Computational Modelling of the Catalytic Cycle of Glutathione Peroxidase Nano Mimic

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Supporting Information

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Table S1: The comparison of the main interatomic distances (Å) of the optimized reactant (R), transition states (TS) and products (P) at the B3LYP/6 31+G(d,p) level of the theory.

Table S2-S4: Cartesian Coordiantes for Each System Studied

Table S1. The comparison of the main interatomic distances (Å) of the optimized reactant (R), transition states (TS) and products (P) at the B3LYP/6 31+G(d,p) level of the theory.

	Step 1→2		
	R	**TS**	**P**
Se_1- O_7	4.47	2.26	1.66
O_7-O_8	1.45	1.81	2.47
O_8-H_9	1.9	1.54	0.97
	***Step* 2 → 3**		
Se_1-S_{14}	6.25	2.83	2.29
S_{14}-H_{15}	1.35	1.96	2.41
H_{15}-O_{16}	2.08	1.03	0.97
O_{16}-H_{18}	0.98	1.11	1.80
H_{18}-O_{19}	1.78	1.31	0.98
O_{19}-H_{21}	0.98	1.12	1.77

H_{21}-O_{22}	1.79	1.46	0.98
O_{22}-H_{23}	0.96	1.11	1.98
H_{23}-N_5	4.23	3.03	1.01
N_5-Se_1	1.87	2.02	3.19
***Step* 3 → 4**			
Se_1-S_{14}	2.29	2.41	4.92
S_{14}-S_{28}	6.21	2.70	2.09
S_{28}-H_{29}	1.35	1.80	2.38
H_{29}-O_{34}	2.09	1.10	0.98
O_{34}-H_{36}	0.98	1.20	1.78
H_{36}-O_{37}	1.78	1.20	0.98
O_{37}-H_{39}	0.98	1.09	1.79
H_{39}-O_{40}	1.73	1.36	0.98
O_{40}-H_{42}	0.98	1.10	1.72
H_{42}-O_{16}	1.64	1.74	0.99
O_{16}-Se_1	1.67	1.71	1.82
***Step* 4 → 1**			
Se_1-O_{11}	1.85	2.19	2.72
O_{11}-H_{34}	1.90	1.57	0.98
H_{34}-O_{33}	0.97	1.13	4.22
O_{33}-H_{31}	1.72	1.45	0.97
H_{31}-O_{30}	0.98	1.16	2.95
O_{30}-H_{10}	6.16	1.57	0.97
H_{10}-N_5	1.00	1.61	2.12
N_5-Se_1	4.00	2.60	1.92

Table S2-S4 Cartesian Coordiantes of the optimized structures at the B3LYP/6-31+G(d,p) level of the theory

S2 : THE OXIDATION of **1** (step **1** → **2)**

Reactants

Atom	**X**	**Y**	**Z**
Se	-0.64481701	0.28736420	-0.80389524
N	-0.39885745	-0.42540022	0.79035879
C	1.21490611	0.70542916	-0.95944670
C	2.07469078	0.65390451	0.41047489
C	0.74752642	0.36562520	1.27085368
O	0.70788231	0.79934359	2.45148371
O	-0.44846486	-0.07546111	-3.78332422
H	-0.53053428	0.82029389	-3.44793253
O	0.59451287	0.09364563	-4.78932554
H	0.14246801	-0.25981323	-5.55895030
C	-1.60681989	-0.29503729	1.61784429
H	-1.88163946	0.73670421	1.68772762
H	-2.40664848	-0.84770478	1.17092945
H	-1.41143691	-0.67922129	2.59719517
C	2.31796677	1.58595666	1.61201373
H	3.35598264	1.33701414	1.53818498
H	2.33739280	1.18351909	2.60325872
H	2.59631571	2.60592762	1.44745034
C	2.84990694	1.61474187	-0.51008553
H	3.89028078	1.58485432	-0.26183363
H	2.48036617	2.61028921	-0.37884109

H	2.71769808	1.31667686	-1.52919203
H	1.69176774	0.01845711	-1.62695878
H	1.24307076	1.69698628	-1.36059658

Transition State

Atom	X	Y	Z
Se	-0.27253109	0.91626671	-0.33100273
N	0.84702902	-0.50354186	-0.09159993
C	-1.82502905	-0.19589189	-0.58143225
C	-1.58621830	-1.40002448	0.15135501
C	-0.05629802	-1.49407813	0.52773365
O	0.37759408	-2.38618884	1.30197307
O	-0.95795932	2.40862358	0.49396755
H	-0.19468468	2.98492542	0.41097345
O	-1.56841915	3.83771978	1.60611061
H	-1.84625385	3.23482922	2.29960239
C	2.01077864	-0.16413530	0.73989871
H	2.61033701	-1.03792048	0.88798385
H	1.67689530	0.20410887	1.68743137
H	2.59218667	0.58845676	0.24952141
C	-1.92514630	-2.62495321	-0.71828712
H	-1.31355710	-2.61926646	-1.59625427
H	-1.74112209	-3.51977418	-0.16121396
H	-2.95624864	-2.58690581	-1.00162501
C	-2.47521653	-1.40002469	1.40884543
H	-2.30691422	-2.29873703	1.96462457
H	-2.23267915	-0.55380107	2.01710624
H	-3.50373681	-1.34753610	1.11851635

H	-2.68017214	0.33118091	-0.21288842
H	-1.98335299	-0.44485695	-1.60995057

Products

Atom	X	Y	Z
Se	1.00255242	1.32278795	-1.50895024
N	0.60261215	0.88374232	0.11408251
C	2.83229290	0.86183835	-1.16176435
C	3.24223873	0.93984204	0.43316285
C	1.80207070	1.58873555	0.63531554
O	1.68016099	2.68735898	1.23675975
O	0.17499018	0.53604072	-2.93900952
H	-2.87684193	-1.26380760	-2.43802878
O	-3.65365933	-0.71306963	-2.31619937
H	-4.14261846	-1.01505671	-1.54722422
C	-0.70992797	1.29610538	0.63186157
H	-0.77582300	1.05225603	1.67161892
H	-0.82769448	2.35201048	0.50499371
H	-1.48165276	0.78420503	0.09585889
C	3.54645906	1.96976419	1.53693382
H	4.33454202	1.60214292	2.16037574
H	2.66883251	2.12885949	2.12800093
H	3.84737649	2.89388541	1.08933058
C	4.61114136	1.13193836	-0.24566303
H	5.38281800	0.76201904	0.39665687
H	4.77268923	2.17267611	-0.43452071
H	4.62903753	0.59458945	-1.17077702
H	3.03533601	-0.14657961	-1.45632626

H	3.41612305	1.54188287	-1.74621435

S3 : THE REDUCTION of SELENOXIDE 2 with METHANTHIOL (step **2 → 3)**

Reactants

Atom	**X**	**Y**	**Z**
Se	1.27659500	0.84271400	-0.92042700
C	1.40721100	-1.13615700	-1.07103500
C	1.84773100	-1.71504900	0.28431000
C	2.55732000	-0.60877400	1.08638600
N	2.30164100	0.66112700	0.64178300
C	2.79594600	1.82667000	1.37776800
H	2.44057500	1.79479900	2.41105500
H	3.88937800	1.83526600	1.38418400
H	2.43356000	2.73539600	0.89614000
C	-3.06204400	-2.03964000	-1.31316200
H	-2.68381500	-3.03068500	-1.56909900
H	-3.51935100	-1.59309400	-2.19732000
H	-2.23126200	-1.42196800	-0.96983100
S	-4.30347800	-2.27487600	0.02198500
H	-4.63617100	-0.97088100	0.19606100
O	-5.22092600	0.98133500	0.60150000
H	-5.60418400	1.44282500	-0.15552000
H	-4.50465400	1.56795800	0.93751900
O	-3.16395200	2.53436800	1.60066000
H	-3.43857500	3.29364300	2.13123400
H	-2.57233100	2.88670600	0.89888800
O	-1.53179300	3.33396600	-0.49493600
H	-0.81204100	2.69549100	-0.60398300

H	-1.10273400	4.20047900	-0.45519000
O	2.31551800	1.38391000	-2.10926000
C	0.62274300	-2.16364600	1.11768200
H	0.11561400	-2.99017000	0.61070500
H	-0.09735900	-1.35009600	1.25265300
H	0.94204600	-2.50897600	2.10446900
C	2.80599400	-2.90094900	0.07113400
H	3.69990000	-2.59582300	-0.48135200
H	2.30280300	-3.69112800	-0.49443900
H	3.11867700	-3.31030800	1.03527300
H	0.45362200	-1.52289900	-1.43405700
H	2.16687400	-1.24415700	-1.84933400
O	3.24239800	-0.81848700	2.08750200

Transition State

Atom	**X**	**Y**	**Z**
Se	-0.09939031	-1.66693644	-0.18597337
C	0.99734459	-1.73263788	1.42644826
C	1.70278598	-0.27362768	1.49557090
C	2.47942923	0.02567878	0.14610849
N	1.66577826	0.30894699	-0.87575452
C	2.29073709	0.12036368	-2.19571019
H	3.07242284	0.83949105	-2.32740796
H	2.70154827	-0.86811212	-2.25927337
H	1.55187219	0.25058337	-2.95947904
C	-4.20265474	-1.17335656	-1.10635262
H	-4.15931231	-2.15646395	-1.52102241
H	-5.21802631	-0.92101109	-0.89707378
H	-3.79946837	-0.47604300	-1.80431006

S	-3.25341113	-1.11712822	0.39528495
H	-3.17299912	0.65386274	1.17997831
O	-3.11699073	1.95462944	1.73616603
H	-3.96741485	2.24860504	2.07953469
H	-2.64342568	2.76947665	0.65350395
O	-2.17436834	3.57873264	-0.42014946
H	-2.33330001	4.49843584	-0.19469563
H	-0.75414661	3.35504707	-0.63660042
O	0.65083770	3.13721396	-0.93169267
H	1.14845094	1.75088926	-0.90429601
H	0.79884368	3.45871860	-1.82434711
O	-0.23183223	-3.02440603	-1.40514249
C	0.58688409	0.77816615	1.65981573
H	0.04774431	0.58461337	2.56373548
H	-0.08114018	0.72162143	0.82508251
H	1.01693616	1.75859100	1.70559217
C	2.66486300	-0.18959217	2.69378969
H	3.44079393	-0.91971818	2.58268209
H	2.12387191	-0.37695249	3.59545073
H	3.09700780	0.78620931	2.73540730
H	0.40023953	-1.89504762	2.30010195
H	1.72151539	-2.52022519	1.35421360
O	3.72440426	-0.07487855	0.03248661

Products

Atom	**X**	**Y**	**Z**
Se	-0.51425900	-0.97253200	-0.48316400
C	0.39467800	-1.02446500	1.30761500
C	1.56379100	-0.01503700	1.39355000

C	2.49321000	-0.27612100	0.18254500
N	2.37737100	0.53411800	-0.88324200
C	3.13185500	0.27110300	-2.10329500
H	4.21167300	0.39990200	-1.94103700
H	2.95777300	-0.75436200	-2.45495500
H	2.79974400	0.97702600	-2.86877500
C	-3.61473500	-1.19916800	-1.09476600
H	-3.36750500	-2.04537500	-1.74355100
H	-4.65423000	-1.29122500	-0.76046900
H	-3.49068900	-0.24955200	-1.62475200
S	-2.59773700	-1.24178000	0.43746200
H	-2.71301100	0.97861900	1.10282700
O	-2.73197100	1.92302400	1.39905600
H	-3.66531000	2.12449800	1.63363500
H	-1.98744000	3.11312800	0.28300400
O	-1.57739200	3.76857400	-0.33165900
H	-1.43640100	4.57844100	0.18297600
H	-0.09712000	3.22603900	-1.15502800
O	0.73850500	2.91235300	-1.57278000
H	1.75699200	1.34303200	-0.88365000
H	0.60279500	3.01164200	-2.52462900
O	-0.05274700	-2.44873800	-1.13512100
C	1.00706100	1.42147500	1.46490700
H	0.41691900	1.53626400	2.37909900
H	0.35089800	1.67248400	0.62468100
H	1.81745500	2.15758400	1.49313900
C	2.33842700	-0.31222900	2.69738700
H	2.75624500	-1.32174700	2.68755300
H	1.67128600	-0.21296100	3.55957800

H	3.16189400	0.40112200	2.82063600
H	-0.35396500	-0.80668800	2.07428000
H	0.72024400	-2.06561600	1.37663100
O	3.25648600	-1.25144800	0.17325600

S4 : THE REDUCTION of 3 (SELENENYLSULFIDE) by METHANTHIOL (step **3** → **4**)

Reactants

Atom	**X**	**Y**	**Z**
Se	-0.79066323	-0.93354560	-0.08643910
C	0.47987302	-1.03748873	1.37593345
C	1.72021480	-0.18893809	1.03960909
C	2.37443751	-0.72386903	-0.24780753
N	1.99935852	-0.24285890	-1.43834786
C	2.43928339	0.74038860	-2.43864305
H	1.74999080	1.55845897	-2.46180753
H	3.41271453	1.10141046	-2.17980905
H	2.47536227	0.27699352	-3.40241861
C	-3.79276319	-2.09447080	-0.93026881
H	-3.33820589	-2.46614358	-1.82477258
H	-4.65455911	-2.68404819	-0.69658889
H	-4.08628429	-1.07589115	-1.07601125
S	-2.62701341	-2.18984134	0.41149566
H	1.29414983	0.46408106	-1.49235339
O	-0.01324274	-1.56921029	-1.61629131
C	1.29776386	1.27705505	0.82984892
H	0.84320653	1.64872783	1.72435268
H	0.59700417	1.33438451	0.02328262
H	2.15955977	1.86663245	0.59616901

C	2.72878481	-0.27144965	2.20046152
H	3.02230593	-1.29002929	2.34620397
H	2.27422748	0.10022313	3.09496528
H	3.59058072	0.31812776	1.96678161
H	0.02531569	-0.66581594	2.27043721
H	0.77339411	-2.05606838	1.52167591
O	3.26187494	-1.61347945	-0.17984673
S	-1.37568843	-4.37172753	-3.73040440
H	-0.35749064	-5.16533937	-3.95301058
C	-2.89034225	-5.29600060	-3.87162447
H	-3.72199999	-4.64778330	-3.68980108
H	-2.96698649	-5.70677849	-4.85665604
H	-2.89253442	-6.08904235	-3.15330701
O	1.50361253	-6.06492901	-3.66118026
H	1.85164016	-6.95933381	-3.68391388
H	2.06696713	-5.48898106	-4.18321049
O	2.88179254	-4.26321531	-5.16766519
H	3.79721518	-3.98114528	-5.23120943
H	2.41784002	-3.70505670	-4.53932848
O	1.78382228	-2.52775838	-3.33434293
H	2.63646597	-2.08772277	-3.36544611
H	1.18378981	-2.02400447	-2.77955195

Transition State

Atom	**X**	**Y**	**Z**
Se	0.10096343	-1.22297419	-0.02488886
C	-0.80817276	-0.65292682	1.59550235
C	-2.21872364	-0.14931897	1.24110378
C	-2.11421334	1.04282018	0.27411798

N	-3.08179718	1.26430609	-0.61993735
C	-2.97547076	2.40150112	-1.54180198
H	-2.42615275	3.19108148	-1.07352436
H	-2.46765882	2.09233803	-2.43219393
H	-3.95374538	2.74927480	-1.79126916
C	2.45240338	-3.47392817	-0.41099905
H	2.36996735	-3.28535682	-1.45948033
H	3.42306859	-3.87020247	-0.19664814
H	1.70549573	-4.17887970	-0.11399791
S	2.22054342	-1.95426845	0.48754587
H	-3.87642846	0.65676119	-0.66131921
O	0.29052958	0.13160546	-1.22053748
C	-3.01083865	-1.28660915	0.57166355
H	-3.08644870	-2.11389167	1.24422176
H	-2.50315220	-1.59406845	-0.31861771
H	-3.99054984	-0.94216220	0.32258675
C	-2.94166106	0.30119267	2.52394144
H	-2.38986958	1.09669477	2.98149861
H	-3.01031507	-0.52009953	3.20370084
H	-3.92541313	0.64319730	2.27799833
H	-0.88463313	-1.48082341	2.27000393
H	-0.25350973	0.13420894	2.05955723
O	-1.11766745	1.80897246	0.32582417
S	4.37435192	0.05450491	-0.28516780
H	3.75742889	1.86211916	-0.27911314
C	5.64203403	0.00762611	0.96339508
H	6.04114966	-0.98303798	1.02852942
H	6.42366839	0.69022195	0.70452446
H	5.22180541	0.28705589	1.90590036

O	3.99668264	2.74772264	0.22488409
H	3.95514828	3.13720785	-0.65199033
H	2.93491420	3.01638593	0.80632009
O	1.87563840	3.19714636	1.24319587
H	1.92512783	2.68375429	2.05165456
H	0.99562463	2.97037906	0.69752899
O	-0.19268643	2.66694162	-0.03616220
H	-0.94879396	2.66858828	0.55570800
H	-0.02581988	1.61977987	-0.53194475

Products

Atom	**X**	**Y**	**Z**
Se	-1.65554300	-1.74369900	-0.24278300
C	-2.25159100	-0.70466300	1.32711300
C	-3.69418700	-0.19063800	1.17306200
C	-3.74069100	0.76849900	-0.03635100
N	-4.70314600	0.58781200	-0.95769500
C	-4.85892900	1.46763400	-2.11021500
H	-5.19155700	2.46412300	-1.80439300
H	-3.91174000	1.56779300	-2.64317700
H	-5.60103300	1.03224700	-2.77719800
C	4.92212900	-2.34497300	-1.25740500
H	4.83496000	-1.87877000	-2.23975600
H	5.95789100	-2.61859900	-1.05123900
H	4.29759700	-3.24216700	-1.22375900
S	4.25728700	-1.23636800	0.04471200
H	-5.35943200	-0.16979800	-0.84972500
O	0.00903400	-1.01311400	-0.42218500
C	-4.64636000	-1.39704900	1.05936300

H	-4.47954000	-2.06965000	1.90570600
H	-4.47844600	-1.97347600	0.14153300
H	-5.69931300	-1.09571900	1.08910100
C	-4.04481900	0.62682100	2.43861900
H	-3.36568800	1.47525500	2.55559800
H	-3.96404200	-0.00833900	3.32568100
H	-5.07070800	1.00704600	2.38566600
H	-2.16970700	-1.32138700	2.22373700
H	-1.53336200	0.11498700	1.38763200
O	-2.92863100	1.71228600	-0.12504300
S	5.41194700	0.49347400	-0.14713700
H	3.86035600	2.17352700	0.92224300
C	6.83797200	0.20865700	0.97220600
H	7.45235700	-0.61701400	0.61116000
H	7.42190300	1.13292200	0.95071200
H	6.49379600	0.01733900	1.98934700
O	3.15127800	2.70590700	1.32491900
H	3.59870100	3.42598000	1.78907900
H	1.96847400	3.17360600	0.08931500
O	1.31951600	3.39351800	-0.61842000
H	0.90033700	4.22129500	-0.35062600
H	0.17040600	2.13585900	-1.14809300
O	-0.46322900	1.44237400	-1.44016000
H	-1.32777000	1.67667700	-1.04401000
H	-0.14657200	-0.09984500	-0.78849500

S5 : THE DEHYDRATION of the SELENENIC ACID (step**4** → **1)**

Reactants

Atom	**X**	**Y**	**Z**
Se	-0.43894100	-1.62103500	-0.72807100
C	-1.33353100	-1.13037100	0.96049700
C	-2.51261400	-0.17655300	0.68841900
C	-1.96543700	1.16141800	0.14282700
N	-2.56765700	1.71085900	-0.92386300
C	-2.16160400	3.00053600	-1.47247400
H	-2.24486600	3.78598500	-0.71617200
H	-1.12569500	2.96281900	-1.82121200
H	-2.81439400	3.23772000	-2.31237800
H	-3.34994400	1.24008800	-1.35196900
O	1.32435600	-1.60340100	-0.15517900
C	-3.50334200	-0.88256500	-0.25870500
H	-3.74524600	-1.87119500	0.14182200
H	-3.09143500	-1.02600100	-1.26578700
H	-4.44594400	-0.33365900	-0.35458200
C	-3.20862700	0.11724400	2.04004400
H	-2.51470300	0.58418400	2.74411200
H	-3.57725000	-0.81468300	2.47970100
H	-4.06336600	0.78671900	1.89777400
H	-1.70138300	-2.03879900	1.44030100
H	-0.56154200	-0.68107700	1.58719300
O	-1.01456200	1.73809500	0.70841200
H	3.45812100	-1.63283500	-0.18381000
O	4.35415200	-1.77088100	0.15590900
H	4.80692600	-0.90338700	0.06029900

H	6.29675700	0.87232400	0.57628400
O	5.64485800	0.70207100	-0.11664800
H	4.96135700	1.41422400	-0.03292000
H	3.38070500	2.96771600	-0.70831800
O	3.64589800	2.55691000	0.12527500
H	2.86036100	2.04323100	0.44653500
H	1.47121100	-2.43694900	0.32056700
O	1.62778900	1.00678300	1.03911800
H	1.65342900	0.10752700	0.66269600
H	0.69549800	1.30037100	0.95257000

Transition State

Atom	**X**	**Y**	**Z**
Se	0.13072700	-0.85385700	-0.85231300
C	-0.51054800	1.02572600	-1.06336200
C	-1.67178900	1.30653600	-0.07196200
C	-2.32482600	-0.05363900	0.25581500
N	-1.43255400	-0.98369700	0.72495200
C	-1.97381400	-2.33763800	0.85935500
H	-2.75002300	-2.52685300	0.11657200
H	-1.16465600	-3.06885800	0.76113700
H	-2.42616200	-2.46919200	1.85067300
H	0.12877300	-0.91075400	1.53657300
O	1.96592500	-0.60561500	-1.79097800
C	-1.15010400	1.94165500	1.23516300
H	-0.77790400	2.95278400	1.03812900
H	-0.33997200	1.36219300	1.67740200
H	-1.95509700	2.01404900	1.97486500
C	-2.68236600	2.25976500	-0.72795300

H	-3.14558000	1.80505000	-1.60810200
H	-2.17741200	3.18114900	-1.03773100
H	-3.47915700	2.52617900	-0.02675600
H	0.34070800	1.69027200	-0.90394100
H	-0.84904400	1.11962400	-2.09626700
O	-3.52513000	-0.28092000	0.04084500
H	2.73393100	1.02383100	-1.28852800
O	3.19472700	1.82606100	-0.96334300
H	3.00694100	1.85322000	-0.00830200
H	3.17335000	2.10253000	2.48197700
O	2.49236300	1.90072900	1.82550600
H	2.03514300	1.11268500	2.15538600
H	1.00263400	-1.34029500	2.85592100
O	1.03375800	-0.86848000	2.00701000
H	1.89087400	-1.21082300	1.27220000
H	1.97890200	-0.60237000	-2.76004500
O	2.88111900	-1.46139500	0.49356300
H	2.69077200	-1.26277200	-0.47681100
H	3.20472700	-2.37209000	0.56648700

Products

Atom	**X**	**Y**	**Z**
Se	0.04305000	0.04858200	-1.14236100
C	-0.53156500	-1.36521100	0.11564300
C	-2.02758100	-1.12454300	0.37640000
C	-2.28319500	0.39600300	0.34932900
N	-1.29745300	1.10067200	-0.29083200
C	-1.52364800	2.46220700	-0.76725400
H	-2.02490700	2.46207900	-1.74222900

H	-2.14987000	2.98253600	-0.04159100
H	-0.56738100	2.98176700	-0.85633700
H	0.37330000	1.31068900	1.24944100
O	2.97393100	-1.22794300	-2.11234700
C	-2.88800800	-1.73930200	-0.75253600
H	-2.77047100	-2.82760600	-0.75143900
H	-2.58823600	-1.36354300	-1.73555800
H	-3.94605800	-1.50927900	-0.60023600
C	-2.43820200	-1.70691300	1.73745400
H	-1.86895400	-1.25082800	2.55342100
H	-2.26186200	-2.78691700	1.75478100
H	-3.50088800	-1.52664500	1.91888700
H	-0.32577200	-2.33388600	-0.34115200
H	0.06689100	-1.26586400	1.02305700
O	-3.28760400	0.93385200	0.82517300
H	4.05098600	-2.67775700	0.69627400
O	3.24682500	-2.19464900	0.46563000
H	3.10192800	-1.52950900	1.18062400
H	2.53774200	-0.77815500	3.25182900
O	2.84751500	-0.36164800	2.43602000
H	2.20548400	0.35747100	2.24629000
H	0.60028400	2.09123800	2.57055100
O	1.06193500	1.67769800	1.82764000
H	2.51012800	2.45254700	-0.87222700
H	3.16605700	-1.91858900	-2.75934500
O	2.64211700	3.07103200	-0.14118200
H	3.14257400	-1.62810400	-1.23199000
H	2.14293600	2.68167800	0.60136000