175090000	0.538959000	-0.384920000
6	4.245567000	-1.118710000	1.359723000
6	5.568706000	0.593344000	-0.386354000
1	3.618808000	1.165754000	-1.072748000
6	5.633630000	-1.065553000	1.360048000
1	3.734445000	-1.798618000	2.036401000
6	6.299058000	-0.205888000	0.485657000
1	6.079605000	1.263065000	-1.071836000
1	6.199409000	-1.696795000	2.039197000
1	7.384457000	-0.162761000	0.485442000
1	-2.487995000	-0.492712000	-2.090422000

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Doordinates (Angstroms)			
	X	Y	Z
25	-0.271215000	-0.359094000	-0.894464000
7	0.490079000	-1.305666000	1.089300000
6	-1.864988000	0.367432000	2.019442000
1	-1.908323000	1.042578000	2.881925000
1	-2.882705000	-0.001663000	1.839293000
6	1.033279000	-3.509036000	-0.939910000
6	-0.666248000	0.316758000	-2.458018000
8	-0.946796000	0.681645000	-3.537972000
15	1.157066000	-1.913967000	-1.855998000
15	-1.320594000	1.224080000	0.470331000
14	0.715983000	-3.067926000	0.879160000
14	-0.763435000	-1.143832000	2.345853000
6	2.112662000	-3.748364000	1.942618000
1	1.949793000	-3.556518000	3.009296000
1	2.224412000	-4.831162000	1.808264000
1	3.064807000	-3.279467000	1.662109000
6	-0.094720000	-1.055489000	4.107674000
1	-0.919283000	-1.086929000	4.831228000
1	0.573559000	-1.895353000	4.330677000
1	0.462857000	-0.128926000	4.291360000
1	0.170845000	-4.068973000	-1.321107000
1	1.923047000	-4.136166000	-1.078245000

6	2.951629000	-1.584036000	-1.671958000
1	3.538745000	-2.447330000	-2.007385000
1	3.235018000	-0.709189000	-2.260432000
1	3.188396000	-1.354560000	-0.631323000
6	1.119248000	-2.398513000	-3.632341000
1	1.370093000	-1.523088000	-4.241603000
1	1.847763000	-3.189438000	-3.843856000
1	0.127519000	-2.740678000	-3.936911000
15	-2.174255000	-1.679985000	-1.086937000
6	-2.646802000	-3.021280000	0.142799000
1	-3.659461000	-2.809830000	0.511287000
1	-2.720666000	-3.975359000	-0.395937000
14	-1.489531000	-3.242682000	1.634135000
6	-3.787771000	-0.790113000	-1.191941000
1	-4.009693000	-0.270617000	-0.255280000
1	-3.742241000	-0.037561000	-1.984497000
1	-4.605796000	-1.487084000	-1.407361000
6	-2.321297000	-2.646254000	-2.654836000
1	-1.572523000	-3.442889000	-2.685923000
1	-3.312706000	-3.103448000	-2.750372000
1	-2.155027000	-1.981845000	-3.508589000
6	-2.118395000	-4.592489000	2.794343000
1	-3.104777000	-4.340593000	3.201027000
1	-2.209769000	-5.552594000	2.272921000
1	-1.433658000	-4.734487000	3.638136000
1	1.235786000	-0.603260000	0.927365000
6	2.214862000	1.687797000	-0.771687000
8	1.474571000	0.605509000	-0.345732000
6	3.698500000	1.437737000	-0.459564000
6	4.740079000	1.634588000	-1.367062000
6	4.028112000	0.961691000	0.816267000
6	6.064354000	1.357949000	-1.019941000
1	4.528337000	1.997798000	-2.368416000
6	5.343711000	0.691277000	1.172515000
1	3.225518000	0.793335000	1.528165000
6	6.373068000	0.884359000	0.249743000
1	6.853962000	1.510692000	-1.751540000
1	5.570493000	0.324262000	2.170763000
1	7.403111000	0.668845000	0.520715000
6	1.957419000	2.076031000	-2.228488000
1	2.186635000	1.255859000	-2.920165000
1	0.898781000	2.321407000	-2.342853000
1	2.534709000	2.960736000	-2.525664000
1	1.956426000	2.595726000	-0.188104000

6	-0.256703000	2.559286000	1.158958000
6	-0.334905000	3.873969000	0.694751000
6	0.710887000	2.249415000	2.120513000
6	0.530742000	4.853315000	1.180092000
1	-1.073110000	4.146820000	-0.052989000
6	1.574808000	3.222993000	2.606253000
1	0.819390000	1.232201000	2.480528000
6	1.488370000	4.532039000	2.135300000
1	0.453442000	5.869273000	0.803302000
1	2.325815000	2.956508000	3.344286000
1	2.168467000	5.292392000	2.507891000
6	-2.801417000	2.207018000	-0.012562000
6	-3.760022000	2.622592000	0.918032000
6	-2.953576000	2.590241000	-1.348761000
6	-4.853299000	3.386296000	0.519494000
1	-3.654451000	2.356384000	1.965814000
6	-4.042631000	3.361911000	-1.747887000
1	-2.221593000	2.279033000	-2.086174000
6	-4.997809000	3.756997000	-0.815717000
1	-5.590246000	3.697789000	1.254255000
1	-4.145745000	3.647044000	-2.790944000
1	-5.850716000	4.353626000	-1.126526000

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Doordinates (Angstroms)			
	X	Y	Z
25	-0.313552000	0.158909000	-0.856804000
7	-1.241630000	-0.455937000	1.240713000
6	1.036735000	1.252314000	2.064771000
1	1.652288000	0.922832000	2.910261000
1	1.182413000	2.331741000	1.976931000
6	-3.361886000	-1.227512000	-0.576278000
6	0.415518000	0.296991000	-2.440736000
8	0.835349000	0.381728000	-3.531599000
15	-2.338325000	-0.417879000	-1.863405000
15	1.580449000	0.466615000	0.471597000
14	-3.000699000	-0.372140000	1.064808000
14	-0.787962000	0.821247000	2.369228000
6	-3.987635000	-1.275390000	2.398201000
1	-3.732980000	-2.342881000	2.412365000
1	-3.811740000	-0.875861000	3.403218000
1	-5.064016000	-1.197299000	2.197283000
6	-0.942870000	0.383170000	4.201176000
1	-0.656810000	1.240135000	4.825342000

1	-1.964997000	0.101658000	4.477672000
1	-0.284246000	-0.452868000	4.470288000
1	-4.419259000	-1.318027000	-0.848602000
1	-2.947007000	-2.234527000	-0.436965000
6	-2.193733000	-1.633135000	-3.225561000
1	-3.151154000	-2.121457000	-3.439009000
1	-1.841115000	-1.126948000	-4.130740000
1	-1.455379000	-2.375234000	-2.927732000
6	-3.605931000	0.695773000	-2.619397000
1	-3.195543000	1.235666000	-3.477588000
1	-4.456308000	0.102425000	-2.975471000
1	-3.985174000	1.424303000	-1.897778000
15	-0.795731000	2.431314000	-0.872642000
6	-2.363622000	2.968642000	-0.032462000
1	-2.303092000	4.035947000	0.219464000
1	-3.202071000	2.866442000	-0.729297000
14	-2.705450000	1.928634000	1.520824000
6	0.311146000	3.747548000	-0.179735000
1	0.243631000	3.780378000	0.911085000
1	1.353585000	3.577102000	-0.460524000
1	0.002741000	4.728599000	-0.559232000
6	-0.973834000	3.163220000	-2.557408000
1	-1.593254000	2.535168000	-3.200029000
1	-1.410896000	4.167069000	-2.509143000
1	0.017355000	3.234233000	-3.018216000
6	-3.883846000	2.844928000	2.679705000
1	-3.440767000	3.783222000	3.034706000
1	-4.823369000	3.094508000	2.172029000
1	-4.131642000	2.239413000	3.558990000
1	-0.756404000	-1.330328000	0.963570000
6	0.615498000	-2.912850000	-0.865237000
8	-0.333047000	-1.923712000	-0.674980000
6	1.354518000	-2.802443000	-2.202807000
1	2.056830000	-3.635789000	-2.342244000
1	0.669197000	-2.780091000	-3.057947000
1	1.929543000	-1.870499000	-2.223931000
6	-0.003144000	-4.320541000	-0.646245000
1	0.828236000	-5.038446000	-0.724048000
6	-1.063228000	-4.719753000	-1.672928000
1	-1.394575000	-5.753332000	-1.510075000
1	-1.944815000	-4.074326000	-1.592902000
1	-0.686656000	-4.655016000	-2.700590000
6	-0.576876000	-4.424423000	0.767729000
1	-0.953004000	-5.433380000	0.980125000

1	0.183983000	-4.180303000	1.519147000
1	-1.405760000	-3.718029000	0.892198000
1	1.406380000	-2.860973000	-0.097697000
6	2.484532000	-1.008469000	1.101157000
6	1.998394000	-1.738946000	2.189881000
6	3.613439000	-1.484784000	0.426317000
6	2.619866000	-2.918088000	2.591079000
1	1.112719000	-1.409667000	2.725268000
6	4.233539000	-2.664914000	0.824342000
1	4.010178000	-0.937797000	-0.424080000
6	3.736649000	-3.388147000	1.905704000
1	2.223758000	-3.472913000	3.436802000
1	5.106053000	-3.021513000	0.284691000
1	4.218055000	-4.311590000	2.213710000
6	3.011115000	1.512648000	-0.031854000
6	3.899570000	2.025986000	0.921590000
6	3.246931000	1.780591000	-1.382370000
6	4.989005000	2.798086000	0.534428000
1	3.743333000	1.816310000	1.976320000
6	4.342131000	2.550734000	-1.772528000
1	2.573573000	1.390555000	-2.136852000
6	5.212583000	3.062987000	-0.816192000
1	5.668686000	3.189095000	1.286233000
1	4.510999000	2.747716000	-2.827274000
1	6.064568000	3.664836000	-1.119339000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.580289000	-0.462194000	0.958937000
7	1.235214000	-1.338905000	-1.168164000
6	-0.600148000	0.751026000	-1.963239000
1	-1.296011000	-0.077299000	-2.151106000
1	-0.884625000	1.582823000	-2.615107000
6	3.289868000	-2.550601000	0.597887000
6	0.013261000	-0.136440000	2.581311000
8	-0.307456000	0.064694000	3.690945000
15	1.741010000	-2.361951000	1.596533000
15	-0.745931000	1.134937000	-0.173651000
14	2.956242000	-1.737081000	-1.083569000
14	1.083753000	-0.019278000	-2.332018000
6	3.556367000	-2.927153000	-2.420257000
1	3.402072000	-2.535978000	-3.431833000

1	4.628384000	-3.131626000	-2.303033000
1	3.027498000	-3.886383000	-2.348517000
6	1.024291000	-0.545077000	-4.146763000
1	0.852373000	0.324362000	-4.794503000
1	1.948392000	-1.028011000	-4.483695000
1	0.198953000	-1.248859000	-4.316200000
1	4.129080000	-2.075014000	1.114356000
1	3.555788000	-3.608757000	0.476611000
6	0.904987000	-3.950149000	1.197576000
1	1.571853000	-4.802893000	1.369783000
1	0.016104000	-4.064662000	1.823173000
1	0.578769000	-3.949192000	0.153830000
6	2.280822000	-2.717396000	3.318939000
1	1.402315000	-2.750706000	3.972534000
1	2.804295000	-3.678001000	3.383465000
1	2.944721000	-1.932916000	3.690208000
15	2.323625000	1.007236000	1.362393000
6	3.292303000	1.679419000	-0.076102000
1	2.857852000	2.648509000	-0.349927000
1	4.328495000	1.878883000	0.228496000
14	3.259057000	0.551829000	-1.602271000
6	1.901732000	2.559003000	2.266850000
1	1.225495000	3.183036000	1.682449000
1	1.402891000	2.306969000	3.208287000
1	2.805396000	3.137615000	2.489854000
6	3.705599000	0.496910000	2.479391000
1	4.260495000	-0.356247000	2.084646000
1	4.409675000	1.323648000	2.626865000
1	3.287837000	0.224230000	3.453809000
6	4.563299000	1.118967000	-2.847067000
1	4.405944000	2.168242000	-3.125055000
1	5.573694000	1.035807000	-2.428797000
1	4.531888000	0.522358000	-3.765924000
1	0.405539000	-1.923721000	-0.958360000
6	-1.978376000	-2.442786000	0.567561000
8	-0.922970000	-1.660463000	0.149522000
6	-3.177230000	-2.223926000	-0.366774000
6	-4.492879000	-2.046971000	0.058701000
6	-2.928968000	-2.216832000	-1.745506000
6	-5.526735000	-1.862731000	-0.861649000
1	-4.726288000	-2.031693000	1.118841000
6	-3.951752000	-2.033384000	-2.667275000
1	-1.906311000	-2.357371000	-2.085932000
6	-5.263579000	-1.852519000	-2.226153000

1	-6.542002000	-1.714205000	-0.502422000
1	-3.730349000	-2.034690000	-3.731989000
1	-6.068488000	-1.707675000	-2.941803000
6	-2.330437000	-2.292610000	2.047912000
1	-3.077078000	-3.032410000	2.363660000
1	-1.429479000	-2.447901000	2.648611000
1	-2.711932000	-1.292984000	2.271489000
1	-1.724312000	-3.519406000	0.437477000
6	-2.550549000	1.171108000	0.161346000
6	-3.497287000	1.325187000	-0.854513000
6	-2.987006000	1.140120000	1.488381000
6	-4.849502000	1.443733000	-0.548924000
1	-3.186653000	1.347279000	-1.894375000
6	-4.339120000	1.267253000	1.796510000
1	-2.264479000	1.016932000	2.289053000
6	-5.274068000	1.419344000	0.777221000
1	-5.574781000	1.547157000	-1.350519000
1	-4.658429000	1.239268000	2.834658000
1	-6.330452000	1.512075000	1.013099000
6	-0.425435000	2.962606000	-0.198858000
6	0.480184000	3.523399000	-1.107135000
6	-1.029053000	3.814835000	0.734048000
6	0.788133000	4.881682000	-1.075052000
1	0.962203000	2.900048000	-1.854561000
6	-0.727298000	5.173162000	0.766447000
1	-1.744547000	3.419817000	1.448493000
6	0.187431000	5.712637000	-0.134626000
1	1.496048000	5.288049000	-1.792234000
1	-1.211743000	5.811530000	1.499798000
1	0.423177000	6.772486000	-0.107894000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.444389000	-0.169012000	-0.902859000
7	1.123789000	0.901250000	1.103560000
6	-0.576879000	-1.268492000	2.159388000
1	-1.259142000	-1.056420000	2.990903000
1	-0.410605000	-2.348162000	2.159524000
6	2.957705000	2.050182000	-0.831249000
6	-0.185297000	-0.745290000	-2.427862000
8	-0.535256000	-1.130763000	-3.478908000
15	2.206918000	0.857748000	-2.003720000

15	-1.316608000	-0.800713000	0.520548000
14	2.833338000	1.311820000	0.898463000
14	1.050705000	-0.315986000	2.380703000
6	3.485170000	2.607445000	2.108128000
1	2.937401000	3.550902000	1.986640000
1	3.391717000	2.299909000	3.155592000
1	4.546162000	2.815199000	1.918391000
6	1.063131000	0.343112000	4.151542000
1	1.044369000	-0.491000000	4.865381000
1	1.956462000	0.938734000	4.369289000
1	0.187019000	0.970092000	4.361111000
1	3.952849000	2.394005000	-1.134840000
1	2.284882000	2.917422000	-0.790740000
6	1.771489000	1.855213000	-3.481063000
1	2.641620000	2.407347000	-3.854260000
1	1.404883000	1.194629000	-4.273959000
1	0.979250000	2.561211000	-3.229210000
6	3.729344000	0.050643000	-2.673191000
1	3.480296000	-0.608466000	-3.510548000
1	4.429035000	0.809552000	-3.043063000
1	4.243297000	-0.538864000	-1.909698000
15	1.543029000	-2.195272000	-0.664243000
6	3.184792000	-2.188826000	0.208038000
1	3.404043000	-3.192613000	0.596071000
1	3.980814000	-1.956675000	-0.507773000
14	3.211209000	-0.911132000	1.612580000
6	0.812257000	-3.674133000	0.182166000
1	0.902417000	-3.585862000	1.268070000
1	-0.244262000	-3.794404000	-0.074523000
1	1.349627000	-4.580286000	-0.119919000
6	1.952061000	-3.036762000	-2.255392000
1	2.378293000	-2.337289000	-2.976777000
1	2.657756000	-3.860081000	-2.096416000
1	1.031300000	-3.441668000	-2.688319000
6	4.597385000	-1.293522000	2.838615000
1	4.454420000	-2.271913000	3.312905000
1	5.572984000	-1.307674000	2.338071000
1	4.641436000	-0.540195000	3.633296000
1	0.404833000	1.571221000	0.777495000
6	-1.029485000	2.657845000	-1.581924000
8	-0.199042000	1.818539000	-0.872397000
6	-1.963870000	1.907209000	-2.535359000
1	-2.613507000	1.226233000	-1.971863000
1	-2.593813000	2.583530000	-3.125102000

1	-1.376827000	1.309037000	-3.236050000
6	-1.813810000	3.595660000	-0.628591000
1	-2.478808000	2.963323000	-0.033178000
6	-2.673782000	4.618942000	-1.376465000
1	-3.110911000	5.344358000	-0.678781000
1	-2.076914000	5.183395000	-2.106715000
1	-3.503551000	4.147769000	-1.913602000
6	-0.862577000	4.316523000	0.327053000
1	-0.154224000	4.946468000	-0.230736000
1	-1.414924000	4.968873000	1.015585000
1	-0.281059000	3.610085000	0.925245000
1	-0.432019000	3.355779000	-2.222422000
6	-2.551683000	0.460277000	1.062616000
6	-3.805399000	0.545984000	0.448816000
6	-2.248235000	1.373026000	2.078240000
6	-4.730612000	1.507607000	0.846872000
1	-4.073515000	-0.149554000	-0.341177000
6	-3.173443000	2.330371000	2.483158000
1	-1.278598000	1.355956000	2.565149000
6	-4.420476000	2.400749000	1.868731000
1	-5.698457000	1.554762000	0.356218000
1	-2.911640000	3.028398000	3.273098000
1	-5.143422000	3.148522000	2.180875000
6	-2.439184000	-2.214738000	0.158555000
6	-3.072151000	-2.932634000	1.180969000
6	-2.694390000	-2.569275000	-1.168951000
6	-3.926334000	-3.988783000	0.882288000
1	-2.900095000	-2.665187000	2.219819000
6	-3.555034000	-3.624086000	-1.469633000
1	-2.220776000	-2.022409000	-1.975944000
6	-4.169004000	-4.337867000	-0.445480000
1	-4.407404000	-4.537367000	1.687112000
1	-3.741402000	-3.884771000	-2.507438000
1	-4.836888000	-5.162085000	-0.679133000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.698527000	-0.146907000	0.897096000
7	1.323160000	-1.126182000	-1.110756000
6	0.667332000	1.746140000	-1.905883000
1	0.160291000	2.152279000	-2.790069000
1	1.380235000	2.506102000	-1.564635000

6	3.251990000	-2.432733000	0.862775000
6	0.261923000	0.559038000	2.434682000
8	0.036459000	1.048074000	3.478523000
15	1.682067000	-2.073322000	1.759875000
15	-0.502825000	1.395574000	-0.507604000
14	2.911586000	-1.963191000	-0.943200000
14	1.652393000	0.182248000	-2.302856000
6	3.016042000	-3.495132000	-2.032595000
1	2.821653000	-3.269958000	-3.087180000
1	4.007096000	-3.959790000	-1.962967000
1	2.279687000	-4.242228000	-1.708852000
6	1.407301000	-0.331775000	-4.103797000
1	1.823608000	0.436978000	-4.767716000
1	1.927157000	-1.271702000	-4.324614000
1	0.353878000	-0.464335000	-4.376293000
1	4.055746000	-1.796233000	1.250541000
1	3.569476000	-3.476349000	0.980630000
6	0.798741000	-3.635358000	1.352984000
1	1.441315000	-4.501978000	1.551050000
1	-0.115992000	-3.723663000	1.936841000
1	0.503655000	-3.631214000	0.300963000
6	2.079076000	-2.378886000	3.532118000
1	1.147539000	-2.382066000	4.108481000
1	2.579493000	-3.343564000	3.673758000
1	2.715869000	-1.586138000	3.933338000
15	2.649845000	1.139006000	1.104972000
6	4.129424000	1.094881000	-0.058203000
1	4.383609000	2.124770000	-0.341474000
1	4.998204000	0.712429000	0.493372000
14	3.874435000	0.050796000	-1.622636000
6	2.466100000	2.973391000	1.263196000
1	2.173396000	3.423715000	0.310445000
1	1.696431000	3.198683000	2.008142000
1	3.407089000	3.434867000	1.583220000
6	3.529488000	0.865299000	2.709647000
1	3.960099000	-0.138665000	2.749184000
1	4.340177000	1.590098000	2.846714000
1	2.819820000	0.968759000	3.536395000
6	5.330506000	0.178181000	-2.816000000
1	5.513018000	1.220046000	-3.104420000
1	6.251751000	-0.207051000	-2.363775000
1	5.141742000	-0.394629000	-3.730937000
6	-0.897178000	3.110002000	0.106801000
6	-1.335684000	4.139424000	-0.956534000

6	-1.851001000	3.150711000	1.311524000
6	-1.989032000	5.379465000	-0.308990000
1	-0.458833000	4.444596000	-1.541111000
6	-1.704749000	4.499488000	2.044503000
1	-2.882634000	3.030052000	0.967265000
6	-1.392601000	5.657403000	1.072435000
1	-1.874029000	6.247930000	-0.967226000
1	-0.911135000	4.425893000	2.797702000
1	-0.306042000	5.783216000	0.970168000
1	0.076563000	3.429622000	0.491126000
1	-1.654448000	2.327146000	2.002536000
1	-2.632226000	4.711103000	2.589835000
1	-1.774218000	6.602422000	1.474874000
1	-3.068872000	5.214936000	-0.199420000
1	-2.042649000	3.696131000	-1.666680000
6	-1.997002000	0.945503000	-1.552821000
6	-1.870127000	-0.436872000	-2.202930000
6	-3.367629000	1.080178000	-0.854262000
6	-2.913395000	-0.628815000	-3.322901000
1	-0.874571000	-0.582345000	-2.629717000
6	-4.466651000	0.269543000	-1.569976000
1	-3.308183000	0.762310000	0.190420000
6	-4.198575000	0.179853000	-3.070330000
1	-2.483536000	-0.342436000	-4.291584000
1	-5.444911000	0.721529000	-1.369760000
1	-4.097993000	1.192106000	-3.486564000
1	-5.044759000	-0.285275000	-3.588437000
1	-4.503415000	-0.745433000	-1.161898000
1	-3.649712000	2.139808000	-0.846255000
1	-1.973031000	1.686164000	-2.364275000
1	-1.973399000	-1.184122000	-1.414683000
1	-3.160115000	-1.695106000	-3.392176000
1	0.439349000	-1.641236000	-1.106843000
6	-1.994849000	-1.302930000	1.504571000
8	-0.905747000	-1.410405000	0.680449000
6	-3.226268000	-2.008682000	0.931801000
6	-4.512654000	-1.687483000	1.374700000
6	-3.085769000	-3.021698000	-0.016630000
6	-5.630638000	-2.348695000	0.873716000
1	-4.639008000	-0.895918000	2.111519000
6	-4.200376000	-3.683818000	-0.527799000
1	-2.083595000	-3.264281000	-0.356582000
6	-5.478602000	-3.349001000	-0.085605000
1	-6.623284000	-2.075893000	1.222821000

1	-4.072044000	-4.463134000	-1.275180000
1	-6.349789000	-3.858935000	-0.487681000
6	-1.790840000	-1.873064000	2.931856000
1	-1.730035000	-2.967384000	2.914559000
1	-0.874960000	-1.474275000	3.374854000
1	-2.627697000	-1.602739000	3.588450000
1	-2.283727000	-0.239146000	1.656624000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.575433000	-0.102918000	-0.848407000
7	1.501481000	0.691408000	1.129218000
6	-0.904341000	-0.846026000	2.082122000
1	-1.518812000	-0.469940000	2.906838000
1	-1.007984000	-1.932381000	2.108800000
6	3.885583000	0.816486000	-0.649537000
6	-0.207644000	-0.428443000	-2.377156000
8	-0.712809000	-0.648786000	-3.412632000
15	2.654855000	0.180134000	-1.882323000
15	-1.489458000	-0.212598000	0.428861000
14	3.264200000	0.524451000	1.110860000
14	0.902483000	-0.364609000	2.404048000
6	4.151168000	1.743936000	2.244435000
1	3.899728000	2.774407000	1.960768000
1	3.876829000	1.613594000	3.297310000
1	5.240520000	1.636211000	2.168470000
6	0.958308000	0.396374000	4.133419000
1	0.558506000	-0.298629000	4.883281000
1	1.976596000	0.662343000	4.439907000
1	0.351995000	1.311355000	4.171319000
1	4.881400000	0.389660000	-0.821249000
1	3.977937000	1.901899000	-0.787000000
6	2.699216000	1.466370000	-3.189462000
1	3.712903000	1.596332000	-3.586139000
1	2.026674000	1.186689000	-4.007123000
1	2.341721000	2.395088000	-2.748152000
6	3.645822000	-1.099568000	-2.783806000
1	3.112424000	-1.387512000	-3.696512000
1	4.617098000	-0.687638000	-3.080717000
1	3.822429000	-2.003762000	-2.196590000
15	1.026808000	-2.394682000	-0.480783000
6	2.639556000	-2.744738000	0.369787000

1	2.698790000	-3.810474000	0.627254000
1	3.477743000	-2.537398000	-0.302568000
14	2.837727000	-1.640037000	1.914489000
6	0.066488000	-3.667517000	0.481401000
1	0.188677000	-3.518837000	1.558159000
1	-0.998373000	-3.656811000	0.246712000
1	0.454585000	-4.663826000	0.240355000
6	1.127385000	-3.366173000	-2.047527000
1	1.628278000	-2.803149000	-2.835838000
1	1.646758000	-4.319909000	-1.899064000
1	0.107867000	-3.574843000	-2.391038000
6	3.859383000	-2.504848000	3.247468000
1	3.367237000	-3.422234000	3.591971000
1	4.851276000	-2.781017000	2.870661000
1	4.000718000	-1.853605000	4.117552000
1	1.083726000	1.535119000	0.685730000
6	-0.136676000	2.912471000	-1.275897000
8	0.798575000	1.952987000	-0.952624000
6	-2.646768000	1.156881000	1.039324000
6	-3.770788000	0.668985000	1.973318000
6	-3.253444000	2.095643000	-0.054618000
6	-4.525372000	1.848407000	2.597125000
1	-4.475718000	0.051933000	1.408100000
6	-4.758474000	2.338234000	0.108775000
1	-2.770207000	3.074404000	0.020249000
6	-5.075487000	2.823947000	1.525402000
1	-5.340610000	1.458725000	3.217637000
1	-5.076896000	3.086977000	-0.625615000
1	-6.156320000	2.958146000	1.643306000
6	-2.617688000	-1.544634000	-0.270730000
6	-3.391994000	-2.482422000	0.667826000
6	-3.591611000	-0.991402000	-1.332642000
6	-3.821935000	-3.755430000	-0.098784000
1	-2.809184000	-2.763685000	1.550322000
6	-4.591019000	-2.072361000	-1.812413000
1	-4.162301000	-0.155882000	-0.921866000
6	-4.047206000	-3.484749000	-1.598833000
1	-3.064605000	-4.540320000	0.020003000
1	-5.534127000	-1.975692000	-1.258390000
1	-3.103687000	-3.594291000	-2.149273000
6	-0.407469000	3.032479000	-2.783015000
1	-1.240958000	3.721440000	-2.977893000
1	0.463384000	3.396529000	-3.340316000
1	-0.676555000	2.052435000	-3.188919000

6	0.255389000	4.283041000	-0.658923000
1	-0.453303000	5.032299000	-1.044274000
6	1.671337000	4.708957000	-1.047772000
1	1.933486000	5.675122000	-0.598765000
1	2.391739000	3.960990000	-0.698792000
1	1.788176000	4.808348000	-2.133181000
6	0.113615000	4.255617000	0.865673000
1	0.309567000	5.241412000	1.306009000
1	-0.898736000	3.954897000	1.166198000
1	0.819760000	3.547239000	1.315419000
1	-1.892280000	-2.156590000	-0.818008000
1	-3.018434000	-0.600910000	-2.179462000
1	-4.834330000	-1.908198000	-2.867486000
1	-4.734181000	-4.229546000	-2.015645000
1	-4.743047000	-4.146692000	0.349819000
1	-4.280999000	-1.966155000	1.044428000
1	-1.962975000	1.763098000	1.653063000
1	-3.039357000	1.734668000	-1.065247000
1	-5.332524000	1.430066000	-0.115151000
1	-4.625051000	3.815570000	1.658283000
1	-3.848037000	2.379404000	3.277606000
1	-3.385160000	0.030004000	2.772384000
1	-1.102927000	2.655851000	-0.827589000

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Doordinates (Angstroms)			
	X	Y	Z
25	-0.589106000	-0.490207000	-0.952899000
7	-1.045977000	-1.513631000	1.145391000
6	0.437313000	0.825161000	1.978108000
1	1.239664000	0.079142000	2.064715000
1	0.649586000	1.615780000	2.703245000
6	-2.976527000	-2.910762000	-0.658868000
6	-0.149921000	0.010155000	-2.574557000
8	0.099056000	0.317274000	-3.676787000
15	-1.490638000	-2.494813000	-1.687674000
15	0.496905000	1.347277000	0.213345000
14	-2.698584000	-2.142031000	1.057574000
14	-1.057015000	-0.239077000	2.374432000
6	-3.098779000	-3.475957000	2.332926000
1	-2.983777000	-3.122501000	3.363596000
1	-4.130916000	-3.830584000	2.215483000
1	-2.436106000	-4.341436000	2.202285000

6	-0.820077000	-0.849957000	4.147129000
1	-0.830194000	-0.009916000	4.853746000
1	-1.601782000	-1.551448000	4.460119000
1	0.147168000	-1.357606000	4.255819000
1	-3.880049000	-2.525742000	-1.136313000
1	-3.106501000	-3.997684000	-0.579549000
6	-0.611603000	-4.109126000	-1.519800000
1	-1.259624000	-4.923193000	-1.866294000
1	0.307592000	-4.122747000	-2.110410000
1	-0.353524000	-4.294113000	-0.472265000
6	-2.033315000	-2.672456000	-3.439790000
1	-1.142296000	-2.822237000	-4.059771000
1	-2.701555000	-3.529712000	-3.578710000
1	-2.528345000	-1.767343000	-3.799143000
15	-2.637580000	0.636807000	-1.190005000
6	-3.459324000	1.296220000	0.341921000
1	-2.989373000	2.233054000	0.658762000
1	-4.509798000	1.531615000	0.125608000
14	-3.308684000	0.041388000	1.762116000
6	-2.568265000	2.104032000	-2.303677000
1	-1.661730000	2.679454000	-2.130867000
1	-2.538345000	1.751668000	-3.340645000
1	-3.444745000	2.748673000	-2.175822000
6	-4.186611000	-0.085902000	-1.924420000
1	-4.711010000	-0.712698000	-1.198852000
1	-4.864368000	0.727700000	-2.207443000
1	-3.980878000	-0.679893000	-2.817761000
6	-4.668092000	0.302744000	3.048643000
1	-4.605704000	1.301846000	3.495831000
1	-5.663372000	0.199502000	2.599799000
1	-4.590449000	-0.431590000	3.858530000
6	-0.206348000	3.087422000	0.247802000
6	0.093291000	3.901909000	1.525259000
6	0.202060000	3.918800000	-0.982542000
6	-0.089031000	5.419476000	1.306128000
1	-0.575301000	3.564685000	2.326719000
6	-0.712244000	5.152282000	-1.124325000
1	1.238683000	4.253330000	-0.860904000
6	-1.158584000	5.695325000	0.248306000
1	-0.342718000	5.905036000	2.255085000
1	-1.596243000	4.899076000	-1.721987000
1	-2.096985000	5.214943000	0.557160000
1	-1.289936000	2.951782000	0.183236000
1	0.192341000	3.323082000	-1.902353000

1	-0.175044000	5.932079000	-1.677121000
1	-1.370188000	6.768011000	0.179433000
1	0.857717000	5.865804000	0.975184000
1	1.117205000	3.708990000	1.870211000
6	2.311531000	1.770109000	-0.071568000
6	3.322520000	1.155811000	0.901801000
6	2.710303000	1.452813000	-1.528268000
6	4.718593000	1.787672000	0.712302000
1	3.013638000	1.301754000	1.941233000
6	4.230087000	1.287889000	-1.704330000
1	2.207963000	0.534038000	-1.832242000
6	4.995927000	2.198476000	-0.746992000
1	4.822097000	2.664501000	1.364387000
1	4.506396000	1.486436000	-2.746521000
1	4.679536000	3.237523000	-0.914459000
1	6.072371000	2.166910000	-0.951154000
1	4.512631000	0.248023000	-1.495877000
1	2.344993000	2.250833000	-2.186671000
1	2.374014000	2.855002000	0.079680000
1	3.363496000	0.078858000	0.733048000
1	5.469941000	1.060503000	1.042018000
1	-0.143094000	-1.939680000	0.883246000
6	2.043281000	-2.311435000	-0.698638000
8	1.186948000	-1.324935000	-0.249868000
6	3.282527000	-2.335768000	0.205192000
6	4.597369000	-2.240745000	-0.249989000
6	3.071958000	-2.417446000	1.587964000
6	5.668152000	-2.193084000	0.646228000
1	4.801954000	-2.184955000	-1.315121000
6	4.130876000	-2.379846000	2.485149000
1	2.050930000	-2.487536000	1.954908000
6	5.440377000	-2.256789000	2.015845000
1	6.682240000	-2.101767000	0.265690000
1	3.939909000	-2.440925000	3.553607000
1	6.271297000	-2.217252000	2.714764000
6	2.384400000	-2.216078000	-2.188178000
1	2.954581000	-3.088507000	-2.533850000
1	1.453592000	-2.164799000	-2.761055000
1	2.958690000	-1.313788000	-2.422611000
1	1.593769000	-3.316742000	-0.564648000

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Doordinates (Angstroms)

	X	Y	Z
25	0.505272000	-0.139865000	-0.902366000
7	1.476039000	0.555318000	1.138148000
6	-0.931131000	-0.929443000	2.120751000
1	-1.525372000	-0.488751000	2.927245000
1	-1.099422000	-2.009667000	2.193638000
6	3.840390000	0.806107000	-0.636644000
6	-0.284289000	-0.292821000	-2.461573000
8	-0.775371000	-0.339571000	-3.523065000
15	2.600065000	0.288421000	-1.910625000
15	-1.481745000	-0.392186000	0.422476000
14	3.235342000	0.354385000	1.093722000
14	0.902538000	-0.554193000	2.386883000
6	4.189514000	1.438995000	2.309046000
1	3.982055000	2.500489000	2.121417000
1	3.939324000	1.229089000	3.354608000
1	5.270214000	1.288217000	2.190517000
6	1.072444000	0.087049000	4.157824000
1	0.658169000	-0.636262000	4.872345000
1	2.111635000	0.278371000	4.447308000
1	0.517771000	1.026834000	4.279333000
1	4.838299000	0.408765000	-0.858459000
1	3.925224000	1.900321000	-0.662882000
6	2.801093000	1.600148000	-3.198191000
1	3.779568000	1.509678000	-3.683943000
1	2.018739000	1.504350000	-3.958179000
1	2.728766000	2.595834000	-2.760430000
6	3.569341000	-0.990603000	-2.840532000
1	3.084443000	-1.181822000	-3.803845000
1	4.575833000	-0.607767000	-3.043048000
1	3.667234000	-1.940108000	-2.312170000
15	1.004907000	-2.427360000	-0.769988000
6	2.560581000	-2.876562000	0.144072000
1	2.570737000	-3.953027000	0.359629000
1	3.438118000	-2.678969000	-0.480559000
14	2.773789000	-1.855389000	1.742211000
6	-0.044044000	-3.751602000	-0.001140000
1	-0.217516000	-3.574892000	1.063570000
1	-1.004331000	-3.832356000	-0.515308000
1	0.465150000	-4.716780000	-0.105036000
6	1.162872000	-3.286299000	-2.399960000
1	1.660284000	-2.666280000	-3.144138000
1	1.694429000	-4.240442000	-2.307556000
1	0.151269000	-3.486215000	-2.770948000

6	3.818239000	-2.813004000	2.992574000
1	3.318362000	-3.739940000	3.298375000
1	4.790845000	-3.085751000	2.566119000
1	4.002727000	-2.219176000	3.894893000
1	1.014897000	1.426073000	0.802911000
6	0.220551000	3.046984000	-1.411810000
8	0.211709000	1.918986000	-0.620811000
6	-2.433930000	1.204272000	0.658868000
6	-2.967214000	1.533137000	2.058923000
6	-3.555931000	1.358122000	-0.402092000
6	-3.421354000	3.006530000	2.143234000
1	-3.800854000	0.866519000	2.314234000
6	-4.634673000	2.372664000	0.022545000
1	-3.102648000	1.663695000	-1.348799000
6	-4.039424000	3.522028000	0.829582000
1	-4.146511000	3.103246000	2.960662000
1	-5.151582000	2.749349000	-0.867472000
1	-4.799381000	4.283002000	1.040236000
6	-2.755244000	-1.719547000	0.095305000
6	-3.994326000	-1.719555000	1.006197000
6	-3.120373000	-1.862782000	-1.403205000
6	-4.763703000	-3.049728000	0.871137000
1	-3.696390000	-1.572393000	2.050536000
6	-4.507041000	-2.495604000	-1.591866000
1	-3.074252000	-0.905186000	-1.928238000
6	-4.729727000	-3.610082000	-0.568355000
1	-4.341998000	-3.790709000	1.561393000
1	-5.287668000	-1.731534000	-1.472645000
1	-3.913992000	-4.339766000	-0.667070000
6	-1.118573000	3.291549000	-2.120060000
1	-1.924546000	3.507335000	-1.411638000
1	-1.052936000	4.131804000	-2.825260000
1	-1.393884000	2.394059000	-2.684798000
6	0.666936000	4.289651000	-0.591687000
1	0.605470000	5.162233000	-1.259819000
6	2.121584000	4.147278000	-0.139631000
1	2.461998000	5.034016000	0.409604000
1	2.228467000	3.281202000	0.522471000
1	2.797065000	4.009265000	-0.993027000
6	-0.223881000	4.549945000	0.624009000
1	0.127880000	5.421275000	1.190458000
1	-1.262872000	4.744387000	0.339114000
1	-0.213116000	3.682989000	1.294664000
1	-2.210393000	-2.623967000	0.374122000

1	-2.361530000	-2.492502000	-1.885594000
1	-4.604170000	-2.879839000	-2.613451000
1	-5.655654000	-4.155485000	-0.782048000
1	-5.802176000	-2.890615000	1.184817000
1	-4.658104000	-0.885887000	0.758894000
1	-1.645645000	1.926519000	0.411948000
1	-4.060460000	0.412816000	-0.603223000
1	-5.396518000	1.867573000	0.633047000
1	-3.270917000	4.014126000	0.222500000
1	-2.563586000	3.634919000	2.410352000
1	-2.198934000	1.375688000	2.821868000
1	0.953718000	2.964806000	-2.231395000

In_E5r

Doordinates (Angstroms)			
	X	Y	Z
25	0.700501000	0.022837000	-1.044385000
7	0.633729000	1.513417000	0.776762000
6	0.895639000	-1.097161000	2.136052000
1	0.301782000	-1.296117000	3.036458000
1	1.735120000	-1.798170000	2.154112000
6	1.181615000	3.358300000	-1.424555000
6	0.379730000	-1.005781000	-2.425648000
8	0.146161000	-1.658124000	-3.368683000
15	1.275304000	1.785728000	-2.370497000
15	-0.065689000	-1.431331000	0.581974000
14	1.599880000	2.946995000	0.370541000
14	1.489279000	0.704018000	2.099631000
6	1.214896000	4.475370000	1.405960000
1	1.431502000	4.331483000	2.469973000
1	1.799868000	5.337003000	1.060425000
1	0.153451000	4.738974000	1.312420000
6	1.179965000	1.418706000	3.821716000
1	1.776397000	0.877840000	4.568175000
1	1.442425000	2.479764000	3.896377000
1	0.126225000	1.317158000	4.112087000
1	1.761587000	4.171817000	-1.869810000
1	0.124826000	3.653628000	-1.413330000
15	2.897780000	-0.664485000	-0.950050000
6	4.108369000	0.617785000	-0.373612000
1	5.066467000	0.147697000	-0.115359000
1	4.310019000	1.305815000	-1.204633000
14	3.420281000	1.627579000	1.084850000

6	3.530082000	-2.098708000	0.031837000
1	3.550886000	-1.854000000	1.098112000
1	2.894924000	-2.978305000	-0.106077000
1	4.552671000	-2.351736000	-0.271525000
6	3.598208000	-1.119179000	-2.594027000
1	3.382314000	-0.335776000	-3.327015000
1	4.682461000	-1.269993000	-2.543187000
1	3.129746000	-2.043254000	-2.948738000
6	4.815491000	2.349893000	2.131670000
1	5.432523000	1.557849000	2.572392000
1	5.472831000	2.985374000	1.526222000
1	4.420542000	2.961186000	2.950922000
1	-0.375301000	1.500421000	0.566860000
6	-2.223727000	0.673825000	-1.710205000
8	-1.060962000	1.086941000	-1.103055000
6	-3.454327000	1.279773000	-1.033331000
6	-4.730889000	0.767494000	-1.281349000
6	-3.335882000	2.366791000	-0.168643000
6	-5.857158000	1.320286000	-0.679632000
1	-4.840692000	-0.088045000	-1.945385000
6	-4.458300000	2.923613000	0.441182000
1	-2.343172000	2.759649000	0.027257000
6	-5.724749000	2.401134000	0.190921000
1	-6.839256000	0.899341000	-0.880243000
1	-4.343724000	3.767221000	1.117921000
1	-6.601419000	2.832868000	0.666503000
6	-2.254978000	1.037508000	-3.208024000
1	-2.159138000	2.124144000	-3.326799000
1	-1.423154000	0.554642000	-3.730578000
1	-3.188005000	0.719916000	-3.689928000
1	0.507795000	2.051854000	-3.520717000
1	2.550313000	1.938780000	-2.974441000
1	-2.346586000	-0.426027000	-1.646983000
6	-1.803913000	-1.204564000	1.139783000
6	-2.820664000	-1.984999000	0.577506000
6	-2.155164000	-0.212827000	2.058920000
6	-4.149070000	-1.785311000	0.936468000
1	-2.573621000	-2.758967000	-0.144046000
6	-3.486166000	-0.007815000	2.413992000
1	-1.395248000	0.423315000	2.503414000
6	-4.486556000	-0.795415000	1.856099000
1	-4.924536000	-2.399734000	0.488250000
1	-3.740168000	0.777174000	3.119883000
1	-5.525684000	-0.627153000	2.121134000

6	0.023884000	-3.266966000	0.475443000
6	-0.320854000	-4.060691000	1.577924000
6	0.453673000	-3.893837000	-0.695300000
6	-0.225822000	-5.445629000	1.512356000
1	-0.678375000	-3.591285000	2.490671000
6	0.548675000	-5.283943000	-0.763813000
1	0.714599000	-3.297516000	-1.562067000
6	0.212657000	-6.060574000	0.339611000
1	-0.496580000	-6.047328000	2.375378000
1	0.884492000	-5.755335000	-1.682852000
1	0.287608000	-7.142998000	0.287442000

In_E5s

Doordinates (Angstroms)			
	X	Y	Z
25	0.666834000	-0.068110000	1.070592000
7	0.263409000	-1.557088000	-0.736268000
6	1.101478000	0.904752000	-2.166025000
1	0.565676000	1.222268000	-3.068614000
1	2.085757000	1.379276000	-2.212211000
6	0.464798000	-3.448667000	1.505274000
6	0.642846000	1.053662000	2.414541000
8	0.617687000	1.780637000	3.331167000
15	0.825700000	-1.889729000	2.421043000
15	0.287645000	1.491281000	-0.610206000
14	0.889624000	-3.159546000	-0.315813000
14	1.251660000	-0.986181000	-2.088252000
6	0.145205000	-4.583781000	-1.302080000
1	0.300948000	-4.468290000	-2.380349000
1	0.589327000	-5.541419000	-1.002488000
1	-0.935951000	-4.652461000	-1.126316000
6	0.747001000	-1.657772000	-3.780419000
1	1.317677000	-1.165095000	-4.578195000
1	0.917029000	-2.736299000	-3.873609000
1	-0.317891000	-1.473375000	-3.973120000
1	0.940892000	-4.326169000	1.953940000
1	-0.620914000	-3.612427000	1.541563000
15	2.968142000	0.054790000	0.954446000
6	3.850766000	-1.471638000	0.378147000
1	4.891469000	-1.233393000	0.120650000
1	3.889489000	-2.188092000	1.209183000
14	2.946702000	-2.300575000	-1.079078000
6	3.887407000	1.301294000	-0.054471000

1	3.841411000	1.047869000	-1.117736000
1	3.462335000	2.300036000	0.079714000
1	4.943420000	1.326654000	0.237927000
6	3.782235000	0.368288000	2.579719000
1	3.396992000	-0.316879000	3.341066000
1	4.869701000	0.250042000	2.514749000
1	3.557499000	1.388728000	2.907123000
6	4.149121000	-3.321540000	-2.117319000
1	4.930686000	-2.686006000	-2.550891000
1	4.644680000	-4.087287000	-1.508689000
1	3.635878000	-3.830154000	-2.941307000
1	-0.700331000	-1.269926000	-0.483795000
6	-2.306264000	-0.845104000	1.806289000
8	-1.345372000	-0.408945000	0.926388000
6	-3.618984000	-1.054941000	1.035590000
6	-4.849081000	-0.527041000	1.429591000
6	-3.586526000	-1.821879000	-0.134942000
6	-6.006636000	-0.756063000	0.683798000
1	-4.917931000	0.081129000	2.326228000
6	-4.734944000	-2.061798000	-0.879303000
1	-2.637472000	-2.229656000	-0.472244000
6	-5.956706000	-1.525400000	-0.473002000
1	-6.949804000	-0.327421000	1.013279000
1	-4.677845000	-2.662939000	-1.783535000
1	-6.858391000	-1.707682000	-1.051526000
6	-2.464195000	0.078589000	3.016953000
1	-3.211199000	-0.290203000	3.731431000
1	-1.508437000	0.149715000	3.542151000
1	-2.743779000	1.089162000	2.696771000
1	0.015718000	-2.017292000	3.571180000
1	2.043812000	-2.245065000	3.048848000
1	-2.060566000	-1.852080000	2.229269000
6	0.764052000	3.268614000	-0.570776000
6	1.327508000	3.833359000	0.574901000
6	0.567010000	4.079680000	-1.696098000
6	1.695539000	5.178816000	0.595905000
1	1.475736000	3.225691000	1.460565000
6	0.935212000	5.419646000	-1.677949000
1	0.112736000	3.661166000	-2.590531000
6	1.502469000	5.972256000	-0.529681000
1	2.129737000	5.603815000	1.496252000
1	0.774727000	6.035660000	-2.558165000
1	1.786793000	7.020540000	-0.513675000
6	-1.486330000	1.613827000	-1.047523000

6	-2.065361000	0.941990000	-2.121628000
6	-2.312135000	2.327274000	-0.171650000
6	-3.445494000	0.980409000	-2.320089000
1	-1.454833000	0.366357000	-2.811626000
6	-3.683775000	2.374173000	-0.373689000
1	-1.876019000	2.828619000	0.688984000
6	-4.257193000	1.694956000	-1.448867000
1	-3.884587000	0.440636000	-3.154178000
1	-4.312892000	2.925348000	0.319436000
1	-5.332763000	1.713033000	-1.595322000

In_F5r

Doordinates (Angstroms)			
	X	Y	Z
25	0.044047000	0.213855000	-0.935532000
7	-1.142216000	0.623704000	1.056550000
6	1.728098000	0.630659000	1.978441000
1	1.999541000	0.119403000	2.910878000
1	2.478074000	1.412476000	1.830125000
6	-3.192748000	1.481596000	-0.908561000
6	0.782535000	-0.372241000	-2.417046000
8	1.228703000	-0.766471000	-3.422622000
15	-1.821612000	0.958676000	-2.032096000
15	1.757430000	-0.523094000	0.522708000
14	-2.458788000	1.789240000	0.804850000
14	0.013116000	1.426324000	2.134053000
6	-3.852907000	1.719628000	2.069122000
1	-3.491950000	1.833383000	3.097202000
1	-4.584046000	2.515935000	1.880533000
1	-4.380867000	0.761606000	1.997393000
6	-0.444636000	1.384147000	3.968276000
1	0.340914000	1.863203000	4.567085000
1	-1.384537000	1.904757000	4.183583000
1	-0.548175000	0.351468000	4.325474000
1	-3.740269000	2.340784000	-1.309579000
1	-3.906834000	0.653107000	-0.826010000
15	0.971755000	2.330014000	-1.213585000
6	-0.058254000	3.754490000	-0.625813000
1	0.537343000	4.677166000	-0.631866000
1	-0.886991000	3.912285000	-1.328030000
14	-0.785052000	3.405722000	1.104778000
6	2.580920000	2.919340000	-0.508013000
1	2.492691000	3.077017000	0.570844000

1	3.386131000	2.205935000	-0.691267000
1	2.860272000	3.875909000	-0.964361000
6	1.287570000	2.771373000	-2.976603000
1	0.422012000	2.524473000	-3.598264000
1	1.513905000	3.837407000	-3.092160000
1	2.138381000	2.188947000	-3.346637000
6	-1.028677000	5.011146000	2.069404000
1	-0.071215000	5.518866000	2.237281000
1	-1.678722000	5.703355000	1.521312000
1	-1.486199000	4.826252000	3.047836000
1	-1.305833000	-0.389315000	0.936951000
6	-1.757660000	-2.475661000	-1.019010000
8	-0.965130000	-1.531289000	-0.407135000
6	-3.246675000	-2.123088000	-0.873345000
6	-4.129513000	-1.956852000	-1.941278000
6	-3.746399000	-1.934853000	0.422052000
6	-5.461460000	-1.594500000	-1.728230000
1	-3.782885000	-2.104767000	-2.960176000
6	-5.075123000	-1.592381000	0.644238000
1	-3.072721000	-2.064989000	1.266244000
6	-5.940801000	-1.410035000	-0.435731000
1	-6.125674000	-1.462861000	-2.578497000
1	-5.441467000	-1.468583000	1.660346000
1	-6.978863000	-1.137524000	-0.267592000
6	-1.350686000	-2.801864000	-2.458597000
1	-1.473884000	-1.946792000	-3.131516000
1	-0.291514000	-3.074988000	-2.473966000
1	-1.926231000	-3.645773000	-2.860364000
6	3.583478000	-0.680330000	0.049955000
6	3.871978000	-0.343456000	-1.431758000
6	4.576552000	0.024529000	0.985155000
6	5.336394000	0.062749000	-1.665685000
1	3.630940000	-1.221304000	-2.041551000
6	6.017419000	-0.454213000	0.712188000
1	4.515232000	1.110835000	0.847007000
6	6.270264000	-0.760342000	-0.779139000
1	5.587703000	-0.063531000	-2.724669000
1	6.222348000	-1.351347000	1.308447000
1	6.091060000	-1.825160000	-0.978776000
6	1.589016000	-2.186013000	1.358578000
6	0.376382000	-2.312894000	2.290077000
6	1.552016000	-3.299999000	0.299145000
6	0.327499000	-3.694930000	2.949583000
1	0.396584000	-1.537823000	3.066172000

6	1.480067000	-4.689365000	0.939204000
1	0.668852000	-3.114354000	-0.319041000
6	0.292942000	-4.805570000	1.897577000
1	1.211008000	-3.829134000	3.591347000
1	2.411066000	-4.885517000	1.491936000
1	0.287109000	-5.790235000	2.380757000
1	3.779419000	-1.751632000	0.175572000
1	3.209094000	0.446521000	-1.791973000
1	5.474980000	1.129497000	-1.439264000
1	7.319512000	-0.570435000	-1.030962000
1	6.716672000	0.315675000	1.060008000
1	4.326086000	-0.166290000	2.034063000
1	2.426636000	-3.249990000	-0.362270000
1	2.501223000	-2.300110000	1.968813000
1	-0.522609000	-2.166410000	1.682896000
1	1.411234000	-5.454001000	0.155740000
1	-0.641539000	-4.724427000	1.324366000
1	-0.551198000	-3.762543000	3.602940000
1	-2.504189000	0.150442000	-2.965054000
1	-1.735217000	2.101187000	-2.865059000
1	-1.645659000	-3.436654000	-0.465807000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.461457000	-0.205639000	-0.998168000
7	1.564277000	0.384367000	0.945476000
6	-0.800243000	-1.169012000	1.955988000
1	-1.373373000	-0.898215000	2.850666000
1	-0.931948000	-2.243035000	1.815073000
6	3.800083000	0.575884000	-1.001936000
6	-0.513967000	-0.318175000	-2.450462000
8	-1.172605000	-0.368398000	-3.416799000
15	2.468750000	-0.066896000	-2.100304000
15	-1.387785000	-0.275902000	0.442328000
14	3.315109000	0.127255000	0.764533000
14	1.038645000	-0.777485000	2.181920000
6	4.372898000	1.149373000	1.943103000
1	4.196013000	2.220059000	1.778903000
1	4.162801000	0.934006000	2.996544000
1	5.439820000	0.961001000	1.769949000
6	1.282421000	-0.178338000	3.955938000
1	0.930796000	-0.930164000	4.673885000

1	2.331886000	0.035310000	4.187760000
1	0.709163000	0.740983000	4.133836000
1	4.792414000	0.217502000	-1.293663000
1	3.802463000	1.667844000	-1.075555000
15	0.779889000	-2.518065000	-0.931533000
6	2.402303000	-3.068908000	-0.208981000
1	2.376757000	-4.149293000	-0.013940000
1	3.196639000	-2.905510000	-0.948062000
14	2.830910000	-2.089496000	1.372620000
6	-0.275737000	-3.818907000	-0.127565000
1	-0.108857000	-3.845215000	0.953107000
1	-1.340761000	-3.654225000	-0.311579000
1	-0.009520000	-4.804355000	-0.526230000
6	0.822687000	-3.262478000	-2.619905000
1	1.448438000	-2.668868000	-3.291699000
1	1.200401000	-4.291062000	-2.598930000
1	-0.192733000	-3.268469000	-3.031049000
6	3.931155000	-3.099135000	2.528786000
1	3.422274000	-4.011004000	2.863273000
1	4.858623000	-3.401646000	2.028324000
1	4.205053000	-2.522177000	3.419571000
1	1.182589000	1.316700000	0.723451000
6	0.462105000	2.955676000	-1.799823000
8	0.805972000	1.892820000	-0.991312000
6	-2.027089000	1.273921000	1.244752000
6	-3.237852000	1.145452000	2.179816000
6	-2.247402000	2.395931000	0.208595000
6	-3.405565000	2.432478000	3.012761000
1	-4.140205000	0.974488000	1.581313000
6	-3.212928000	3.477271000	0.716286000
1	-1.270076000	2.822231000	0.002672000
6	-3.021236000	3.699027000	2.216985000
1	-4.446670000	2.503393000	3.350359000
1	-3.046096000	4.408529000	0.162293000
1	-3.606679000	4.556792000	2.566063000
6	-2.873206000	-1.247502000	-0.151712000
6	-3.700106000	-2.030171000	0.878080000
6	-3.827676000	-0.424117000	-1.047274000
6	-4.520054000	-3.126047000	0.161476000
1	-3.073637000	-2.489710000	1.648389000
6	-5.137580000	-1.192940000	-1.339104000
1	-4.086570000	0.522020000	-0.564812000
6	-4.934578000	-2.705983000	-1.263505000
1	-3.935340000	-4.053386000	0.113047000

1	-5.904060000	-0.907087000	-0.606747000
1	-4.161779000	-3.000238000	-1.985537000
6	0.824919000	2.783867000	-3.284444000
1	0.408495000	3.607887000	-3.879069000
1	1.908843000	2.769382000	-3.451451000
1	0.407169000	1.848992000	-3.669745000
6	1.086846000	4.276736000	-1.254951000
1	0.909698000	5.056084000	-2.011633000
6	2.595690000	4.152651000	-1.039067000
1	3.032505000	5.113042000	-0.738357000
1	2.795275000	3.424936000	-0.245317000
1	3.119133000	3.821801000	-1.943464000
6	0.428033000	4.735800000	0.047641000
1	0.895246000	5.652839000	0.428869000
1	-0.639384000	4.942577000	-0.091675000
1	0.529724000	3.962886000	0.819550000
1	-2.393270000	-1.984061000	-0.808452000
1	-3.316976000	-0.173132000	-1.981906000
1	-5.525533000	-0.902287000	-2.321155000
1	-5.848036000	-3.232739000	-1.560917000
1	-5.412350000	-3.352946000	0.757238000
1	-4.372117000	-1.339958000	1.400602000
1	-1.172886000	1.575592000	1.872495000
1	-2.599615000	1.998666000	-0.748654000
1	-4.254977000	3.186688000	0.523353000
1	-1.967320000	3.949715000	2.397047000
1	-2.789022000	2.366473000	3.917913000
1	-3.149320000	0.283800000	2.850229000
1	-0.636270000	3.123046000	-1.807546000
1	2.611901000	0.721971000	-3.254926000
1	3.136300000	-1.208453000	-2.616219000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.510371000	-0.334401000	1.060654000
7	-0.286894000	-1.605086000	-0.738293000
6	1.365611000	0.507892000	-2.095103000
1	1.005758000	0.990546000	-3.012270000
1	2.455502000	0.587563000	-2.114697000
6	-0.638005000	-3.562975000	1.440971000
6	0.798878000	0.710472000	2.440477000
8	0.950198000	1.385904000	3.382000000

15	0.139759000	-2.169778000	2.373672000
15	0.726025000	1.357131000	-0.570645000
14	-0.201012000	-3.340430000	-0.387333000
14	0.853790000	-1.318339000	-2.062487000
6	-1.381856000	-4.402412000	-1.402160000
1	-1.241871000	-4.255658000	-2.478779000
1	-1.234680000	-5.468574000	-1.188953000
1	-2.425851000	-4.159366000	-1.165843000
6	0.209029000	-1.759699000	-3.783964000
1	0.949345000	-1.486006000	-4.546769000
1	0.005130000	-2.830645000	-3.896312000
1	-0.718027000	-1.220404000	-4.015631000
1	-0.373850000	-4.542935000	1.851163000
1	-1.728052000	-3.459247000	1.524638000
15	2.754100000	-0.959363000	0.941147000
6	3.080049000	-2.707074000	0.410961000
1	4.150612000	-2.848204000	0.211431000
1	2.821062000	-3.390820000	1.228847000
14	2.025140000	-3.150313000	-1.115390000
6	4.068733000	-0.174040000	-0.106898000
1	3.965550000	-0.492981000	-1.148435000
1	4.025372000	0.916389000	-0.072571000
1	5.059225000	-0.489206000	0.241319000
6	3.622146000	-0.870460000	2.566892000
1	3.018714000	-1.336411000	3.351514000
1	4.600567000	-1.362426000	2.530187000
1	3.767842000	0.180112000	2.840769000
6	2.882550000	-4.449858000	-2.183367000
1	3.825393000	-4.065782000	-2.591233000
1	3.115387000	-5.350884000	-1.603479000
1	2.252419000	-4.749517000	-3.028468000
1	-1.117978000	-1.046070000	-0.476307000
6	-2.547751000	-0.334409000	1.806606000
8	-1.535173000	-0.020648000	0.926378000
6	-3.894711000	-0.158780000	1.090252000
6	-4.910768000	0.686333000	1.537919000
6	-4.109404000	-0.860270000	-0.103176000
6	-6.098861000	0.831891000	0.819252000
1	-4.783194000	1.250566000	2.456362000
6	-5.287942000	-0.720196000	-0.825985000
1	-3.326832000	-1.517492000	-0.476208000
6	-6.292248000	0.133217000	-0.366681000
1	-6.869867000	1.503591000	1.187586000
1	-5.424979000	-1.272577000	-1.752096000

1	-7.214558000	0.250156000	-0.928759000
6	-2.463198000	0.456629000	3.114856000
1	-3.264810000	0.189491000	3.815343000
1	-1.507775000	0.250014000	3.603116000
1	-2.503321000	1.535236000	2.921921000
6	1.802323000	2.896115000	-0.369054000
6	2.577073000	2.961943000	0.968300000
6	2.722442000	3.211792000	-1.556905000
6	3.813280000	3.872820000	0.881268000
1	1.899589000	3.335358000	1.743265000
6	3.266680000	4.651550000	-1.458568000
1	3.557736000	2.500311000	-1.576626000
6	3.521382000	5.087098000	-0.000375000
1	4.113688000	4.181981000	1.888636000
1	2.557084000	5.342639000	-1.929017000
1	2.636539000	5.600452000	0.398397000
6	-0.792996000	2.213402000	-1.241952000
6	-1.760053000	1.296300000	-2.001722000
6	-1.544875000	2.936686000	-0.111685000
6	-2.944193000	2.088393000	-2.564703000
1	-1.248214000	0.776374000	-2.820369000
6	-2.742375000	3.724455000	-0.652343000
1	-1.874177000	2.164000000	0.591166000
6	-3.689122000	2.825281000	-1.450672000
1	-2.582192000	2.812548000	-3.310524000
1	-2.383245000	4.540579000	-1.297886000
1	-4.514524000	3.414723000	-1.868757000
1	1.062900000	3.705222000	-0.345125000
1	2.878371000	1.966552000	1.304219000
1	4.664296000	3.319631000	0.459335000
1	4.343068000	5.810471000	0.040872000
1	4.196496000	4.718172000	-2.036245000
1	2.192458000	3.087326000	-2.507184000
1	-0.878342000	3.615259000	0.436630000
1	-0.408789000	2.962558000	-1.956091000
1	-2.138370000	0.545835000	-1.302626000
1	-3.280594000	4.192980000	0.180824000
1	-4.133017000	2.085235000	-0.774406000
1	-3.626998000	1.406900000	-3.086783000
1	-0.664379000	-2.100866000	3.533582000
1	1.218656000	-2.853429000	2.984882000
1	-2.521527000	-1.410958000	2.102783000

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Doordinates (Angstroms)

	X	Y	Z
25	0.442163000	-0.172520000	-1.032548000
7	1.674405000	0.331569000	0.917544000
6	-0.729924000	-1.096353000	1.990539000
1	-1.241047000	-0.753082000	2.897649000
1	-0.923324000	-2.170001000	1.921738000
6	3.819024000	0.545172000	-1.092954000
6	-0.580524000	-0.235320000	-2.453914000
8	-1.271093000	-0.266324000	-3.398260000
15	2.412252000	0.051080000	-2.186464000
15	-1.372129000	-0.270774000	0.455690000
14	3.399446000	0.019433000	0.675712000
14	1.135946000	-0.822673000	2.140116000
6	4.546280000	0.962320000	1.838538000
1	4.402577000	2.044123000	1.721845000
1	4.366293000	0.717668000	2.891193000
1	5.598722000	0.741652000	1.619840000
6	1.480023000	-0.298182000	3.921823000
1	1.112973000	-1.051247000	4.630994000
1	2.547431000	-0.149504000	4.120211000
1	0.966560000	0.645849000	4.147469000
1	4.780802000	0.169670000	-1.457199000
1	3.880302000	1.641343000	-1.091639000
15	0.760976000	-2.480766000	-1.096489000
6	2.357943000	-3.095984000	-0.373163000
1	2.307629000	-4.181534000	-0.216914000
1	3.156021000	-2.926892000	-1.108101000
14	2.840775000	-2.193699000	1.237988000
6	-0.366313000	-3.777386000	-0.396932000
1	-0.508895000	-3.662914000	0.680373000
1	-1.345445000	-3.737873000	-0.882040000
1	0.056807000	-4.771863000	-0.578280000
6	0.832837000	-3.172128000	-2.807796000
1	1.551756000	-2.626949000	-3.425348000
1	1.107323000	-4.233121000	-2.802440000
1	-0.151710000	-3.065765000	-3.275609000
6	3.930735000	-3.294697000	2.319402000
1	3.398587000	-4.205125000	2.620565000
1	4.839187000	-3.602037000	1.787896000
1	4.237951000	-2.770823000	3.231801000
1	1.250557000	1.243581000	0.645370000

6	0.965857000	2.900240000	-1.491069000
8	0.440983000	1.881133000	-0.727897000
6	-2.006601000	1.340212000	1.136072000
6	-3.127338000	1.241890000	2.181322000
6	-2.389590000	2.348439000	0.019224000
6	-3.312641000	2.592631000	2.897457000
1	-4.061290000	0.960349000	1.681121000
6	-3.431985000	3.371706000	0.492463000
1	-1.466143000	2.838832000	-0.281061000
6	-3.146013000	3.789667000	1.935188000
1	-4.306142000	2.615399000	3.361373000
1	-3.414248000	4.242040000	-0.173839000
1	-3.796191000	4.616517000	2.242536000
6	-2.867530000	-1.299600000	-0.010116000
6	-3.656504000	-2.008219000	1.101624000
6	-3.869356000	-0.581203000	-0.940467000
6	-4.439793000	-3.194332000	0.497618000
1	-3.012720000	-2.370428000	1.907740000
6	-5.148369000	-1.425636000	-1.157962000
1	-4.164228000	0.379903000	-0.511056000
6	-4.887953000	-2.917795000	-0.952186000
1	-3.815971000	-4.096845000	0.521579000
1	-5.923672000	-1.107711000	-0.448681000
1	-4.114351000	-3.247023000	-1.658509000
6	0.227900000	3.039906000	-2.828764000
1	-0.823483000	3.301859000	-2.655781000
1	0.673487000	3.795254000	-3.487296000
1	0.242604000	2.083464000	-3.359189000
6	0.960038000	4.231273000	-0.691609000
1	-0.090557000	4.526868000	-0.550214000
6	1.678283000	5.360515000	-1.436057000
1	1.720497000	6.270621000	-0.825180000
1	2.712949000	5.076364000	-1.673624000
1	1.180523000	5.622741000	-2.375083000
6	1.583641000	4.036241000	0.691212000
1	1.642782000	4.986132000	1.237153000
1	1.003380000	3.333451000	1.294987000
1	2.606678000	3.641579000	0.603478000
1	-2.392905000	-2.081631000	-0.611653000
1	-3.385567000	-0.366804000	-1.898307000
1	-5.550964000	-1.237723000	-2.159000000
1	-5.785006000	-3.500921000	-1.188501000
1	-5.314879000	-3.403560000	1.124585000
1	-4.350544000	-1.294150000	1.560529000

1	-1.115451000	1.742671000	1.641081000
1	-2.747174000	1.840815000	-0.881050000
1	-4.447264000	2.955052000	0.428120000
1	-2.116472000	4.168987000	1.984873000
1	-2.584987000	2.673957000	3.714416000
1	-2.933164000	0.460026000	2.923414000
1	2.043525000	2.727914000	-1.737766000
1	2.540398000	0.957219000	-3.262785000
1	3.005850000	-1.049058000	-2.849065000

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Doordinates (Angstroms)			
	X	Y	Z
25	-0.437550000	-1.290292000	-0.541772000
7	1.019427000	-0.658006000	1.156438000
6	-1.384869000	-1.452562000	-2.011145000
8	-1.967274000	-1.510532000	-3.018660000
6	2.823948000	-2.010227000	-0.641553000
1	3.606266000	-2.760835000	-0.811639000
1	3.174048000	-1.065467000	-1.076602000
6	-1.626539000	0.131901000	2.207889000
6	-1.142411000	-2.684303000	0.304580000
8	-1.609439000	-3.626811000	0.811835000
15	-1.832870000	0.214844000	0.384000000
15	1.248560000	-2.440399000	-1.481023000
14	0.195087000	-0.117933000	2.642680000
14	2.426760000	-1.757984000	1.177693000
6	0.942581000	1.490992000	3.257778000
1	0.385067000	1.863405000	4.126870000
1	1.985723000	1.358515000	3.567318000
1	0.922472000	2.265448000	2.485329000
6	0.313905000	-1.408064000	3.996990000
1	1.341308000	-1.557281000	4.348643000
1	-0.275357000	-1.062660000	4.856444000
1	-0.094190000	-2.376192000	3.688843000
6	3.895960000	-1.003588000	2.100177000
1	4.249634000	-1.671969000	2.894661000
1	4.739018000	-0.823612000	1.423247000
1	3.639407000	-0.044324000	2.563044000
6	1.985956000	-3.407200000	1.965540000
1	2.673154000	-4.172815000	1.582152000
1	2.099964000	-3.392588000	3.053806000
1	0.965809000	-3.730193000	1.737440000

1	-2.107708000	0.951523000	2.753682000
1	-2.156240000	-0.786470000	2.493934000
1	1.280780000	0.166894000	0.609201000
1	0.292402000	-0.088232000	-1.337294000
6	1.573320000	1.902956000	-3.316902000
6	2.711884000	1.430346000	-2.449604000
8	3.474197000	0.555773000	-2.829892000
1	1.584666000	2.992090000	-3.433399000
1	1.647601000	1.428423000	-4.297002000
1	0.623302000	1.619296000	-2.850473000
6	-3.660609000	0.059995000	0.197874000
6	-4.213098000	-1.134165000	-0.271092000
6	-4.520305000	1.101164000	0.569592000
6	-5.594919000	-1.285967000	-0.369031000
1	-3.562884000	-1.950757000	-0.565616000
6	-5.899252000	0.950165000	0.473755000
1	-4.110622000	2.041212000	0.929511000
6	-6.439809000	-0.245068000	0.001998000
1	-6.007851000	-2.218674000	-0.742094000
1	-6.553639000	1.767385000	0.763859000
1	-7.516687000	-0.361738000	-0.079445000
6	-1.604534000	1.987893000	-0.052014000
6	-1.433713000	3.015538000	0.877019000
6	-1.643303000	2.315053000	-1.413988000
6	-1.299678000	4.340418000	0.457808000
1	-1.408028000	2.799951000	1.940313000
6	-1.523655000	3.634729000	-1.833639000
1	-1.765451000	1.524771000	-2.150032000
6	-1.345482000	4.653553000	-0.896233000
1	-1.167984000	5.126414000	1.196446000
1	-1.562689000	3.868218000	-2.893809000
1	-1.245013000	5.684760000	-1.222253000
6	2.908863000	2.064517000	-1.106291000
6	2.007306000	2.996265000	-0.581400000
6	4.057311000	1.735152000	-0.377532000
6	2.268627000	3.607192000	0.640684000
1	1.098933000	3.249498000	-1.118198000
6	4.312148000	2.339946000	0.847479000
1	4.750516000	1.012888000	-0.797095000
6	3.420396000	3.283635000	1.354548000
1	1.565530000	4.334324000	1.034992000
1	5.208653000	2.082231000	1.403496000
1	3.618950000	3.763545000	2.308554000
6	1.218123000	-4.279832000	-1.425733000

1	0.340764000	-4.630246000	-1.980960000
1	2.116650000	-4.718966000	-1.874361000
1	1.122267000	-4.639586000	-0.398030000
6	1.593215000	-2.182256000	-3.263142000
1	2.493150000	-2.724276000	-3.574408000
1	0.742391000	-2.533213000	-3.856560000
1	1.739400000	-1.117709000	-3.455920000

In_TSB4s

Doordinates (Angstroms)			
	X	Y	Z
25	-0.681081000	-0.003328000	-0.798590000
7	-1.977086000	0.546171000	1.001991000
6	0.380249000	-0.749135000	-1.996553000
8	1.063252000	-1.285198000	-2.767564000
6	-3.680496000	-1.405903000	-0.226930000
1	-4.662944000	-1.731373000	-0.590111000
1	-3.276175000	-2.184316000	0.435988000
6	0.171877000	2.572219000	1.148695000
6	-1.183888000	1.381338000	-1.789017000
8	-1.534374000	2.273082000	-2.451893000
15	0.975901000	1.288345000	0.097018000
15	-2.447552000	-1.235851000	-1.569865000
14	-1.431735000	1.966785000	1.934563000
14	-3.712319000	0.210443000	0.721244000
6	-1.212530000	1.448841000	3.728576000
1	-0.748675000	2.248483000	4.319320000
1	-2.187308000	1.230654000	4.182300000
1	-0.595772000	0.549996000	3.839602000
6	-2.657983000	3.382639000	1.841067000
1	-3.616266000	3.162727000	2.324051000
1	-2.225219000	4.247858000	2.360359000
1	-2.852644000	3.690788000	0.808172000
6	-4.611608000	-0.007041000	2.358371000
1	-4.150762000	-0.797043000	2.963666000
1	-4.620094000	0.914935000	2.952502000
1	-5.657392000	-0.292427000	2.188122000
6	-4.511185000	1.583846000	-0.280540000
1	-5.352622000	1.170725000	-0.850826000
1	-4.912358000	2.377829000	0.357453000
1	-3.818980000	2.041783000	-0.994451000
1	0.861331000	3.034038000	1.864628000
1	-0.119748000	3.360827000	0.442519000

1	-1.604943000	-0.279296000	1.474467000
1	-0.325236000	-1.375794000	0.128155000
6	-0.297286000	-2.729111000	1.018610000
8	-1.351529000	-3.355266000	0.797043000
6	1.983365000	2.340199000	-1.039789000
6	1.905841000	2.210044000	-2.426608000
6	2.849043000	3.303305000	-0.502197000
6	2.670001000	3.026606000	-3.260361000
1	1.250134000	1.469499000	-2.868821000
6	3.607376000	4.120515000	-1.330726000
1	2.940539000	3.408003000	0.575934000
6	3.518379000	3.983402000	-2.716193000
1	2.596030000	2.909094000	-4.337466000
1	4.272778000	4.861877000	-0.897582000
1	4.112832000	4.619705000	-3.365473000
6	2.343496000	0.649046000	1.149550000
6	2.307244000	0.698111000	2.545333000
6	3.468421000	0.096217000	0.526705000
6	3.366974000	0.204104000	3.304004000
1	1.453895000	1.131903000	3.056663000
6	4.538191000	-0.371695000	1.281598000
1	3.515453000	0.036564000	-0.557158000
6	4.488479000	-0.326639000	2.673503000
1	3.317991000	0.248669000	4.388268000
1	5.408327000	-0.784574000	0.780051000
1	5.321316000	-0.698969000	3.262837000
6	0.997387000	-3.249311000	0.414887000
6	0.932631000	-4.138124000	-0.661374000
6	2.247922000	-2.941522000	0.952598000
6	2.087296000	-4.689363000	-1.202204000
1	-0.036045000	-4.403300000	-1.066746000
6	3.406544000	-3.503426000	0.420718000
1	2.333472000	-2.261439000	1.793556000
1	2.016152000	-5.374418000	-2.042600000
1	4.368901000	-3.257091000	0.859703000
6	-0.170180000	-2.021379000	2.366840000
1	0.505888000	-1.164982000	2.353776000
1	-1.165631000	-1.716040000	2.703471000
1	0.203035000	-2.746415000	3.101857000
6	3.332635000	-4.374722000	-0.660610000
1	4.236687000	-4.810617000	-1.076685000
6	-2.203760000	-2.947383000	-2.166432000
1	-3.138287000	-3.353127000	-2.570266000
1	-1.434876000	-2.973087000	-2.944898000

1	-1.886900000	-3.547562000	-1.310668000
6	-3.407517000	-0.527898000	-2.970055000
1	-2.760713000	-0.471098000	-3.852621000
1	-4.274175000	-1.153440000	-3.212203000
1	-3.753151000	0.484226000	-2.746112000

In_TSB5r

Doordinates (Angstroms)			
	X	Y	Z
25	-0.200447000	-0.679595000	-0.822892000
7	0.895014000	-1.016577000	1.087966000
6	-0.883603000	-0.095048000	-2.350793000
8	-1.306873000	0.279633000	-3.365393000
6	3.104597000	-1.492694000	-0.691181000
1	3.890648000	-2.167828000	-1.050191000
1	3.550619000	-0.500145000	-0.551912000
6	-1.821195000	-0.553506000	2.143216000
6	-0.888912000	-2.299080000	-0.980882000
8	-1.325403000	-3.374297000	-1.043149000
15	-1.993616000	0.054031000	0.421466000
15	1.742211000	-1.329851000	-1.900385000
14	-0.010775000	-0.948269000	2.571986000
14	2.314253000	-2.018350000	0.946285000
6	0.697326000	0.372452000	3.720005000
1	0.058307000	0.544823000	4.595510000
1	1.683752000	0.066180000	4.091334000
1	0.826610000	1.332266000	3.205725000
6	-0.052310000	-2.580283000	3.517377000
1	0.932639000	-2.876720000	3.896979000
1	-0.721185000	-2.494596000	4.383910000
1	-0.430791000	-3.394979000	2.888378000
6	3.552733000	-1.765316000	2.347835000
1	3.799298000	-0.707215000	2.484101000
1	3.170479000	-2.148234000	3.302299000
1	4.489221000	-2.298464000	2.138804000
6	1.903182000	-3.860282000	0.883079000
1	2.704583000	-4.426440000	0.390674000
1	1.787157000	-4.276321000	1.890971000
1	0.970101000	-4.053623000	0.342792000
1	-2.322279000	0.091374000	2.874293000
1	-2.350395000	-1.515674000	2.155072000
1	1.078995000	0.218277000	0.683544000
6	1.680229000	-2.975535000	-2.712564000

1	0.897447000	-2.971779000	-3.478576000
1	2.636630000	-3.223535000	-3.186259000
1	1.436117000	-3.754193000	-1.984921000
6	2.434546000	-0.307116000	-3.256188000
1	3.351504000	-0.757229000	-3.652578000
1	1.705762000	-0.207402000	-4.067458000
1	2.673925000	0.687528000	-2.875078000
6	5.624018000	1.911626000	0.034840000
6	5.079168000	2.355386000	-1.164773000
6	3.697760000	2.503710000	-1.297632000
6	2.838206000	2.198862000	-0.241831000
6	3.403064000	1.771568000	0.965872000
6	4.778231000	1.626923000	1.106832000
1	6.698650000	1.795228000	0.140460000
1	5.727892000	2.592640000	-2.003474000
1	3.295532000	2.865467000	-2.239337000
1	2.749831000	1.538307000	1.803620000
1	5.193872000	1.291244000	2.052816000
6	1.317630000	2.300592000	-0.332022000
8	0.712259000	1.066138000	-0.051799000
6	0.792041000	2.843697000	-1.652303000
1	1.181883000	3.847698000	-1.854906000
1	1.051373000	2.186229000	-2.488907000
1	-0.297408000	2.907137000	-1.597463000
6	-2.145825000	1.874546000	0.548212000
6	-1.617358000	2.596741000	1.619220000
6	-2.752779000	2.571177000	-0.502589000
6	-1.687595000	3.988128000	1.638532000
1	-1.143013000	2.080322000	2.447161000
6	-2.827505000	3.960350000	-0.482109000
1	-3.171329000	2.027550000	-1.345788000
6	-2.290499000	4.673427000	0.587520000
1	-1.269399000	4.534660000	2.479044000
1	-3.303532000	4.484677000	-1.305597000
1	-2.346578000	5.758006000	0.603606000
6	-3.719147000	-0.400814000	-0.019733000
6	-4.006236000	-1.081347000	-1.204072000
6	-4.774896000	-0.056498000	0.834991000
6	-5.320777000	-1.417396000	-1.527367000
1	-3.206106000	-1.351885000	-1.884680000
6	-6.084614000	-0.391528000	0.515035000
1	-4.570029000	0.484047000	1.755663000
6	-6.359882000	-1.074988000	-0.669574000
1	-5.527227000	-1.946920000	-2.452888000

1	-6.892410000	-0.117368000	1.187459000
1	-7.383891000	-1.336068000	-0.920790000
1	1.003741000	3.010526000	0.452132000

In_TSB5s

Doordinates (Angstroms)			
	X	Y	Z
25	-0.773817000	0.247476000	-0.868314000
7	-1.958529000	0.039447000	1.008176000
6	0.232882000	0.112984000	-2.319911000
8	0.847432000	0.021901000	-3.301533000
6	-3.604046000	-1.621321000	-0.653027000
1	-4.588345000	-1.835489000	-1.085576000
1	-3.188790000	-2.561005000	-0.269198000
6	-0.044008000	2.101124000	1.812594000
6	-1.501024000	1.776113000	-1.380599000
8	-2.027274000	2.766897000	-1.680522000
15	0.809286000	1.395398000	0.355153000
15	-2.434346000	-0.987476000	-1.909987000
14	-1.430611000	0.946439000	2.399589000
14	-3.636009000	-0.388187000	0.782120000
6	-0.834258000	-0.197148000	3.773914000
1	-0.441662000	0.367301000	4.629540000
1	-1.668790000	-0.807065000	4.143115000
1	-0.050605000	-0.884942000	3.437349000
6	-2.756341000	2.077840000	3.119500000
1	-3.610184000	1.533557000	3.538983000
1	-2.325540000	2.676320000	3.933156000
1	-3.136705000	2.777544000	2.365647000
6	-4.377768000	-1.272567000	2.274533000
1	-3.795414000	-2.165352000	2.534373000
1	-4.424991000	-0.634532000	3.165172000
1	-5.402993000	-1.600799000	2.058582000
6	-4.728769000	1.083147000	0.341632000
1	-5.652178000	0.749897000	-0.149315000
1	-5.022880000	1.644297000	1.236236000
1	-4.219370000	1.781098000	-0.332242000
1	0.634688000	2.449119000	2.599299000
1	-0.554104000	2.993050000	1.422877000
1	-1.259114000	-1.002037000	0.762198000
6	-3.509147000	-0.107346000	-3.106650000
1	-2.895688000	0.303883000	-3.915522000
1	-4.262515000	-0.774753000	-3.539490000

1	-4.019589000	0.725000000	-2.612554000
6	-1.940363000	-2.478252000	-2.854259000
1	-2.822181000	-3.022174000	-3.210605000
1	-1.319839000	-2.203985000	-3.713929000
1	-1.359191000	-3.130106000	-2.196523000
6	0.399842000	-2.380177000	0.857052000
8	-0.526230000	-1.681094000	0.073132000
6	2.270479000	0.497207000	1.000353000
6	2.530607000	0.313422000	2.359800000
6	3.176228000	-0.011183000	0.061289000
6	3.675625000	-0.367056000	2.772665000
1	1.841618000	0.691658000	3.108306000
6	4.326305000	-0.672043000	0.473169000
1	2.981501000	0.112097000	-1.000730000
6	4.577100000	-0.854415000	1.831847000
1	3.862931000	-0.509039000	3.833301000
1	5.015133000	-1.064289000	-0.268245000
1	5.470135000	-1.381722000	2.154468000
6	1.649890000	2.858752000	-0.382969000
6	1.458871000	3.216077000	-1.717802000
6	2.496378000	3.643934000	0.411180000
6	2.091460000	4.338604000	-2.250579000
1	0.816373000	2.619974000	-2.354656000
6	3.124277000	4.765278000	-0.116616000
1	2.672989000	3.370759000	1.448532000
6	2.921441000	5.116107000	-1.451355000
1	1.931129000	4.600286000	-3.292351000
1	3.775576000	5.365914000	0.511751000
1	3.412239000	5.992320000	-1.865106000
1	0.863692000	-1.703972000	1.592750000
6	1.533100000	-2.968089000	0.035019000
6	2.594437000	-3.616757000	0.673700000
6	1.556245000	-2.862789000	-1.352997000
6	3.653606000	-4.141068000	-0.057991000
1	2.605631000	-3.689921000	1.758812000
6	2.620186000	-3.378259000	-2.091696000
1	0.737714000	-2.358502000	-1.849670000
6	3.673178000	-4.020027000	-1.447630000
1	4.473345000	-4.635659000	0.456343000
1	2.623764000	-3.272294000	-3.173344000
1	4.503927000	-4.422959000	-2.020311000
6	-0.354829000	-3.472673000	1.623047000
1	0.303274000	-4.037756000	2.291904000
1	-1.148296000	-3.018337000	2.227967000

1	-0.813909000	-4.172916000	0.915982000
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In_TSC4r

Doordinates (Angstroms)			
	X	Y	Z
25	-0.262886000	-0.611410000	0.838800000
7	-1.318940000	0.571875000	-0.796282000
6	1.105167000	-0.356565000	-2.218187000
1	1.602633000	0.360842000	-2.878783000
1	1.409304000	-1.344785000	-2.573864000
6	-3.483112000	0.209299000	1.170287000
6	0.594267000	-1.056775000	2.299405000
8	1.128099000	-1.279833000	3.317312000
15	-2.290026000	-0.922095000	1.969078000
15	1.625961000	-0.215138000	-0.441461000
14	-3.056817000	0.172462000	-0.659910000
14	-0.778898000	-0.146942000	-2.331551000
6	-4.207232000	1.337126000	-1.599440000
1	-3.821576000	1.589402000	-2.593368000
1	-5.194423000	0.875930000	-1.731695000
1	-4.351680000	2.273443000	-1.048750000
6	-1.109200000	0.945137000	-3.835681000
1	-0.642634000	0.522469000	-4.734749000
1	-2.176310000	1.071615000	-4.047426000
1	-0.682123000	1.944537000	-3.677211000
1	-4.529833000	-0.009828000	1.412225000
1	-3.230382000	1.209746000	1.555540000
6	-2.250973000	-0.487532000	3.748178000
1	-3.258401000	-0.503580000	4.179119000
1	-1.620026000	-1.204160000	4.285023000
1	-1.845527000	0.524497000	3.840114000
6	-3.346107000	-2.443871000	2.067640000
1	-2.785793000	-3.339684000	2.347466000
1	-4.121340000	-2.282635000	2.825534000
1	-3.853299000	-2.626244000	1.116918000
15	-0.362216000	-2.796145000	0.011525000
6	-1.918307000	-3.238453000	-0.905701000
1	-1.732107000	-4.104401000	-1.554058000
1	-2.704258000	-3.538936000	-0.209471000
14	-2.483257000	-1.741235000	-1.929330000
6	0.782894000	-3.618223000	-1.196491000
1	0.628199000	-3.226526000	-2.206065000
1	1.832507000	-3.492301000	-0.928971000

1	0.560126000	-4.691296000	-1.219442000
6	-0.215508000	-4.065302000	1.343851000
1	-0.697875000	-3.735094000	2.265832000
1	-0.633483000	-5.030236000	1.035806000
1	0.849708000	-4.203503000	1.561894000
6	-3.604130000	-2.261118000	-3.358426000
1	-3.092493000	-2.953802000	-4.037026000
1	-4.507194000	-2.762630000	-2.990521000
1	-3.922032000	-1.390344000	-3.943714000
1	-0.448971000	1.035746000	1.547433000
1	-1.029196000	1.519757000	-0.558696000
6	-0.750199000	2.336632000	2.160114000
8	-1.862488000	2.302938000	2.768586000
6	2.633268000	1.329663000	-0.353877000
6	2.813203000	2.244687000	-1.390289000
6	3.300403000	1.551038000	0.858568000
6	3.640141000	3.355614000	-1.221451000
1	2.302754000	2.119826000	-2.339733000
6	4.117157000	2.660907000	1.032394000
1	3.179753000	0.843817000	1.675880000
6	4.288211000	3.571374000	-0.010553000
1	3.766760000	4.059149000	-2.039739000
1	4.619164000	2.816367000	1.982756000
1	4.925647000	4.440542000	0.121920000
6	3.077209000	-1.365327000	-0.366911000
6	3.968500000	-1.444725000	-1.443720000
6	3.333593000	-2.134469000	0.769985000
6	5.070111000	-2.291628000	-1.396738000
1	3.804829000	-0.836749000	-2.329649000
6	4.442821000	-2.977865000	0.823181000
1	2.662809000	-2.088690000	1.619289000
6	5.310099000	-3.063321000	-0.260808000
1	5.748380000	-2.342893000	-2.243803000
1	4.624883000	-3.567764000	1.717018000
1	6.170743000	-3.724910000	-0.222326000
6	-0.735093000	3.226643000	0.907569000
6	0.422932000	3.751732000	0.330984000
6	-1.968132000	3.575022000	0.341690000
6	0.350365000	4.566535000	-0.799119000
1	1.393589000	3.539036000	0.763763000
6	-2.044067000	4.363691000	-0.800624000
1	-2.869015000	3.220291000	0.830113000
6	-0.878568000	4.861926000	-1.380763000
1	1.264322000	4.971372000	-1.223200000

1	-3.013165000	4.602991000	-1.230436000
1	-0.929976000	5.489565000	-2.266327000
6	0.506104000	2.394377000	3.030387000
1	0.562384000	3.380529000	3.510176000
1	0.422300000	1.633684000	3.810503000
1	1.427089000	2.216420000	2.472700000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.355679000	-0.165286000	-0.789697000
7	1.244326000	0.604168000	1.161990000
6	-1.128946000	-0.900624000	2.129653000
1	-1.728181000	-0.482006000	2.944419000
1	-1.310234000	-1.978126000	2.155973000
6	3.485593000	0.987411000	-0.708142000
6	-0.394794000	-0.259979000	-2.377122000
8	-0.858121000	-0.256918000	-3.449312000
15	2.487469000	-0.037923000	-1.839925000
15	-1.628883000	-0.294931000	0.450626000
14	3.016631000	0.389050000	1.007365000
14	0.717694000	-0.551666000	2.410978000
6	4.016142000	1.331524000	2.298534000
1	3.771178000	1.054076000	3.329617000
1	5.088235000	1.149389000	2.151074000
1	3.852594000	2.411322000	2.190967000
6	0.888685000	0.092950000	4.175714000
1	0.466740000	-0.624869000	4.891015000
1	1.930473000	0.270499000	4.463007000
1	0.343964000	1.038560000	4.296404000
1	4.559257000	0.966720000	-0.931127000
1	3.103519000	2.018266000	-0.862231000
15	0.605008000	-2.488286000	-0.634295000
6	2.115338000	-3.059114000	0.291375000
1	1.927487000	-4.054381000	0.714139000
1	2.958434000	-3.175742000	-0.394414000
14	2.559432000	-1.839714000	1.680957000
6	-0.572452000	-3.719462000	0.097484000
1	-0.639679000	-3.617538000	1.183805000
1	-1.572951000	-3.620774000	-0.326396000
1	-0.203386000	-4.728476000	-0.119630000
6	0.731472000	-3.292954000	-2.290133000
1	1.276278000	-2.669866000	-3.000821000
1	1.208344000	-4.277294000	-2.225417000

1	-0.283475000	-3.423122000	-2.681932000
6	3.691490000	-2.633537000	2.981272000
1	3.947026000	-3.665030000	2.712647000
1	4.628704000	-2.075249000	3.084564000
1	3.214766000	-2.658727000	3.967425000
1	0.504526000	1.794530000	-0.988684000
1	0.877176000	1.552352000	1.167337000
6	0.718018000	3.004829000	-1.318086000
8	1.837093000	3.154017000	-1.965097000
6	-2.746391000	1.142220000	0.760070000
6	-3.049864000	1.678702000	2.012107000
6	-3.331919000	1.713519000	-0.375795000
6	-3.914102000	2.766344000	2.126373000
1	-2.602395000	1.275600000	2.914994000
6	-4.199886000	2.792877000	-0.263176000
1	-3.101018000	1.313987000	-1.360442000
6	-4.491351000	3.325573000	0.991301000
1	-4.130722000	3.178551000	3.107720000
1	-4.640643000	3.224405000	-1.156882000
1	-5.164575000	4.172929000	1.081444000
6	-2.964929000	-1.477866000	-0.035188000
6	-3.806163000	-2.045723000	0.928424000
6	-3.188378000	-1.780497000	-1.380432000
6	-4.825934000	-2.916049000	0.557968000
1	-3.668810000	-1.809350000	1.980144000
6	-4.214514000	-2.646405000	-1.753993000
1	-2.556501000	-1.350858000	-2.147972000
6	-5.031123000	-3.222269000	-0.785995000
1	-5.465978000	-3.351746000	1.319854000
1	-4.370335000	-2.870180000	-2.805422000
1	-5.826631000	-3.902449000	-1.075927000
6	-0.545016000	3.282626000	-2.152932000
1	-0.552154000	4.332109000	-2.473891000
1	-0.517461000	2.658879000	-3.052196000
1	-1.472014000	3.071821000	-1.610249000
6	0.748116000	3.768697000	0.048665000
1	1.610302000	3.348328000	0.590539000
6	-0.492796000	3.641694000	0.922779000
1	-0.331768000	4.087944000	1.912982000
1	-1.358096000	4.142824000	0.473543000
1	-0.783104000	2.599630000	1.068878000
6	1.076955000	5.242719000	-0.199888000
1	1.261421000	5.768257000	0.746031000
1	1.963167000	5.322202000	-0.833455000

1	0.245594000	5.754538000	-0.701803000
6	2.487705000	0.761921000	-3.483399000
1	2.024115000	1.748610000	-3.347716000
1	3.509941000	0.894765000	-3.855847000
1	1.922179000	0.146853000	-4.191734000
6	3.709600000	-1.396446000	-2.154703000
1	4.143322000	-1.755506000	-1.217934000
1	3.290467000	-2.245264000	-2.700147000
1	4.527016000	-0.981543000	-2.755192000

In_TSC4s

Doordinates (Angstroms)			
	X	Y	Z
25	-0.477707000	-0.337557000	-0.625068000
7	-1.457431000	-0.251259000	1.463376000
6	-0.188701000	2.415866000	1.290016000
1	0.304020000	2.832258000	2.176066000
1	-0.431618000	3.260024000	0.640777000
6	-2.798374000	-2.553223000	0.251771000
6	0.497429000	-0.714591000	-2.034341000
8	1.115510000	-1.035068000	-2.973189000
15	-2.032017000	-1.956447000	-1.297110000
15	0.926288000	1.260139000	0.347122000
14	-3.072070000	-0.990049000	1.258954000
14	-1.761395000	1.477774000	1.776265000
6	-3.916423000	-1.443029000	2.884303000
1	-4.162460000	-0.574666000	3.505094000
1	-4.852022000	-1.981693000	2.687508000
1	-3.276517000	-2.109106000	3.477533000
6	-2.107666000	1.881473000	3.587999000
1	-2.294756000	2.956343000	3.708414000
1	-2.979788000	1.349447000	3.982162000
1	-1.248849000	1.629401000	4.223968000
1	-3.690601000	-3.169000000	0.089338000
1	-2.033644000	-3.161951000	0.759660000
6	-1.346116000	-3.426992000	-2.141667000
1	-2.128287000	-4.164875000	-2.352860000
1	-0.869873000	-3.127044000	-3.080925000
1	-0.608224000	-3.867879000	-1.462925000
6	-3.580316000	-1.733655000	-2.294103000
1	-3.397848000	-1.282901000	-3.272899000
1	-4.034842000	-2.717807000	-2.455590000
1	-4.307687000	-1.120719000	-1.755504000

15	-1.627733000	1.291742000	-1.804505000
6	-3.424539000	1.526023000	-1.367973000
1	-3.729637000	2.555933000	-1.595658000
1	-4.052112000	0.879167000	-1.987758000
14	-3.704986000	1.159963000	0.473967000
6	-1.188971000	3.088061000	-1.951304000
1	-1.441780000	3.640309000	-1.042140000
1	-0.123948000	3.221041000	-2.156315000
1	-1.759355000	3.531861000	-2.775496000
6	-1.653788000	0.955117000	-3.621160000
1	-1.756654000	-0.110242000	-3.833905000
1	-2.457582000	1.505602000	-4.122934000
1	-0.695220000	1.280910000	-4.039735000
6	-5.345026000	1.881049000	1.073177000
1	-5.388156000	2.964307000	0.909407000
1	-6.190899000	1.432369000	0.538588000
1	-5.494487000	1.697378000	2.143252000
1	0.252302000	-1.752263000	0.146589000
1	-0.756387000	-0.759639000	1.996225000
6	0.793440000	-3.003594000	0.733259000
8	0.072216000	-3.992952000	0.414590000
6	2.196353000	0.924404000	1.653228000
6	1.810611000	0.658252000	2.972276000
6	3.561497000	0.917729000	1.350451000
6	2.756118000	0.387685000	3.957521000
1	0.759257000	0.657645000	3.249728000
6	4.510452000	0.659689000	2.336002000
1	3.894307000	1.113029000	0.336376000
6	4.112336000	0.388482000	3.641967000
1	2.431162000	0.180357000	4.973073000
1	5.565663000	0.666543000	2.077845000
1	4.852625000	0.183269000	4.409522000
6	1.910721000	2.406619000	-0.709217000
6	2.179934000	3.721588000	-0.310210000
6	2.434914000	1.953582000	-1.922670000
6	2.932178000	4.568964000	-1.116985000
1	1.802210000	4.091598000	0.638720000
6	3.196471000	2.799172000	-2.727857000
1	2.257487000	0.935027000	-2.244555000
6	3.440059000	4.110066000	-2.331271000
1	3.125708000	5.588651000	-0.796156000
1	3.597060000	2.426822000	-3.666277000
1	4.028692000	4.770951000	-2.960962000
6	2.172693000	-2.907621000	0.081544000

6	2.369877000	-3.503861000	-1.166293000
6	3.261344000	-2.296363000	0.705132000
6	3.611012000	-3.462932000	-1.789993000
1	1.534422000	-4.001641000	-1.645599000
6	4.509610000	-2.258420000	0.086219000
1	3.148922000	-1.841724000	1.683363000
6	4.689351000	-2.836322000	-1.166389000
1	3.739709000	-3.924960000	-2.765321000
1	5.342711000	-1.775835000	0.590793000
1	5.661767000	-2.806415000	-1.650583000
6	0.746344000	-2.609499000	2.211784000
1	-0.285416000	-2.701260000	2.566447000
1	1.347419000	-3.328767000	2.782929000
1	1.129373000	-1.609401000	2.420057000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.403629000	0.098317000	-0.768507000
7	1.120868000	0.437709000	1.396215000
6	-0.665385000	-1.877369000	1.743414000
1	-1.319381000	-1.965620000	2.618142000
1	-0.562960000	-2.885788000	1.338396000
6	3.039128000	2.017930000	-0.150802000
6	-0.340109000	0.147539000	-2.354048000
8	-0.808746000	0.195284000	-3.425106000
15	2.328649000	1.165557000	-1.602018000
15	-1.397792000	-0.825412000	0.402885000
14	2.867883000	0.795965000	1.262323000
14	1.023130000	-1.149826000	2.205370000
6	3.616393000	1.547596000	2.822059000
1	3.480156000	0.926882000	3.713947000
1	4.693846000	1.706427000	2.688102000
1	3.165957000	2.528402000	3.021592000
6	1.114238000	-1.071246000	4.090150000
1	0.916628000	-2.062021000	4.519105000
1	2.095893000	-0.748641000	4.452869000
1	0.369152000	-0.379311000	4.503529000
1	4.051078000	2.403869000	-0.321709000
1	2.362112000	2.869893000	0.043673000
6	2.061243000	2.457162000	-2.867829000
1	3.005593000	2.949672000	-3.126813000
1	1.628499000	2.013104000	-3.770783000

1	1.377894000	3.195212000	-2.428556000
6	3.871414000	0.384794000	-2.273140000
1	3.676922000	-0.303542000	-3.099932000
1	4.531630000	1.177445000	-2.643002000
1	4.412742000	-0.150887000	-1.488566000
15	1.290729000	-1.987110000	-1.265909000
6	2.948691000	-2.385774000	-0.521341000
1	3.065644000	-3.473891000	-0.431108000
1	3.747553000	-2.046569000	-1.186359000
14	3.108887000	-1.566236000	1.183524000
6	0.480319000	-3.624338000	-0.945736000
1	0.599930000	-3.927189000	0.097935000
1	-0.586486000	-3.594804000	-1.183856000
1	0.953897000	-4.393308000	-1.566686000
6	1.550144000	-2.231814000	-3.077601000
1	1.906355000	-1.319552000	-3.559560000
1	2.255362000	-3.046992000	-3.274901000
1	0.587085000	-2.487046000	-3.532531000
6	4.487405000	-2.366701000	2.195756000
1	4.295776000	-3.433623000	2.360184000
1	5.451945000	-2.278408000	1.681523000
1	4.591846000	-1.889381000	3.176735000
1	-0.055393000	1.868094000	-0.516115000
1	0.491391000	1.187866000	1.672842000
6	-0.343915000	3.188121000	-0.322653000
8	0.612038000	3.943629000	-0.721090000
6	-2.544685000	0.257467000	1.357613000
6	-2.379850000	0.529248000	2.718516000
6	-3.588192000	0.891790000	0.672527000
6	-3.225244000	1.420755000	3.376476000
1	-1.583805000	0.057840000	3.285811000
6	-4.430949000	1.783399000	1.326111000
1	-3.746012000	0.687045000	-0.383025000
6	-4.249031000	2.054797000	2.681346000
1	-3.076125000	1.620802000	4.433568000
1	-5.229736000	2.270213000	0.774609000
1	-4.904842000	2.754096000	3.191371000
6	-2.639627000	-1.967403000	-0.343888000
6	-3.473177000	-2.735729000	0.480068000
6	-2.772368000	-2.084788000	-1.728806000
6	-4.404110000	-3.609742000	-0.067864000
1	-3.399637000	-2.644603000	1.560648000
6	-3.710134000	-2.958080000	-2.280303000
1	-2.145341000	-1.495142000	-2.386244000

6	-4.523248000	-3.724520000	-1.452869000
1	-5.040749000	-4.200369000	0.584600000
1	-3.801356000	-3.035939000	-3.359816000
1	-5.251257000	-4.407132000	-1.881661000
6	-0.562512000	3.228560000	1.198665000
1	0.395166000	3.084333000	1.711989000
1	-0.898345000	4.235117000	1.471862000
1	-1.302053000	2.511588000	1.562398000
6	-1.681768000	3.255969000	-1.127306000
1	-2.200588000	2.300757000	-0.991729000
6	-1.408823000	3.463122000	-2.612692000
1	-2.345202000	3.441860000	-3.184709000
1	-0.920660000	4.429230000	-2.777254000
1	-0.755009000	2.687587000	-3.015231000
6	-2.590531000	4.377375000	-0.608258000
1	-3.471660000	4.484790000	-1.253670000
1	-2.950880000	4.184065000	0.407716000
1	-2.059987000	5.337475000	-0.607372000

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Doordinates (Angstroms)			
	X	Y	Z
25	-0.315779000	-0.413396000	-0.931335000
7	0.862003000	-0.957141000	0.918997000
6	-1.724680000	0.046063000	2.117657000
1	-1.911832000	0.721676000	2.960056000
1	-2.587851000	-0.627853000	2.048304000
6	1.727170000	-3.120123000	-1.039774000
6	-0.935763000	0.192043000	-2.455368000
8	-1.304039000	0.560507000	-3.505797000
15	1.324061000	-1.633854000	-2.040091000
15	-1.609621000	0.904025000	0.495303000
14	1.534965000	-2.586258000	0.783414000
14	-0.176139000	-1.048659000	2.335166000
6	3.204926000	-2.779880000	1.639709000
1	3.141316000	-2.555299000	2.710942000
1	3.606555000	-3.795114000	1.532147000
1	3.931735000	-2.082822000	1.201244000
6	0.674158000	-0.605641000	3.964962000
1	-0.037526000	-0.593370000	4.799918000
1	1.456429000	-1.334813000	4.207833000
1	1.156155000	0.379211000	3.917551000
1	0.990978000	-3.904217000	-1.255602000
1	2.720644000	-3.522478000	-1.275267000

6	2.985845000	-0.861387000	-2.154315000
1	3.690306000	-1.543269000	-2.645463000
1	2.927385000	0.067246000	-2.726452000
1	3.359189000	-0.610275000	-1.159936000
6	1.167342000	-2.224961000	-3.777874000
1	1.197755000	-1.357188000	-4.446481000
1	1.990628000	-2.898129000	-4.042204000
1	0.220417000	-2.739561000	-3.949541000
15	-1.831591000	-2.174756000	-0.865584000
6	-1.756761000	-3.472281000	0.489870000
1	-2.738440000	-3.501608000	0.982060000
1	-1.643706000	-4.453668000	0.008987000
14	-0.415463000	-3.316742000	1.845555000
6	-3.630949000	-1.768646000	-0.804295000
1	-3.886303000	-1.234421000	0.114962000
1	-3.893840000	-1.121717000	-1.646806000
1	-4.234686000	-2.682005000	-0.856666000
6	-1.888531000	-3.278238000	-2.345517000
1	-0.950591000	-3.831480000	-2.447493000
1	-2.706379000	-4.003756000	-2.268596000
1	-2.036432000	-2.675414000	-3.247587000
6	-0.621142000	-4.751581000	3.062059000
1	-1.604619000	-4.724823000	3.546479000
1	-0.524887000	-5.719878000	2.556097000
1	0.139902000	-4.711501000	3.849524000
1	1.356537000	0.130389000	0.398234000
6	1.957505000	2.130973000	-0.622426000
8	1.328020000	0.889894000	-0.504240000
6	3.449039000	1.974320000	-0.324329000
6	4.462266000	2.380106000	-1.192173000
6	3.818751000	1.364839000	0.881788000
6	5.805600000	2.171050000	-0.875389000
1	4.213669000	2.858372000	-2.134934000
6	5.154349000	1.150437000	1.201291000
1	3.044857000	1.037197000	1.571605000
6	6.157412000	1.551822000	0.318553000
1	6.576718000	2.490510000	-1.571347000
1	5.413690000	0.668548000	2.140316000
1	7.202688000	1.383557000	0.562105000
6	1.639754000	2.722959000	-1.988702000
1	2.051367000	2.110404000	-2.798763000
1	0.553781000	2.748379000	-2.112494000
1	2.021198000	3.745728000	-2.089432000
1	1.568110000	2.831757000	0.131462000

6	-0.903435000	2.545278000	0.937226000
6	-1.034399000	3.597691000	0.024749000
6	-0.190328000	2.769517000	2.116828000
6	-0.463226000	4.838830000	0.281130000
1	-1.583207000	3.446912000	-0.900907000
6	0.384868000	4.012684000	2.375691000
1	-0.071463000	1.977523000	2.848743000
6	0.251933000	5.050230000	1.458443000
1	-0.572156000	5.640318000	-0.443839000
1	0.937884000	4.166373000	3.297967000
1	0.704138000	6.017401000	1.657282000
6	-3.343819000	1.422528000	0.138880000
6	-4.288095000	1.600177000	1.155652000
6	-3.726010000	1.677878000	-1.181797000
6	-5.585710000	2.007110000	0.857889000
1	-4.015047000	1.420168000	2.191421000
6	-5.020393000	2.096233000	-1.480281000
1	-3.013488000	1.538809000	-1.987659000
6	-5.955658000	2.255783000	-0.461962000
1	-6.308967000	2.132832000	1.658752000
1	-5.297423000	2.287986000	-2.513009000
1	-6.968509000	2.572187000	-0.694171000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.289138000	-0.278448000	-0.869554000
7	1.271276000	0.502104000	1.042102000
6	-1.117687000	-0.914524000	2.137415000
1	-1.721363000	-0.470894000	2.937387000
1	-1.300837000	-1.991112000	2.177424000
6	3.603256000	0.609463000	-0.775606000
6	-0.491414000	-0.451984000	-2.430124000
8	-0.957189000	-0.542329000	-3.501170000
15	2.324381000	0.020553000	-1.968498000
15	-1.622814000	-0.325686000	0.460335000
14	3.009761000	0.238428000	0.985502000
14	0.734694000	-0.524968000	2.352827000
6	4.034874000	1.342310000	2.127934000
1	3.843496000	2.401133000	1.909279000
1	3.815714000	1.178064000	3.188823000
1	5.107739000	1.163206000	1.979708000
6	0.919366000	0.191322000	4.095802000

1	0.511819000	-0.498387000	4.846561000
1	1.965883000	0.383097000	4.358324000
1	0.379770000	1.143205000	4.189951000
1	4.591940000	0.194107000	-1.004158000
1	3.685683000	1.701050000	-0.862750000
6	2.293162000	1.315360000	-3.267527000
1	3.293511000	1.501040000	-3.674876000
1	1.628237000	1.003344000	-4.079853000
1	1.896201000	2.228745000	-2.827600000
6	3.243427000	-1.269844000	-2.917218000
1	2.651813000	-1.577786000	-3.785722000
1	4.191939000	-0.861513000	-3.284469000
1	3.463609000	-2.156832000	-2.317934000
15	0.622778000	-2.566226000	-0.619924000
6	2.199083000	-3.032960000	0.232006000
1	2.164865000	-4.094664000	0.511879000
1	3.039506000	-2.921488000	-0.461401000
14	2.546641000	-1.933619000	1.760013000
6	-0.480091000	-3.724217000	0.319234000
1	-0.332652000	-3.606279000	1.396355000
1	-1.535685000	-3.562672000	0.088647000
1	-0.224862000	-4.758952000	0.062466000
6	0.667788000	-3.529010000	-2.193408000
1	1.228625000	-3.003637000	-2.967852000
1	1.108333000	-4.521280000	-2.041991000
1	-0.358857000	-3.655475000	-2.555159000
6	3.602575000	-2.906248000	2.993553000
1	3.071217000	-3.792770000	3.360899000
1	4.536431000	-3.247865000	2.530588000
1	3.866463000	-2.290739000	3.861338000
1	0.841487000	1.454294000	0.338315000
6	-0.272468000	3.007808000	-0.895863000
8	0.545357000	1.875422000	-0.764932000
6	-0.889785000	3.057657000	-2.289208000
1	-1.539838000	3.934704000	-2.398829000
1	-0.130166000	3.089869000	-3.077489000
1	-1.495706000	2.160781000	-2.452528000
6	0.503620000	4.290230000	-0.518575000
1	-0.199349000	5.124195000	-0.662917000
6	1.736184000	4.547515000	-1.384944000
1	2.216202000	5.493878000	-1.107616000
1	2.473854000	3.748451000	-1.249384000
1	1.489327000	4.606223000	-2.451075000
6	0.893710000	4.261468000	0.961554000

1	1.376372000	5.198740000	1.264756000
1	0.014362000	4.111488000	1.598743000
1	1.592649000	3.441746000	1.166972000
1	-1.106695000	2.958825000	-0.186891000
6	-2.492771000	1.250553000	0.841593000
6	-2.168709000	2.031914000	1.953307000
6	-3.442526000	1.734103000	-0.066217000
6	-2.776443000	3.270094000	2.152468000
1	-1.422207000	1.695958000	2.665973000
6	-4.045819000	2.971324000	0.128811000
1	-3.708084000	1.142924000	-0.938843000
6	-3.711663000	3.745717000	1.238767000
1	-2.509756000	3.865297000	3.021364000
1	-4.777025000	3.332515000	-0.588564000
1	-4.181403000	4.713140000	1.390700000
6	-3.092387000	-1.371101000	0.072495000
6	-4.077455000	-1.591995000	1.043683000
6	-3.254378000	-1.942769000	-1.190821000
6	-5.192295000	-2.371638000	0.758758000
1	-3.976006000	-1.141219000	2.027455000
6	-4.373576000	-2.723370000	-1.479902000
1	-2.503568000	-1.781274000	-1.955623000
6	-5.342319000	-2.940511000	-0.505823000
1	-5.948384000	-2.532812000	1.521933000
1	-4.484401000	-3.160644000	-2.468002000
1	-6.214992000	-3.547395000	-0.729743000

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Doordinates (Angstroms)			
	X	Y	Z
25	-0.644417000	-0.337215000	-1.014250000
7	-1.020927000	-1.465868000	0.989950000
6	0.694971000	0.672137000	1.939526000
1	1.474215000	-0.094459000	2.039970000
1	0.929043000	1.476360000	2.643569000
6	-3.220501000	-2.556088000	-0.696055000
6	-0.155836000	0.128189000	-2.631389000
8	0.123038000	0.400467000	-3.736612000
15	-1.768835000	-2.214493000	-1.777835000
15	0.712431000	1.208275000	0.183763000
14	-2.715531000	-1.914457000	1.024844000
14	-0.896293000	-0.291262000	2.285434000
6	-3.178419000	-3.280391000	2.248873000

1	-2.937613000	-3.021095000	3.285849000
1	-4.253538000	-3.498125000	2.202512000
1	-2.641708000	-4.207725000	2.007210000
6	-0.662308000	-0.995099000	4.028860000
1	-0.411107000	-0.197931000	4.740639000
1	-1.554377000	-1.505421000	4.409441000
1	0.163038000	-1.719618000	4.039891000
1	-4.107051000	-2.042433000	-1.077110000
1	-3.458193000	-3.627637000	-0.675534000
6	-0.883462000	-3.817829000	-1.596618000
1	-1.535727000	-4.652064000	-1.880104000
1	0.008507000	-3.843594000	-2.227823000
1	-0.577485000	-3.952099000	-0.555081000
6	-2.396591000	-2.400210000	-3.496975000
1	-1.553559000	-2.366457000	-4.196053000
1	-2.923153000	-3.352327000	-3.627082000
1	-3.078493000	-1.586111000	-3.754060000
15	-2.461367000	1.077578000	-1.165876000
6	-3.303294000	1.564144000	0.414022000
1	-2.863277000	2.509301000	0.753274000
1	-4.363587000	1.772334000	0.216283000
14	-3.136296000	0.279560000	1.812439000
6	-2.156959000	2.710304000	-1.966173000
1	-1.330995000	3.239314000	-1.490053000
1	-1.895202000	2.547653000	-3.017339000
1	-3.052756000	3.340185000	-1.920367000
6	-3.936073000	0.633239000	-2.190311000
1	-4.459059000	-0.244574000	-1.805646000
1	-4.647715000	1.466635000	-2.211363000
1	-3.618759000	0.432195000	-3.218124000
6	-4.401098000	0.688955000	3.161693000
1	-4.237174000	1.691238000	3.576181000
1	-5.424855000	0.656081000	2.768899000
1	-4.339709000	-0.028735000	3.987906000
1	0.123792000	-1.825297000	0.439726000
6	2.002286000	-2.417875000	-0.688927000
8	0.977876000	-1.543130000	-0.300295000
6	3.167638000	-2.262453000	0.287470000
6	4.483816000	-2.025029000	-0.102453000
6	2.887605000	-2.351536000	1.656885000
6	5.493379000	-1.869091000	0.848907000
1	4.734193000	-1.937499000	-1.154964000
6	3.887386000	-2.194039000	2.608391000
1	1.864425000	-2.541830000	1.974186000

6	5.200965000	-1.949139000	2.205169000
1	6.511131000	-1.673164000	0.522127000
1	3.645579000	-2.265762000	3.665667000
1	5.986627000	-1.825183000	2.945352000
6	2.368892000	-2.190905000	-2.148577000
1	3.070438000	-2.951550000	-2.510688000
1	1.462226000	-2.236293000	-2.758885000
1	2.814531000	-1.202939000	-2.291938000
1	1.649573000	-3.458598000	-0.591997000
6	2.497219000	1.280951000	-0.257070000
6	3.492100000	1.393869000	0.718427000
6	2.873714000	1.289806000	-1.602971000
6	4.830623000	1.508397000	0.356812000
1	3.230474000	1.387568000	1.771872000
6	4.213089000	1.410919000	-1.967072000
1	2.117854000	1.197853000	-2.375744000
6	5.195315000	1.518371000	-0.987058000
1	5.590722000	1.581141000	1.129043000
1	4.484734000	1.414605000	-3.019063000
1	6.241050000	1.607343000	-1.267795000
6	0.365724000	3.016401000	0.355912000
6	-0.502938000	3.490151000	1.345620000
6	0.906449000	3.940285000	-0.546244000
6	-0.835711000	4.840663000	1.421580000
1	-0.930655000	2.802380000	2.069721000
6	0.578948000	5.290915000	-0.469530000
1	1.591871000	3.606786000	-1.319546000
6	-0.298778000	5.746229000	0.511245000
1	-1.514456000	5.183621000	2.197484000
1	1.012265000	5.989122000	-1.180017000
1	-0.555132000	6.799935000	0.570804000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.349906000	-0.267761000	-0.899503000
7	1.199542000	0.664055000	1.019856000
6	-0.900101000	-1.101375000	2.160951000
1	-1.544952000	-0.729209000	2.965179000
1	-0.931460000	-2.192022000	2.228921000
6	3.370998000	1.309396000	-0.821010000
6	-0.446153000	-0.573754000	-2.430373000
8	-0.945929000	-0.745138000	-3.476189000
15	2.292453000	0.408789000	-2.008274000

15	-1.505099000	-0.628058000	0.481109000
14	2.950107000	0.709316000	0.925886000
14	0.877863000	-0.440005000	2.338891000
6	3.803897000	1.915855000	2.107308000
1	3.362438000	2.916473000	2.009076000
1	3.717676000	1.618943000	3.158375000
1	4.873859000	2.000970000	1.877059000
6	0.977854000	0.298288000	4.078950000
1	0.721147000	-0.451438000	4.838479000
1	1.974919000	0.683654000	4.318554000
1	0.271590000	1.132812000	4.185303000
1	4.431562000	1.258154000	-1.093387000
1	3.085319000	2.371490000	-0.833509000
6	2.144748000	1.560249000	-3.440139000
1	3.137318000	1.837503000	-3.813827000
1	1.588470000	1.071231000	-4.247101000
1	1.611424000	2.470329000	-3.163581000
6	3.508940000	-0.739979000	-2.792491000
1	3.066537000	-1.209886000	-3.676442000
1	4.391915000	-0.178509000	-3.118258000
1	3.840014000	-1.525762000	-2.111029000
15	1.072709000	-2.467490000	-0.683010000
6	2.675559000	-2.729013000	0.213204000
1	2.736866000	-3.770533000	0.556311000
1	3.517775000	-2.582885000	-0.471044000
14	2.885593000	-1.524578000	1.682617000
6	0.104320000	-3.770896000	0.208115000
1	0.174433000	-3.629551000	1.289957000
1	-0.949553000	-3.761838000	-0.079892000
1	0.520587000	-4.757961000	-0.024121000
6	1.293310000	-3.393296000	-2.262800000
1	1.845230000	-2.803828000	-2.996024000
1	1.812640000	-4.345275000	-2.103937000
1	0.302996000	-3.601304000	-2.682869000
6	4.131814000	-2.258299000	2.905395000
1	3.769611000	-3.204779000	3.325266000
1	5.096094000	-2.455993000	2.421418000
1	4.312776000	-1.571106000	3.740104000
1	0.485817000	1.493565000	0.384630000
6	-0.114970000	3.024015000	-1.159311000
8	-0.210682000	1.770649000	-0.557786000
6	-0.921923000	3.009960000	-2.456128000
1	-1.994035000	2.973817000	-2.229323000
1	-0.726310000	3.889885000	-3.079512000

1	-0.677090000	2.116283000	-3.037030000
6	-0.600316000	4.117594000	-0.184218000
1	-1.637692000	3.867337000	0.072001000
6	-0.573507000	5.507806000	-0.826421000
1	-0.820963000	6.281155000	-0.089675000
1	0.423956000	5.740085000	-1.224936000
1	-1.292255000	5.597368000	-1.647532000
6	0.224716000	4.119492000	1.104077000
1	1.279644000	4.345530000	0.891637000
1	-0.141547000	4.882882000	1.801470000
1	0.184665000	3.154489000	1.616378000
1	0.942421000	3.265207000	-1.399208000
6	-2.542235000	0.860363000	0.783025000
6	-3.419694000	1.252800000	-0.233934000
6	-2.472841000	1.632427000	1.941995000
6	-4.223568000	2.375908000	-0.085037000
1	-3.469361000	0.677800000	-1.155546000
6	-3.276597000	2.762408000	2.092865000
1	-1.783935000	1.372879000	2.739827000
6	-4.157878000	3.134692000	1.083957000
1	-4.901669000	2.662780000	-0.883827000
1	-3.206677000	3.351649000	3.002914000
1	-4.784911000	4.013774000	1.201380000
6	-2.837528000	-1.861703000	0.161223000
6	-3.712140000	-2.250506000	1.183245000
6	-3.000343000	-2.416860000	-1.110171000
6	-4.715056000	-3.182777000	0.943279000
1	-3.610681000	-1.816598000	2.174505000
6	-4.008402000	-3.349158000	-1.353986000
1	-2.334770000	-2.125289000	-1.915249000
6	-4.863563000	-3.737024000	-0.327672000
1	-5.384387000	-3.476312000	1.746964000
1	-4.120266000	-3.773792000	-2.347544000
1	-5.645607000	-4.467199000	-0.515191000

In_TSD4r

Doordinates (Angstroms)			
	X	Y	Z
25	0.676816000	-0.449334000	-0.796059000
7	1.047049000	0.959062000	0.986559000
6	-0.655387000	-1.141613000	2.219609000
1	-1.427823000	-0.870476000	2.950400000
1	-0.418494000	-2.195199000	2.395319000

6	3.175467000	1.761582000	-0.895584000
6	0.156326000	-1.173622000	-2.307818000
8	-0.165619000	-1.590925000	-3.351797000
15	2.722633000	0.228559000	-1.781509000
15	-1.263515000	-0.951353000	0.468509000
14	2.780790000	1.380180000	0.902742000
14	0.882878000	-0.064850000	2.441388000
6	3.260610000	2.865500000	1.964971000
1	2.982980000	2.747455000	3.018066000
1	4.344557000	3.031595000	1.922774000
1	2.777757000	3.777550000	1.590972000
6	0.694309000	0.906172000	4.051848000
1	0.483835000	0.220446000	4.882876000
1	1.597967000	1.467943000	4.313140000
1	-0.135188000	1.622680000	3.998818000
1	4.207218000	2.083245000	-1.081625000
1	2.491305000	2.540902000	-1.263513000
6	2.677949000	0.601123000	-3.575926000
1	3.644020000	0.983784000	-3.924480000
1	2.431078000	-0.310016000	-4.132055000
1	1.916141000	1.367661000	-3.740486000
6	4.396838000	-0.580056000	-1.718211000
1	4.409606000	-1.604761000	-2.096288000
1	5.079089000	0.012746000	-2.338127000
1	4.796515000	-0.576099000	-0.701076000
15	1.744769000	-2.427281000	-0.173172000
6	3.242940000	-2.247248000	0.928912000
1	3.327597000	-3.128547000	1.578215000
1	4.157259000	-2.228470000	0.328837000
14	3.109870000	-0.691591000	2.009873000
6	1.051222000	-3.943564000	0.649580000
1	0.699671000	-3.747725000	1.665829000
1	0.228853000	-4.360368000	0.062092000
1	1.836168000	-4.706887000	0.703805000
6	2.363951000	-3.349040000	-1.654807000
1	2.687981000	-2.677926000	-2.450614000
1	3.179234000	-4.035278000	-1.399341000
1	1.530599000	-3.937769000	-2.053282000
6	4.341535000	-0.757349000	3.441718000
1	4.143555000	-1.610804000	4.100871000
1	5.370162000	-0.853686000	3.073937000
1	4.289962000	0.153926000	4.048489000
1	0.125174000	1.133371000	-1.462193000
1	0.351987000	1.673871000	0.775171000

6	-0.106285000	2.405152000	-2.300750000
8	0.990979000	2.894422000	-2.689939000
6	-2.746585000	0.131015000	0.821262000
6	-2.429774000	1.482546000	1.466883000
6	-3.658098000	0.340882000	-0.400604000
6	-3.712502000	2.087365000	2.078973000
1	-1.670306000	1.391764000	2.250469000
6	-4.717457000	1.438777000	-0.153030000
1	-3.046909000	0.606820000	-1.271078000
6	-4.988342000	1.639016000	1.338721000
1	-3.790808000	1.801732000	3.135360000
1	-4.366519000	2.387782000	-0.568634000
1	-5.361936000	0.698909000	1.766947000
6	-2.110785000	-2.596960000	0.195640000
6	-3.304019000	-2.912859000	1.109223000
6	-2.465159000	-2.849545000	-1.291156000
6	-3.659841000	-4.409451000	1.023880000
1	-3.082121000	-2.651049000	2.150409000
6	-3.618990000	-3.853948000	-1.445997000
1	-2.715660000	-1.917414000	-1.807943000
6	-3.499472000	-4.969697000	-0.407002000
1	-3.022851000	-4.977244000	1.713046000
1	-4.584705000	-3.345816000	-1.322013000
1	-2.513984000	-5.442723000	-0.517499000
6	-0.826562000	3.267153000	-1.267609000
6	-2.171879000	3.615016000	-1.387858000
6	-0.076496000	3.872389000	-0.253212000
6	-2.755489000	4.527789000	-0.507376000
1	-2.776286000	3.183482000	-2.179682000
6	-0.661656000	4.748023000	0.652533000
1	0.988024000	3.668836000	-0.199765000
6	-2.009967000	5.084656000	0.525348000
1	-3.801965000	4.794980000	-0.628281000
1	-0.062339000	5.189511000	1.444353000
1	-2.468429000	5.784392000	1.218303000
6	-0.988247000	1.732894000	-3.350876000
1	-1.383878000	2.500961000	-4.029184000
1	-0.379189000	1.044844000	-3.939155000
1	-1.819271000	1.169760000	-2.917639000
1	-3.307431000	-0.444801000	1.568047000
1	-2.021611000	2.152526000	0.707756000
1	-3.631893000	3.179463000	2.053909000
1	-5.784034000	2.378412000	1.484986000
1	-5.644493000	1.189209000	-0.681307000

1	-4.158037000	-0.602967000	-0.644961000
1	-1.577811000	-3.240703000	-1.799318000
1	-3.614221000	-4.265003000	-2.461517000
1	-4.239780000	-5.755919000	-0.591315000
1	-4.691279000	-4.548276000	1.368801000
1	-4.173515000	-2.313505000	0.815440000
1	-1.334910000	-3.312986000	0.473198000

In_TSD4ra

Doordinates (Angstroms)			

	X	Y	Z

25	0.496222000	-0.276380000	-0.789586000
7	1.176253000	0.874536000	1.081025000
6	-0.822455000	-1.034809000	2.171724000
1	-1.508622000	-0.799120000	2.994609000
1	-0.739742000	-2.122083000	2.150225000
6	3.284873000	1.487231000	-0.883679000
6	-0.252079000	-0.882825000	-2.255462000
8	-0.748221000	-1.279619000	-3.238133000
15	2.547186000	0.128539000	-1.862727000
15	-1.467561000	-0.473312000	0.514741000
14	2.948081000	1.021159000	0.908067000
14	0.890993000	-0.255833000	2.432805000
6	3.721751000	2.315376000	2.041918000
1	3.489477000	2.151081000	3.099895000
1	4.814170000	2.309852000	1.936931000
1	3.374099000	3.321004000	1.772912000
6	0.943376000	0.550386000	4.142414000
1	0.714924000	-0.192940000	4.917152000
1	1.931710000	0.965640000	4.369205000
1	0.214577000	1.363816000	4.242972000
1	4.339736000	1.673876000	-1.119267000
1	2.704870000	2.392893000	-1.128422000
6	2.445685000	0.700959000	-3.600398000
1	3.443398000	0.889542000	-4.012579000
1	1.945532000	-0.059837000	-4.209622000
1	1.877870000	1.637592000	-3.606967000
6	4.056674000	-0.945303000	-2.012621000
1	3.847152000	-1.927221000	-2.446011000
1	4.777642000	-0.438190000	-2.663754000
1	4.539344000	-1.082417000	-1.041636000
15	1.212656000	-2.459300000	-0.292496000
6	2.834715000	-2.600852000	0.608839000

1	2.883434000	-3.559881000	1.140715000
1	3.664906000	-2.603671000	-0.100332000
14	2.987366000	-1.163652000	1.837220000
6	0.363379000	-3.824615000	0.650869000
1	0.433836000	-3.662089000	1.730204000
1	-0.689732000	-3.938221000	0.382984000
1	0.869367000	-4.771552000	0.429506000
6	1.479025000	-3.436666000	-1.838199000
1	1.895436000	-2.819594000	-2.636466000
1	2.135367000	-4.296038000	-1.660637000
1	0.508430000	-3.806534000	-2.186931000
6	4.248906000	-1.556860000	3.187477000
1	3.986260000	-2.477999000	3.721156000
1	5.250158000	-1.694689000	2.761743000
1	4.309492000	-0.748982000	3.925335000
1	0.286353000	1.424031000	-1.362062000
1	0.594172000	1.699779000	0.967441000
6	0.093671000	2.705729000	-2.062001000
8	1.197219000	3.172933000	-2.477670000
6	-2.714946000	0.803428000	1.116091000
6	-2.126866000	1.837363000	2.091343000
6	-3.498881000	1.524258000	-0.010666000
6	-3.249464000	2.613844000	2.807467000
1	-1.497386000	1.363141000	2.847103000
6	-4.018943000	2.905035000	0.427036000
1	-2.884448000	1.627201000	-0.910695000
6	-4.461114000	2.873341000	1.888927000
1	-3.570944000	2.055402000	3.695052000
1	-3.236342000	3.663372000	0.309244000
1	-5.208704000	2.078684000	2.016164000
6	-2.561083000	-1.881280000	-0.036151000
6	-3.348319000	-2.618841000	1.065587000
6	-3.502230000	-1.542651000	-1.201810000
6	-4.475555000	-3.491318000	0.471074000
1	-2.662323000	-3.252259000	1.640484000
6	-3.922408000	-2.842668000	-1.912533000
1	-4.392565000	-1.040621000	-0.809130000
6	-4.090165000	-4.010901000	-0.916334000
1	-4.699486000	-4.321596000	1.150216000
1	-4.862985000	-2.669298000	-2.448531000
1	-3.149777000	-4.572911000	-0.833984000
6	-0.874015000	2.177156000	-3.128952000
1	-1.186851000	3.009712000	-3.771923000
1	-0.369291000	1.441857000	-3.757903000

1	-1.762397000	1.706590000	-2.695567000
1	-3.432225000	0.209656000	1.701155000
1	-1.482596000	2.535506000	1.547592000
1	-2.841624000	3.565428000	3.168887000
1	-4.955316000	3.810142000	2.167999000
1	-4.843413000	3.207748000	-0.228032000
1	-4.357744000	0.910007000	-0.294422000
1	-3.037878000	-0.855231000	-1.914716000
1	-3.171796000	-3.102654000	-2.667337000
1	-4.838529000	-4.721137000	-1.284348000
1	-5.399513000	-2.904867000	0.386187000
1	-3.778278000	-1.905166000	1.779441000
1	-1.820520000	-2.572527000	-0.451844000
6	-0.591865000	3.515438000	-0.931805000
1	-1.226731000	2.834606000	-0.362922000
6	-1.476977000	4.616014000	-1.534321000
1	-1.836845000	5.296514000	-0.752577000
1	-0.904961000	5.212812000	-2.254525000
1	-2.354473000	4.208614000	-2.047381000
6	0.440352000	4.153626000	-0.005985000
1	-0.044385000	4.620085000	0.861262000
1	1.175235000	3.432293000	0.361824000
1	1.005535000	4.922151000	-0.541327000

In_TSD4s

Doordinates (Angstroms)			
	X	Y	Z
25	0.497062000	0.436055000	-0.536456000
7	1.559215000	-0.238943000	1.405282000
6	0.310907000	-2.761240000	0.418850000
1	-0.090450000	-3.519280000	1.103458000
1	0.520682000	-3.276038000	-0.520556000
6	2.855328000	2.330279000	0.830175000
6	-0.497370000	1.095412000	-1.822001000
8	-1.109851000	1.585834000	-2.689367000
15	2.003611000	2.206465000	-0.784772000
15	-0.917705000	-1.401385000	0.079972000
14	3.158457000	0.560992000	1.373184000
14	1.884523000	-1.977884000	1.136339000
6	4.032608000	0.574079000	3.044960000
1	4.167906000	-0.425790000	3.472033000
1	5.024001000	1.035743000	2.954380000
1	3.458393000	1.173082000	3.763528000
6	2.367665000	-2.939099000	2.692724000

1	2.567557000	-3.987463000	2.434174000
1	3.276394000	-2.540548000	3.157573000
1	1.580804000	-2.936547000	3.456605000
1	3.741538000	2.975619000	0.807489000
1	2.123341000	2.759956000	1.534062000
6	1.246461000	3.848165000	-1.092432000
1	2.015705000	4.621747000	-1.195931000
1	0.639095000	3.818997000	-2.002697000
1	0.616801000	4.098942000	-0.237230000
6	3.485473000	2.371050000	-1.892586000
1	3.253405000	2.197348000	-2.946707000
1	3.883511000	3.387672000	-1.798199000
1	4.278895000	1.684261000	-1.587559000
15	1.669217000	-0.812973000	-2.156252000
6	3.499141000	-1.008041000	-1.875296000
1	3.873713000	-1.872957000	-2.437787000
1	4.036593000	-0.137997000	-2.257718000
14	3.805130000	-1.242657000	-0.018812000
6	1.406510000	-2.551963000	-2.773852000
1	1.791174000	-3.287653000	-2.061803000
1	0.356202000	-2.775122000	-2.975361000
1	1.960493000	-2.679311000	-3.710910000
6	1.572742000	-0.011822000	-3.818469000
1	1.638601000	1.075099000	-3.745437000
1	2.361240000	-0.378942000	-4.484936000
1	0.600605000	-0.248969000	-4.263733000
6	5.456364000	-2.100672000	0.310442000
1	5.510600000	-3.068465000	-0.201942000
1	6.295083000	-1.490641000	-0.046019000
1	5.608080000	-2.279651000	1.380862000
1	-0.173987000	1.661661000	0.564111000
1	0.868489000	0.069713000	2.086058000
6	-0.683703000	2.812536000	1.525719000
8	0.262063000	3.578478000	1.838661000
6	-2.030680000	-1.741572000	1.566485000
6	-1.328355000	-1.637475000	2.928534000
6	-3.371167000	-0.969276000	1.585758000
6	-2.170724000	-2.314194000	4.028455000
1	-0.343203000	-2.109199000	2.904678000
6	-3.963523000	-0.861544000	3.002331000
1	-3.258162000	0.035941000	1.170499000
6	-3.686090000	-2.134474000	3.800818000
1	-1.930721000	-3.383699000	4.071307000
1	-3.524591000	-0.002636000	3.526854000

1	-4.087443000	-2.992908000	3.245452000
6	-1.967239000	-2.095989000	-1.299515000
6	-2.595808000	-3.472706000	-1.050998000
6	-3.031546000	-1.088022000	-1.808354000
6	-3.113829000	-4.074657000	-2.371628000
1	-1.875374000	-4.158899000	-0.590866000
6	-4.204434000	-1.796915000	-2.508014000
1	-3.419853000	-0.468347000	-0.995565000
6	-3.705638000	-2.999953000	-3.309330000
1	-2.295418000	-4.597630000	-2.881898000
1	-4.940923000	-2.136796000	-1.767360000
1	-2.939721000	-2.653823000	-4.016508000
1	-2.270077000	-2.806245000	1.441614000
1	-1.162117000	-0.589829000	3.183413000
1	-1.885632000	-1.891056000	4.998796000
1	-4.212521000	-2.115141000	4.761185000
1	-5.039407000	-0.666862000	2.934567000
1	-4.085185000	-1.490343000	0.936552000
1	-2.555501000	-0.399053000	-2.509638000
1	-4.725837000	-1.085548000	-3.158017000
1	-4.512279000	-3.427110000	-3.914819000
1	-3.871880000	-4.833122000	-2.143081000
1	-3.426947000	-3.374249000	-0.341837000
1	-1.238520000	-2.217476000	-2.107141000
6	-1.784804000	3.376923000	0.629126000
6	-2.698430000	2.579507000	-0.059346000
6	-1.929958000	4.763591000	0.571990000
6	-3.738446000	3.148073000	-0.785073000
1	-2.554994000	1.504169000	-0.062919000
6	-2.968110000	5.340689000	-0.156132000
1	-1.215480000	5.379628000	1.109272000
6	-3.878369000	4.534334000	-0.834579000
1	-4.429398000	2.509440000	-1.329126000
1	-3.067370000	6.422472000	-0.192143000
1	-4.688300000	4.982288000	-1.403934000
6	-1.212876000	1.893033000	2.619740000
1	-0.372770000	1.440062000	3.154649000
1	-1.770453000	2.510131000	3.336977000
1	-1.876115000	1.121855000	2.234114000

In_TSD4sa

Doordinates (Angstroms)

X

Y

Z

25	0.496196000	-0.276337000	-0.789650000
7	1.176341000	0.874116000	1.081187000
6	-0.822654000	-1.035123000	2.171506000
1	-1.508813000	-0.799478000	2.994410000
1	-0.740077000	-2.122406000	2.149830000
6	3.285138000	1.486904000	-0.883291000
6	-0.252358000	-0.882254000	-2.255624000
8	-0.748894000	-1.278476000	-3.238327000
15	2.547302000	0.128516000	-1.862651000
15	-1.467649000	-0.473298000	0.514594000
14	2.948200000	1.020537000	0.908344000
14	0.890888000	-0.256438000	2.432770000
6	3.721945000	2.314449000	2.042493000
1	3.489781000	2.149843000	3.100445000
1	4.814352000	2.309009000	1.937391000
1	3.374214000	3.320138000	1.773811000
6	0.943309000	0.549474000	4.142521000
1	0.714790000	-0.193974000	4.917120000
1	1.931662000	0.964629000	4.369410000
1	0.214554000	1.362930000	4.243200000
1	4.340040000	1.673435000	-1.118795000
1	2.705284000	2.392703000	-1.127890000
6	2.445979000	0.701308000	-3.600212000
1	3.443745000	0.889795000	-4.012308000
1	1.945715000	-0.059268000	-4.209618000
1	1.878343000	1.638050000	-3.606605000
6	4.056656000	-0.945496000	-2.012679000
1	3.847044000	-1.927292000	-2.446299000
1	4.777731000	-0.438327000	-2.663650000
1	4.539245000	-1.082882000	-1.041692000
15	1.212340000	-2.459433000	-0.293029000
6	2.834320000	-2.601391000	0.608391000
1	2.882855000	-3.560529000	1.140091000
1	3.664561000	-2.604211000	-0.100722000
14	2.987140000	-1.164460000	1.837071000
6	0.362825000	-3.824862000	0.649945000
1	0.433161000	-3.662572000	1.729324000
1	-0.690263000	-3.938307000	0.381903000
1	0.868748000	-4.771802000	0.428443000
6	1.478686000	-3.436446000	-1.838959000
1	1.895188000	-2.819208000	-2.637051000
1	2.134938000	-4.295928000	-1.661595000
1	0.508066000	-3.806129000	-2.187822000
6	4.248573000	-1.558143000	3.187290000

1	3.985758000	-2.479346000	3.720776000
1	5.249817000	-1.696051000	2.761561000
1	4.309269000	-0.750423000	3.925312000
1	0.286622000	1.424357000	-1.361824000
1	0.594380000	1.699462000	0.967735000
6	0.094304000	2.706172000	-2.061461000
8	1.197987000	3.173253000	-2.476958000
6	-2.714849000	0.803582000	1.116007000
6	-2.126670000	1.837288000	2.091435000
6	-3.498493000	1.524695000	-0.010771000
6	-3.249180000	2.613959000	2.807496000
1	-1.497379000	1.362856000	2.847222000
6	-4.018423000	2.905494000	0.427030000
1	-2.883885000	1.627655000	-0.910678000
6	-4.460717000	2.873701000	1.888880000
1	-3.570831000	2.055562000	3.695048000
1	-3.235732000	3.663759000	0.309375000
1	-5.208417000	2.079125000	2.015973000
6	-2.561419000	-1.881051000	-0.036399000
6	-3.348620000	-2.618626000	1.065371000
6	-3.502685000	-1.542156000	-1.201885000
6	-4.476200000	-3.490711000	0.470953000
1	-2.662668000	-3.252333000	1.640001000
6	-3.923178000	-2.842033000	-1.912674000
1	-4.392887000	-1.040034000	-0.809017000
6	-4.091140000	-4.010298000	-0.916543000
1	-4.700281000	-4.320973000	1.150066000
1	-4.863739000	-2.668420000	-2.448619000
1	-3.150899000	-4.572575000	-0.834347000
1	-3.432311000	0.209872000	1.700911000
1	-1.482186000	2.535343000	1.547823000
1	-2.841192000	3.565464000	3.168962000
1	-4.954825000	3.810536000	2.168009000
1	-4.842807000	3.208366000	-0.228073000
1	-4.357401000	0.910620000	-0.294759000
1	-3.038341000	-0.854731000	-1.914792000
1	-3.172659000	-3.102133000	-2.667530000
1	-4.839747000	-4.720298000	-1.284516000
1	-5.399997000	-2.903981000	0.386244000
1	-3.778241000	-1.904974000	1.779453000
1	-1.821008000	-2.572352000	-0.452273000
6	-0.873411000	2.178087000	-3.128634000
1	-1.185963000	3.010867000	-3.771453000
1	-0.368807000	1.442802000	-3.757698000

1	-1.761961000	1.707646000	-2.695460000
6	-0.591154000	3.515833000	-0.931179000
1	-1.226250000	2.835038000	-0.362509000
6	0.441111000	4.153574000	-0.005102000
1	1.006571000	4.922046000	-0.540231000
1	-0.043619000	4.620002000	0.862165000
1	1.175756000	3.431984000	0.362678000
6	-1.475911000	4.616772000	-1.533553000
1	-2.353415000	4.209718000	-2.046872000
1	-1.835753000	5.297146000	-0.751686000
1	-0.903631000	5.213632000	-2.253498000

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Doordinates (Angstroms)			
	X	Y	Z
25	-0.109487000	-0.699687000	-0.952257000
7	1.108030000	-0.631184000	0.928363000
6	-1.719874000	-0.461117000	1.995593000
1	-2.238425000	0.059762000	2.807125000
1	-2.233119000	-1.420130000	1.862501000
6	2.608622000	-2.716581000	-0.707435000
6	-0.876134000	-0.521936000	-2.523111000
8	-1.329979000	-0.431384000	-3.599234000
15	1.834507000	-1.565183000	-1.912052000
15	-1.774742000	0.399983000	0.371945000
14	2.270601000	-1.958394000	1.014368000
14	0.108693000	-0.840580000	2.365399000
6	3.918913000	-1.448452000	1.777715000
1	3.778715000	-0.964876000	2.751881000
1	4.590506000	-2.304360000	1.918913000
1	4.427066000	-0.728358000	1.122991000
6	0.670891000	0.205865000	3.833666000
1	0.059122000	0.025003000	4.726198000
1	1.715208000	-0.003085000	4.095133000
1	0.600624000	1.275421000	3.593993000
1	2.111595000	-3.692015000	-0.762257000
1	3.674859000	-2.877506000	-0.912142000
6	3.255194000	-0.426904000	-2.162596000
1	4.125728000	-0.984998000	-2.527294000
1	3.002046000	0.344077000	-2.892428000
1	3.517057000	0.070173000	-1.227183000
6	1.884928000	-2.406978000	-3.551931000
1	1.737826000	-1.649192000	-4.330123000

1	2.853260000	-2.892503000	-3.718597000
1	1.092089000	-3.148595000	-3.662053000
15	-1.006384000	-2.819816000	-0.595253000
6	-0.537680000	-3.836084000	0.919545000
1	-1.467713000	-4.128394000	1.426752000
1	-0.097110000	-4.776982000	0.561356000
14	0.651377000	-3.103892000	2.239648000
6	-2.846033000	-3.015929000	-0.539500000
1	-3.262296000	-2.588807000	0.375861000
1	-3.296473000	-2.506791000	-1.398193000
1	-3.125489000	-4.075006000	-0.571908000
6	-0.709335000	-4.087349000	-1.909110000
1	0.354562000	-4.319091000	-2.000954000
1	-1.241945000	-5.017846000	-1.682497000
1	-1.065766000	-3.705807000	-2.871923000
6	0.856409000	-4.385639000	3.617172000
1	-0.102235000	-4.603474000	4.103406000
1	1.252320000	-5.329792000	3.223307000
1	1.549264000	-4.029873000	4.388029000
1	1.313177000	0.487859000	0.236524000
6	1.532046000	2.369455000	-1.074253000
8	1.100311000	1.087807000	-0.735128000
6	2.988035000	2.574756000	-0.657554000
6	3.972732000	3.061094000	-1.517311000
6	3.356721000	2.249090000	0.654290000
6	5.292032000	3.205528000	-1.087093000
1	3.721852000	3.320491000	-2.541409000
6	4.670411000	2.389791000	1.087511000
1	2.609901000	1.858624000	1.341603000
6	5.647249000	2.867877000	0.214383000
1	6.043638000	3.578215000	-1.777822000
1	4.932129000	2.122842000	2.107858000
1	6.675380000	2.976784000	0.547956000
6	1.239190000	2.633670000	-2.546674000
1	1.855442000	2.014222000	-3.205189000
1	0.193519000	2.381851000	-2.748137000
1	1.397425000	3.686985000	-2.805738000
1	0.955247000	3.118754000	-0.505699000
6	-1.340830000	2.159752000	0.848676000
6	-1.721753000	3.169158000	-0.252766000
6	-1.802326000	2.716004000	2.205218000
6	-1.537179000	4.635585000	0.207840000
1	-1.133888000	2.961786000	-1.150696000
6	-0.960487000	3.955459000	2.578315000

1	-2.861335000	2.991070000	2.148863000
6	-0.522100000	4.768600000	1.344377000
1	-1.240321000	5.257981000	-0.643820000
1	-1.544960000	4.588445000	3.256815000
1	0.458400000	4.419902000	0.998651000
6	-3.588578000	0.385170000	-0.061093000
6	-4.523926000	1.201238000	0.841432000
6	-3.838411000	0.692750000	-1.559896000
6	-5.993907000	0.815464000	0.581966000
1	-4.281513000	1.042528000	1.897901000
6	-5.263407000	1.214292000	-1.808516000
1	-3.108892000	1.408729000	-1.951538000
6	-6.261315000	0.490013000	-0.903938000
1	-6.260654000	-0.050584000	1.200118000
1	-5.312850000	2.293528000	-1.610214000
1	-7.292193000	0.750125000	-1.168706000
1	-2.499753000	5.031830000	0.557440000
1	-0.390386000	5.822797000	1.612661000
1	-0.070063000	3.640437000	3.136746000
1	-2.769355000	3.033768000	-0.538010000
1	-1.715300000	1.979471000	3.008048000
1	-0.246296000	2.097347000	0.882399000
1	-3.680867000	-0.227178000	-2.133018000
1	-3.859710000	-0.663893000	0.100072000
1	-5.524184000	1.081418000	-2.864410000
1	-6.161914000	-0.590811000	-1.074324000
1	-6.640074000	1.639614000	0.907303000
1	-4.385280000	2.270700000	0.649731000

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Doordinates (Angstroms)			

	X	Y	Z
25	0.392747000	-0.351751000	-0.843775000
7	1.351441000	0.493631000	1.048994000
6	-1.091843000	-0.855559000	2.165861000
1	-1.701228000	-0.410563000	2.961935000
1	-1.260660000	-1.934627000	2.218330000
6	3.743979000	0.416132000	-0.694601000
6	-0.377653000	-0.567538000	-2.407620000
8	-0.826911000	-0.684032000	-3.482466000
15	2.502005000	-0.225610000	-1.898475000
15	-1.593086000	-0.258724000	0.486656000
14	3.079501000	0.165519000	1.060501000
14	0.754514000	-0.461547000	2.392412000

6	4.110949000	1.299122000	2.169720000
1	3.919533000	2.350648000	1.917315000
1	3.893372000	1.170900000	3.235766000
1	5.183363000	1.114125000	2.025606000
6	0.939251000	0.316872000	4.109956000
1	0.526229000	-0.346351000	4.881578000
1	1.986554000	0.509836000	4.368627000
1	0.405894000	1.274242000	4.172897000
1	4.731251000	-0.033040000	-0.855208000
1	3.855639000	1.496987000	-0.848388000
6	2.572330000	0.971582000	-3.287185000
1	3.589676000	1.069079000	-3.682919000
1	1.903761000	0.643830000	-4.090172000
1	2.228284000	1.935567000	-2.919578000
6	3.457470000	-1.584403000	-2.716213000
1	2.950531000	-1.893382000	-3.636144000
1	4.452365000	-1.217091000	-2.992322000
1	3.581462000	-2.464055000	-2.080431000
15	0.655400000	-2.652394000	-0.524807000
6	2.176243000	-3.113333000	0.433678000
1	2.093740000	-4.154108000	0.775034000
1	3.047928000	-3.078202000	-0.228703000
14	2.526701000	-1.952331000	1.915728000
6	-0.500637000	-3.859746000	0.282071000
1	-0.678423000	-3.632749000	1.335780000
1	-1.458502000	-3.888267000	-0.243838000
1	-0.063902000	-4.863458000	0.223555000
6	0.807240000	-3.613218000	-2.096715000
1	1.385204000	-3.075383000	-2.847207000
1	1.263333000	-4.595451000	-1.926730000
1	-0.197724000	-3.763097000	-2.506864000
6	3.521196000	-2.908504000	3.213441000
1	2.944473000	-3.749369000	3.618170000
1	4.446070000	-3.316003000	2.787151000
1	3.798147000	-2.260109000	4.052780000
1	1.003139000	1.445263000	0.238942000
6	0.104394000	2.965160000	-1.189969000
8	0.817388000	1.798029000	-0.882624000
6	-0.387166000	2.937721000	-2.634663000
1	-1.066848000	3.777377000	-2.826547000
1	0.428838000	2.992564000	-3.361932000
1	-0.928619000	2.006232000	-2.822924000
6	0.930379000	4.233293000	-0.860937000
1	0.325137000	5.090391000	-1.193005000

6	2.272359000	4.290358000	-1.591321000
1	2.792113000	5.230798000	-1.372812000
1	2.920291000	3.467874000	-1.270040000
1	2.156686000	4.227886000	-2.678930000
6	1.146786000	4.373526000	0.648426000
1	1.778502000	5.239831000	0.879037000
1	0.196886000	4.511294000	1.178112000
1	1.634537000	3.482352000	1.062082000
1	-0.794762000	3.021956000	-0.566279000
6	-2.533635000	1.288120000	0.959569000
6	-1.722243000	2.263381000	1.823065000
6	-3.172681000	1.968181000	-0.274543000
6	-2.583653000	3.451560000	2.312740000
1	-1.316587000	1.743706000	2.695281000
6	-3.457583000	3.463812000	-0.050051000
1	-2.539073000	1.841568000	-1.159070000
6	-3.799782000	3.734144000	1.413071000
1	-2.927798000	3.265863000	3.337180000
1	-2.577097000	4.061788000	-0.321450000
1	-4.134147000	4.768308000	1.552395000
6	-3.002226000	-1.414185000	0.067261000
6	-4.252898000	-1.322612000	0.951476000
6	-3.387480000	-1.380738000	-1.429883000
6	-5.138092000	-2.569918000	0.751498000
1	-3.983213000	-1.229730000	2.009772000
6	-4.801957000	-1.938044000	-1.672278000
1	-3.317072000	-0.367126000	-1.837586000
6	-5.101795000	-3.082810000	-0.703973000
1	-4.809087000	-3.366168000	1.430298000
1	-5.550509000	-1.146148000	-1.533758000
1	-6.048525000	-3.572713000	-0.956426000
1	-2.567266000	-2.395894000	0.271261000
1	-4.823509000	-0.421754000	0.693559000
1	-6.168594000	-2.324764000	1.035063000
1	-4.320607000	-3.847878000	-0.813231000
1	-4.894573000	-2.270536000	-2.712193000
1	-2.659088000	-1.976923000	-1.988863000
1	-3.346483000	0.929757000	1.603227000
1	-0.854833000	2.619920000	1.268521000
1	-1.952560000	4.348114000	2.358501000
1	-4.642725000	3.093252000	1.706343000
1	-4.267909000	3.789033000	-0.712130000
1	-4.115908000	1.454804000	-0.499168000

In_TSD5s

Doordinates (Angstroms)			
	X	Y	Z

25	-0.483578000	-0.453256000	-0.973116000
7	0.241081000	-1.654807000	0.800190000
6	-0.466211000	0.904349000	2.243804000
1	0.325781000	1.425919000	2.790234000
1	-1.403173000	1.164485000	2.748533000
6	-0.777782000	-3.819286000	-1.051250000
6	-0.711320000	0.471985000	-2.447628000
8	-0.867623000	1.054896000	-3.451200000
15	-0.261433000	-2.433773000	-2.163959000
15	-0.555498000	1.467377000	0.474062000
14	-0.571837000	-3.210561000	0.747270000
14	-0.242707000	-0.974094000	2.348642000
6	0.314712000	-4.607625000	1.666985000
1	0.430879000	-4.403134000	2.737655000
1	-0.231690000	-5.554651000	1.568574000
1	1.319067000	-4.759999000	1.248868000
6	0.949849000	-1.328070000	3.769239000
1	0.545656000	-0.972047000	4.725549000
1	1.166373000	-2.397113000	3.874792000
1	1.902512000	-0.807981000	3.602798000
1	-1.812458000	-4.105257000	-1.256689000
1	-0.167699000	-4.712903000	-1.234638000
6	1.295014000	-3.174258000	-2.836976000
1	1.044627000	-4.050313000	-3.447618000
1	1.837530000	-2.459355000	-3.462173000
1	1.953033000	-3.504415000	-2.028911000
6	-1.253593000	-2.567777000	-3.715378000
1	-0.662302000	-2.131871000	-4.528788000
1	-1.479958000	-3.608807000	-3.972077000
1	-2.181733000	-1.996712000	-3.652658000
15	-2.786958000	-0.847737000	-0.687680000
6	-3.317432000	-0.943053000	1.081973000
1	-3.229326000	0.045300000	1.548096000
1	-4.378195000	-1.223853000	1.133644000
14	-2.230388000	-2.183288000	2.078131000
6	-3.896944000	0.411211000	-1.457592000
1	-3.444063000	1.400206000	-1.433634000
1	-4.044883000	0.147673000	-2.511097000
1	-4.876088000	0.445636000	-0.966556000
6	-3.761231000	-2.332477000	-1.243809000

1	-3.547969000	-3.198165000	-0.611681000
1	-4.829825000	-2.107642000	-1.146472000
1	-3.568139000	-2.603360000	-2.283824000
6	-3.293367000	-3.043430000	3.385726000
1	-3.743818000	-2.318803000	4.074749000
1	-4.108872000	-3.612266000	2.922428000
1	-2.694332000	-3.741371000	3.981665000
1	1.195317000	-1.067595000	0.191091000
6	2.821539000	-0.714148000	-1.181144000
8	1.661753000	-0.251248000	-0.544032000
6	4.027019000	-0.555324000	-0.251655000
6	5.256636000	-0.042125000	-0.666951000
6	3.900410000	-0.965598000	1.081393000
6	6.321697000	0.081581000	0.226266000
1	5.394450000	0.279899000	-1.694736000
6	4.957099000	-0.842892000	1.975670000
1	2.956604000	-1.383866000	1.421998000
6	6.175191000	-0.311994000	1.551466000
1	7.266073000	0.493324000	-0.119487000
1	4.830992000	-1.162894000	3.006774000
1	7.001410000	-0.211038000	2.249625000
6	2.994410000	-0.054143000	-2.544400000
1	3.760639000	-0.558476000	-3.144894000
1	2.042478000	-0.101737000	-3.081984000
1	3.273079000	1.001261000	-2.452215000
1	2.730520000	-1.795915000	-1.354830000
6	0.843651000	2.701539000	0.313479000
6	2.104850000	2.339161000	1.136622000
6	1.212869000	2.934617000	-1.157123000
6	3.386571000	2.909592000	0.508701000
1	1.993757000	2.740960000	2.151733000
6	2.151251000	4.146219000	-1.305547000
1	1.685843000	2.022517000	-1.522968000
6	3.129806000	4.278118000	-0.119818000
1	4.175997000	2.959428000	1.267096000
1	2.710872000	4.043023000	-2.243652000
1	4.067336000	4.739868000	-0.449761000
6	-2.021871000	2.637774000	0.527904000
6	-2.088389000	3.539145000	1.789336000
6	-2.127524000	3.499793000	-0.740356000
6	-2.843825000	4.856350000	1.531828000
1	-2.599841000	2.992797000	2.590476000
6	-3.493726000	4.207161000	-0.820817000
1	-1.331124000	4.252976000	-0.723641000

6	-4.009973000	4.630768000	0.569481000
1	-3.198135000	5.268703000	2.483388000
1	-3.396602000	5.085703000	-1.469451000
1	-4.660460000	3.848199000	0.983429000
1	-2.901627000	1.982950000	0.547786000
1	-1.085287000	3.766270000	2.169211000
1	-1.960541000	2.904228000	-1.643939000
1	-2.162638000	5.604273000	1.104991000
1	-4.627165000	5.532131000	0.487691000
1	-4.228041000	3.548496000	-1.300165000
1	0.448754000	3.647987000	0.708335000
1	0.326745000	3.083823000	-1.778982000
1	1.560362000	5.066534000	-1.399103000
1	2.708091000	4.946758000	0.643505000
1	3.749580000	2.221113000	-0.263035000
1	2.211540000	1.255185000	1.213839000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.422455000	-0.340980000	-0.864701000
7	1.386197000	0.444582000	1.049268000
6	-1.050081000	-0.894585000	2.170511000
1	-1.627157000	-0.425625000	2.974289000
1	-1.242724000	-1.968729000	2.251521000
6	3.722307000	0.581246000	-0.701076000
6	-0.369510000	-0.504665000	-2.424926000
8	-0.840245000	-0.572419000	-3.494394000
15	2.528287000	-0.116872000	-1.917258000
15	-1.565810000	-0.333393000	0.484683000
14	3.111911000	0.135558000	1.038032000
14	0.802355000	-0.528549000	2.382209000
6	4.166115000	1.168635000	2.223862000
1	3.972503000	2.239849000	2.082862000
1	3.977334000	0.935205000	3.277450000
1	5.234050000	0.996381000	2.035807000
6	0.968046000	0.262862000	4.094874000
1	0.570979000	-0.399227000	4.875555000
1	2.003899000	0.502764000	4.358698000
1	0.394255000	1.199318000	4.130286000
1	4.758490000	0.297787000	-0.920615000
1	3.675011000	1.678560000	-0.748196000
6	2.696266000	0.953334000	-3.413271000

1	3.733680000	0.958493000	-3.767184000
1	2.056271000	0.556690000	-4.208844000
1	2.394612000	1.982234000	-3.219181000
6	3.533525000	-1.514891000	-2.597687000
1	3.097245000	-1.871231000	-3.535726000
1	4.545723000	-1.157530000	-2.816815000
1	3.612029000	-2.358225000	-1.910071000
15	0.719073000	-2.643155000	-0.626149000
6	2.180367000	-3.183014000	0.387950000
1	2.009787000	-4.202519000	0.758826000
1	3.074132000	-3.241170000	-0.242573000
14	2.575097000	-2.009522000	1.844496000
6	-0.513707000	-3.809641000	0.119505000
1	-0.685591000	-3.603807000	1.178637000
1	-1.465315000	-3.759898000	-0.415332000
1	-0.135425000	-4.834916000	0.033692000
6	0.894761000	-3.588142000	-2.205660000
1	1.507811000	-3.057800000	-2.933000000
1	1.320252000	-4.583960000	-2.035648000
1	-0.101659000	-3.706959000	-2.645976000
6	3.612250000	-2.963306000	3.110058000
1	3.049817000	-3.803510000	3.535629000
1	4.522235000	-3.371429000	2.653157000
1	3.917863000	-2.314082000	3.938735000
1	0.874660000	1.408216000	0.352419000
6	0.847648000	2.943351000	-1.230121000
8	0.293055000	1.836203000	-0.580334000
6	0.142638000	3.130556000	-2.572872000
1	-0.857062000	3.558162000	-2.426794000
1	0.698584000	3.792608000	-3.246030000
1	0.023125000	2.161060000	-3.064597000
6	0.759992000	4.206414000	-0.349169000
1	-0.307242000	4.393146000	-0.171796000
6	1.354250000	5.427713000	-1.056789000
1	1.354609000	6.300273000	-0.393072000
1	2.395595000	5.239762000	-1.352718000
1	0.793732000	5.700644000	-1.956872000
6	1.443310000	3.999404000	1.003419000
1	2.512570000	3.786869000	0.865451000
1	1.364149000	4.900948000	1.622594000
1	1.007505000	3.166708000	1.562578000
1	1.925490000	2.779292000	-1.416608000
6	-2.252874000	1.375406000	0.780929000
6	-2.937229000	1.906063000	-0.496206000

6	-3.135317000	1.678086000	2.000294000
6	-3.726880000	3.206299000	-0.227587000
1	-2.159779000	2.062307000	-1.249913000
6	-3.162806000	3.201056000	2.244585000
1	-4.154713000	1.321044000	1.824090000
6	-3.122897000	4.004861000	0.928034000
1	-3.761697000	3.814716000	-1.138834000
1	-4.066402000	3.453595000	2.813274000
1	-2.084452000	4.250214000	0.679382000
6	-3.013386000	-1.455602000	0.117375000
6	-4.314753000	-1.193058000	0.885232000
6	-3.287906000	-1.599701000	-1.398212000
6	-5.257760000	-2.408868000	0.770978000
1	-4.109148000	-0.984635000	1.940234000
6	-4.705855000	-2.128667000	-1.679391000
1	-3.140357000	-0.650177000	-1.920295000
6	-5.139238000	-3.116122000	-0.595713000
1	-5.033640000	-3.123159000	1.572453000
1	-5.419383000	-1.294205000	-1.708423000
1	-6.089151000	-3.594733000	-0.857948000
1	-1.325005000	1.948176000	0.893536000
1	-3.631884000	1.162152000	-0.901915000
1	-2.784842000	1.177869000	2.908209000
1	-2.308350000	3.487935000	2.870046000
1	-3.644204000	4.961014000	1.050297000
1	-4.769462000	2.963641000	0.019221000
1	-2.650456000	-2.422612000	0.480378000
1	-4.805155000	-0.301644000	0.478081000
1	-6.290013000	-2.074983000	0.930916000
1	-4.394302000	-3.921713000	-0.537856000
1	-4.737461000	-2.595700000	-2.669929000
1	-2.545202000	-2.284965000	-1.824085000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.127300000	-0.598587000	1.015637000
7	-1.383400000	-0.295682000	-0.667512000
6	1.214854000	-0.293926000	-2.137887000
1	1.429635000	0.398949000	-2.958435000
1	1.898567000	-1.135545000	-2.271698000
6	-3.134319000	-1.485249000	1.412070000
6	1.121551000	-0.412279000	2.449524000
8	1.710360000	-0.238148000	3.444122000

15	-1.508399000	-1.604859000	2.252747000
15	1.567762000	0.416737000	-0.463951000
14	-2.762313000	-1.420441000	-0.430479000
14	-0.585019000	-0.892055000	-2.152325000
6	-4.311326000	-0.914869000	-1.374725000
1	-4.223586000	-1.060986000	-2.456610000
1	-5.176218000	-1.494763000	-1.029242000
1	-4.527821000	0.145059000	-1.192217000
6	-1.398014000	-0.233886000	-3.723287000
1	-0.815708000	-0.504360000	-4.613194000
1	-2.415274000	-0.614171000	-3.864807000
1	-1.460905000	0.861794000	-3.685176000
1	-3.839212000	-2.269002000	1.706757000
1	-3.543041000	-0.515399000	1.718646000
15	0.939469000	-2.715854000	0.531956000
6	-0.298969000	-3.898038000	-0.187539000
1	0.212498000	-4.771668000	-0.612286000
1	-0.952502000	-4.271301000	0.610371000
14	-1.382271000	-3.015291000	-1.480044000
6	2.350241000	-3.148603000	-0.588256000
1	2.048080000	-3.079734000	-1.637509000
1	3.208243000	-2.491473000	-0.427386000
1	2.663179000	-4.182120000	-0.401589000
6	1.529519000	-3.613104000	2.031624000
1	0.811454000	-3.521724000	2.851125000
1	1.696497000	-4.675730000	1.821957000
1	2.474620000	-3.169581000	2.362996000
6	-2.072600000	-4.223540000	-2.755016000
1	-1.265941000	-4.720998000	-3.306411000
1	-2.673338000	-5.003091000	-2.271971000
1	-2.711809000	-3.712113000	-3.483428000
1	-0.716409000	0.837065000	1.589957000
1	-1.569506000	0.703415000	-0.561306000
6	-1.604897000	1.703655000	2.332064000
8	-2.299402000	1.058695000	3.170590000
6	1.504627000	2.233873000	-0.760543000
6	0.957929000	2.827086000	-1.900441000
6	2.007452000	3.062372000	0.251274000
6	0.916944000	4.215423000	-2.029037000
1	0.541734000	2.220608000	-2.698727000
6	1.963388000	4.445871000	0.126228000
1	2.430632000	2.618318000	1.149415000
6	1.414215000	5.027782000	-1.016057000
1	0.487174000	4.659202000	-2.922760000

1	2.352483000	5.071545000	0.924024000
1	1.374882000	6.108544000	-1.113696000
6	3.402547000	0.236956000	-0.347336000
6	4.216815000	0.642476000	-1.412806000
6	4.005624000	-0.302614000	0.789752000
6	5.597449000	0.496620000	-1.347430000
1	3.767291000	1.084093000	-2.298629000
6	5.391293000	-0.444979000	0.860269000
1	3.394885000	-0.617626000	1.627273000
6	6.188349000	-0.050801000	-0.208830000
1	6.215022000	0.813579000	-2.183032000
1	5.843140000	-0.866578000	1.753479000
1	7.267262000	-0.164553000	-0.155737000
6	-2.379165000	2.288486000	1.139014000
6	-1.777952000	2.999782000	0.098009000
6	-3.764054000	2.115732000	1.110299000
6	-2.533994000	3.483095000	-0.967938000
1	-0.708308000	3.169013000	0.112872000
6	-4.527359000	2.605221000	0.052715000
1	-4.224349000	1.603292000	1.948921000
6	-3.912539000	3.281066000	-0.999606000
1	-2.040898000	4.024383000	-1.770937000
1	-5.604939000	2.461307000	0.051625000
1	-4.503685000	3.659366000	-1.829098000
6	-0.519148000	2.629012000	2.892655000
1	-1.009966000	3.477135000	3.388150000
1	0.059883000	2.079084000	3.638422000
1	0.160785000	3.013119000	2.128881000
1	-1.756938000	-1.184675000	3.566715000
1	-1.442764000	-2.998682000	2.494262000

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Doordinates (Angstroms)			

	X	Y	Z
25	0.294018000	-0.182621000	-0.967071000
7	1.450611000	0.407511000	0.917643000
6	-0.899617000	-1.049329000	2.042614000
1	-1.417881000	-0.696410000	2.940752000
1	-1.131699000	-2.114222000	1.964734000
6	3.608093000	0.591472000	-1.139331000
6	-0.635160000	-0.173802000	-2.458090000
8	-1.210459000	-0.085896000	-3.470871000
15	2.257698000	-0.105402000	-2.165720000

15	-1.495868000	-0.255491000	0.477942000
14	3.198329000	0.103005000	0.632675000
14	0.974926000	-0.785626000	2.164355000
6	4.313345000	1.061446000	1.809629000
1	4.128782000	0.827575000	2.863439000
1	5.368742000	0.848709000	1.599246000
1	4.163965000	2.140280000	1.673694000
6	1.345404000	-0.214984000	3.924825000
1	0.957657000	-0.938817000	4.652921000
1	2.416531000	-0.095345000	4.119609000
1	0.862586000	0.749821000	4.129156000
1	4.607868000	0.287933000	-1.466543000
1	3.512529000	1.678255000	-1.258621000
15	0.543857000	-2.499266000	-0.946507000
6	2.163600000	-3.130786000	-0.285615000
1	2.081687000	-4.199711000	-0.049491000
1	2.938597000	-3.039058000	-1.055699000
14	2.689910000	-2.119403000	1.236283000
6	-0.544275000	-3.733284000	-0.093819000
1	-0.350203000	-3.746294000	0.982770000
1	-1.603320000	-3.519206000	-0.255559000
1	-0.331339000	-4.736754000	-0.479382000
6	0.478867000	-3.233180000	-2.637156000
1	1.103525000	-2.666091000	-3.332522000
1	0.807968000	-4.278371000	-2.633890000
1	-0.552120000	-3.191114000	-3.004717000
6	3.832228000	-3.099206000	2.374791000
1	3.338252000	-4.005210000	2.745113000
1	4.742634000	-3.409307000	1.848476000
1	4.135207000	-2.503304000	3.243292000
1	0.399390000	1.593512000	-1.163738000
1	1.136070000	1.371786000	1.004513000
6	0.833084000	2.803948000	-1.724368000
8	1.757083000	2.620445000	-2.582534000
6	-2.284093000	1.307025000	1.048998000
6	-2.171057000	1.834818000	2.336512000
6	-3.005813000	2.026451000	0.087979000
6	-2.764549000	3.055734000	2.657349000
1	-1.604956000	1.314622000	3.103286000
6	-3.604815000	3.237694000	0.408415000
1	-3.088823000	1.637400000	-0.924171000
6	-3.482546000	3.758575000	1.696414000
1	-2.659491000	3.457307000	3.661171000
1	-4.158483000	3.781802000	-0.351079000

1	-3.944164000	4.709363000	1.945763000
6	-3.036675000	-1.206424000	0.114324000
6	-3.997980000	-1.397411000	1.115122000
6	-3.272792000	-1.739818000	-1.153614000
6	-5.160730000	-2.113114000	0.855345000
1	-3.841897000	-0.970649000	2.102780000
6	-4.440376000	-2.455107000	-1.418053000
1	-2.542432000	-1.600444000	-1.941766000
6	-5.384210000	-2.644999000	-0.414589000
1	-5.898080000	-2.250782000	1.641092000
1	-4.607904000	-2.861915000	-2.411108000
1	-6.295096000	-3.200076000	-0.619668000
6	-0.524091000	3.268321000	-2.273358000
1	-0.417917000	4.286836000	-2.670692000
1	-0.814882000	2.613913000	-3.098974000
1	-1.315829000	3.264921000	-1.519423000
1	2.359221000	0.520255000	-3.413150000
1	2.848194000	-1.342660000	-2.522718000
6	1.299020000	3.555303000	-0.438818000
1	2.109737000	2.943455000	-0.018983000
6	0.231018000	3.757969000	0.628632000
1	0.670491000	4.114544000	1.569264000
1	-0.514776000	4.497269000	0.314991000
1	-0.309477000	2.831425000	0.833219000
6	1.924692000	4.892951000	-0.843984000
1	2.371636000	5.394585000	0.023965000
1	2.697997000	4.734610000	-1.600058000
1	1.170766000	5.571259000	-1.263835000

In_TSE4s

Doordinates (Angstroms)			
	X	Y	Z
25	-0.351651000	-0.307202000	-0.802544000
7	-1.549514000	-0.754810000	1.142155000
6	-0.941390000	2.131935000	1.416665000
1	-0.655787000	2.556659000	2.386472000
1	-1.283416000	2.969000000	0.802751000
6	-2.303370000	-3.063932000	-0.537750000
6	0.836991000	-0.187800000	-2.080023000
8	1.638189000	-0.156381000	-2.931698000
15	-1.287659000	-2.122632000	-1.747817000
15	0.482898000	1.354854000	0.514695000
14	-2.937023000	-1.796954000	0.696815000

14	-2.290740000	0.813774000	1.578867000
6	-3.696214000	-2.706367000	2.163604000
1	-4.107417000	-2.031208000	2.921735000
1	-4.508601000	-3.362468000	1.826763000
1	-2.946191000	-3.342659000	2.650843000
6	-2.960730000	0.891666000	3.344997000
1	-3.399259000	1.880441000	3.533096000
1	-3.741766000	0.147025000	3.533970000
1	-2.171302000	0.737877000	4.091879000
1	-3.076518000	-3.682445000	-1.004163000
1	-1.597533000	-3.722220000	-0.013825000
15	-1.832604000	1.027997000	-1.940546000
6	-3.635848000	0.617517000	-1.758319000
1	-4.263876000	1.437248000	-2.131243000
1	-3.866161000	-0.263481000	-2.370279000
14	-3.995459000	0.209737000	0.060314000
6	-1.983733000	2.869537000	-1.790046000
1	-2.528230000	3.139125000	-0.879684000
1	-0.999875000	3.345872000	-1.757490000
1	-2.539851000	3.275975000	-2.642622000
6	-1.613291000	0.937212000	-3.770847000
1	-1.549846000	-0.103899000	-4.100553000
1	-2.439676000	1.427655000	-4.298005000
1	-0.676550000	1.431473000	-4.049269000
6	-5.794739000	0.541151000	0.526158000
1	-6.054680000	1.592095000	0.352933000
1	-6.477021000	-0.072733000	-0.073421000
1	-5.982555000	0.319157000	1.582757000
1	0.654123000	-1.505357000	-0.158973000
1	-0.790958000	-1.144376000	1.697800000
6	1.365405000	-3.028402000	0.231781000
8	0.677341000	-3.915415000	-0.294930000
6	1.601828000	0.884746000	1.901844000
6	1.142622000	0.628964000	3.197831000
6	2.963354000	0.708584000	1.629898000
6	2.019007000	0.209822000	4.197403000
1	0.093890000	0.756279000	3.448709000
6	3.841946000	0.309441000	2.631099000
1	3.341519000	0.876624000	0.625195000
6	3.372704000	0.052675000	3.918086000
1	1.640270000	0.013735000	5.196565000
1	4.896303000	0.186019000	2.400993000
1	4.059128000	-0.266680000	4.696734000
6	1.375742000	2.842175000	-0.109298000

6	1.787444000	3.846845000	0.776671000
6	1.620492000	3.007978000	-1.473232000
6	2.419113000	4.992111000	0.306890000
1	1.619451000	3.726974000	1.843978000
6	2.255124000	4.156170000	-1.946934000
1	1.318092000	2.237004000	-2.172373000
6	2.653059000	5.149764000	-1.059280000
1	2.733333000	5.761517000	1.006322000
1	2.439998000	4.268177000	-3.011338000
1	3.147490000	6.043972000	-1.427863000
6	2.691361000	-2.684051000	-0.411465000
6	2.841015000	-2.889288000	-1.784407000
6	3.797835000	-2.274607000	0.333594000
6	4.059912000	-2.658668000	-2.407699000
1	1.982290000	-3.226863000	-2.355228000
6	5.026067000	-2.052685000	-0.286909000
1	3.710896000	-2.130984000	1.404723000
6	5.159404000	-2.237934000	-1.659436000
1	4.156324000	-2.807232000	-3.479518000
1	5.881497000	-1.740461000	0.306649000
1	6.115477000	-2.062485000	-2.144876000
6	1.229059000	-2.791369000	1.728329000
1	0.189970000	-2.969683000	2.019143000
1	1.844110000	-3.534813000	2.253691000
1	1.542986000	-1.795054000	2.042961000
1	-0.477993000	-3.113427000	-2.331248000
1	-2.213894000	-2.007515000	-2.817329000

In_TSE4sa

Doordinates (Angstroms)			
	X	Y	Z
25	0.297210000	0.074629000	-0.913277000
7	1.453396000	0.489431000	1.005935000
6	-0.541722000	-1.563000000	1.893352000
1	-1.074305000	-1.466948000	2.846155000
1	-0.572319000	-2.623823000	1.630874000
6	3.579942000	1.286072000	-1.002101000
6	-0.655513000	0.166485000	-2.378288000
8	-1.249135000	0.309212000	-3.378090000
15	2.098590000	0.921794000	-2.040828000
15	-1.349847000	-0.638843000	0.504258000
14	3.221009000	0.567640000	0.699043000
14	1.255492000	-0.972322000	2.020580000
6	4.127772000	1.568649000	2.007264000

1	3.987765000	1.178437000	3.020858000
1	5.205140000	1.596425000	1.803192000
1	3.758965000	2.601706000	1.985797000
6	1.628955000	-0.678675000	3.850076000
1	1.368214000	-1.566676000	4.440290000
1	2.686364000	-0.461850000	4.037664000
1	1.046013000	0.163031000	4.246014000
1	4.498466000	0.890074000	-1.447442000
1	3.664694000	2.371357000	-0.909978000
15	1.048492000	-2.063046000	-1.375953000
6	2.793609000	-2.452981000	-0.876791000
1	2.981479000	-3.532607000	-0.948364000
1	3.478237000	-1.964460000	-1.582758000
14	3.148594000	-1.777977000	0.870994000
6	0.265104000	-3.627530000	-0.769137000
1	0.484598000	-3.788908000	0.290357000
1	-0.820011000	-3.604603000	-0.900453000
1	0.664245000	-4.484465000	-1.323863000
6	1.058103000	-2.473692000	-3.174445000
1	1.531500000	-1.677295000	-3.755033000
1	1.586075000	-3.414699000	-3.365932000
1	0.025627000	-2.573941000	-3.526001000
6	4.448902000	-2.796363000	1.784435000
1	4.113649000	-3.830132000	1.929027000
1	5.391948000	-2.827606000	1.226395000
1	4.657868000	-2.370152000	2.772138000
1	-0.129565000	1.687574000	-0.628214000
1	1.005432000	1.371985000	1.244435000
6	0.274959000	3.192792000	-0.464740000
8	1.526856000	3.273350000	-0.366316000
6	-2.349450000	0.623365000	1.397562000
6	-2.022914000	1.081189000	2.675708000
6	-3.438760000	1.205122000	0.736868000
6	-2.762719000	2.095012000	3.281482000
1	-1.179388000	0.661708000	3.215919000
6	-4.179341000	2.215347000	1.339981000
1	-3.710642000	0.865611000	-0.259466000
6	-3.841666000	2.666030000	2.615699000
1	-2.489416000	2.439172000	4.274977000
1	-5.020491000	2.654759000	0.811817000
1	-4.416963000	3.458133000	3.085893000
6	-2.707475000	-1.781444000	0.000885000
6	-3.523424000	-2.390011000	0.963255000
6	-2.945838000	-2.049385000	-1.348071000

6	-4.543048000	-3.255148000	0.583656000
1	-3.365032000	-2.181133000	2.018236000
6	-3.971760000	-2.912656000	-1.731640000
1	-2.327705000	-1.582739000	-2.106050000
6	-4.768960000	-3.519344000	-0.767148000
1	-5.166452000	-3.721406000	1.341263000
1	-4.144087000	-3.107459000	-2.786213000
1	-5.566407000	-4.194458000	-1.064033000
6	-0.535609000	3.493267000	0.796229000
1	-0.043126000	3.068328000	1.675896000
1	-0.545268000	4.583425000	0.933877000
1	-1.565380000	3.140491000	0.755002000
1	1.980976000	2.078633000	-2.831420000
1	2.689440000	0.113044000	-3.043945000
6	-0.386344000	3.651902000	-1.787492000
1	0.084259000	3.069900000	-2.586348000
6	-1.893243000	3.414686000	-1.851939000
1	-2.440408000	4.094851000	-1.187300000
1	-2.264531000	3.577400000	-2.870475000
1	-2.136268000	2.386851000	-1.564469000
6	-0.040608000	5.126970000	-2.022306000
1	1.043629000	5.272421000	-2.003586000
1	-0.422546000	5.466251000	-2.992902000
1	-0.483614000	5.770280000	-1.251106000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.710935000	-0.249843000	1.065164000
7	-0.197953000	-1.498042000	-0.637344000
6	1.058829000	0.724984000	-2.146303000
1	0.502859000	1.171758000	-2.978890000
1	2.115955000	0.954350000	-2.308048000
6	-0.165938000	-3.519189000	1.498681000
6	0.931511000	0.763305000	2.479614000
8	1.040230000	1.394642000	3.459262000
15	0.630578000	-2.121511000	2.385111000
15	0.548082000	1.443626000	-0.520485000
14	0.125713000	-3.202569000	-0.350098000
14	0.761599000	-1.150790000	-2.060584000
6	-0.992229000	-4.414819000	-1.274980000
1	-0.887440000	-4.333795000	-2.362464000
1	-0.766199000	-5.452413000	-0.997429000

1	-2.046450000	-4.227648000	-1.031264000
6	-0.004057000	-1.619447000	-3.728189000
1	0.647084000	-1.297562000	-4.551787000
1	-0.160943000	-2.698396000	-3.837421000
1	-0.976450000	-1.128087000	-3.865361000
1	0.158107000	-4.497810000	1.864998000
1	-1.247856000	-3.439269000	1.660951000
15	2.975418000	-0.548707000	0.764838000
6	3.441882000	-2.212796000	0.100376000
1	4.479468000	-2.190628000	-0.259795000
1	3.412038000	-2.941043000	0.921210000
14	2.256046000	-2.810498000	-1.279660000
6	4.051563000	0.503510000	-0.305541000
1	3.851586000	0.308647000	-1.362981000
1	3.877876000	1.564969000	-0.108677000
1	5.108007000	0.280981000	-0.116605000
6	3.954699000	-0.446090000	2.323333000
1	3.491231000	-1.050163000	3.109252000
1	4.986232000	-0.785283000	2.175898000
1	3.971465000	0.593592000	2.668042000
6	3.172588000	-4.022504000	-2.408493000
1	4.025312000	-3.540858000	-2.902618000
1	3.557301000	-4.880332000	-1.843547000
1	2.509520000	-4.409794000	-3.190799000
1	-1.140301000	-0.948428000	0.129739000
6	-2.443343000	0.234594000	1.596874000
8	-1.386581000	-0.596904000	1.209345000
6	-3.749829000	-0.169325000	0.931429000
6	-4.844377000	0.699315000	0.968053000
6	-3.890799000	-1.392778000	0.278612000
6	-6.047153000	0.358768000	0.360018000
1	-4.740755000	1.665845000	1.456150000
6	-5.093983000	-1.737883000	-0.335654000
1	-3.046074000	-2.072977000	0.238058000
6	-6.176558000	-0.864271000	-0.298352000
1	-6.882557000	1.053264000	0.389731000
1	-5.182818000	-2.693267000	-0.846234000
1	-7.113316000	-1.129960000	-0.780220000
6	-2.567613000	0.164947000	3.120214000
1	-2.791500000	-0.862622000	3.429029000
1	-1.626158000	0.475376000	3.584022000
1	-3.365941000	0.819876000	3.486882000
1	-0.077732000	-2.045654000	3.602928000
1	1.790324000	-2.751409000	2.896722000

1	-2.234341000	1.277656000	1.317655000
6	-1.127567000	2.095119000	-0.929662000
6	-1.535862000	3.371703000	-0.529886000
6	-2.041504000	1.280450000	-1.608883000
6	-2.820375000	3.827676000	-0.818104000
1	-0.849961000	4.021294000	0.005918000
6	-3.320378000	1.739676000	-1.904004000
1	-1.772854000	0.265623000	-1.886236000
6	-3.713483000	3.016275000	-1.512133000
1	-3.118816000	4.823553000	-0.502382000
1	-4.018505000	1.085954000	-2.417914000
1	-4.716011000	3.370249000	-1.734396000
6	1.518936000	3.005460000	-0.439121000
6	1.780955000	3.743370000	-1.600729000
6	2.001342000	3.483497000	0.781850000
6	2.515778000	4.922123000	-1.544053000
1	1.402830000	3.396870000	-2.558394000
6	2.734480000	4.668312000	0.840992000
1	1.807378000	2.933107000	1.695229000
6	2.997228000	5.386788000	-0.320975000
1	2.711975000	5.479306000	-2.455655000
1	3.102246000	5.025618000	1.798587000
1	3.570641000	6.308212000	-0.275531000

In_TSE5ra

Doordinates (Angstroms)			
	X	Y	Z
25	0.222687000	-0.268591000	-1.014198000
7	1.466490000	0.351646000	0.819433000
6	-0.852108000	-1.012379000	2.092098000
1	-1.322374000	-0.584144000	2.985338000
1	-1.112759000	-2.074293000	2.080071000
6	3.565770000	0.487640000	-1.251332000
6	-0.756777000	-0.298339000	-2.470874000
8	-1.357871000	-0.303503000	-3.474171000
15	2.117972000	-0.022930000	-2.271223000
15	-1.494455000	-0.260091000	0.532690000
14	3.172317000	0.015685000	0.544631000
14	1.036138000	-0.764461000	2.100568000
6	4.380317000	0.991414000	1.621645000
1	4.246369000	2.069157000	1.460444000
1	4.241827000	0.797985000	2.690990000
1	5.420500000	0.745669000	1.371547000

6	1.478735000	-0.233289000	3.864125000
1	1.109336000	-0.969647000	4.590133000
1	2.559542000	-0.137286000	4.017322000
1	1.025548000	0.734436000	4.116670000
1	4.506473000	0.080377000	-1.634452000
1	3.645566000	1.580919000	-1.282627000
15	0.483315000	-2.558402000	-1.009882000
6	2.120811000	-3.144072000	-0.377267000
1	2.078241000	-4.224756000	-0.185276000
1	2.873087000	-2.997413000	-1.163490000
14	2.687407000	-2.195543000	1.186696000
6	-0.603838000	-3.750303000	-0.108268000
1	-0.428069000	-3.688694000	0.969579000
1	-1.660424000	-3.544664000	-0.300019000
1	-0.383826000	-4.776736000	-0.423605000
6	0.408721000	-3.327562000	-2.683514000
1	1.068646000	-2.796165000	-3.375620000
1	0.699629000	-4.383768000	-2.655790000
1	-0.611600000	-3.253656000	-3.074697000
6	3.817998000	-3.307880000	2.219674000
1	3.293846000	-4.216476000	2.540762000
1	4.701466000	-3.618919000	1.648899000
1	4.167007000	-2.788379000	3.119410000
1	1.010446000	1.378979000	0.207703000
6	-0.039417000	3.045649000	-0.990745000
8	0.637392000	1.824995000	-0.847755000
6	-0.904976000	3.015075000	-2.243151000
1	-1.369406000	3.991879000	-2.428051000
1	-0.316026000	2.732164000	-3.122794000
1	-1.702742000	2.275224000	-2.126711000
6	0.973268000	4.212262000	-0.978148000
1	0.382759000	5.140255000	-1.002773000
6	1.908463000	4.203317000	-2.188159000
1	2.674400000	4.983636000	-2.102318000
1	2.418737000	3.236747000	-2.268622000
1	1.368749000	4.374863000	-3.126005000
6	1.770363000	4.195559000	0.327225000
1	2.419324000	5.075475000	0.412335000
1	1.102344000	4.179646000	1.197442000
1	2.402175000	3.301318000	0.381907000
1	-0.704688000	3.213487000	-0.133112000
1	2.088691000	0.934740000	-3.305565000
1	2.686250000	-1.077045000	-3.027262000
6	-2.068987000	1.392515000	1.098141000

6	-1.411113000	2.085454000	2.118550000
6	-3.118564000	2.027636000	0.424988000
6	-1.790590000	3.381920000	2.457254000
1	-0.580435000	1.629816000	2.647288000
6	-3.496214000	3.324125000	0.759769000
1	-3.644965000	1.507922000	-0.371349000
6	-2.831780000	4.006744000	1.776694000
1	-1.265718000	3.904462000	3.252062000
1	-4.312074000	3.801946000	0.225027000
1	-3.123932000	5.020108000	2.036439000
6	-3.109881000	-1.107033000	0.289145000
6	-4.028181000	-1.206820000	1.342738000
6	-3.440872000	-1.667430000	-0.945932000
6	-5.243621000	-1.857143000	1.164709000
1	-3.794902000	-0.762456000	2.307015000
6	-4.660228000	-2.319737000	-1.127108000
1	-2.743792000	-1.596189000	-1.773168000
6	-5.561559000	-2.417129000	-0.072772000
1	-5.947647000	-1.924290000	1.989228000
1	-4.901290000	-2.750285000	-2.094736000
1	-6.512031000	-2.924016000	-0.212443000

In_TSE5s

Doordinates (Angstroms)			
	X	Y	Z
25	0.678704000	-0.187694000	1.071731000
7	-0.162244000	-1.552802000	-0.574919000
6	0.976733000	0.684973000	-2.193530000
1	0.377509000	1.084880000	-3.020007000
1	2.020000000	0.931770000	-2.414357000
6	0.033043000	-3.541096000	1.602073000
6	0.873003000	0.906198000	2.430599000
8	0.961336000	1.604609000	3.364694000
15	0.607241000	-2.009046000	2.454895000
15	0.537418000	1.455462000	-0.574434000
14	0.225497000	-3.237867000	-0.262373000
14	0.750189000	-1.197114000	-2.030677000
6	-0.884872000	-4.507166000	-1.114733000
1	-0.881360000	-4.402186000	-2.205142000
1	-0.564891000	-5.530275000	-0.878543000
1	-1.923893000	-4.403192000	-0.774881000
6	-0.029567000	-1.753519000	-3.664127000
1	0.577576000	-1.412732000	-4.513263000
1	-0.123246000	-2.842219000	-3.745222000

1	-1.034079000	-1.326034000	-3.784320000
1	0.542405000	-4.437098000	1.970613000
1	-1.038154000	-3.673762000	1.803179000
15	2.951290000	-0.489888000	0.808302000
6	3.464892000	-2.147093000	0.163143000
1	4.510197000	-2.107308000	-0.171960000
1	3.427714000	-2.872748000	0.986632000
14	2.319619000	-2.781413000	-1.236121000
6	3.991981000	0.572905000	-0.284795000
1	3.757211000	0.391791000	-1.337730000
1	3.826064000	1.631959000	-0.071811000
1	5.053596000	0.347757000	-0.131505000
6	3.940877000	-0.332792000	2.356288000
1	3.520437000	-0.954420000	3.152339000
1	4.987082000	-0.617884000	2.198542000
1	3.908211000	0.708314000	2.695579000
6	3.286999000	-3.968514000	-2.348503000
1	4.123595000	-3.459366000	-2.842596000
1	3.700733000	-4.805297000	-1.772755000
1	2.643154000	-4.387087000	-3.130652000
1	-1.080809000	-0.905827000	0.049799000
6	-2.451537000	-0.607043000	1.742276000
8	-1.425808000	-0.149423000	0.908315000
6	-3.750665000	-0.597616000	0.938416000
6	-4.822247000	0.249442000	1.212982000
6	-3.844350000	-1.447343000	-0.169924000
6	-5.957854000	0.251446000	0.401752000
1	-4.778171000	0.930030000	2.057514000
6	-4.972382000	-1.451318000	-0.981291000
1	-3.006720000	-2.098015000	-0.412977000
6	-6.038882000	-0.598267000	-0.695840000
1	-6.779711000	0.924275000	0.631818000
1	-5.021625000	-2.121041000	-1.835868000
1	-6.924270000	-0.597999000	-1.325781000
6	-2.486471000	0.226170000	3.014769000
1	-3.289860000	-0.091582000	3.689569000
1	-1.533908000	0.122869000	3.541537000
1	-2.617623000	1.286415000	2.774616000
1	-0.179135000	-1.996886000	3.630827000
1	1.791433000	-2.473574000	3.071522000
1	-2.268442000	-1.660404000	2.036807000
6	1.490369000	3.030256000	-0.581797000
6	2.043064000	3.533230000	0.598765000
6	1.656624000	3.757237000	-1.766781000

6	2.750448000	4.735006000	0.596033000
1	1.923454000	2.987613000	1.528226000
6	2.368040000	4.951821000	-1.772699000
1	1.222632000	3.388982000	-2.692306000
6	2.917575000	5.443471000	-0.589540000
1	3.171898000	5.113756000	1.522738000
1	2.491866000	5.501359000	-2.701492000
1	3.470791000	6.378266000	-0.593551000
6	-1.167534000	2.084678000	-0.840501000
6	-2.072946000	1.420513000	-1.670956000
6	-1.614225000	3.180226000	-0.097173000
6	-3.394865000	1.844631000	-1.762767000
1	-1.764819000	0.542565000	-2.231192000
6	-2.936383000	3.605134000	-0.187347000
1	-0.929251000	3.706423000	0.562746000
6	-3.831160000	2.937620000	-1.020066000
1	-4.090284000	1.301064000	-2.394967000
1	-3.267018000	4.459041000	0.397487000
1	-4.866171000	3.260732000	-1.083528000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.236135000	-0.294777000	-1.044375000
7	1.473900000	0.452724000	0.729854000
6	-0.710055000	-1.029716000	2.122477000
1	-1.191984000	-0.603002000	3.009988000
1	-0.884793000	-2.108598000	2.168140000
6	3.537762000	0.658918000	-1.376437000
6	-0.809436000	-0.442513000	-2.446557000
8	-1.486150000	-0.510568000	-3.398203000
15	2.086025000	0.055295000	-2.344482000
15	-1.446001000	-0.418016000	0.546554000
14	3.197323000	0.253702000	0.447599000
14	1.154156000	-0.638725000	2.067611000
6	4.323599000	1.376047000	1.466052000
1	4.099646000	2.430445000	1.258150000
1	4.202146000	1.220407000	2.543512000
1	5.379972000	1.204323000	1.222895000
6	1.595847000	0.010662000	3.790639000
1	1.259235000	-0.689892000	4.565899000
1	2.673079000	0.157392000	3.926947000
1	1.108242000	0.976398000	3.979795000

1	4.483835000	0.263360000	-1.759723000
1	3.585576000	1.751821000	-1.466283000
15	0.715106000	-2.551785000	-0.997274000
6	2.405888000	-2.982150000	-0.381864000
1	2.467390000	-4.060428000	-0.182063000
1	3.132257000	-2.769598000	-1.177291000
14	2.898890000	-1.965723000	1.166021000
6	-0.251425000	-3.792369000	-0.027107000
1	-0.055094000	-3.677923000	1.042738000
1	-1.325356000	-3.677874000	-0.196065000
1	0.041110000	-4.808960000	-0.314594000
6	0.654337000	-3.388071000	-2.639575000
1	1.227429000	-2.827155000	-3.383814000
1	1.047341000	-4.409778000	-2.587540000
1	-0.384823000	-3.429426000	-2.983603000
6	4.122116000	-2.963614000	2.209363000
1	3.663611000	-3.888571000	2.580288000
1	5.008427000	-3.244014000	1.627170000
1	4.461001000	-2.388434000	3.078689000
1	0.815815000	1.384744000	0.182054000
6	0.451936000	2.908640000	-1.414291000
8	0.064570000	1.784204000	-0.681910000
6	-0.377774000	2.981863000	-2.692273000
1	-1.433225000	3.150365000	-2.446928000
1	-0.040640000	3.780741000	-3.361642000
1	-0.307874000	2.034953000	-3.234453000
6	0.304080000	4.168050000	-0.534920000
1	-0.745347000	4.192902000	-0.210839000
6	0.619125000	5.453618000	-1.305484000
1	0.620781000	6.319333000	-0.632663000
1	1.611697000	5.399100000	-1.773716000
1	-0.113027000	5.654224000	-2.094246000
6	1.184137000	4.077965000	0.713780000
1	1.035685000	4.953033000	1.358001000
1	0.961828000	3.186225000	1.306153000
1	2.248546000	4.046715000	0.439390000
1	1.523429000	2.842626000	-1.705197000
1	2.042458000	0.957901000	-3.431280000
1	2.668902000	-1.016223000	-3.060027000
6	-2.147123000	1.223352000	0.975839000
6	-3.071008000	1.782067000	0.085968000
6	-1.742877000	1.969588000	2.081816000
6	-3.591408000	3.050397000	0.307404000
1	-3.377482000	1.223838000	-0.795332000

6	-2.259322000	3.246420000	2.302909000
1	-1.010024000	1.574173000	2.778907000
6	-3.187298000	3.788358000	1.420330000
1	-4.310693000	3.466688000	-0.392278000
1	-1.930512000	3.816158000	3.167519000
1	-3.592542000	4.781233000	1.593138000
6	-2.994617000	-1.400650000	0.395330000
6	-3.885579000	-1.487667000	1.472715000
6	-3.309952000	-2.060707000	-0.793675000
6	-5.060209000	-2.222360000	1.363590000
1	-3.664244000	-0.965482000	2.400217000
6	-4.487892000	-2.799167000	-0.905199000
1	-2.635440000	-1.996030000	-1.640598000
6	-5.362835000	-2.882415000	0.172483000
1	-5.744709000	-2.277071000	2.205328000
1	-4.718971000	-3.305438000	-1.838021000
1	-6.282934000	-3.453164000	0.085511000

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Doordinates (Angstroms)			
	X	Y	Z
25	-0.396062000	-0.599419000	1.004046000
7	-1.574603000	0.344791000	-0.743186000
6	0.676215000	-1.016796000	-2.169660000
1	1.173150000	-0.494747000	-2.997427000
1	0.862721000	-2.085005000	-2.320101000
6	-3.695057000	0.276197000	1.345214000
6	0.562533000	-0.966110000	2.429316000
8	1.146291000	-1.174107000	3.419990000
15	-2.335802000	-0.571891000	2.241363000
15	1.373043000	-0.518077000	-0.518187000
14	-3.329505000	0.069882000	-0.486251000
14	-1.179480000	-0.658237000	-2.175288000
6	-4.431692000	1.244292000	-1.465438000
1	-4.287161000	1.160954000	-2.547667000
1	-5.488406000	1.038683000	-1.253584000
1	-4.239054000	2.286606000	-1.181815000
6	-1.584877000	0.176100000	-3.821791000
1	-1.264447000	-0.463291000	-4.654738000
1	-2.653279000	0.376637000	-3.955723000
1	-1.053206000	1.131543000	-3.918526000
1	-4.691574000	-0.062156000	1.646696000
1	-3.582019000	1.335171000	1.608761000

15	-0.813290000	-2.868528000	0.663392000
6	-2.465653000	-3.284445000	-0.079874000
1	-2.466141000	-4.315274000	-0.457072000
1	-3.229266000	-3.241193000	0.706564000
14	-2.937378000	-2.044142000	-1.440660000
6	0.209112000	-4.084972000	-0.290155000
1	0.295814000	-3.818455000	-1.346794000
1	1.211514000	-4.156979000	0.141087000
1	-0.249622000	-5.078247000	-0.227115000
6	-0.844517000	-3.837794000	2.235762000
1	-1.431626000	-3.333838000	3.007188000
1	-1.260465000	-4.838797000	2.074014000
1	0.178024000	-3.940282000	2.614231000
6	-4.142933000	-2.794961000	-2.684191000
1	-3.701267000	-3.658229000	-3.195781000
1	-5.057623000	-3.136573000	-2.185708000
1	-4.431748000	-2.063899000	-3.447486000
1	-0.368754000	1.124303000	1.502337000
1	-1.209593000	1.294401000	-0.667956000
6	-0.755769000	2.308500000	2.318245000
8	-1.942094000	2.214430000	2.749843000
6	2.266276000	1.037123000	-1.022739000
6	1.367423000	2.135548000	-1.598545000
6	3.128781000	1.618771000	0.112373000
6	2.230122000	3.195609000	-2.318333000
1	0.632274000	1.734009000	-2.305499000
6	3.604293000	3.055441000	-0.199004000
1	2.552623000	1.611426000	1.046106000
6	3.638941000	3.322434000	-1.704458000
1	2.321979000	2.940372000	-3.381561000
1	2.923040000	3.776421000	0.261878000
1	4.323880000	2.607849000	-2.180689000
6	2.801374000	-1.716422000	-0.358702000
6	3.916294000	-1.578806000	-1.405962000
6	3.392775000	-1.771724000	1.071074000
6	4.819429000	-2.827713000	-1.395046000
1	3.499342000	-1.439144000	-2.410132000
6	4.839272000	-2.296556000	1.077381000
1	3.357678000	-0.791689000	1.556954000
6	5.017468000	-3.393873000	0.027631000
1	4.384841000	-3.600218000	-2.041275000
1	5.540378000	-1.477935000	0.865797000
1	4.280935000	-4.185446000	0.222738000
6	-0.558530000	3.380867000	1.247870000

6	0.532295000	4.249458000	1.228724000
6	-1.576889000	3.576412000	0.308829000
6	0.617593000	5.268691000	0.278960000
1	1.323539000	4.144082000	1.964482000
6	-1.479539000	4.563795000	-0.663765000
1	-2.464338000	2.954642000	0.374855000
6	-0.377310000	5.419756000	-0.680882000
1	1.470128000	5.942829000	0.288401000
1	-2.272593000	4.684535000	-1.397268000
1	-0.303528000	6.203882000	-1.429083000
6	0.366496000	2.179536000	3.349348000
1	0.377965000	3.079313000	3.979431000
1	0.148978000	1.321876000	3.988527000
1	1.355547000	2.039288000	2.903117000
1	2.932049000	0.715780000	-1.833999000
1	0.803638000	2.595844000	-0.783261000
1	1.714951000	4.160687000	-2.268544000
1	4.048173000	4.318624000	-1.906523000
1	4.590631000	3.226109000	0.246588000
1	3.998025000	0.970494000	0.272448000
1	2.766369000	-2.428329000	1.683926000
1	5.090473000	-2.667136000	2.077266000
1	6.003166000	-3.863624000	0.116001000
1	5.789691000	-2.566983000	-1.834081000
1	4.518785000	-0.688368000	-1.190615000
1	2.325977000	-2.681566000	-0.555008000
1	-2.383394000	-0.042345000	3.539239000
1	-2.970737000	-1.805040000	2.528058000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.389948000	-0.186319000	-0.992082000
7	1.618657000	0.335093000	0.845682000
6	-0.852554000	-0.878102000	2.087072000
1	-1.323790000	-0.367838000	2.936627000
1	-1.141264000	-1.931961000	2.165595000
6	3.936516000	-0.134045000	-1.110599000
6	-0.529486000	-0.176948000	-2.490760000
8	-1.084315000	-0.084447000	-3.515949000
15	2.409998000	-0.227421000	-2.147512000
15	-1.455910000	-0.210030000	0.456784000
14	3.353238000	-0.110609000	0.679061000
14	1.028633000	-0.718149000	2.170061000

6	4.475651000	0.986003000	1.711546000
1	4.212050000	0.999209000	2.774188000
1	5.521672000	0.667544000	1.626516000
1	4.406345000	2.011156000	1.327093000
6	1.465451000	-0.060329000	3.887469000
1	1.032235000	-0.703960000	4.663893000
1	2.545271000	-0.012602000	4.066124000
1	1.059484000	0.949361000	4.033956000
1	4.604323000	-0.978941000	-1.310819000
1	4.457594000	0.795460000	-1.344323000
15	0.602325000	-2.530162000	-0.924206000
6	2.196754000	-3.157196000	-0.200142000
1	2.138453000	-4.241270000	-0.037978000
1	3.002659000	-2.997861000	-0.928245000
14	2.654189000	-2.232501000	1.411129000
6	-0.510247000	-3.780444000	-0.122509000
1	-0.641710000	-3.599035000	0.947390000
1	-1.489703000	-3.786329000	-0.607636000
1	-0.077477000	-4.779722000	-0.246195000
6	0.565732000	-3.318804000	-2.595255000
1	1.243042000	-2.824976000	-3.294986000
1	0.824813000	-4.382464000	-2.542179000
1	-0.447932000	-3.226005000	-3.000650000
6	3.599829000	-3.343697000	2.608702000
1	2.997237000	-4.209282000	2.908847000
1	4.520145000	-3.723718000	2.149999000
1	3.880229000	-2.799287000	3.517501000
1	0.478038000	1.588981000	-1.145919000
1	1.408099000	1.331269000	0.832371000
6	1.524165000	2.780255000	-1.441486000
8	2.682863000	2.347480000	-1.202573000
6	-2.375306000	1.293848000	1.062198000
6	-1.472587000	2.316615000	1.752725000
6	-3.194848000	1.969790000	-0.054855000
6	-2.307606000	3.405733000	2.465680000
1	-0.806550000	1.835489000	2.479006000
6	-3.674306000	3.386056000	0.340709000
1	-2.595732000	2.017251000	-0.972898000
6	-3.713730000	3.561079000	1.858950000
1	-2.399371000	3.170901000	3.532970000
1	-3.001729000	4.142114000	-0.078254000
1	-4.394049000	2.814703000	2.290807000
6	-2.886040000	-1.370115000	0.118576000
6	-4.066781000	-1.307752000	1.098424000

6	-3.377637000	-1.317063000	-1.345292000
6	-4.954847000	-2.559171000	0.939375000
1	-3.714094000	-1.239552000	2.134144000
6	-4.799264000	-1.888509000	-1.494067000
1	-3.351213000	-0.296928000	-1.740024000
6	-5.021409000	-3.048609000	-0.523146000
1	-4.572492000	-3.364509000	1.578417000
1	-5.542018000	-1.105410000	-1.290508000
1	-4.247512000	-3.808339000	-0.700595000
6	1.106166000	3.007101000	-2.896072000
1	1.560754000	3.946328000	-3.242150000
1	1.475027000	2.206382000	-3.537358000
1	0.023692000	3.076489000	-3.020872000
1	-3.070405000	0.909685000	1.819262000
1	-0.831076000	2.763139000	0.994207000
1	-1.775417000	4.362916000	2.402826000
1	-4.127675000	4.541022000	2.121472000
1	-4.661618000	3.577330000	-0.093759000
1	-4.064531000	1.345086000	-0.287239000
1	-2.681891000	-1.893588000	-1.965774000
1	-4.963369000	-2.206883000	-2.529483000
1	-5.981758000	-3.540105000	-0.713742000
1	-5.963303000	-2.327564000	1.302110000
1	-4.662355000	-0.406747000	0.911231000
1	-2.434814000	-2.351110000	0.275525000
6	0.999006000	3.847798000	-0.452999000
1	0.962896000	3.372757000	0.534787000
6	-0.373882000	4.412484000	-0.799314000
1	-0.776356000	4.998886000	0.035144000
1	-0.318898000	5.078166000	-1.668968000
1	-1.082815000	3.613979000	-1.034130000
6	2.037688000	4.973507000	-0.359646000
1	1.721761000	5.727161000	0.371837000
1	3.008767000	4.573169000	-0.058150000
1	2.163507000	5.480151000	-1.324756000
1	2.705205000	0.618839000	-3.227175000
1	2.692337000	-1.425948000	-2.849849000

In_TSF4s

Doordinates (Angstroms)			
X Y Z			
25	-0.285564000	0.115746000	-0.728978000
7	-0.982156000	0.820482000	1.327265000

6	1.974750000	1.364062000	1.457166000
1	2.545181000	1.118388000	2.361788000
1	2.540125000	2.145073000	0.938260000
6	-3.553963000	1.007350000	-0.098823000
6	0.097683000	-0.848251000	-2.141042000
8	0.272750000	-1.560825000	-3.053635000
15	-2.418733000	0.502277000	-1.454842000
15	1.793607000	-0.094344000	0.319701000
14	-2.468002000	1.811338000	1.206233000
14	0.245598000	1.990976000	1.887839000
6	-3.443770000	1.898801000	2.814073000
1	-2.916587000	2.425640000	3.616246000
1	-4.405250000	2.403799000	2.658567000
1	-3.654342000	0.879838000	3.162060000
6	0.206213000	2.314578000	3.749605000
1	1.030075000	2.980962000	4.036134000
1	-0.725509000	2.779902000	4.088298000
1	0.329078000	1.377587000	4.307938000
1	-4.393480000	1.613522000	-0.451918000
1	-3.955341000	0.099710000	0.362691000
15	0.260493000	2.127862000	-1.748082000
6	-0.717115000	3.610348000	-1.191788000
1	-0.220516000	4.536877000	-1.507420000
1	-1.693157000	3.597408000	-1.692741000
14	-1.017188000	3.585653000	0.689522000
6	1.920090000	2.948267000	-1.843766000
1	2.322749000	3.177866000	-0.853915000
1	2.629357000	2.307897000	-2.375783000
1	1.835852000	3.888152000	-2.400980000
6	-0.046511000	2.116185000	-3.571177000
1	-1.047571000	1.747688000	-3.808900000
1	0.073452000	3.115689000	-4.004837000
1	0.673565000	1.438891000	-4.042944000
6	-1.274296000	5.330293000	1.365436000
1	-0.391512000	5.955873000	1.187748000
1	-2.129484000	5.819865000	0.884630000
1	-1.461847000	5.314191000	2.444998000
1	-0.901769000	-1.371965000	-0.115294000
1	-1.137303000	-0.103957000	1.750801000
6	-1.960181000	-2.334456000	0.734416000
8	-2.269987000	-1.691820000	1.766133000
6	2.213675000	-1.473017000	1.504800000
6	1.244469000	-1.524353000	2.695494000
6	2.343717000	-2.821480000	0.772678000

6	1.571126000	-2.680420000	3.679351000
1	1.290675000	-0.572208000	3.235253000
6	2.422708000	-4.032599000	1.733585000
1	1.505991000	-2.941049000	0.077468000
6	2.687156000	-3.603883000	3.176796000
1	1.845999000	-2.275258000	4.659727000
1	1.481171000	-4.594546000	1.708570000
1	3.658238000	-3.094656000	3.241105000
6	3.369672000	0.044564000	-0.677577000
6	4.684070000	-0.151213000	0.090838000
6	3.350687000	-0.807863000	-1.967185000
6	5.871876000	0.371497000	-0.743471000
1	4.657641000	0.368801000	1.055391000
6	4.768852000	-1.066027000	-2.507270000
1	2.840873000	-1.762233000	-1.806588000
6	5.670307000	0.143224000	-2.256570000
1	6.013623000	1.441983000	-0.551207000
1	5.205402000	-1.946101000	-2.016264000
1	5.203378000	1.028219000	-2.710512000
1	3.199495000	-1.213468000	1.910847000
1	0.216833000	-1.616765000	2.336026000
1	0.667475000	-3.281826000	3.839205000
1	2.756462000	-4.484110000	3.826412000
1	3.200178000	-4.726704000	1.395527000
1	3.249263000	-2.794246000	0.156872000
1	2.760252000	-0.279546000	-2.724096000
1	4.718714000	-1.301983000	-3.576034000
1	6.639061000	0.018852000	-2.752838000
1	6.788336000	-0.128463000	-0.408348000
1	4.832107000	-1.214411000	0.313045000
1	3.362561000	1.094997000	-0.980550000
1	-3.169994000	-0.457333000	-2.160844000
1	-2.675000000	1.565950000	-2.354731000
6	-3.003165000	-2.537720000	-0.354859000
6	-2.674342000	-2.999970000	-1.632792000
6	-4.345436000	-2.336270000	-0.036353000
6	-3.665691000	-3.223815000	-2.580774000
1	-1.631935000	-3.137098000	-1.902630000
6	-5.342513000	-2.553666000	-0.985970000
1	-4.594484000	-2.008300000	0.968731000
6	-5.005186000	-2.994711000	-2.262143000
1	-3.392691000	-3.565972000	-3.575224000
1	-6.383858000	-2.384172000	-0.725788000
1	-5.779490000	-3.163416000	-3.005360000

6	-1.044125000	-3.546393000	0.867125000
1	-0.302447000	-3.377543000	1.643043000
1	-1.672818000	-4.392345000	1.176935000
1	-0.545442000	-3.816630000	-0.065757000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.389955000	-0.186348000	-0.992097000
7	1.618659000	0.335225000	0.845591000
6	-0.852459000	-0.877995000	2.087115000
1	-1.323688000	-0.367689000	2.936648000
1	-1.141141000	-1.931857000	2.165721000
6	3.936533000	-0.133955000	-1.110704000
6	-0.529513000	-0.177072000	-2.490755000
8	-1.084373000	-0.084585000	-3.515940000
15	2.409986000	-0.227398000	-2.147577000
15	-1.455872000	-0.210047000	0.456795000
14	3.353262000	-0.110364000	0.678957000
14	1.028729000	-0.717966000	2.170047000
6	4.475534000	0.986422000	1.711397000
1	4.211639000	0.999881000	2.773946000
1	5.521550000	0.667917000	1.626708000
1	4.406344000	2.011489000	1.326698000
6	1.465598000	-0.060083000	3.887416000
1	1.032372000	-0.703660000	4.663876000
1	2.545424000	-0.012411000	4.066038000
1	1.059688000	0.949633000	4.033875000
1	4.604316000	-0.978889000	-1.310855000
1	4.457629000	0.795519000	-1.344530000
15	0.602454000	-2.530180000	-0.924075000
6	2.196946000	-3.157077000	-0.200030000
1	2.138711000	-4.241145000	-0.037801000
1	3.002814000	-2.997744000	-0.928175000
14	2.654374000	-2.232261000	1.411174000
6	-0.510021000	-3.780482000	-0.122269000
1	-0.641530000	-3.598981000	0.947608000
1	-1.489464000	-3.786509000	-0.607421000
1	-0.077157000	-4.779732000	-0.245844000
6	0.565876000	-3.318924000	-2.595071000
1	1.243306000	-2.825229000	-3.294777000
1	0.824827000	-4.382608000	-2.541904000
1	-0.447742000	-3.226023000	-3.000553000

6	3.600186000	-3.343315000	2.608745000
1	2.997725000	-4.208969000	2.908945000
1	4.520526000	-3.723227000	2.150002000
1	3.880572000	-2.798845000	3.517513000
1	0.477896000	1.588941000	-1.146012000
1	1.408093000	1.331412000	0.832128000
6	1.524060000	2.780267000	-1.441467000
8	2.682738000	2.347483000	-1.202431000
6	-2.375449000	1.293757000	1.062123000
6	-1.472938000	2.316652000	1.752734000
6	-3.194995000	1.969580000	-0.055005000
6	-2.308208000	3.405611000	2.465638000
1	-0.806875000	1.835624000	2.479058000
6	-3.674571000	3.385831000	0.340452000
1	-2.595855000	2.017030000	-0.973033000
6	-3.714252000	3.560856000	1.858685000
1	-2.400131000	3.170669000	3.532890000
1	-3.001954000	4.141911000	-0.078404000
1	-4.394588000	2.814430000	2.290427000
6	-2.885896000	-1.370263000	0.118608000
6	-4.066624000	-1.308031000	1.098478000
6	-3.377525000	-1.317259000	-1.345254000
6	-4.954543000	-2.559550000	0.939434000
1	-3.713923000	-1.239801000	2.134190000
6	-4.799154000	-1.888699000	-1.493971000
1	-3.351092000	-0.297148000	-1.740038000
6	-5.021213000	-3.048871000	-0.523121000
1	-4.571991000	-3.364885000	1.578355000
1	-5.541899000	-1.105625000	-1.290308000
1	-4.247313000	-3.808565000	-0.700690000
1	-3.070561000	0.909525000	1.819138000
1	-0.831438000	2.763303000	0.994284000
1	-1.776115000	4.362857000	2.402964000
1	-4.128312000	4.540770000	2.121139000
1	-4.661815000	3.577060000	-0.094189000
1	-4.064628000	1.344801000	-0.287375000
1	-2.681808000	-1.893822000	-1.965730000
1	-4.963324000	-2.206997000	-2.529395000
1	-5.981564000	-3.540372000	-0.713681000
1	-5.962981000	-2.328119000	1.302321000
1	-4.662305000	-0.407094000	0.911306000
1	-2.434571000	-2.351210000	0.275544000
6	1.106150000	3.007100000	-2.896082000
1	1.561169000	3.946040000	-3.242303000

1	1.474531000	2.206136000	-3.537264000
1	0.023737000	3.077006000	-3.020853000
6	0.998803000	3.847766000	-0.452990000
1	0.962603000	3.372706000	0.534788000
6	2.037438000	4.973530000	-0.359471000
1	2.163510000	5.480031000	-1.324626000
1	1.721180000	5.727255000	0.371845000
1	3.008523000	4.573366000	-0.057597000
6	-0.374071000	4.412438000	-0.799393000
1	-1.083003000	3.613934000	-1.034085000
1	-0.776502000	4.998952000	0.034976000
1	-0.319106000	5.077994000	-1.669121000
1	2.705106000	0.619004000	-3.227181000
1	2.692380000	-1.425863000	-2.850023000

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Doordinates (Angstroms)			
	X	Y	Z
25	0.853666000	-0.246128000	1.073062000
7	0.215889000	-1.631335000	-0.642495000
6	0.870090000	0.857521000	-2.120583000
1	0.253349000	1.199716000	-2.957759000
1	1.858197000	1.307776000	-2.263018000
6	0.794566000	-3.656923000	1.407832000
6	0.836848000	0.782440000	2.498369000
8	0.784734000	1.414953000	3.480538000
15	1.251705000	-2.132948000	2.329792000
15	0.228146000	1.402733000	-0.474711000
14	0.928948000	-3.222551000	-0.436100000
14	0.989358000	-1.033602000	-2.090078000
6	0.061097000	-4.629395000	-1.356002000
1	0.039130000	-4.474976000	-2.440419000
1	0.555549000	-5.591288000	-1.168319000
1	-0.978201000	-4.721160000	-1.012979000
6	0.259806000	-1.629271000	-3.734132000
1	0.742125000	-1.119608000	-4.578743000
1	0.380064000	-2.706926000	-3.892450000
1	-0.814555000	-1.405518000	-3.781958000
1	1.362433000	-4.535742000	1.727533000
1	-0.267502000	-3.855918000	1.595870000
15	3.121595000	-0.024848000	0.749716000
6	3.917645000	-1.499028000	-0.043919000
1	4.907855000	-1.223113000	-0.431450000
1	4.094200000	-2.250834000	0.736963000

14	2.866335000	-2.315672000	-1.423978000
6	3.970638000	1.321044000	-0.190488000
1	3.662376000	1.338096000	-1.239028000
1	3.745745000	2.292327000	0.260626000
1	5.056696000	1.176341000	-0.158120000
6	4.090594000	0.153301000	2.310844000
1	3.798027000	-0.604777000	3.042059000
1	5.167962000	0.070241000	2.127565000
1	3.882749000	1.135214000	2.749918000
6	4.033465000	-3.239316000	-2.595242000
1	4.747548000	-2.552728000	-3.066770000
1	4.612075000	-4.002171000	-2.060002000
1	3.477159000	-3.742594000	-3.394492000
1	-0.831327000	-1.369401000	0.199581000
6	-2.366497000	-0.787788000	1.773987000
8	-1.114263000	-1.139312000	1.262076000
6	-3.525597000	-1.297944000	0.925124000
6	-4.838678000	-0.999264000	1.309895000
6	-3.332463000	-2.015411000	-0.256904000
6	-5.923762000	-1.395811000	0.536925000
1	-5.015584000	-0.433852000	2.221860000
6	-4.419759000	-2.414271000	-1.035261000
1	-2.330169000	-2.256792000	-0.595404000
6	-5.718083000	-2.106169000	-0.645014000
1	-6.932268000	-1.144883000	0.853874000
1	-4.243026000	-2.965241000	-1.955083000
1	-6.563148000	-2.413046000	-1.254635000
6	-2.436045000	-1.297640000	3.215033000
1	-2.361331000	-2.390657000	3.233573000
1	-1.598652000	-0.876571000	3.781279000
1	-3.366195000	-1.003148000	3.712030000
1	0.578136000	-2.274564000	3.562363000
1	2.536188000	-2.494758000	2.802328000
1	-2.453933000	0.307730000	1.811542000
6	-1.622231000	1.538824000	-0.732032000
6	-2.279327000	2.477557000	0.294235000
6	-2.108870000	1.862969000	-2.164099000
6	-3.817060000	2.322108000	0.310966000
1	-1.877964000	2.292201000	1.296856000
6	-3.549665000	2.412088000	-2.181734000
1	-1.450092000	2.582583000	-2.658868000
6	-4.370750000	1.826814000	-1.034324000
1	-4.118860000	1.628970000	1.102533000
1	-3.532479000	3.506435000	-2.083158000

1	-5.428009000	2.098194000	-1.129232000
6	0.907565000	3.138383000	-0.381312000
6	0.439025000	4.123566000	-1.461905000
6	0.814680000	3.761706000	1.032403000
6	1.349185000	5.369357000	-1.493134000
1	0.447428000	3.646841000	-2.447526000
6	0.896406000	5.297237000	0.992336000
1	-0.103360000	3.462637000	1.543368000
6	1.869026000	5.757537000	-0.093009000
1	2.199568000	5.184041000	-2.160840000
1	-0.095861000	5.722562000	0.789703000
1	2.844692000	5.286398000	0.089353000
1	-1.960492000	0.522808000	-0.499894000
1	-2.066588000	0.941294000	-2.756816000
1	-4.014234000	2.196503000	-3.150448000
1	-4.326518000	0.731033000	-1.079570000
1	-4.265716000	3.291913000	0.558420000
1	-2.019364000	3.514004000	0.049674000
1	1.969561000	2.960100000	-0.585358000
1	-0.597766000	4.421787000	-1.270033000
1	1.635297000	3.365944000	1.641291000
1	0.790139000	6.205824000	-1.928975000
1	2.035133000	6.838904000	-0.036763000
1	1.199406000	5.675441000	1.975044000

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Doordinates (Angstroms)			

	X	Y	Z

25	0.312950000	-0.343317000	-1.014232000
7	1.587260000	0.272803000	0.776957000
6	-0.837942000	-0.881461000	2.127399000
1	-1.297953000	-0.390363000	2.994177000
1	-1.118336000	-1.938598000	2.185181000
6	3.776292000	-0.127719000	-1.246976000
6	-0.663270000	-0.376773000	-2.476393000
8	-1.248843000	-0.373097000	-3.488676000
15	2.237568000	-0.283013000	-2.264336000
15	-1.453714000	-0.185930000	0.527498000
14	3.265808000	-0.218419000	0.583861000
14	1.053679000	-0.699684000	2.137437000
6	4.516711000	0.817648000	1.548091000
1	4.509249000	1.854699000	1.187349000
1	4.299608000	0.840362000	2.621732000

1	5.535601000	0.429759000	1.421181000
6	1.529510000	-0.058168000	3.855902000
1	1.119009000	-0.712035000	4.636807000
1	2.615054000	-0.016846000	4.002618000
1	1.136188000	0.952240000	4.028600000
1	4.476382000	-0.930680000	-1.502525000
1	4.289376000	0.814288000	-1.467310000
15	0.465199000	-2.648120000	-0.919147000
6	2.033065000	-3.284581000	-0.163280000
1	1.928042000	-4.355721000	0.055377000
1	2.826382000	-3.203093000	-0.918978000
14	2.599120000	-2.319886000	1.397256000
6	-0.737128000	-3.800960000	-0.114855000
1	-0.844355000	-3.599125000	0.953900000
1	-1.717200000	-3.709751000	-0.592350000
1	-0.399119000	-4.836944000	-0.233062000
6	0.472185000	-3.470498000	-2.572727000
1	1.216137000	-3.019607000	-3.234854000
1	0.681850000	-4.542804000	-2.485872000
1	-0.508850000	-3.341537000	-3.042850000
6	3.593872000	-3.478787000	2.516986000
1	2.989544000	-4.335611000	2.839865000
1	4.477864000	-3.871799000	2.000565000
1	3.937755000	-2.955821000	3.416758000
1	1.221430000	1.353078000	0.101794000
6	0.496427000	3.034716000	-1.322336000
8	0.883552000	1.745284000	-0.943874000
6	0.023998000	3.015311000	-2.771769000
1	-0.276405000	4.017650000	-3.100680000
1	0.805715000	2.649063000	-3.445885000
1	-0.836626000	2.347901000	-2.875967000
6	1.628949000	4.054563000	-1.067469000
1	1.272060000	5.017812000	-1.461475000
6	2.928029000	3.692797000	-1.786739000
1	3.684072000	4.473719000	-1.642069000
1	3.333608000	2.757265000	-1.389134000
1	2.784640000	3.568506000	-2.865653000
6	1.879471000	4.226352000	0.432877000
1	2.672697000	4.959943000	0.620805000
1	0.977089000	4.576245000	0.948994000
1	2.183435000	3.279004000	0.895533000
1	-0.357630000	3.371862000	-0.715324000
1	2.345902000	0.798591000	-3.159773000
1	2.624400000	-1.292628000	-3.177905000

6	-2.116730000	1.459919000	1.105662000
6	-1.081695000	2.330262000	1.827891000
6	-2.791804000	2.237420000	-0.044391000
6	-1.754487000	3.555983000	2.486160000
1	-0.556014000	1.756066000	2.596344000
6	-2.945782000	3.740322000	0.269119000
1	-2.216936000	2.106927000	-0.968990000
6	-3.052695000	3.979850000	1.774429000
1	-1.972677000	3.341586000	3.539226000
1	-2.079540000	4.295929000	-0.112584000
1	-3.902683000	3.406413000	2.168318000
6	-3.026842000	-1.157089000	0.258769000
6	-4.139655000	-0.933641000	1.291862000
6	-3.576843000	-1.027550000	-1.181710000
6	-5.213168000	-2.033656000	1.172887000
1	-3.734058000	-0.923918000	2.310310000
6	-5.080754000	-1.342884000	-1.257177000
1	-3.391571000	-0.029358000	-1.589751000
6	-5.444996000	-2.469782000	-0.290150000
1	-4.915945000	-2.902873000	1.772344000
1	-5.666883000	-0.448775000	-1.005477000
1	-6.484878000	-2.784029000	-0.431797000
1	-2.883077000	1.210189000	1.850500000
1	-0.317389000	2.645234000	1.117930000
1	-3.781615000	1.802572000	-0.229079000
1	-3.822042000	4.141131000	-0.252409000
1	-3.268434000	5.033548000	1.984606000
1	-1.044898000	4.392762000	2.483171000
1	-2.694202000	-2.191021000	0.394425000
1	-4.602064000	0.047760000	1.130507000
1	-6.149537000	-1.662314000	1.606358000
1	-4.824317000	-3.345630000	-0.524306000
1	-5.349092000	-1.607864000	-2.286005000
1	-3.025609000	-1.719315000	-1.828040000

In_TSF5s

Doordinates (Angstroms)			
	X	Y	Z
25	-0.531446000	0.397237000	1.058384000
7	0.619645000	1.414985000	-0.609192000
6	-1.294894000	-0.352704000	-2.137683000
1	-0.959079000	-0.916973000	-3.016582000
1	-2.370978000	-0.202901000	-2.258268000

6	1.074222000	3.438458000	1.510808000
6	-1.016705000	-0.561037000	2.450760000
8	-1.274956000	-1.173367000	3.412351000
15	0.098006000	2.146458000	2.401899000
15	-0.971461000	-1.261236000	-0.559699000
14	0.808390000	3.143227000	-0.348896000
14	-0.412848000	1.332365000	-2.027016000
6	2.277484000	3.938173000	-1.232000000
1	2.252028000	3.767663000	-2.314026000
1	2.299469000	5.022659000	-1.064868000
1	3.222963000	3.527921000	-0.853223000
6	0.452830000	1.585694000	-3.693234000
1	-0.256866000	1.449741000	-4.520075000
1	0.887007000	2.586839000	-3.797545000
1	1.264725000	0.859258000	-3.829103000
1	0.817226000	4.449416000	1.843228000
1	2.139756000	3.292036000	1.728509000
15	-2.601367000	1.422798000	0.820730000
6	-2.540069000	3.173458000	0.223623000
1	-3.552191000	3.508523000	-0.040689000
1	-2.201368000	3.823860000	1.040383000
14	-1.341397000	3.374030000	-1.262011000
6	-3.973644000	0.852126000	-0.284309000
1	-3.732213000	1.053611000	-1.331637000
1	-4.169147000	-0.215290000	-0.168759000
1	-4.893508000	1.397181000	-0.043101000
6	-3.566354000	1.551560000	2.388257000
1	-2.943900000	1.947355000	3.195996000
1	-4.445229000	2.195297000	2.270032000
1	-3.901813000	0.552584000	2.688549000
6	-1.944387000	4.784228000	-2.371302000
1	-2.927823000	4.559837000	-2.802178000
1	-2.034286000	5.722062000	-1.809837000
1	-1.248239000	4.957154000	-3.200031000
1	1.340228000	0.531191000	0.037023000
6	2.608623000	0.012754000	1.720733000
8	1.516310000	-0.259676000	0.883062000
6	3.910959000	-0.267192000	0.967841000
6	4.901973000	-1.125345000	1.445627000
6	4.113856000	0.348165000	-0.274217000
6	6.055998000	-1.374960000	0.702199000
1	4.778566000	-1.622246000	2.402707000
6	5.262070000	0.103815000	-1.018625000
1	3.348969000	1.009187000	-0.675437000

6	6.239986000	-0.764149000	-0.532981000
1	6.808398000	-2.055269000	1.091769000
1	5.393193000	0.589732000	-1.981698000
1	7.137203000	-0.960308000	-1.113202000
6	2.455191000	-0.769025000	3.017360000
1	3.242571000	-0.522971000	3.738778000
1	1.489073000	-0.531120000	3.469331000
1	2.474555000	-1.847541000	2.825259000
1	0.867920000	1.928577000	3.568461000
1	-0.887749000	2.942209000	3.028877000
1	2.627861000	1.087981000	1.981745000
6	-2.334096000	-2.560530000	-0.386816000
6	-3.139799000	-2.460105000	0.929997000
6	-3.264987000	-2.683191000	-1.602051000
6	-4.535471000	-3.094226000	0.810363000
1	-2.574398000	-2.961022000	1.723417000
6	-4.111253000	-3.970380000	-1.521494000
1	-3.924856000	-1.808320000	-1.652251000
6	-4.489076000	-4.340938000	-0.072097000
1	-4.917028000	-3.335083000	1.808888000
1	-5.019865000	-3.832782000	-2.119867000
1	-5.449464000	-4.867689000	-0.054430000
6	0.400202000	-2.431197000	-1.049399000
6	1.585360000	-1.807728000	-1.794794000
6	0.874746000	-3.211359000	0.206308000
6	2.552381000	-2.892704000	-2.307382000
1	1.243956000	-1.204882000	-2.643092000
6	2.343779000	-3.645639000	0.095728000
1	0.751023000	-2.586242000	1.096198000
6	2.671776000	-4.082489000	-1.331579000
1	2.225973000	-3.255371000	-3.290513000
1	2.993670000	-2.807864000	0.373615000
1	1.973162000	-4.878769000	-1.624068000
1	-0.077103000	-3.137364000	-1.747546000
1	2.112010000	-1.137836000	-1.117256000
1	0.245297000	-4.100722000	0.339326000
1	3.536728000	-2.431320000	-2.451878000
1	3.676216000	-4.517116000	-1.386086000
1	2.545646000	-4.453833000	0.808846000
1	-1.774827000	-3.502562000	-0.342905000
1	-3.235762000	-1.421361000	1.254789000
1	-5.243029000	-2.373953000	0.375254000
1	-2.689404000	-2.684625000	-2.533951000
1	-3.560128000	-4.800296000	-1.979560000

1	-3.747243000	-5.035940000	0.343243000
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In_TSF5sa

Doordinates (Angstroms)			
	X	Y	Z
25	0.386136000	-0.373177000	-1.040097000
7	1.600681000	0.311360000	0.762347000
6	-0.783125000	-0.963716000	2.089633000
1	-1.267793000	-0.532579000	2.971686000
1	-0.999730000	-2.036209000	2.118545000
6	3.805423000	0.178802000	-1.208643000
6	-0.577314000	-0.471125000	-2.507230000
8	-1.161010000	-0.507254000	-3.519724000
15	2.340486000	-0.278695000	-2.237497000
15	-1.425176000	-0.285827000	0.497120000
14	3.304440000	-0.093485000	0.603148000
14	1.092076000	-0.672964000	2.125125000
6	4.499859000	0.938598000	1.641084000
1	4.355510000	2.007809000	1.438889000
1	4.364047000	0.785170000	2.717034000
1	5.542048000	0.692063000	1.400177000
6	1.466562000	0.061224000	3.829223000
1	1.106071000	-0.598152000	4.629529000
1	2.534877000	0.234590000	3.999137000
1	0.954708000	1.027282000	3.938792000
1	4.704965000	-0.367262000	-1.510615000
1	4.017978000	1.246752000	-1.344663000
15	0.631733000	-2.665602000	-0.929311000
6	2.191537000	-3.261992000	-0.122511000
1	2.091296000	-4.323692000	0.140337000
1	2.998489000	-3.204713000	-0.865650000
14	2.723550000	-2.225065000	1.401667000
6	-0.576882000	-3.820412000	-0.139999000
1	-0.667899000	-3.642895000	0.934093000
1	-1.561188000	-3.703550000	-0.603380000
1	-0.254193000	-4.857799000	-0.285121000
6	0.685653000	-3.514228000	-2.569358000
1	1.421803000	-3.055560000	-3.234690000
1	0.922904000	-4.578749000	-2.462274000
1	-0.294782000	-3.419529000	-3.048989000
6	3.785790000	-3.301875000	2.540716000
1	3.226594000	-4.175628000	2.897498000
1	4.679486000	-3.669323000	2.021929000
1	4.118360000	-2.737138000	3.419292000

1	1.083618000	1.304787000	0.114107000
6	1.100712000	2.748843000	-1.540187000
8	0.452009000	1.766940000	-0.780694000
6	0.429229000	2.863257000	-2.905801000
1	-0.571199000	3.302738000	-2.806843000
1	1.010769000	3.482527000	-3.597238000
1	0.313708000	1.872325000	-3.352481000
6	1.103094000	4.089039000	-0.775793000
1	0.049695000	4.378206000	-0.653741000
6	1.821550000	5.193891000	-1.555148000
1	1.879896000	6.113741000	-0.961583000
1	2.850116000	4.896124000	-1.801039000
1	1.310648000	5.441317000	-2.491130000
6	1.724347000	3.937542000	0.613944000
1	1.699251000	4.889711000	1.157218000
1	1.203293000	3.190416000	1.219646000
1	2.776044000	3.628510000	0.536838000
1	2.163351000	2.475647000	-1.702075000
1	2.466088000	0.584235000	-3.351014000
1	2.837669000	-1.429387000	-2.889953000
6	-1.883457000	1.464058000	0.945496000
6	-2.612720000	2.167489000	-0.215890000
6	-2.603813000	1.787548000	2.262535000
6	-3.132515000	3.562165000	0.203726000
1	-1.911235000	2.240562000	-1.051649000
6	-2.376713000	3.274818000	2.606548000
1	-3.676816000	1.596455000	2.155499000
6	-2.303900000	4.158052000	1.343596000
1	-3.132421000	4.235532000	-0.661145000
1	-3.185758000	3.618261000	3.262989000
1	-1.261218000	4.246388000	1.016861000
6	-2.996984000	-1.254787000	0.249479000
6	-4.148802000	-0.942051000	1.212699000
6	-3.487364000	-1.239977000	-1.218036000
6	-5.222332000	-2.046701000	1.144998000
1	-3.785317000	-0.841708000	2.241212000
6	-4.984119000	-1.580437000	-1.328317000
1	-3.297820000	-0.271653000	-1.690374000
6	-5.382952000	-2.619366000	-0.279693000
1	-4.960407000	-2.855071000	1.838698000
1	-5.585594000	-0.673706000	-1.180923000
1	-6.412585000	-2.958462000	-0.438048000
1	-0.886456000	1.917750000	0.999657000
1	-4.592042000	0.023367000	0.943054000

1	-6.177036000	-1.635266000	1.493957000
1	-4.744828000	-3.505218000	-0.402863000
1	-5.207361000	-1.938100000	-2.339537000
1	-2.677389000	-2.278478000	0.479317000
1	-2.900057000	-1.967199000	-1.790279000
1	-3.465058000	1.566337000	-0.553740000
1	-4.177366000	3.485955000	0.533740000
1	-2.641647000	5.175295000	1.571798000
1	-1.444404000	3.381173000	3.174949000
1	-2.261017000	1.169504000	3.097625000
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