Electronic Supplementary Information for Dalton Transactions

Paper Ref.: B919779F

Supporting Information

for

On the mechanism of carbonyl hydrogenation catalyzed by iron catalyst

Honghong Zhang, Dezhan Chen*, Yuhua Zhang, Guiqiu Zhang, Jianbiao Liu

Cartesian coordinates of all relevant complexes optimized at B3LYP/BSI level.

Cat (Figure 2)

Atom	X	Y	Z
C	-0.347264	3.186464	-0.750341
C	1.004506	3.002798	-1.456930
C	1.744945	1.739190	-0.973895
C	0.796269	0.568477	-0.846596
C	-0.610198	0.697032	-0.895090
C	-1.301498	2.023116	-1.069176
C	1.135636	-0.844037	-0.737976
C	-0.112381	-1.547439	-0.807789
C	-1.205543	-0.632537	-0.829008
H	-0.806988	4.132748	-1.054858
H	-0.190622	3.241139	0.334777
H	1.641211	3.880222	-1.301810
H	0.830503	2.928325	-2.538838
H	2.243569	1.939369	-0.018612
H	2.541112	1.486586	-1.685880
H	-1.638995	2.106162	-2.113069

H	-2.203547	2.079946	-0.451463
Fe	-0.050751	-0.259637	0.936662
O	-0.305692	-2.885113	-0.866840
H	0.479894	-3.344470	-0.537409
H	-0.115372	-1.508649	1.742723
C	1.214126	0.216330	2.058890
C	-1.367360	0.270386	1.971346
O	2.062402	0.501756	2.788269
O	-2.248010	0.583339	2.648738
Si	2.827906	-1.628278	-0.690747
Si	-3.011899	-1.123779	-0.910080
H	2.661886	-3.046943	-0.262734
H	3.463717	-1.632360	-2.035984
H	3.729987	-0.935616	0.260164
H	-3.291003	-2.267134	-0.010911
H	-3.842148	0.040920	-0.508646
H	-3.384815	-1.499426	-2.301033

Int1a (Figure 2)

Atom	X	Y	Z
C	2.690265	-0.569002	-0.581649
C	2.555564	0.814754	-0.324609
C	1.470682	-1.040443	-1.216932
C	0.650054	0.115725	-1.419347
C	1.258809	1.268373	-0.820684
Fe	1.007389	-0.222304	0.701908
O	-0.500093	0.042221	-2.113437
H	-1.171337	0.682692	-1.784602
H	-0.464845	-0.394265	0.817023
C	1.088989	-1.690518	1.655665
C	0.822024	0.850793	2.077009
O	1.119920	-2.673338	2.263137
O	0.662587	1.578988	2.960183
C	-3.477944	1.561143	-0.440635

C	-4.181129	2.833456	-0.012041
H	-4.288306	2.871717	1.077036
H	-3.596599	3.688608	-0.350610
H	-5.186703	2.888162	-0.442742
O	-2.430741	1.653855	-1.083157
C	3.660723	1.642756	0.278769
C	3.948783	-1.351188	-0.279697
H	3.784577	-2.039430	0.557258
H	4.201347	-1.980441	-1.141698
C	5.126805	-0.408807	0.035241
C	4.711593	0.747622	0.957078
H	5.515432	0.010522	-0.902781
H	5.586226	1.349052	1.228138
H	4.141189	2.222552	-0.522982
H	4.298553	0.343833	1.890712
H	5.944584	-0.982898	0.484119
H	3.263119	2.377092	0.987387
Si	0.674731	3.049441	-0.912106
H	-0.196634	3.456087	0.217888
H	1.881626	3.919802	-0.889505
H	-0.042989	3.272801	-2.191109
Si	1.046531	-2.755522	-1.827337
H	1.292120	-2.878212	-3.290710
H	1.914141	-3.743466	-1.133592
H	-0.373635	-3.091037	-1.560893
C	-4.064963	0.242557	-0.076451
C	-5.302723	0.149126	0.584434
C	-3.367835	-0.937379	-0.393134
C	-5.833490	-1.094806	0.917546
H	-5.856733	1.045881	0.840235
C	-3.899670	-2.178291	-0.055083
H	-2.409946	-0.875474	-0.895651
C	-5.131977	-2.259913	0.599073
H	-6.790849	-1.155866	1.426156
H	-3.350521	-3.082346	-0.299602

H	-5.544345	-3.229869	0.861976

TS1a (Figure 2)

Atom	X	Y	Z
C	1.953852	-1.187611	-0.561230
C	2.455629	0.142847	-0.474596
C	0.670681	-1.149746	-1.227770
C	0.454460	0.217482	-1.641581
C	1.504691	1.049740	-1.082696
Fe	0.611905	0.035203	0.562701
O	-0.593167	0.614561	-2.311220
H	-1.151364	1.409491	-1.741623
H	-0.822735	0.769499	0.578986
C	0.021037	-1.243598	1.635399
C	1.145119	1.098300	1.871067
O	-0.345728	-2.097397	2.317861
O	1.523270	1.798200	2.705909
C	-1.919837	1.591511	0.255196
C	-1.886827	2.511353	1.475456
H	-1.910613	1.967674	2.421620
H	-0.997129	3.141626	1.435638
H	-2.770959	3.156648	1.425269
O	-1.658350	2.189938	-0.866984
C	3.817177	0.460362	0.084328
C	2.738858	-2.394658	-0.098210
H	2.292050	-2.819849	0.807890
H	2.672233	-3.179909	-0.860229
C	4.216821	-2.040162	0.158560
C	4.371876	-0.711052	0.912513
H	4.742841	-1.964258	-0.802713
H	5.426351	-0.527164	1.144105
H	4.489242	0.656318	-0.763809
H	3.841831	-0.767112	1.872416
H	4.696062	-2.853703	0.713337

H	3.799083	1.383041	0.674103
Si	1.688849	2.899415	-1.358192
H	1.305166	3.698344	-0.167314
H	3.126186	3.177018	-1.637303
H	0.882382	3.314301	-2.527062
Si	-0.469960	-2.557983	-1.709647
H	-0.287653	-2.894964	-3.147085
H	-0.106821	-3.755843	-0.905701
H	-1.886760	-2.211627	-1.464256
C	-3.020169	0.542814	0.245325
C	-3.331205	-0.224206	1.378141
C	-3.777262	0.369262	-0.920279
C	-4.375514	-1.145546	1.345106
H	-2.749608	-0.112542	2.288273
C	-4.825292	-0.551734	-0.952457
H	-3.544279	0.972621	-1.789998
C	-5.126746	-1.312025	0.177862
H	-4.603277	-1.734633	2.228830
H	-5.406819	-0.672918	-1.861902
H	-5.941677	-2.029798	0.152732

Int2a (Figure 2)

Atom	X	Y	Z
C	1.905235	-1.174099	-0.619526
C	2.436009	0.157282	-0.536555
C	0.603347	-1.109800	-1.218473
C	0.405788	0.269807	-1.703739
C	1.482999	1.079920	-1.089205
Fe	0.668235	0.045688	0.582638
O	-0.590224	0.681805	-2.340003
H	-1.434389	1.775340	-1.400425
H	-0.954647	0.813536	0.636124
C	0.237377	-1.267104	1.707134
C	1.274127	1.132446	1.857699

O	0.008805	-2.150455	2.411651
O	1.722686	1.829670	2.657688
C	-1.909573	1.464449	0.468636
C	-2.037430	2.319207	1.730002
H	-2.129310	1.699487	2.625176
H	-1.168418	2.974144	1.829026
H	-2.933923	2.940011	1.643390
O	-1.721272	2.306209	-0.610216
C	3.830557	0.437584	-0.044652
C	2.701924	-2.395345	-0.216130
H	2.300829	-2.829235	0.706653
H	2.577828	-3.167063	-0.984478
C	4.196952	-2.066406	-0.036867
C	4.411209	-0.755178	0.732971
H	4.670008	-1.978319	-1.024195
H	5.478765	-0.589025	0.911369
H	4.456103	0.634678	-0.927735
H	3.932572	-0.823126	1.718666
H	4.693754	-2.897754	0.474133
H	3.861576	1.353015	0.555712
Si	1.687660	2.930651	-1.335422
H	1.501898	3.684303	-0.068611
H	3.077639	3.193013	-1.807176
H	0.733848	3.414430	-2.356197
Si	-0.579644	-2.492079	-1.666782
H	-0.462333	-2.818852	-3.113251
H	-0.209624	-3.705548	-0.887722
H	-1.978425	-2.124122	-1.358709
C	-3.056193	0.472812	0.302129
C	-3.260397	-0.550444	1.238595
C	-3.944046	0.594712	-0.771626
C	-4.329465	-1.434102	1.104934
H	-2.578789	-0.663673	2.077669
C	-5.015488	-0.291382	-0.906808
H	-3.795083	1.390078	-1.493103

C	-5.211911	-1.306988	0.028369
H	-4.472445	-2.223061	1.837895
H	-5.695764	-0.185472	-1.747099
H	-6.044083	-1.996735	-0.079154

Int3a (Figure 2)

Atom	X	Y	Z
Fe	-0.337036	-0.036752	-0.132491
Si	-2.083484	3.148675	-0.124251
Si	-1.022252	-1.704048	2.938217
O	-1.035547	1.518159	2.508884
O	1.071960	0.815518	1.133949
O	0.969965	-2.632039	-0.565706
O	0.361422	1.082389	-2.753218
C	-1.557037	0.832510	1.586939
C	-1.957650	1.324427	0.260941
C	-2.425964	0.193260	-0.500062
C	-3.166271	0.191036	-1.820691
C	-3.869161	-1.156153	-2.078296
C	-2.976594	-2.351232	-1.714166
C	-2.650220	-2.352492	-0.212019
C	-2.187884	-0.997385	0.255197
C	-1.564843	-0.638165	1.503015
C	2.355761	1.462332	0.933399
C	3.265248	0.480108	0.217144
C	3.659576	-0.679984	0.901698
C	4.489366	-1.620408	0.296020
C	4.944657	-1.412588	-1.009152
C	4.564438	-0.260889	-1.697137
C	3.729532	0.680117	-1.087639
C	0.504601	-1.593766	-0.391776
C	0.133238	0.642466	-1.711552
H	0.524858	1.276810	1.830354
H	-2.482110	0.419071	-2.645641

H	-3.904382	1.001258	-1.815481
H	-4.787828	-1.206306	-1.478223
H	-4.178167	-1.211302	-3.127559
H	-2.044464	-2.305952	-2.292721
H	-3.470732	-3.291142	-1.982250
H	-3.558043	-2.606932	0.354739
H	-1.915580	-3.125737	0.032998
H	2.762980	1.609113	1.942994
H	3.304493	-0.843228	1.915927
H	4.784213	-2.512417	0.841099
H	5.594977	-2.142210	-1.482884
H	4.917435	-0.089274	-2.709964
H	3.448271	1.571977	-1.637625
H	-0.989047	-3.128206	2.505183
H	-1.974912	-1.589741	4.074423
H	0.330999	-1.322868	3.411432
H	-0.818111	3.866902	0.159504
H	-3.170510	3.778698	0.671507
H	-2.405455	3.322853	-1.567167
C	2.190864	2.830457	0.281735
H	3.161208	3.326864	0.180816
H	1.732303	2.758081	-0.707671
H	1.548499	3.460337	0.902573

INT4 (Figure 2)

Atom	X	Y	Z
C	-0.648389	3.116269	-0.688755
C	0.704088	3.070422	-1.413535
C	1.558936	1.873606	-0.956660
C	0.746296	0.603283	-0.857836
C	-0.696838	0.604893	-0.878448
C	-1.490418	1.874444	-1.023965
C	1.208515	-0.741743	-0.767135
C	0.020533	-1.626509	-0.849056

C	-1.168063	-0.741491	-0.820338
H	-1.201640	4.018549	-0.969422
H	-0.485145	3.168236	0.395680
H	1.261406	3.998426	-1.248956
H	0.526045	3.000067	-2.495066
H	2.020692	2.095183	0.012399
H	2.389944	1.712477	-1.652476
H	-1.824481	1.936449	-2.070477
H	-2.401406	1.834604	-0.418825
Fe	-0.026239	-0.339352	0.898131
O	0.017848	-2.855534	-0.657339
C	1.255926	0.191864	2.022652
C	-1.364782	0.191058	1.951540
O	2.102713	0.587676	2.696677
O	-2.246125	0.581841	2.582891
Si	2.945704	-1.440597	-0.701233
Si	-2.907435	-1.436104	-0.839907
H	3.113341	-2.342427	0.463505
H	3.245094	-2.187914	-1.949294
H	3.910657	-0.314706	-0.578737
H	-3.119291	-2.375712	0.287097
H	-3.876147	-0.313343	-0.717443
H	-3.162949	-2.141359	-2.122038

TS1b (Figure 4)

Atom	X	Y	Z
C	1.963181	-1.056673	-0.604607
C	2.430772	0.256571	-0.306386
C	0.734078	-0.943558	-1.358483
C	0.522308	0.463510	-1.602352
C	1.511057	1.226419	-0.862093
Fe	0.514991	-0.003852	0.557279
O	-0.485439	0.933128	-2.289946
H	-1.079580	1.651287	-1.680129

H	-0.920848	0.729104	0.551969
C	-0.177972	-1.410449	1.387686
C	0.918521	0.872768	2.041979
O	-0.616324	-2.342220	1.904152
O	1.201157	1.458131	2.994009
C	-1.923747	1.629033	0.316946
O	-1.659807	2.322951	-0.745208
C	3.736977	0.509590	0.398145
C	2.736187	-2.306487	-0.247090
H	2.230779	-2.855300	0.555789
H	2.744726	-2.982125	-1.110328
C	4.181861	-1.973652	0.171004
C	4.247617	-0.756726	1.105811
H	4.779347	-1.762938	-0.726187
H	5.275602	-0.594849	1.446816
H	4.469717	0.824448	-0.359117
H	3.642483	-0.947391	2.001849
H	4.634075	-2.849073	0.648878
H	3.653233	1.345043	1.101058
Si	1.661640	3.101150	-0.858007
H	1.111879	3.715528	0.375184
H	3.112752	3.435129	-0.919605
H	0.989752	3.658293	-2.052650
Si	-0.345397	-2.285120	-2.101249
H	-0.102838	-2.391024	-3.564437
H	0.018352	-3.583918	-1.474566
H	-1.779818	-2.010994	-1.859868
C	-3.113676	0.706050	0.338008
C	-3.594703	0.213537	1.558172
C	-3.762107	0.357130	-0.852468
C	-4.709498	-0.622036	1.589894
H	-3.096786	0.492321	2.484837
C	-4.877319	-0.479639	-0.819916
H	-3.390940	0.755226	-1.790481
C	-5.351637	-0.971943	0.398518

H	-5.080801	-0.995811	2.539728
H	-5.380171	-0.744600	-1.745587
H	-6.221956	-1.621527	0.421364
H	-1.774233	2.152298	1.275129

Int5 (Figure 6)

Atom	X	Y	Z
C	-0.707129	2.801755	-1.394272
C	0.649305	2.594994	-2.084241
C	1.532248	1.571223	-1.342606
C	0.736372	0.365571	-0.888923
C	-0.700638	0.331430	-0.910601
C	-1.522090	1.498311	-1.390933
C	1.215172	-0.926297	-0.486039
C	0.065678	-1.878340	-0.606882
C	-1.134776	-0.988433	-0.540202
H	-1.275742	3.586267	-1.904508
H	-0.550875	3.144116	-0.362909
H	1.187425	3.544965	-2.167755
H	0.472613	2.245106	-3.110105
H	2.027223	2.049274	-0.490657
H	2.339035	1.230015	-2.001608
H	-1.843912	1.272744	-2.418396
H	-2.439420	1.602533	-0.803142
Fe	-0.027791	-0.061327	1.017448
O	0.100139	-3.102946	-0.607577
C	1.227341	0.907879	1.851019
C	-1.380209	0.835353	1.773876
O	2.051213	1.542332	2.344377
O	-2.265342	1.419201	2.221386
Si	2.975349	-1.540348	-0.310109

Si	-2.866820	-1.692661	-0.455586
H	3.066710	-2.532235	0.787756
H	3.451458	-2.163290	-1.573496
H	3.864648	-0.389118	0.004918
H	-2.959594	-2.703250	0.625117
H	-3.828695	-0.593308	-0.168649
H	-3.252035	-2.320695	-1.747143
H	0.389442	-1.325785	2.029833
H	-0.420877	-1.340086	2.020162

TS2 (Figure 6)

Atom	X	Y	Z
C	-0.656594	3.187157	-0.560856
C	0.694745	3.171091	-1.290105
C	1.555575	1.957704	-0.888414
C	0.734743	0.689848	-0.822434
C	-0.691555	0.689104	-0.842701
C	-1.497646	1.956053	-0.935506
C	1.200722	-0.683698	-0.810466
C	0.021332	-1.532793	-0.900608
C	-1.160503	-0.685302	-0.862470
H	-1.211470	4.098123	-0.808524
H	-0.490806	3.201864	0.524575
H	1.250362	4.093427	-1.091118
H	0.512242	3.143418	-2.372741
H	2.046639	2.147069	0.072877
H	2.366379	1.815845	-1.612048
H	-1.843649	2.054617	-1.975156
H	-2.402595	1.892673	-0.323000
Fe	-0.022681	-0.367176	0.887338
O	0.017862	-2.811178	-0.652481
H	-0.034470	-1.948832	1.523138
C	1.285103	0.165548	1.993986
C	-1.384047	0.165828	1.925156
O	2.152712	0.498703	2.670181

O	-2.284385	0.494459	2.559534
Si	2.935229	-1.396281	-0.821594
Si	-2.893406	-1.394442	-0.955737
H	3.158860	-2.333645	0.303521
H	3.182751	-2.099941	-2.105832
H	3.903248	-0.271932	-0.702450
H	-3.159294	-2.361446	0.134511
H	-3.865979	-0.273169	-0.844883
H	-3.093315	-2.063558	-2.266609
H	-0.015472	-2.416946	0.704214

Int6a (Figure 7)

Atom	X	Y	Z
C	2.921244	0.489249	0.037309
C	2.399928	-0.511160	0.920901
C	1.969385	1.561918	-0.042281
C	0.981650	1.364296	1.049823
C	1.128798	-0.065435	1.437082
Fe	1.091506	-0.275268	-0.678854
O	0.113953	2.173933	1.411042
H	-1.498098	1.364511	1.207772
H	-3.266012	2.183220	-0.046638
C	1.676441	-0.288188	-2.370691
C	0.610670	-2.000485	-0.689839
O	2.092176	-0.283082	-3.443942
O	0.326436	-3.113751	-0.650284
C	-3.384125	1.308468	0.612762
C	-3.987214	1.784643	1.942868
H	-3.323098	2.509993	2.425650
H	-4.959999	2.261387	1.785309
H	-4.123514	0.933707	2.617081
O	-2.113983	0.699350	0.832826
C	3.187887	-1.736008	1.302400
C	4.299682	0.397539	-0.581391
H	4.230168	0.227993	-1.661005

H	4.798877	1.366524	-0.465604
C	5.148332	-0.709713	0.075435
C	4.341527	-1.993678	0.319213
H	5.533804	-0.347782	1.037949
H	4.991845	-2.779974	0.716594
H	3.597995	-1.567574	2.308766
H	3.939966	-2.365576	-0.632738
H	6.021750	-0.917391	-0.551535
H	2.538564	-2.613755	1.385852
Si	0.109892	-0.906579	2.776269
H	-0.765531	-1.977922	2.239409
H	1.055165	-1.548477	3.735260
H	-0.693631	0.097565	3.505243
Si	2.056045	3.167513	-1.000405
H	2.563690	4.273100	-0.145267
H	2.993374	2.995951	-2.143774
H	0.720228	3.535603	-1.527557
H	-0.268058	0.437153	-1.334872
H	-0.576408	0.169666	-0.638580
C	-4.289673	0.311853	-0.088662
C	-5.311614	0.766113	-0.931370
C	-4.151546	-1.065538	0.122588
C	-6.183333	-0.133249	-1.546509
H	-5.423135	1.833325	-1.111331
C	-5.019420	-1.967248	-0.496335
H	-3.356793	-1.423200	0.768512
C	-6.038922	-1.505159	-1.330879
H	-6.969144	0.236647	-2.199466
H	-4.898356	-3.033725	-0.325855
H	-6.712772	-2.207994	-1.812752

TS3a (Figure 7)

Atom	X	Y	Z
C	2.684176	0.779688	0.168087

C	2.697524	-0.630617	0.387534
C	1.532825	1.336029	0.838931
C	0.951477	0.272425	1.667426
C	1.564834	-0.983906	1.216994
Fe	0.943888	-0.111637	-0.631261
O	-0.009383	0.402277	2.479814
H	-1.295022	-0.185966	1.847281
H	-2.563517	1.528805	0.817650
C	0.903669	0.973242	-2.041861
C	0.915320	-1.610522	-1.593766
O	0.897576	1.697611	-2.937468
O	0.919121	-2.592516	-2.195170
C	-3.014748	0.571123	1.110896
O	-1.976233	-0.439184	1.134335
C	3.822878	-1.509715	-0.091062
C	3.792005	1.509240	-0.561162
H	3.440575	1.880752	-1.530016
H	4.066694	2.399868	0.016074
C	5.030829	0.612261	-0.755851
C	4.653851	-0.814238	-1.181742
H	5.592125	0.561069	0.186878
H	5.556618	-1.400473	-1.383907
H	4.469794	-1.725563	0.772282
H	4.080021	-0.781898	-2.117208
H	5.699680	1.069920	-1.492425
H	3.448017	-2.478107	-0.437226
Si	1.111610	-2.651337	1.932161
H	1.705793	-3.724191	1.089801
H	1.648088	-2.799261	3.312437
H	-0.359085	-2.830592	1.970037
Si	0.969615	3.112570	0.974295
H	1.370624	3.707489	2.277326
H	1.597609	3.911316	-0.112920
H	-0.505012	3.217141	0.842218
H	-0.661300	-0.027968	-0.677250

H	-1.108881	-0.260869	0.072969
C	-3.596010	0.706736	2.520392
H	-4.377334	1.472343	2.532308
H	-4.036808	-0.241324	2.842177
H	-2.814486	0.995915	3.229964
C	-4.052572	0.176789	0.080341
C	-4.679139	1.160338	-0.693652
C	-4.433916	-1.161542	-0.081648
C	-5.676197	0.817308	-1.608281
H	-4.383737	2.201180	-0.581885
C	-5.424835	-1.505999	-1.001266
H	-3.941108	-1.929014	0.506645
C	-6.050897	-0.518022	-1.764741
C	-6.152520	1.591331	-2.203312
C	-5.708198	-2.547798	-1.122387
C	-6.821949	-0.788023	-2.480609

Int7a (Figure 7)

Atom	X	Y	Z
C	2.912644	0.645250	0.173172
C	2.751696	-0.739905	0.418631
C	1.803575	1.352840	0.790917
C	1.030240	0.366975	1.481614
C	1.547713	-0.945586	1.213723
Fe	1.055065	-0.041521	-0.661394
O	-0.001311	0.698677	2.281248
H	-0.812175	0.169312	2.063720
H	-2.794778	1.530520	0.920327
C	0.953097	1.066470	-2.023164
C	0.808499	-1.492814	-1.625367
O	0.867353	1.814012	-2.898165
O	0.631652	-2.456087	-2.236135
C	-3.242106	0.561536	1.183488

O	-2.196774	-0.431682	1.264386
C	3.763868	-1.768061	-0.016146
C	4.108416	1.223845	-0.550062
H	3.821981	1.580822	-1.545948
H	4.470578	2.104398	-0.006529
C	5.240163	0.184884	-0.670840
C	4.712164	-1.197122	-1.084074
H	5.752563	0.093263	0.296489
H	5.545361	-1.890318	-1.241807
H	4.350548	-2.067486	0.865142
H	4.179372	-1.115940	-2.040524
H	5.987364	0.540458	-1.388385
H	3.272240	-2.676856	-0.378449
Si	0.936750	-2.555827	1.946385
H	1.283397	-3.678547	1.037482
H	1.590461	-2.805163	3.260418
H	-0.530766	-2.516773	2.143944
Si	1.453971	3.191232	0.867605
H	1.860854	3.747170	2.186055
H	2.248087	3.873269	-0.187716
H	0.015228	3.475412	0.651453
H	-0.435059	0.086566	-0.644560
H	-1.765904	-0.488358	0.390667
C	-3.849720	0.659448	2.581686
H	-4.642718	1.412024	2.597053
H	-4.279602	-0.302552	2.875753
H	-3.086102	0.942234	3.312864
C	-4.265520	0.192006	0.124092
C	-4.845352	1.184810	-0.674191
C	-4.668258	-1.139236	-0.047929
C	-5.817891	0.858303	-1.620852
H	-4.531282	2.219576	-0.556728
C	-5.635042	-1.467722	-0.998326
H	-4.209599	-1.914121	0.558874
C	-6.214822	-0.469725	-1.785188

H	-6.257331	1.639079	-2.235149
H	-5.935507	-2.503958	-1.125890
H	-6.966537	-0.726692	-2.525966

Int6b (Figure 7)

Atom	X	Y	Z
C	-2.842442	0.433244	-0.140915
C	-2.307244	-0.754352	-0.770676
C	-1.915734	1.524245	-0.360424
C	-0.919380	1.068226	-1.369589
C	-1.049980	-0.417995	-1.418517
Fe	-0.934816	-0.086501	0.706791
O	-0.035164	1.793752	-1.933140
H	1.546816	1.179414	-1.615949
H	3.387057	2.348371	-0.533120
C	-1.461095	0.327507	2.361234
C	-0.408833	-1.739546	1.134836
O	-1.847747	0.607678	3.436535
O	-0.086047	-2.843441	1.376476
C	3.500149	1.364207	-1.016673
O	2.221147	0.676276	-1.077446
C	-3.073318	-2.054270	-0.823503
C	-4.210962	0.470702	0.512858
C	-4.124888	0.566507	1.602631
C	-4.737969	1.372380	0.172615
C	-5.048829	-0.786778	0.160224
C	-4.209734	-2.083195	0.225681
H	-5.456693	-0.681506	-0.856326
H	-4.850471	-2.955478	0.044244
H	-3.509508	-2.144807	-1.831273
H	-3.784815	-2.198568	1.233647
H	-5.905360	-0.853160	0.843083
H	-2.407845	-2.917669	-0.700290
Si	-0.032690	-1.536300	-2.544020

H	0.857833	-2.445160	-1.781612
H	-0.977996	-2.387726	-3.318287
H	0.761164	-0.721392	-3.485682
Si	-2.084546	3.327749	0.134028
H	-2.658762	4.122430	-0.982198
H	-3.007697	3.424754	1.294682
H	-0.771969	3.896499	0.515508
H	0.485549	0.790115	1.121224
H	0.797530	0.409727	0.489531
H	3.875256	1.539468	-2.039430
C	4.506513	0.528865	-0.244222
C	4.284960	-0.840803	0.001561
C	5.701515	1.124182	0.216135
C	5.245037	-1.604361	0.693829
H	3.362178	-1.290282	-0.350105
C	6.663187	0.361855	0.904037
H	5.881135	2.184267	0.039595
C	6.437578	-1.007958	1.145733
H	5.062255	-2.660866	0.878501
H	7.579373	0.833074	1.253274
H	7.178499	-1.598419	1.679967

TS3b (Figure 7)

Atom	X	Y	Z
C	-2.616724	0.693540	-0.279585
C	-2.570689	-0.733016	-0.270812
C	-1.506163	1.182766	-1.062140
C	-0.893789	0.025224	-1.724974
C	-1.442247	-1.167410	-1.067440
Fe	-0.818217	0.013165	0.599544
O	0.046173	0.063738	-2.572087
H	1.348869	-0.370431	-1.899571
H	2.630458	1.510717	-1.122249

C	-0.795722	1.306844	1.821741
C	-0.689463	-1.316891	1.777912
O	-0.800335	2.162808	2.592552
O	-0.627197	-2.195081	2.520025
C	3.063031	0.521295	-1.317377
O	2.056411	-0.499231	-1.172455
C	-3.643814	-1.570533	0.373858
C	-3.742007	1.483007	0.354825
H	-3.391367	2.012400	1.247358
H	-4.064137	2.262404	-0.345548
C	-4.936662	0.577989	0.714140
C	-4.488096	-0.742793	1.356390
H	-5.506707	0.351451	-0.196947
H	-5.359275	-1.326664	1.671920
H	-4.294464	-1.954970	-0.425656
H	-3.901580	-0.533294	2.260722
H	-5.616017	1.119254	1.381074
H	-3.216036	-2.450314	0.864992
Si	-0.939611	-2.907163	-1.536111
H	-1.461836	-3.860782	-0.520764
H	-1.512027	-3.281830	-2.857791
H	0.535371	-3.035809	-1.601404
Si	-1.027718	2.936858	-1.493345
H	-1.495198	3.304260	-2.856856
H	-1.658706	3.869338	-0.520339
H	0.444069	3.119206	-1.434579
H	0.779441	0.182843	0.576309
H	1.214056	-0.177733	-0.134529
C	4.219261	0.253671	-0.385430
C	4.840099	1.310502	0.289373
C	4.709192	-1.047601	-0.211117
C	5.939573	1.076271	1.117623
H	4.461387	2.322672	0.167676
C	5.801089	-1.283414	0.623387

H	4.221932	-1.871561	-0.723062
C	6.421630	-0.222012	1.287286
H	6.411489	1.906067	1.635970
H	6.169530	-2.296884	0.755062
H	7.272679	-0.407527	1.936273
H	3.392910	0.506671	-2.364062

Int7b (Figure 7)

Atom	X	Y	Z
C	-2.750443	0.637638	-0.249147
C	-2.629571	-0.772955	-0.234537
C	-1.670535	1.182837	-1.054534
C	-0.960332	0.061483	-1.588748
C	-1.482473	-1.161099	-1.045665
Fe	-0.857330	0.067685	0.591557
O	0.024191	0.208046	-2.495545
H	0.825223	-0.318296	-2.243919
H	2.867211	1.208221	-1.636819
C	-0.658745	1.410030	1.709959
C	-0.580061	-1.180065	1.801658
O	-0.513012	2.306783	2.421446
O	-0.386291	-2.012683	2.576887
C	3.292925	0.197759	-1.581563
O	2.253739	-0.777924	-1.391404
C	-3.631173	-1.668917	0.446517
C	-3.885436	1.379087	0.421090
H	-3.524930	1.919373	1.303818
H	-4.272047	2.144281	-0.262471
C	-5.021476	0.416686	0.819630
C	-4.488580	-0.878961	1.449666
H	-5.608256	0.160154	-0.072840
H	-5.320435	-1.503740	1.792305
H	-4.284986	-2.102477	-0.324874
H	-3.885579	-0.637470	2.334778

H	-5.705311	0.924438	1.508127
H	-3.136302	-2.513765	0.936777
Si	-0.951026	-2.898445	-1.496925
H	-1.214847	-3.814166	-0.357565
H	-1.727132	-3.384906	-2.670572
H	0.491447	-2.929484	-1.832175
Si	-1.296001	2.963507	-1.499438
H	-1.792534	3.277442	-2.866169
H	-1.995626	3.854103	-0.536777
H	0.159765	3.237643	-1.444178
H	0.631841	0.149103	0.469959
H	1.850472	-0.613665	-0.516875
C	4.355447	0.132915	-0.507597
C	4.848982	1.303693	0.078280
C	4.871952	-1.104089	-0.096415
C	5.849613	1.244407	1.050877
H	4.446859	2.267159	-0.226127
C	5.865039	-1.165148	0.879978
H	4.481418	-2.015387	-0.539920
C	6.358842	0.009649	1.454018
H	6.222755	2.161097	1.498526
H	6.255926	-2.129225	1.193014
H	7.132904	-0.038967	2.214512
H	3.718273	-0.035607	-2.563815

Electronic Supplementary Information for Dalton Transactions