Electronic Supplementary Information for Dalton Transactions

Table ESI. Cartesian coordinates for optimized structures using DFT in neutral and acid conditions

Neutral conditions

Step1

Reactants

C	-0.241177	2.751603	0.022287
N	0.060232	1.454625	0.222638
C	1.359687	1.041754	0.225284
C	2.393543	1.954158	0.030632
C	2.088293	3.300421	-0.176441
C	0.749152	3.701815	-0.181688
Pt	-1.313045	0.021233	0.510584
N	0.360236	-1.080694	0.608656
C	0.369858	-2.412342	0.807970
C	1.557284	-3.128563	0.856091
C	2.768416	-2.449033	0.695655
C	2.751101	-1.068689	0.488730
C	1.530313	-0.400272	0.444398
C	4.041513	-3.247072	0.753156
O	5.124868	-2.475665	0.593961
C	6.394460	-3.168019	0.636656
C	3.143055	4.349076	-0.397303
O	4.378795	3.833894	-0.357792
C	5.454858	4.779392	-0.560789
O	-2.683057	-1.417525	0.812318
C	-3.923164	-0.978591	0.836402
C	-4.092049	0.450076	0.619232
C	-5.302854	1.159640	0.596576
C	-6.609251	0.708693	0.770538
C	-7.077351	-0.583481	1.015295
C	-6.318801	-1.748310	1.143755
C	-4.938768	-1.920146	1.064501
O	-2.984627	1.133243	0.424447
O	4.055478	-4.446019	0.925129
O	2.877075	5.515713	-0.585649
H	-0.601664	-2.878433	0.925675
H	1.555562	-4.200636	1.016129
H	3.682387	-0.532355	0.360196
H	3.426567	1.631161	0.033842
H	0.497355	4.743755	-0.342693
H	-1.296946	2.997004	0.031165
H	-4.562592	-2.931425	1.198780
H	-6.881761	-2.658946	1.334415
H	-8.153150	-0.695161	1.117299
H	-7.371251	1.481777	0.705490
H	-5.172030	2.223755	0.415557
H	6.441844	-3.910893	-0.162469
H	6.517765	-3.663038	1.602267
H	5.425737	5.550139	0.212353
H	5.361900	5.245656	-1.543980
H	6.369994	4.193064	-0.492492

H	7.148690	-2.395257	0.495584
O	0.330522	-0.268518	-2.490461
H	0.356238	-0.369775	-3.454569
H	-0.607408	-0.347122	-2.254515

Transition state

C	0.697295	1.216160	1.959894
N	0.589033	0.405713	0.885972
C	1.032274	-0.886421	0.951073
C	1.593511	-1.384349	2.125271
C	1.705602	-0.553322	3.240532
C	1.250723	0.766205	3.149012
Pt	-0.166948	0.986298	-0.853932
N	0.304260	-0.914439	-1.311594
C	0.045436	-1.516696	-2.490686
C	0.346094	-2.850173	-2.718859
C	0.930018	-3.600642	-1.693108
C	1.179741	-2.985723	-0.466578
C	0.855276	-1.640706	-0.292046
C	1.248731	-5.044937	-1.964633
O	1.791172	-5.646973	-0.899564
C	2.126433	-7.044434	-1.075568
C	2.299428	-1.012600	4.542426
O	2.696434	-2.290864	4.489051
C	3.282308	-2.812661	5.705217
O	-2.356852	1.605383	-1.798633
C	-2.749116	2.699125	-1.243881
C	-1.780956	3.403523	-0.391701
C	-1.953998	4.655443	0.213688
C	-3.052021	5.520081	0.240782
C	-4.311070	5.366799	-0.325988
C	-4.757225	4.281239	-1.089919
C	-4.079373	3.136089	-1.480764
O	-0.611662	2.828478	-0.179943
O	1.027628	-5.571295	-3.032871
O	2.394578	-0.289166	5.509160
H	-0.424425	-0.899858	-3.246461
H	0.131703	-3.315150	-3.674414
H	1.616754	-3.557821	0.341920
H	1.945843	-2.406517	2.179191
H	1.334320	1.426440	4.004848
H	0.329443	2.225240	1.818592
H	-4.634811	2.430919	-2.094637
H	-5.785435	4.344675	-1.439687
H	-5.023031	6.170535	-0.160759
H	-2.889961	6.440348	0.797470
H	-1.068772	4.992507	0.748132
H	2.860118	-7.153634	-1.877011
H	1.228529	-7.615035	-1.321813
H	2.558176	-2.759746	6.520941
H	4.171356	-2.235770	5.968592
H	3.540865	-3.846201	5.479791
H	2.541623	-7.362916	-0.120643
O	-0.154705	1.848044	-2.984582
H	0.269749	1.400372	-3.734714
H	-1.134124	1.846226	-3.102830

Products

C	-0.494844	2.177683	-0.222690
N	0.079109	0.962482	-0.160936
C	1.431502	0.854378	-0.012954
C	2.230990	1.990841	0.091648

C	1.637522	3.253595	0.034561
C	0.253230	3.344032	-0.130343
Pt	-0.913298	-0.806248	-0.173158
N	0.961040	-1.485711	-0.109551
C	1.306732	-2.785930	-0.208308
C	2.631597	-3.194646	-0.163012
C	3.636351	-2.234226	-0.021158
C	3.277863	-0.886910	0.047644
C	1.932407	-0.528633	-0.007113
C	5.064835	-2.702468	0.031891
O	5.921609	-1.682140	0.161929
C	7.321428	-2.047079	0.220168
C	2.425798	4.530092	0.140883
O	3.734831	4.298564	0.300432
C	4.568200	5.476708	0.412256
O	-3.953322	-1.957773	0.988383
C	-4.641053	-0.911508	0.589807
C	-3.993807	0.118105	-0.220099
C	-4.697078	1.182416	-0.841878
C	-6.013836	1.615939	-0.760989
C	-7.068838	1.117415	0.006615
C	-7.019057	0.005940	0.840006
C	-5.961793	-0.874428	1.066546
O	-2.713418	0.123195	-0.443385
O	5.370654	-3.872117	-0.037110
O	1.908570	5.623832	0.085185
H	0.488846	-3.482520	-0.343835
H	2.892123	-4.244149	-0.240396
H	4.048275	-0.131423	0.132704
H	3.303087	1.907831	0.215380
H	-0.221966	4.317088	-0.181500
H	-1.570551	2.174951	-0.346274
H	-6.175598	-1.716213	1.720506
H	-7.937105	-0.239233	1.368496
H	-8.016100	1.644964	-0.058598
H	-6.242612	2.485815	-1.372564
H	-4.049289	1.767797	-1.489882
H	7.610814	-2.562145	-0.698243
H	7.501101	-2.699693	1.077056
H	4.262252	6.069529	1.276844
H	4.483255	6.081046	-0.493341
H	5.582606	5.100788	0.536549
H	7.859718	-1.106493	0.326221
O	-1.806498	-2.600995	-0.115475
H	-1.445607	-3.109267	0.631445
H	-3.085320	-2.177108	0.458593

Step2 – Same side

Reactants

C	0.616089	2.024387	0.382566
N	-0.035815	0.853521	0.266409
C	-1.377859	0.847948	0.011935
C	-2.079869	2.037644	-0.162469
C	-1.400559	3.254246	-0.062359
C	-0.034886	3.242039	0.223822
Pt	0.816064	-0.988096	0.347266
N	-1.104558	-1.517071	0.179462
C	-1.558525	-2.783659	0.272894
C	-2.903149	-3.091172	0.127559
C	-3.813768	-2.059025	-0.113751
C	-3.345933	-0.745856	-0.176080

C	-1.984580	-0.491122	-0.017446
C	-5.265887	-2.416829	-0.277755
O	-6.026578	-1.336385	-0.491092
C	-7.441498	-1.592536	-0.659669
C	-2.080024	4.583240	-0.243832
O	-3.387485	4.446284	-0.502141
C	-4.117671	5.680900	-0.692512
O	3.592657	-2.233705	-1.086010
C	4.277815	-1.125442	-0.930298
C	3.844499	-0.142505	0.055631
C	4.604704	0.983287	0.445180
C	5.797882	1.515437	-0.038023
C	6.595968	1.088888	-1.098275
C	6.384842	-0.040608	-1.886934
C	5.384208	-1.002879	-1.791141
O	2.726288	-0.318629	0.714882
O	-5.666819	-3.557975	-0.218718
O	-1.489537	5.637469	-0.162443
H	-0.813575	-3.540252	0.485506
H	-3.251260	-4.115138	0.201865
H	-4.044732	0.064673	-0.337688
H	-3.141573	2.032377	-0.372589
H	0.506351	4.175935	0.322543
H	1.665671	1.962206	0.629371
H	5.457615	-1.840787	-2.479893
H	7.117990	-0.220792	-2.669437
H	7.472644	1.689027	-1.325016
H	6.135214	2.410398	0.479865
H	4.151373	1.519563	1.276635
H	-7.843390	-2.069429	0.236727
H	-7.602435	-2.242279	-1.522476
H	-3.701862	6.234222	-1.537243
H	-4.057429	6.293423	0.209615
H	-5.145226	5.380100	-0.891410
H	-7.893871	-0.614744	-0.817762
O	1.621200	-2.825694	0.348911
H	1.178365	-3.388814	-0.308192
H	2.843186	-2.437684	-0.391364
H	2.509916	0.583701	2.463241
O	2.347976	1.436134	2.905424
H	2.434228	1.262376	3.855107

Transition state

C	-0.258105	2.300284	-0.797628
N	0.181821	1.037634	-0.633449
C	1.458785	0.807364	-0.213626
C	2.325355	1.867426	0.049381
C	1.873225	3.177181	-0.117671
C	0.559733	3.392557	-0.547056
Pt	-0.917029	-0.592508	-1.039178
N	0.770185	-1.466427	-0.417265
C	0.959285	-2.799064	-0.300385
C	2.156709	-3.339219	0.139168
C	3.209102	-2.483405	0.478948
C	3.013550	-1.107231	0.369889
C	1.788473	-0.614421	-0.076720
C	4.498470	-3.092772	0.951597
O	5.415817	-2.161546	1.242647
C	6.691170	-2.665857	1.705267
C	2.739067	4.377969	0.144244
O	3.975131	4.031638	0.526250
C	4.876362	5.131967	0.793327

O	-3.709493	-2.049994	0.476190
C	-4.168727	-0.947764	1.040268
C	-3.789454	0.347710	0.468276
C	-4.254957	1.594980	0.965371
C	-5.088198	1.929256	2.023185
C	-5.729033	1.099845	2.950227
C	-5.671940	-0.287395	2.992403
C	-4.992231	-1.170511	2.150106
O	-3.024551	0.361542	-0.567847
O	4.658754	-4.289599	1.047662
O	2.337980	5.513792	0.016508
H	0.119826	-3.428816	-0.562211
H	2.282946	-4.412808	0.222284
H	3.814033	-0.428563	0.635530
H	3.340934	1.687506	0.378086
H	0.195861	4.404550	-0.683303
H	-1.282543	2.399435	-1.134254
H	-5.116108	-2.228374	2.368044
H	-6.243240	-0.764890	3.784935
H	-6.335042	1.590199	3.706781
H	-5.262250	2.995968	2.147100
H	-3.875541	2.428641	0.379099
H	7.141837	-3.299941	0.938878
H	6.553842	-3.243105	2.622065
H	4.483411	5.748104	1.604905
H	4.995208	5.743060	-0.103845
H	5.820059	4.668720	1.077402
H	7.300733	-1.782259	1.888302
O	-2.088052	-2.129203	-1.535921
H	-1.671068	-3.002866	-1.565433
H	-3.132058	-1.945533	-0.353953
H	-2.905823	0.512501	-2.438816
O	-2.099698	0.344824	-2.968767
H	-2.267725	-0.509397	-3.405922

Product

C	-0.931179	-2.731633	-0.444871
N	-0.942234	-1.386174	-0.450452
C	-2.070232	-0.711404	-0.082849
C	-3.220982	-1.399731	0.295254
C	-3.213987	-2.796635	0.298063
C	-2.049099	-3.469997	-0.077343
Pt	0.613464	-0.191427	-0.987092
N	-0.722532	1.211519	-0.529848
C	-0.465079	2.531590	-0.591355
C	-1.434520	3.468321	-0.254970
C	-2.694925	3.028329	0.155442
C	-2.948337	1.655773	0.224551
C	-1.943652	0.756129	-0.122197
C	-3.727963	4.062899	0.511191
O	-4.884285	3.505342	0.892985
C	-5.934552	4.433602	1.253486
C	-4.412549	-3.616109	0.691512
O	-5.457036	-2.847465	1.024755
C	-6.655391	-3.558335	1.416403
O	4.292708	1.645424	0.011013
C	5.207222	0.859439	0.562671
C	4.912325	-0.581675	0.539147
C	5.786544	-1.585030	1.045668
C	7.019892	-1.489019	1.665088
C	7.783535	-0.353039	1.981634
C	7.457056	0.968725	1.723333

C	6.321703	1.498920	1.093876
O	3.792416	-0.884322	0.026453
O	-3.510235	5.252410	0.449527
O	-4.403324	-4.827140	0.696111
H	0.539443	2.784773	-0.913429
H	-1.222127	4.530122	-0.306816
H	-3.920075	1.305904	0.548343
H	-4.117701	-0.867762	0.586065
H	-2.027066	-4.553850	-0.076907
H	0.002641	-3.195167	-0.741092
H	6.288938	2.580519	0.988634
H	8.183906	1.710453	2.046333
H	8.731173	-0.533433	2.481357
H	7.461284	-2.440811	1.953642
H	5.384691	-2.587318	0.916115
H	-6.178447	5.070680	0.400710
H	-5.612157	5.054368	2.092110
H	-6.451509	-4.180805	2.290192
H	-7.002109	-4.186831	0.593379
H	-7.385248	-2.784795	1.650427
H	-6.784515	3.812494	1.532082
O	2.035993	1.143646	-1.405585
H	2.227376	1.142516	-2.358593
H	3.531304	1.137907	-0.394411
H	2.770704	-1.549654	-0.824916
O	1.938934	-1.761246	-1.393633
H	2.226338	-1.735336	-2.323327

Step2 – Opposite side

Reactants

C	0.556636	2.147411	-0.497308
N	-0.048386	0.952860	-0.360738
C	-1.396282	0.885552	-0.149834
C	-2.159859	2.047967	-0.070707
C	-1.536235	3.290004	-0.209361
C	-0.157039	3.336468	-0.425675
Pt	0.888909	-0.819917	-0.466364
N	-0.989339	-1.463308	-0.172378
C	-1.339262	-2.759411	-0.069683
C	-2.653193	-3.136328	0.179563
C	-3.628605	-2.148053	0.331303
C	-3.257303	-0.804983	0.227616
C	-1.926704	-0.482036	-0.025918
C	-5.043045	-2.581592	0.606922
O	-5.868107	-1.536472	0.746576
C	-7.251507	-1.866153	1.018323
C	-2.287968	4.591894	-0.140007
O	-3.596623	4.403527	0.066432
C	-4.396690	5.607991	0.143777
O	3.223633	-1.794456	1.254067
C	3.920059	-0.740531	1.169335
C	3.718894	0.187337	0.033142
C	4.509304	1.292363	-0.276465
C	5.616551	1.877503	0.367960
C	6.212240	1.530010	1.562397
C	5.842588	0.457424	2.399352
C	4.866363	-0.498268	2.224028
O	2.748992	-0.071371	-0.850118
O	-5.364596	-3.746020	0.687932
O	-1.742807	5.666365	-0.261754
H	-0.533007	-3.474090	-0.188319

H	-2.925589	-4.182610	0.259814
H	-4.004528	-0.031321	0.349400
H	-3.228624	1.999880	0.093938
H	0.340783	4.293042	-0.536857
H	1.625296	2.113343	-0.668803
H	4.791913	-1.261757	2.994549
H	6.427514	0.353577	3.310804
H	7.048485	2.139225	1.893964
H	6.038101	2.736778	-0.148673
H	4.206943	1.776413	-1.203532
H	-7.323659	-2.432547	1.949152
H	-7.661776	-2.458362	0.197681
H	-4.319693	6.166810	-0.791220
H	-4.052674	6.231428	0.971686
H	-5.416635	5.265321	0.310871
H	-7.763966	-0.909114	1.103160
O	1.733270	-2.699270	-0.555132
H	2.239449	-2.720631	-1.422808
H	2.440614	-2.514167	0.174416
H	3.242669	-1.240904	-2.399274
O	3.195946	-2.170070	-2.702940
H	2.866195	-2.148933	-3.614833

Transition state

C	0.036359	2.382684	-0.550265
N	-0.347706	1.094439	-0.482729
C	-1.643996	0.782893	-0.189080
C	-2.594296	1.786885	-0.009062
C	-2.205552	3.123646	-0.111792
C	-0.865465	3.423125	-0.374154
Pt	0.864746	-0.498377	-0.766281
N	-0.788251	-1.440255	-0.218537
C	-0.863863	-2.776185	-0.041057
C	-2.061093	-3.390817	0.295154
C	-3.212214	-2.613301	0.455341
C	-3.121142	-1.229998	0.289634
C	-1.895748	-0.656367	-0.041348
C	-4.496629	-3.308816	0.807632
O	-5.517505	-2.448691	0.924149
C	-6.794702	-3.040399	1.259052
C	-3.165828	4.267530	0.065740
O	-4.411895	3.842943	0.309752
C	-5.401238	4.883471	0.492324
O	4.282155	-1.087277	-0.993286
C	4.739460	-0.457098	0.110655
C	3.838230	0.535158	0.710304
C	4.168853	1.286616	1.890303
C	5.308428	1.332141	2.661245
C	6.529907	0.638525	2.512170
C	6.844151	-0.278521	1.532759
C	6.037712	-0.761025	0.479857
O	2.720436	0.771963	0.151855
O	-4.571313	-4.508001	0.960896
O	-2.822173	5.426657	-0.008863
H	0.067754	-3.312722	-0.177583
H	-2.111553	-4.465115	0.432210
H	-4.001452	-0.614065	0.422822
H	-3.624585	1.542518	0.215802
H	-0.545137	4.456985	-0.434951
H	1.093104	2.548794	-0.722070
H	6.497190	-1.505039	-0.166134
H	7.842038	-0.708036	1.575176

H	7.299325	0.857361	3.247470
H	5.263863	2.015494	3.506785
H	3.354174	1.941507	2.190246
H	-6.728708	-3.551467	2.221933
H	-7.089554	-3.754336	0.487050
H	-5.465628	5.498996	-0.407391
H	-5.130652	5.510183	1.344740
H	-6.338706	4.360341	0.674768
H	-7.494422	-2.207309	1.307083
O	1.976579	-2.168065	-0.921918
H	1.902799	-2.487844	-1.839222
H	3.369014	-1.562902	-0.859443
H	3.192591	-0.011726	-2.135130
O	2.312964	0.174963	-2.540153
H	2.308105	1.125698	-2.737264

Products

C	0.700540	-2.629764	-0.358215
N	0.835396	-1.291238	-0.335979
C	2.056435	-0.728634	-0.101516
C	3.179408	-1.526523	0.104689
C	3.045771	-2.917011	0.075836
C	1.785718	-3.473597	-0.155472
Pt	-0.660158	0.033133	-0.665474
N	0.831126	1.312623	-0.304000
C	0.679236	2.649529	-0.251932
C	1.754319	3.489630	0.007540
C	3.016305	2.932062	0.226309
C	3.161776	1.543031	0.191145
C	2.051344	0.744601	-0.072350
C	4.166057	3.862802	0.501400
O	5.312705	3.198678	0.693780
C	6.472198	4.021681	0.964597
C	4.206785	-3.849917	0.286881
O	5.351224	-3.186067	0.494447
C	6.521149	-4.011376	0.705987
O	-4.507013	0.538984	-1.237205
C	-5.379670	0.252171	-0.262060
C	-4.846710	-0.410881	0.931267
C	-5.609601	-0.632187	2.119477
C	-6.953377	-0.468622	2.386862
C	-7.991718	-0.029340	1.542773
C	-7.868855	0.402053	0.235689
C	-6.706441	0.547721	-0.542078
O	-3.628142	-0.789797	0.931059
O	4.038110	5.066414	0.537314
O	4.089534	-5.055023	0.265410
H	-0.331440	3.006395	-0.414913
H	1.624021	4.565234	0.044040
H	4.132763	1.101009	0.373802
H	4.150765	-1.085290	0.287649
H	1.665637	-4.550828	-0.175592
H	-0.302455	-2.997056	-0.542980
H	-6.844831	0.977481	-1.531265
H	-8.787988	0.708074	-0.258110
H	-8.991143	-0.026956	1.968938
H	-7.258000	-0.748969	3.392925
H	-4.998479	-1.042033	2.919893
H	6.312417	4.603170	1.875049
H	6.653553	4.698045	0.126649
H	6.694117	-4.644375	-0.166897
H	6.380909	-4.638164	1.589209

H	7.343921	-3.312775	0.850353
H	7.298393	3.323131	1.087961
O	-2.078051	1.426717	-0.945113
H	-2.005700	1.758426	-1.857490
H	-3.585380	0.824772	-0.917845
H	-2.585115	-1.248571	-1.787303
O	-2.141796	-1.385104	-0.930412
H	-2.875894	-1.127820	-0.172509

Acid conditions

Step1

Reactants

C	-0.073416	2.669375	-0.073485
N	-0.239847	1.333673	-0.086627
C	-1.494417	0.796052	-0.103153
C	-2.620254	1.616263	-0.108800
C	-2.454848	3.003600	-0.094082
C	-1.161597	3.533325	-0.075452
Pt	1.276764	0.014016	-0.086221
N	-0.256640	-1.241367	-0.130321
C	-0.118450	-2.586773	-0.152125
C	-1.211162	-3.432944	-0.165206
C	-2.502842	-2.865650	-0.160235
C	-2.642308	-1.467238	-0.141685
C	-1.504315	-0.671132	-0.123400
C	-3.673734	-3.718428	-0.173593
O	-4.843759	-3.174233	-0.177846
C	-6.081725	-3.963159	-0.190059
C	-3.613717	3.967756	-0.099204
O	-4.790855	3.334517	-0.132773
C	-5.960512	4.196034	-0.145964
O	2.787753	-1.300157	-0.085736
C	3.983628	-0.737105	-0.079359
C	3.992272	0.709480	-0.055823
C	5.110415	1.553764	-0.043975
C	6.467240	1.233168	-0.052976
C	7.077979	-0.021970	-0.074691
C	6.456271	-1.274349	-0.093073
C	5.099727	-1.587824	-0.094598
O	2.798525	1.284782	-0.044381
O	-3.480216	-5.006699	-0.182062
O	-3.452972	5.166201	-0.075681
H	0.901572	-2.954427	-0.158329
H	-1.060338	-4.505566	-0.180664
H	-3.625136	-1.013346	-0.135519
H	-3.620240	1.201008	-0.125887
H	-1.019693	4.608525	-0.065556
H	0.952758	3.018801	-0.062801
H	4.840343	-2.643555	-0.111746
H	7.124769	-2.131503	-0.109099
H	8.164358	-0.026864	-0.078270
H	7.140246	2.086771	-0.041735
H	4.855762	2.610614	-0.026975
H	-6.134276	-4.574198	0.715123
H	-6.126825	-4.556808	-1.107135
H	-5.937719	4.837177	-1.029179

H	-5.976955	4.812075	0.755094
H	-6.813922	3.520760	-0.174473
H	-6.876616	-3.220862	-0.186311
O	-0.970863	-0.572024	2.891468
H	-1.210818	0.165448	3.475117
H	-0.225222	-0.992652	3.348416
H	-4.290565	-5.553382	-0.194467

Transition state

C	-0.373604	2.396627	-0.434163
N	0.078424	1.129032	-0.347445
C	1.403778	0.883609	-0.109055
C	2.300275	1.937128	0.061674
C	1.838997	3.251799	-0.021461
C	0.483230	3.477522	-0.279476
Pt	-1.087213	-0.478887	-0.506887
N	0.667941	-1.377517	-0.290302
C	0.846928	-2.721363	-0.291784
C	2.085129	-3.296476	-0.081560
C	3.195813	-2.454831	0.143938
C	3.010334	-1.061144	0.144600
C	1.740680	-0.540771	-0.075212
C	4.508690	-3.022167	0.369108
O	5.507265	-2.228545	0.569835
C	6.870335	-2.720085	0.806652
C	2.736932	4.449941	0.150634
O	4.003369	4.094640	0.388476
C	4.935842	5.194751	0.567109
O	-2.815518	-1.556684	0.753406
C	-3.863217	-0.799484	0.802963
C	-3.868879	0.359558	-0.084759
C	-4.930641	1.237744	-0.327911
C	-6.204826	1.299091	0.244931
C	-6.759677	0.505740	1.243320
C	-6.156010	-0.576647	1.899080
C	-4.900553	-1.136044	1.709057
O	-2.748955	0.606179	-0.753986
O	4.612216	-4.321160	0.356254
O	2.318048	5.581923	0.074736
H	-0.038099	-3.314394	-0.484661
H	2.182311	-4.375342	-0.094383
H	3.847801	-0.396169	0.314858
H	3.349842	1.753598	0.255837
H	0.111788	4.493744	-0.355152
H	-1.433130	2.503640	-0.632634
H	-4.650918	-1.995615	2.326290
H	-6.761422	-1.058634	2.663091
H	-7.771737	0.752035	1.551761
H	-6.840493	2.092039	-0.141239
H	-4.708319	1.984776	-1.086386
H	7.215991	-3.274537	-0.070053
H	6.889038	-3.317643	1.722119
H	4.629430	5.804629	1.419018
H	4.960653	5.808686	-0.335143
H	5.901366	4.725717	0.748365
H	7.465119	-1.818911	0.936771
O	-1.954818	-2.405321	-1.482927
H	-2.405607	-2.233070	-2.329003
H	-2.647107	-2.524438	-0.789965
H	5.511348	-4.672810	0.509479

Products

C	-0.462342	2.299818	-0.213787
N	0.071971	1.067509	-0.197961
C	1.422464	0.908813	-0.069588
C	2.263002	2.012488	0.051096
C	1.710822	3.297136	0.038370
C	0.328761	3.438437	-0.097557
Pt	-0.968328	-0.670950	-0.408571
N	0.850750	-1.410440	-0.234577
C	1.107734	-2.738714	-0.224585
C	2.393499	-3.226551	-0.069217
C	3.451002	-2.307939	0.083174
C	3.175678	-0.928511	0.084087
C	1.863756	-0.496295	-0.073024
C	4.812755	-2.785959	0.243137
O	5.763124	-1.926521	0.381166
C	7.169686	-2.320403	0.548457
C	2.542595	4.549108	0.161894
O	3.844485	4.273163	0.284350
C	4.717143	5.428706	0.408027
O	-3.523161	-1.839005	1.168877
C	-4.371026	-0.888846	0.810656
C	-3.983985	0.112020	-0.173178
C	-4.876198	1.050836	-0.744132
C	-6.201825	1.370269	-0.472316
C	-7.051129	0.858780	0.510956
C	-6.745350	-0.150204	1.420458
C	-5.581814	-0.910535	1.523842
O	-2.750938	0.229323	-0.615694
O	4.999851	-4.073449	0.237163
O	2.047445	5.652233	0.147498
H	0.234920	-3.372703	-0.346874
H	2.563406	-4.296623	-0.069380
H	3.975431	-0.209495	0.209596
H	3.335325	1.898550	0.151332
H	-0.112603	4.429023	-0.111862
H	-1.539083	2.342179	-0.327198
H	-5.592298	-1.697310	2.274199
H	-7.529022	-0.414688	2.125754
H	-8.046118	1.290458	0.571110
H	-6.619759	2.151901	-1.102003
H	-4.403356	1.634296	-1.530411
H	7.502755	-2.864917	-0.339106
H	7.277857	-2.899109	1.469634
H	4.444936	6.004424	1.294606
H	4.627337	6.056421	-0.480513
H	5.722202	5.020572	0.499232
H	7.706173	-1.378175	0.632767
O	-1.810097	-2.481830	-0.582222
H	-2.220465	-2.563194	-1.461660
H	-2.860664	-2.136043	0.442791
H	5.926493	-4.366982	0.344587

Step 2 – Same side

Reactants

C	0.575550	2.159608	0.327798
N	-0.035370	0.965243	0.266494
C	-1.383688	0.900484	0.046548
C	-2.136902	2.054535	-0.144551
C	-1.500884	3.300140	-0.102528
C	-0.130035	3.347521	0.145047
Pt	0.865481	-0.848007	0.533237

N	-1.006040	-1.445786	0.320456
C	-1.361594	-2.749516	0.349247
C	-2.669399	-3.147942	0.127351
C	-3.637446	-2.160050	-0.137034
C	-3.258709	-0.807081	-0.175253
C	-1.929223	-0.466436	0.056276
C	-5.021005	-2.541421	-0.374046
O	-5.887149	-1.620399	-0.616088
C	-7.307244	-1.910023	-0.868352
C	-2.234507	4.602237	-0.300060
O	-3.540781	4.411709	-0.515041
C	-4.320862	5.620899	-0.714076
O	3.274939	-2.266735	-1.083999
C	4.078728	-1.222721	-1.007838
C	3.830074	-0.160794	-0.045873
C	4.691624	0.933726	0.179039
C	5.881041	1.331226	-0.429773
C	6.562072	0.757178	-1.501112
C	6.194201	-0.399087	-2.189038
C	5.118906	-1.250273	-1.956518
O	2.769455	-0.187755	0.744359
O	-5.308262	-3.808306	-0.327429
O	-1.670556	5.671139	-0.261519
H	-0.548118	-3.439952	0.550873
H	-2.921872	-4.201021	0.161394
H	-3.990230	-0.036958	-0.384730
H	-3.204869	2.011516	-0.319027
H	0.376621	4.304802	0.198902
H	1.630273	2.149148	0.566843
H	5.058840	-2.128058	-2.595129
H	6.846598	-0.698737	-3.005325
H	7.467376	1.258014	-1.832211
H	6.320442	2.235797	-0.016207
H	4.334852	1.581352	0.977442
H	-7.744278	-2.380421	0.016416
H	-7.397761	-2.524581	-1.767899
H	-3.946889	6.163684	-1.584217
H	-4.253095	6.255215	0.171785
H	-5.342437	5.280463	-0.874321
H	-7.756347	-0.933583	-1.034396
O	1.570177	-2.712014	0.748308
H	2.004578	-2.782542	1.617192
H	2.651429	-2.449902	-0.290192
H	2.802120	1.015058	2.486262
O	2.611095	1.957615	2.622659
H	2.844721	2.151325	3.544023
H	-6.245166	-4.037584	-0.490131

Transition state

C	-0.181307	2.446084	-0.894537
N	0.190329	1.165414	-0.718871
C	1.428979	0.874541	-0.221380
C	2.315994	1.892235	0.124604
C	1.929751	3.223694	-0.046779
C	0.663583	3.500299	-0.568541
Pt	-0.945922	-0.463744	-1.156436
N	0.676132	-1.372985	-0.556969
C	0.802034	-2.725852	-0.525425
C	1.953531	-3.333217	-0.069131
C	3.024437	-2.527447	0.378211
C	2.883369	-1.126650	0.351601
C	1.705070	-0.564824	-0.117639

C	4.247243	-3.134242	0.847744
O	5.213394	-2.372721	1.246792
C	6.489938	-2.910035	1.728659
C	2.820408	4.388931	0.303280
O	4.003503	3.988393	0.778688
C	4.923230	5.053844	1.139481
O	-3.357706	-2.114912	0.717919
C	-3.952631	-1.044047	1.216612
C	-3.797321	0.229079	0.520200
C	-4.380529	1.446688	0.946612
C	-5.200988	1.759277	2.025232
C	-5.681655	0.932351	3.043690
C	-5.436808	-0.430534	3.193450
C	-4.681255	-1.283908	2.389655
O	-3.112777	0.236083	-0.582358
O	4.315872	-4.436847	0.842338
O	2.464795	5.535542	0.156130
H	-0.065102	-3.271216	-0.883781
H	2.017803	-4.414817	-0.064953
H	3.690918	-0.488787	0.688703
H	3.299738	1.672216	0.520451
H	0.353565	4.529399	-0.713357
H	-1.168996	2.600989	-1.310422
H	-4.648476	-2.326703	2.695315
H	-5.905372	-0.907352	4.050789
H	-6.314541	1.400005	3.792503
H	-5.507597	2.801285	2.079263
H	-4.141905	2.271685	0.279337
H	6.978642	-3.469232	0.926074
H	6.319220	-3.514766	2.623552
H	4.479575	5.677896	1.917498
H	5.146063	5.663182	0.261587
H	5.817007	4.550167	1.503525
H	7.077773	-2.030341	1.980600
O	-1.882828	-2.205812	-1.438582
H	-2.379097	-2.210343	-2.274291
H	-2.900928	-2.003378	-0.175843
H	-2.972336	0.745883	-2.329912
O	-2.100887	0.726331	-2.787143
H	-2.214906	0.316431	-3.661589
H	5.158276	-4.813266	1.163981

Products

C	0.598452	2.706333	-0.437693
N	0.755578	1.370690	-0.434045
C	1.961966	0.831244	-0.082415
C	3.039305	1.644136	0.262024
C	2.880835	3.033002	0.248171
C	1.639974	3.566720	-0.105561
Pt	-0.685058	-0.002372	-0.875527
N	0.798092	-1.233096	-0.432022
C	0.670292	-2.575569	-0.485545
C	1.739855	-3.412219	-0.206547
C	2.976287	-2.830462	0.130215
C	3.099403	-1.432105	0.186529
C	1.988773	-0.641203	-0.098138
C	4.125858	-3.679386	0.414422
O	5.245775	-3.126531	0.720865
C	6.461967	-3.901119	1.018543
C	3.989200	3.990010	0.605430
O	5.117609	3.349583	0.928508
C	6.236458	4.204680	1.287265

O	-3.790275	-1.582945	0.950408
C	-4.895487	-0.843229	1.015691
C	-5.107595	0.113179	-0.064363
C	-6.207334	0.995954	-0.150446
C	-7.305577	1.174978	0.682723
C	-7.640038	0.515697	1.870726
C	-6.917177	-0.491362	2.501948
C	-5.709657	-1.083681	2.122770
O	-4.212149	0.103208	-1.000172
O	3.950865	-4.964124	0.339681
O	3.832674	5.188934	0.588742
H	-0.318846	-2.928106	-0.766344
H	1.607156	-4.486365	-0.255725
H	4.045392	-0.972842	0.444009
H	3.997155	1.224835	0.544434
H	1.498845	4.642141	-0.114652
H	-0.388422	3.066170	-0.705220
H	-5.325305	-1.860194	2.779446
H	-7.346404	-0.879523	3.422344
H	-8.564918	0.823396	2.350265
H	-8.009068	1.936774	0.354843
H	-6.171058	1.622144	-1.038696
H	6.746379	-4.480695	0.136437
H	6.288424	-4.522041	1.901298
H	5.974692	4.810982	2.156442
H	6.488983	4.855059	0.447751
H	7.055292	3.524826	1.516232
H	7.215984	-3.147069	1.231916
O	-1.922472	-1.524240	-1.152287
H	-2.638833	-1.284156	-1.766799
H	-3.264673	-1.409123	0.124302
H	-3.141774	0.906950	-1.150206
O	-2.163518	1.357800	-1.348974
H	-2.149629	1.564868	-2.301767
H	4.736843	-5.513267	0.534606

Step2 – Opposite side

Reactants

C	-0.243224	2.411679	0.236146
N	0.222227	1.153787	0.168661
C	1.565216	0.927788	0.063742
C	2.468593	1.987029	0.022068
C	1.987381	3.298075	0.089369
C	0.611769	3.509035	0.199054
Pt	-0.915628	-0.541899	0.250112
N	0.864902	-1.361304	0.080610
C	1.053335	-2.698801	-0.001231
C	2.315177	-3.242037	-0.159257
C	3.428711	-2.380981	-0.238201
C	3.219698	-0.991847	-0.157638
C	1.929686	-0.497314	-0.002986
C	4.783449	-2.890894	-0.403985
O	5.757848	-2.059830	-0.389732
C	7.155585	-2.514482	-0.564926
C	2.889956	4.505607	0.049934
O	4.176738	4.162561	-0.060957
C	5.115805	5.270629	-0.108325
O	-3.520874	-1.570168	-1.356167
C	-4.306961	-0.574788	-1.014833
C	-3.879797	0.402576	-0.018602
C	-4.720873	1.396377	0.532303

C	-6.020114	1.800287	0.237707
C	-6.882326	1.342651	-0.757812
C	-6.622969	0.314414	-1.663106
C	-5.508806	-0.514605	-1.749286
O	-2.651383	0.440912	0.451786
O	5.087988	-4.147005	-0.567432
O	2.456943	5.632998	0.113193
H	0.143670	-3.288748	0.066902
H	2.389789	-4.324716	-0.201727
H	4.059858	-0.312505	-0.224355
H	3.535320	1.818693	-0.059462
H	0.225137	4.520878	0.253629
H	-1.318900	2.508506	0.324268
H	-5.553553	-1.295470	-2.504477
H	-7.409021	0.100751	-2.383008
H	-7.846951	1.835843	-0.836488
H	-6.396401	2.609467	0.858892
H	-4.226029	1.952959	1.324699
H	7.246715	-2.998269	-1.537738
H	7.404496	-3.198120	0.246995
H	5.043408	5.855976	0.810220
H	4.894744	5.905715	-0.968171
H	6.097761	4.810428	-0.203150
H	7.736638	-1.597642	-0.513022
O	-1.837198	-2.311021	0.292191
H	-2.221426	-2.454193	1.192668
H	-2.838897	-1.915344	-0.626578
H	-3.086419	-2.188227	3.496086
O	-2.842273	-2.830826	2.812543
H	-3.451647	-3.577040	2.926368
H	4.322709	-4.751554	-0.600362

Transition state

C	0.051754	2.419870	-0.611492
N	-0.325294	1.131559	-0.540402
C	-1.614028	0.814351	-0.217946
C	-2.565292	1.811832	-0.012328
C	-2.184345	3.151793	-0.119513
C	-0.852469	3.456495	-0.410662
Pt	0.890946	-0.474151	-0.839667
N	-0.730377	-1.406784	-0.284491
C	-0.792146	-2.751974	-0.098936
C	-1.967316	-3.380394	0.255773
C	-3.138412	-2.612624	0.442673
C	-3.054711	-1.215588	0.284399
C	-1.848877	-0.627835	-0.068949
C	-4.409026	-3.217328	0.796501
O	-5.417413	-2.452449	1.008482
C	-6.740148	-3.012878	1.358088
C	-3.144461	4.297840	0.082597
O	-4.381273	3.870507	0.349326
C	-5.372475	4.914292	0.553419
O	4.267991	-0.990321	-0.998861
C	4.703746	-0.412829	0.155207
C	3.756650	0.471136	0.826292
C	4.043219	1.135500	2.064588
C	5.188739	1.191290	2.829927
C	6.449065	0.592748	2.615478
C	6.811991	-0.223698	1.563828
C	6.021742	-0.671679	0.484901
O	2.619768	0.707969	0.284816
O	-4.615069	-4.500024	0.918060

O	-2.789973	5.451327	0.002604
H	0.144488	-3.276469	-0.255067
H	-1.932731	-4.458357	0.384689
H	-3.932877	-0.600978	0.436926
H	-3.591488	1.570386	0.235754
H	-0.539018	4.492756	-0.476051
H	1.101512	2.598304	-0.810630
H	6.515111	-1.333560	-0.222621
H	7.835467	-0.589380	1.564538
H	7.211938	0.802445	3.360074
H	5.110816	1.798268	3.729179
H	3.193467	1.710956	2.423542
H	-6.650343	-3.568094	2.292069
H	-7.076272	-3.654502	0.543128
H	-5.450894	5.529316	-0.344921
H	-5.083716	5.536705	1.402402
H	-6.305056	4.388924	0.751291
H	-7.374251	-2.137338	1.469508
O	1.959377	-2.166418	-1.002933
H	1.940365	-2.446179	-1.936937
H	3.417279	-1.539459	-0.869229
H	3.209982	0.043192	-2.055034
O	2.311614	0.223999	-2.439956
H	2.290358	1.161588	-2.695967
H	-3.837585	-5.056790	0.726264

Products

C	-0.615003	2.619964	-0.492505
N	-0.784142	1.289690	-0.418788
C	-2.007075	0.764327	-0.114397
C	-3.100051	1.593643	0.123171
C	-2.932593	2.980610	0.047969
C	-1.672974	3.495985	-0.262161
Pt	0.678679	-0.069830	-0.751736
N	-0.828619	-1.309280	-0.351360
C	-0.714070	-2.655463	-0.325817
C	-1.793512	-3.474771	-0.044652
C	-3.043015	-2.884228	0.230213
C	-3.149742	-1.482143	0.222967
C	-2.031331	-0.708319	-0.070409
C	-4.222061	-3.688338	0.530800
O	-5.287680	-3.093614	0.914880
C	-6.524693	-3.850380	1.216533
C	-4.058552	3.954031	0.288951
O	-5.206858	3.328936	0.569933
C	-6.344767	4.198272	0.814581
O	4.465875	-0.577097	-1.138841
C	5.318733	-0.267523	-0.164720
C	4.820833	0.402635	1.013388
C	5.550655	0.653566	2.188585
C	6.897707	0.470348	2.483982
C	7.927379	0.011480	1.658441
C	7.809497	-0.425178	0.341080
C	6.660342	-0.562665	-0.438879
O	3.557772	0.794911	1.054085
O	-4.275054	-4.986176	0.438124
O	-3.898981	5.150942	0.225628
H	0.283465	-3.034466	-0.524224
H	-1.618917	-4.546541	-0.020980
H	-4.099335	-1.009243	0.438518
H	-4.076386	1.191586	0.364297
H	-1.529753	4.569489	-0.321265

H	0.389625	2.947097	-0.739347
H	6.798400	-0.992512	-1.427839
H	8.731090	-0.739311	-0.142237
H	8.924476	-0.004102	2.089405
H	7.190293	0.764965	3.488668
H	4.940646	1.099219	2.970346
H	-6.324288	-4.526242	2.048136
H	-6.829233	-4.394211	0.322046
H	-6.541271	4.808178	-0.069178
H	-6.139058	4.845189	1.669470
H	-7.178035	3.528935	1.021502
H	-7.241933	-3.079956	1.486547
O	2.070401	-1.505409	-1.005398
H	2.086975	-1.753505	-1.947595
H	3.526140	-0.894391	-0.875068
H	2.609682	1.097210	-1.825566
O	2.095780	1.298154	-1.023265
H	3.086197	0.949501	0.158478
H	-3.460707	-5.403285	0.098420