

Supporting Information

How Does Multiple Substrate Binding Lead to Substrate Inhibition of CYP2D6 Metabolizing Dextromethorphan? A Theoretical Study

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This supporting information contains six supplementary figures (Figure S1-S6), one supplementary table (Table S1) and the cartesian coordinates of all states in the QM calculation.

Six supplementary figures

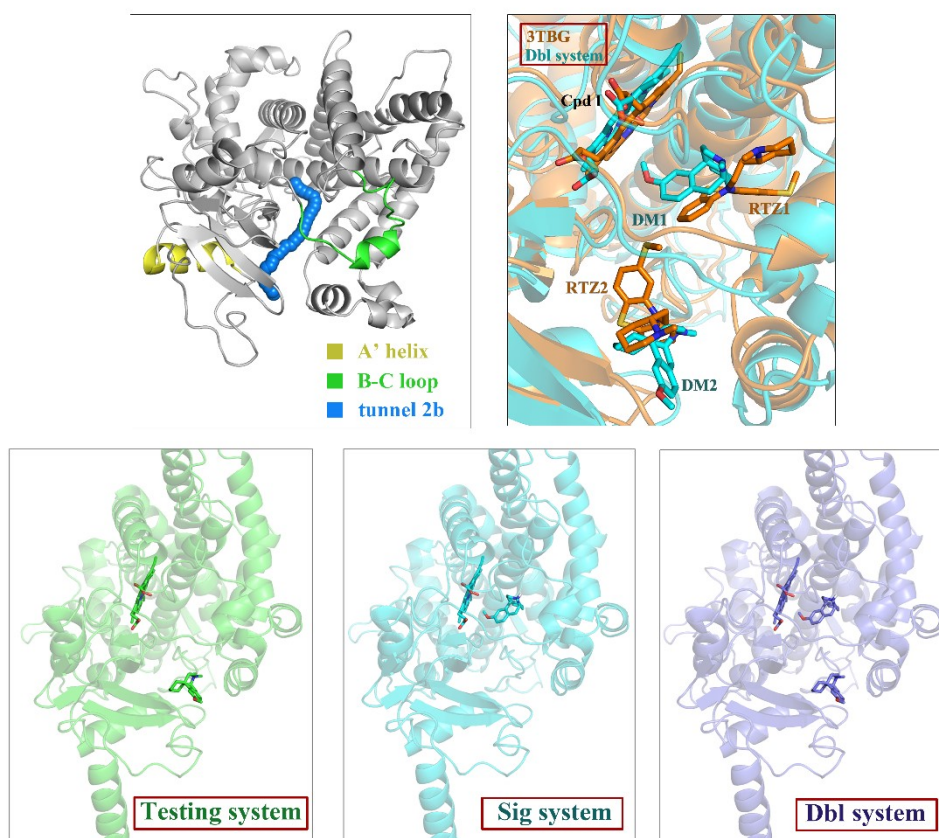


Figure S1. The upper figure shows the location of tunnel 2b of CYP2D6, and the comparison of the positions of two molecules bound in **Dbl system** and crystal structure (PDB code: 3TBG). The key secondary structure, A' helix and B-C loop has been drawn in yellow and blue, respectively. The lower three figures show the initial structure of **Sig system**, **Dbl system** and **Testing system**.

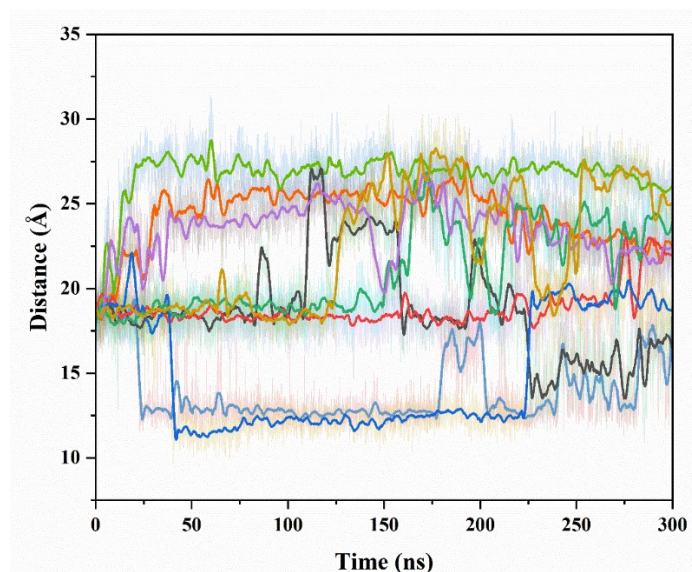


Figure S2. The distance between the reactive sites for the **Testing system**. The results of the nine parallel trajectories are shown in different colors.

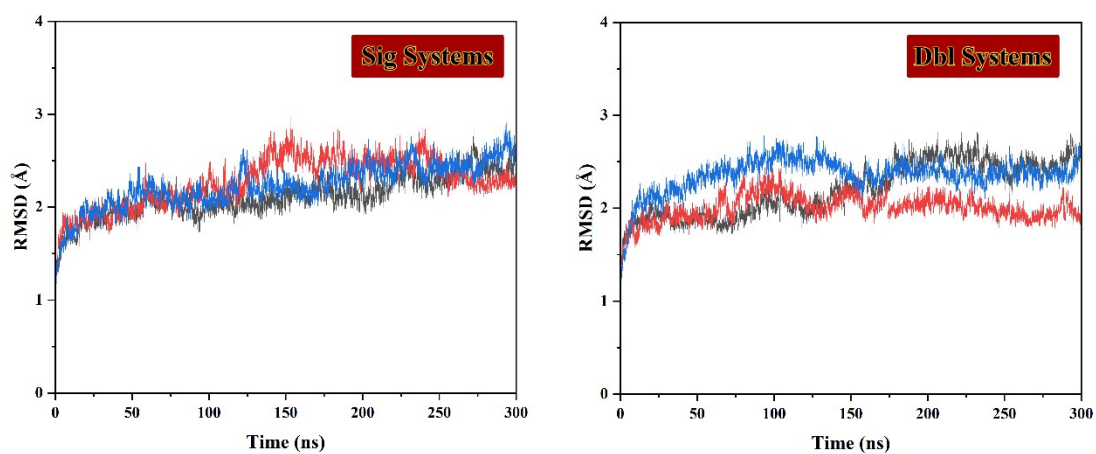


Figure S3. The RMSD for the **Sig system** and **Dbl system**. The results of three parallel trajectories for these two systems are shown in red, blue and black, respectively.

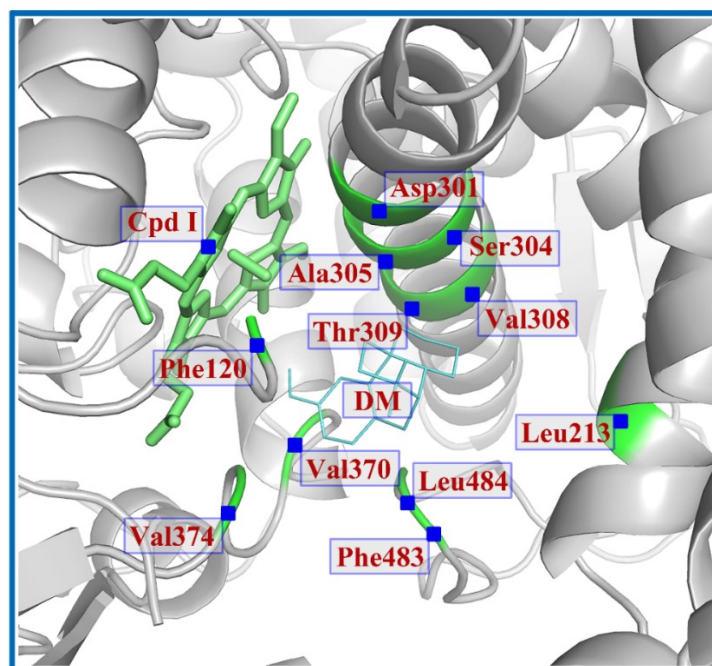


Figure S4. The position of residues that contribute significantly in the residue decomposition energy results.

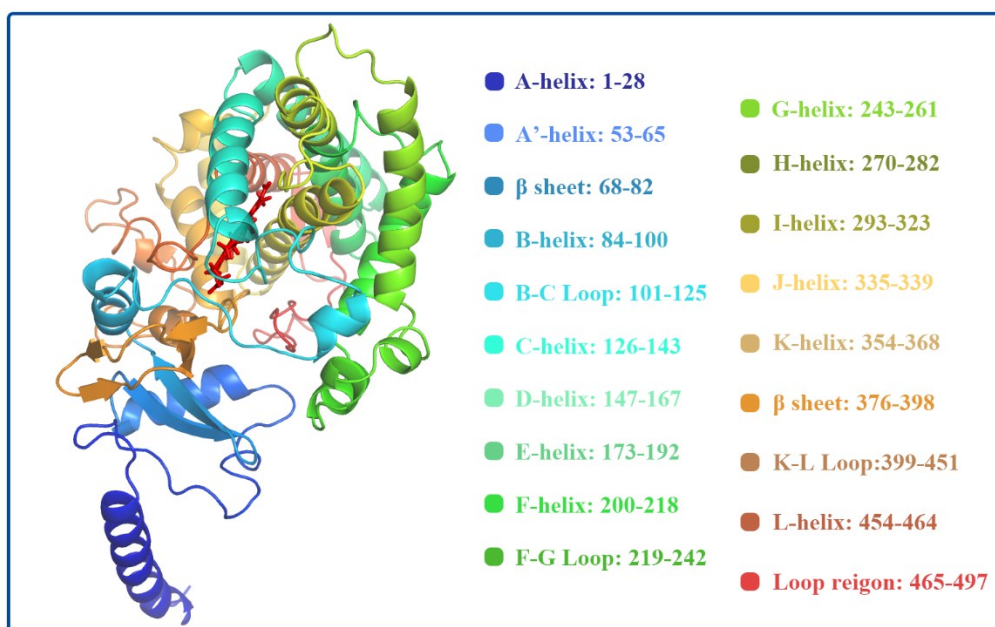


Figure S5. The residue numbers that corresponds to different secondary structures for CYP2D6.

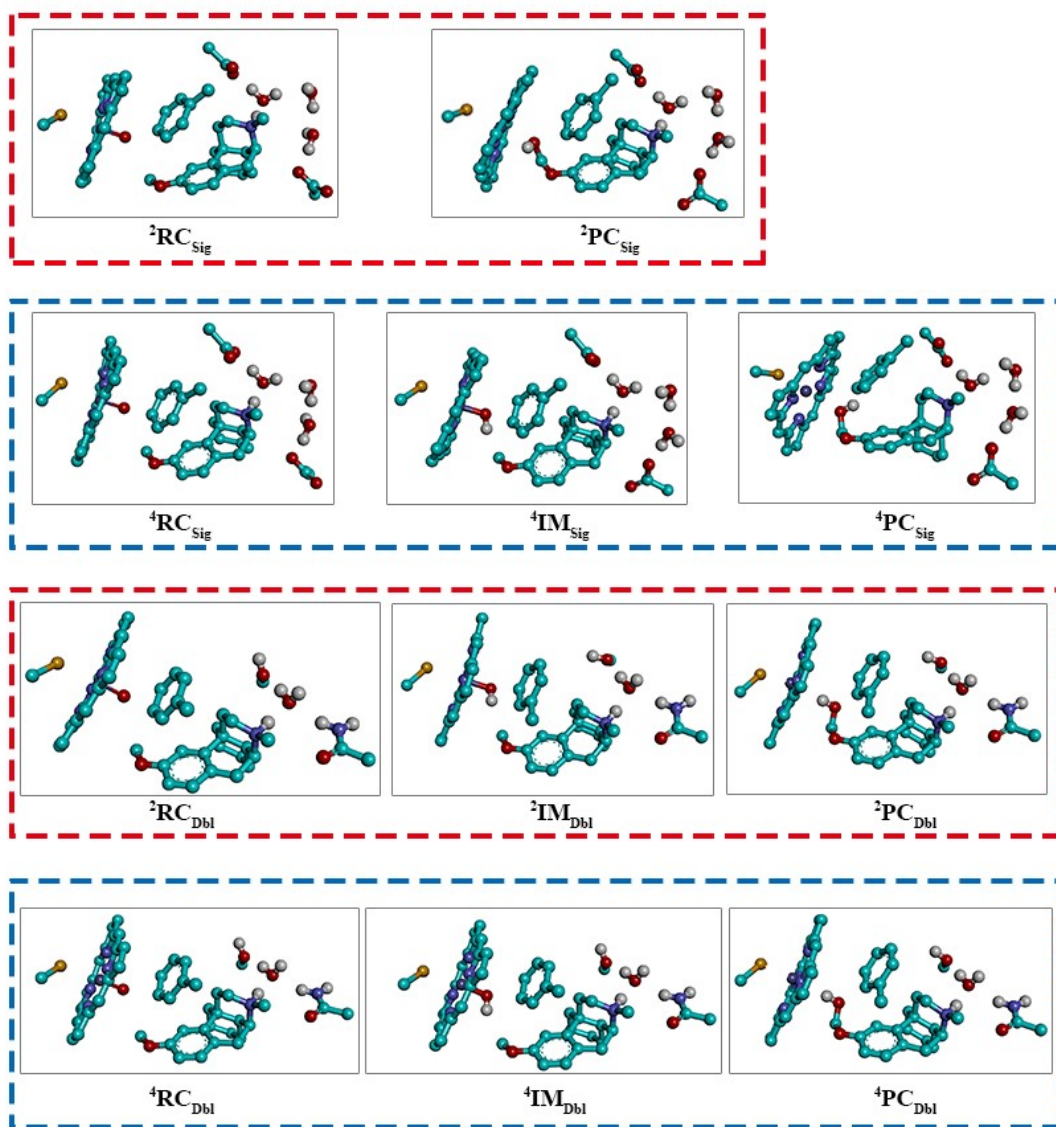


Figure S6. The corresponding structures of reactant complex (RC), intermediate (IM), and product complex (PC) of the Sig system and Dbl system.

One supplementary table

Table S1. Binding free energy (kcal/mol).

	Sig system	Dbl system
E_{ele}	-94.59 ± 6.03	-82.47 ± 4.91
E_{vdw}	-39.42 ± 1.36	-38.36 ± 1.77
G_{gb}	107.09 ± 5.95	98.56 ± 4.73
G_{sa}	-4.74 ± 0.12	-4.92 ± 0.18
ΔG_{gas}	-134.02 ± 6.49	-120.83 ± 5.26
ΔG_{sol}	102.35 ± 5.90	93.64 ± 4.70
$\Delta G_{\text{binding}}$	-31.67 ± 1.76	-27.19 ± 2.06

E_{ele} , E_{vdw} : electrostatic, and van der waals energy in the gas phase

G_{gb} : polar contribution to solvation energy

G_{sa} : nonpolar solvation energy

G_{gas} : gas phase energy contributions

G_{sol} : solvation free energy components

The cartesian coordinates of all states in the QM calculation in this study

The cartesian coordinates of the reactant complex in doublet spin state of **Sig** system

$^2\text{RC}_{\text{Sig}}$

C	-2.21593	3.20451	-2.66898
C	-1.14743	2.235	-2.22399
C	-0.48195	2.40568	-1.00309
C	-0.81507	1.11764	-3.00628
C	0.48288	1.48944	-0.576
C	0.14641	0.2017	-2.58392
C	0.8004	0.38495	-1.36432
H	-2.53735	3.87243	-1.86641
H	-3.09646	2.66643	-3.03969
H	-0.74886	3.24987	-0.375
H	-1.33496	0.95865	-3.94893
H	0.99497	1.63336	0.3706
H	0.37468	-0.66949	-3.19045
H	1.55998	-0.31074	-1.03248
C	-9.60848	-3.48059	1.37266
C	-9.30424	-2.65158	0.11679
O	-10.06261	-2.76556	-0.86637
O	-8.29631	-1.86938	0.18892
H	-9.86511	-2.80051	2.19231
H	-8.71409	-4.03383	1.67833
C	-1.894	5.66134	1.07957
C	-3.09974	4.6772	0.87429
O	-3.55844	4.07393	1.89372
O	-3.52838	4.55634	-0.30219

H	-2.19649	6.6635	0.75954
H	-1.05989	5.35543	0.43942
C	8.02244	0.22853	-1.64984
S	7.3654	0.71785	-0.02854
H	7.99558	-0.86544	-1.71546
H	9.05028	0.57337	-1.77928
N	4.85719	-1.17804	-1.47822
N	5.51402	-1.64228	1.26264
N	4.10693	1.56165	-0.78311
C	3.88683	0.49002	-2.99211
C	5.62845	-3.30305	-0.5622
C	5.67777	-0.61291	3.4798
C	4.09938	3.24551	1.00551
C	4.4426	-0.75987	-2.71702
C	5.69078	-2.91358	0.76974
C	5.39952	0.71418	3.13381
C	3.76289	2.79628	-0.2738
O	3.20023	-0.50902	0.63253
C	4.62574	-1.83677	-3.67823
C	5.96902	-3.8274	1.85224
C	5.47668	1.85016	4.03891
C	3.06187	3.57662	-1.29963
C	5.13696	-2.92051	-3.0127
C	5.95313	-3.10608	3.00459
C	5.06678	2.96773	3.36428
C	3.04277	2.79419	-2.41568
C	5.25217	-2.48983	-1.62193
C	5.68816	-1.71744	2.62564
C	4.70493	2.49235	2.01691
C	3.69612	1.53933	-2.09119

N	4.96383	1.14343	1.9069
Fe	4.70976	-0.06019	0.2668
H	3.53557	0.65641	-4.00518
H	5.85673	-4.34074	-0.78304
H	5.91731	-0.79984	4.52212
H	3.84662	4.27417	1.24315
O	0.47083	-3.18377	-1.25719
N	-4.98875	0.92663	-0.39922
C	-3.27483	-0.88727	1.10346
C	-4.82146	-0.97696	1.14518
C	-5.39836	-0.51173	-0.19497
C	-2.88898	0.59289	0.86861
C	-2.73319	-1.34015	2.47413
C	-5.32251	-2.37744	1.5301
C	-2.7238	-1.69888	-0.07485
C	-4.9466	-1.43561	-1.32421
C	-3.50876	1.1619	-0.39856
C	-3.21028	-2.74129	2.87039
C	-4.74351	-2.80968	2.8811
C	-3.50283	-1.89294	-1.22834
C	-1.38956	-2.13715	-0.06491
C	-5.65106	1.60693	-1.53685
C	-2.92289	-2.53387	-2.33316
C	-0.82583	-2.76174	-1.17709
C	-1.60725	-2.96954	-2.32089
C	1.28643	-3.07773	-0.0951
H	-5.1661	-0.27329	1.91545
H	-6.48859	-0.50635	-0.14878
H	-1.80414	0.69085	0.78049
H	-3.20328	1.20163	1.7237

H	-3.09136	-0.61687	3.21848
H	-1.64029	-1.27483	2.49928
H	-5.00758	-3.10216	0.76995
H	-6.41711	-2.37613	1.52907
H	-5.12508	-0.97018	-2.29992
H	-5.6217	-2.29913	-1.29406
H	-3.37867	2.2447	-0.43919
H	-3.08643	0.70881	-1.29519
H	-2.80589	-3.00897	3.85429
H	-2.81707	-3.47429	2.15436
H	-5.08061	-3.82363	3.128
H	-5.12759	-2.14923	3.67158
H	-0.77884	-1.95135	0.80737
H	-6.73072	1.48971	-1.42146
H	-5.32128	1.18489	-2.48739
H	-5.37284	2.66219	-1.48221
H	-3.52437	-2.68468	-3.22696
H	-1.15851	-3.45506	-3.18117
H	2.26687	-3.46442	-0.37722
H	0.8762	-3.67587	0.72978
H	1.41034	-2.04204	0.23161
H	-5.33618	1.49978	0.45929
O	-5.68525	2.47399	1.49793
H	-6.47475	2.9747	1.2284
H	-4.91636	3.13923	1.61682
O	-8.63019	3.35731	0.11695
H	-8.32069	3.59639	-0.76443
H	-8.83513	2.39884	0.04884
O	-9.00622	0.63123	0.27252
H	-8.76486	0.56875	1.20504

H	-8.79629	-0.2914	-0.03854
H	-10.43528	-4.17426	1.2046
H	-1.57029	5.68698	2.12239
H	-1.8536	3.81496	-3.50822
H	5.38682	-3.90235	-3.38828
H	4.37657	-1.75646	-4.72867
H	2.5911	3.01157	-3.37404
H	2.65619	4.56782	-1.15604
H	5.8069	1.78012	5.06756
H	6.144	-4.88776	1.72672
H	6.12363	-3.44352	4.01813
H	4.97493	3.98628	3.71291
H	7.38195	0.61709	-2.44668

The cartesian coordinates of the transition state in doublet spin state of **Sig system**

²TS_{Sig}

C	-2.28784	3.68966	-2.45007
C	-1.30366	2.56573	-2.24325
C	-0.50198	2.51584	-1.09444
C	-1.16053	1.53893	-3.1888
C	0.4167	1.48277	-0.89974
C	-0.2438	0.50434	-2.99978
C	0.55448	0.47691	-1.85552
H	-2.63711	4.12174	-1.50795
H	-3.16312	3.34109	-3.01058
H	-0.61995	3.2904	-0.34143
H	-1.78639	1.55109	-4.07891
H	1.03201	1.44379	-0.00711
H	-0.16272	-0.29056	-3.73632

H	1.27481	-0.31556	-1.69717
C	-9.80058	-3.63467	-0.08729
C	-8.3574	-3.0508	-0.12633
O	-7.40054	-3.8449	-0.03472
O	-8.25884	-1.78265	-0.25777
H	-10.34248	-3.34779	-0.99573
H	-10.34752	-3.20893	0.76142
C	-2.18933	5.42444	1.69389
C	-3.36606	4.4787	1.27735
O	-3.88482	3.74449	2.17556
O	-3.70121	4.49767	0.06758
H	-2.27179	6.37253	1.15642
H	-1.24004	4.95698	1.40444
C	7.91829	0.59976	-1.44608
S	7.03923	1.03114	0.0893
H	7.90982	-0.47796	-1.62293
H	8.94517	0.97101	-1.38766
N	4.71303	-0.84989	-1.69116
N	5.15227	-1.81875	0.93172
N	3.96088	1.7542	-0.55673
C	3.87353	1.09782	-2.9281
C	5.43198	-3.11396	-1.14812
C	5.30822	-1.16548	3.29452
C	3.80738	3.07582	1.50711
C	4.41091	-0.19141	-2.85416
C	5.40471	-2.97594	0.23726
C	5.03305	0.20388	3.19198
C	3.56274	2.87131	0.14756
O	2.79598	-0.39259	0.41184
C	4.68531	-1.05659	-3.98981

C	5.69966	-4.05105	1.15378
C	5.07251	1.15558	4.29321
C	2.90716	3.81775	-0.75768
C	5.14445	-2.25497	-3.50904
C	5.64986	-3.53024	2.40932
C	4.67473	2.37497	3.81798
C	2.96983	3.25976	-1.99868
C	5.13309	-2.11315	-2.05889
C	5.33196	-2.11118	2.2639
C	4.36905	2.15206	2.39427
C	3.62403	1.97053	-1.87105
N	4.63739	0.84629	2.05085
Fe	4.47964	-0.06046	0.20404
H	3.59408	1.44956	-3.91611
H	5.69998	-4.08929	-1.54155
H	5.53996	-1.53391	4.28958
H	3.52533	4.04203	1.91393
O	0.99636	-2.85092	-0.99581
N	-5.09765	0.5063	-0.40838
C	-2.99571	-0.75199	1.19036
C	-4.49545	-1.12055	1.33914
C	-5.2034	-0.95111	-0.00438
C	-2.90919	0.72793	0.74706
C	-2.32799	-0.9017	2.5725
C	-4.69396	-2.53063	1.91655
C	-2.34261	-1.61641	0.10466
C	-4.62123	-1.91295	-1.03726
C	-3.69286	1.02279	-0.52686
C	-2.51503	-2.29815	3.17659
C	-4.00462	-2.65658	3.2793

C	-3.11841	-2.10473	-0.96577
C	-0.95566	-1.84409	0.10729
C	-5.92305	0.84912	-1.59238
C	-2.48075	-2.80594	-1.99939
C	-0.35299	-2.56492	-0.92113
C	-1.11393	-3.04194	-1.99076
C	1.83023	-2.70586	0.09008
H	-4.93575	-0.40075	2.04284
H	-6.27767	-1.15639	0.08152
H	-1.86861	1.00369	0.56279
H	-3.27459	1.3797	1.54834
H	-2.79039	-0.15947	3.23534
H	-1.26687	-0.63307	2.52264
H	-4.26422	-3.27401	1.23622
H	-5.76165	-2.7622	1.97243
H	-4.90694	-1.61754	-2.05256
H	-5.14511	-2.86379	-0.86627
H	-3.76897	2.10496	-0.66265
H	-3.23192	0.57171	-1.40772
H	-2.03988	-2.34269	4.16438
H	-2.00633	-3.03935	2.54645
H	-4.12643	-3.67334	3.67153
H	-4.4883	-1.9803	3.99819
H	-0.34176	-1.41787	0.89006
H	-6.94737	0.51465	-1.413
H	-5.51358	0.3827	-2.48961
H	-5.89784	1.93514	-1.70465
H	-3.08027	-3.17804	-2.82654
H	-0.62176	-3.59031	-2.78678
H	2.72474	-3.30691	-0.07211

H	1.34654	-2.86907	1.05698
H	2.35104	-1.48928	0.19111
H	-5.52003	1.11431	0.37885
O	-5.95969	2.2058	1.32485
H	-6.74271	2.7247	1.07958
H	-5.2221	2.8479	1.59573
O	-8.83925	3.31935	-0.02723
H	-8.28541	3.45318	-0.80593
H	-8.98575	2.34748	-0.02169
O	-9.19086	0.61005	-0.38925
H	-9.75133	0.51095	-1.16699
H	-8.89844	-0.3335	-0.19954
H	-9.77582	-4.72263	-0.00058
H	-2.17627	5.59341	2.77353
H	-1.83189	4.49129	-3.04913
H	5.43681	-3.14349	-4.05017
H	4.53158	-0.76748	-5.02163
H	2.57144	3.65043	-2.92508
H	2.47499	4.76255	-0.45996
H	5.36674	0.90129	5.30356
H	5.92333	-5.0671	0.85685
H	5.8303	-4.0255	3.35408
H	4.56306	3.31295	4.34253
H	7.4234	1.09483	-2.28926

The cartesian coordinates of the product complex in doublet spin state of **Sig system**

${}^2\text{PC}_{\text{Sig}}$

C	-2.32934	3.82166	-2.31078
C	-1.44433	2.60361	-2.316

C	-0.48993	2.41099	-1.30649
C	-1.54834	1.62507	-3.31454
C	0.33056	1.28359	-1.29163
C	-0.73153	0.49313	-3.30652
C	0.21365	0.32139	-2.2958
H	-2.68278	4.08709	-1.30809
H	-3.20543	3.67009	-2.95065
H	-0.4047	3.15157	-0.51571
H	-2.29153	1.74977	-4.0989
H	1.05264	1.13906	-0.4961
H	-0.84275	-0.2619	-4.08012
H	0.83399	-0.56722	-2.27724
C	-9.80408	-3.72806	-0.63738
C	-8.36474	-3.13576	-0.49177
O	-7.41626	-3.93059	-0.3573
O	-8.26615	-1.85842	-0.52936
H	-10.24928	-3.39718	-1.58291
H	-10.44354	-3.35062	0.16856
C	-2.30809	5.23044	1.95608
C	-3.484	4.32343	1.45964
O	-4.05015	3.56688	2.31127
O	-3.77016	4.39342	0.2406
H	-2.41082	6.23024	1.52546
H	-1.36228	4.80961	1.59326
C	7.89067	0.75076	-1.39339
S	6.92229	0.80905	0.19026
H	7.97806	-0.27391	-1.7599
H	8.87961	1.13945	-1.14041
N	4.82367	-0.6436	-1.80974
N	5.25759	-1.80713	0.75777

N	3.92879	1.78604	-0.4863
C	3.85566	1.32588	-2.90806
C	5.57442	-2.934	-1.41913
C	5.2568	-1.39159	3.17179
C	3.77525	2.96299	1.66608
C	4.44867	0.06216	-2.93078
C	5.52666	-2.90434	-0.03012
C	4.99059	-0.01853	3.15464
C	3.52422	2.85478	0.29572
O	2.54415	-0.74961	-0.00955
C	4.6747	-0.74724	-4.11506
C	5.73469	-4.07094	0.79559
C	4.94014	0.83402	4.33419
C	2.83897	3.86256	-0.53443
C	5.17507	-1.95897	-3.71336
C	5.60662	-3.68521	2.09547
C	4.55367	2.08434	3.94221
C	2.89738	3.37975	-1.80977
C	5.24763	-1.88086	-2.26035
C	5.34546	-2.24036	2.06647
C	4.33967	1.98128	2.48514
C	3.58537	2.1013	-1.78048
N	4.65598	0.71299	2.04293
Fe	4.81795	0.06798	0.1164
H	3.54026	1.73511	-3.86218
H	5.83659	-3.88021	-1.88121
H	5.41462	-1.8416	4.14721
H	3.47315	3.88904	2.14543
O	1.23957	-2.6499	-0.38586
N	-5.12189	0.35035	-0.46588

C	-3.0231	-0.62243	1.3198
C	-4.50077	-1.0877	1.42067
C	-5.13884	-1.08189	0.03293
C	-2.99972	0.8134	0.74658
C	-2.43933	-0.60043	2.74759
C	-4.63511	-2.45581	2.10559
C	-2.24954	-1.52715	0.35762
C	-4.42295	-2.0613	-0.89835
C	-3.7497	0.9488	-0.57405
C	-2.55969	-1.9525	3.46017
C	-4.02194	-2.41875	3.50991
C	-2.92017	-2.16465	-0.70143
C	-0.85268	-1.64916	0.46751
C	-5.92631	0.54861	-1.69632
C	-2.16835	-2.9319	-1.60265
C	-0.13234	-2.42589	-0.43203
C	-0.79321	-3.07597	-1.47643
C	2.07565	-1.98671	0.52129
H	-5.0311	-0.34815	2.03491
H	-6.19993	-1.35829	0.0709
H	-1.96734	1.12579	0.56704
H	-3.41876	1.51219	1.47708
H	-2.99783	0.15714	3.31107
H	-1.40016	-0.25225	2.73876
H	-4.11956	-3.22077	1.51416
H	-5.68963	-2.74939	2.13239
H	-4.63975	-1.82589	-1.94608
H	-4.91151	-3.02994	-0.73016
H	-3.88748	2.00962	-0.79507
H	-3.22744	0.4631	-1.40018

H	-2.14803	-1.87714	4.47424
H	-1.95802	-2.70087	2.92811
H	-4.0918	-3.40702	3.98009
H	-4.59804	-1.72677	4.13977
H	-0.3412	-1.10698	1.25143
H	-6.91444	0.11176	-1.54266
H	-5.42793	0.08531	-2.54949
H	-6.01055	1.62391	-1.86691
H	-2.68135	-3.43076	-2.42144
H	-0.21699	-3.67703	-2.17196
H	2.91416	-2.66391	0.69151
H	1.58414	-1.7471	1.46616
H	2.78564	-0.91754	-0.9365
H	-5.59334	0.96631	0.28413
O	-6.04117	2.01796	1.28138
H	-6.84369	2.52324	1.07189
H	-5.33649	2.66734	1.61353
O	-8.91143	3.20833	-0.02423
H	-8.32375	3.40562	-0.76379
H	-9.05607	2.23898	-0.10729
O	-9.23135	0.53237	-0.60033
H	-9.77806	0.46162	-1.39056
H	-8.93562	-0.41624	-0.44229
H	-9.77538	-4.81887	-0.60533
H	-2.27365	5.28568	3.04687
H	-1.7875	4.68915	-2.71423
H	5.44196	-2.82058	-4.30847
H	4.44941	-0.42037	-5.12211
H	2.48443	3.82112	-2.70678
H	2.39501	4.77582	-0.16558

H	5.16526	0.49224	5.33643
H	5.94028	-5.06034	0.40859
H	5.69883	-4.27722	2.99556
H	4.38195	2.9694	4.53774
H	7.43257	1.37859	-2.16033

The cartesian coordinates of the reactant complex in quartet spin state of **Sig system**

⁴RC_{Sig}

C	-2.20558	3.20617	-2.65641
C	-1.13502	2.23259	-2.22507
C	-0.46773	2.38794	-1.00305
C	-0.80066	1.12721	-3.02337
C	0.50146	1.46923	-0.59102
C	0.1657	0.20934	-2.61651
C	0.82243	0.37799	-1.39632
H	-2.52104	3.87026	-1.84839
H	-3.08942	2.67162	-3.02426
H	-0.73626	3.22234	-0.36249
H	-1.32201	0.97964	-3.96705
H	1.01393	1.6003	0.35719
H	0.39541	-0.65238	-3.23602
H	1.58463	-0.3202	-1.07569
C	-9.62129	-3.46633	1.36367
C	-9.30257	-2.63764	0.11059
O	-10.04784	-2.75369	-0.88183
O	-8.29634	-1.85387	0.19637
H	-9.88816	-2.78611	2.17994
H	-8.73039	-4.01897	1.68056
C	-1.88238	5.65578	1.09675

C	-3.09114	4.67608	0.88924
O	-3.55287	4.07299	1.90728
O	-3.51698	4.55621	-0.28839
H	-2.16764	6.6514	0.74291
H	-1.03652	5.32488	0.48474
C	8.02356	0.20149	-1.62831
S	7.2717	0.90679	-0.13184
H	7.97758	-0.8906	-1.60125
H	9.05462	0.54269	-1.74374
N	4.85426	-1.19795	-1.46116
N	5.47266	-1.68124	1.27732
N	4.13695	1.55509	-0.76424
C	3.96075	0.50251	-2.98687
C	5.54844	-3.34744	-0.54177
C	5.71535	-0.63418	3.47869
C	4.07049	3.21931	1.0408
C	4.48777	-0.76116	-2.70612
C	5.61654	-2.95582	0.79121
C	5.42706	0.69269	3.13906
C	3.7626	2.78028	-0.24803
O	3.18533	-0.51203	0.64041
C	4.6717	-1.83453	-3.67152
C	5.90368	-3.86792	1.87282
C	5.50913	1.82608	4.04713
C	3.07126	3.56208	-1.27914
C	5.13166	-2.93756	-3.00039
C	5.93899	-3.13554	3.0177
C	5.06809	2.94001	3.38652
C	3.09244	2.79553	-2.40616
C	5.2174	-2.52168	-1.60393

C	5.68519	-1.74636	2.63337
C	4.68942	2.46665	2.04362
C	3.75318	1.54408	-2.08417
N	4.96313	1.12089	1.92282
Fe	4.70479	-0.0872	0.28601
H	3.63688	0.67927	-4.00734
H	5.75468	-4.39011	-0.76068
H	5.98291	-0.81809	4.51483
H	3.80039	4.24142	1.2869
O	0.46945	-3.17541	-1.27786
N	-4.98652	0.93392	-0.39652
C	-3.27231	-0.8871	1.09693
C	-4.81896	-0.97604	1.1401
C	-5.39719	-0.50493	-0.19745
C	-2.88599	0.59388	0.86827
C	-2.72911	-1.34637	2.46485
C	-5.32058	-2.37772	1.51993
C	-2.723	-1.69348	-0.08581
C	-4.94742	-1.42453	-1.33093
C	-3.5063	1.16831	-0.39611
C	-3.20663	-2.74889	2.85563
C	-4.73989	-2.81611	2.8682
C	-3.50352	-1.88225	-1.23918
C	-1.38877	-2.13185	-0.07964
C	-5.64923	1.61883	-1.53128
C	-2.92488	-2.51778	-2.3478
C	-0.8266	-2.75169	-1.19527
C	-1.60924	-2.95358	-2.33925
C	1.28492	-3.07577	-0.11521
H	-5.16232	-0.27534	1.91366

H	-6.48741	-0.49919	-0.1499
H	-1.80109	0.69169	0.78
H	-3.19956	1.19917	1.7261
H	-3.08584	-0.62615	3.21287
H	-1.63613	-1.28185	2.48881
H	-5.00735	-3.09951	0.75628
H	-6.4152	-2.37519	1.5206
H	-5.12752	-0.95548	-2.3046
H	-5.62252	-2.28811	-1.30287
H	-3.37565	2.25122	-0.43268
H	-3.08495	0.71826	-1.2948
H	-2.80099	-3.02119	3.83776
H	-2.81499	-3.479	2.1358
H	-5.07746	-3.83082	3.1113
H	-5.12231	-2.15873	3.66204
H	-0.77708	-1.95043	0.79288
H	-6.72885	1.50167	-1.41551
H	-5.32023	1.20004	-2.48351
H	-5.37034	2.6737	-1.47293
H	-3.52744	-2.66422	-3.24159
H	-1.16168	-3.43517	-3.20235
H	2.26474	-3.46322	-0.3985
H	0.87339	-3.67649	0.70718
H	1.41045	-2.04162	0.21578
H	-5.33329	1.50433	0.46394
O	-5.68246	2.47768	1.50449
H	-6.4707	2.98034	1.23499
H	-4.91269	3.14103	1.6261
O	-8.62335	3.37119	0.12094
H	-8.31369	3.61238	-0.75985

H	-8.82928	2.41302	0.05023
O	-9.00671	0.64574	0.27122
H	-8.77303	0.58547	1.20588
H	-8.79382	-0.27826	-0.03526
H	-10.44555	-4.16059	1.18582
H	-1.58126	5.70495	2.14546
H	-1.84803	3.8208	-3.49462
H	5.36567	-3.92282	-3.37715
H	4.4568	-1.73883	-4.72822
H	2.66051	3.02019	-3.37194
H	2.64639	4.54457	-1.13179
H	5.86079	1.75642	5.06867
H	6.05686	-4.93209	1.75144
H	6.13411	-3.46683	4.02885
H	4.96954	3.95581	3.74119
H	7.43916	0.53338	-2.49477

The cartesian coordinates of the transition state in quartet spin state of **Sig system**

⁴TS_{Sig}

C	-2.28736	3.68571	-2.46003
C	-1.30136	2.56586	-2.23726
C	-0.50258	2.52954	-1.08596
C	-1.1547	1.52892	-3.17111
C	0.41602	1.49895	-0.87703
C	-0.23792	0.49714	-2.9679
C	0.55678	0.48252	-1.82091
H	-2.64073	4.12617	-1.52378
H	-3.16023	3.32933	-3.01927
H	-0.62211	3.31266	-0.34205

H	-1.77816	1.53055	-4.06301
H	1.02876	1.47019	0.01787
H	-0.1547	-0.30637	-3.69463
H	1.27656	-0.3079	-1.65124
C	-9.80428	-3.62485	-0.06806
C	-8.36147	-3.04249	-0.10677
O	-7.40545	-3.83732	-0.01005
O	-8.25994	-1.77537	-0.24289
H	-10.34492	-3.33935	-0.97765
H	-10.35149	-3.19688	0.77933
C	-2.18657	5.43578	1.67744
C	-3.36664	4.49739	1.26834
O	-3.87859	3.7579	2.16472
O	-3.7167	4.52142	0.0619
H	-2.24793	6.37322	1.11921
H	-1.23951	4.94861	1.41486
C	7.917	0.59282	-1.44735
S	7.01694	1.06624	0.06016
H	7.9437	-0.49352	-1.56208
H	8.9276	1.00756	-1.43308
N	4.69817	-0.85802	-1.68565
N	5.16398	-1.81022	0.93986
N	3.95593	1.74987	-0.55986
C	3.86196	1.08456	-2.93052
C	5.43769	-3.11428	-1.13556
C	5.30674	-1.15253	3.30125
C	3.80626	3.08339	1.49815
C	4.39579	-0.20571	-2.85127
C	5.4123	-2.97015	0.24942
C	5.02942	0.21567	3.1922

C	3.56173	2.87317	0.13992
O	2.79477	-0.42159	0.44741
C	4.67501	-1.07395	-3.98437
C	5.70048	-4.04442	1.16915
C	5.07226	1.17136	4.28999
C	2.90819	3.81664	-0.76954
C	5.14072	-2.26771	-3.49895
C	5.64691	-3.52136	2.42395
C	4.67605	2.38968	3.81097
C	2.9685	3.25189	-2.0081
C	5.1275	-2.11955	-2.04865
C	5.33425	-2.10114	2.27328
C	4.36659	2.16133	2.38864
C	3.61837	1.96162	-1.8758
N	4.63185	0.85453	2.04936
Fe	4.46864	-0.05615	0.20805
H	3.58233	1.43404	-3.91924
H	5.7083	-4.09023	-1.52563
H	5.53596	-1.51689	4.29838
H	3.52646	4.05197	1.90085
O	0.99748	-2.86072	-1.02782
N	-5.09443	0.49876	-0.40033
C	-2.9824	-0.76346	1.184
C	-4.48125	-1.13261	1.34043
C	-5.19729	-0.96012	0.00161
C	-2.90016	0.71793	0.74482
C	-2.30686	-0.91627	2.56199
C	-4.67622	-2.54425	1.91528
C	-2.33493	-1.62542	0.09244
C	-4.62036	-1.91857	-1.03727

C	-3.68968	1.0144	-0.52494
C	-2.49017	-2.31431	3.16347
C	-3.97903	-2.67351	3.27372
C	-3.1168	-2.11036	-0.97446
C	-0.94794	-1.85528	0.08771
C	-5.92409	0.84261	-1.58152
C	-2.48539	-2.81027	-2.01261
C	-0.35064	-2.57503	-0.94491
C	-1.11889	-3.04866	-2.01097
C	1.83256	-2.73289	0.06403
H	-4.91767	-0.41498	2.04898
H	-6.27105	-1.16477	0.09317
H	-1.86099	0.99628	0.55719
H	-3.26435	1.36617	1.54958
H	-2.76557	-0.17599	3.22974
H	-1.24613	-0.64771	2.50634
H	-4.24967	-3.28525	1.23044
H	-5.74353	-2.77638	1.97656
H	-4.91229	-1.62032	-2.04997
H	-5.14249	-2.86996	-0.86594
H	-3.76594	2.09604	-0.66272
H	-3.2333	0.5625	-1.40757
H	-2.00942	-2.36123	4.14841
H	-1.98471	-3.05342	2.52845
H	-4.09832	-3.69139	3.66381
H	-4.45898	-1.99945	3.99725
H	-0.32867	-1.4324	0.86806
H	-6.94708	0.50524	-1.40056
H	-5.51529	0.37951	-2.48062
H	-5.90216	1.92897	-1.69057

H	-3.0896	-3.1803	-2.83738
H	-0.63188	-3.59661	-2.81052
H	2.72358	-3.33644	-0.10641
H	1.34537	-2.91486	1.02599
H	2.36055	-1.50946	0.19227
H	-5.51441	1.1054	0.38608
O	-5.95916	2.21828	1.32136
H	-6.74139	2.73562	1.07044
H	-5.22396	2.86005	1.58903
O	-8.83835	3.3287	-0.03405
H	-8.29231	3.45934	-0.81878
H	-8.98647	2.35714	-0.0244
O	-9.19185	0.61831	-0.38592
H	-9.7531	0.51449	-1.16248
H	-8.89946	-0.32368	-0.19073
H	-9.78063	-4.71262	0.02103
H	-2.18814	5.6265	2.75353
H	-1.83178	4.48277	-3.06521
H	5.43892	-3.1567	-4.03616
H	4.52103	-0.78894	-5.01737
H	2.56992	3.63897	-2.93599
H	2.47864	4.76402	-0.47618
H	5.36846	0.92028	5.30062
H	5.92035	-5.06213	0.8749
H	5.81979	-4.01558	3.37069
H	4.56735	3.32998	4.33206
H	7.38041	1.00853	-2.30874

The cartesian coordinates of the intermediate state in quartet spin state of **Sig system**

⁴IM_{Sig}

C	-2.24881	3.60089	-2.56036
C	-1.28513	2.47143	-2.28743
C	-0.42518	2.50926	-1.18078
C	-1.22491	1.34787	-3.1258
C	0.46631	1.4659	-0.92188
C	-0.33696	0.30177	-2.87263
C	0.51724	0.36059	-1.77068
H	-2.61547	4.07107	-1.64319
H	-3.11358	3.24477	-3.13135
H	-0.47377	3.36121	-0.50758
H	-1.89628	1.29136	-3.98026
H	1.12399	1.49191	-0.05981
H	-0.32629	-0.56992	-3.52089
H	1.2132	-0.44189	-1.55997
C	-9.78057	-3.54445	0.24796
C	-8.3485	-2.96827	0.08856
O	-7.3825	-3.73895	0.25189
O	-8.27017	-1.72868	-0.21972
H	-10.34199	-3.40352	-0.68276
H	-10.31601	-2.99598	1.03116
C	-2.10142	5.5477	1.48683
C	-3.29215	4.61164	1.11488
O	-3.76759	3.86333	2.02388
O	-3.69108	4.64401	-0.07638
H	-2.18001	6.4871	0.93414
H	-1.16359	5.06059	1.19333
C	7.94855	0.50427	-1.4902
S	7.13674	1.01249	0.0538
H	7.93429	-0.58326	-1.59712

H	8.97167	0.8853	-1.52821
N	4.73132	-0.93706	-1.63329
N	5.22258	-1.76732	1.0308
N	4.02811	1.73869	-0.62919
C	3.89689	0.95151	-2.96107
C	5.44484	-3.17599	-0.9794
C	5.39167	-0.99104	3.35478
C	3.88509	3.16037	1.36786
C	4.42323	-0.33781	-2.82568
C	5.43808	-2.9655	0.39794
C	5.11728	0.37226	3.18485
C	3.63323	2.88952	0.02101
O	2.84627	-0.40519	0.502
C	4.6821	-1.26307	-3.91697
C	5.71922	-3.99552	1.36883
C	5.16502	1.37688	4.23798
C	2.96253	3.78453	-0.92428
C	5.13921	-2.43646	-3.37675
C	5.69303	-3.40604	2.59501
C	4.76484	2.57023	3.70386
C	3.01033	3.16105	-2.13501
C	5.14282	-2.22	-1.93687
C	5.40184	-1.99067	2.3754
C	4.45003	2.27923	2.29614
C	3.66898	1.88172	-1.94829
N	4.7144	0.95951	2.01743
Fe	4.55829	-0.03274	0.21968
H	3.60627	1.25267	-3.96255
H	5.69584	-4.17356	-1.32557
H	5.62668	-1.30851	4.36655

H	3.60445	4.14491	1.72929
O	0.72342	-3.12243	-1.20218
N	-5.14682	0.55259	-0.39747
C	-3.00602	-0.73498	1.12814
C	-4.50781	-1.0163	1.39306
C	-5.29269	-0.8772	0.08941
C	-2.87985	0.7186	0.61344
C	-2.24909	-0.85607	2.46637
C	-4.73504	-2.38367	2.05667
C	-2.47454	-1.6825	0.04464
C	-4.83472	-1.91671	-0.92742
C	-3.73076	0.99394	-0.61971
C	-2.46204	-2.21099	3.15039
C	-3.95681	-2.48149	3.37304
C	-3.34356	-2.18052	-0.94683
C	-1.1052	-1.98533	-0.0316
C	-6.01152	0.8696	-1.56103
C	-2.81495	-2.96478	-1.98187
C	-0.61417	-2.78541	-1.05935
C	-1.46365	-3.27486	-2.05065
C	1.56317	-3.09427	-0.13661
H	-4.86423	-0.24043	2.08483
H	-6.36665	-1.02406	0.24495
H	-1.84227	0.93727	0.35367
H	-3.16679	1.41821	1.40681
H	-2.62592	-0.06143	3.12283
H	-1.18262	-0.64612	2.3295
H	-4.39885	-3.18233	1.38725
H	-5.80568	-2.55367	2.20109
H	-5.18068	-1.65842	-1.9338

H	-5.39414	-2.82758	-0.66836
H	-3.76767	2.0693	-0.80854
H	-3.34672	0.48119	-1.50324
H	-1.92008	-2.23549	4.10382
H	-2.0385	-3.007	2.52421
H	-4.1031	-3.47014	3.82437
H	-4.35196	-1.74595	4.08807
H	-0.41238	-1.55665	0.68085
H	-7.03576	0.56849	-1.33181
H	-5.64709	0.35802	-2.45286
H	-5.96389	1.94954	-1.71832
H	-3.48905	-3.34522	-2.74527
H	-1.05531	-3.88902	-2.84613
H	2.53811	-3.50624	-0.37133
H	1.13201	-3.21731	0.85307
H	2.62172	-1.30875	0.19931
H	-5.50548	1.21004	0.37908
O	-5.89336	2.33759	1.31981
H	-6.6681	2.86247	1.06102
H	-5.1362	2.97373	1.53481
O	-8.77913	3.39725	-0.06201
H	-8.24653	3.48658	-0.86156
H	-8.92115	2.42732	0.00483
O	-9.14956	0.67503	-0.2796
H	-9.74964	0.58362	-1.02857
H	-8.86822	-0.27607	-0.10343
H	-9.74723	-4.6063	0.49975
H	-2.07002	5.73404	2.56314
H	-1.76713	4.3791	-3.16948
H	5.42131	-3.35384	-3.87361

H	4.52078	-1.02868	-4.96145
H	2.5971	3.50087	-3.07495
H	2.53031	4.7424	-0.67155
H	5.46489	1.17373	5.2582
H	5.91591	-5.03144	1.12631
H	5.86852	-3.8542	3.56395
H	4.65719	3.53288	4.18294
H	7.38402	0.92914	-2.329

The cartesian coordinates of the product complex in quartet spin state of **Sig system**

⁴PC_{Sig}

C	-2.28495	3.79955	-2.35004
C	-1.3299	2.64962	-2.17067
C	-0.50174	2.58277	-1.04327
C	-1.22824	1.62317	-3.12198
C	0.41804	1.5448	-0.89003
C	-0.32034	0.57683	-2.96437
C	0.52174	0.53984	-1.85198
H	-2.6466	4.19215	-1.39487
H	-3.15214	3.49582	-2.94748
H	-0.58536	3.35585	-0.28496
H	-1.87816	1.6477	-3.99395
H	1.07739	1.54981	-0.02599
H	-0.27028	-0.21684	-3.70411
H	1.24202	-0.26058	-1.73654
C	-9.79777	-3.65493	-0.43751
C	-8.36054	-3.05338	-0.38564
O	-7.40793	-3.82549	-0.16497
O	-8.26562	-1.79341	-0.59447

H	-10.24828	-3.45421	-1.41631
H	-10.43078	-3.16883	0.31345
C	-2.22032	5.31033	1.88129
C	-3.38925	4.3765	1.41743
O	-3.94603	3.64242	2.29216
O	-3.6781	4.40297	0.19606
H	-2.25977	6.25247	1.32896
H	-1.26499	4.82362	1.64782
C	7.92068	0.67973	-1.43811
S	7.07077	0.88308	0.17927
H	7.89292	-0.36349	-1.76262
H	8.96191	0.98922	-1.31905
N	4.78732	-0.73103	-1.78281
N	5.2187	-1.83343	0.7907
N	3.89469	1.73652	-0.50657
C	3.85156	1.23355	-2.92092
C	5.53115	-3.01496	-1.35678
C	5.28528	-1.34306	3.19346
C	3.79973	2.98995	1.60943
C	4.4255	-0.0381	-2.91282
C	5.48328	-2.95009	0.03048
C	5.01659	0.0295	3.15044
C	3.53296	2.84124	0.24653
O	2.25117	-0.95116	0.49652
C	4.67011	-0.85656	-4.08634
C	5.72983	-4.08584	0.88709
C	5.02057	0.91611	4.30092
C	2.89738	3.84678	-0.61533
C	5.16833	-2.0658	-3.67104
C	5.63395	-3.65488	2.17418

C	4.63518	2.16466	3.88945
C	2.94889	3.33637	-1.87893
C	5.21111	-1.97444	-2.21531
C	5.34403	-2.21984	2.10904
C	4.36389	2.02382	2.448
C	3.58122	2.03315	-1.81198
N	4.64603	0.7355	2.03233
Fe	4.80424	0.03701	0.1186
H	3.56273	1.63409	-3.88691
H	5.80083	-3.96857	-1.79823
H	5.48012	-1.76638	4.17392
H	3.53176	3.94044	2.05975
O	1.11965	-2.66947	-0.65965
N	-5.10684	0.47146	-0.47302
C	-3.09421	-0.75584	1.24838
C	-4.59178	-1.15909	1.28972
C	-5.20641	-0.99486	-0.09882
C	-2.99481	0.72452	0.80731
C	-2.52919	-0.89495	2.67692
C	-4.79446	-2.57891	1.8407
C	-2.34971	-1.59797	0.20849
C	-4.52796	-1.92924	-1.10004
C	-3.70669	1.01082	-0.51126
C	-2.72323	-2.29896	3.26141
C	-4.20634	-2.69732	3.25045
C	-3.02949	-2.09196	-0.91865
C	-0.96009	-1.78068	0.30899
C	-5.88432	0.82062	-1.68655
C	-2.29152	-2.76769	-1.90154
C	-0.2469	-2.45933	-0.67685

C	-0.92035	-2.95845	-1.79442
C	1.86098	-2.30459	0.48298
H	-5.09817	-0.45602	1.96485
H	-6.27947	-1.22444	-0.09274
H	-1.94621	1.00691	0.67889
H	-3.40339	1.37719	1.58552
H	-3.05984	-0.16749	3.30375
H	-1.47458	-0.59682	2.71195
H	-4.29199	-3.3032	1.18998
H	-5.85608	-2.84094	1.81041
H	-4.74424	-1.62184	-2.12912
H	-5.04246	-2.89196	-0.97972
H	-3.78947	2.09297	-0.64319
H	-3.19001	0.56955	-1.3653
H	-2.32254	-2.3355	4.28207
H	-2.1491	-3.02316	2.66879
H	-4.32889	-3.71984	3.62694
H	-4.76027	-2.03972	3.93507
H	-0.4475	-1.3659	1.16809
H	-6.91071	0.47184	-1.55417
H	-5.43294	0.36652	-2.57004
H	-5.86616	1.90786	-1.78785
H	-2.81344	-3.15333	-2.7742
H	-0.35528	-3.48096	-2.55896
H	2.78819	-2.8725	0.43452
H	1.29989	-2.56451	1.39007
H	1.47017	-0.38382	0.55718
H	-5.56074	1.05551	0.31233
O	-5.98055	2.10891	1.31301
H	-6.77366	2.62852	1.10318

H	-5.25836	2.74647	1.62883
O	-8.85282	3.28771	0.00141
H	-8.28671	3.46427	-0.75983
H	-8.9954	2.31613	-0.04825
O	-9.19565	0.60101	-0.50754
H	-9.76926	0.55322	-1.28057
H	-8.89184	-0.35236	-0.39694
H	-9.77286	-4.73142	-0.25738
H	-2.25808	5.4932	2.95812
H	-1.79458	4.6158	-2.8999
H	5.44688	-2.93183	-4.2538
H	4.4639	-0.53392	-5.09891
H	2.56495	3.7756	-2.7897
H	2.48849	4.78713	-0.27459
H	5.28412	0.60176	5.30281
H	5.94502	-5.08384	0.5288
H	5.76327	-4.21487	3.09032
H	4.50328	3.06889	4.4657
H	7.44901	1.30076	-2.20399

The cartesian coordinates of the reactant complex in doublet spin state of **Dbl system**

²RC_{Dbl}

C	2.36984	-1.55464	4.13056
H	3.17942	-0.91374	4.49445
H	2.81404	-2.45117	3.68644
C	1.48387	-0.83055	3.14244
C	1.34377	0.56487	3.17451
H	1.8948	1.13845	3.91685
C	0.49682	1.22162	2.27793

H	0.39416	2.30222	2.32646
C	-0.23434	0.4954	1.3354
H	-0.92489	0.98424	0.65612
C	-0.10845	-0.89312	1.30502
H	-0.69764	-1.47484	0.60903
C	0.752	-1.54628	2.18719
H	0.85296	-2.62693	2.13295
C	11.74399	0.44811	0.29781
H	12.03127	0.0348	1.26735
H	12.29247	1.37613	0.12285
C	10.22733	0.62404	0.27313
O	9.45454	-0.29676	0.54042
N	9.77477	1.86488	-0.05765
H	8.77477	2.01681	-0.12979
H	10.40324	2.59941	-0.33967
C	4.57089	4.25438	-1.37438
H	5.10557	3.49423	-1.94565
H	5.02178	5.23232	-1.57544
O	4.6928	3.89152	0.00684
H	4.24074	4.54605	0.55343
C	-7.61947	-1.08952	1.58378
H	-8.39463	-0.82066	2.3065
H	-8.08866	-1.657	0.7739
S	-6.94115	0.46115	0.8896
N	-4.41633	2.46342	0.25138
C	-4.83645	3.44617	-0.62631
C	-3.91882	3.10477	1.35535
C	-4.61927	4.79637	-0.01568
C	-4.05424	4.54335	1.19922
C	-3.32555	2.48817	2.45664

H	-2.94975	3.14847	3.23202
C	-3.13659	1.12257	2.66875
N	-3.58293	0.11257	1.85297
C	-3.18746	-1.07201	2.44253
C	-2.43234	-0.80061	3.65837
C	-2.42781	0.55724	3.80045
C	-3.51673	-2.34832	1.98888
H	-3.18599	-3.18509	2.59558
C	-4.23325	-2.63856	0.83358
C	-4.61577	-3.98411	0.36754
C	-5.21887	-2.31418	-1.12095
N	-4.63934	-1.66148	-0.06453
C	-5.21735	-3.75333	-0.84924
C	-5.69607	-1.69081	-2.28919
H	-6.07675	-2.35933	-3.05575
C	-5.73903	-0.32365	-2.60551
C	-6.2015	0.23217	-3.87576
N	-5.36935	0.70647	-1.77318
C	-5.58394	1.89241	-2.46463
C	-5.35464	3.15995	-1.90361
H	-5.60785	4.0141	-2.52467
Fe	-4.34771	0.39689	0.00304
C	-6.11239	1.59842	-3.83322
O	-2.89736	0.38355	-0.71756
O	-0.36475	-3.14909	-1.34564
N	5.62321	-0.25379	0.79701
C	3.51869	-0.03101	-1.24407
C	5.02692	-0.10961	-1.5953
C	5.75526	-0.95907	-0.55103
C	3.38342	0.62462	0.15364

C	2.83198	0.86861	-2.29087
C	5.26495	-0.61968	-3.02462
C	2.91721	-1.43688	-1.16078
C	5.21052	-2.38869	-0.5283
C	4.18621	-0.09769	1.22651
C	3.04651	0.37605	-3.72561
C	4.54271	0.26695	-4.04645
C	3.70966	-2.51088	-0.7265
C	1.54802	-1.6372	-1.39263
C	6.4857	-0.8498	1.85994
C	3.10112	-3.7576	-0.51269
C	0.95626	-2.88409	-1.18002
C	1.74612	-3.9522	-0.72754
C	-1.19446	-2.18208	-1.99774
H	5.43304	0.91167	-1.53876
H	6.83343	-0.96648	-0.73688
H	2.33756	0.62723	0.46759
H	3.71219	1.66904	0.09838
H	3.25995	1.87382	-2.19277
H	1.76755	0.97722	-2.06321
H	4.88997	-1.64456	-3.11689
H	6.34131	-0.65017	-3.23171
H	5.52053	-2.91135	0.38237
H	5.7246	-2.9198	-1.33892
H	4.18991	0.46163	2.16389
H	3.79082	-1.09354	1.42547
H	2.55604	1.05612	-4.42997
H	2.57272	-0.60445	-3.84969
H	4.69103	-0.13092	-5.05537
H	4.99139	1.27069	-4.0366

H	0.92889	-0.80796	-1.70312
H	6.38845	-0.23426	2.75601
H	7.52089	-0.84161	1.5104
H	6.15026	-1.86084	2.08562
H	3.70939	-4.59345	-0.17552
H	1.27703	-4.91562	-0.56141
H	-0.79084	-1.92849	-2.98527
H	-1.3241	-1.27186	-1.4049
H	-2.1693	-2.65691	-2.10798
H	6.00484	0.70799	0.6556
O	6.74233	2.30551	0.63297
H	7.17162	2.55668	1.46079
H	6.05375	2.98984	0.45175
H	12.02369	-0.28322	-0.46535
H	1.79951	-1.88042	5.00835
H	3.5227	4.26059	-1.68924
H	-6.84012	-1.6915	2.05251
H	-4.87391	5.73766	-0.48049
H	-3.74791	5.26131	1.9492
H	-1.96995	1.14461	4.58464
H	-1.99952	-1.55448	4.29964
H	-4.42952	-4.91312	0.88474
H	-5.63504	-4.48802	-1.52642
H	-6.55262	-0.37625	-4.69979
H	-6.37096	2.33446	-4.57968

The cartesian coordinates of the transition state in doublet spin state of **Dbl system**

²TS_{Dbl}

C	-2.54142	-2.18532	-3.72639
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H	-2.63855	-2.97629	-2.9761
H	-2.01629	-2.61674	-4.58643
C	-1.79195	-0.99231	-3.1708
C	-1.99352	0.29132	-3.7007
H	-2.70285	0.42699	-4.51415
C	-1.28742	1.38997	-3.20683
H	-1.45418	2.37389	-3.63666
C	-0.36116	1.22334	-2.17409
H	0.21193	2.06613	-1.80181
C	-0.1502	-0.04704	-1.63847
H	0.59484	-0.17923	-0.86124
C	-0.86714	-1.14062	-2.12912
H	-0.70076	-2.12335	-1.6994
C	-11.86955	0.07162	0.07668
H	-12.43517	1.0008	0.1748
H	-12.08633	-0.5698	0.93571
C	-10.3602	0.28577	-0.00588
O	-9.58129	-0.62694	-0.27856
N	-9.92317	1.55194	0.2426
H	-8.92559	1.73335	0.24592
H	-10.55542	2.28561	0.51805
C	-4.74261	4.17303	1.1334
H	-5.14247	3.37895	1.7655
H	-5.24947	5.11182	1.38238
O	-4.99098	3.7839	-0.2231
H	-4.65872	4.46558	-0.82015
C	7.48894	-1.25171	-1.48845
H	8.2728	-1.05564	-2.22461
H	7.94679	-1.72989	-0.61676
S	6.79302	0.36231	-0.96943

N	4.20829	2.37756	-0.48143
C	4.6359	3.45484	0.26461
C	3.71066	2.87764	-1.65326
C	4.40281	4.7229	-0.49718
C	3.83343	4.32807	-1.67053
C	3.14088	2.12	-2.67712
H	2.75861	2.67389	-3.52918
C	2.97542	0.73342	-2.72797
N	3.43421	-0.17146	-1.80197
C	3.0263	-1.41894	-2.23212
C	2.25317	-1.29547	-3.45791
C	2.2573	0.03411	-3.77361
C	3.37349	-2.62885	-1.63124
H	3.0395	-3.53589	-2.12491
C	4.13004	-2.7716	-0.47297
C	4.57294	-4.04255	0.12037
C	5.18468	-2.20689	1.38881
N	4.53204	-1.69164	0.29835
C	5.22008	-3.6662	1.27566
C	5.68088	-1.44399	2.46463
H	6.1087	-2.014	3.28437
C	5.69471	-0.04837	2.62917
C	6.17411	0.65861	3.81579
N	5.27321	0.87082	1.69816
C	5.47188	2.13215	2.24519
C	5.19272	3.32288	1.55236
H	5.44535	4.24646	2.06527
Fe	4.22931	0.33283	-0.02507
C	6.04426	2.00906	3.62232
O	2.67659	0.43403	0.74351

O	0.97913	-2.55432	1.18893
N	-5.57462	-0.47212	-0.47503
C	-3.23995	0.12071	1.22827
C	-4.66455	-0.11645	1.79401
C	-5.41443	-1.10814	0.90101
C	-3.38807	0.68635	-0.20793
C	-2.54118	1.16699	2.11928
C	-4.64075	-0.55648	3.26518
C	-2.47606	-1.20467	1.14872
C	-4.69137	-2.45754	0.84578
C	-4.23977	-0.19093	-1.11519
C	-2.4991	0.75496	3.59502
C	-3.91146	0.48112	4.12819
C	-3.17361	-2.38918	0.86176
C	-1.07719	-1.23866	1.26211
C	-6.51413	-1.21324	-1.3701
C	-2.44918	-3.57146	0.64584
C	-0.3758	-2.43133	1.08068
C	-1.0664	-3.60324	0.7447
C	1.7327	-1.61598	1.88885
H	-5.19993	0.8443	1.7479
H	-6.44014	-1.24813	1.25458
H	-2.4078	0.7915	-0.67476
H	-3.83393	1.68599	-0.15943
H	-3.10272	2.10387	2.03047
H	-1.53905	1.38573	1.73876
H	-4.12671	-1.5197	3.35433
H	-5.66622	-0.70425	3.62419
H	-5.03723	-3.05348	-0.00478
H	-5.02555	-3.01607	1.72858

H	-4.43552	0.30281	-2.06819
H	-3.76406	-1.14853	-1.32086
H	-2.01706	1.54098	4.18546
H	-1.88532	-0.14586	3.70809
H	-3.86906	0.13776	5.16659
H	-4.48769	1.41723	4.13136
H	-0.5229	-0.33096	1.45657
H	-6.54689	-0.6897	-2.32688
H	-7.50968	-1.20644	-0.9182
H	-6.15364	-2.22747	-1.53284
H	-2.98527	-4.48865	0.41523
H	-0.5057	-4.51879	0.59377
H	1.18098	-1.12335	2.69394
H	2.22239	-0.57423	1.14553
H	2.65803	-2.08955	2.20744
H	-6.03536	0.45492	-0.34232
O	-6.91628	1.96891	-0.58653
H	-7.36318	2.04462	-1.43911
H	-6.29916	2.7359	-0.51774
H	-12.19594	-0.45993	-0.81963
H	-3.54355	-1.90799	-4.06942
H	-3.66982	4.27292	1.32542
H	6.71833	-1.90347	-1.90217
H	4.65601	5.7142	-0.15002
H	3.52128	4.95193	-2.49831
H	1.78218	0.52035	-4.61471
H	1.80887	-2.1195	-3.99752
H	4.40059	-5.02829	-0.28496
H	5.69183	-4.31222	2.00567
H	6.56344	0.15725	4.69315

H	6.30011	2.83068	4.27459
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The cartesian coordinates of the intermediate state in doublet spin state of **Dbl system**

$^2\text{IM}_{\text{Dbl}}$

C	-2.37772	-1.77405	-3.70036
H	-2.57279	-2.56746	-2.97096
H	-1.75359	-2.20921	-4.48939
C	-1.69045	-0.59156	-3.05044
C	-2.01518	0.72253	-3.41574
H	-2.76979	0.89119	-4.18088
C	-1.37071	1.81379	-2.82638
H	-1.62654	2.82265	-3.13975
C	-0.3873	1.60713	-1.85624
H	0.13724	2.44616	-1.40979
C	-0.04953	0.30381	-1.48651
H	0.73785	0.14279	-0.75701
C	-0.69568	-0.78131	-2.08071
H	-0.40874	-1.78832	-1.79824
C	-11.60658	0.64824	0.24068
H	-12.14469	1.58834	0.37864
H	-11.8789	-0.04194	1.04393
C	-10.08952	0.81281	0.23242
O	-9.32686	-0.12311	-0.01837
N	-9.61782	2.05652	0.51515
H	-8.61474	2.19749	0.55942
H	-10.23125	2.80828	0.78521
C	-4.33313	4.44092	1.44167

H	-5.32863	4.4943	1.88484
H	-3.8771	5.4352	1.4724
O	-4.51258	4.00049	0.08805
H	-3.65098	3.89322	-0.33483
C	7.68665	-1.2999	-1.4706
H	8.57167	-1.13737	-2.08964
H	7.97475	-1.90573	-0.60453
S	7.0986	0.31954	-0.85599
N	4.55061	2.40144	-0.28423
C	5.03768	3.42853	0.49197
C	4.01199	2.96932	-1.40693
C	4.82118	4.73272	-0.20589
C	4.1844	4.41292	-1.36682
C	3.36341	2.28322	-2.43292
H	2.95536	2.89226	-3.23386
C	3.16859	0.90503	-2.55673
N	3.65239	-0.06108	-1.70854
C	3.24316	-1.27621	-2.21914
C	2.44666	-1.06955	-3.41572
C	2.42244	0.28034	-3.62801
C	3.58181	-2.52541	-1.69515
H	3.23726	-3.39783	-2.24116
C	4.31284	-2.74393	-0.53232
C	4.67681	-4.05178	0.02877
C	5.32214	-2.29546	1.38858
N	4.73112	-1.71308	0.29795
C	5.29664	-3.74849	1.22078
C	5.83716	-1.5954	2.49851
H	6.22091	-2.21529	3.30368
C	5.92337	-0.21018	2.71302

C	6.43126	0.42411	3.92868
N	5.55867	0.76673	1.8176
C	5.82306	1.99289	2.4114
C	5.6059	3.22172	1.76602
H	5.9034	4.11177	2.31283
Fe	4.52276	0.34095	0.07515
C	6.37632	1.7844	3.78391
O	2.93665	0.41218	0.89471
O	0.22036	-3.23476	0.46414
N	-5.89016	-0.25891	-0.74218
C	-3.65226	-0.19975	1.15604
C	-5.12973	-0.30891	1.61109
C	-5.93954	-1.06461	0.55416
C	-3.61651	0.589	-0.17493
C	-2.87611	0.5881	2.23004
C	-5.26464	-0.94656	3.00319
C	-3.0709	-1.58776	0.87659
C	-5.41636	-2.49185	0.38646
C	-4.48954	-0.03811	-1.2508
C	-2.98498	-0.04248	3.62127
C	-4.45363	-0.16731	4.04558
C	-3.90494	-2.62896	0.4345
C	-1.68404	-1.78534	0.91108
C	-6.79482	-0.78849	-1.8044
C	-3.3258	-3.84421	0.03792
C	-1.12993	-2.99974	0.51286
C	-1.95237	-4.03992	0.06893
C	1.09423	-2.43894	1.14756
H	-5.52956	0.71352	1.67675
H	-7.00246	-1.07286	0.81054

H	-2.59558	0.64047	-0.55792
H	-3.95074	1.61423	0.01286
H	-3.30604	1.59822	2.26615
H	-1.83152	0.71979	1.933
H	-4.90037	-1.97915	2.97462
H	-6.32265	-0.98713	3.28747
H	-5.80997	-2.95104	-0.52558
H	-5.85816	-3.07557	1.20305
H	-4.56593	0.60909	-2.12586
H	-4.10051	-1.00307	-1.57332
H	-2.4285	0.55945	4.34689
H	-2.51899	-1.03494	3.6099
H	-4.53119	-0.65945	5.02013
H	-4.88401	0.83668	4.16517
H	-1.02413	-0.97436	1.18539
H	-6.79518	-0.07539	-2.63067
H	-7.79915	-0.87586	-1.38908
H	-6.42124	-1.74704	-2.16192
H	-3.96836	-4.65171	-0.30327
H	-1.50285	-4.97595	-0.2426
H	0.75187	-1.99128	2.07586
H	2.47186	-0.41455	0.68134
H	2.12033	-2.75524	1.01866
H	-6.25109	0.6926	-0.50676
O	-6.59005	2.39365	-0.36229
H	-7.07305	2.77866	-1.10488
H	-5.815	2.98895	-0.20517
H	-11.91299	0.18991	-0.70233
H	-3.32646	-1.48335	-4.16144
H	-3.72266	3.73866	2.01891

H	6.90478	-1.82006	-2.02584
H	5.12077	5.69912	0.17344
H	3.85525	5.08494	-2.14899
H	1.92466	0.82212	-4.42091
H	1.99929	-1.85644	-4.00652
H	4.47648	-5.01383	-0.41887
H	5.71022	-4.44281	1.9416
H	6.78388	-0.12947	4.78993
H	6.67023	2.56526	4.46952

The cartesian coordinates of the product complex in doublet spin state of **Dbl system**

${}^2\text{PC}_{\text{Dbl}}$

C	-2.39509	1.73669	3.67515
H	-2.39654	2.4638	2.85715
H	-1.73871	2.13291	4.45878
C	-1.9192	0.38218	3.19875
C	-2.50914	-0.79896	3.67132
H	-3.31385	-0.73672	4.40034
C	-2.07308	-2.04987	3.22826
H	-2.53583	-2.95139	3.62068
C	-1.03587	-2.13929	2.29638
H	-0.68732	-3.10932	1.95326
C	-0.43627	-0.97138	1.82078
H	0.36315	-1.01689	1.09044
C	-0.87209	0.2746	2.27404
H	-0.38531	1.16825	1.90187
C	-11.63903	-0.3896	-0.39909
H	-12.20099	-1.31309	-0.55331
H	-11.88936	0.31864	-1.1939

C	-10.12587	-0.59537	-0.38706
O	-9.33816	0.30634	-0.09579
N	-9.68729	-1.84099	-0.71609
H	-8.68802	-2.00326	-0.7707
H	-10.31883	-2.56207	-1.0252
C	-4.41595	-4.23825	-1.71984
H	-5.35328	-4.08555	-2.25712
H	-4.09318	-5.27518	-1.85724
O	-4.68718	-3.96542	-0.33813
H	-3.86059	-3.96935	0.16123
C	7.672	1.20344	1.47121
H	8.62921	0.92088	1.91588
H	7.84306	1.84793	0.60763
S	6.89879	-0.40167	0.95386
N	4.58066	-2.37798	0.16291
C	5.01098	-3.39836	-0.6712
C	4.00213	-2.99196	1.24746
C	4.72503	-4.73083	-0.04621
C	4.10338	-4.4377	1.12866
C	3.33148	-2.34452	2.28055
H	2.89565	-2.97982	3.0453
C	3.13307	-0.97442	2.44038
N	3.62776	0.02057	1.61383
C	3.24429	1.22513	2.21075
C	2.41983	0.97296	3.38315
C	2.37541	-0.38803	3.52065
C	3.62376	2.48163	1.74605
H	3.27806	3.34188	2.30967
C	4.38074	2.72599	0.60453
C	4.70993	4.0572	0.07036

C	5.4023	2.34177	-1.32046
N	4.82638	1.71414	-0.24191
C	5.33973	3.79054	-1.12422
C	5.89938	1.68137	-2.45867
H	6.2965	2.32563	-3.23773
C	5.93095	0.30578	-2.74041
C	6.42976	-0.28334	-3.98268
N	5.50956	-0.69648	-1.89653
C	5.77479	-1.90096	-2.54336
C	5.55836	-3.15295	-1.9425
H	5.83434	-4.02423	-2.52933
Fe	4.85279	-0.32447	0.014
C	6.34239	-1.64871	-3.90811
O	1.46044	0.51288	-0.52675
O	0.62506	2.70866	-0.23003
N	-5.87929	0.40186	0.59767
C	-3.56748	0.22705	-1.2024
C	-4.99757	0.55281	-1.70338
C	-5.75992	1.316	-0.61817
C	-3.68371	-0.64936	0.06783
C	-2.84902	-0.56912	-2.30987
C	-4.98681	1.31242	-3.0397
C	-2.83372	1.50624	-0.79904
C	-5.07155	2.6474	-0.30028
C	-4.53951	-0.00729	1.14975
C	-2.80764	0.18024	-3.64501
C	-4.22635	0.52595	-4.11423
C	-3.55246	2.60455	-0.30148
C	-1.4331	1.52755	-0.7835
C	-6.78591	0.93338	1.65688

C	-2.83925	3.70706	0.19378
C	-0.73698	2.63399	-0.29484
C	-1.45087	3.73309	0.2022
C	1.39595	1.80969	-1.03654
H	-5.5143	-0.40397	-1.87045
H	-6.79731	1.48498	-0.91991
H	-2.69408	-0.82906	0.49304
H	-4.10778	-1.62006	-0.2024
H	-3.4064	-1.50402	-2.45169
H	-1.84536	-0.86103	-1.98713
H	-4.50277	2.28586	-2.90686
H	-6.01718	1.50643	-3.36017
H	-5.43843	3.06303	0.64363
H	-5.41392	3.35453	-1.06552
H	-4.73002	-0.70327	1.96693
H	-4.0682	0.88364	1.5613
H	-2.29602	-0.42861	-4.39762
H	-2.22225	1.09984	-3.52944
H	-4.19379	1.10341	-5.04352
H	-4.77072	-0.40166	-4.3394
H	-0.87485	0.65559	-1.09178
H	-6.87828	0.17063	2.43173
H	-7.76334	1.12192	1.21298
H	-6.35495	1.83404	2.09164
H	-3.38666	4.56446	0.5776
H	-0.90309	4.58801	0.58269
H	0.93859	1.74425	-2.02895
H	2.13536	0.47098	0.17355
H	2.3801	2.27546	-1.09354
H	-6.31231	-0.48757	0.27093

O	-6.65148	-2.23164	0.15492
H	-7.17272	-2.60034	0.87934
H	-5.92398	-2.87939	-0.01382
H	-11.93735	0.0631	0.54904
H	-3.40346	1.68149	4.09673
H	-3.65786	-3.56143	-2.12541
H	7.06112	1.72033	2.21319
H	4.96681	-5.68827	-0.48418
H	3.72593	-5.13049	1.86978
H	1.86062	-0.96228	4.27901
H	1.97508	1.73654	4.00493
H	4.4713	5.00347	0.53187
H	5.72785	4.50716	-1.83726
H	6.80328	0.30462	-4.81183
H	6.62272	-2.40556	-4.62508

The cartesian coordinates of the reactant complex in quartet spin state of **Dbl system**

⁴RC_{Dbl}

C	2.3728	-1.55637	4.12476
H	3.19037	-0.92388	4.48553
H	2.80603	-2.45614	3.67644
C	1.48843	-0.82196	3.14275
C	1.35482	0.57392	3.18437
H	1.90963	1.13999	3.92965
C	0.50979	1.24061	2.29342
H	0.41256	2.32138	2.34919
C	-0.22604	0.52402	1.34707
H	-0.91502	1.02031	0.67172
C	-0.10658	-0.86475	1.30706

H	-0.69988	-1.43859	0.60812
C	0.75199	-1.52784	2.18374
H	0.84797	-2.60853	2.12199
C	11.74491	0.44617	0.28688
H	12.0333	0.03362	1.2564
H	12.29336	1.37393	0.1104
C	10.22828	0.62252	0.26393
O	9.45551	-0.29709	0.53524
N	9.77574	1.8625	-0.07021
H	8.77574	2.01452	-0.14182
H	10.40411	2.5958	-0.35566
C	4.57111	4.25309	-1.38079
H	5.10467	3.49233	-1.95232
H	5.02239	5.23067	-1.58274
O	4.6943	3.8907	0.00044
H	4.24228	4.54511	0.5472
C	-7.61794	-1.09027	1.58383
H	-8.39737	-0.82351	2.30261
H	-8.08181	-1.65827	0.77112
S	-6.9388	0.46107	0.89183
N	-4.41676	2.46213	0.24891
C	-4.83543	3.44553	-0.62831
C	-3.92039	3.10261	1.3541
C	-4.61825	4.79554	-0.0168
C	-4.05494	4.54139	1.19862
C	-3.32884	2.48596	2.45606
H	-2.95432	3.14619	3.2321
C	-3.1384	1.12046	2.66739
N	-3.58361	0.11032	1.85148
C	-3.18526	-1.07374	2.43966

C	-2.42961	-0.80198	3.65539
C	-2.42788	0.55575	3.79846
C	-3.51381	-2.34998	1.98525
H	-3.18312	-3.18714	2.59143
C	-4.23045	-2.63939	0.83002
C	-4.61508	-3.98499	0.3654
C	-5.21801	-2.31538	-1.12385
N	-4.63575	-1.66212	-0.06914
C	-5.21796	-3.75426	-0.85082
C	-5.69636	-1.69212	-2.29157
H	-6.07893	-2.3602	-3.05754
C	-5.73917	-0.3248	-2.60702
C	-6.20342	0.23177	-3.87613
N	-5.36634	0.7048	-1.77506
C	-5.58324	1.89179	-2.46588
C	-5.35372	3.15932	-1.90569
H	-5.6074	4.01319	-2.52691
Fe	-4.34579	0.39462	-0.00285
C	-6.11373	1.59813	-3.83385
O	-2.88673	0.38821	-0.70551
O	-0.37076	-3.15006	-1.32943
N	5.62347	-0.25355	0.79508
C	3.51517	-0.0343	-1.24269
C	5.0227	-0.11496	-1.59641
C	5.75231	-0.96234	-0.55132
C	3.38308	0.6249	0.15369
C	2.82736	0.86347	-2.29035
C	5.2577	-0.62874	-3.02489
C	2.9127	-1.43952	-1.15489
C	5.20638	-2.39141	-0.52373

C	4.18745	-0.09516	1.22688
C	3.0389	0.36736	-3.72431
C	4.53442	0.2561	-4.04755
C	3.70499	-2.51279	-0.71839
C	1.54309	-1.6397	-1.38446
C	6.48748	-0.84749	1.85792
C	3.0958	-3.75823	-0.49924
C	0.95065	-2.8854	-1.16657
C	1.74029	-3.95247	-0.71127
C	-1.19983	-2.18718	-1.98837
H	5.42965	0.90617	-1.54311
H	6.8301	-0.97122	-0.73932
H	2.33784	0.62927	0.46966
H	3.71262	1.66889	0.09507
H	3.25641	1.86855	-2.19534
H	1.76344	0.97354	-2.06099
H	4.88161	-1.65349	-3.11396
H	6.33365	-0.66073	-3.23387
H	5.51793	-2.91203	0.38757
H	5.71816	-2.92504	-1.33414
H	4.19335	0.46672	2.1627
H	3.79173	-1.09015	1.42931
H	2.54782	1.04623	-4.4294
H	2.56399	-0.61299	-3.84526
H	4.68058	-0.14433	-5.05577
H	4.98404	1.25944	-4.04089
H	0.92414	-0.81112	-1.69713
H	6.39219	-0.22966	2.75263
H	7.52207	-0.84071	1.5066
H	6.15185	-1.85777	2.08671

H	3.70395	-4.59343	-0.16024
H	1.27068	-4.91492	-0.54109
H	-0.79536	-1.94009	-2.97719
H	-1.32978	-1.27311	-1.40152
H	-2.17463	-2.66265	-2.09624
H	6.00562	0.70762	0.6507
O	6.74354	2.30387	0.62509
H	7.17557	2.55551	1.45133
H	6.05535	2.98886	0.44482
H	12.02349	-0.28583	-0.47607
H	1.80415	-1.87834	5.00504
H	3.52258	4.25981	-1.69451
H	-6.83959	-1.69125	2.05551
H	-4.87185	5.73718	-0.48145
H	-3.74916	5.25866	1.94948
H	-1.97034	1.1436	4.58246
H	-1.99472	-1.55553	4.29562
H	-4.42958	-4.91373	0.88335
H	-5.63758	-4.48888	-1.52687
H	-6.55593	-0.37652	-4.69968
H	-6.3731	2.33445	-4.57972

The cartesian coordinates of the transition state in quartet spin state of **Dbl** system

⁴TS_{Dbl}

C	-2.54181	-2.17576	-3.75845
H	-3.54119	-1.88105	-4.09507
H	-2.64703	-2.98285	-3.02674
C	-1.78087	-1.00273	-3.17587
C	-1.95973	0.29166	-3.68773
H	-2.66008	0.44953	-4.50497

C	-1.24247	1.37268	-3.17162
H	-1.39221	2.36526	-3.58762
C	-0.32645	1.17736	-2.1348
H	0.25636	2.00556	-1.74552
C	-0.13737	-0.10389	-1.6174
H	0.60228	-0.25744	-0.83934
C	-0.86693	-1.1797	-2.12873
H	-0.71843	-2.17081	-1.71106
C	-11.87713	0.05543	0.04176
H	-12.20345	-0.45898	-0.86467
H	-12.44332	0.98225	0.15721
C	-10.36769	0.27133	-0.03673
O	-9.58703	-0.64121	-0.3051
N	-9.93305	1.53878	0.20891
H	-8.93588	1.72272	0.2103
H	-10.56726	2.27312	0.47789
C	-4.7561	4.15998	1.12488
H	-5.1492	3.36007	1.75377
H	-5.27335	5.09275	1.37521
O	-4.99684	3.7722	-0.23346
H	-4.66853	4.45876	-0.82716
C	7.48463	-1.24077	-1.50363
H	8.30178	-1.01829	-2.19499
H	7.89766	-1.7768	-0.64353
S	6.79985	0.35584	-0.92173
N	4.19208	2.38106	-0.48233
C	4.61865	3.45578	0.26825
C	3.70241	2.88486	-1.65761
C	4.39081	4.72634	-0.49144
C	3.82703	4.33532	-1.66863

C	3.14012	2.13294	-2.68891
H	2.76013	2.69157	-3.53888
C	2.97831	0.74557	-2.74817
N	3.44087	-0.15984	-1.82668
C	3.029	-1.40674	-2.25571
C	2.25149	-1.28195	-3.48
C	2.25645	0.04835	-3.79361
C	3.37282	-2.61797	-1.65586
H	3.03975	-3.52324	-2.15352
C	4.12411	-2.76657	-0.49437
C	4.56948	-4.04144	0.08993
C	5.17311	-2.21356	1.37304
N	4.52087	-1.69264	0.28648
C	5.21337	-3.67211	1.24951
C	5.66647	-1.4532	2.45265
H	6.09772	-2.02385	3.27009
C	5.67552	-0.05853	2.62099
C	6.15932	0.64545	3.80673
N	5.24672	0.86527	1.69473
C	5.45117	2.12565	2.24482
C	5.17314	3.31906	1.55635
H	5.42832	4.2404	2.07193
Fe	4.21791	0.34437	-0.02944
C	6.02975	1.99715	3.61889
O	2.63965	0.41493	0.68565
O	0.9889	-2.54804	1.24367
N	-5.56047	-0.47322	-0.47025
C	-3.22908	0.13062	1.23514
C	-4.65546	-0.10176	1.79848
C	-5.40315	-1.09975	0.91075

C	-3.37315	0.68509	-0.20582
C	-2.53256	1.18363	2.12003
C	-4.63649	-0.53031	3.27307
C	-2.46512	-1.19546	1.16945
C	-4.67979	-2.44962	0.86668
C	-4.2234	-0.19797	-1.10893
C	-2.49547	0.78334	3.59917
C	-3.90956	0.51394	4.13006
C	-3.162	-2.38201	0.8899
C	-1.06676	-1.22926	1.29045
C	-6.49869	-1.22035	-1.36198
C	-2.43723	-3.56674	0.6889
C	-0.36533	-2.42421	1.12484
C	-1.05504	-3.59861	0.79577
C	1.74117	-1.60195	1.93409
H	-5.19037	0.85877	1.74337
H	-6.42956	-1.23759	1.26307
H	-2.39163	0.78579	-0.67095
H	-3.81844	1.68544	-0.16611
H	-3.09291	2.12016	2.02199
H	-1.52909	1.39855	1.74089
H	-4.12317	-1.493	3.37142
H	-5.66315	-0.67479	3.63003
H	-5.02165	-3.0504	0.01789
H	-5.01849	-3.003	1.75098
H	-4.41597	0.28903	-2.06604
H	-3.74806	-1.15757	-1.30651
H	-2.01524	1.57398	4.1849
H	-1.88229	-0.11668	3.72146
H	-3.87044	0.17883	5.17127

H	-4.48563	1.45014	4.12411
H	-0.51284	-0.32004	1.47876
H	-6.52652	-0.70567	-2.3237
H	-7.49624	-1.20736	-0.91433
H	-6.14013	-2.2369	-1.51393
H	-2.97265	-4.48566	0.4637
H	-0.49431	-4.51605	0.65687
H	1.18882	-1.1004	2.73328
H	2.22323	-0.57344	1.16371
H	2.6682	-2.07008	2.25617
H	-6.02229	0.45416	-0.34536
O	-6.92541	1.96071	-0.60716
H	-7.35872	2.02794	-1.46743
H	-6.31047	2.72905	-0.53575
H	-12.09352	-0.60266	0.88802
H	-2.02061	-2.5922	-4.6282
H	-3.68494	4.27066	1.31991
H	6.72104	-1.8515	-1.98701
H	4.6441	5.71628	-0.14052
H	3.52063	4.9619	-2.49651
H	1.77895	0.53657	-4.63224
H	1.80429	-2.10494	-4.01868
H	4.40122	-5.02447	-0.32363
H	5.68602	-4.32222	1.97529
H	6.55269	0.14098	4.68051
H	6.28873	2.81633	4.2729

The cartesian coordinates of the intermediate state in quartet spin state of **Dbl system**

$^4\text{IM}_{\text{Dbl}}$

C	-2.38754	-1.59749	-4.05854
H	-3.2305	-1.00327	-4.42565
H	-2.78402	-2.49379	-3.57093
C	-1.50814	-0.80025	-3.11864
C	-1.40217	0.59458	-3.23232
H	-1.97293	1.11032	-4.00169
C	-0.56575	1.32388	-2.38327
H	-0.49129	2.40193	-2.49688
C	0.18898	0.67255	-1.40484
H	0.87316	1.21086	-0.75755
C	0.09753	-0.71398	-1.2909
H	0.70996	-1.22557	-0.55855
C	-0.75089	-1.44006	-2.12873
H	-0.82155	-2.51857	-2.01436
C	-11.74883	0.47312	-0.23144
H	-12.0192	0.01235	-1.18433
H	-12.2973	1.4101	-0.11386
C	-10.23317	0.64597	-0.18655
O	-9.45925	-0.29047	-0.39038
N	-9.78106	1.90056	0.08676
H	-8.78201	2.0509	0.17302
H	-10.41113	2.64959	0.32381
C	-4.56319	4.27909	1.38423
H	-5.08886	3.53294	1.98193
H	-5.03727	5.25492	1.5354
O	-4.65767	3.85223	0.01865
H	-4.19968	4.48512	-0.54847
C	7.60769	-1.12977	-1.53583
H	8.6421	-0.91962	-1.82021
H	7.59793	-1.89022	-0.75136

S	6.92266	0.4556	-0.90232
N	4.40803	2.46692	-0.26228
C	4.83278	3.44377	0.62611
C	3.93164	3.09772	-1.38593
C	4.62582	4.7816	0.00262
C	4.07515	4.53344	-1.22196
C	3.34788	2.47124	-2.48879
H	2.97193	3.12602	-3.2685
C	3.16389	1.09901	-2.69435
N	3.62623	0.1014	-1.87688
C	3.20485	-1.10403	-2.40939
C	2.41742	-0.85081	-3.60389
C	2.42131	0.50361	-3.78905
C	3.51302	-2.37474	-1.92942
H	3.16259	-3.21346	-2.52231
C	4.22429	-2.67175	-0.7655
C	4.59872	-4.00262	-0.28119
C	5.22683	-2.33297	1.18981
N	4.63021	-1.70934	0.12932
C	5.213	-3.77186	0.93271
C	5.71459	-1.68032	2.34258
H	6.11326	-2.33527	3.11192
C	5.7483	-0.30914	2.65158
C	6.22186	0.26008	3.91332
N	5.36173	0.72248	1.83592
C	5.57326	1.90755	2.49383
C	5.34102	3.17061	1.90756
H	5.59767	4.03438	2.51348
Fe	4.42868	0.43068	-0.04351
C	6.11772	1.62313	3.85326

O	2.79211	0.34197	0.72918
O	0.29983	-3.28245	1.12388
N	-5.66998	-0.26036	-0.76599
C	-3.48342	-0.04199	1.18788
C	-4.97784	-0.057	1.60024
C	-5.77637	-0.91118	0.61173
C	-3.3851	0.57722	-0.22844
C	-2.71888	0.85608	2.18091
C	-5.17682	-0.51376	3.05363
C	-2.93573	-1.47081	1.11479
C	-5.28784	-2.3602	0.6243
C	-4.24598	-0.1498	-1.25015
C	-2.89535	0.41278	3.63646
C	-4.38068	0.37411	4.01799
C	-3.78517	-2.53236	0.7582
C	-1.56251	-1.71232	1.26545
C	-6.57545	-0.87731	-1.78085
C	-3.23644	-3.806	0.54652
C	-1.03914	-2.98608	1.0521
C	-1.87671	-4.04305	0.68429
C	1.16952	-2.47367	1.79226
H	-5.34847	0.97604	1.52663
H	-6.84658	-0.87155	0.83523
H	-2.35269	0.55082	-0.58089
H	-3.68773	1.6297	-0.18068
H	-3.10965	1.87517	2.0688
H	-1.66127	0.91509	1.90775
H	-4.83761	-1.54921	3.16581
H	-6.24426	-0.49657	3.30351
H	-5.65762	-2.90783	-0.248

H	-5.78015	-2.83858	1.47971
H	-4.27085	0.38595	-2.20091
H	-3.88412	-1.16034	-1.44
H	-2.34993	1.09097	4.30083
H	-2.45682	-0.58293	3.77208
H	-4.50473	0.01361	5.04399
H	-4.78938	1.39442	3.99318
H	-0.88659	-0.89856	1.48723
H	-6.50699	-0.28489	-2.69499
H	-7.59718	-0.85385	-1.39474
H	-6.25316	-1.89545	-1.99383
H	-3.89223	-4.62722	0.2693
H	-1.44915	-5.02512	0.51703
H	0.79244	-1.91584	2.64439
H	2.6186	-0.55834	1.05533
H	2.18248	-2.85557	1.76654
H	-6.02945	0.7135	-0.64461
O	-6.74381	2.31341	-0.59664
H	-7.17525	2.57969	-1.41871
H	-6.0391	2.98248	-0.41708
H	-12.04558	-0.21831	0.56188
H	-1.82457	-1.93236	-4.93756
H	-3.51973	4.32216	1.71157
H	7.05289	-1.48838	-2.40513
H	4.87783	5.72553	0.46405
H	3.78463	5.25694	-1.9728
H	1.94008	1.06871	-4.5755
H	1.95663	-1.61477	-4.2133
H	4.40908	-4.93897	-0.7848
H	5.63022	-4.5086	1.60767

H	6.59009	-0.334	4.74011
H	6.38121	2.36526	4.59258

The cartesian coordinates of the product complex in quartet spin state of **Dbl system**

⁴PC_{Dbl}

C	2.4213	-1.7512	3.68056
H	3.43459	-1.66232	4.08457
H	2.43413	-2.47211	2.85707
C	1.88733	-0.41237	3.22389
C	2.42189	0.78583	3.71834
H	3.22504	0.7479	4.45082
C	1.93222	2.02271	3.29233
H	2.35271	2.93775	3.70055
C	0.89832	2.08038	2.35475
H	0.50987	3.03862	2.02194
C	0.35581	0.89474	1.85497
H	-0.43466	0.91754	1.11449
C	0.84261	-0.3379	2.29311
H	0.40137	-1.2472	1.90281
C	11.66856	0.32426	-0.41151
H	11.97874	-0.10942	0.54139
H	12.22543	1.24643	-0.59055
C	10.15524	0.52665	-0.38651
O	9.37494	-0.35564	-0.02658
N	9.70811	1.74898	-0.7876
H	8.70786	1.90083	-0.84675
H	10.33202	2.44701	-1.15903
C	4.45598	4.18601	-1.75037
H	5.2907	3.79636	-2.33543

H	4.34218	5.25422	-1.96202
O	4.78453	3.96908	-0.37199
H	4.01456	4.1521	0.18038
C	-7.64646	-1.20255	1.4782
H	-8.53647	-1.02758	2.08696
H	-7.92271	-1.76665	0.58549
S	-6.98926	0.45707	1.02463
N	-4.28122	2.26119	0.5674
C	-4.61517	3.47359	-0.01639
C	-3.65152	2.55674	1.75587
C	-4.20133	4.59811	0.88006
C	-3.6117	3.99593	1.95226
C	-3.06005	1.63627	2.62203
H	-2.55805	2.05263	3.4897
C	-3.02386	0.24435	2.50691
N	-3.62839	-0.4845	1.50425
C	-3.44016	-1.8213	1.8129
C	-2.63817	-1.93174	3.00696
C	-2.38652	-0.65565	3.43676
C	-3.97283	-2.89608	1.09617
H	-3.75454	-3.8887	1.47649
C	-4.72064	-2.81661	-0.07631
C	-5.18651	-3.95537	-0.88439
C	-5.64056	-1.91441	-1.88972
N	-5.01891	-1.60591	-0.70026
C	-5.7481	-3.36787	-1.99891
C	-6.01616	-0.97381	-2.86845
H	-6.46495	-1.39316	-3.76447
C	-5.88427	0.42894	-2.86169
C	-6.30157	1.32557	-3.94048

N	-5.38364	1.17453	-1.82852
C	-5.49885	2.50195	-2.17786
C	-5.16639	3.56222	-1.30873
H	-5.34921	4.56468	-1.68534
Fe	-4.90821	0.3074	0.07085
C	-6.06865	2.61565	-3.5484
O	-1.4886	-0.49286	-0.58693
O	-0.66281	-2.69787	-0.35158
N	5.84349	-0.39639	0.64883
C	3.54618	-0.18416	-1.1631
C	4.97879	-0.50847	-1.65849
C	5.7289	-1.29267	-0.57977
C	3.65439	0.66942	0.12448
C	2.84157	0.63492	-2.26277
C	4.97513	-1.24561	-3.0072
C	2.80459	-1.46937	-0.79443
C	5.0327	-2.62523	-0.28533
C	4.50083	0.00385	1.20032
C	2.80774	-0.09022	-3.61159
C	4.22849	-0.43631	-4.07445
C	3.51406	-2.57863	-0.30813
C	1.40423	-1.49344	-0.81155
C	6.75121	-0.93982	1.70061
C	2.79199	-3.69224	0.14809
C	0.69928	-2.61389	-0.36912
C	1.40405	-3.72137	0.12258
C	-1.41082	-1.76695	-1.14474
H	5.50181	0.44796	-1.80553
H	6.76765	-1.46261	-0.87678
H	2.66145	0.84281	0.54516

H	4.08111	1.64576	-0.12297
H	3.40487	1.56847	-2.38317
H	1.8367	0.92654	-1.94338
H	4.48484	-2.21848	-2.89489
H	6.00717	-1.43995	-3.32223
H	5.38549	-3.05092	0.65962
H	5.38337	-3.32608	-1.05261
H	4.68587	0.68216	2.03392
H	4.02493	-0.89437	1.58976
H	2.30685	0.53549	-4.35763
H	2.21589	-1.00814	-3.51865
H	4.20084	-0.99702	-5.01411
H	4.78033	0.49192	-4.27848
H	0.85154	-0.61562	-1.11257
H	6.83329	-0.19246	2.49153
H	7.73209	-1.11059	1.25604
H	6.32931	-1.85402	2.11574
H	3.33243	-4.5574	0.52438
H	0.84959	-4.58604	0.4699
H	-0.92777	-1.66703	-2.12218
H	-2.18071	-0.48945	0.10089
H	-2.39323	-2.2298	-1.24474
H	6.27772	0.49718	0.33027
O	6.68796	2.18365	0.13467
H	7.26273	2.55273	0.81729
H	5.98048	2.85544	-0.02329
H	11.9124	-0.39777	-1.19618
H	1.79475	-2.17782	4.47265
H	3.54267	3.65625	-2.0363
H	-6.91617	-1.7662	2.06203

H	-4.34424	5.64821	0.66987
H	-3.1726	4.47343	2.81889
H	-1.81882	-0.34531	4.30322
H	-2.32841	-2.86308	3.46114
H	-5.07599	-4.99991	-0.63511
H	-6.19116	-3.8705	-2.84966
H	-6.72663	0.99145	-4.87845
H	-6.26221	3.53703	-4.07834