

Supporting Information of

**DFT Study of CO<sub>2</sub> Hydrogenation Catalyzed by a Cobalt-Base System: an  
Unexpected Formate Anion Assisted Deprotonation Mechanism**

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## 1 Some optimized structures of intermediates

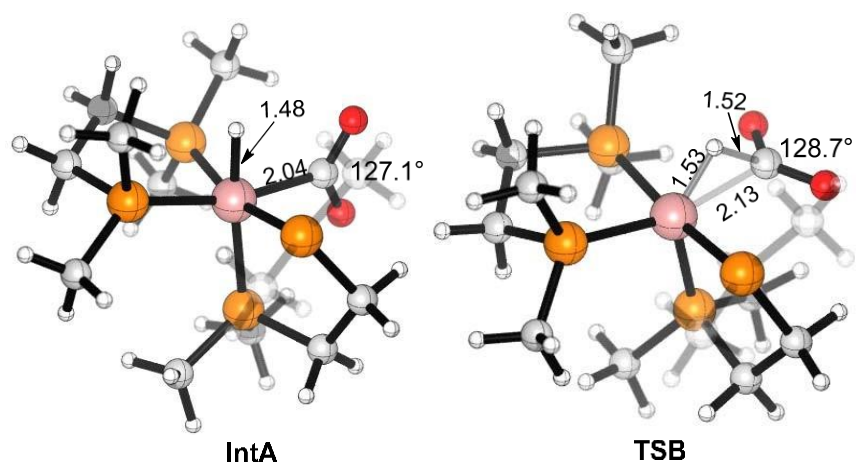


Figure S1. Optimized structures of intermediate and transition state involve in hydrogenation step.

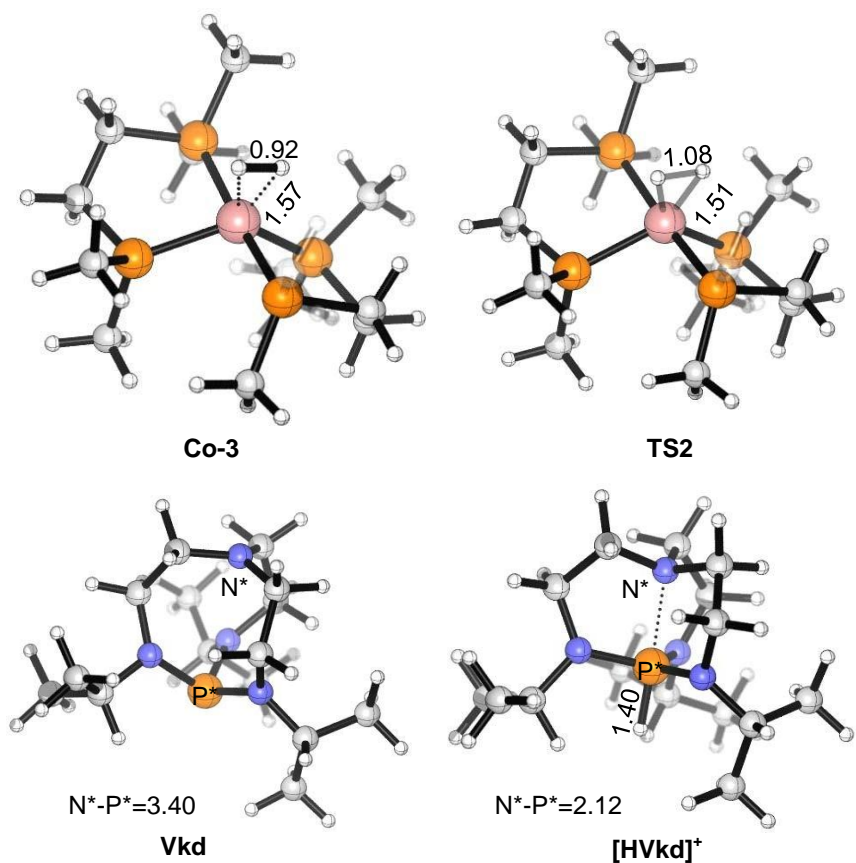


Figure S2. Optimized Structures of intermediates and transition state involve in oxidative addition and deprotonation step in scheme 1.

## 2 The Calculation of Hydricity of Monohydride and Dihydride in Different Solvent

Table S1. The Calculated Hydricity in different solvent

Species	THF	Acetonitrile
<b>Co-1</b> (monohydride)	33.7	31.9
<b>Co-2</b> (dihydride)	96.5	81.3

## 3 The Cartesian Coordinates (xyz) for all optimized structures are presented

Co-1-HCOOH

E= -2177.234188 a.u.

27	0.084292	-0.037977	-0.187518
1	-0.119822	0.553340	-1.558092
15	2.135809	-0.511049	-0.873081
6	2.380945	-0.802576	-2.680179
1	3.442623	-0.783731	-2.956807
1	1.846888	-0.036351	-3.250945
1	1.966818	-1.777999	-2.956060
6	3.323514	-1.769158	-0.218962
1	4.282667	-1.738609	-0.750775
1	2.899182	-2.774323	-0.321824
1	3.512703	-1.586227	0.843212
6	3.142823	1.037543	-0.613617
1	3.994615	1.081454	-1.303725
1	3.550188	0.980132	0.404800
6	2.247620	2.270414	-0.744343
1	2.762851	3.180747	-0.413643
1	1.954698	2.417900	-1.791462
6	1.195139	2.570367	1.899869
1	1.699993	3.542931	1.859886
1	1.875820	1.839696	2.348762

1	0.318470	2.665354	2.548815
6	-0.258249	3.517858	-0.307138
1	0.372669	4.413380	-0.250425
1	-1.129785	3.668224	0.338459
1	-0.612905	3.390318	-1.333767
15	0.671210	2.015499	0.216684
15	-0.098423	-0.899762	1.813504
6	1.344402	-1.300036	2.888593
1	1.023519	-1.711191	3.853124
1	1.941923	-0.400717	3.070979
1	1.978710	-2.038445	2.389052
6	-1.194997	-0.082404	3.049906
1	-1.306257	-0.690756	3.955552
1	-2.180424	0.095825	2.609754
1	-0.773642	0.887786	3.330996
6	-0.891859	-2.573115	1.658027
1	-0.104378	-3.269424	1.342389
1	-1.277431	-2.923345	2.623276
6	-1.985565	-2.499055	0.592403
1	-2.855341	-1.952715	0.978879
1	-2.332940	-3.493893	0.288678
6	-0.651025	-2.867630	-1.932962
1	-1.401265	-3.636189	-2.155683
1	0.208224	-3.339905	-1.445114
1	-0.310643	-2.426637	-2.875770
6	-2.878861	-1.178060	-1.785797
1	-3.416092	-2.103953	-2.024677
1	-2.636122	-0.658500	-2.717612
1	-3.538148	-0.533447	-1.198945
15	-1.328997	-1.528858	-0.853462

6	-3.400484	2.128131	-0.543773
8	-3.067368	2.261492	-1.703294
8	-2.762554	1.454034	0.392657
1	-4.319465	2.578509	-0.136556
1	-1.888800	1.030824	0.076495

Co-1

E= -1987.496489 a.u.

27	0.041973	0.007032	-0.291470
15	-1.478783	1.574327	-0.153142
6	-1.698777	2.876405	1.141008
1	-2.644829	3.416675	1.010576
1	-0.875915	3.597984	1.089556
1	-1.692580	2.422965	2.136740
6	-1.795491	2.601479	-1.655636
1	-2.667308	3.257074	-1.539155
1	-1.953716	1.941987	-2.515183
1	-0.913649	3.216519	-1.866587
6	-3.111534	0.680433	0.022266
1	-3.263465	0.518046	1.098073
1	-3.946056	1.297346	-0.335312
6	-3.059669	-0.669431	-0.698402
1	-3.044042	-0.517191	-1.785263
1	-3.939692	-1.282129	-0.464297
15	-1.477721	-1.563073	-0.264272
6	-2.012378	-2.488621	1.245766
1	-2.942348	-3.045428	1.076404
1	-2.168618	-1.788307	2.073684
1	-1.233436	-3.198380	1.542748
6	-1.527236	-2.937127	-1.494912

1	-2.494666	-3.454610	-1.505516
1	-0.741130	-3.663760	-1.261497
1	-1.325845	-2.531858	-2.492022
15	1.981221	0.042014	-1.205837
6	2.440180	-1.182391	-2.506187
1	3.497981	-1.111292	-2.787795
1	1.825241	-1.009287	-3.396132
1	2.230724	-2.194398	-2.144405
6	2.554636	1.591668	-2.034550
1	3.554050	1.491765	-2.476162
1	2.563097	2.406777	-1.303025
1	1.840771	1.857238	-2.821936
6	3.316718	-0.223155	0.065029
1	3.440138	-1.306968	0.186619
1	4.280391	0.185400	-0.262683
6	2.843265	0.401442	1.378193
1	2.888333	1.496154	1.312778
1	3.461953	0.094585	2.230574
15	1.057249	-0.052152	1.642045
6	1.227932	-1.672557	2.512201
1	1.966243	-1.622718	3.321519
1	1.532063	-2.442626	1.796336
1	0.263802	-1.966466	2.938706
6	0.636809	1.018828	3.081312
1	1.346882	0.876247	3.904842
1	-0.369316	0.778665	3.441701
1	0.653238	2.071024	2.780777
1	-0.377776	0.020503	-1.733437

E= -1986.802909 a.u.

27	-0.000001	-0.000002	0.000001
15	-1.615796	-1.496692	0.084905
6	-1.676585	-3.014464	-0.942930
1	-2.629669	-3.535634	-0.800469
1	-0.864583	-3.696644	-0.676314
1	-1.574006	-2.749737	-1.999913
6	-1.875000	-2.144957	1.783334
1	-2.780863	-2.758718	1.841635
1	-1.961739	-1.309507	2.485275
1	-1.014431	-2.749733	2.085173
6	-3.244605	-0.702964	-0.298359
1	-3.338972	-0.655858	-1.390159
1	-4.073119	-1.312044	0.079537
6	-3.244584	0.702954	0.298573
1	-3.338871	0.655846	1.390379
1	-4.073126	1.312034	-0.079261
15	-1.615804	1.496687	-0.084804
6	-1.875143	2.144992	-1.783196
1	-2.781028	2.758729	-1.841416
1	-1.961905	1.309560	-2.485156
1	-1.014613	2.749802	-2.085076
6	-1.676515	3.014442	0.943064
1	-2.629621	3.535599	0.800700
1	-0.864550	3.696637	0.676375
1	-1.573827	2.749701	2.000033
15	1.615803	1.496689	0.084771
6	1.676516	3.014421	-0.943131
1	2.629622	3.535581	-0.800777
1	0.864551	3.696623	-0.676457

1	1.573828	2.749657	-2.000094
6	1.875140	2.145032	1.783150
1	2.781030	2.758763	1.841360
1	1.961892	1.309615	2.485129
1	1.014614	2.749856	2.085013
6	3.244584	0.702947	-0.298584
1	3.338874	0.655813	-1.390389
1	4.073125	1.312037	0.079237
6	3.244604	-0.702956	0.298383
1	3.338966	-0.655823	1.390182
1	4.073119	-1.312046	-0.079495
15	1.615797	-1.496693	-0.084870
6	1.875003	-2.144982	-1.783291
1	2.780879	-2.758724	-1.841588
1	1.961716	-1.309543	-2.485248
1	1.014446	-2.749784	-2.085112
6	1.676588	-3.014452	0.942985
1	2.629670	-3.535625	0.800525
1	0.864582	-3.696633	0.676383
1	1.574016	-2.749710	1.999965

## CO2

E= -188.526181a.u.

6	0.000000	0.000000	0.000000
8	0.000000	0.000000	1.165177
8	0.000000	0.000000	-1.165177

## Co-3

E= -1987.991157 a.u.

27	0.000057	-0.000058	-0.464011
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1	-0.185239	0.421635	-1.964163
1	0.185700	-0.422255	-1.963973
15	-0.791559	1.802983	0.570003
6	-0.487402	3.416601	-0.253479
1	-0.972170	4.241210	0.281453
1	-0.872563	3.374706	-1.277463
1	0.587843	3.614191	-0.303466
6	-0.399475	2.192696	2.321255
1	-0.993334	3.043355	2.675166
1	0.660478	2.436098	2.435044
1	-0.620414	1.319598	2.943734
6	-2.649010	1.716751	0.620775
1	-3.080861	2.722548	0.582318
1	-2.928526	1.276906	1.585847
6	-3.154556	0.837801	-0.524196
1	-4.215547	0.588582	-0.410170
1	-3.026666	1.345268	-1.487847
6	-2.835064	-1.700750	0.770516
1	-3.909549	-1.835782	0.606302
1	-2.679837	-1.214315	1.738219
1	-2.360272	-2.685824	0.797560
6	-2.610767	-1.566269	-2.080215
1	-3.686073	-1.774038	-2.079810
1	-2.062292	-2.511486	-2.147896
1	-2.359469	-0.960466	-2.956305
15	-2.107718	-0.680210	-0.563858
15	0.791402	-1.802777	0.570737
6	0.398888	-2.191906	2.322019
1	0.992593	-3.042499	2.676345
1	-0.661113	-2.435183	2.435631

1	0.619747	-1.318626	2.944273
6	0.487365	-3.416639	-0.252305
1	0.971911	-4.241110	0.283040
1	0.872839	-3.375103	-1.276186
1	-0.587882	-3.614161	-0.302558
6	2.648843	-1.716603	0.621887
1	2.928183	-1.276496	1.586891
1	3.080663	-2.722429	0.583808
6	3.154664	-0.838016	-0.523238
1	3.026970	-1.345770	-1.486765
1	4.215638	-0.588797	-0.409061
6	2.834994	1.700952	0.770594
1	3.909534	1.835816	0.606603
1	2.679474	1.214880	1.738433
1	2.360309	2.686087	0.797177
6	2.611293	1.565585	-2.080131
1	3.686605	1.773323	-2.079550
1	2.062858	2.510794	-2.148234
1	2.360177	0.959512	-2.956088
15	2.107883	0.680016	-0.563608

Co-4

E= -1988.003474 a.u.

27	0.000020	-0.000015	-0.507339
1	0.325925	-0.955876	-1.587877
1	-0.325814	0.955793	-1.587944
15	0.763285	-1.589648	0.885753
6	0.686180	-3.295424	0.222241
1	1.271006	-3.980980	0.845334
1	1.073282	-3.312835	-0.800528

1	-0.351750	-3.639374	0.202212
6	0.200369	-1.833937	2.611830
1	0.662603	-2.728648	3.043277
1	-0.887348	-1.952789	2.641685
1	0.477238	-0.971640	3.223740
6	2.580852	-1.295115	1.074208
1	3.088166	-2.206570	1.409133
1	2.709106	-0.536845	1.856630
6	3.147743	-0.789053	-0.253766
1	4.186958	-0.458167	-0.151755
1	3.121968	-1.583370	-1.009420
6	2.783528	2.075505	-0.079905
1	3.866725	2.118870	-0.237951
1	2.578936	2.070617	0.995098
1	2.333925	2.971484	-0.517735
6	2.582827	0.791283	-2.618087
1	3.662755	0.956017	-2.697577
1	2.056919	1.648178	-3.050072
1	2.306994	-0.103179	-3.184096
15	2.079166	0.583604	-0.876669
15	-0.763353	1.589696	0.885615
6	-0.200598	1.834040	2.611737
1	-0.662880	2.728760	3.043117
1	0.887115	1.952905	2.641684
1	-0.477512	0.971758	3.223646
6	-0.686181	3.295451	0.222057
1	-1.271056	3.981025	0.845085
1	-1.073203	3.312833	-0.800743
1	0.351749	3.639402	0.202104
6	-2.580942	1.295200	1.073913

1	-2.709285	0.536980	1.856368
1	-3.088275	2.206685	1.408732
6	-3.147714	0.789067	-0.254081
1	-3.121853	1.583336	-1.009785
1	-4.186945	0.458207	-0.152148
6	-2.783517	-2.075477	-0.079930
1	-3.866705	-2.118854	-0.238031
1	-2.578980	-2.070496	0.995084
1	-2.333889	-2.971496	-0.517655
6	-2.582620	-0.791483	-2.618222
1	-3.662542	-0.956217	-2.697789
1	-2.056681	-1.648424	-3.050079
1	-2.306732	0.102924	-3.184293
15	-2.079100	-0.583649	-0.876783

Co-F-TS6

E= -2177.223725 a.u.

27	-0.109022	0.038594	-0.261122
15	0.336550	-1.076427	1.591215
6	2.032810	-1.576804	2.114544
1	1.986731	-2.358360	2.882781
1	2.579602	-0.725108	2.527171
1	2.579969	-1.956408	1.246614
6	-0.308682	-0.432557	3.198574
1	-0.030879	-1.074923	4.043550
1	-1.400416	-0.364171	3.149609
1	0.086274	0.573826	3.376621
6	-0.474718	-2.750736	1.518850
1	0.229221	-3.425386	1.015906
1	-0.645347	-3.148583	2.526194

6	-1.768518	-2.649916	0.714127
1	-2.535604	-2.112617	1.286354
1	-2.174955	-3.634777	0.455280
15	-1.419608	-1.646944	-0.802828
6	-0.687801	-2.879857	-1.948691
1	-1.332052	-3.760667	-2.051676
1	0.300235	-3.181360	-1.591699
1	-0.555070	-2.414764	-2.931046
6	-3.098131	-1.475537	-1.530560
1	-3.559575	-2.460905	-1.662093
1	-3.028530	-0.987364	-2.507426
1	-3.741479	-0.873764	-0.881021
15	-1.697249	1.565989	-0.208517
6	-2.796246	1.983030	-1.634635
1	-3.305437	2.940477	-1.468677
1	-3.557630	1.212985	-1.784063
1	-2.196437	2.051420	-2.548232
6	-2.956732	1.449752	1.139603
1	-3.722658	2.231498	1.062983
1	-2.453649	1.544750	2.107743
1	-3.447635	0.470799	1.108847
6	-0.973009	3.255539	0.114028
1	-0.808171	3.727998	-0.862153
1	-1.683807	3.883948	0.663101
6	0.356509	3.107929	0.850938
1	0.188294	2.832059	1.899532
1	0.941410	4.035391	0.837179
15	1.274263	1.713696	0.055300
6	1.885819	2.455055	-1.504544
1	2.413999	3.399769	-1.328454

1	1.047097	2.626290	-2.185788
1	2.569533	1.734780	-1.965551
6	2.813558	1.636224	1.048606
1	3.360330	2.583318	0.975980
1	3.451931	0.832051	0.671671
1	2.578454	1.449121	2.100811
1	0.668099	-0.201965	-1.621304
6	3.520129	-1.385249	-1.468445
8	3.917351	-0.240015	-1.693258
8	2.307657	-1.780485	-1.310325
1	4.260877	-2.207992	-1.385433
1	1.401529	-0.885351	-1.286273

Co-Int1A

E= -2176.044138 a.u.

27	-0.057653	-0.075277	-0.350483
15	-1.039240	1.931004	0.174939
6	-0.653277	3.161318	1.490080
1	-1.365546	3.993621	1.446903
1	0.356862	3.560695	1.355358
1	-0.717826	2.702119	2.479575
6	-1.173716	3.045591	-1.281992
1	-1.749374	3.948601	-1.047352
1	-1.660031	2.512169	-2.104275
1	-0.176098	3.341538	-1.622625
6	-2.818912	1.567193	0.538525
1	-2.877051	1.277806	1.595969
1	-3.435368	2.464294	0.407206
6	-3.296131	0.419687	-0.352127
1	-3.367633	0.751717	-1.394922

1	-4.287024	0.060598	-0.050678
15	-2.063343	-0.963187	-0.308135
6	-2.612596	-1.926132	1.153919
1	-3.668534	-2.205112	1.062699
1	-2.478743	-1.335718	2.065642
1	-2.013542	-2.837004	1.238383
6	-2.632028	-2.028298	-1.681396
1	-3.705835	-2.229149	-1.590989
1	-2.083722	-2.973989	-1.668819
1	-2.429548	-1.533202	-2.634338
15	1.944530	0.599864	-0.914685
6	2.424116	0.694683	-2.672348
1	3.501995	0.855082	-2.785506
1	1.887146	1.522009	-3.148298
1	2.122090	-0.238449	-3.155298
6	2.521571	2.220656	-0.266697
1	3.570729	2.396949	-0.530723
1	2.424196	2.240007	0.823164
1	1.916554	3.033788	-0.679463
6	3.155555	-0.564867	-0.149573
1	3.113477	-1.486210	-0.736864
1	4.173686	-0.163752	-0.216977
6	2.762858	-0.847269	1.308860
1	3.264924	-0.141012	1.979939
1	3.081558	-1.852020	1.601717
15	0.920931	-0.688927	1.618697
6	0.505606	-2.211234	2.554889
1	1.271055	-2.405212	3.315392
1	0.451937	-3.047010	1.856606
1	-0.456251	-2.086691	3.061128

6	0.915362	0.508550	3.021369
1	1.539680	0.143649	3.845611
1	-0.106050	0.640277	3.394433
1	1.296138	1.482096	2.700110
1	-0.510054	0.317569	-1.702290
6	0.505346	-1.831168	-1.215595
8	0.804662	-2.745283	-0.406035
8	0.521229	-1.893611	-2.462351

#### Formate

E= -189.234019 a.u.

6	0.000000	0.000000	0.325275
8	0.000000	1.132684	-0.212743
8	0.000000	-1.132684	-0.212743
1	0.000000	0.000000	1.452233

#### Formic

E= -189.718249 a.u.

6	0.000000	0.422969	0.000000
8	1.161194	0.090018	0.000000
8	-1.031008	-0.423290	0.000000
1	-0.353750	1.461462	0.000000
1	-0.687743	-1.333100	0.000000

#### H2

E= -1.174756 a.u.

1	0.000000	0.000000	0.371730
1	0.000000	0.000000	-0.371730

#### TS1



E= -2176.018343 a.u.

27	-0.101193	0.041324	0.126805
1	0.830815	1.272283	0.409820
15	1.049484	-0.205867	-1.761060
6	0.571028	-1.098811	-3.306563
1	1.385770	-1.097120	-4.041083
1	-0.305582	-0.621261	-3.758283
1	0.316458	-2.137914	-3.079155
6	1.799292	1.299657	-2.524478
1	2.411479	1.051803	-3.400398
1	2.433205	1.812565	-1.794852
1	1.007524	1.992199	-2.828805
6	2.578989	-1.171702	-1.291593
1	2.333723	-2.235203	-1.414340
1	3.410761	-0.951327	-1.972472
6	2.960087	-0.889034	0.165121
1	3.327700	0.138177	0.269172
1	3.756546	-1.561952	0.506834
15	1.455302	-1.033604	1.255994
6	1.417799	-2.860829	1.532385
1	2.418652	-3.244187	1.763497
1	1.039642	-3.377809	0.644623
1	0.759868	-3.097826	2.374367
6	2.123878	-0.498940	2.885470
1	3.051553	-1.024440	3.143948
1	1.377132	-0.696621	3.662465
1	2.315811	0.576941	2.861409
15	-1.734981	1.471793	0.253114
6	-1.907391	2.683867	1.629527
1	-2.858894	3.226161	1.568952

1	-1.088458	3.408143	1.593846
1	-1.855175	2.154789	2.586575
6	-1.960346	2.580260	-1.204376
1	-2.802954	3.271532	-1.079062
1	-2.127047	1.966688	-2.096599
1	-1.043409	3.157481	-1.353040
6	-3.377745	0.604575	0.329967
1	-3.591570	0.405745	1.387763
1	-4.184895	1.237349	-0.057492
6	-3.256855	-0.711673	-0.437455
1	-3.216552	-0.523089	-1.517682
1	-4.101997	-1.384033	-0.247091
15	-1.649031	-1.503709	0.040744
6	-2.122576	-2.364360	1.602367
1	-3.088454	-2.872121	1.496148
1	-2.180572	-1.642295	2.422052
1	-1.366986	-3.111913	1.859675
6	-1.596802	-2.936788	-1.113341
1	-2.426732	-3.627236	-0.922467
1	-0.653372	-3.481226	-1.001670
1	-1.671635	-2.579331	-2.144521
6	1.667451	2.728924	0.626060
8	1.007483	3.530209	0.051695
8	2.608445	2.389693	1.266268

TS2

E= -1987.990781 a.u.

27	-0.000001	0.000001	-0.506138
1	-0.199443	0.500189	-1.917547
1	0.199431	-0.500148	-1.917565

15	-0.762508	1.768527	0.617870
6	-0.431996	3.410145	-0.135416
1	-0.894517	4.217084	0.443981
1	-0.836902	3.419435	-1.152469
1	0.644067	3.595247	-0.199621
6	-0.366601	2.046519	2.387725
1	-0.930701	2.895395	2.790817
1	0.701802	2.244062	2.514170
1	-0.621097	1.146195	2.956533
6	-2.621762	1.718926	0.640002
1	-3.029108	2.735487	0.633307
1	-2.930327	1.249806	1.581851
6	-3.126505	0.896721	-0.548130
1	-4.194625	0.668041	-0.460887
1	-2.969438	1.435799	-1.489645
6	-2.862255	-1.649425	0.715932
1	-3.939570	-1.757469	0.549343
1	-2.700082	-1.163500	1.682730
1	-2.415513	-2.646656	0.750540
6	-2.641339	-1.507191	-2.138059
1	-3.719350	-1.699736	-2.131892
1	-2.105908	-2.459101	-2.215378
1	-2.385569	-0.897976	-3.010427
15	-2.114275	-0.642618	-0.619498
15	0.762512	-1.768541	0.617854
6	0.366610	-2.046587	2.387701
1	0.930646	-2.895532	2.790737
1	-0.701807	-2.244043	2.514156
1	0.621202	-1.146314	2.956549
6	0.432019	-3.410151	-0.135456

1	0.894928	-4.217058	0.443675
1	0.836512	-3.419257	-1.152675
1	-0.644037	-3.595456	-0.199223
6	2.621764	-1.718915	0.639997
1	2.930313	-1.249789	1.581849
1	3.029124	-2.735470	0.633307
6	3.126511	-0.896704	-0.548128
1	2.969453	-1.435780	-1.489645
1	4.194629	-0.668019	-0.460874
6	2.862240	1.649453	0.715925
1	3.939556	1.757497	0.549345
1	2.700057	1.163545	1.682730
1	2.415498	2.646685	0.750511
6	2.641319	1.507209	-2.138058
1	3.719325	1.699782	-2.131888
1	2.105864	2.459108	-2.215372
1	2.385565	0.897992	-3.010429
15	2.114272	0.642627	-0.619498

TS3

E= -3139.556748 a.u.

27	-1.821083	-0.033525	0.077112
1	0.154942	-0.041893	-0.162057
1	-1.206697	-0.670680	1.272222
15	-1.585994	-2.002519	-0.882990
6	-1.419602	-2.302444	-2.692885
1	-1.367428	-3.379188	-2.891066
1	-0.542560	-1.822693	-3.126701
1	-2.308914	-1.906311	-3.192872
6	-0.371073	-3.184846	-0.168146

1	-0.395915	-4.144221	-0.696869
1	-0.624992	-3.355469	0.883649
1	0.643592	-2.781362	-0.213777
6	-3.159670	-2.956696	-0.627961
1	-3.870119	-2.617606	-1.392851
1	-2.986639	-4.027408	-0.790363
6	-3.707047	-2.666367	0.760403
1	-3.039477	-3.079805	1.527132
1	-4.698327	-3.109316	0.913464
15	-3.766326	-0.830137	1.026006
6	-5.499245	-0.453532	0.504356
1	-6.223694	-1.042466	1.079889
1	-5.637019	-0.669853	-0.559458
1	-5.710562	0.609449	0.663300
6	-4.013736	-0.840634	2.856671
1	-4.652662	-1.685553	3.140204
1	-4.497052	0.076987	3.200250
1	-3.049672	-0.942670	3.364734
15	-1.680823	1.877159	1.189921
6	-2.796597	2.174939	2.625199
1	-2.688836	3.212064	2.964086
1	-2.542417	1.509807	3.455037
1	-3.839072	2.008949	2.341673
6	-0.130331	2.563218	1.953244
1	-0.260275	2.652960	3.036448
1	0.079975	3.561891	1.560572
1	0.730320	1.919052	1.771418
6	-2.285351	3.255477	0.089746
1	-3.371144	3.310417	0.238515
1	-1.868060	4.218511	0.404480

6	-1.981074	2.947357	-1.370210
1	-0.918479	3.096384	-1.583969
1	-2.546015	3.597560	-2.049052
15	-2.365203	1.167756	-1.717776
6	-4.141056	1.273599	-2.203239
1	-4.277658	1.936663	-3.065738
1	-4.734994	1.653318	-1.366723
1	-4.515149	0.277621	-2.461871
6	-1.624580	0.990047	-3.395827
1	-1.792390	1.907401	-3.972042
1	-2.087106	0.159574	-3.935589
1	-0.550327	0.805324	-3.334679
7	2.156582	-0.287928	1.620182
15	1.886315	-0.106829	-0.034035
6	3.198921	0.450279	2.328858
7	2.744202	-1.372042	-0.780892
7	2.609826	1.320364	-0.562302
6	4.636473	-0.031280	2.098395
6	3.846423	-2.044305	-0.087320
6	3.986603	1.361411	-1.061996
7	5.070057	-0.019717	0.723518
6	5.161261	-1.262433	-0.002017
6	5.080915	1.223759	-0.003611
1	2.982167	0.399949	3.399646
1	3.135816	1.509189	2.051738
1	5.290792	0.611696	2.709899
1	4.752647	-1.050294	2.483308
1	4.031820	-3.001232	-0.584403
1	3.532534	-2.281240	0.926403
1	4.132840	2.315621	-1.573150

1	4.134906	0.587693	-1.823835
1	5.896511	-1.930816	0.475363
1	5.545277	-1.049758	-1.006327
1	4.997993	2.043705	0.718176
1	6.044122	1.355964	-0.524209
6	1.806153	2.544041	-0.751072
1	0.811561	2.314303	-0.363439
6	1.293823	-1.214735	2.389246
1	0.528097	-1.547226	1.687488
6	2.724446	-1.618040	-2.241614
1	3.760170	-1.512355	-2.596034
6	1.630724	2.931998	-2.223205
1	1.064387	3.867568	-2.291989
1	2.589668	3.100990	-2.724498
1	1.084567	2.163857	-2.775984
6	2.381157	3.717081	0.045260
1	2.515954	3.458747	1.099636
1	3.350732	4.031089	-0.358482
1	1.708265	4.579833	-0.013629
6	0.555355	-0.529211	3.541493
1	-0.175178	-1.229967	3.961490
1	1.228386	-0.233554	4.354509
1	0.012996	0.350626	3.196705
6	2.024351	-2.455177	2.915793
1	2.322745	-3.134437	2.113204
1	2.914178	-2.182551	3.495182
1	1.358030	-3.017295	3.579744
6	2.266903	-3.041726	-2.576458
1	2.454775	-3.243887	-3.637036
1	2.799184	-3.801730	-1.996647

1	1.197240	-3.165361	-2.392797
6	1.873193	-0.604938	-3.002527
1	0.893874	-0.482644	-2.529840
1	2.351271	0.373770	-3.062758
1	1.707522	-0.959743	-4.024739

TS4

E= -2176.504007 a.u.

27	0.045738	0.030865	-0.374889
15	-2.165497	0.165873	-0.844986
6	-3.006951	1.709338	-1.333625
1	-4.077518	1.505793	-1.443706
1	-2.618764	2.056420	-2.295138
1	-2.877123	2.494317	-0.583743
6	-2.631857	-0.974062	-2.190409
1	-3.715070	-0.933212	-2.346576
1	-2.330722	-1.991536	-1.932643
1	-2.123843	-0.676563	-3.112581
6	-3.115563	-0.404701	0.625926
1	-3.246429	0.461457	1.286521
1	-4.112997	-0.732876	0.313003
6	-2.355875	-1.517557	1.345210
1	-2.326254	-2.427519	0.739246
1	-2.825713	-1.757208	2.305486
15	-0.607238	-0.997378	1.624267
6	-0.742592	-0.013645	3.168815
1	-1.030367	-0.677348	3.991537
1	-1.504333	0.764122	3.070596
1	0.214447	0.453537	3.419146
6	0.204628	-2.508793	2.255241



1	-0.488531	-3.027081	2.927469
1	1.098870	-2.244882	2.826925
1	0.467804	-3.168599	1.427031
15	2.280649	-0.168646	-0.119682
6	3.058795	-1.668810	0.557342
1	4.142587	-1.601874	0.415073
1	2.685309	-2.551658	0.031888
1	2.847471	-1.763367	1.624018
6	3.164708	0.115071	-1.687829
1	4.247671	0.127879	-1.526111
1	2.847377	1.061406	-2.133851
1	2.911124	-0.699131	-2.374476
6	2.778121	1.204548	0.989014
1	2.440425	0.950485	2.000043
1	3.867081	1.315995	1.012236
6	2.100230	2.476116	0.484535
1	2.592440	2.831755	-0.427202
1	2.146039	3.286815	1.219251
15	0.327425	2.164898	0.052054
6	-0.636859	2.871944	1.430239
1	-0.556502	3.963851	1.394059
1	-0.241641	2.523242	2.385556
1	-1.690807	2.592670	1.347723
6	0.044736	3.353005	-1.303218
1	0.467922	4.319491	-1.008077
1	-1.020294	3.488791	-1.498904
1	0.535490	3.006361	-2.216062
1	0.314508	0.643719	-1.683225
1	0.199620	-1.241198	-2.019998
6	0.423548	-2.306740	-1.655291

8	1.403783	-2.841838	-2.192151
8	-0.368120	-2.742273	-0.783226

TS6

E= -3139.561928 a.u.

27	2.179075	0.021412	0.040393
1	0.520372	-0.148435	0.066055
1	-0.528793	0.009313	0.179751
15	2.290676	1.591193	1.610927
6	1.762769	1.381007	3.363427
1	1.572826	2.355761	3.828013
1	2.542283	0.873733	3.938891
1	0.849155	0.781113	3.413073
6	3.815007	2.601805	1.864460
1	3.642392	3.453625	2.533932
1	4.179921	2.973404	0.900648
1	4.599545	1.967417	2.291816
6	1.075591	2.882272	1.058002
1	0.086359	2.425870	1.168854
1	1.107371	3.772923	1.697165
6	1.339940	3.230364	-0.404578
1	2.169256	3.943984	-0.469736
1	0.477779	3.706272	-0.883952
15	1.855917	1.706673	-1.353937
6	0.583003	1.476295	-2.660891
1	0.336487	2.425582	-3.149354
1	-0.322994	1.027737	-2.248527
1	0.979748	0.787687	-3.414709
6	3.196481	2.453672	-2.372696
1	2.815731	3.347468	-2.880362

1	3.567061	1.759657	-3.131222
1	4.030857	2.747162	-1.728388
15	3.637809	-0.914536	-1.303573
6	3.310022	-1.246305	-3.088942
1	4.137974	-1.801965	-3.544956
1	3.171922	-0.314503	-3.645249
1	2.391899	-1.835037	-3.182593
6	5.323637	-0.162599	-1.398764
1	5.992024	-0.761160	-2.029448
1	5.741484	-0.102834	-0.388013
1	5.277357	0.852367	-1.800531
6	4.082493	-2.624016	-0.729024
1	3.349366	-3.322519	-1.150800
1	5.069241	-2.915718	-1.105911
6	4.011784	-2.639466	0.794288
1	4.837021	-2.059564	1.225203
1	4.062810	-3.654202	1.205664
15	2.428879	-1.806937	1.268951
6	1.229999	-3.166911	0.948104
1	1.557695	-4.098999	1.423076
1	1.130566	-3.327355	-0.129281
1	0.248773	-2.898883	1.345240
6	2.539860	-1.870854	3.101690
1	2.715800	-2.901401	3.430057
1	1.618936	-1.508873	3.565498
1	3.372566	-1.247875	3.442450
7	-2.443849	-1.100832	-1.208734
15	-2.231261	-0.070762	0.103812
6	-3.502804	-0.925616	-2.192047
7	-2.965991	-0.768719	1.448056

7	-3.039737	1.369430	-0.191430
6	-4.879398	-1.351159	-1.666991
6	-3.948287	-1.842374	1.312619
6	-4.418554	1.593857	0.243477
7	-5.236203	-0.653040	-0.457652
6	-5.309044	-1.352960	0.799889
6	-5.466444	0.767764	-0.506454
1	-3.244568	-1.487378	-3.095319
1	-3.550096	0.128686	-2.486025
1	-5.625991	-1.179726	-2.460117
1	-4.877614	-2.425504	-1.455919
1	-4.074569	-2.316291	2.291653
1	-3.573776	-2.616814	0.637039
1	-4.651712	2.652538	0.105809
1	-4.509767	1.386210	1.316924
1	-5.978983	-2.225749	0.728409
1	-5.746939	-0.674170	1.540833
1	-5.483460	1.074707	-1.558018
1	-6.451584	1.024150	-0.082048
6	-2.264630	2.524940	-0.673650
1	-1.230259	2.176123	-0.737832
6	-1.524390	-2.250808	-1.328350
1	-1.032684	-2.348143	-0.354538
6	-2.439507	-0.491685	2.799380
1	-3.246261	-0.762998	3.489147
6	-2.281068	3.703431	0.304577
1	-1.529766	4.441113	0.002995
1	-3.249378	4.215164	0.318396
1	-2.050068	3.376715	1.322838
6	-2.705039	2.958628	-2.071424

1	-2.568885	2.150355	-2.797194
1	-3.762921	3.248325	-2.073984
1	-2.122713	3.824147	-2.408090
6	-0.437980	-2.004224	-2.377412
1	0.165307	-2.909016	-2.519489
1	-0.879496	-1.738400	-3.345656
1	0.228313	-1.201501	-2.052548
6	-2.241255	-3.577016	-1.601710
1	-3.014071	-3.794667	-0.859701
1	-2.704211	-3.592802	-2.594602
1	-1.508460	-4.390413	-1.570398
6	-1.216777	-1.355178	3.107347
1	-0.893544	-1.226293	4.147054
1	-1.435448	-2.416690	2.945963
1	-0.388979	-1.065213	2.449786
6	-2.127052	0.985740	3.033307
1	-1.291979	1.326534	2.411849
1	-2.995348	1.619224	2.830852
1	-1.835882	1.133942	4.078793

TS7

E= -2177.227317 a.u.

27	0.064621	-0.008231	-0.212390
1	-0.001769	0.477130	-1.627999
15	2.129135	-0.761231	-0.688368
6	2.455558	-1.146025	-2.460864
1	3.524319	-1.298993	-2.654210
1	2.090352	-0.325853	-3.086335
1	1.915494	-2.053427	-2.750224
6	3.082044	-2.126687	0.107089

1	4.078285	-2.236358	-0.338834
1	2.543809	-3.074138	-0.008115
1	3.201378	-1.929379	1.176576
6	3.277732	0.675348	-0.407633
1	4.207523	0.562395	-0.978341
1	3.543333	0.668395	0.658083
6	2.555436	1.978895	-0.755770
1	3.134425	2.857920	-0.447965
1	2.397982	2.049271	-1.839245
6	1.251384	2.667705	1.702609
1	1.863338	3.574421	1.630227
1	1.784041	1.927619	2.309035
1	0.317571	2.924728	2.212271
6	0.098649	3.448551	-0.747930
1	0.758711	4.322060	-0.688461
1	-0.843679	3.684144	-0.244972
1	-0.123333	3.228370	-1.795464
15	0.873262	1.983294	0.034837
15	-0.335375	-0.651671	1.863626
6	0.989020	-1.251089	2.994080
1	0.583086	-1.511144	3.978770
1	1.749906	-0.473523	3.121975
1	1.467972	-2.137510	2.568332
6	-1.243961	0.466705	3.007729
1	-1.611639	-0.083877	3.881427
1	-2.079902	0.931623	2.479203
1	-0.573812	1.257579	3.357724
6	-1.452454	-2.138066	1.793653
1	-0.808311	-3.020082	1.685360
1	-2.010157	-2.252936	2.730244

6	-2.378149	-2.019323	0.581861
1	-3.123174	-1.231141	0.743364
1	-2.913032	-2.955815	0.383861
6	-0.690585	-3.123709	-1.455793
1	-1.494184	-3.852614	-1.615298
1	0.019758	-3.527544	-0.726883
1	-0.161849	-2.978400	-2.403308
6	-2.581190	-1.152006	-2.171538
1	-3.316617	-1.960889	-2.252469
1	-2.065892	-1.042091	-3.131623
1	-3.087986	-0.207203	-1.959015
15	-1.345826	-1.503929	-0.867137
6	-3.181797	2.162258	-0.634537
8	-2.982750	2.230880	-1.846025
8	-2.536411	1.474545	0.243554
1	-4.016080	2.743779	-0.186492
1	-1.449394	0.870050	-0.089030

TS8

E= -1341.31641 a.u.

6	1.782495	1.989776	0.016063
6	1.741390	3.263665	-0.829343
6	2.562444	2.197938	1.316612
7	0.435042	1.446414	0.264727
15	0.233405	-0.200459	-0.010759
6	-0.541758	2.256738	0.978379
7	-0.320797	-0.358429	-1.590620
7	-0.941840	-0.780107	1.040090
6	-1.794052	2.561433	0.150259
6	-0.105065	-1.574039	-2.402091

6	-1.002693	0.744569	-2.267107
6	-0.482827	-1.357189	2.316452
6	-2.350617	-0.886317	0.681302
7	-2.454733	1.377876	-0.339825
6	0.941982	-2.516837	-1.817629
6	-1.410715	-2.327326	-2.671408
6	-2.410555	1.057136	-1.744334
6	-0.613930	-2.882263	2.326614
6	-1.179933	-0.725103	3.522694
6	-3.068953	0.463362	0.589283
1	2.316232	1.230757	-0.567427
1	1.235411	3.087342	-1.783863
1	2.761467	3.601354	-1.043616
1	1.225864	4.081253	-0.311425
1	2.596592	1.268319	1.895063
1	3.592392	2.503617	1.099747
1	2.106633	2.975795	1.941251
1	-0.067654	3.196385	1.277167
1	-0.844506	1.753468	1.904693
1	-2.476692	3.165383	0.771063
1	-1.515878	3.178558	-0.711768
1	0.284168	-1.224702	-3.368217
1	-1.061903	0.499753	-3.333124
1	-0.393985	1.651659	-2.185035
1	0.584268	-1.118661	2.396175
1	-2.855567	-1.514440	1.420900
1	-2.450437	-1.400521	-0.280756
1	1.073673	-3.358509	-2.506013
1	1.910861	-2.024214	-1.695951
1	0.630317	-2.929601	-0.850500



1	-1.241719	-3.118641	-3.411161
1	-2.186645	-1.663105	-3.066593
1	-1.788393	-2.796997	-1.756184
1	-2.809280	1.888901	-2.349274
1	-3.067301	0.197301	-1.916893
1	-0.184188	-3.297011	3.245333
1	-0.085244	-3.320037	1.473115
1	-1.663580	-3.195926	2.278564
1	-0.780449	-1.150993	4.449825
1	-1.019619	0.357282	3.549866
1	-2.259577	-0.914695	3.511171
1	-3.077709	0.937474	1.576792
1	-4.120212	0.268264	0.317521
6	3.828498	-1.146594	0.180952
8	3.906141	-0.570605	-0.906656
8	2.756521	-1.418111	0.839125
1	4.754347	-1.489519	0.685018
1	1.677970	-0.922652	0.345380

TSA

E= -2176.023101 a.u.

27	-0.002506	-0.027698	-0.291654
15	-1.273633	1.754269	-0.541772
6	-1.105380	3.440245	0.200845
1	-1.978714	4.068199	-0.015477
1	-0.217860	3.930861	-0.215097
1	-0.979328	3.387930	1.285934
6	-1.657954	2.267904	-2.272996
1	-2.436616	3.039687	-2.312151
1	-1.984991	1.397483	-2.850102

1	-0.750927	2.657864	-2.747221
6	-2.959015	1.243384	0.059749
1	-2.936667	1.285265	1.156975
1	-3.739212	1.935847	-0.281717
6	-3.233570	-0.185700	-0.415814
1	-3.400335	-0.186462	-1.501051
1	-4.135866	-0.602318	0.048713
15	-1.757387	-1.300259	-0.105957
6	-2.246111	-2.096513	1.489181
1	-3.231124	-2.572851	1.414694
1	-2.277774	-1.353823	2.291966
1	-1.510018	-2.860580	1.759692
6	-2.206970	-2.677413	-1.250310
1	-3.276044	-2.913185	-1.176240
1	-1.640168	-3.582046	-1.005677
1	-1.973602	-2.395772	-2.281132
15	2.040074	0.481377	-0.815319
6	3.266350	-0.521715	-1.766747
1	4.219236	0.012465	-1.867517
1	2.871742	-0.730500	-2.765893
1	3.457538	-1.477176	-1.267699
6	2.207697	2.064930	-1.754080
1	3.256553	2.326933	-1.939553
1	1.731874	2.876244	-1.193241
1	1.694088	1.967638	-2.716375
6	3.025525	0.857393	0.723593
1	3.520561	-0.072697	1.030779
1	3.812464	1.594410	0.522992
6	2.070407	1.326411	1.822634
1	1.707177	2.339094	1.605633

1	2.555241	1.347752	2.806345
15	0.586345	0.212192	1.817200
6	1.194764	-1.218609	2.805681
1	1.545041	-0.896454	3.793940
1	2.009913	-1.718878	2.277838
1	0.389198	-1.947638	2.936305
6	-0.485209	1.003798	3.093257
1	0.083755	1.219334	4.005429
1	-1.311350	0.335300	3.356041
1	-0.911236	1.937770	2.719481
1	-0.193488	-0.271469	-1.757587
6	1.078237	-2.754693	-0.833850
8	1.348658	-3.106939	0.259339
8	0.960713	-2.773137	-2.004780

TSB

E= -2176.032813 a.u.

27	-0.018968	-0.073542	-0.402813
15	-0.709607	2.014337	0.145718
6	0.115760	3.133756	1.361059
1	-0.631342	3.795452	1.814468
1	0.864732	3.760860	0.872285
1	0.603954	2.561733	2.155863
6	-1.091105	3.219305	-1.193143
1	-1.526642	4.146469	-0.801692
1	-1.786746	2.767075	-1.907331
1	-0.169658	3.457782	-1.735323
6	-2.351205	1.825841	0.979511
1	-2.156101	1.391008	1.967882
1	-2.824531	2.803446	1.131838

6	-3.218999	0.894430	0.143131
1	-3.557874	1.413215	-0.761737
1	-4.115835	0.570536	0.682895
15	-2.214293	-0.574498	-0.400458
6	-2.847035	-1.904584	0.691270
1	-3.928153	-2.029850	0.563748
1	-2.643305	-1.658344	1.738414
1	-2.341469	-2.837261	0.433366
6	-3.030383	-0.938658	-2.000153
1	-4.117018	-0.999576	-1.868618
1	-2.649731	-1.880933	-2.396039
1	-2.800833	-0.137853	-2.710180
15	2.123312	0.502399	-0.746437
6	2.856664	0.332007	-2.414904
1	3.944841	0.456985	-2.373431
1	2.437129	1.108435	-3.064143
1	2.608062	-0.650610	-2.816406
6	2.756949	2.177803	-0.321619
1	3.820374	2.240009	-0.579111
1	2.651015	2.374909	0.747769
1	2.222027	2.952339	-0.879982
6	3.147199	-0.536746	0.390868
1	3.188871	-1.537259	-0.047776
1	4.167334	-0.142599	0.469311
6	2.452617	-0.568983	1.756895
1	2.517964	0.415240	2.239446
1	2.926544	-1.291844	2.431286
15	0.646084	-0.962188	1.547383
6	0.634649	-2.791012	1.728329
1	1.113142	-3.099407	2.665489

1	1.161773	-3.240273	0.881856
1	-0.394827	-3.159830	1.714126
6	-0.035157	-0.464782	3.184466
1	0.544690	-0.900726	4.006698
1	-1.070937	-0.808976	3.275053
1	-0.025621	0.624715	3.288164
1	-0.033625	-0.540031	-1.858247
6	0.316292	-1.938242	-1.385130
8	-0.680898	-2.685519	-1.390654
8	1.505150	-2.224575	-1.624417

VKDH-formate

E= -1341.341835 a.u.

6	-0.421439	-1.949213	-1.650473
6	-0.264850	-3.462552	-1.799847
6	-1.811374	-1.476571	-2.086649
7	-0.085720	-1.510946	-0.285311
15	0.702836	-0.032014	-0.071263
6	-0.892048	-2.062866	0.795468
7	2.231979	-0.011334	0.651485
7	-0.140384	1.416114	-0.264670
6	-0.351880	-1.471502	2.085769
6	3.440514	-0.413443	-0.101959
6	2.351576	-0.055809	2.097616
6	0.231368	2.342579	-1.345225
6	-0.926603	1.957322	0.833243
7	-0.029755	-0.058503	1.795563
6	3.323416	-1.803975	-0.734408
6	3.879931	0.649302	-1.109942
6	1.043687	0.474555	2.658895

6	1.168298	3.450319	-0.854087
6	-1.000922	2.916409	-2.044396
6	-1.233086	0.802717	1.768965
1	0.315882	-1.481646	-2.312352
1	0.713325	-3.793326	-1.433937
1	-0.349631	-3.738616	-2.856374
1	-1.043730	-4.008091	-1.255297
1	-1.910542	-0.393580	-1.956038
1	-1.977935	-1.715013	-3.143307
1	-2.602280	-1.959449	-1.502847
1	-0.784705	-3.151171	0.833617
1	-1.956206	-1.825358	0.672802
1	-1.071644	-1.529853	2.906392
1	0.569335	-1.977105	2.382979
1	4.227301	-0.474634	0.657504
1	3.175760	0.583568	2.430786
1	2.559985	-1.075165	2.454607
1	0.777299	1.748804	-2.085805
1	-1.878123	2.350813	0.467225
1	-0.388277	2.764425	1.349762
1	4.300571	-2.127333	-1.110239
1	2.979814	-2.537346	0.002967
1	2.623612	-1.811481	-1.577045
1	4.838779	0.364492	-1.557480
1	4.007370	1.618941	-0.617908
1	3.155914	0.768196	-1.923355
1	0.873245	0.182763	3.698577
1	1.022018	1.564022	2.588382
1	1.541635	4.032928	-1.703425
1	2.027446	3.025084	-0.323824

1	0.653102	4.142658	-0.178702
1	-0.692088	3.480142	-2.931491
1	-1.678024	2.116724	-2.361128
1	-1.559356	3.600458	-1.396408
1	-2.076901	0.223268	1.385249
1	-1.470505	1.136274	2.782956
6	-4.297220	-0.011497	-0.035069
8	-4.097214	1.223229	0.040559
8	-4.051684	-0.897627	0.822378
1	-4.759010	-0.375400	-0.991335
1	1.216167	-0.015566	-1.376939

VKD-H

E= -1152.083652 a.u.

6	-2.585685	0.275545	-1.294214
6	-3.603865	-0.815325	-1.625633
6	-3.246989	1.636422	-1.077295
7	-1.746274	-0.113930	-0.147317
15	-0.072020	-0.102994	-0.273104
6	-2.372114	-0.174835	1.163108
7	0.648872	-1.573841	-0.683672
7	0.868023	1.109776	0.410248
6	-1.566546	-1.163345	1.983038
6	1.828755	-1.647314	-1.579516
6	0.518204	-2.664762	0.275520
6	1.082897	2.390679	-0.284333
6	1.435341	0.930796	1.736505
7	-0.146448	-0.874034	1.704477
6	1.734343	-0.742756	-2.807339
6	3.140730	-1.410325	-0.825971

6	0.684707	-2.091935	1.675379
6	2.571472	2.694549	-0.448354
6	0.336620	3.533291	0.406974
6	0.399514	0.191383	2.565223
1	-1.914553	0.360614	-2.154447
1	-3.103268	-1.778845	-1.766747
1	-4.133096	-0.562361	-2.550656
1	-4.357576	-0.927195	-0.837729
1	-2.496132	2.401358	-0.849875
1	-3.784651	1.941989	-1.981183
1	-3.970971	1.606053	-0.254821
1	-3.402604	-0.526279	1.074565
1	-2.397670	0.812880	1.644109
1	-1.766970	-1.093485	3.055903
1	-1.783915	-2.179087	1.648034
1	1.827208	-2.678903	-1.949624
1	1.276505	-3.426428	0.082954
1	-0.462443	-3.144386	0.166652
1	0.653156	2.275486	-1.285367
1	1.647563	1.897028	2.198737
1	2.382331	0.376141	1.690608
1	2.523372	-1.031874	-3.508961
1	0.771039	-0.854078	-3.316153
1	1.887419	0.314536	-2.564119
1	3.994541	-1.549684	-1.498286
1	3.257580	-2.111748	0.007573
1	3.180486	-0.389751	-0.429239
1	0.378412	-2.783943	2.465460
1	1.726532	-1.806959	1.837825
1	2.703140	3.620928	-1.017338



1	3.080310	1.886416	-0.984393
1	3.063135	2.829680	0.521981
1	0.423060	4.452639	-0.182113
1	-0.726569	3.293090	0.516580
1	0.746061	3.742291	1.402127
1	-0.414410	0.874222	2.821444
1	0.811206	-0.233786	3.485332
1	-0.051432	0.450145	-1.556978

VKD

E= -1151.586015 a.u.

6	-2.624303	-0.321392	-1.320664
6	-3.688044	-1.292949	-0.803570
6	-3.254154	0.960675	-1.877494
7	-1.589413	-0.060735	-0.310990
15	0.017133	0.005987	-0.929017
6	-1.991605	0.632074	0.902240
7	0.677374	-1.466978	-0.345349
7	0.767354	1.215471	0.032830
6	-1.655570	-0.109859	2.201682
6	1.756963	-2.169504	-1.058006
6	0.045150	-2.236933	0.718662
6	0.988903	2.506226	-0.630381
6	1.526231	0.926280	1.237350
7	-0.258702	-0.395858	2.431794
6	2.110977	-1.567321	-2.416249
6	3.022579	-2.280467	-0.198582
6	0.240725	-1.721833	2.151399
6	2.412494	2.654648	-1.180334
6	0.610015	3.688164	0.265912

6	0.679118	0.700797	2.495169
1	-2.111596	-0.820565	-2.152846
1	-3.226749	-2.223795	-0.456979
1	-4.401895	-1.537930	-1.598632
1	-4.257936	-0.863528	0.028992
1	-2.478264	1.626227	-2.273383
1	-3.954568	0.729611	-2.688608
1	-3.808616	1.505998	-1.104492
1	-3.075575	0.788292	0.880186
1	-1.535011	1.630039	0.945594
1	-2.047661	0.501008	3.032512
1	-2.200773	-1.061348	2.223468
1	1.402240	-3.193998	-1.251237
1	0.435442	-3.261321	0.675013
1	-1.033327	-2.302578	0.528108
1	0.305406	2.523231	-1.488771
1	2.214795	1.754766	1.436298
1	2.150337	0.037227	1.083465
1	2.892452	-2.183738	-2.875079
1	1.254736	-1.544225	-3.096292
1	2.504189	-0.548267	-2.322674
1	3.756242	-2.939373	-0.679164
1	2.800934	-2.694442	0.790996
1	3.486775	-1.296341	-0.063130
1	-0.253785	-2.450560	2.816746
1	1.307154	-1.738820	2.405835
1	2.522423	3.599446	-1.725619
1	2.643267	1.833351	-1.868048
1	3.158948	2.646901	-0.377166
1	0.715676	4.631724	-0.281864

1	-0.427694	3.603975	0.605613
1	1.255076	3.748866	1.150830
1	0.116308	1.614028	2.722800
1	1.380883	0.541402	3.331966