DFT Explorations of Parathion and Paraoxon Hydrolysis as a Function of the Underlying Alkaline Environment

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Supplementary Information

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Physical Parameters for the Various Reactions Analyzed

Table S1. Various physical parameters for parathion + $1OH^-$ + 10 water molecules and how they evolve through the potential energy surface for the transformation of pentacoordinated parathion to paraoxon. All bond distances are listed in Å. P-OCH_2CH_3 refers to the phosphorous-ethoxide bond distance, P-S is the phosphorous sulfur bond distance, P-OH is the distance between the incoming hydroxide and phosphorous center, and P-nitrophenolate is the bond distance between the phosphorous and nitrophenolate group. HB – OH is the number of hydrogen bonds the hydroxide anion participates in, and HB – OP is the number of hydrogen bonds to the other oxygens that are attached to phosphorous.

State	Reactant	TS	Product
P-OCH_2CH_3	1.67	1.63	1.57
P-OCH_2CH_3	1.7	1.69	1.57
P-S	2.03	2.15	3.75
P-OH	1.73	1.63	1.49
P-Nitrophenolate	1.7	1.69	1.62
HB - OH	3	2	3
HB - OP	4	2	0

Table S2. Various physical parameters for parathion + $1OH^-$ + 10 water molecules and how they evolve through the potential energy surface for the transformation of pentacoordinated parathion to 4-nitrophenol. All bond distances are listed in Å. See Table S1 for other physical parameter definitions.

State	Reactant	TS	Product
P-OCH_2CH_3	1.71	1.66	1.63
P-OCH_2CH_3	1.64	1.61	1.63
P-S	2.00	1.97	1.98
P-OH	1.65	1.62	1.52
P-Nitrophenolate	1.85	2.26	3.58
HB - OH	1	1	2
HB - OP	3	5	3

Table S3. Various physical parameters for parathion + $2OH^-$ + 9 water molecules, pentacoordinate to hexacoordinate parathion. P-OH incoming refers to the second OH^- approaching to the phosphorous center, while P-OH connected refers to the hydroxide that already attached to the phosphorous center in the pentacoordinated step. All bond distances are listed in Å. See Table S1 for other physical parameter definitions.

State	Reactant	TS	Product
P-OCH_2CH_3	1.65	1.7	1.75
P-OCH_2CH_3	1.67	1.68	1.69
P-S	2.02	2.06	2.15
P-OH incoming	3.58	2.49	1.75
P-OH connected	1.63	1.71	1.74
P-Nitrophenolate	1.89	1.76	1.9
HB - OH	8	5	5
HB - OP	8	6	9

Table S4. Various physical parameters for parathion + $2OH^-$ + 9 water molecules, hexacoordinate parathion to the formation . P-OH incoming refers to the OH^- that formed the hexacoordinated parathion, while P-OH connected refers to the hydroxide that already attached to the phosphorous center in the pentacoordinated step. All bond distances are listed in Å. See Table S1 for other physical parameter definitions.

State	Reactant	TS	Product
P-OCH_2CH_3	1.75	1.75	1.8
P-OCH_2CH_3	1.69	1.67	1.65
P-S	2.15	2.12	2.04
P-OH (2nd OH in)	1.75	1.72	1.57
P-OH connected	1.74	1.74	1.8
P-Nitrophenolate	1.9	2.15	3.5
HB - OH	5	4	4
HB - OP	9	8	8

Table S5. Various physical parameters for paraoxon + $2OH^-$ + 9 water molecules for the reaction pentacoordinate paraoxon to 4-nitrophenol. HB - nitrophenolate group are hydrogen bonds specifically to the nitrophenolate group, while HB – OP refers to hydrogen bonds to all other O-P oxygens. All bond distances are listed in Å. See Table S1 for other physical parameter definitions.

State	Reactant	TS	Product
P-OCH_2CH_3	1.69	1.64	1.62
P-OCH_2CH_3	1.85	1.59	1.6
P-O	1.52	1.51	1.51
P-OH	1.65	1.62	1.53
P-Nitrophenolate	1.85	2.20	3.36
HB - Nitrophenolate group	1	1	1
HB - OP	7	7	8

Table S6. Various physical parameters for paraoxon + $1OH^-$ + 10 water molecules for the reaction pentacoordinate paraoxon to 4-nitrophenol. All bond distances are listed in Å. See Table S1 for other physical parameter definitions.

State	Reactant	TS	Product
P-OCH_2CH_3	1.69	1.67	1.63
P-OCH_2CH_3	1.65	1.64	1.64
P-O	1.49	1.5	1.49
P-OH	1.64	1.62	1.52
P-Nitrophenolate	1.93	2.10	3.56
HB - Nitrophenolate group	3	3	5
HB - OP	3	3	4

Reaction Pathways Examined

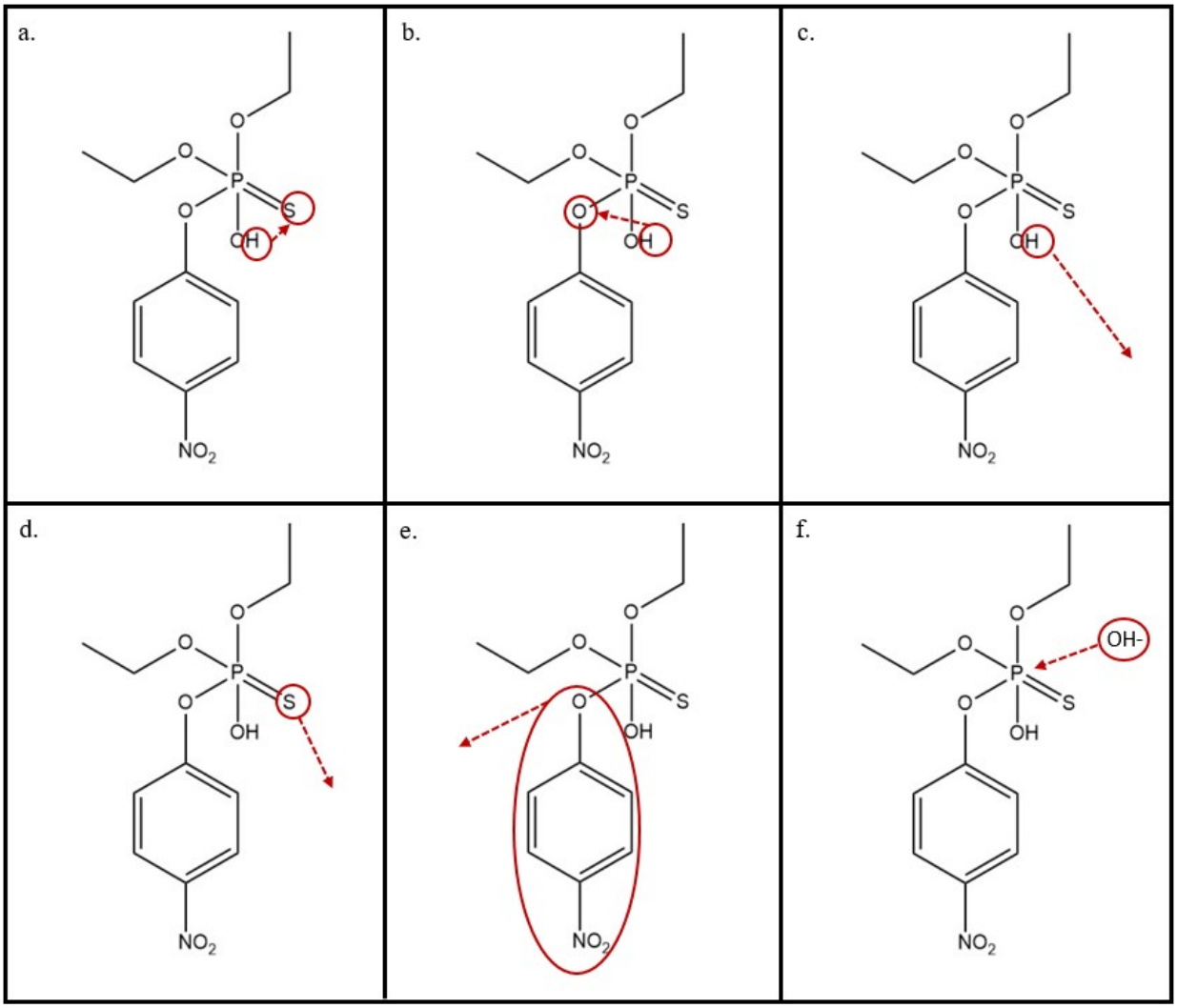

Figure S1: Pathways tested with rPES starting from the parathion pentacoordinate intermediate. These pathways include a) transferring the H from a P-OH moiety to the sulfur group, b) bringing that H to the oxygen of the nitrophenolate group, c) removing a H from the P-OH group, d) removing the sulfur group, e) removing the nitrophenolate group, and f) adding a second hydroxide to the phosphorous center (only available in the HA case).

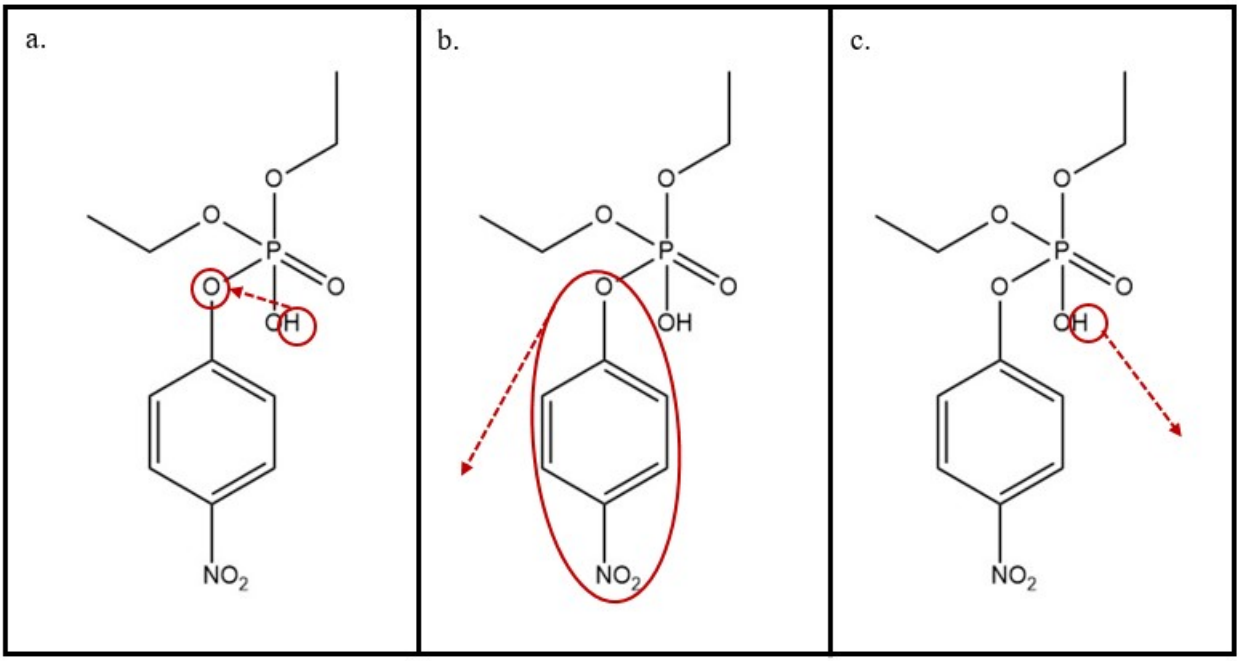

Figure S2: Pathways tested with rPES starting from the paraoxon pentacoordinate intermediate. These pathways include a) bringing the H of the P-OH group to the oxygen of the nitrophenolate group, b) removing the nitrophenolate group, and c) removing the H atom

Relative Energetics of the Parathion Pentacoordinated Intermediates

Table S7: Relative energetics of the parathion pentacoordinate intermediate in the HA (Parathion + 2OH + 9 water molecules). Reaction types are indicated as well as the corresponding figure of the intermediate and their place in that reaction pathway. Relative energy is given with respect to the lowest energy parathion pentacoordinate intermediate, which in this case is the intermediate in Figure 2(a).

Reaction Type	Place in Reaction Pathway	Figure for Reference	Relative Energy (kcal/mol)
parathion to parathion pentacoordinate intermediate	product	Figure 2(a)	0.0
parathion pentacoordinate intermediate to paraoxon	reactant	Figure 3(a)	19.7
parathion pentacoordinate intermediate to nitrophenolate	reactant	Figure 4(a)	14.0
parathion pentacoordinate intermediate to parathion hexacoordinated intermediate	reactant	Figure 5	0.7

Table S8: Relative energetics of the parathion pentacoordinate intermediate in the LA (Parathion + 1OH + 10 water molecules). Reaction types are indicated as well as the corresponding figure of the intermediate and their place in that reaction pathway. Relative energy is given with respect to the lowest energy parathion pentacoordinate intermediate, which in this case is the intermediate in Figure 4(b).

Reaction Type	Place in Reaction Pathway	Figure for Reference	Relative Energy (kcal/mol)
parathion to parathion pentacoordinate intermediate	product	Figure 2(b)	4.5
parathion pentacoordinate intermediate to paraoxon	reactant	Figure 3(b)	6.5
parathion pentacoordinate intermediate to 4-nitrophenol	reactant	Figure 4(b)	0.0

Discussion of Parathion Pentacoordinated Intermediates with Solvent Removed

Table S9: Relative energetics and configurational information for the parathion pentacoordinate intermediate in HA (Parathion + 2OH + 9 water molecules) with the extra hydroxide and water molecules removed. Reaction types are indicated as well as the corresponding figure of the intermediate and their place in that reaction pathway. Relative energy is given with respect to the lowest energy parathion pentacoordinate intermediate, which in this case is the intermediate in Figure 2(a).

Reaction Type	Place in Reaction Pathway	Figure for Reference	relative energy (kcal/mol)	S-P-O- (nitro-phenol)	Groups in the Trigonal Plane of the Trigonal Bipyramidal Structure		
parathion to parathion pentacoordinate intermediate	product	Figure 2(a)	0.0	94.6°	O-ethane	OH	S
parathion pentacoordinate intermediate to paraoxon	reactant	Figure 3(a)	13.8	174.1°	O-ethane	O-ethane	OH
parathion pentacoordinate intermediate to nitrophenolate	reactant	Figure 4(a)	3.8	94.1°	O-ethane	O-ethane	S
parathion pentacoordinate intermediate to parathion hexacoordinate intermediate	reactant	Figure 5	3.6	93.4°	O-ethane	OH	S

Table S10: Relative energetics and configurational information for the parathion pentacoordinate intermediate in HA (Parathion + 1OH + 10 water molecules) with the water molecules removed. Reaction types are indicated as well as the corresponding figure of the intermediate and their place in that reaction pathway. Relative energy is given with respect to the lowest energy parathion pentacoordinate intermediate, which in this case is the intermediate in Figure 4(b).

Reaction Type	Place in	Figure for	Relative	S-P-O-	Groups in the Trigonal

	Reaction Pathway	Reference	Energy (kcal/mol)	(nitro-phenol)	Plane of the Trigonal Bipyramidal Structure		
parathion to parathion pentacoordinate intermediate	product	Figure 2(b)	4.6	94.0°	O-ethane	O-ethane	S
parathion pentacoordinate intermediate to paraoxon	reactant	Figure 3(b)	7.8	118.9°	O-ethane	O-(nitro-phenol)	S
parathion pentacoordinate intermediate to 4-nitrophenol	reactant	Figure 4(b)	0.0	96.6°	O-ethane	OH	S

In order to determine the source of the large range of energetics in the HA pentacoordinate intermediates, all pentacoordinate parathion intermediates (HA and LA) were stripped of their solvent and, in the HA case, second OH group. A single point calculation was then performed (with the addition of thermal corrections for consistency) and the relative energetics were calculated (relative energetics here refers to the difference in energy between the lowest energy parathion pentacoordinate intermediate and the other pentacoordinate intermediates, in their respective alkaline environment). It is interesting to note, while looking at Table S10, that in the LA environment, removing solvent calculation yields relative energies that increase in their range. With solvent, the highest energy pentacoordinated intermediate was 6.5 kcal/mol and without solvent, the highest energy structure is 7.8 kcal/mol. This indicates that there is enough water present in these calculations to lend to a stabilizing effect. In contrast, in the HA environment, removing solvent leads to a decrease in the relative energy range. In the calculations with solvent, the highest relative energy structure is 19.7 kcal/mol (table S9) while without solvent it is 13.8 kcal/mol. The decrease in range of relative energies indicates that in the HA environment there are not enough water molecules to see a stabilization effect. As such, the high relative energies of the pentacoordinate intermediate is an artifact created by the limited solvation model. Furthermore,

the highest energy pentacoordinate intermediate listed in table S9 also has a very large S-P-O-nitrophenol angle (174.1° while most other angles are in tables S9 and S10 are around 93°-96°) indicating that sterics may also play a role in the high configuration. Furthermore, as seen in table S10, the highest energy intermediate also has a large S-P-O(nitrophenol) bond angle at 118.9°. Interestingly, this is the only structure that has the oxygen attached to the nitrophenol group in the trigonal plane of the trigonal bipyramidal structure. These important cases show a high energetic environment where sterics play a role. While it is likely that there is not enough water in the HA environment to fully stabilize the system, there is also the converse affect that including several water molecules increases the amount of local minima on the potential energy surface. It is likely that these sterically hindered intermediates are, in fact, local minima on the potential energy surface. It would be computationally intractable for this work to include complete solvation and sample the complete configurational space. However, while we cannot directly compare the routes from the pentacoordinate intermediates to their various products, we can still determine the effect that changing the alkaline environment plays on the isolated reaction steps.

System of Equations for Kinetics of Low Alkaline Conditions

Chemical Species in Low Alkaline Environment System	
Compound	**Abbreviation**
parathion	PARA
paraoxon	PARX
nitrophenol	NPH
OH	OH
penta-coordinated intermediate (first step)	PENTa
penta-coordinated intermediate (second step)	PENTb

$$\frac{d}{dt}\mathrm{PARA}(t) = +k_{-1}\cdot\mathrm{PENTa}(t) - k_1\cdot\mathrm{PARA}(t)\cdot\mathrm{OH}(t) \tag{1}$$

$$\frac{d}{dt}\mathrm{PARX}(t) = +k_2\cdot\mathrm{PENTa}(t) + k_{-4}\cdot\mathrm{PENTb}(t) - k_{-2}\cdot\mathrm{PARX}(t)\cdot\mathrm{HS}(t) - k_4\cdot\mathrm{PARX}(t)\cdot\mathrm{OH}(t) \tag{2}$$

$$\frac{d}{dt}\mathrm{OH}(t) = +k_{-1}\cdot\mathrm{PENTa}(t) + k_{-4}\cdot\mathrm{PENTb}(t) - k_1\cdot\mathrm{PARA}(t)\cdot\mathrm{OH}(t) - k_4\cdot\mathrm{PARX}(t)\cdot\mathrm{OH}(t) \tag{3}$$

$$\frac{d}{dt}\mathrm{NPOH}(t) = +k_3\cdot\mathrm{PENTa}(t) + k_5\cdot\mathrm{PENTb}(t) - k_{-3}\cdot\mathrm{NPOH}(t)\cdot\mathrm{DPT}(t) - k_{-5}\cdot\mathrm{NPOH}(t)\cdot\mathrm{DP}(t) \tag{4}$$

$$\begin{aligned}\frac{d}{dt}\mathrm{PENTa}(t) = &+ k_1\cdot\mathrm{PARA}(t)\cdot\mathrm{OH}(t) + k_{-2}\cdot\mathrm{PARX}(t)\cdot\mathrm{HS}(t) + k_{-3}\cdot\mathrm{NPOH}(t)\cdot\mathrm{DPT}(t)\\ &- k_{-1}\cdot\mathrm{PENTa}(t) - k_2\cdot\mathrm{PENTa}(t) - k_3\cdot\mathrm{PENTa}(t)\end{aligned} \tag{5}$$

$$\frac{d}{dt}\mathrm{PENTb}(t) = +k_4\cdot\mathrm{PARX}(t)\cdot\mathrm{OH}(t) + k_{-5}\cdot\mathrm{NPOH}(t)\cdot\mathrm{DP}(t) - k_{-4}\cdot\mathrm{PENTb}(t) - k_5\cdot\mathrm{PENTb}(t) \tag{6}$$

$$\frac{d}{dt}\mathrm{DP}(t) = +k_5\cdot\mathrm{PENTb}(t) - k_{-5}\cdot\mathrm{NPOH}(t)\cdot\mathrm{DP}(t) \tag{7}$$

XYZ Structures

Parathion + 2OH$^-$ + 9 Water Molecules

Parathion to the parathion pentacoordinate intermediate - Figure 2(a)			
Reactant			
63			
C	2.70839	2.6327	-1.9878
C	3.25936	1.56625	-1.0719
O	3.20911	0.28828	-1.7893
P	2.71618	-0.9933	-1.0014
S	2.74087	-2.6257	-2.0432
O	3.65055	-0.9554	0.28658
C	3.24516	-1.5852	1.52563
C	4.10008	-0.9984	2.62289
O	1.28555	-0.5168	-0.4431
C	0.08691	-1.1663	-0.2738
C	-0.4886	-1.0628	0.98943
C	-1.7699	-1.5514	1.18676
C	-2.4314	-2.1326	0.1125
C	-1.8544	-2.2581	-1.1448
C	-0.5718	-1.766	-1.3443
N	-3.8086	-2.5774	0.29743
O	-4.2409	-2.652	1.43449
O	-4.4577	-2.8623	-0.6961
H	2.73779	3.59951	-1.478
H	1.67228	2.40366	-2.2409
H	3.29924	2.70383	-2.9044
H	2.68047	1.48429	-0.1458
H	4.31033	1.7342	-0.8248
H	3.38582	-2.6657	1.41891
H	2.19392	-1.3591	1.71355
H	5.16094	-1.1826	2.4379
H	3.81619	-1.4414	3.57941
H	3.91187	0.07679	2.66985
H	0.06088	-0.574	1.78512
H	-2.269	-1.4495	2.14212
H	-2.4197	-2.6947	-1.9576
H	-0.1056	-1.7957	-2.3205

O	0.13081	2.17269	0.12557
H	-0.8081	1.96117	0.43729
O	-2.296	1.79918	0.97468
H	-2.4653	2.5966	1.4956
O	-4.1572	0.22484	0.24261
H	-4.9026	0.80693	0.05382
H	-3.4427	0.84724	0.62749
O	-0.6413	3.81993	-1.9955
H	-1.5877	3.63204	-1.7953
H	-0.1894	3.46204	-1.2078
O	-0.7262	1.29219	3.20874
H	-1.3526	1.23803	2.45383
H	0.17932	1.30727	2.75532
O	-0.6598	3.96733	2.29787
H	-0.3069	3.59306	1.473
H	-0.7134	3.17301	2.85954
O	-3.1019	0.33082	-2.333
H	-2.1305	0.42394	-2.2604
H	-3.418	0.12782	-1.4265
O	-3.1237	2.92663	-1.3061
H	-2.8081	2.52224	-0.4503
H	-3.2362	2.1387	-1.8712
O	1.28513	-0.6469	3.90961
H	1.58414	0.00914	3.22667
H	0.38082	-0.3346	4.05741
O	1.59316	1.20512	2.00076
H	2.08849	1.96183	2.33966
H	0.76148	1.75681	0.81888
O	-0.3858	1.06151	-2.3543
H	-0.546	1.99329	-2.5964
H	-0.0714	1.18669	-1.4321
Transition State			
63			
C	2.03302	2.89562	-2.6938
C	2.3639	2.21244	-1.3847
O	1.93806	0.84	-1.5272
P	2.4163	-0.4328	-0.6823
S	2.57662	-1.8393	-2.1134
O	3.86441	-0.278	-0.0083
C	4.86663	-1.3213	-0.0318
C	5.9637	-0.8739	0.90808

O	1.31698	-1.1142	0.3374
C	0.04157	-1.4711	0.03284
C	-0.5552	-2.3725	0.91931
C	-1.8776	-2.7375	0.73966
C	-2.5758	-2.2021	-0.3371
C	-1.9906	-1.316	-1.2328
C	-0.669	-0.9411	-1.0466
N	-3.9767	-2.5561	-0.5139
O	-4.4866	-3.3142	0.29594
O	-4.5739	-2.0876	-1.4695
H	2.31152	3.95086	-2.6378
H	0.95717	2.82276	-2.8734
H	2.56819	2.43429	-3.5266
H	1.82174	2.66912	-0.5597
H	3.43646	2.22746	-1.1684
H	5.21987	-1.4546	-1.0557
H	4.41087	-2.2534	0.30877
H	6.38342	0.082	0.58581
H	6.76321	-1.6186	0.91707
H	5.56678	-0.7697	1.92016
H	0.0288	-2.7475	1.75117
H	-2.3715	-3.42	1.41932
H	-2.5774	-0.9048	-2.0443
H	-0.2038	-0.2327	-1.7212
O	-0.2124	2.04806	0.50398
H	-0.9344	1.48127	0.98031
O	-1.9923	0.77371	1.75557
H	-2.0075	1.22651	2.61106
O	-4.2099	-0.2134	0.95465
H	-4.8265	0.45257	1.28281
H	-3.3104	0.09644	1.32466
O	-1.5607	4.30057	-0.4132
H	-2.3632	3.92348	0.0073
H	-0.8693	3.73017	-0.0282
O	0.43151	-0.0547	2.91697
H	-0.4264	-0.0543	2.44045
H	1.07115	0.31337	2.25659
O	-0.2963	2.63772	3.37135
H	-0.2649	2.7473	2.40696
H	0.03026	1.72474	3.47014
O	-3.9821	1.13739	-1.4732

H	-3.0291	1.30058	-1.6341
H	-4.0276	0.47779	-0.7489
O	-3.5776	2.79384	0.7261
H	-2.9741	2.10154	1.09077
H	-3.8989	2.37776	-0.0973
O	3.1099	-1.1927	2.67665
H	3.03394	-0.4485	2.05283
H	2.18086	-1.3139	2.92043
O	2.09186	0.96385	1.04178
H	2.78773	1.61845	1.17444
H	0.68361	1.63476	0.69765
O	-1.3631	1.97256	-1.9595
H	-1.5616	2.91421	-1.7986
H	-0.8282	1.78425	-1.1538
Product			
63			
C	-2.0003	-0.3275	3.47976
C	-2.4357	0.13872	2.10892
O	-1.9582	-0.8294	1.15801
P	-2.3119	-0.6636	-0.4275
S	-2.2557	-2.2637	-1.6335
O	-3.9913	-0.573	-0.1541
C	-4.6848	-1.644	0.46488
C	-6.0747	-1.1582	0.83105
O	-0.5191	-0.2278	-0.6715
C	0.54821	-0.9839	-0.4203
C	1.78542	-0.4712	-0.8618
C	2.96581	-1.1361	-0.6042
C	2.91744	-2.3441	0.09226
C	1.70999	-2.8777	0.53859
C	0.52768	-2.2019	0.28996
N	4.14825	-3.0522	0.36882
O	5.20201	-2.5642	-0.0201
O	4.08932	-4.1121	0.98038
H	-2.3367	0.38368	4.23839
H	-0.9113	-0.3913	3.50893
H	-2.4307	-1.307	3.70435
H	-1.9935	1.11508	1.87218
H	-3.5237	0.22171	2.03112
H	-4.1419	-1.9732	1.3617
H	-4.737	-2.4956	-0.2235

H	-6.0194	-0.3211	1.53237
H	-6.6488	-1.9633	1.29645
H	-6.6076	-0.8238	-0.0626
H	1.78927	0.47315	-1.3932
H	3.91114	-0.7148	-0.9223
H	1.70929	-3.8121	1.08609
H	-0.4086	-2.6004	0.65388
O	-0.7875	2.89473	0.24869
H	0.14038	2.8261	-0.1709
O	1.46666	2.94702	-0.9584
H	1.32324	3.79345	-1.4071
O	3.81183	1.8836	-1.0809
H	4.46366	2.59146	-1.0263
H	2.91371	2.34985	-1.0974
O	0.13566	3.33865	2.79481
H	1.00636	3.61279	2.42023
H	-0.4301	3.32775	1.9991
O	-0.0938	1.76641	-2.7343
H	0.59439	2.11735	-2.0975
H	-0.7114	1.2993	-2.1481
O	-0.8169	4.482	-2.1459
H	-0.9811	4.17736	-1.2377
H	-0.7122	3.63778	-2.6156
O	3.46357	1.16297	1.58047
H	2.52866	0.87843	1.63918
H	3.63014	1.27624	0.62084
O	2.46874	3.74161	1.4542
H	2.10058	3.52547	0.56275
H	2.94147	2.91384	1.67861
O	0.21547	-0.9396	-3.6418
H	-0.3979	-1.3102	-2.9883
H	0.2594	0.00066	-3.3992
O	-2.4395	0.88705	-0.9806
H	-3.383	1.11092	-0.9943
H	-1.3113	2.16637	-0.1201
O	0.73069	0.77685	1.99385
H	0.51746	1.65088	2.39099
H	0.21283	0.75657	1.17567
Parathion pentacoordinate intermediate to paraoxon - Figure 3(a)			
Reactant			

63			
C	-0.9271	-1.6978	3.10084
C	-0.1676	-1.8471	1.79949
O	-1.0483	-1.375	0.75315
P	-0.8657	-1.4596	-0.868
S	-2.9097	-0.8697	-1.1365
O	-0.1421	-0.2945	-1.7261
C	-0.6925	0.97051	-2.1423
C	0.45462	1.95166	-2.2489
O	0.78633	-2.1278	-0.6682
C	1.92868	-1.4646	-0.4894
C	2.01832	-0.1555	0.02649
C	3.25298	0.44037	0.21004
C	4.40848	-0.2683	-0.1158
C	4.35016	-1.5671	-0.6186
C	3.11393	-2.158	-0.8034
N	5.70167	0.35737	0.0757
O	5.73609	1.4998	0.51283
O	6.70578	-0.2827	-0.2076
H	-0.2951	-2.033	3.92794
H	-1.8331	-2.3076	3.07553
H	-1.203	-0.6533	3.27258
H	0.08287	-2.8888	1.60204
H	0.74091	-1.2424	1.81013
H	-1.4194	1.32797	-1.4167
H	-1.2048	0.83057	-3.097
H	0.89737	2.13123	-1.2651
H	0.06315	2.89868	-2.6297
H	1.23113	1.59069	-2.9285
H	1.11292	0.38498	0.2823
H	3.32344	1.447	0.60715
H	5.26551	-2.0924	-0.8609
H	3.03293	-3.1652	-1.1961
O	-3.5957	-2.6275	1.42456
H	-4.497	-2.9666	1.35932
O	-0.6316	1.39935	1.06456
H	-1.1879	0.61612	0.94786
O	-1.5376	-4.5363	0.88735
H	-2.251	-3.917	1.12551
H	-1.231	-4.2126	0.02977
O	-3.4928	0.21033	1.97629

H	-3.4322	-0.7413	2.16103
H	-3.3466	0.2299	1.01393
O	-2.6416	3.56904	-2.2761
H	-2.0795	4.09587	-2.8533
H	-2.1431	3.52364	-1.3784
O	-3.5752	1.32123	-3.5905
H	-3.2437	2.1169	-3.1243
H	-3.3988	0.6095	-2.9546
O	1.36647	3.30144	1.24348
H	0.68173	3.78832	1.744
H	0.96335	2.42143	1.18395
O	-1.7067	1.82616	3.49333
H	-2.5069	1.39273	3.14527
H	-1.1081	1.68533	2.72525
O	-1.3728	3.46494	-0.0767
H	-1.0465	2.22735	0.54077
H	-0.4686	3.71809	-0.311
O	-1.0227	4.38745	2.37225
H	-1.3678	3.65218	2.90774
H	-1.2997	4.14087	1.44616
O	-1.0988	-2.919	-1.5884
H	-2.0307	-2.9261	-1.8646
H	-3.4429	-2.1366	0.58118
Transition State			
63			
C	-0.4984	1.70394	-2.9313
C	0.32872	1.70673	-1.6667
O	-0.4762	1.08492	-0.6266
P	-0.1911	1.20531	0.97584
S	-2.3758	1.00085	1.45829
O	0.29815	-0.124	1.74925
C	-0.4669	-1.3278	1.97372
C	0.53542	-2.4108	2.31642
O	1.52022	1.5629	0.73706
C	2.47137	0.68822	0.37509
C	2.21992	-0.5389	-0.2707
C	3.27699	-1.3578	-0.6302
C	4.57991	-0.9552	-0.3507
C	4.85417	0.25771	0.27556
C	3.79708	1.07321	0.6356
N	5.68383	-1.8215	-0.7285

O	5.42535	-2.8859	-1.2712
O	6.82191	-1.4467	-0.4864
H	0.0886	2.13682	-3.7453
H	-1.4108	2.28577	-2.7972
H	-0.7797	0.68383	-3.2049
H	0.5967	2.71561	-1.3507
H	1.24405	1.12792	-1.8039
H	-1.0354	-1.5845	1.07413
H	-1.1696	-1.1599	2.78924
H	1.23127	-2.5798	1.4912
H	0.00563	-3.3444	2.52113
H	1.1087	-2.1385	3.20592
H	1.20491	-0.8468	-0.5013
H	3.10222	-2.3032	-1.1286
H	5.87917	0.54396	0.47449
H	3.96884	2.02492	1.12554
O	-1.2494	4.22626	-0.5091
H	-1.727	5.02667	-0.2565
O	-1.4506	-1.3847	-1.56
H	-1.1828	-0.551	-1.1464
O	1.63065	4.43323	0.03135
H	0.71939	4.61598	-0.2402
H	1.54333	3.62199	0.55453
O	-3.3677	2.39131	-1.2659
H	-2.6709	3.06875	-1.2401
H	-3.1514	1.85399	-0.4774
O	-3.087	-3.145	2.35878
H	-2.3525	-3.7418	2.53134
H	-3.0508	-2.9444	1.34567
O	-3.167	-1.0016	4.06286
H	-3.1685	-1.7903	3.47718
H	-3.0053	-0.2801	3.43615
O	-2.8232	-3.3737	-3.0841
H	-3.6474	-2.9642	-2.7553
H	-2.1486	-2.7347	-2.8121
O	-3.4106	0.08958	-2.8941
H	-3.3779	0.94284	-2.4198
H	-2.6876	-0.4401	-2.4969
O	-3.0273	-2.6808	-0.1216
H	-2.0918	-1.8744	-0.8898
H	-2.8852	-3.5257	-0.57

O	-4.9302	-1.9938	-1.8059
H	-4.5919	-1.1498	-2.1601
H	-4.3042	-2.2013	-1.0535
O	-0.3424	2.63209	1.63662
H	-1.5986	2.29803	1.85367
H	-1.0698	3.75727	0.32845
Product			
63			
C	-2.042	1.51031	-2.5657
C	-0.7984	2.03871	-1.8925
O	-0.4523	1.11078	-0.8146
P	0.16535	1.68739	0.53156
S	-3.0572	0.1949	2.09919
O	0.44921	0.4306	1.41419
C	0.44428	-0.9645	0.97354
C	1.6237	-1.6541	1.61195
O	1.62143	2.27623	0.12153
C	2.67712	1.41581	-0.1209
C	2.64337	0.53387	-1.1999
C	3.72489	-0.31	-1.4156
C	4.80978	-0.2347	-0.5512
C	4.85793	0.65023	0.52004
C	3.7712	1.485	0.73778
N	5.9528	-1.1229	-0.7802
O	5.8951	-1.8967	-1.7201
O	6.90051	-1.0404	-0.0182
H	-2.3447	2.19825	-3.3586
H	-2.855	1.42562	-1.8407
H	-1.8619	0.52471	-3.0003
H	-0.9559	3.03484	-1.4691
H	0.05862	2.07214	-2.5703
H	0.49565	-0.9953	-0.1168
H	-0.5037	-1.3903	1.30398
H	2.56297	-1.1697	1.32853
H	1.65535	-2.6917	1.26937
H	1.50657	-1.6375	2.69675
H	1.78276	0.50613	-1.8586
H	3.73482	-1.0118	-2.2395
H	5.72543	0.67293	1.16682
H	3.75447	2.18531	1.56427
O	-3.1659	3.3879	0.0669

H	-3.7204	3.77991	0.75425
O	-1.7143	-1.4917	-1.4343
H	-1.375	-0.662	-1.0779
O	-0.9834	5.1742	-0.4162
H	-1.8846	4.81449	-0.4138
H	-0.559	4.62359	0.25737
O	-4.8768	1.12525	-0.3619
H	-4.4318	1.97869	-0.4885
H	-4.3847	0.76437	0.4115
O	-0.8654	-3.6952	2.50831
H	0.02398	-4.012	2.32046
H	-1.2956	-3.5352	1.58395
O	-0.6693	-1.3323	3.92066
H	-0.7265	-2.2001	3.46809
H	-1.2802	-0.7859	3.39589
O	-2.2234	-3.9616	-2.6917
H	-3.0458	-3.9133	-2.1658
H	-1.8428	-3.0808	-2.5557
O	-4.2919	-0.9992	-2.1002
H	-4.5565	-0.2364	-1.5505
H	-3.3337	-1.1216	-1.9008
O	-1.9111	-3.3051	0.23762
H	-1.7701	-2.1946	-0.6414
H	-1.5843	-3.9934	-0.3584
O	-4.3243	-3.5137	-0.856
H	-4.4847	-2.6164	-1.2081
H	-3.5057	-3.4165	-0.2965
O	-0.6045	2.78553	1.16209
H	-2.3216	1.31567	2.20328
H	-2.4527	2.93818	0.55786
Parathion pentacoordinate intermediate to nitrophenolate - Figure 4(a)			
Reactant			
63			
C	-2.655	-1.0312	1.92793
C	-1.6797	-1.8425	1.09693
O	-1.4801	-1.2784	-0.2175
P	-0.5766	0.06442	-0.4585
S	0.08153	0.37997	-2.3368
O	-0.169	0.87043	0.88606
C	-0.6819	2.14812	1.30803

C	0.34784	2.75221	2.23706
O	0.84164	-1.031	-0.005
C	2.13475	-0.7097	-0.0189
C	2.62839	0.6109	-0.0489
C	3.99352	0.83714	-0.0389
C	4.87443	-0.242	0.00023
C	4.41271	-1.557	0.02045
C	3.05019	-1.7847	0.00389
N	6.30156	0.00647	0.01407
O	6.69126	1.16645	-0.0109
O	7.0592	-0.9543	0.05071
H	-2.8333	-1.5466	2.87614
H	-3.6089	-0.9227	1.40565
H	-2.2623	-0.0365	2.15182
H	-2.079	-2.8359	0.88925
H	-0.7142	-1.952	1.59264
H	-1.6439	1.9989	1.8083
H	-0.8407	2.7938	0.44747
H	0.57732	2.07307	3.0617
H	-0.0385	3.68438	2.65864
H	1.2631	2.97	1.68194
H	1.95154	1.4544	-0.0896
H	4.38455	1.84712	-0.0631
H	5.11935	-2.3772	0.0419
H	2.65835	-2.7964	0.01612
O	0.19501	-3.7669	-0.4934
H	0.31479	-2.8057	-0.5694
O	-2.0171	1.02286	-0.6315
H	-2.3666	0.84504	-1.5167
O	1.14611	-3.4172	2.07958
H	0.73295	-3.6853	1.23261
H	1.36159	-2.4904	1.92027
O	-4.417	-3.447	-0.0245
H	-4.2431	-3.4162	0.92298
H	-3.1953	-3.7589	-0.7719
O	-0.739	5.24965	-0.1647
H	-0.6489	5.40635	0.78172
H	-1.6134	4.81083	-0.2739
O	1.19116	3.3775	-0.9925
H	0.52159	4.04081	-0.7365
H	0.71311	2.70333	-1.4984

O	-4.0159	1.97041	1.10287
H	-4.8583	1.51277	0.8694
H	-3.3478	1.43772	0.63698
O	-4.4041	-1.1723	-0.9098
H	-4.4428	-2.1902	-0.4765
H	-3.5044	-0.8725	-0.7243
O	-2.9461	3.76802	-0.6782
H	-2.4474	3.00739	-1.0127
H	-3.4699	3.35089	0.03957
O	-6.0573	0.41087	0.26812
H	-5.4282	-0.2241	-0.214
H	-6.5384	0.86645	-0.4315
O	-2.3527	-3.8055	-1.3896
H	-2.2461	-2.8758	-1.6326
H	-0.7527	-3.9034	-0.741
Transition State			
63			
C	-2.7316	-1.1902	2.0196
C	-1.6607	-1.8769	1.19583
O	-1.5348	-1.2305	-0.083
P	-0.6277	0.0883	-0.3499
S	0.12227	0.24014	-2.3197
O	-0.1777	0.85819	1.00276
C	-0.753	2.0956	1.46403
C	0.31137	2.82	2.25947
O	0.82586	-1.0222	0.05873
C	2.11414	-0.686	0.02271
C	2.58801	0.64223	-0.0264
C	3.94986	0.88782	-0.0453
C	4.84695	-0.1779	-0.0144
C	4.40499	-1.4994	0.02502
C	3.04647	-1.7478	0.03618
N	6.2702	0.09154	-0.0284
O	6.64226	1.25684	-0.0696
O	7.04232	-0.8578	0.00196
H	-2.9079	-1.7461	2.94496
H	-3.6626	-1.1378	1.44874
H	-2.4344	-0.1705	2.27886
H	-1.9382	-2.9038	0.95284
H	-0.6947	-1.8907	1.70174
H	-1.6292	1.86125	2.07522

H	-1.0861	2.69304	0.61701
H	0.7011	2.18514	3.05904
H	-0.1153	3.71749	2.71678
H	1.13071	3.11409	1.59975
H	1.89795	1.47637	-0.0595
H	4.32625	1.90287	-0.084
H	5.12414	-2.3088	0.04082
H	2.67023	-2.7649	0.06683
O	0.22934	-3.7311	-0.5168
H	0.36351	-2.769	-0.5449
O	-1.8276	1.04784	-0.8402
H	-1.1955	0.94024	-2.0994
O	1.15133	-3.4679	2.0693
H	0.73358	-3.7098	1.21642
H	1.34897	-2.532	1.94319
O	-4.2972	-3.3217	-0.1529
H	-4.1241	-3.3185	0.79483
H	-3.1024	-3.6183	-0.8741
O	-0.9174	5.1625	-0.1147
H	-0.9398	5.24808	0.84472
H	-1.7459	4.67911	-0.354
O	0.98505	3.31584	-0.9503
H	0.33225	3.98104	-0.6518
H	0.48489	2.67511	-1.4724
O	-3.8485	1.84543	0.98771
H	-4.6985	1.36884	0.84489
H	-3.2023	1.36049	0.43924
O	-4.3332	-1.0125	-1.0158
H	-4.3154	-2.01	-0.6044
H	-3.4505	-0.6425	-0.8661
O	-2.9659	3.61461	-0.8842
H	-2.4545	2.82992	-1.1513
H	-3.4801	3.2369	-0.1394
O	-6.0124	0.31452	0.39886
H	-5.3902	-0.226	-0.1945
H	-6.5737	0.8101	-0.2078
O	-2.2464	-3.6688	-1.4968
H	-2.1104	-2.7309	-1.6879
H	-0.7127	-3.8396	-0.8132
Product			
63			

C	-2.8275	-1.204	1.80848
C	-1.7008	-1.894	1.06772
O	-1.4903	-1.3325	-0.2568
P	-1.2264	0.20243	-0.5085
S	0.10332	0.24822	-2.1115
O	-0.5304	0.758	0.80503
C	-0.8638	2.09369	1.2764
C	0.22258	2.51683	2.23463
O	1.2846	-1.283	0.02147
C	2.50873	-0.9096	0.02075
C	2.87223	0.47774	-0.0332
C	4.1875	0.8743	-0.0375
C	5.20864	-0.089	0.01797
C	4.89886	-1.457	0.08533
C	3.58457	-1.8575	0.08933
N	6.57207	0.32562	0.01081
O	6.82921	1.52897	-0.0508
O	7.45685	-0.5301	0.06661
H	-3.0451	-1.757	2.72641
H	-3.7252	-1.1797	1.18612
H	-2.5654	-0.1798	2.08862
H	-1.9455	-2.933	0.85099
H	-0.7486	-1.8547	1.59831
H	-1.8468	2.04851	1.75448
H	-0.92	2.776	0.42739
H	0.31375	1.80374	3.05736
H	-0.0259	3.49638	2.65204
H	1.17337	2.59308	1.70417
H	2.07447	1.21261	-0.0665
H	4.45287	1.92451	-0.082
H	5.70629	-2.1784	0.13386
H	3.32077	-2.9092	0.15133
O	0.33509	-3.8908	-0.3546
H	0.61952	-2.9559	-0.3919
O	-2.469	0.96388	-0.875
H	-0.763	0.94888	-2.8641
O	1.21476	-3.1794	2.17432
H	0.79959	-3.7253	1.48219
H	1.34797	-2.3623	1.66602
O	-4.2641	-3.2714	-0.3983
H	-4.1875	-3.3618	0.55762

H	-3.0056	-3.6084	-1.0495
O	-0.904	5.08008	-0.4044
H	-0.8671	5.39417	0.50609
H	-1.7765	4.62802	-0.4842
O	1.29454	3.37507	-0.771
H	0.52698	3.97509	-0.691
H	1.00588	2.67788	-1.3725
O	-4.177	1.90812	1.1869
H	-5.0372	1.42643	1.15368
H	-3.6243	1.39159	0.57717
O	-4.8293	-0.9587	-0.93
H	-4.5577	-2.0006	-0.6729
H	-4.0063	-0.4568	-1.0108
O	-3.2043	3.67979	-0.7214
H	-2.8762	2.853	-1.1114
H	-3.6833	3.3442	0.06146
O	-6.2745	0.24774	0.81245
H	-5.7356	-0.2581	0.11227
H	-6.9779	0.68522	0.3203
O	-2.1181	-3.7577	-1.5869
H	-1.8869	-2.853	-1.8305
H	-0.5754	-3.9066	-0.7258
Parathion pentacoordinate intermediate to hexacoordinate to 4-nitrophenol - Figure 5			
Reactant			
63			
C	-3.3869	0.55892	-2.431
C	-2.7679	1.6102	-1.5321
O	-1.4246	1.17979	-1.2514
P	-0.332	2.00923	-0.3344
S	0.83293	3.41173	-1.1951
O	-1.5677	2.99216	0.25769
C	-1.3	3.9417	1.27862
C	-2.2127	5.13545	1.07178
O	0.71434	0.58083	-0.9821
C	1.94692	0.2611	-0.653
C	2.49508	-0.8857	-1.2792
C	3.77304	-1.3161	-0.9935
C	4.53974	-0.595	-0.0758
C	4.03446	0.54441	0.5512
C	2.75204	0.97319	0.26866

N	5.87939	-1.0364	0.22806
O	6.30628	-2.0389	-0.3335
O	6.54003	-0.393	1.03558
H	-4.3969	0.86949	-2.7111
H	-3.4515	-0.4003	-1.9086
H	-2.7953	0.42316	-3.3393
H	-3.3203	1.70373	-0.5958
H	-2.7367	2.59172	-2.0137
H	-0.2517	4.2603	1.23908
H	-1.484	3.47613	2.25445
H	-1.9967	5.61204	0.1119
H	-2.0726	5.87146	1.86797
H	-3.2594	4.81959	1.07224
H	1.87152	-1.4222	-1.9858
H	4.1889	-2.1967	-1.4673
H	4.65499	1.08143	1.25822
H	2.35426	1.85049	0.75899
O	-0.7164	-1.3527	-2.4871
H	-0.5533	-0.4574	-2.1305
O	-0.0201	1.38605	1.13338
H	-0.8437	1.40855	1.73208
O	-2.1793	1.08054	2.49643
H	-1.9381	0.44188	3.18683
H	-2.4548	0.45366	1.75561
O	1.03759	-1.2034	1.99515
H	0.83767	-0.2879	1.73568
H	0.7073	-1.7157	1.22844
O	-0.4183	-2.4701	0.03515
H	-0.2339	-2.1922	-0.8796
H	-1.2319	-1.9382	0.28078
O	-4.4296	-2.1437	0.00385
H	-3.6859	-1.4991	0.23436
H	-4.0581	-2.5811	-0.7868
H	-2.4818	-3.8716	-1.4255
O	-1.5275	-1.664	2.96976
H	-1.7736	-1.3041	2.07565
H	-0.5534	-1.6599	2.91116
O	-1.7628	-4.8502	-0.1038
H	-1.0643	-4.1699	-0.037
O	-3.2394	-3.7287	1.90251
H	-3.7501	-3.1616	1.27739

H	-2.6048	-3.1265	2.33304
O	-2.3736	-0.7636	0.65628
H	-1.9664	-0.2383	-0.0462
H	-2.3427	-4.5965	0.65001
H	-0.2928	-1.3818	-3.3523
O	-2.8831	-3.2318	-2.0537
H	-2.2133	-2.5375	-2.1713
Transition State - 1			
63			
C	3.49772	-0.6658	-2.859
C	2.96616	-1.3986	-1.6405
O	1.66511	-0.8841	-1.3705
P	0.56883	-1.7061	-0.3727
S	0.12954	-3.4313	-1.4058
O	1.86053	-2.0976	0.60617
C	1.78827	-3.1474	1.55737
C	3.17554	-3.7508	1.68182
O	-0.5054	-0.5305	-1.13
C	-1.7897	-0.2797	-0.8606
C	-2.1632	1.07065	-0.7436
C	-3.4879	1.41873	-0.544
C	-4.4415	0.40788	-0.4665
C	-4.0995	-0.9386	-0.5913
C	-2.7757	-1.2815	-0.7941
N	-5.8329	0.76507	-0.2533
O	-6.1217	1.9504	-0.1662
O	-6.6572	-0.1348	-0.1699
H	4.48229	-1.0564	-3.1304
H	3.5981	0.40346	-2.6509
H	2.82521	-0.7928	-3.7118
H	3.60964	-1.2314	-0.7752
H	2.89496	-2.4759	-1.8299
H	1.07658	-3.9145	1.22892
H	1.44655	-2.754	2.5204
H	3.49083	-4.1749	0.72435
H	3.18427	-4.5433	2.43506
H	3.90066	-2.9867	1.97467
H	-1.3901	1.83262	-0.7851
H	-3.7893	2.45358	-0.4407
H	-4.8728	-1.6947	-0.5376
H	-2.4797	-2.3167	-0.9187

O	1.08169	1.61331	-2.1595
H	1.23428	0.69623	-1.8198
O	-0.5251	-1.8316	0.93431
H	-0.9625	-2.689	0.83127
O	0.0091	-1.1216	3.6128
H	0.5508	-0.3097	3.62276
H	-0.0344	-1.3488	2.66324
O	-1.6734	0.78497	2.41667
H	-1.4493	0.09726	3.06478
H	-1.059	0.55586	1.69511
O	0.54683	3.37	-0.0886
H	0.77724	2.78388	-0.8365
H	1.18847	3.14499	0.61462
O	3.40325	0.98006	0.40525
H	2.46622	0.63248	0.49195
H	3.4486	1.46247	-0.4431
H	3.37997	3.58575	-1.2817
O	1.02315	1.45555	3.14902
H	0.99029	1.01198	2.18047
H	0.1024	1.74489	3.23846
O	2.82354	4.99674	-0.2415
H	1.88326	4.79995	-0.3963
O	2.66184	3.13414	1.80751
H	3.07025	2.35216	1.35419
H	2.09643	2.71746	2.49478
O	0.86279	0.40879	0.90479
H	0.47458	1.06657	0.31278
H	2.95226	4.57505	0.62813
H	0.32323	1.53456	-2.7497
O	3.55614	2.76185	-1.7812
H	2.70384	2.5207	-2.1818
Intermediate -as product			
63			
C	3.75066	-0.1595	-2.8507
C	3.05698	-1.1126	-1.8919
O	1.88258	-0.4746	-1.4203
P	0.71645	-1.2621	-0.3836
S	0.32419	-2.9287	-1.6841
O	1.9839	-1.9159	0.52586
C	1.86371	-3.1261	1.24073
C	3.2023	-3.8419	1.19695

O	-0.4717	-0.1176	-1.3236
C	-1.7609	0.02774	-1.0579
C	-2.2331	1.30638	-0.687
C	-3.5774	1.52391	-0.4413
C	-4.4669	0.45901	-0.5677
C	-4.0342	-0.8168	-0.936
C	-2.692	-1.0298	-1.1822
N	-5.8741	0.68061	-0.3088
O	-6.2404	1.8073	0.00102
O	-6.6425	-0.2675	-0.41
H	4.66187	-0.6159	-3.2468
H	4.02237	0.76876	-2.3378
H	3.09437	0.09222	-3.6887
H	3.71163	-1.3493	-1.0465
H	2.78827	-2.0506	-2.3896
H	1.08901	-3.759	0.79368
H	1.5714	-2.9194	2.27961
H	3.4557	-4.0929	0.16279
H	3.17193	-4.7641	1.7842
H	3.99383	-3.2021	1.59743
H	-1.51	2.10907	-0.5729
H	-3.9462	2.49915	-0.148
H	-4.7566	-1.6185	-1.0295
H	-2.3188	-2.0036	-1.4802
O	1.36158	1.99656	-2.0833
H	1.53154	1.03935	-1.8528
O	-0.5437	-1.7442	0.71871
H	-0.9473	-2.5233	0.30543
O	-0.5042	-2.0887	3.52398
H	0.07143	-1.3282	3.71767
H	-0.4275	-2.1486	2.55206
O	-2.0326	0.04689	2.46673
H	-1.8715	-0.7273	3.03317
H	-1.6823	-0.2698	1.61554
O	0.50845	3.07075	0.29806
H	0.88475	2.72292	-0.5385
H	1.10438	2.75106	1.00848
O	3.64836	0.91666	0.54256
H	2.8485	0.41502	0.29694
H	3.71848	1.63114	-0.1283
H	3.41492	3.77597	-0.4963

O	0.64119	0.47624	3.24467
H	0.82191	0.20456	2.30598
H	-0.3064	0.69685	3.17595
O	2.65019	4.81654	0.79922
H	1.74197	4.61848	0.51209
O	2.34548	2.47182	2.30417
H	2.89424	1.84562	1.7683
H	1.78746	1.90869	2.87409
O	0.87252	0.14695	0.64752
H	0.3637	0.88199	0.27668
H	2.73717	4.21885	1.56236
H	0.53844	1.97752	-2.5857
O	3.70934	3.10127	-1.1434
H	2.92856	2.91901	-1.6939
Intermediate -as reactant			
63			
C	3.75059	-0.1588	-2.8508
C	3.05718	-1.1122	-1.8921
O	1.88257	-0.4745	-1.4205
P	0.71695	-1.2622	-0.3835
S	0.3244	-2.9288	-1.6841
O	1.98459	-1.9161	0.52546
C	1.86483	-3.1264	1.24027
C	3.20297	-3.8429	1.1945
O	-0.4716	-0.1176	-1.3231
C	-1.7608	0.02754	-1.0575
C	-2.2332	1.30614	-0.6867
C	-3.5775	1.52351	-0.4411
C	-4.4669	0.45852	-0.5674
C	-4.034	-0.8173	-0.9357
C	-2.6918	-1.0301	-1.1817
N	-5.8742	0.67998	-0.3087
O	-6.2405	1.80654	0.00147
O	-6.6425	-0.2681	-0.4103
H	4.662	-0.6148	-3.2469
H	4.02189	0.7695	-2.3378
H	3.09426	0.09276	-3.6888
H	3.71184	-1.3488	-1.0467
H	2.78876	-2.0503	-2.3898
H	1.08918	-3.7589	0.79427
H	1.57408	-2.9197	2.27958

H	3.45481	-4.0937	0.15991
H	3.17285	-4.7652	1.7815
H	3.9954	-3.2037	1.59413
H	-1.5103	2.10899	-0.5727
H	-3.9464	2.49875	-0.148
H	-4.7563	-1.6191	-1.0291
H	-2.3184	-2.0039	-1.4796
O	1.36054	1.99694	-2.0835
H	1.53062	1.03986	-1.8529
O	-0.543	-1.7443	0.71899
H	-0.9465	-2.5235	0.30582
O	-0.5018	-2.0902	3.52418
H	0.07375	-1.3296	3.71816
H	-0.4253	-2.1494	2.5522
O	-2.0318	0.04492	2.46792
H	-1.8699	-0.7293	3.03411
H	-1.6818	-0.2715	1.61646
O	0.50644	3.07034	0.29884
H	0.88287	2.7229	-0.5377
H	1.10313	2.7516	1.00905
O	3.64803	0.91932	0.54088
H	2.84787	0.41852	0.29448
H	3.7187	1.63467	-0.1291
H	3.41238	3.77884	-0.4966
O	0.64237	0.47534	3.24516
H	0.82334	0.20386	2.3065
H	-0.3054	0.6952	3.17631
O	2.64717	4.81819	0.79957
H	1.73891	4.61956	0.51299
O	2.34476	2.47261	2.30411
H	2.89355	1.84697	1.76758
H	1.7877	1.90894	2.87442
O	0.87325	0.14677	0.64761
H	0.36359	0.88157	0.27743
H	2.73503	4.22049	1.56258
H	0.53727	1.97783	-2.5858
O	3.70717	3.10424	-1.1436
H	2.92619	2.92085	-1.6935
Transition State - 2			
63			
C	4.10667	-0.2009	-2.4836

C	3.00043	-1.1811	-2.1259
O	2.04149	-0.4831	-1.3459
P	0.8405	-1.2864	-0.3628
S	0.41949	-2.8694	-1.711
O	2.05252	-1.9409	0.58465
C	1.86727	-3.1419	1.31277
C	3.20587	-3.8501	1.40364
O	-0.4829	0.03109	-1.432
C	-1.7566	0.12945	-1.1628
C	-2.2927	1.3788	-0.7442
C	-3.6358	1.52583	-0.463
C	-4.4839	0.42367	-0.5925
C	-3.9966	-0.8225	-1.0009
C	-2.655	-0.9677	-1.2843
N	-5.885	0.57186	-0.2966
O	-6.2997	1.67274	0.05265
O	-6.616	-0.408	-0.404
H	4.8557	-0.6882	-3.1136
H	4.59211	0.17366	-1.5792
H	3.69721	0.65277	-3.0328
H	3.3949	-2.0216	-1.5437
H	2.53072	-1.5901	-3.0257
H	1.13576	-3.7821	0.80698
H	1.48089	-2.9128	2.31419
H	3.55803	-4.115	0.4025
H	3.11996	-4.7642	1.99731
H	3.95287	-3.2025	1.87056
H	-1.6038	2.20998	-0.6213
H	-4.0419	2.47569	-0.1363
H	-4.6829	-1.6558	-1.0937
H	-2.2486	-1.9198	-1.6082
O	1.41472	1.95763	-2.1256
H	1.69848	1.05356	-1.8259
O	-0.4915	-1.7242	0.66077
H	-0.9139	-2.4743	0.21397
O	-0.6671	-2.1125	3.45614
H	-0.1176	-1.3399	3.6766
H	-0.5279	-2.1762	2.49227
O	-2.1877	-0.0031	2.31615
H	-2.0174	-0.7885	2.86465
H	-1.8269	-0.2825	1.45734

O	0.48057	3.05972	0.24282
H	0.91361	2.71303	-0.5639
H	1.02664	2.73271	0.9894
O	3.67901	1.02544	0.61089
H	2.98163	0.44663	0.25117
H	3.74034	1.76338	-0.0366
H	3.31892	3.8857	-0.3888
O	0.44958	0.45707	3.17244
H	0.70098	0.18562	2.25478
H	-0.4966	0.65947	3.04361
O	2.50202	4.86701	0.91536
H	1.61761	4.63859	0.57916
O	2.20347	2.46089	2.33304
H	2.78224	1.8519	1.80827
H	1.62575	1.88714	2.87058
O	0.90927	0.15328	0.57533
H	0.3521	0.82317	0.14964
H	2.58193	4.24332	1.6583
H	0.50096	1.77624	-2.3899
O	3.6542	3.23045	-1.036
H	2.90106	3.03531	-1.6169
Product			
63			
C	4.54957	1.13334	-1.4041
C	3.51211	0.10127	-1.8183
O	2.39438	0.23491	-0.9636
P	1.24475	-1.1201	-0.6695
S	0.70138	-1.3065	-2.6312
O	2.556	-1.9437	-0.1068
C	2.71386	-3.3537	-0.2506
C	4.20087	-3.6481	-0.2839
O	-0.8992	1.62927	-0.3393
C	-2.1674	1.20897	-0.3645
C	-2.4985	-0.1332	-0.1057
C	-3.8207	-0.5371	-0.1077
C	-4.8128	0.40034	-0.3888
C	-4.5076	1.73362	-0.6622
C	-3.1851	2.13662	-0.6478
N	-6.2013	-0.02	-0.3948
O	-6.4546	-1.1905	-0.1461
O	-7.0599	0.81381	-0.6488

H	5.4249	1.09709	-2.0581
H	4.86663	0.95049	-0.3732
H	4.11798	2.13896	-1.4559
H	3.9253	-0.9115	-1.7399
H	3.20456	0.25645	-2.861
H	2.23633	-3.6948	-1.177
H	2.23787	-3.8651	0.59072
H	4.67075	-3.1699	-1.1472
H	4.36965	-4.726	-0.3494
H	4.68346	-3.2764	0.62342
H	-1.6976	-0.8343	0.0941
H	-4.0822	-1.5653	0.11054
H	-5.3054	2.4337	-0.8763
H	-2.9148	3.16737	-0.8488
O	1.29214	2.47758	-1.9138
H	1.65692	1.63125	-1.552
O	0.15656	-2.4662	-0.162
H	0.01793	-3.0221	-0.9409
O	0.4343	-3.637	2.36734
H	0.36361	-2.7577	2.78081
H	0.46489	-3.3856	1.42326
O	-2.1479	-2.8959	1.48628
H	-1.5795	-3.4651	2.03206
H	-1.5494	-2.7144	0.73873
O	-0.0298	3.48469	1.63405
H	-0.4862	2.99274	0.93273
H	0.28054	2.77246	2.2483
O	3.07741	0.9691	1.67396
H	2.72535	0.72158	0.79564
H	3.55889	1.81121	1.53007
H	3.49004	3.75613	0.73284
O	-0.3991	-0.9832	2.68222
H	-0.0256	-0.7723	1.78196
H	-1.2689	-1.3669	2.4803
O	2.06833	4.21125	0.0566
H	1.35394	4.00809	0.70441
O	0.89026	1.49159	3.17505
H	1.68283	1.24572	2.63653
H	0.30188	0.71864	3.12749
O	0.56846	-0.1858	0.39381
H	-0.2309	0.84755	-0.0357

H	1.85125	3.63363	-0.7091
H	0.34754	2.40715	-1.7113
O	4.297	3.39428	1.19502
H	4.96236	3.29547	0.50538

Parathion + 1OH^- + 10 Water Molecules

Parathion to the parathion pentacoordinate intermediate - Figure 2(b)			
Reactant			
64			
C	0.23381	-1.6658	2.76002
C	-0.4757	-0.4816	2.13643
O	-0.1023	-0.2685	0.74047
P	-0.5399	-1.2746	-0.4085
S	-0.3947	-0.489	-2.1735
O	0.22205	-2.6468	-0.1689
C	1.68023	-2.6171	-0.1958
C	2.18102	-3.9347	0.33796
O	-2.0115	-1.812	0.01466
C	-3.1571	-1.0508	-0.1023
C	-4.3366	-1.7622	-0.3145
C	-5.5368	-1.0753	-0.4029
C	-5.5181	0.30994	-0.2811
C	-4.3465	1.02517	-0.0705
C	-3.1428	0.33903	0.02581
N	-6.7819	1.04092	-0.3793
O	-7.8025	0.39745	-0.557
O	-6.75	2.25587	-0.2785
H	0.01802	-1.6726	3.83168
H	1.31605	-1.5867	2.62321
H	-0.1115	-2.6114	2.33626
H	-0.1985	0.45378	2.62149
H	-1.5634	-0.5895	2.18329
H	2.02911	-1.7906	0.42967
H	1.99877	-2.4485	-1.2288
H	1.86716	-4.0705	1.37521
H	3.27183	-3.9237	0.30171
H	1.80873	-4.7665	-0.2643
H	-4.2962	-2.8407	-0.4072
H	-6.4721	-1.5943	-0.5675
H	-4.378	2.10354	0.02029

H	-2.2228	0.89649	0.19201
O	1.61586	2.75201	-0.69
H	2.05036	1.82695	-0.8786
O	2.67187	0.4917	-0.9951
H	1.95051	0.01331	-1.427
O	4.4296	-1.5608	-0.5047
H	5.27969	-1.1712	-0.788
H	3.78168	-0.8439	-0.6915
O	6.47891	0.02409	-1.5257
H	6.34533	0.75516	-0.9001
H	5.86002	0.27758	-2.2404
O	4.96696	2.07743	-0.4208
H	4.23106	1.44327	-0.4506
H	4.681	2.73779	0.23204
O	0.73123	2.52599	2.62542
H	1.44621	3.15409	2.43943
H	0.08486	2.64783	1.89695
O	-0.8562	2.61338	0.39787
H	-0.0243	2.59459	-0.1329
H	-1.2497	3.4756	0.21868
O	4.39475	1.14045	-3.0119
H	3.69746	0.82007	-2.3898
H	4.66774	1.96137	-2.5769
O	3.81237	-1.7824	2.20917
H	3.39343	-0.9052	2.24286
H	4.14279	-1.8098	1.28953
O	3.25381	3.36565	1.42395
H	3.25855	2.42354	1.68581
H	2.6675	3.3421	0.6351
O	2.58663	0.6704	1.66794
H	2.47603	0.51978	0.69164
H	1.76664	1.09808	1.9839
H	1.6923	3.26622	-1.5023
Transition State			
64			
C	-0.28	-1.3978	-2.8662
C	0.29468	-0.1597	-2.212
O	-0.2361	0.05204	-0.8783
P	0.06721	-0.9001	0.37478
S	0.45302	-0.1441	2.15882
O	-0.6558	-2.3111	0.25769

C	-2.0016	-2.5782	-0.1913
C	-2.0259	-3.9724	-0.7738
O	1.51974	-1.5604	-0.1253
C	2.74244	-0.974	0.01435
C	3.81085	-1.8322	0.28817
C	5.09564	-1.3242	0.38931
C	5.2841	0.04324	0.21757
C	4.23146	0.90963	-0.0556
C	2.94582	0.39942	-0.1602
N	6.63473	0.58654	0.32581
O	7.54873	-0.1877	0.56085
O	6.78491	1.78862	0.1761
H	0.09738	-1.4681	-3.8896
H	-1.3724	-1.3511	-2.9004
H	0.02679	-2.298	-2.3268
H	0.00802	0.74903	-2.7432
H	1.38503	-0.1972	-2.1656
H	-2.2944	-1.8397	-0.936
H	-2.6711	-2.4893	0.66457
H	-1.3636	-4.0477	-1.6396
H	-3.0447	-4.1953	-1.1003
H	-1.7239	-4.7163	-0.033
H	3.61392	-2.8898	0.41716
H	5.94095	-1.9662	0.60115
H	4.42326	1.96696	-0.1877
H	2.11784	1.06723	-0.3844
O	-1.2071	2.36607	0.63754
H	-1.5377	1.39228	0.73875
O	-2.1516	0.01154	0.73205
H	-2.3056	-0.2533	1.64961
O	-4.6652	-0.9855	0.03766
H	-4.9735	-1.0757	0.9563
H	-3.754	-0.6465	0.1588
O	-5.0848	-0.4577	2.76968
H	-5.15	0.4487	2.42484
H	-4.218	-0.4397	3.20776
O	-4.0924	1.85912	1.59533
H	-3.5607	1.22249	1.07587
H	-4.1551	2.63331	1.013
O	-1.3713	2.9236	-2.8175
H	-1.9905	3.45525	-2.2919

H	-0.5352	2.93715	-2.3039
O	0.78528	2.68976	-1.1391
H	0.13465	2.47862	-0.4245
H	1.17242	3.53709	-0.8881
O	-2.5946	0.64749	3.6298
H	-1.6593	0.54957	3.39205
H	-2.9301	1.38127	3.08514
O	-4.0287	-1.6237	-2.6101
H	-3.6423	-0.7309	-2.5824
H	-4.4408	-1.6766	-1.7315
O	-3.3537	3.36573	-0.7058
H	-3.5151	2.50288	-1.131
H	-2.5439	3.18336	-0.1794
O	-2.8569	0.82651	-1.87
H	-2.3919	0.49808	-1.0789
H	-2.2134	1.40393	-2.3358
H	-0.9419	2.65709	1.51811
Product			
64			
C	0.21879	-0.8381	3.11467
C	-0.4499	0.18011	2.21244
O	0.14987	0.20029	0.90379
P	0.15318	-1.0225	-0.2011
S	-0.4596	-0.8271	-2.1358
O	0.64955	-2.4518	0.38957
C	2.01255	-2.7721	0.70589
C	1.995	-4.127	1.38198
O	-1.4409	-1.5886	0.37873
C	-2.6172	-1.0088	0.13093
C	-3.7418	-1.8544	0.0918
C	-5.0098	-1.3395	-0.1026
C	-5.1562	0.03672	-0.2651
C	-4.0617	0.89803	-0.2299
C	-2.7934	0.38029	-0.0346
N	-6.483	0.58683	-0.4703
O	-7.434	-0.1824	-0.489
O	-6.5945	1.79635	-0.6159
H	-0.1696	-0.7387	4.13175
H	1.30204	-0.6803	3.1351
H	0.01588	-1.8513	2.75933
H	-0.2997	1.20026	2.57511

H	-1.5238	0.00754	2.13577
H	2.43087	-2.0101	1.37169
H	2.6093	-2.7994	-0.2113
H	1.4087	-4.0881	2.30345
H	3.01532	-4.4277	1.63177
H	1.56006	-4.8824	0.72343
H	-3.5872	-2.9197	0.21919
H	-5.8804	-1.9825	-0.1345
H	-4.2142	1.96347	-0.3507
H	-1.9418	1.05023	0.01055
O	0.9685	2.06858	-1.33
H	1.40539	1.25726	-0.9941
O	1.76592	-0.4576	-0.5381
H	2.04381	-0.7008	-1.4491
O	4.45679	-0.485	0.14869
H	4.78023	-1.0017	-0.6174
H	3.48213	-0.5294	0.10108
O	5.26674	-1.205	-2.3965
H	5.48487	-0.2731	-2.5449
H	4.40258	-1.2904	-2.8322
O	4.25823	1.45737	-1.8398
H	4.37918	0.95151	-1.0111
H	4.02473	2.35579	-1.5484
O	1.46747	4.00824	2.07835
H	2.01197	4.33228	1.34395
H	0.60752	3.795	1.65741
O	-0.6791	3.00624	0.7022
H	-0.132	2.59	0.00183
H	-1.2034	3.67412	0.24379
O	2.72611	-0.3791	-3.0785
H	1.81859	-0.2513	-3.3927
H	3.08778	0.49048	-2.7973
O	3.81927	-0.537	2.88079
H	3.39101	0.28565	2.58412
H	4.3304	-0.7771	2.09292
O	3.07435	3.5651	-0.3673
H	3.05435	2.81414	0.26084
H	2.27477	3.40636	-0.898
O	2.5247	1.56807	1.52412
H	1.79108	1.03281	1.16684
H	2.1059	2.33909	1.96963

H	0.36062	1.71634	-1.9987
Parathion pentacoordinate intermediate to paraoxon - Figure 3(b)			
Reactant			
64			
C	-4.9474	2.24049	-0.1403
C	-4.4786	0.80678	-0.2935
O	-3.0476	0.83025	-0.456
P	-2.0996	-0.4841	-0.0744
S	-2.0957	-1.0322	1.8809
O	-3.3397	-1.4557	-0.6613
C	-3.3286	-2.8625	-0.4843
C	-4.3127	-3.4661	-1.4692
O	-1.1079	-1.3316	-1.167
C	0.2385	-1.4789	-1.0291
C	1.09529	-0.8358	-1.9268
C	2.46467	-0.9998	-1.8044
C	2.95438	-1.8045	-0.7802
C	2.11816	-2.4804	0.09931
C	0.74543	-2.3282	-0.0418
N	4.39886	-1.9161	-0.6095
O	5.11852	-1.4364	-1.469
O	4.81614	-2.4869	0.38543
H	-6.0247	2.25621	0.04141
H	-4.746	2.82602	-1.0411
H	-4.4447	2.71851	0.70491
H	-4.9313	0.32181	-1.1602
H	-4.7267	0.21824	0.5943
H	-3.6124	-3.1008	0.54772
H	-2.322	-3.2624	-0.6556
H	-5.3129	-3.0549	-1.3091
H	-4.3603	-4.5508	-1.3438
H	-4.0095	-3.2461	-2.4958
H	0.67563	-0.1831	-2.6829
H	3.15199	-0.4866	-2.4649
H	2.53661	-3.1043	0.87953
H	0.05672	-2.8466	0.6155
O	-2.1956	3.41996	-1.3436
H	-2.6099	2.54756	-1.2237
O	-0.8027	0.66257	-0.0186
H	-1.0722	1.44503	0.51221

O	1.43059	0.45305	1.65993
H	0.95023	0.6172	2.50826
H	0.7206	0.31665	0.99696
O	1.57571	3.10364	0.8592
H	1.65976	2.22425	1.27735
H	0.62937	3.32829	0.96751
O	3.94738	0.82584	0.38365
H	3.23722	0.57847	1.0001
H	3.45959	1.04409	-0.4311
O	4.25948	3.63984	0.11757
H	3.39899	3.84357	0.51616
H	4.38602	2.71028	0.37961
O	0.8612	-2.0047	3.13127
H	-0.0102	-2.0001	2.69855
H	1.38566	-1.4401	2.54061
O	-0.0454	0.54482	3.93117
H	0.25544	-0.3685	4.08863
H	-0.8735	0.4078	3.43726
O	-0.182	2.00465	-2.4378
H	0.76841	2.21635	-2.4049
H	-0.3282	1.45963	-1.6388
O	2.43784	2.26964	-1.5569
H	3.1876	2.88671	-1.5795
H	-1.4094	3.19476	-1.8862
O	-1.1536	3.14481	1.05031
H	-1.5878	3.43897	0.20358
H	-1.6992	3.44766	1.78446
H	1.98013	2.56821	-0.7345
Transition State			
64			
C	-3.5333	1.31112	-3.41
C	-3.67	0.31443	-2.2773
O	-2.5605	0.55349	-1.396
P	-2.1994	-0.2467	-0.0221
S	-2.8339	0.57788	1.85496
O	-3.6018	-1.1699	-0.1659
C	-3.867	-2.2379	0.73367
C	-3.9542	-3.5469	-0.0298
O	-1.3652	-1.6995	-0.2217
C	-0.0144	-1.8216	-0.3432
C	0.67207	-1.1931	-1.3869

C	2.03989	-1.3655	-1.5046
C	2.69452	-2.1761	-0.581
C	2.02361	-2.8311	0.44323
C	0.65052	-2.6561	0.55542
N	4.14227	-2.3253	-0.6861
O	4.7042	-1.8204	-1.6435
O	4.72046	-2.9524	0.18683
H	-4.3589	1.19333	-4.1156
H	-2.59	1.15904	-3.9391
H	-3.5469	2.33305	-3.0214
H	-3.6315	-0.7168	-2.6348
H	-4.604	0.44964	-1.7272
H	-4.8137	-2.0208	1.24257
H	-3.0909	-2.3034	1.5061
H	-4.7202	-3.4828	-0.807
H	-4.214	-4.3676	0.64445
H	-2.994	-3.7663	-0.5018
H	0.13418	-0.5495	-2.0741
H	2.60229	-0.8639	-2.2821
H	2.57193	-3.4543	1.13808
H	0.08649	-3.1311	1.35057
O	-1.9344	3.3186	-0.8549
H	-2.3971	2.46453	-0.8587
O	-0.8597	0.65548	0.20263
H	-1.5309	1.12097	1.37914
O	1.47045	0.34477	1.57179
H	1.14485	0.84645	2.35935
H	0.70822	0.38131	0.94471
O	2.01102	2.95434	0.67988
H	2.0623	2.07215	1.08895
H	1.09774	3.25161	0.88807
O	4.01754	0.38452	0.36001
H	3.24632	0.23147	0.93542
H	3.60324	0.60664	-0.4934
O	4.73286	3.10343	-0.085
H	3.91565	3.46559	0.28998
H	4.71205	2.18636	0.24185
O	-0.3938	-1.1545	3.27154
H	-1.228	-0.9859	2.80688
H	0.29471	-1.0141	2.60155
O	0.18455	1.67726	3.5142

H	-0.3465	0.88296	3.68908
H	-0.3308	2.24376	2.90977
O	-0.0518	1.88619	-2.1762
H	0.9146	1.93676	-2.2527
H	-0.2338	1.38889	-1.3488
O	2.72378	1.87624	-1.6818
H	3.54531	2.37943	-1.7954
H	-1.1868	3.11461	-1.4554
O	-0.5727	3.41297	1.44389
H	-1.1275	3.30985	0.62325
H	-0.7498	4.30637	1.76296
H	2.34264	2.31469	-0.8839
Product			
64			
C	3.69619	-0.3227	3.41631
C	3.42662	-1.141	2.17651
O	2.24497	-0.5633	1.553
P	1.6786	-1.0289	0.16933
S	4.64045	1.22068	-0.3332
O	2.91782	-1.6365	-0.5819
C	2.74256	-2.2979	-1.8678
C	2.89219	-3.7905	-1.6865
O	0.74733	-2.3319	0.42069
C	-0.6327	-2.1847	0.36739
C	-1.3046	-1.6342	1.45282
C	-2.6791	-1.4547	1.3701
C	-3.3301	-1.8491	0.2084
C	-2.6692	-2.4279	-0.8681
C	-1.2939	-2.5955	-0.7861
N	-4.772	-1.6167	0.10137
O	-5.3194	-1.0055	1.00237
O	-5.3488	-2.0481	-0.881
H	4.60264	-0.6856	3.90551
H	2.86331	-0.3981	4.11878
H	3.83339	0.72572	3.14089
H	3.21596	-2.1889	2.40686
H	4.24664	-1.0724	1.45987
H	3.50824	-1.8699	-2.5141
H	1.7664	-2.0305	-2.2852
H	3.86684	-4.0239	-1.253
H	2.81483	-4.2854	-2.6573

H	2.10947	-4.178	-1.0308
H	-0.7484	-1.318	2.32712
H	-3.2347	-0.9915	2.17427
H	-3.2223	-2.7171	-1.7522
H	-0.7296	-3.0264	-1.6054
O	2.34761	2.41617	1.5745
H	2.98441	1.8617	1.06718
O	0.90186	0.03774	-0.5236
H	5.07449	2.4906	-0.4299
O	-1.2427	1.12103	-1.9816
H	-0.5726	1.69774	-2.4359
H	-0.6977	0.49301	-1.4799
O	-1.6283	3.16647	-0.1794
H	-1.5531	2.46842	-0.8649
H	-0.708	3.48427	-0.0474
O	-3.8665	0.90126	-0.8829
H	-3.0821	0.93591	-1.457
H	-3.4974	0.90076	0.02023
O	-4.4449	3.49776	0.10916
H	-3.534	3.79576	-0.0375
H	-4.466	2.66989	-0.403
O	2.58033	0.73816	-2.7425
H	3.3186	0.95836	-2.1281
H	1.90315	0.42808	-2.1199
O	0.71133	2.75857	-2.7796
H	1.48123	2.1739	-2.9345
H	0.89165	3.1656	-1.908
O	-0.1178	1.15243	1.92929
H	-1.0347	1.31033	2.20379
H	-0.1622	0.96164	0.98088
O	-2.8475	1.68925	1.64828
H	-3.663	2.1905	1.79753
H	1.64227	1.82112	1.88722
O	1.0126	3.7798	-0.2047
H	1.55651	3.26997	0.46935
H	1.27401	4.70414	-0.1259
H	-2.3415	2.30007	1.05254
Parathion pentacoordinate intermediate to 4-nitrophenol - Figure 4(b)			
Reactant			
64			

C	-3.4919	-0.6529	1.93383
C	-2.4093	-1.4904	1.28274
O	-1.7567	-0.695	0.28714
P	-0.1578	-1.0832	-0.1897
S	-0.0396	0.33887	-1.596
O	0.4651	-0.8071	1.29797
C	0.05383	0.3379	2.07172
C	1.22289	0.74129	2.94316
O	1.47873	-1.8748	-0.5499
C	2.63605	-1.1833	-0.5097
C	3.17779	-0.6674	-1.6978
C	4.37723	0.02562	-1.6779
C	5.03114	0.19249	-0.4605
C	4.52881	-0.3265	0.72872
C	3.32911	-1.0183	0.7001
N	6.28844	0.92761	-0.4321
O	6.72342	1.37089	-1.4844
O	6.85195	1.06849	0.64302
H	-4.0372	-1.2458	2.67333
H	-4.1959	-0.3046	1.17445
H	-3.0663	0.21961	2.43834
H	-2.8457	-2.3763	0.80683
H	-1.681	-1.8457	2.02263
H	-0.8208	0.06587	2.66993
H	-0.2208	1.15432	1.39853
H	1.54822	-0.094	3.57007
H	0.92059	1.56423	3.59716
H	2.04809	1.0761	2.31091
H	2.63424	-0.8149	-2.6226
H	4.8082	0.43535	-2.5826
H	5.07595	-0.186	1.65244
H	2.91245	-1.4479	1.60267
O	-0.6952	-2.6097	-0.4845
H	0.029	-3.1535	-0.829
O	-3.2934	0.38405	-2.1868
H	-3.2604	-0.5918	-2.1968
O	1.37382	-3.4436	1.92344
H	0.94465	-2.64	2.24466
H	1.58085	-3.1866	1.01269
O	-5.5848	-2.0446	-0.3504
H	-5.503	-2.377	0.55031

H	-4.7395	-2.261	-0.7898
O	-0.2186	3.56228	0.78319
H	-0.2697	3.68577	1.7377
H	-1.0204	3.0415	0.55667
O	2.20416	2.22835	0.15683
H	1.36576	2.68526	0.3584
H	1.91179	1.42948	-0.3036
O	-4.8785	2.49721	1.37412
H	-4.9248	3.20491	0.70963
H	-5.2153	1.73907	0.84853
O	-5.4363	0.70305	-0.5975
H	-5.7127	-0.2264	-0.4729
H	-4.5772	0.61538	-1.0774
O	-2.4393	2.05305	0.23089
H	-2.2052	1.10462	0.20624
H	-3.2034	2.14306	0.84305
O	-4.4966	3.3123	-1.3194
H	-5.1111	2.58364	-1.4855
H	-3.6659	2.85729	-1.0965
O	-3.2062	-2.3766	-1.7682
H	-3.2312	-3.0267	-2.4806
H	-2.3464	-2.4953	-1.3221
H	-2.4118	0.62231	-1.8515
Transition State			
64			
C	-3.5771	-0.7145	1.97151
C	-2.5158	-1.5356	1.27241
O	-1.871	-0.6899	0.29692
P	-0.3245	-1.0303	-0.183
S	-0.0177	0.3512	-1.5498
O	0.41288	-0.9087	1.24657
C	0.10044	0.22928	2.09216
C	1.27668	0.4404	3.01587
O	1.64838	-2.0218	-0.6391
C	2.74292	-1.3048	-0.5845
C	3.25386	-0.6644	-1.7422
C	4.39513	0.11182	-1.6834
C	5.05049	0.26331	-0.46
C	4.58437	-0.3571	0.70035
C	3.4437	-1.1323	0.63674
N	6.23799	1.08235	-0.3935

O	6.63744	1.61995	-1.42
O	6.80238	1.20926	0.68707
H	-4.1136	-1.3345	2.69413
H	-4.2893	-0.3301	1.23818
H	-3.131	0.13037	2.50439
H	-2.9569	-2.3895	0.74871
H	-1.7708	-1.9214	1.97701
H	-0.8169	0.00576	2.64476
H	-0.0676	1.11258	1.46821
H	1.48939	-0.4685	3.58555
H	1.04161	1.24306	3.72
H	2.15202	0.7279	2.43069
H	2.71931	-0.7963	-2.6756
H	4.78702	0.60561	-2.5642
H	5.11959	-0.219	1.63207
H	3.05853	-1.632	1.5187
O	-0.6818	-2.5674	-0.5437
H	0.11952	-2.9963	-0.8954
O	-3.3016	0.46614	-2.1762
H	-3.2347	-0.5081	-2.1803
O	1.43432	-3.5555	1.7065
H	0.96428	-2.8681	2.19275
H	1.58788	-3.1088	0.8517
O	-5.6122	-1.967	-0.441
H	-5.5996	-2.3977	0.42064
H	-4.7685	-2.2023	-0.8712
O	-0.1226	3.45597	0.68995
H	-0.1669	3.67315	1.6281
H	-0.9601	2.97824	0.50602
O	2.32327	2.08337	0.35785
H	1.45071	2.51771	0.40184
H	2.14282	1.24107	-0.0807
O	-4.8689	2.56205	1.46062
H	-4.9446	3.27563	0.80493
H	-5.2063	1.80354	0.93735
O	-5.4147	0.78231	-0.5347
H	-5.7158	-0.1444	-0.4577
H	-4.5646	0.69665	-1.0284
O	-2.4699	2.09902	0.26808
H	-2.309	1.13962	0.23698
H	-3.2149	2.23387	0.89736

O	-4.5589	3.40836	-1.229
H	-5.1669	2.67021	-1.379
H	-3.7162	2.96425	-1.0338
O	-3.2173	-2.3225	-1.849
H	-3.2979	-2.8963	-2.6209
H	-2.3622	-2.5408	-1.4386
H	-2.421	0.7478	-1.8817
Product			
64			
C	-3.0007	-1.0413	2.22128
C	-1.9881	-1.6176	1.25852
O	-1.6865	-0.5992	0.27124
P	-0.248	-0.7024	-0.4863
S	-0.1853	0.76128	-1.8105
O	0.79799	-0.4579	0.73452
C	0.53877	0.5881	1.70093
C	1.80945	0.8126	2.48874
O	2.26239	-3.2453	-0.3043
C	3.01098	-2.1198	-0.3658
C	2.94323	-1.2716	-1.4794
C	3.64046	-0.0755	-1.4803
C	4.40336	0.25372	-0.365
C	4.52569	-0.6002	0.7273
C	3.83644	-1.8014	0.71818
N	5.06793	1.54713	-0.3276
O	5.1534	2.18337	-1.3649
O	5.51527	1.93214	0.7428
H	-3.2745	-1.7924	2.96628
H	-3.8951	-0.7383	1.67432
H	-2.5917	-0.1699	2.7405
H	-2.3875	-2.4864	0.72838
H	-1.0653	-1.9222	1.76478
H	-0.2828	0.2589	2.34697
H	0.23099	1.49803	1.17691
H	2.15048	-0.1215	2.94511
H	1.61949	1.53857	3.28363
H	2.5868	1.20283	1.82873
H	2.30692	-1.54	-2.3156
H	3.57499	0.61564	-2.3118
H	5.13101	-0.3055	1.57557
H	3.86543	-2.4695	1.57114

O	-0.0526	-2.1345	-0.9457
H	1.38236	-3.026	-0.7036
O	-3.4358	0.22655	-2.0795
H	-3.1608	-0.7109	-2.0933
O	1.25396	-2.7844	2.35998
H	1.20955	-1.9565	1.85733
H	1.54128	-3.4045	1.67542
O	-4.9238	-2.5043	-0.2004
H	-4.799	-3.0672	0.57115
H	-4.1148	-2.6026	-0.7374
O	-0.2471	3.7364	0.37553
H	-0.2629	4.02175	1.29618
H	-1.0355	3.16177	0.28378
O	2.25074	2.49827	-0.251
H	1.42606	2.9815	-0.0532
H	1.91721	1.65798	-0.5952
O	-4.8069	2.19052	1.83011
H	-5.1254	2.82484	1.16583
H	-5.0244	1.34453	1.38631
O	-5.2016	0.23763	-0.0539
H	-5.3518	-0.7253	0.00593
H	-4.4452	0.28914	-0.6849
O	-2.5491	2.14969	0.29423
H	-2.3166	1.20841	0.22605
H	-3.1912	2.20174	1.03674
O	-5.0589	2.94601	-0.8917
H	-5.4905	2.07954	-0.9264
H	-4.1177	2.71797	-0.8004
O	-2.6571	-2.4924	-1.8517
H	-2.7181	-3.0299	-2.6504
H	-1.7199	-2.5321	-1.5637
H	-2.595	0.70169	-1.9834

Paraoxon + 2OH$^-$ + 9 Water Molecules

Paraoxon to the paraoxon pentacoordinate intermediate - Figure 6(a)			
Reactant			
63			
C	-0.9251	0.89781	2.1809
C	-0.2228	-0.3091	1.6025
O	0.264	0.06062	0.28725

P	0.75501	-0.9983	-0.7646
O	1.86892	-0.5837	-1.6553
O	0.84595	-2.4108	-0.0647
C	2.09294	-3.1372	0.11067
C	2.25946	-3.4768	1.57158
O	-0.5493	-1.2043	-1.7251
C	-1.8198	-1.2228	-1.1873
C	-2.4667	-2.444	-1.0122
C	-3.7548	-2.4529	-0.4931
C	-4.3464	-1.239	-0.1581
C	-3.705	-0.0159	-0.3271
C	-2.4248	-0.0119	-0.859
N	-5.6991	-1.2523	0.40088
O	-6.2529	-2.3307	0.54
O	-6.2061	-0.1841	0.70002
H	-1.3653	0.62672	3.14473
H	-1.7143	1.25128	1.51226
H	-0.2063	1.70266	2.33947
H	-0.9089	-1.1568	1.49927
H	0.64661	-0.6065	2.19163
H	2.91669	-2.5162	-0.237
H	2.00602	-4.0298	-0.5137
H	2.33027	-2.5484	2.13995
H	3.18434	-4.0434	1.70752
H	1.42157	-4.0782	1.9331
H	-1.9593	-3.3638	-1.2786
H	-4.295	-3.3783	-0.3407
H	-4.1796	0.91452	-0.0405
H	-1.8641	0.90774	-0.9923
O	-0.3387	2.56763	-1.2288
H	-0.1569	1.96033	-1.9537
O	3.35202	1.77735	-1.0728
H	2.81497	1.06523	-1.4575
O	2.92097	-0.4877	1.09106
H	3.06229	0.09573	0.3337
O	5.12025	-1.6877	1.06049
H	4.18612	-1.2262	1.14399
H	5.08417	-2.047	0.1615
O	5.75887	0.58926	-0.4011
H	5.61243	-0.0801	0.30052
H	4.92189	1.09149	-0.4732

O	-2.5814	3.10179	0.05379
H	-2.1112	3.58793	0.75261
H	-1.8009	2.76731	-0.4694
O	-1.0873	4.99421	-1.5612
H	-0.6838	4.06276	-1.5834
H	-1.989	4.77311	-1.2861
O	4.59673	-1.5114	-1.8298
H	3.66367	-1.2441	-1.7919
H	5.08069	-0.7258	-1.5067
O	2.14887	1.26051	2.66185
H	2.91937	1.80636	2.85571
H	2.51287	0.48298	2.03508
O	-0.4778	4.72461	1.17751
H	0.26261	4.09141	1.07781
H	-0.6273	5.00984	0.25441
O	1.45885	2.83192	0.48039
H	1.52751	2.16439	1.19693
H	0.7029	2.57767	-0.1974
H	2.71557	2.25482	-0.4767
Transition State			
63			
C	-0.931	0.78855	2.41382
C	-0.3396	-0.3841	1.66497
O	0.17647	0.13111	0.41787
P	0.72397	-0.8263	-0.7175
O	1.79595	-0.3818	-1.6544
O	0.59421	-2.3383	-0.2597
C	1.68943	-3.2682	-0.0996
C	1.7982	-3.6785	1.35064
O	-0.6013	-0.7939	-1.7267
C	-1.8649	-0.8898	-1.2086
C	-2.4676	-2.1418	-1.0733
C	-3.7565	-2.2246	-0.5653
C	-4.406	-1.0489	-0.2027
C	-3.8172	0.20535	-0.3353
C	-2.5324	0.28221	-0.8491
N	-5.7605	-1.1357	0.34016
O	-6.2665	-2.241	0.45125
O	-6.3202	-0.0985	0.65645
H	-1.4338	0.42997	3.3162
H	-1.6483	1.32166	1.78368

H	-0.1328	1.47452	2.70307
H	-1.1002	-1.1417	1.44496
H	0.48689	-0.8492	2.20731
H	2.60987	-2.805	-0.4511
H	1.43978	-4.1184	-0.7394
H	2.04848	-2.8081	1.95845
H	2.58995	-4.4239	1.4611
H	0.85716	-4.1135	1.6976
H	-1.9163	-3.0302	-1.358
H	-4.2562	-3.1772	-0.4447
H	-4.3539	1.09619	-0.0345
H	-2.0194	1.23005	-0.9621
O	0.0151	2.56492	-1.2014
H	0.04716	1.78853	-1.7703
O	3.62588	1.62217	-0.8591
H	3.03367	1.03495	-1.3584
O	2.61041	-0.778	0.85084
H	3.01892	-0.0925	0.30356
O	4.71276	-2.2081	1.00333
H	3.83076	-1.6824	1.0169
H	4.75306	-2.4805	0.07425
O	5.80533	0.07411	-0.1916
H	5.51205	-0.6087	0.44497
H	5.06233	0.70715	-0.269
O	-2.0108	3.32588	0.31281
H	-1.4726	3.88832	0.89577
H	-1.2919	2.88916	-0.2263
O	-0.7011	4.98578	-1.6388
H	-0.3264	4.04893	-1.6625
H	-1.5465	4.79995	-1.2029
O	4.37142	-1.6785	-1.8487
H	3.48818	-1.2832	-1.7472
H	4.97145	-1.0194	-1.4491
O	2.17769	0.8816	2.70573
H	3.0432	1.26869	2.8799
H	2.35697	0.14772	1.99816
O	0.20026	4.97638	1.05528
H	0.81256	4.2104	1.01748
H	0.0086	5.14733	0.11272
O	1.70796	2.7052	0.5912
H	1.64066	2.01636	1.28194

H	0.97589	2.5273	-0.1604
H	2.99139	2.11669	-0.2689
Product			
63			
C	-0.5388	1.42466	2.56475
C	-0.3403	0.11574	1.82972
O	0.15308	0.43384	0.52136
P	0.65029	-0.7587	-0.4958
O	1.57184	-0.3783	-1.657
O	-0.1264	-2.1664	-0.2799
C	0.39625	-3.3855	0.26176
C	0.27962	-3.4484	1.77177
O	-0.779	-0.3288	-1.5454
C	-2.0336	-0.3656	-1.0928
C	-2.82	-1.5209	-1.2761
C	-4.1404	-1.5524	-0.8658
C	-4.6826	-0.4187	-0.2611
C	-3.9328	0.73999	-0.0659
C	-2.6123	0.76605	-0.4829
N	-6.0669	-0.4457	0.17334
O	-6.7141	-1.4687	-0.007
O	-6.5308	0.55534	0.70263
H	-1.0036	1.24296	3.53692
H	-1.1732	2.09301	1.97719
H	0.42775	1.91056	2.72728
H	-1.2854	-0.4306	1.7248
H	0.37784	-0.52	2.35389
H	1.42721	-3.5325	-0.0597
H	-0.2205	-4.1644	-0.1957
H	0.95562	-2.7337	2.24428
H	0.53452	-4.454	2.118
H	-0.7455	-3.2276	2.0822
H	-2.3608	-2.3851	-1.7413
H	-4.7546	-2.4338	-1.0029
H	-4.3912	1.60131	0.40465
H	-2.0035	1.65311	-0.3399
O	1.5136	2.42515	-1.6438
H	1.4263	1.483	-1.8833
O	3.88944	0.49469	-0.2666
H	3.40264	0.42354	-1.1023
O	1.91819	-1.2266	0.57187

H	2.70569	-0.6973	0.30277
O	3.77955	-3.3633	0.48504
H	3.12721	-2.7404	0.84715
H	3.63638	-3.2375	-0.4755
O	5.72595	-1.4941	-0.4469
H	5.28325	-2.1552	0.11354
H	5.23392	-0.67	-0.2573
O	-0.7014	3.52657	-0.198
H	-0.0967	3.85656	0.50009
H	-0.1378	2.88415	-0.6692
O	1.07514	5.16114	-1.6763
H	1.42912	4.30561	-1.9745
H	0.20971	4.88188	-1.331
O	3.5681	-2.3107	-2.0822
H	2.87017	-1.6362	-1.9543
H	4.39207	-1.9011	-1.7578
O	2.75847	0.35227	2.93574
H	2.79247	1.13823	2.35528
H	2.44408	-0.3326	2.32701
O	1.46907	4.60397	1.14152
H	1.93997	3.72094	1.09983
H	1.58762	4.97315	0.24987
O	2.46213	2.19584	0.85809
H	1.63316	1.69426	0.91165
H	1.96479	2.41079	-0.7587
H	3.37257	1.2536	0.24502
Paraoxon intermediate to 4-nitrophenol - Figure 7(a)			
Reactant			
63			
C	-3.6984	-0.8918	0.05623
C	-3.1545	-2.275	0.3746
O	-1.8085	-2.3091	0.84323
P	-0.5017	-1.727	-0.0628
O	0.56008	-2.3686	0.96783
C	0.294	-2.7528	2.33082
C	1.60972	-2.6508	3.07162
O	0.97477	-1.5182	-1.1629
C	2.03953	-0.7747	-0.9187
C	2.23023	-0.0017	0.24933
C	3.39101	0.73437	0.40591

C	4.36904	0.71545	-0.5878
C	4.20384	-0.0349	-1.7526
C	3.04781	-0.7707	-1.9104
N	5.57729	1.48842	-0.4102
O	5.71013	2.13848	0.61951
O	6.4223	1.46243	-1.297
H	-4.7695	-0.9773	-0.1509
H	-3.2184	-0.446	-0.8165
H	-3.557	-0.2165	0.90305
H	-3.2577	-2.9372	-0.4946
H	-3.744	-2.7182	1.18388
H	-0.0929	-3.7761	2.32488
H	-0.4458	-2.0853	2.76925
H	2.37307	-3.2776	2.60362
H	1.47993	-2.9759	4.10725
H	1.94714	-1.6119	3.06812
H	1.47578	0.02276	1.0251
H	3.54988	1.33048	1.29648
H	4.97754	-0.0324	-2.5102
H	2.88698	-1.3669	-2.8017
O	-3.15	-1.8518	-2.9785
H	-3.0731	-2.2736	-3.8425
O	-2.4204	2.0143	0.7965
H	-1.9326	1.20466	0.56686
O	-1.3592	-5.0574	0.39097
H	-1.573	-4.2021	0.79783
H	-1.1479	-4.7844	-0.5105
O	-1.5467	0.44489	-2.644
H	-2.0952	-0.3362	-2.8483
H	-1.1892	0.27033	-1.75
O	-0.9171	2.85557	3.17743
H	-1.7806	2.47595	2.95955
H	-0.7359	3.35715	2.3204
O	-0.0886	0.27422	2.71016
H	-0.2316	1.22223	2.91363
H	-0.4466	0.16978	1.8141
O	-3.9373	4.4771	0.7721
H	-3.4516	4.67357	-0.0524
H	-3.7101	3.55072	0.93877
O	-3.4401	2.24319	-1.7427
H	-2.806	1.64332	-2.1874

H	-3.2064	2.13516	-0.7936
O	-0.9491	4.02149	0.86002
H	-1.7377	2.82882	0.75723
H	-1.645	4.60998	1.18832
O	-2.1778	4.69457	-1.442
H	-2.5678	3.84534	-1.7327
H	-1.549	4.43453	-0.7224
O	-0.9865	-2.6721	-1.3279
H	-0.3105	-2.6113	-2.021
H	-2.5604	-2.3585	-2.3968
O	-0.8068	-0.2348	-0.0438
Transition State			
63			
C	-3.6564	-1.4507	-0.2767
C	-2.9328	-2.614	0.37443
O	-1.6858	-2.2612	0.99955
P	-0.4478	-1.6064	0.14114
O	0.70623	-1.9051	1.19351
C	0.46763	-2.14	2.60374
C	1.74731	-1.7764	3.32031
O	1.31292	-1.2592	-1.1308
C	2.35997	-0.5341	-0.9238
C	2.47132	0.37442	0.17036
C	3.61107	1.12783	0.34789
C	4.6772	1.0102	-0.5522
C	4.60269	0.13317	-1.6411
C	3.46645	-0.6218	-1.8212
N	5.85881	1.7979	-0.3586
O	5.90996	2.56193	0.60257
O	6.78366	1.68378	-1.1602
H	-4.6175	-1.8072	-0.6577
H	-3.0955	-1.0331	-1.1151
H	-3.8363	-0.6512	0.44479
H	-2.7489	-3.418	-0.3475
H	-3.5369	-3.0297	1.18439
H	0.21194	-3.196	2.72467
H	-0.3549	-1.5124	2.94413
H	2.58918	-2.3557	2.93323
H	1.64331	-1.9836	4.38848
H	1.94447	-0.7116	3.18153
H	1.64921	0.46787	0.86911

H	3.69553	1.81855	1.17876
H	5.43989	0.06029	-2.3249
H	3.3852	-1.3099	-2.656
O	-2.5316	-2.5489	-3.0779
H	-2.2722	-3.0249	-3.8759
O	-2.9968	1.57769	0.6672
H	-2.2974	0.92254	0.50326
O	-0.6293	-4.9464	0.92378
H	-1.1046	-4.2012	1.31537
H	-0.4167	-4.6054	0.04531
O	-1.4662	0.05923	-2.8692
H	-1.8228	-0.8344	-3.033
H	-1.0768	0.01412	-1.9761
O	-1.9498	2.69839	3.15749
H	-2.6197	2.06835	2.85445
H	-1.8909	3.28608	2.33562
O	-0.0264	0.88126	2.42982
H	-0.6436	1.57168	2.75516
H	-0.3095	0.70865	1.51985
O	-5.066	3.56182	0.24669
H	-4.5109	3.8847	-0.4891
H	-4.6415	2.7236	0.48113
O	-3.6447	1.55303	-2.021
H	-2.8994	1.05106	-2.4103
H	-3.4942	1.48934	-1.0527
O	-2.1283	3.89527	0.87241
H	-2.5513	2.54588	0.69348
H	-2.9964	4.27513	1.07301
O	-3.0508	4.23745	-1.6349
H	-3.1593	3.31627	-1.9459
H	-2.5218	4.14949	-0.8023
O	-0.52	-2.7075	-1.0509
H	0.26165	-2.5383	-1.6185
H	-1.9485	-2.8883	-2.3817
O	-0.8466	-0.1809	-0.1427
Product			
63			
C	3.13522	2.48546	1.26373
C	1.69247	2.75632	1.63896
O	0.88296	1.56139	1.56765
P	0.44263	0.99932	0.11747

O	-0.6962	-0.0362	0.53662
C	-0.3539	-1.2983	1.13906
C	-1.4207	-2.2957	0.74501
O	-2.0741	0.81813	-2.0964
C	-3.1306	0.41856	-1.3839
C	-3.9496	-0.5768	-1.9429
C	-5.0623	-1.0306	-1.2596
C	-5.3578	-0.4804	-0.0136
C	-4.5626	0.51339	0.55627
C	-3.449	0.96496	-0.1273
N	-6.524	-0.9524	0.70729
O	-7.2113	-1.8244	0.19335
O	-6.7716	-0.459	1.79915
H	3.73667	3.37697	1.46134
H	3.22958	2.23633	0.20525
H	3.53234	1.65145	1.84764
H	1.25112	3.52281	0.99312
H	1.60705	3.08964	2.67515
H	-0.3052	-1.1523	2.22275
H	0.62843	-1.6225	0.77901
H	-2.4111	-1.9264	1.02622
H	-1.2491	-3.252	1.24688
H	-1.3805	-2.4442	-0.3359
H	-3.6846	-0.9837	-2.912
H	-5.701	-1.8007	-1.6735
H	-4.825	0.91889	1.52553
H	-2.812	1.72646	0.312
O	1.80957	3.78033	-1.5388
H	1.57796	4.3261	-2.2989
O	3.55985	-0.8066	1.10477
H	2.82514	-0.3544	0.65538
O	-1.497	3.34448	1.57585
H	-1.0704	2.67162	2.12162
H	-1.1277	3.1534	0.69704
O	3.43967	1.58219	-2.1733
H	3.04357	2.46372	-2.0361
H	2.78398	1.00678	-1.7366
O	1.50754	-3.8939	-0.2447
H	1.13162	-3.9051	0.64144
H	2.48987	-3.5812	-0.1236
O	0.48643	-1.9842	-1.9438

H	0.79178	-2.6982	-1.3443
H	0.90961	-1.1921	-1.5781
O	6.01017	-1.9958	1.94091
H	6.20795	-2.0411	0.98497
H	5.21152	-1.4488	1.96053
O	5.38396	0.61365	-0.3755
H	4.80993	1.02981	-1.047
H	4.75207	0.15618	0.22615
O	3.86328	-3.0539	0.02483
H	3.63497	-1.7343	0.63398
H	4.29431	-3.4809	0.77709
O	6.11739	-2.043	-0.882
H	5.92852	-1.0848	-0.8927
H	5.22956	-2.4605	-0.6906
O	-0.2529	2.11478	-0.6548
H	-1.4731	1.40113	-1.5639
H	1.00569	3.26056	-1.3388
O	1.59333	0.29549	-0.5624

Paraoxon + 1OH$^-$ + 10 Water Molecules

Paraoxon to the paraoxon pentacoordinate intermediate - Figure 6(b)			
Reactant			
64			
C	-0.8463	0.82987	3.06195
C	-0.7561	-0.387	2.171
O	-0.3084	0.06832	0.87011
P	0.47484	-0.8176	-0.1635
O	1.71694	-0.2821	-0.7717
O	0.65439	-2.2444	0.50289
C	1.97477	-2.826	0.68282
C	2.03286	-3.4459	2.05853
O	-0.6046	-1.0656	-1.3458
C	-1.9614	-1.0192	-1.0842
C	-2.6273	-2.1912	-0.7378
C	-3.9956	-2.1412	-0.5038
C	-4.6429	-0.9169	-0.6217
C	-3.9805	0.25831	-0.9637
C	-2.6159	0.2041	-1.2035
N	-6.0846	-0.8614	-0.3688
O	-6.6543	-1.8975	-0.0698

O	-6.6423	0.21824	-0.4701
H	-1.2163	0.53736	4.0477
H	-1.523	1.56185	2.6175
H	0.14216	1.2822	3.172
H	-1.7335	-0.8601	2.02843
H	-0.0462	-1.1224	2.54952
H	2.72697	-2.0424	0.56718
H	2.10296	-3.5679	-0.1094
H	1.93619	-2.6637	2.81415
H	2.99367	-3.9491	2.19227
H	1.23475	-4.1801	2.18907
H	-2.0744	-3.12	-0.6561
H	-4.5554	-3.0271	-0.2332
H	-4.527	1.19021	-1.0305
H	-2.0313	1.08524	-1.452
O	0.03459	2.19418	-1.0544
H	0.41017	1.64676	-1.7521
O	3.5229	1.77852	-0.8989
H	2.8958	1.10245	-1.2052
O	4.52957	0.05385	1.07838
H	4.96086	-0.7102	0.64076
H	4.24057	0.64129	0.35231
O	5.78854	-1.8462	-0.4536
H	6.17948	-1.1071	-0.9482
H	5.01759	-2.0594	-1.0183
O	5.59508	0.46614	-2.0765
H	5.05114	1.16543	-1.6646
H	6.06268	0.88145	-2.8094
O	-2.0641	2.75986	0.62602
H	-1.4931	3.36978	1.13058
H	-1.3969	2.26501	0.10435
O	-0.8346	4.59181	-1.2518
H	-0.4053	3.67648	-1.3297
H	-1.6849	4.33455	-0.8662
O	3.71786	-1.6306	-2.2454
H	2.95848	-1.2604	-1.7632
H	4.27073	-0.8572	-2.4595
O	2.15514	-0.1286	2.20158
H	2.25435	-0.1048	3.15981
H	3.07789	-0.1414	1.83503
O	0.0086	4.51077	1.42181

H	0.66932	3.7875	1.35569
H	-0.1573	4.739	0.48454
O	1.64767	2.40034	0.7914
H	1.64604	1.57547	1.31044
H	0.93627	2.25046	-0.0169
H	2.95229	2.20891	-0.1947
Transition State			
64			
C	-0.488	-0.1422	3.44241
C	-0.3017	-1.0857	2.27487
O	-0.1883	-0.2763	1.07772
P	0.63878	-0.6912	-0.2193
O	1.93474	-0.1065	-0.6842
O	0.93868	-2.2431	0.12471
C	2.27225	-2.7836	0.15618
C	2.44589	-3.6023	1.41782
O	-0.4263	-0.9161	-1.4301
C	-1.7789	-0.7946	-1.23
C	-2.4518	-1.7581	-0.4781
C	-3.8228	-1.6465	-0.2986
C	-4.4814	-0.5766	-0.8931
C	-3.8228	0.38351	-1.6532
C	-2.4507	0.27264	-1.8213
N	-5.9261	-0.4513	-0.7036
O	-6.4902	-1.2891	-0.0192
O	-6.4964	0.48455	-1.2397
H	-0.5367	-0.7183	4.37007
H	-1.4118	0.42698	3.32925
H	0.35394	0.55113	3.49799
H	-1.1694	-1.7404	2.144
H	0.59496	-1.689	2.38629
H	2.99687	-1.9678	0.11975
H	2.39346	-3.4021	-0.739
H	2.43162	-2.9461	2.29115
H	3.40722	-4.122	1.39074
H	1.65203	-4.3474	1.51172
H	-1.8934	-2.5836	-0.0486
H	-4.3779	-2.3716	0.28235
H	-4.3776	1.20617	-2.0861
H	-1.8828	1.01837	-2.3613
O	-0.0603	1.56023	-0.5575

H	0.47272	1.77657	-1.3333
O	3.1885	2.25523	-0.4877
H	2.68325	1.43693	-0.6856
O	4.76401	0.48816	1.01944
H	5.22612	-0.0638	0.35324
H	4.34028	1.19734	0.49924
O	6.0732	-0.7171	-1.0756
H	6.20426	0.16695	-1.4566
H	5.30237	-1.0264	-1.5949
O	5.15867	1.67223	-2.2617
H	4.55724	2.13932	-1.6495
H	5.42264	2.31555	-2.9284
O	-2.7126	1.17954	1.39525
H	-2.2314	1.90847	1.83992
H	-1.9913	0.72725	0.92882
O	-2.0735	3.18681	-0.5304
H	-1.2824	2.55828	-0.6078
H	-2.7276	2.60223	-0.1172
O	3.80985	-0.7853	-2.6297
H	3.08374	-0.6796	-1.9887
H	4.13188	0.12356	-2.7679
O	2.48611	-0.2542	2.18428
H	2.71098	-0.3722	3.11428
H	3.34925	-0.0901	1.7265
O	-1.1584	3.37861	2.11337
H	-0.2559	3.00305	2.03965
H	-1.4018	3.57494	1.18613
O	1.30189	2.291	1.42493
H	1.61774	1.4478	1.80216
H	0.72488	1.99204	0.60451
H	2.66544	2.60421	0.26822
Product			
64			
C	-2.9372	-2.2266	2.49527
C	-1.5879	-1.6088	2.18762
O	-1.4969	-1.4953	0.75429
P	-0.4699	-0.481	-0.0212
O	-0.7103	1.01531	-0.2517
O	0.52991	-0.3471	1.32956
C	0.59596	0.84682	2.09254
C	1.30645	0.52047	3.39208

O	0.77783	-1.2697	-0.8255
C	2.09444	-0.9973	-0.6208
C	2.58064	0.3165	-0.6179
C	3.93991	0.53996	-0.4807
C	4.79492	-0.5536	-0.3632
C	4.32921	-1.8638	-0.3797
C	2.96634	-2.0826	-0.5093
N	6.22622	-0.3169	-0.2223
O	6.62047	0.839	-0.2043
O	6.96475	-1.2852	-0.1284
H	-3.0915	-2.2567	3.57693
H	-3.0053	-3.2428	2.10198
H	-3.7263	-1.6204	2.0421
H	-0.7612	-2.2257	2.54958
H	-1.521	-0.6177	2.63361
H	-0.4102	1.24314	2.2774
H	1.15202	1.61507	1.53747
H	0.74753	-0.2314	3.95638
H	1.40813	1.41628	4.01007
H	2.30492	0.12445	3.18676
H	1.89471	1.15224	-0.7179
H	4.34477	1.54406	-0.4698
H	5.02633	-2.6868	-0.288
H	2.55951	-3.087	-0.5218
O	-1.4415	-0.9467	-1.4225
H	-1.2236	-0.3164	-2.1227
O	-2.675	1.99883	-1.6365
H	-1.9259	1.58107	-1.122
O	-3.1061	3.41956	0.71868
H	-2.3584	4.0523	0.76558
H	-3.0535	3.05616	-0.1866
O	-1.0434	5.21075	0.39214
H	-1.2809	5.27056	-0.5487
H	-0.2849	4.59462	0.3475
O	-1.2627	4.24526	-2.238
H	-1.9006	3.50465	-2.2323
H	-1.2356	4.57449	-3.1428
O	-2.4193	-4.0855	-0.1424
H	-3.3385	-3.756	-0.2188
H	-1.9308	-3.2709	0.06414
O	-2.6081	-3.15	-2.7542

H	-2.1357	-2.3683	-2.4132
H	-2.4001	-3.8046	-2.0646
O	0.73023	3.2817	-0.4756
H	0.24138	2.4625	-0.2434
H	0.30797	3.55205	-1.3107
O	-3.0952	0.98302	1.80984
H	-3.755	1.03089	2.51137
H	-2.9916	1.91389	1.48713
O	-4.771	-2.8453	-0.9631
H	-4.6713	-1.9211	-0.6638
H	-4.2432	-2.8742	-1.7836
O	-3.9394	-0.2231	-0.5063
H	-3.7168	0.14111	0.38162
H	-3.0847	-0.5961	-0.8117
H	-3.4075	1.3687	-1.5175
Paraoxon pentacoordinate intermediate to 4-nitrophenol - Figure 7(b)			
Reactant			
64			
C	5.3795	-1.6863	-0.0345
C	3.93872	-2.136	-0.2453
O	3.37885	-1.6501	-1.4621
P	2.27334	-0.3671	-1.462
O	1.94823	-0.3372	-2.9184
O	1.25556	-1.0957	-0.3896
C	0.85203	-2.4537	-0.6556
C	-0.4716	-2.6969	0.03903
O	1.21111	1.17965	-1.0119
C	-0.0963	1.24074	-1.1178
C	-0.7655	2.22217	-0.3425
C	-2.14	2.25404	-0.2787
C	-2.87	1.34075	-1.0456
C	-2.2454	0.41943	-1.8861
C	-0.8648	0.36319	-1.9201
N	-4.2915	1.26238	-0.8721
O	-4.7708	1.7022	0.18046
O	-4.974	0.73327	-1.7345
H	5.82694	-2.2601	0.78153
H	5.46239	-0.6287	0.24013
H	5.96577	-1.8646	-0.9394
H	3.32079	-1.8363	0.61174

H	3.91269	-3.2302	-0.2987
H	1.62127	-3.1401	-0.2902
H	0.75912	-2.5922	-1.7377
H	-0.3728	-2.5685	1.11993
H	-0.8014	-3.7204	-0.1558
H	-1.2408	-2.0118	-0.327
H	-0.1596	2.90113	0.24911
H	-2.6582	2.96465	0.35515
H	-2.8507	-0.2777	-2.4537
H	-0.353	-0.3592	-2.5436
O	3.35298	0.63537	-0.7405
H	4.26245	0.32201	-0.8456
O	-2.9105	-0.2085	1.63004
H	-1.9401	-0.0778	1.71012
O	-6.3662	-0.7653	0.41236
H	-5.6468	-1.0804	-0.1664
H	-6.2297	0.19245	0.42978
O	-4.803	-2.2348	2.23602
H	-5.5075	-1.7049	1.81863
H	-4.083	-1.5895	2.33253
O	-0.1702	0.03211	1.77551
H	0.19444	-0.1135	0.88263
H	0.30507	-0.655	2.30154
O	5.27814	1.90043	0.82805
H	4.97859	1.37597	1.58334
H	4.47169	2.40716	0.607
O	2.74051	3.1725	0.40647
H	2.20928	3.06819	1.21347
H	2.35139	2.51964	-0.2028
O	-3.888	-1.8343	-0.4077
H	-3.3949	-1.1584	0.09689
H	-4.1324	-2.4377	0.31602
O	1.152	2.26442	2.54552
H	0.84437	2.63109	3.38176
H	0.52194	1.55091	2.29154
O	1.60295	-1.6701	2.86473
H	2.30475	-1.0394	2.58824
H	1.78101	-2.4966	2.40238
O	3.15608	0.42706	2.08899
H	3.0908	0.56743	1.12701
H	2.5878	1.12941	2.46481

H	-3.3119	0.66961	1.58424
Transition State			
64			
C	5.43671	-1.7303	0.00263
C	3.98611	-2.1574	-0.1641
O	3.43295	-1.7165	-1.4062
P	2.33878	-0.4603	-1.4536
O	1.99141	-0.4272	-2.8984
O	1.29921	-1.0875	-0.3591
C	0.84345	-2.4399	-0.5856
C	-0.4694	-2.6244	0.14399
O	1.16236	1.22581	-1.0463
C	-0.1296	1.27037	-1.1565
C	-0.841	2.25775	-0.4134
C	-2.2137	2.25189	-0.3592
C	-2.9185	1.29786	-1.1053
C	-2.2593	0.37025	-1.9174
C	-0.8801	0.35083	-1.9416
N	-4.3298	1.18106	-0.9292
O	-4.8288	1.65509	0.10259
O	-4.9978	0.58791	-1.764
H	5.87558	-2.2512	0.85764
H	5.54511	-0.6571	0.19327
H	6.01054	-1.9898	-0.89
H	3.38014	-1.7935	0.67588
H	3.92704	-3.2507	-0.1638
H	1.60301	-3.1396	-0.2243
H	0.71837	-2.5965	-1.662
H	-0.3409	-2.4865	1.22028
H	-0.8427	-3.6363	-0.0317
H	-1.2176	-1.914	-0.2158
H	-0.2598	2.96991	0.16423
H	-2.7561	2.96547	0.25086
H	-2.8421	-0.358	-2.4698
H	-0.3428	-0.3753	-2.5398
O	3.32313	0.60928	-0.7307
H	4.26198	0.36884	-0.7616
O	-2.8855	-0.168	1.60594
H	-1.9199	0.00069	1.66642
O	-6.3495	-0.8306	0.46107
H	-5.6372	-1.1653	-0.1157

H	-6.2232	0.12843	0.4269
O	-4.7391	-2.1848	2.332
H	-5.4537	-1.6833	1.89662
H	-4.0247	-1.5286	2.38906
O	-0.1443	0.1622	1.7503
H	0.23884	0.03337	0.86371
H	0.32021	-0.529	2.27982
O	5.25191	1.86795	0.70178
H	4.97309	1.39076	1.49599
H	4.45365	2.39878	0.50332
O	2.72863	3.16966	0.33217
H	2.20902	3.14343	1.15238
H	2.27466	2.52391	-0.2431
O	-3.8718	-1.9076	-0.3431
H	-3.3822	-1.1932	0.10796
H	-4.0915	-2.4681	0.42195
O	1.14516	2.41415	2.53599
H	0.82131	2.80157	3.35646
H	0.51829	1.69772	2.28557
O	1.58508	-1.553	2.9039
H	2.28859	-0.9244	2.62708
H	1.77567	-2.3887	2.46372
O	3.11852	0.53948	2.09293
H	3.00434	0.66506	1.13389
H	2.57667	1.25367	2.48403
H	-3.3168	0.69286	1.51902
Product			
64			
C	4.4941	-2.6365	0.03875
C	3.1099	-2.7494	-0.5715
O	2.99328	-1.9016	-1.7203
P	2.30467	-0.4413	-1.5129
O	2.41414	0.28548	-2.8058
O	0.75319	-0.8603	-1.1871
C	-0.0568	-1.3685	-2.2515
C	-1.4004	-1.7477	-1.6695
O	1.83474	2.99992	-0.7261
C	0.56643	2.6333	-0.6219
C	-0.1485	2.75605	0.58837
C	-1.4758	2.38159	0.65614
C	-2.0971	1.87952	-0.4883

C	-1.4124	1.75702	-1.7023
C	-0.0886	2.13723	-1.7684
N	-3.4706	1.46735	-0.4141
O	-4.1041	1.7202	0.6167
O	-3.9663	0.86657	-1.3545
H	4.57651	-3.2831	0.91664
H	4.68984	-1.6066	0.3461
H	5.25259	-2.936	-0.6887
H	2.33402	-2.4944	0.16056
H	2.91619	-3.7688	-0.9168
H	0.44517	-2.2353	-2.6973
H	-0.1556	-0.5936	-3.0196
H	-1.2852	-2.5099	-0.8934
H	-2.0627	-2.1373	-2.4453
H	-1.874	-0.8699	-1.219
H	0.34882	3.15257	1.46567
H	-2.0344	2.47461	1.57965
H	-1.9269	1.36033	-2.57
H	0.48824	2.01736	-2.678
O	2.76872	0.15349	-0.1982
H	4.34762	0.74621	0.39793
O	-2.9239	-0.8267	1.18048
H	-1.9467	-0.751	1.28183
O	-6.1872	-0.3595	0.44007
H	-5.7478	-0.856	-0.2753
H	-5.659	0.45015	0.50688
O	-5.0612	-2.516	1.87065
H	-5.6006	-1.7451	1.61067
H	-4.1702	-2.1307	1.9168
O	-0.2227	-0.5654	1.36344
H	0.11093	-0.4654	0.44825
H	0.1653	-1.4166	1.68423
O	4.94867	1.01036	1.12593
H	4.70107	0.37338	1.81552
H	3.72482	2.29815	1.48701
O	2.90971	2.83263	1.60465
H	2.30473	2.2502	2.1083
H	2.2775	2.98841	0.1868
O	-4.457	-2.1338	-0.8563
H	-3.7745	-1.5416	-0.4972
H	-4.6906	-2.65	-0.064

O	1.20952	1.09713	2.93802
H	0.74237	1.33223	3.74751
H	0.57202	0.60623	2.36459
O	1.0806	-2.6633	2.43568
H	1.94243	-2.1898	2.45628
H	1.23418	-3.4944	1.9731
O	3.06217	-0.8275	2.28425
H	2.85857	-0.5617	1.35348
H	2.54847	-0.1821	2.80685
H	-3.2932	-0.0331	1.58899