Supplementary Information – HyDRA challenge

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1 Computational Details

All the computational calculations were carried out using Gaussian09[1] suite of programs. All the geometries were modeled using MOLDEN software.[2] All the geometries were optimized using DFT-B3LYP method with empirical dispersion (D3) [3] correction with basis set Def2TZVPP.[4]

Acknowledgement

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Reference

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2 Additional computed data (optional)

2.1 OH-stretching fundamentals for test set

Code	CAS	fundamentals (cm^{-1})	Description (method and basis set used)
CON	502-49-8	3637.7	B3LYP-D3/Def2TZVPP
		3635.7	B3LYP-D3/6-311++G**
		3774.7	MP2/6-311++G**
DMI	80-73-9	3611.8	B3LYP-D3/Def2TZVPP
		3620.1	B3LYP-D3/6-311++G**
		3726.1	MP2/6-311++G**
FAH	50-0-0	3720	B3LYP-D3/Def2TZVPP
		3712.8	B3LYP-D3/6-311++G**
		3805.2	MP2/6-311++G**
MLA	547-64-8	3659.9	B3LYP-D3/Def2TZVPP
		3690.1	B3LYP-D3/6-311++G**
		3801.9	MP2/6-311++G**
PCD	125132-75-4		B3LYP-D3/Def2TZVPP
PYR	110-86-1	3549.1	B3LYP-D3/Def2TZVPP
		3550.7	B3LYP-D3/6-311++G**
		3664.5	MP2/6-311++G**
THF	109-99-9	3611.2	B3LYP-D3/Def2TZVPP
		3612.0	B3LYP-D3/6-311++G**
		3693.0	MP2/6-311++G**
THT	110-01-0	3589.3	B3LYP-D3/Def2TZVPP
		3742.8	MP2/6-311++G**
TPH	434-45-7	3735.8	B3LYP-D3/Def2TZVPP
		3747.6	B3LYP-D3/6-311++G**
		3836.9	MP2/6-311++G**
TFE	75-89-8	3762.3	B3LYP-D3/Def2TZVPP
		3776.9	B3LYP-D3/6-311++G**

2.2 IR intensities and Raman scattering activities

No further information has been made available.

2.3 Isotopolog information

No further information has been made available.

2.4 Relative energies for local minima and spectral properties

No further information has been made available.

2.5 Other computed quantities for the training and test sets

No further information has been made available.

Coordinates of the Molecules are given below.

CON

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DFT2-D3 Energy: -291893.7866494

C	-0.86956	-0.49992	-1.43425
C	0.32096	-1.46798	-1.36406
C	1.27890	1.65612	0.50307
C	0.79656	-1.85259	0.04552
C	1.20624	0.38593	1.36259
C	1.78670	-0.90196	0.74526
H	-1.76181	-0.95842	-1.00877
H	1.16425	-1.08073	-1.94182
H	-0.07347	-2.00202	0.69112
H	0.77970	2.46165	1.04340
H	0.17125	0.20154	1.66118
H	-1.08969	-0.29281	-2.48962
H	0.00594	-2.37715	-1.88085
H	2.32240	1.95494	0.37714
H	1.28942	-2.82464	-0.03568
H	1.74423	0.60320	2.28815
H	2.24790	-1.47530	1.55238
H	2.60340	-0.65369	0.05813
C	-0.69971	0.85767	-0.79439
C	0.63976	1.54918	-0.89760
H	1.30061	1.02099	-1.58236
H	0.47379	2.55147	-1.29585
O	-1.61156	1.38712	-0.18488
O	-2.45393	-0.76077	1.47964
H	-3.00812	-0.56248	2.23762
H	-2.40497	0.06389	0.97090

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B3lyp Energy: -291846.0144633

C	-0.77408	0.94884	0.82643
C	0.55333	1.72216	0.89418

C	1.28266	-1.82833	-0.11322
C	1.41626	1.74336	-0.38112
C	1.58442	-0.76074	-1.17800
C	2.30050	0.51792	-0.68942
H	-1.42197	1.35087	0.04199
H	1.15768	1.37945	1.74168
H	0.77280	1.94482	-1.24705
H	0.72996	-2.64416	-0.58771
H	0.65657	-0.48285	-1.69255
H	-1.32067	1.11413	1.76663
H	0.28801	2.75792	1.13013
H	2.22259	-2.25498	0.25332
H	2.08460	2.60787	-0.30138
H	2.20413	-1.24200	-1.94125
H	2.99993	0.83046	-1.47141
H	2.92448	0.28694	0.18402
C	-0.74777	-0.56142	0.66776
C	0.47165	-1.34393	1.11136
H	1.10044	-0.74096	1.76843
H	0.12475	-2.21341	1.67556
O	-1.70713	-1.14970	0.19409
O	-3.73040	0.50399	-0.96054
H	-4.40544	0.01344	-1.43721
H	-3.13941	-0.16907	-0.57933

26

MP2 Energy: -289980.9377404

C	-0.63377	-0.81619	-1.38350
C	0.73885	-1.48385	-1.22571
C	0.84204	1.88692	0.45831
C	1.24279	-1.65942	0.21491
C	0.96658	0.66605	1.37886
C	1.91383	-0.44445	0.88098
H	-1.40765	-1.41061	-0.88730
H	1.49708	-0.95757	-1.81886
H	0.41336	-2.00054	0.84892
H	0.10153	2.57310	0.88381
H	-0.02574	0.23585	1.56461
H	-0.88907	-0.78720	-2.45459
H	0.64799	-2.47985	-1.67588
H	1.79956	2.42060	0.41885
H	1.98006	-2.47204	0.20064

H	1.31916	1.02960	2.35127
H	2.46976	-0.82856	1.74427
H	2.66905	-0.02341	0.20087
C	-0.78351	0.61555	-0.91230
C	0.40740	1.54563	-0.97996
H	1.22949	1.09275	-1.53862
H	0.10014	2.46089	-1.49720
O	-1.85310	1.02684	-0.47255
O	-2.43063	-0.96367	1.49901
H	-3.24526	-0.96383	2.00622
H	-2.55493	-0.25601	0.85166

DME

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DFT2-D3 Energy: -287367.1410739

C	0.04344	-0.32510	-0.04034
N	1.37976	-0.63666	-0.18219
C	2.20437	0.50919	0.15647
C	1.22788	1.67081	-0.05818
N	-0.05788	1.03119	0.16472
C	-1.28740	1.76029	-0.05967
H	1.38943	2.49454	0.63681
H	2.53735	0.45585	1.20146
C	1.85953	-1.98397	0.01207
H	-1.37160	2.09436	-1.10041
H	-2.13998	1.12801	0.17266
H	-1.31147	2.63719	0.58826
H	2.17403	-2.15604	1.04868
H	1.05575	-2.67484	-0.22928
H	2.70819	-2.17825	-0.64483
H	3.08563	0.57335	-0.48159
H	1.29528	2.06364	-1.08096
O	-0.87578	-1.13203	-0.08898
O	-3.65841	-0.72021	-0.00216
H	-2.71613	-0.95177	-0.07748
H	-3.97303	-1.21720	0.75605

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B3LYP-freq Energy: -287334.8778465

C	0.04085	-0.31645	-0.03544
N	1.37283	-0.65734	-0.18534
C	2.22381	0.47640	0.14999

C	1.26860	1.65949	-0.06609
N	-0.03302	1.04557	0.16774
C	-1.25620	1.79748	-0.05059
H	1.45216	2.48345	0.62675
H	2.55803	0.41946	1.19672
C	1.82207	-2.02025	0.01230
H	-1.34259	2.13410	-1.09264
H	-2.11723	1.17605	0.18877
H	-1.26485	2.67412	0.60160
H	2.13523	-2.19903	1.05055
H	0.99722	-2.69033	-0.22591
H	2.66365	-2.23838	-0.64987
H	3.10570	0.52239	-0.49271
H	1.33935	2.04603	-1.09343
O	-0.89725	-1.10593	-0.07603
O	-3.68245	-0.67965	0.01612
H	-2.74296	-0.93388	-0.03522
H	-4.11955	-1.40695	0.46676

21

MP2 Energy: -285583.0758334

C	0.04661	-0.31690	-0.09719
N	1.39099	-0.63335	-0.22915
C	2.19083	0.48146	0.25491
C	1.25056	1.65559	-0.02074
N	-0.04876	1.03332	0.18935
C	-1.25787	1.76827	-0.14674
H	1.40332	2.49643	0.66042
H	2.38761	0.38415	1.33426
C	1.82194	-1.99616	0.01884
H	-1.29618	2.00291	-1.21982
H	-2.13187	1.17598	0.12222
H	-1.27174	2.70046	0.42335
H	1.94095	-2.19069	1.09456
H	1.06865	-2.67373	-0.38429
H	2.77553	-2.17273	-0.48493
H	3.13957	0.55654	-0.28247
H	1.35495	2.00284	-1.06051
O	-0.88222	-1.11163	-0.21670
O	-3.65758	-0.67534	0.13925
H	-2.73314	-0.93464	0.00153
H	-4.02722	-1.40508	0.63946

FAH

7

DFT2-D3 Energy: -119874.0304392

C	-1.29010	0.47547	0.01987
O	-0.93792	-0.67596	-0.00822
H	-2.36026	0.74865	0.01148
H	-0.55928	1.30068	0.05486
O	1.82418	0.15161	-0.06983
H	2.49345	-0.24565	0.49161
H	1.07662	-0.46170	-0.05280

7

B3LYP-Form-wat Energy: -119859.3578258

C	1.36560	0.44395	0.00019
O	0.89293	-0.66624	-0.00006
H	2.45957	0.60301	-0.00076
H	0.72676	1.34495	0.00133
O	-1.85276	0.18836	-0.00057
H	-2.62005	-0.39015	0.00335
H	-1.08123	-0.39849	-0.00008

7

MP2 Energy: -119201.5975817

C	-1.31269	0.47211	0.01554
O	-0.92741	-0.68245	-0.00668
H	-2.38693	0.71791	-0.02073
H	-0.60389	1.31390	0.07188
O	1.83119	0.17174	-0.04655
H	2.55866	-0.34723	0.30071
H	1.07808	-0.43152	-0.01923

MLA

18

DFT2-D3 Energy: -288389.4495937

C	0.39169	2.34721	0.17552
C	-0.30709	1.09319	-0.33965
O	-1.61622	1.10002	0.15858
C	0.45203	-0.18309	0.03852
O	1.74842	-0.09811	-0.28099
C	2.54582	-1.27078	-0.03242
O	-0.03839	-1.17653	0.52714

O -2.69233 -1.48654 -0.28092
H -0.18260 3.21809 -0.13539
H 0.42583 2.33101 1.26502
H 1.40407 2.42500 -0.21337
H -0.29501 1.10919 -1.44075
H -2.09401 0.29638 -0.11040
H 3.54879 -1.01554 -0.35949
H 2.53790 -1.51653 1.02808
H 2.16016 -2.11788 -0.59748
H -3.36987 -1.70122 0.36512
H -1.84173 -1.65839 0.15632
18
B3LYP-water Energy: -288347.7695607
C 0.43438 2.35302 0.15287
C -0.29066 1.09933 -0.33399
O -1.59251 1.12525 0.19254
C 0.45249 -0.19315 0.03289
O 1.75924 -0.11558 -0.25538
C 2.54191 -1.30551 -0.02473
O -0.06106 -1.19534 0.48378
O -2.74074 -1.43487 -0.27151
H -0.13778 3.22890 -0.15665
H 0.49489 2.35249 1.24374
H 1.44032 2.41533 -0.26142
H -0.30883 1.10751 -1.43688
H -2.09468 0.33659 -0.08109
H 3.55518 -1.04537 -0.32131
H 2.50739 -1.58266 1.02916
H 2.16265 -2.13070 -0.62850
H -3.45583 -1.75104 0.28846
H -1.91141 -1.68893 0.16682
18
MP2 Energy: -286706.4298555
C 0.42530 2.34272 0.13500
C -0.30933 1.09287 -0.33542
O -1.60156 1.12960 0.21343
C 0.44268 -0.17585 0.06370
O 1.72703 -0.11661 -0.32846
C 2.49275 -1.30180 -0.04933
O -0.03361 -1.13997 0.63247
O -2.64458 -1.46342 -0.32543

H	-0.16114	3.21896	-0.14963
H	0.51881	2.32661	1.22446
H	1.41838	2.40638	-0.31215
H	-0.34025	1.08397	-1.43676
H	-2.08122	0.33004	-0.05509
H	3.48923	-1.09702	-0.43522
H	2.52445	-1.48795	1.02519
H	2.05262	-2.16409	-0.55290
H	-3.41099	-1.90078	0.05217
H	-1.89649	-1.74045	0.22017

PYR

14

DFT2-D3 Energy: -203855.8506597

C	0.25164	0.99733	-0.01220
C	-1.05536	1.46923	-0.02085
C	-2.09365	0.54686	-0.00462
C	-1.78410	-0.80711	0.01862
C	-0.44595	-1.18186	0.02517
N	0.55557	-0.30160	0.01128
H	-3.12418	0.87656	-0.01119
H	1.09312	1.68002	-0.02747
H	-1.24894	2.53272	-0.04108
H	-2.55965	-1.56033	0.03029
H	-0.16408	-2.22811	0.04067
O	3.42901	-0.49298	-0.11560
H	2.45606	-0.55251	-0.07694
H	3.71847	-0.60761	0.79224

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B3LYP-pyridine Energy: -203828.0947544

C	0.19279	1.14183	-0.00795
C	-1.14684	1.52129	-0.03682
C	-2.12032	0.52619	-0.01852
C	-1.71554	-0.80505	0.02656
C	-0.35142	-1.08473	0.05236
N	0.59049	-0.13476	0.03757
H	-3.17341	0.78303	-0.04062
H	0.98180	1.88747	-0.02450
H	-1.41456	2.57033	-0.07439
H	-2.43702	-1.61303	0.03970

H 0.00482 -2.10987 0.08374
O 3.41866 -0.83358 -0.13407
H 2.47203 -0.59864 -0.07002
H 3.72647 -0.87988 0.77526
14
MP2 Energy: -202566.9986878
C 0.19233 1.14782 0.07528
C -1.14837 1.52432 -0.04722
C -2.12570 0.52593 -0.07505
C -1.71796 -0.80752 0.01640
C -0.35313 -1.08527 0.13620
N 0.59538 -0.13203 0.17039
H -3.17761 0.78032 -0.16889
H 0.98060 1.89685 0.09665
H -1.41333 2.57472 -0.11869
H -2.43791 -1.61985 -0.00427
H 0.00164 -2.11101 0.20597
O 3.40019 -0.83130 -0.24051
H 2.46929 -0.59820 -0.08306
H 3.76254 -0.89416 0.64513

TFE
12
DFT2-D3-Mono-F-ethanol Energy: -207628.1626441
C -1.33053 -0.58308 -0.16611
C -0.99871 0.76876 0.42366
H -1.92913 1.34148 0.47261
H -0.64740 0.62858 1.45459
O -0.09011 1.51643 -0.34940
H 0.79556 1.12900 -0.25817
F -0.23604 -1.47143 -0.01984
O 2.24093 -0.07591 -0.01953
H 2.73498 -0.10872 0.80341
H 1.64446 -0.83517 -0.00149
H -1.53084 -0.50425 -1.23457
H -2.17453 -1.04638 0.34832
12
B3LYP-Mono-F-ethanol Energy: -207600.2369579
C -1.31963 -0.61459 -0.18200
C -1.04642 0.75211 0.40999

H	-1.99439	1.30093	0.40872
H	-0.73700	0.63420	1.45843
O	-0.12479	1.52306	-0.32838
H	0.76651	1.15281	-0.21183
F	-0.19825	-1.47274	-0.00056
O	2.24216	-0.03019	-0.01687
H	2.93214	-0.09662	0.64954
H	1.72625	-0.84604	0.03583
H	-1.49157	-0.55498	-1.25796
H	-2.16038	-1.10374	0.31637

THF

16

DFT2-D3 Energy: -193921.1480112

C	-0.33005	-1.03378	0.74688
O	0.21607	0.27466	0.98234
C	-0.51862	1.24475	0.20191
C	-1.52525	0.45566	-0.64768
C	-0.93253	-0.95944	-0.64878
H	0.48299	-1.75225	0.84051
H	-1.09206	-1.25727	1.50249
H	-1.00148	1.95168	0.87892
H	0.20237	1.78459	-0.41438
H	-2.50789	0.45203	-0.17312
H	-1.63647	0.87381	-1.64663
H	-1.67369	-1.73561	-0.83473
H	-0.13951	-1.04451	-1.39269
O	2.52882	-0.00005	-0.56483
H	3.38028	0.13050	-0.14233
H	1.86496	0.15700	0.12793

16

B3LYP-THF Energy: -193892.8983381

C	0.32842	-1.11913	-0.49446
O	-0.37003	0.13117	-0.67143
C	0.42245	1.22102	-0.14460
C	1.76976	0.61386	0.26128
C	1.39589	-0.84589	0.56337
H	-0.40391	-1.87310	-0.20041
H	0.77724	-1.41466	-1.45071
H	0.51011	1.98898	-0.91677

H	-0.10894	1.64446	0.71394
H	2.47817	0.65944	-0.57104
H	2.21600	1.13009	1.11305
H	2.24254	-1.53121	0.49155
H	0.96704	-0.93312	1.56561
O	-2.93577	-0.02042	0.46466
H	-3.63066	0.15615	-0.17520
H	-2.10045	0.06785	-0.02945

16

MP2-freq Energy: -192705.6778776

C	-0.47858	-1.00690	0.79410
O	0.19459	0.23874	0.99869
C	-0.57986	1.23122	0.30343
C	-1.31457	0.50012	-0.84531
C	-0.87691	-0.96827	-0.67654
H	0.22123	-1.80355	1.05250
H	-1.36046	-1.06570	1.44861
H	-1.28739	1.68792	1.00561
H	0.11952	1.99239	-0.04781
H	-2.39752	0.59756	-0.72985
H	-1.03718	0.89801	-1.82337
H	-1.66821	-1.68004	-0.92469
H	0.00317	-1.18136	-1.28843
O	2.52035	-0.02029	-0.52723
H	3.34592	0.15390	-0.07103
H	1.84091	0.11636	0.15276

THT

16

DFT-D3 Energy: -396595.5466866

C	-0.43310	-0.03840	-1.39045
C	-0.60839	0.37218	1.26981
C	-1.42287	-0.79903	0.71953
C	-0.70409	-1.28070	-0.54148
H	-1.31545	0.26526	-1.95292
H	0.39591	-0.17650	-2.08127
H	0.25147	0.02105	1.83807
H	-1.19744	1.04226	1.89252
H	-1.51464	-1.59067	1.46500
H	-2.43091	-0.46171	0.46666

H 0.24354 -1.74874 -0.27149
H -1.29715 -2.00879 -1.09779
S 0.00224 1.30580 -0.20250
O 2.54583 -0.68578 0.27781
H 3.45655 -0.38344 0.30940
H 2.01638 0.11042 0.10492
16
MP2-THT-water Energy: -395182.1528193
C 0.50713 0.04288 1.37647
C 0.55585 0.29496 -1.29068
C 1.40210 -0.84031 -0.71266
C 0.72050 -1.25168 0.59169
H 1.42960 0.35751 1.87166
H -0.28557 -0.05550 2.12133
H -0.32249 -0.10605 -1.80272
H 1.12134 0.92509 -1.97999
H 1.47092 -1.67322 -1.41974
H 2.41576 -0.48040 -0.50149
H -0.24704 -1.71420 0.37160
H 1.32560 -1.96074 1.16609
S 0.02088 1.30618 0.14197
O -2.59989 -0.67556 -0.22138
H -3.49593 -0.37460 -0.05372
H -2.06057 0.11261 -0.06243

TPH
20
DFT2-D3 Energy: -476522.1899945
C 0.74804 -1.60379 -0.02703
C 0.60369 -0.20931 -0.00161
C 1.74874 0.60171 0.02939
C 3.00736 0.02482 0.03311
C 3.14253 -1.36090 0.00518
C 2.01304 -2.17187 -0.02477
H -0.11545 -2.24963 -0.05084
H 1.64741 1.67737 0.05279
H 3.88470 0.65661 0.05676
H 4.12783 -1.80820 0.00687
H 2.11703 -3.24801 -0.04645
C -0.71332 0.45663 -0.00857

O	-0.88434	1.65374	-0.02532
C	-2.00025	-0.43219	0.00828
F	-3.09975	0.31252	0.02814
F	-2.05048	-1.22167	-1.08493
F	-2.01812	-1.23155	1.09518
O	0.96008	3.91189	-0.08935
H	0.74425	4.57316	0.57215
H	0.20448	3.30937	-0.10330

20

B3lYP Energy: -476453.6084718

C	-0.77323	-1.60783	0.01542
C	-0.61081	-0.21153	-0.00262
C	-1.74846	0.61660	-0.02138
C	-3.01732	0.05432	-0.02128
C	-3.17032	-1.33306	-0.00207
C	-2.04868	-2.16076	0.01655
H	0.08337	-2.26708	0.03018
H	-1.63355	1.69318	-0.03679
H	-3.88821	0.69887	-0.03557
H	-4.16338	-1.76843	-0.00133
H	-2.16644	-3.23777	0.03150
C	0.71505	0.44249	-0.00289
O	0.89559	1.64075	-0.00336
C	2.00024	-0.45061	-0.00286
F	3.10299	0.29370	-0.01486
F	2.04252	-1.23921	1.09517
F	2.03137	-1.25727	-1.08822
O	-0.91301	3.92004	0.06145
H	-0.63202	4.77154	-0.28472
H	-0.13109	3.35054	0.02993

20

MP2 Energy: -473942.9229998

C	0.71774	-1.62864	-0.08455
C	0.59067	-0.22769	-0.02333
C	1.73989	0.58153	0.07036
C	3.00253	-0.01141	0.08478
C	3.13204	-1.40532	0.02053
C	1.98955	-2.20804	-0.07186
H	-0.15392	-2.26799	-0.15851
H	1.64179	1.66131	0.11978
H	3.88632	0.61598	0.15724

H	4.11790	-1.86239	0.03202
H	2.08566	-3.28877	-0.12439
C	-0.72485	0.45700	-0.04267
O	-0.86912	1.66588	-0.11044
C	-2.01186	-0.40669	0.02822
F	-3.09791	0.35285	0.09311
F	-2.11340	-1.19089	-1.06191
F	-1.99394	-1.20482	1.11088
O	1.06709	3.89652	-0.07109
H	0.83340	4.71816	0.36618
H	0.23824	3.40577	-0.10770

PCD

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DFT2-D3.log Energy: -435566.8601568

C	-2.79449	-1.25832	0.07716
C	-2.36995	-0.27816	1.17342
C	-1.06608	0.43451	0.79801
C	0.05774	-0.59811	0.57854
C	-0.34153	-1.59955	-0.53352
C	-1.68283	-2.26282	-0.23829
C	1.45813	-0.05902	0.35147
C	1.73091	1.21290	-0.15752
C	3.04447	1.62647	-0.36936
C	4.10741	0.78087	-0.08232
C	3.85015	-0.48862	0.42634
C	2.54146	-0.89815	0.63903
O	-1.28079	1.27647	-0.35030
O	-0.44805	-0.93321	-1.80860
H	0.91580	1.88328	-0.38303
H	3.23236	2.61828	-0.75983
H	5.12585	1.10653	-0.24744
H	4.66846	-1.15608	0.66311
H	2.35413	-1.88586	1.04415
H	0.09526	-1.18617	1.50099
H	-3.14482	0.47009	1.33812
H	-2.22078	-0.81118	2.11788
H	-1.95468	-2.89113	-1.08778
H	-1.53646	-2.92610	0.61938
H	-3.69789	-1.79021	0.37858
H	-3.05720	-0.70101	-0.82369

H	-0.77082	1.11459	1.59886
H	0.43092	-2.37109	-0.60766
H	-1.21348	0.71546	-1.13736
H	0.42929	-0.62496	-2.06068
O	-3.80296	2.54075	-0.07369
H	-2.90952	2.19749	-0.24253
H	-3.70433	3.49413	-0.02814