Supplementary Material (ESI) for Dalton Transactions

A DFT Study of the Possible Role of Vinylidene and Carbene Intermediates in the Mechanism of the Enzyme Acetylene Hydratase.

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Table S1. Structures (Å) for Scheme 1, 2 and 3.

Scheme 1

Reactant

1	74	0	1.297287	-0.039146	0.138075
2	6	0	-4.627604	-1.006781	-1.101387
3	16	0	3.526070	0.569181	0.630941
4	6	0	3.689651	2.292553	0.276246
5	1	0	4.654077	2.743743	0.498333
6	6	0	2.679662	2.980860	-0.282246
7	1	0	2.761056	4.031618	-0.550240
8	16	0	1.159904	2.174714	-0.685050
9	16	0	2.068152	-2.257552	-0.123590
10	6	0	0.967447	-3.060843	-1.259752
11	1	0	1.160477	-4.112390	-1.459867
12	6	0	-0.013497	-2.383073	-1.876359
13	1	0	-0.673318	-2.836658	-2.611757
14	16	0	-0.224591	-0.646951	-1.580715
15	6	0	-0.846003	-1.525622	2.292320
16	16	0	0.131089	0.045213	2.165753
17	1	0	-0.816765	-1.845899	3.337655
18	1	0	-0.407424	-2.293483	1.655228
19	1	0	-1.881955	-1.340928	1.998239
20	6	0	-4.317688	3.113100	-1.372406
21	6	0	-5.167107	3.648681	-2.042371
22	1	0	-3.566838	2.614692	-0.784659

23	1	0	-5.915862	4.126167	-2.631754
24	8	0	-2.445615	1.099260	0.188545
25	1	0	-1.967255	0.600418	-0.506891
26	1	0	-1.740420	1.231210	0.854834
27	1	0	-3.573464	-1.254072	-1.275306
28	1	0	-4.761951	0.051741	-1.353375
29	1	0	-5.254184	-1.618215	-1.752468
30	6	0	-5.007481	-1.268469	0.348797
31	8	0	-5.864992	-2.057557	0.683235
32	8	0	-4.322628	-0.560548	1.266546
33	1	0	-3.663788	0.053545	0.843414

Transition Structure

1	74	0	-0.225300	-1.207122	0.229585
2	6	0	2.179398	4.236977	-1.238788
3	8	0	-0.290902	2.646290	0.076312
4	1	0	-0.594518	3.317275	-0.576929
5	1	0	-0.884070	1.849887	0.043652
6	16	0	-1.959267	0.035034	-0.767249
7	6	0	-1.450876	0.279526	-2.530252
8	1	0	-2.247725	0.836181	-3.032708
9	1	0	-1.314848	-0.694153	-3.003705
10	1	0	-0.513810	0.837674	-2.576834
11	16	0	-1.291364	-2.832161	1.578482
12	6	0	-1.308690	-2.216916	3.235949
13	1	0	-1.813104	-2.831643	3.978099
14	6	0	-0.681252	-1.071988	3.552160
15	1	0	-0.634741	-0.687467	4.568406
16	16	0	0.188775	-0.155214	2.314204
17	16	0	1.808444	-0.285968	-0.531615
18	16	0	0.290559	-2.952275	-1.268708

19	6	0	1.776168	-2.491597	-2.117536
20	6	0	2.422991	-1.358277	-1.801022
21	1	0	2.144842	-3.188640	-2.866608
22	1	0	3.356086	-1.062886	-2.275257
23	1	0	2.363962	4.765758	-0.298533
24	1	0	1.986402	3.189378	-0.981725
25	1	0	3.057460	4.291852	-1.885307
26	6	0	0.979122	4.807337	-1.980136
27	8	0	0.971075	4.979805	-3.182740
28	8	0	-0.119421	5.057607	-1.237069
29	1	0	0.049828	5.088252	-0.177773
30	6	0	-0.163090	3.541003	1.640675
31	1	0	0.161189	5.492018	2.242688
32	6	0	0.029806	4.782709	1.431347
33	1	0	-0.226586	2.650618	2.244982

Product

1	74	0	1.285534	-0.042465	0.052618
2	6	0	-4.632014	-0.629840	-1.435509
3	16	0	3.341804	1.069470	0.428023
4	6	0	3.175302	2.712308	-0.202924
5	1	0	4.024964	3.376445	-0.060873
6	6	0	2.069565	3.086780	-0.867561
7	1	0	1.953172	4.074769	-1.307025
8	16	0	0.748733	1.939300	-1.131218
9	16	0	2.495058	-2.063623	0.087027
10	6	0	1.590659	-3.231736	-0.892289
11	1	0	2.009886	-4.232798	-0.963689
12	6	0	0.472069	-2.867923	-1.540096
13	1	0	-0.085299	-3.550824	-2.177177
14	16	0	-0.131373	-1.204201	-1.443028

15	6	0	-0.525748	-1.639897	2.389708
16	16	0	0.118092	0.068506	2.085479
17	1	0	-1.230899	-1.585711	3.224662
18	1	0	0.308546	-2.296618	2.643656
19	1	0	-1.025128	-2.021305	1.497499
20	6	0	-2.813537	2.316065	0.213213
21	6	0	-3.965815	2.968810	0.047513
22	1	0	-1.853640	2.700696	-0.123453
23	1	0	-3.973428	3.934051	-0.445278
24	8	0	-2.756546	1.081378	0.800181
25	1	0	-1.824338	0.806819	0.952466
26	1	0	-4.226641	0.052864	0.851026
27	1	0	-3.622414	-1.027897	-1.279588
28	1	0	-4.524225	0.450176	-1.590103
29	1	0	-5.071748	-1.085997	-2.323544
30	6	0	-5.523412	-0.906218	-0.236830
31	8	0	-6.569487	-1.515897	-0.300585
32	8	0	-5.088836	-0.416955	0.942861
33	1	0	-4.908862	2.558227	0.396161

Scheme 2

Reactant

1	6	0	3.903211	-1.247407	0.945327
2	16	0	2.366786	-0.843833	1.855829
3	74	0	0.635834	0.068116	0.394474
4	16	0	-0.546581	1.685452	-1.114567
5	6	0	0.678465	2.701200	-1.808263
6	6	0	1.946968	2.698887	-1.349573
7	16	0	2.437878	1.648248	-0.039491
8	6	0	-0.111250	0.134401	2.349028

9	8	0	-3.660962	-1.810566	2.284076
10	6	0	-0.987702	0.677385	1.570249
11	16	0	1.679326	-1.148276	-1.581640
12	6	0	0.599661	-2.426462	-2.050139
13	6	0	-0.567359	-2.668642	-1.420777
14	16	0	-1.050700	-1.714831	-0.038515
15	8	0	-4.200257	0.590012	0.609862
16	6	0	-4.217647	0.630262	-0.611012
17	6	0	-5.009219	1.647654	-1.398659
18	8	0	-3.529919	-0.183068	-1.409882
19	1	0	3.698469	-1.976251	0.155314
20	1	0	4.617058	-1.655322	1.669130
21	1	0	4.327651	-0.350375	0.484888
22	1	0	0.357207	3.391029	-2.586946
23	1	0	2.707685	3.371476	-1.739693
24	1	0	-5.467486	1.188212	-2.279170
25	1	0	-5.769205	2.102621	-0.761242
26	1	0	-4.318562	2.423204	-1.749568
27	1	0	-2.865338	-0.704402	-0.882290
28	1	0	0.909720	-3.031712	-2.901095
29	1	0	-1.252650	-3.452674	-1.733751
30	1	0	0.135073	-0.103670	3.375806
31	1	0	-1.953063	1.159832	1.510048
32	1	0	-3.842611	-0.993335	1.786263
33	1	0	-2.804642	-2.092101	1.925829

Transition Structure

1	6	0	-0.108203	-1.942341	3.381087
2	16	0	0.540432	-2.078390	1.662764
3	74	0	-0.374235	-0.305485	0.192160
4	6	0	1.020579	-1.260256	-1.172068

5	6	0	0.259324	-0.237927	-1.741047
6	16	0	-1.370325	0.988694	2.128009
7	6	0	-0.021686	1.739687	2.939534
8	6	0	1.216267	1.812930	2.401505
9	16	0	1.535870	1.229587	0.786522
10	16	0	-1.851272	-2.222540	-0.248393
11	6	0	-2.967727	-1.655609	-1.466355
12	6	0	-3.145687	-0.334274	-1.720242
13	16	0	-2.318732	0.894713	-0.809733
14	8	0	1.378013	2.056494	-2.534618
15	6	0	2.665935	1.979182	-2.677056
16	8	0	3.376698	0.993882	-2.416864
17	6	0	3.292501	3.258248	-3.188927
18	1	0	0.095075	-0.960140	3.809955
19	1	0	0.395937	-2.713227	3.975604
20	1	0	-1.185507	-2.125981	3.401737
21	1	0	-3.905315	0.003540	-2.424716
22	1	0	-3.566681	-2.410045	-1.975409
23	1	0	3.323348	3.983077	-2.367053
24	1	0	4.309887	3.069008	-3.536855
25	1	0	2.684481	3.691372	-3.988073
26	1	0	0.939733	1.155924	-2.100474
27	1	0	-0.235179	2.214877	3.896699
28	1	0	2.034257	2.316182	2.912903
29	1	0	1.053822	-2.316155	-1.420031
30	1	0	-0.361649	-0.314488	-2.635798
31	8	0	2.592086	-0.970063	-0.927344
32	1	0	2.866628	-0.209253	-1.563505
33	1	0	2.626801	-0.572166	-0.019497

Product

1	6	0	2.231439	-2.473163	1.851740
2	16	0	1.219574	-0.956765	2.068874
3	74	0	0.569503	0.253288	-0.004833
4	16	0	1.057332	1.660483	-1.961361
5	6	0	2.162864	2.907568	-1.500281
6	6	0	2.709362	2.933969	-0.260181
7	16	0	2.325912	1.701343	0.898518
8	6	0	-0.688217	1.061510	1.785507
9	8	0	-1.562170	0.123647	2.373581
10	6	0	-1.101412	1.693764	0.595885
11	16	0	1.482982	-1.734487	-1.110258
12	6	0	0.416603	-2.142828	-2.424468
13	6	0	-0.808797	-1.587588	-2.520230
14	16	0	-1.344436	-0.401151	-1.351884
15	8	0	-3.773151	-0.971023	1.251668
16	6	0	-4.523637	-0.187902	0.472272
17	6	0	-5.413990	-1.006905	-0.436801
18	8	0	-4.487013	1.028651	0.469734
19	1	0	1.720179	-3.217421	1.235334
20	1	0	2.418168	-2.878792	2.851958
21	1	0	3.190767	-2.233480	1.383470
22	1	0	2.427216	3.637779	-2.263399
23	1	0	3.435652	3.687203	0.038732
24	1	0	-4.802012	-1.371535	-1.269963
25	1	0	-5.820063	-1.878503	0.085252
26	1	0	-6.219586	-0.384294	-0.830998
27	1	0	-2.100863	1.508771	0.213985
28	1	0	0.766707	-2.899953	-3.123361
29	1	0	-1.504976	-1.844353	-3.315958
30	1	0	-0.047080	1.559625	2.510523

31	1	0	-0.710216	2.684302	0.380497
32	1	0	-3.045794	-0.433294	1.673733
33	1	0	-1.002210	-0.655486	2.590117

Scheme 3

React (Eta acetylene complex)

1	6	0	-5.439617	0.982994	-0.589619
2	6	0	-4.472649	-0.058697	-1.080075
3	8	0	-4.101038	-0.188705	-2.229551
4	8	0	-4.012291	-0.820353	-0.062792
5	6	0	-0.642452	-1.990384	-0.578301
6	6	0	-1.033105	-1.016816	-1.338249
7	74	0	0.530750	-0.322612	-0.113169
8	16	0	1.576808	1.349653	1.479267
9	6	0	0.658718	1.318258	2.947838
10	6	0	-0.433781	0.538923	3.102873
11	16	0	-1.009661	-0.467115	1.803462
12	16	0	1.884770	-2.209792	0.857625
13	6	0	3.514633	-1.977383	0.308966
14	6	0	3.833267	-1.055691	-0.623331
15	16	0	2.609874	-0.031088	-1.340414
16	16	0	-0.081044	1.541368	-1.611804
17	6	0	1.007393	2.997579	-1.383408
18	8	0	-2.709351	2.399760	0.398857
19	1	0	4.265120	-2.651193	0.719345
20	1	0	4.847044	-0.931978	-0.997512
21	1	0	-0.996480	0.499791	4.032769
22	1	0	1.006634	1.964953	3.752088
23	1	0	0.672709	3.770061	-2.083929
24	1	0	0.951776	3.365279	-0.354559

25	1	0	2.046538	2.736702	-1.603569
26	1	0	-3.240329	-1.323075	-0.392971
27	1	0	-0.757544	-3.038061	-0.333346
28	1	0	-1.701156	-0.730284	-2.141557
29	1	0	-6.074917	0.593208	0.211082
30	1	0	-6.044017	1.351857	-1.420585
31	1	0	-4.821612	1.795060	-0.182926
32	1	0	-2.057747	2.274808	-0.318982
33	1	0	-2.436477	1.709441	1.026683

Int1 ($C_2H_3^+$ intermediate)

1	6	0	-5.449343	-0.856818	0.272225
2	6	0	-4.212118	-1.004969	-0.626936
3	8	0	-3.741032	0.080672	-1.101613
4	8	0	-3.774265	-2.165015	-0.831723
5	6	0	-0.962366	-1.624542	-1.402023
6	6	0	-0.896667	-0.257205	-1.475285
7	74	0	0.598875	0.035713	-0.174254
8	16	0	1.758697	1.594526	1.362409
9	6	0	0.810213	1.553644	2.816979
10	6	0	-0.435175	1.030884	2.856301
11	16	0	-1.186186	0.377423	1.427304
12	16	0	0.985335	-1.936075	1.321820
13	6	0	2.321487	-2.809304	0.657973
14	6	0	3.006083	-2.368681	-0.424445
15	16	0	2.543864	-0.907092	-1.242780
16	16	0	1.060729	1.751749	-1.871882
17	6	0	2.508732	2.791678	-1.451997
18	8	0	-4.169235	2.313285	0.456582
19	1	0	2.584829	-3.740763	1.155950
20	1	0	3.866122	-2.900558	-0.824323

21	1	0	-1.035343	1.037547	3.762501
22	1	0	1.264890	2.011081	3.693431
23	1	0	2.711811	3.421160	-2.324069
24	1	0	2.303034	3.420412	-0.580406
25	1	0	3.389109	2.174778	-1.245843
26	1	0	-1.987697	-2.049828	-1.268248
27	1	0	-0.109858	-2.295074	-1.470591
28	1	0	-1.829521	0.291824	-1.658056
29	1	0	-5.599330	-1.752662	0.882132
30	1	0	-6.340156	-0.711558	-0.354297
31	1	0	-5.349902	0.032044	0.902850
32	1	0	-4.111574	1.569838	-0.195841
33	1	0	-3.340957	2.200860	0.946977

Int1 (conformationally changed from the previous structure)

1	6	0	5.331941	-0.001507	-0.949212
2	6	0	4.289268	-0.931648	-0.302289
3	8	0	3.573256	-0.376979	0.611876
4	8	0	4.217943	-2.109990	-0.690205
5	6	0	0.959435	-1.286974	-0.319699
6	6	0	1.078239	-2.408980	-1.051361
7	74	0	-0.688844	-0.140239	0.194384
8	16	0	0.004884	0.245366	2.432140
9	6	0	0.755819	1.922427	2.548511
10	16	0	-2.017603	-1.134085	-1.591739
11	6	0	-3.033628	-2.364674	-0.909767
12	6	0	-3.076832	-2.575724	0.422812
13	16	0	-2.125219	-1.616541	1.514296
14	16	0	-1.834257	2.006368	0.208671
15	6	0	-1.288489	2.986789	-1.100970
16	6	0	-0.300955	2.543937	-1.916842

17	16	0	0.466373	1.016365	-1.633233
18	8	0	3.222581	2.283115	0.455891
19	1	0	-3.737507	-3.312368	0.873546
20	1	0	-3.658598	-2.918877	-1.606232
21	1	0	0.047890	3.122475	-2.769068
22	1	0	-1.773835	3.950758	-1.232523
23	1	0	1.598278	2.039376	1.856915
24	1	0	1.104288	2.029621	3.580595
25	1	0	-0.017184	2.668095	2.337442
26	1	0	2.026658	-2.946067	-1.012832
27	1	0	0.278840	-2.791222	-1.684168
28	1	0	1.883113	-0.932846	0.195750
29	1	0	3.445294	1.315219	0.591757
30	1	0	2.597686	2.235054	-0.284511
31	1	0	4.925190	1.004902	-1.088763
32	1	0	6.200142	0.096560	-0.282645
33	1	0	5.677680	-0.412095	-1.903005

Int2 (vinylidene complex)

1	6	0	5.422155	0.526778	-1.121283
2	6	0	4.397341	-0.282586	-0.352185
3	8	0	3.474237	0.515134	0.206273
4	8	0	4.407477	-1.493013	-0.261748
5	6	0	0.601513	-2.074394	-0.916252
6	6	0	1.409526	-3.046072	-1.293011
7	74	0	-0.541430	-0.646017	-0.323098
8	16	0	0.975398	-0.710884	1.634248
9	6	0	0.625675	0.613873	2.865379
10	16	0	-2.342301	-1.769133	-1.519957
11	6	0	-3.759715	-1.771350	-0.513782
12	6	0	-3.701951	-1.365473	0.773718

13	16	0	-2.200526	-0.849496	1.480845
14	16	0	-0.891749	1.806734	0.026376
15	6	0	-0.363931	2.627786	-1.419174
16	6	0	0.169683	1.960313	-2.460250
17	16	0	0.343399	0.224804	-2.425134
18	8	0	2.283145	3.137152	0.994953
19	1	0	-4.573014	-1.378353	1.425377
20	1	0	-4.674741	-2.154692	-0.960518
21	1	0	0.494133	2.463256	-3.368706
22	1	0	-0.503039	3.706963	-1.434603
23	1	0	1.020430	1.569782	2.510196
24	1	0	1.126329	0.333664	3.798104
25	1	0	-0.447074	0.699946	3.051610
26	1	0	2.270859	-3.317365	-0.682029
27	1	0	1.267356	-3.579687	-2.233736
28	1	0	2.738873	-0.021185	0.635823
29	1	0	2.804037	2.379109	0.677668
30	1	0	1.386345	2.918848	0.688421
31	1	0	4.939086	0.991381	-1.988118
32	1	0	5.821287	1.333881	-0.498291
33	1	0	6.229535	-0.125603	-1.457938

Int2 (conformationally changed from the previous structure)

1	74	0	0.760449	0.303796	0.146077
2	16	0	2.215488	0.067362	2.074181
3	6	0	3.951499	-0.294175	1.596209
4	1	0	4.399763	0.553576	1.070037
5	1	0	4.515134	-0.478248	2.517380
6	1	0	3.992864	-1.173522	0.946209
7	16	0	2.503712	1.883397	-0.552230
8	6	0	1.886769	2.827627	-1.875816

9	6	0	0.585758	2.757507	-2.235063
10	16	0	-0.519691	1.705690	-1.405946
11	16	0	-0.871511	-1.527495	-0.085772
12	6	0	-0.131972	-2.856836	-0.947753
13	6	0	1.132646	-2.767398	-1.398528
14	16	0	2.119976	-1.353099	-1.141083
15	1	0	-0.757367	-3.727801	-1.131175
16	1	0	1.592321	-3.568913	-1.974229
17	1	0	2.589236	3.495048	-2.370641
18	1	0	0.170393	3.384480	-3.021553
19	6	0	-0.571740	0.734131	1.466223
20	6	0	-1.502872	1.069821	2.339520
21	1	0	-1.270681	1.161478	3.401929
22	1	0	-2.531138	1.263095	2.031286
23	1	0	-4.068728	-0.970432	1.542792
24	8	0	-4.459845	-0.229322	0.981825
25	6	0	-4.846220	-0.766335	-0.177382
26	8	0	-4.872568	-1.971041	-0.395369
27	6	0	-5.219557	0.277574	-1.201347
28	1	0	-4.297470	0.734109	-1.580679
29	1	0	-5.819599	1.071668	-0.747021
30	1	0	-5.758093	-0.187669	-2.028540
31	1	0	-3.823107	-2.773315	1.123191
32	8	0	-3.370292	-2.460449	1.934685
33	1	0	-2.458528	-2.283149	1.619410

Int3 (Vinylidene with water bound to carbon)

1	74	0	0.623361	0.021233	0.007267
2	16	0	1.605324	-0.029511	2.231580
3	6	0	3.436656	-0.112241	2.172709
4	1	0	3.843419	0.763397	1.656371

5	1	0	3.812882	-0.136849	3.202124
6	1	0	3.762420	-1.014489	1.644238
7	16	0	2.425945	1.543707	-0.577826
8	6	0	1.731023	2.913408	-1.416402
9	6	0	0.401566	3.025936	-1.591737
10	16	0	-0.679783	1.775029	-1.008872
11	16	0	-0.868855	-1.561360	-1.175938
12	6	0	0.085976	-2.952377	-1.701957
13	6	0	1.410603	-2.974294	-1.487942
14	16	0	2.248528	-1.686197	-0.640579
15	1	0	-0.444053	-3.735994	-2.237991
16	1	0	2.032551	-3.796271	-1.839248
17	1	0	2.433120	3.660813	-1.781610
18	1	0	-0.054680	3.871497	-2.102514
19	6	0	-1.017981	0.044547	1.406962
20	6	0	-1.636368	0.942336	2.215553
21	1	0	-1.240518	1.950309	2.262552
22	1	0	-2.340583	0.639434	2.990768
23	1	0	-3.011926	1.177604	0.901702
24	8	0	-3.822008	1.225271	0.288744
25	6	0	-4.398530	0.051184	0.171479
26	8	0	-4.123608	-0.950955	0.841211
27	6	0	-5.436540	0.012212	-0.916977
28	1	0	-4.912817	-0.125174	-1.870472
29	1	0	-5.986486	0.955221	-0.970025
30	1	0	-6.114958	-0.828381	-0.761579
31	1	0	-2.685014	-1.177524	1.457653
32	8	0	-1.679472	-1.316482	1.595441
33	1	0	-1.378385	-1.808491	0.743095

Int4 (carbene complex)

1	6	0	3.549282	-0.219711	2.067854
2	16	0	1.718491	-0.285202	2.200758
3	74	0	0.603300	-0.007813	0.053541
4	16	0	2.416852	-1.313890	-1.014945
5	6	0	1.731664	-2.804857	-1.610206
6	6	0	0.421831	-3.090360	-1.503043
7	16	0	-0.684950	-1.924349	-0.806584
8	16	0	2.172929	1.853539	-0.189510
9	6	0	1.517037	2.964525	-1.365275
10	6	0	0.274625	2.799745	-1.863252
11	16	0	-0.728342	1.464808	-1.354339
12	6	0	-0.954403	0.001258	1.343755
13	6	0	-1.410035	1.257134	2.040423
14	8	0	-1.694858	-1.043089	1.812072
15	8	0	-4.039182	-0.938499	0.256819
16	6	0	-4.690585	0.227374	0.124442
17	8	0	-4.695140	1.108545	0.961935
18	6	0	-5.385525	0.312891	-1.214464
19	1	0	-0.167005	3.503967	-2.565491
20	1	0	2.152006	3.800272	-1.652263
21	1	0	2.426317	-3.484038	-2.101696
22	1	0	-0.016074	-4.001423	-1.904492
23	1	0	3.963051	-0.443006	3.057469
24	1	0	3.904536	-0.954225	1.338374
25	1	0	3.882486	0.775272	1.758038
26	1	0	-0.844859	2.127437	1.709066
27	1	0	-2.480356	1.423336	1.855579
28	1	0	-1.263192	1.129798	3.122667
29	1	0	-5.861765	-0.637742	-1.471734
30	1	0	-6.118859	1.121100	-1.201770

31	1	0	-4.629096	0.522613	-1.979642
32	1	0	-3.421291	-0.890954	1.024651
33	1	0	-1.379697	-1.836411	1.315139

Int4 (conformationally changed from the previous structure)

1	6	0	-0.711015	2.709386	1.271570
2	6	0	-0.772053	1.209902	1.110490
3	8	0	-1.805590	0.740767	1.870752
4	74	0	0.524528	0.201748	-0.023488
5	16	0	0.807119	-0.917932	2.149453
6	6	0	1.747253	-2.492372	2.096985
7	16	0	0.944713	1.765919	-1.875012
8	6	0	2.433491	2.618413	-1.581429
9	6	0	3.181516	2.360395	-0.486327
10	16	0	2.687419	1.179998	0.690471
11	16	0	-1.413158	-0.241545	-1.412842
12	6	0	-0.971610	-1.532555	-2.516722
13	6	0	0.159544	-2.241354	-2.334377
14	16	0	1.239981	-1.942680	-0.993856
15	8	0	-3.226844	-1.651936	1.587949
16	6	0	-4.000016	-1.153475	0.788635
17	6	0	-4.760408	-1.935658	-0.248248
18	8	0	-4.236844	0.166351	0.705647
19	1	0	-0.569954	2.950940	2.335415
20	1	0	0.101459	3.147975	0.694506
21	1	0	-1.663147	3.157608	0.946928
22	1	0	-1.779679	-0.244073	1.896203
23	1	0	2.757275	-2.324734	1.711562
24	1	0	1.817212	-2.865436	3.124481
25	1	0	1.248525	-3.231222	1.463862
26	1	0	4.123302	2.873309	-0.297334

27	1	0	2.730545	3.351446	-2.329351
28	1	0	-1.653185	-1.731757	-3.341313
29	1	0	0.438710	-3.056840	-2.999524
30	1	0	-4.180718	-1.892653	-1.177354
31	1	0	-5.744671	-1.498687	-0.439294
32	1	0	-4.851464	-2.977506	0.064549
33	1	0	-3.532422	0.614601	1.235109

Int5 (Hydride complex)

1	6	0	-0.163796	2.571625	2.054567
2	6	0	-0.845236	1.336855	1.447192
3	8	0	-1.955476	1.033568	1.871781
4	74	0	0.435224	0.365142	-0.078181
5	16	0	0.373280	-0.967564	1.997371
6	6	0	1.620326	-2.311390	2.010937
7	16	0	1.215430	2.155691	-1.586128
8	6	0	2.916932	2.378978	-1.348193
9	6	0	3.581854	1.713174	-0.376926
10	16	0	2.741192	0.641147	0.698627
11	16	0	-1.469579	-0.195101	-1.476242
12	6	0	-1.142970	-1.679786	-2.330908
13	6	0	0.053177	-2.291965	-2.220146
14	16	0	1.328652	-1.667932	-1.220502
15	8	0	-3.132051	-1.349831	1.366115
16	6	0	-4.165545	-1.324980	0.523348
17	6	0	-4.380376	-2.693928	-0.090633
18	8	0	-4.834995	-0.345156	0.255818
19	1	0	0.608864	2.221960	2.748866
20	1	0	0.327811	3.181395	1.292279
21	1	0	-0.912849	3.158952	2.599184
22	1	0	-2.800127	-0.426240	1.550915

23	1	0	2.636377	-1.914771	1.933632
24	1	0	1.512226	-2.828988	2.970214
25	1	0	1.451031	-3.005810	1.183811
26	1	0	4.650053	1.838381	-0.213691
27	1	0	3.408868	3.102192	-1.995660
28	1	0	-1.921875	-2.035246	-3.001803
29	1	0	0.287666	-3.194083	-2.782552
30	1	0	-3.569053	-2.884859	-0.802196
31	1	0	-5.340134	-2.728522	-0.610843
32	1	0	-4.332840	-3.475649	0.674507
33	1	0	-0.702243	1.610766	-0.336370

Int5 (conformationally changed from the previous structure)

1	6	0	-5.535117	1.228668	-0.069905
2	74	0	0.466918	-0.017249	-0.056947
3	16	0	1.502418	-1.320287	-1.910524
4	6	0	0.218887	-2.157134	-2.728587
5	6	0	-1.078106	-1.974595	-2.406189
6	16	0	-1.539314	-0.852216	-1.158250
7	1	0	0.518191	-2.810044	-3.546718
8	1	0	-1.887164	-2.454158	-2.952743
9	16	0	1.073489	-1.849175	1.493108
10	6	0	2.619569	-2.697353	0.985619
11	1	0	2.767204	-3.526111	1.686777
12	1	0	3.482319	-2.028269	1.041506
13	1	0	2.535972	-3.076037	-0.036817
14	16	0	2.799401	0.592840	0.393829
15	6	0	3.141890	2.106635	-0.386895
16	6	0	2.150827	2.833767	-0.948744
17	16	0	0.508351	2.272268	-0.931518
18	1	0	2.327734	3.812892	-1.389470

19	1	0	4.176147	2.443946	-0.376858
20	1	0	-0.939118	0.910338	0.211368
21	6	0	-0.696409	0.119872	1.828735
22	6	0	-0.117352	1.201866	2.754083
23	1	0	-0.159442	2.174104	2.252015
24	1	0	0.930118	0.985465	2.982391
25	1	0	-0.714634	1.229575	3.672662
26	8	0	-1.676198	-0.508560	2.209865
27	1	0	-3.240362	-0.427512	1.476224
28	8	0	-4.135125	-0.293403	1.061743
29	6	0	-4.295716	1.003369	0.772374
30	8	0	-3.540764	1.893274	1.112791
31	1	0	-5.787790	2.290505	-0.079724
32	1	0	-6.376919	0.637070	0.303498
33	1	0	-5.327842	0.898737	-1.094497

Prod (Acetaldehyde)

1	6	0	-5.181863	0.458203	0.274016
2	74	0	0.817672	-0.334108	-0.703087
3	16	0	0.813792	-1.646280	-2.677901
4	6	0	-0.853506	-1.712388	-3.259237
5	6	0	-1.823058	-1.002269	-2.657838
6	16	0	-1.452388	0.032577	-1.272845
7	1	0	-2.849859	-0.992116	-3.017387
8	1	0	-1.037593	-2.324636	-4.139565
9	16	0	3.107434	0.071558	-1.123280
10	6	0	3.493946	1.654315	-0.424457
11	6	0	2.537351	2.414057	0.134086
12	16	0	0.852249	1.861328	0.192332
13	1	0	2.736980	3.407471	0.530755
14	1	0	4.526379	1.986425	-0.511816

15	16	0	0.767699	-1.835331	1.077784
16	6	0	2.172888	-1.347419	2.177404
17	1	0	2.237485	-0.261348	2.261828
18	1	0	1.997732	-1.791057	3.163030
19	1	0	3.108158	-1.725253	1.758042
20	1	0	-1.621074	1.479499	2.345469
21	6	0	-1.381804	1.194786	3.382846
22	8	0	-2.132636	0.468039	4.019062
23	6	0	-0.110979	1.758904	3.943395
24	1	0	0.719919	1.483089	3.283134
25	1	0	0.059169	1.404674	4.963194
26	1	0	-0.164873	2.855688	3.924481
27	1	0	-5.848827	-0.393720	0.433408
28	1	0	-5.739771	1.328732	-0.076539
29	1	0	-4.444912	0.179104	-0.488624
30	6	0	-4.423445	0.807991	1.532601
31	8	0	-4.112566	1.941153	1.853111
32	8	0	-4.093203	-0.284206	2.237163
33	1	0	-3.477167	-0.011172	2.970010