Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Mechanistic Studies: Enantioselective Palladium(II)-Catalyzed Intramolecular Aminoarylation of Alkenes by Dual N-H and Aryl C-H Bond Cleavage

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Contents:

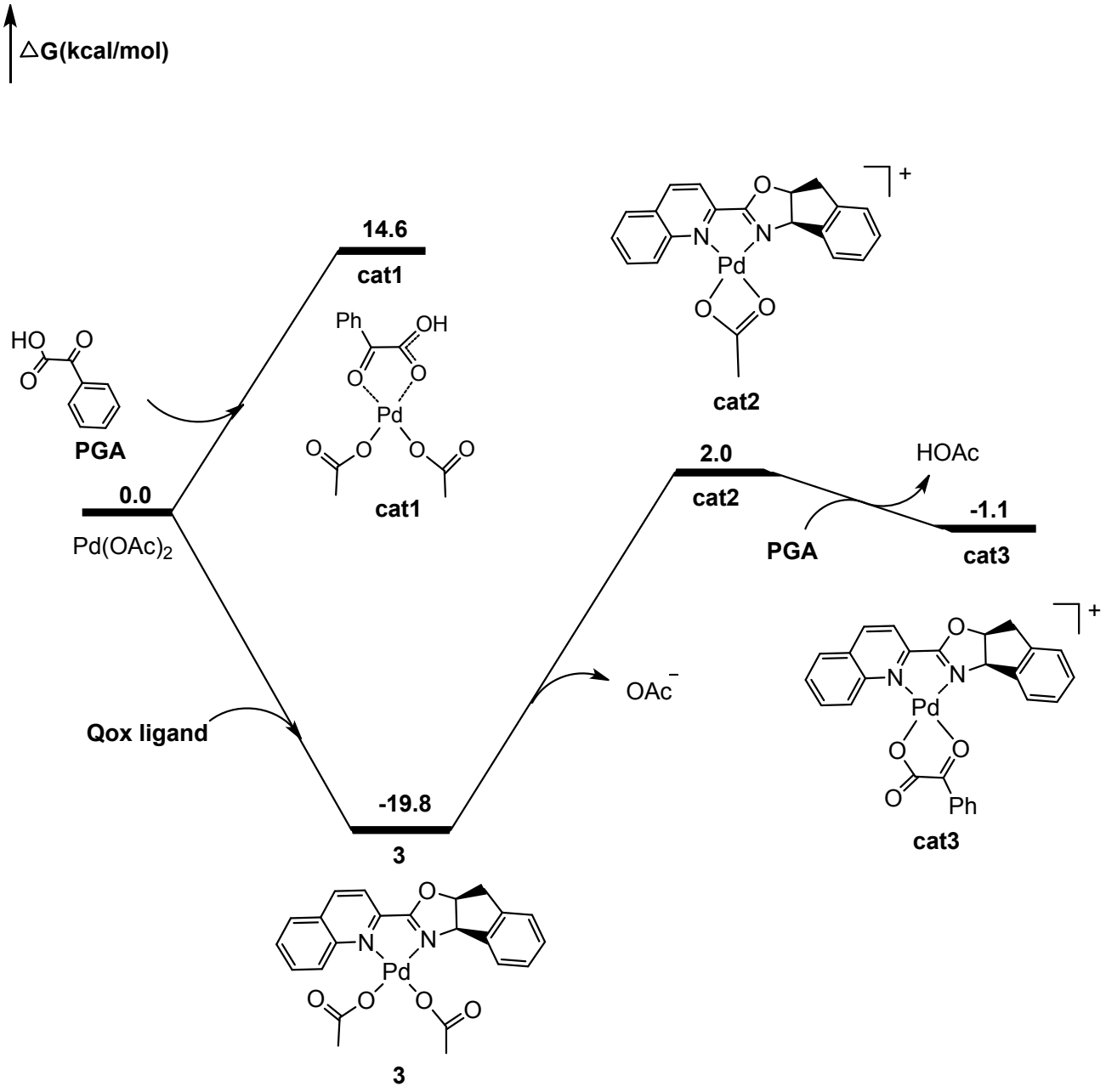

Fig. S1 The Gibbs free energy changes for the formation of the possible catalysts **3**, **cat1**, **cat2** and **cat3** from the $Pd(OAc)_2$.

In the experiment reported by Liu group[1], the authors proposed the active catalyst was the cationic complex **cat3**, which may facilitate the reaction. In fact, as shown in Fig. S1, our calculation result suggests that the cationic complex **cat3** is difficult to be generated because the formation of **cat3** is endergonic by 18.7 kcal/mol relative to **3**. Thus, the active catalyst should be the thermodynamically most stable species **3**.

1. W. Zhang, P. H. Chen and G. S. Liu, *Angew. Chem., Int. Ed.* 2017, **56**, 5336.

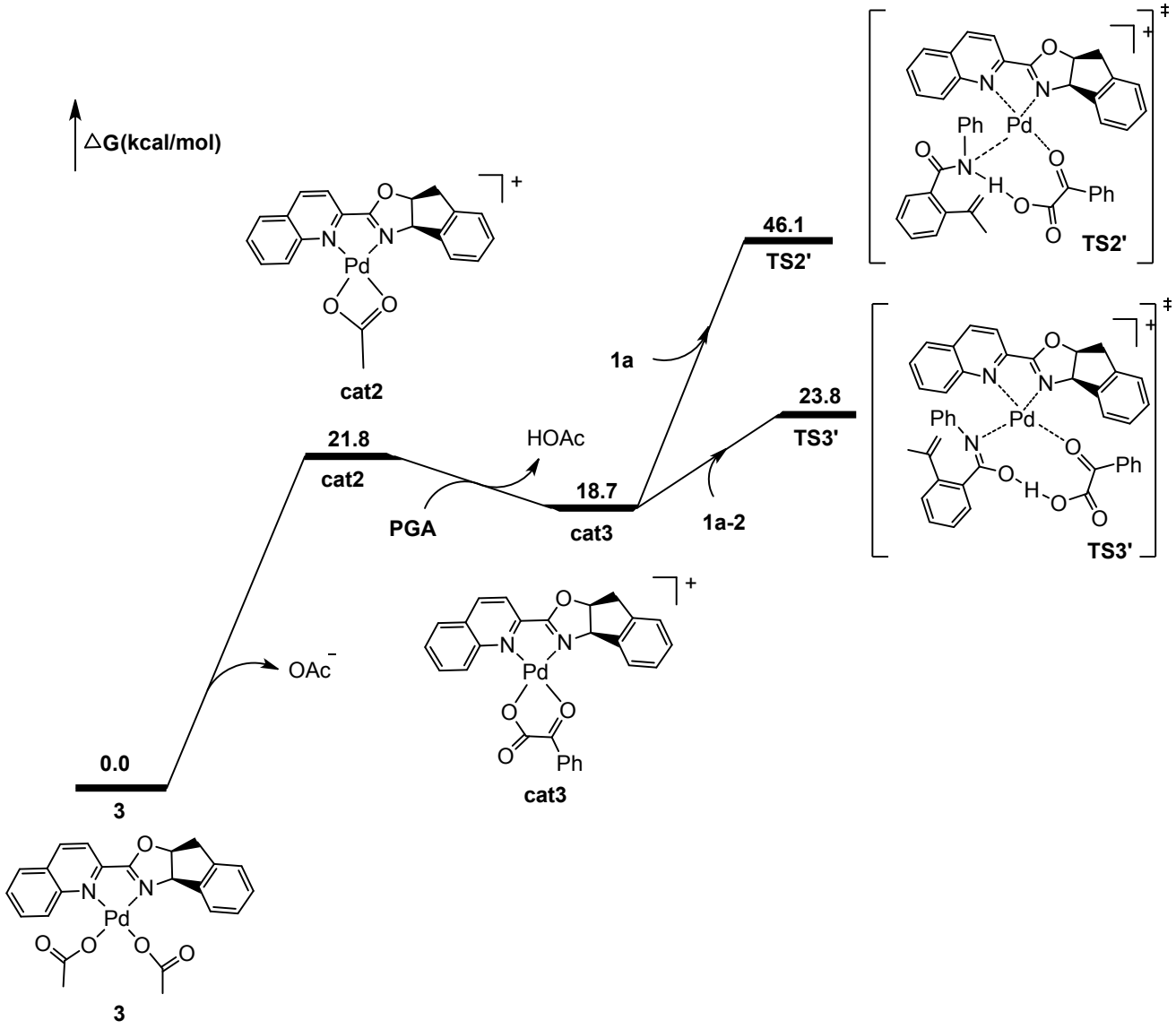

Fig. S2 The energy profile for N-H and O-H deprotonation in which PGA replacing acetate acts as the proton acceptor.

As shown in Fig. 2, the PGA assisted N-H deprotonation via the transition state **TS2'** requires a very high activation energy of 46.1 kcal/mol, suggesting that the PGA assisted N-H deprotonation would not take place. In addition, O-H deprotonation of the tautomer **1a-2** catalyzed by $[(L^*)Pd(PGA)]^+$ has been considered, and the calculated activation energy (**TS3'**, ΔG = 23.8 kcal/mol) is much higher than that of **TS1a** and **TS1b**.

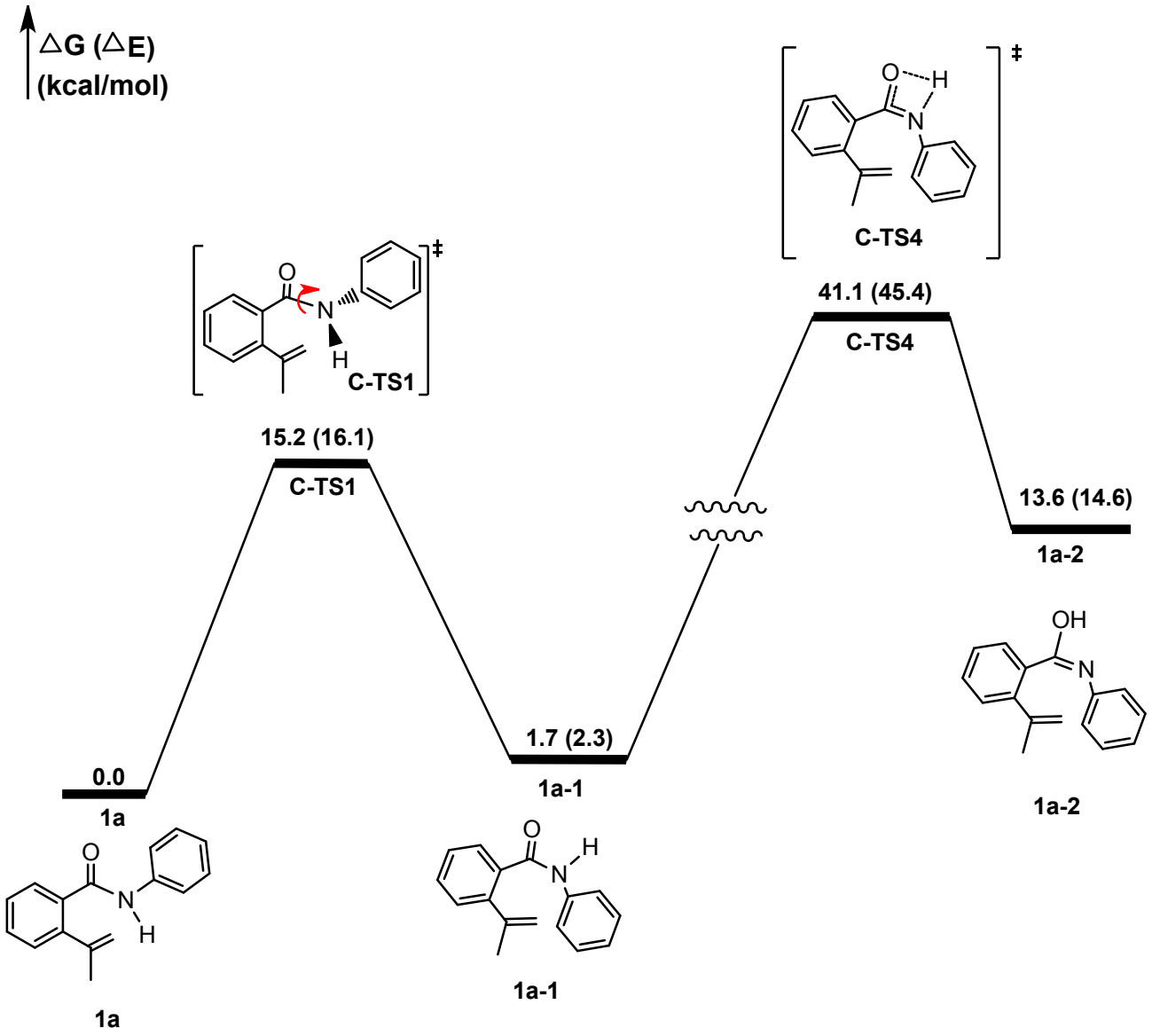

Fig. S3 The energy profile for the intramolecular hydrogen transfer of **1a**. Free energies (Electronic energies in parentheses) are relative to substrate **1a**.

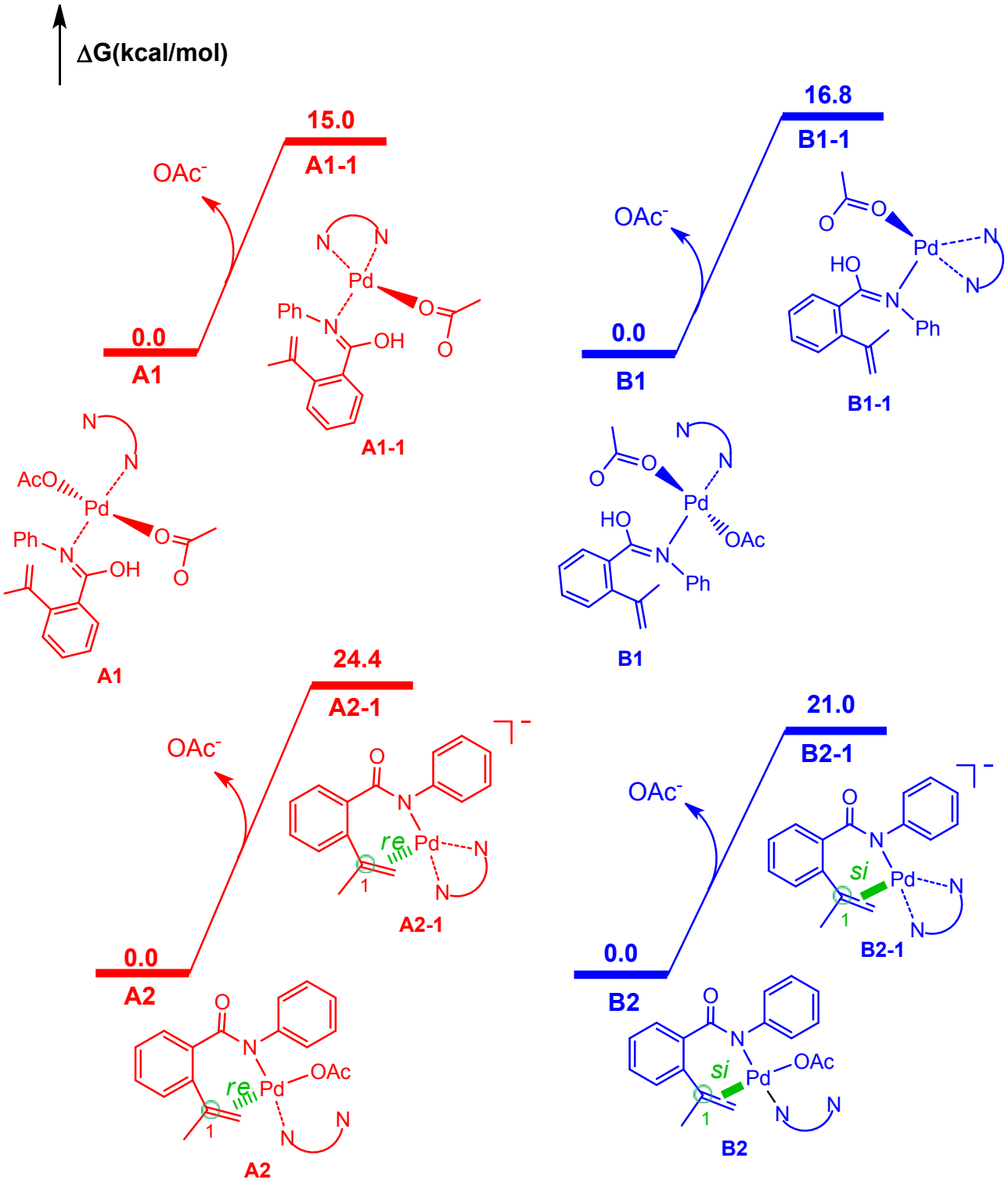

Fig. S4 The energy profiles for the formation of **A1-1**, **B1-1**, **A2-1** and **B2-1** from **A1**, **B1**, **A2** and **B2**, respectively.

In **A1**, **B1**, **A2** and **B2** the Qox ligand acts as monodentate ligand. If the OAc^- ligand dissociates from the palladium center and simultaneously the Qox ligand becomes bidentate ligand, the **A1-1, B1-1, A2-1 and B2-1** will be formed from the above four species, respectively. However, as shown in Fig. S4, the calculated Gibbs free energy changes for the above processes are 15.0, 16.8, 24.4 and 21.0 kcal/mol**,** respectively, which suggests that these processes are endothermic and difficult to take place. It may be because that the palladium center is positively charged, and the interaction between

the palladium center and the anion ligand OAc^- is stronger than that between the palladium center and the neutral ligand.

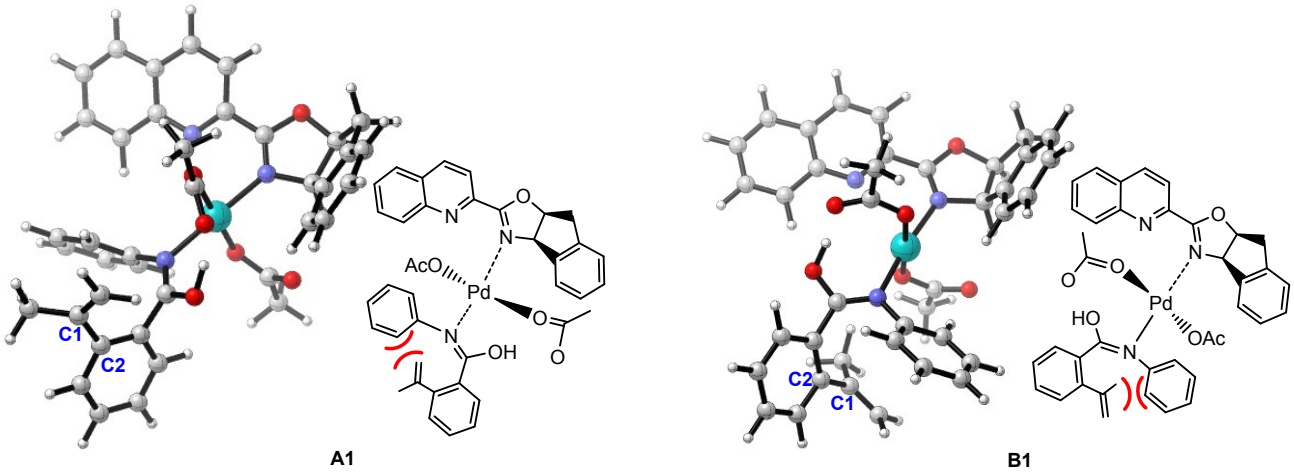

Fig. S5 The optimized structures of **A1** and **B1**.

A1 and **B1** are different in energy because they have different conformations. However, interconversion between the two structures is hardly to take place. This is because that the isopropenyl group on the substrate moiety adopts opposite orientation in **A1** relative to that in **B1** (Fig. S5), and steric repulsion between the isopropenyl group and the imidic acid moiety hinder the C1-C2 bond from rotating, and thus interconversion between **A1**and **B1** becomes difficult.

Table S1: The M06/SDD-6-311+G(d,p)/SMD(THF)//B3LYP/SDD-6-31G(d) computed energies, enthalpies, free energies of all stationary points discussed in the text.

species	E0	ZPE	E	H	G
3	-1501.596389	0.392652	-1501.175970	-1501.175025	-1501.264872
1a	-748.365582	0.270554	-748.079362	-748.078418	-748.139138
1a-1	-748.361913	0.269824	-748.076213	-748.075268	-748.136439
cat1	-1118.735179	0.229911	-1118.483596	-1118.482652	-1118.560983
cat2	-1272.988716	0.341998	-1272.624691	-1272.623746	-1272.70012
cat3	-1577.920731	0.405431	-1577.488609	-1577.487665	-1577.575215
C1	-1496.737956	0.541596	-1496.162866	-1496.161922	-1496.266972
C2	-1282.345555	0.396750	-1281.922260	-1281.921316	-1282.010758
1a-2	-748.342265	0.269254	-748.057158	-748.056213	-748.117473
C3	-1496.709948	0.539158	-1496.137601	-1496.136657	-1496.240643
C4	-1282.330198	0.395189	-1281.908578	-1281.907633	-1281.996856
A1	-2249.970280	0.662178	-2249.262792	-2249.261848	-2249.393314
A2	-2020.919641	0.599418	-2020.280888	-2020.279944	-2020.396409
A2-1	-1792.309005	0.548613	-1791.726665	-1791.725721	-1791.827494
A3	-2020.931350	0.600008	-2020.292645	-2020.291701	-2020.406887
A4	-2020.927720	0.600293	-2020.288574	-2020.287630	-2020.403863
A5	-1791.890496	0.537732	-1791.320415	-1791.319471	-1791.418048
A6	-1791.911966	0.537833	-1791.341295	-1791.340350	-1791.442915
B1	-2249.967986	0.662268	-2249.260460	-2249.259515	-2249.391348
B2	-2020.915027	0.599703	-2020.276121	-2020.275177	-2020.390102
B2-1	-1792.306694	0.548613	-1791.724944	-1791.724000	-1791.826512
B3	-2020.928440	0.600228	-2020.289596	-2020.288652	-2020.403758
B4	-2020.930306	0.600294	-2020.291174	-2020.290230	-2020.406515
B5	-1791.889317	0.537666	-1791.319229	-1791.318285	-1791.417311
B6	-1791.911177	0.537820	-1791.340488	-1791.339544	-1791.442651
C-TS1	-748.339859	0.268383	-748.056177	-748.055232	-748.114844
C-TS2	-1496.706731	0.532883	-1496.141196	-1496.140252	-1496.242065
C-TS3	-1282.329290	0.391175	-1281.912173	-1281.911229	-1281.998685
C-TS4	-748.293200	0.264485	-748.012989	-748.012045	-748.073564
HOAc	-229.039435	0.062040	-228.972832	-228.971888	-229.004618
PGA	-533.964289	0.125286	-533.829874	-533.828930	-533.874752
Qox	-916.762815	0.286109	-916.461190	-916.460245	-916.521586
R-2a	-747.194569	0.250554	-746.930738	-746.929794	-746.983506
S-2a	-747.194568	0.250554	-746.930737	-746.929793	-746.983504
TS1'	-2249.933247	0.658346	-2249.230132	-2249.229188	-2249.358792
TS2'	-2326.258620	0.670141	-2325.544177	-2325.543233	-2325.670725
TS3'	-2326.297548	0.671555	-2325.582338	-2325.581394	-2325.706271
TS1a	-2249.967784	0.658540	-2249.264337	-2249.263393	-2249.394091
TS1b	-2249.965696	0.658438	-2249.262393	-2249.261448	-2249.391534
TS2a	-2020.908627	0.598113	-2020.271842	-2020.270898	-2020.385041
TS2b	-2020.905534	0.598295	-2020.268627	-2020.267683	-2020.381496

TS3a	-2020.906642	0.595911	-2020.272911	-2020.271967	-2020.383682
TS3b	-2020.906888	0.595740	-2020.273204	-2020.272260	-2020.385240
TS4a	-1791.855194	0.535319	-1791.287415	-1791.286471	-1791.387056
TS4b	-1791.854670	0.535265	-1791.286935	-1791.285991	-1791.386976

E0 is the electronic energy. ZPE is the Zero-point vibrational energy. U, H and G are the thermal energy, enthalpy and Gibbs free energy obtained by adding the thermal corrections from frequency calculations to E0. All energies are in Hartree.

The Cartesian Coordinates of the stationary points discussed in the text.

1a

Atom	X	Y	Z
C	3.590701	0.684195	-0.248129
C	2.216962	0.559929	0.014697
C	1.644598	-0.734811	0.006897
C	2.465764	-1.847676	-0.226499
C	3.825495	-1.704075	-0.483748
C	4.389712	-0.428794	-0.503376
H	4.032667	1.676276	-0.229261
H	2.003639	-2.828780	-0.205187
H	4.438925	-2.581213	-0.669690
H	5.449676	-0.298042	-0.704271
C	0.182267	-1.067464	0.206301
O	-0.154589	-2.150650	0.675305
N	-0.709323	-0.115744	-0.229840
H	-0.306660	0.731686	-0.612419
C	-2.119558	-0.139296	-0.193602
C	-2.786151	0.993472	-0.690803
C	-2.868909	-1.217630	0.303256
C	-4.176470	1.051255	-0.691709
H	-2.207410	1.829928	-1.077624
C	-4.262094	-1.142463	0.294768
H	-2.356804	-2.089766	0.683311
C	-4.925905	-0.018397	-0.197676
H	-4.673297	1.936086	-1.080795
H	-4.833107	-1.982727	0.681300
H	-6.011324	0.024420	-0.198286
C	1.464596	1.812168	0.355005
C	1.323123	2.791864	-0.550356
H	1.706537	2.693876	-1.562592
H	0.829356	3.727726	-0.299774
C	0.967197	1.948092	1.776733
H	0.298930	1.125169	2.052737
H	1.812009	1.917703	2.476605
H	0.430866	2.890848	1.921827

1a-1

Atom	X	Y	Z
C	-2.207473	-0.914780	1.435015
C	-1.437831	0.054163	0.772139
C	-1.431935	0.042038	-0.639571
C	-2.219852	-0.879828	-1.340042
C	-2.971583	-1.837197	-0.661908
C	-2.955147	-1.859525	0.732905
H	-2.228527	-0.903277	2.520934
H	-2.226990	-0.842314	-2.425580
H	-3.569340	-2.553756	-1.218249
H	-3.538753	-2.598023	1.276140
C	-0.651199	1.026570	-1.467041
O	-1.215401	1.791336	-2.242351
N	0.723364	1.077191	-1.338583
H	1.109454	1.857223	-1.859893
C	1.665628	0.205697	-0.741522
C	2.874168	0.760020	-0.294559
C	1.466881	-1.177827	-0.637549
C	3.861964	-0.051842	0.257340
H	3.029421	1.833257	-0.374450
C	2.453381	-1.978793	-0.062374
H	0.554511	-1.626612	-1.011022
C	3.653955	-1.426397	0.386067
H	4.792839	0.395083	0.595939
H	2.284367	-3.049542	0.015350
H	4.420916	-2.059633	0.822583
C	-0.718736	1.086446	1.581779
C	0.188363	0.725388	2.497604
H	0.478288	-0.311811	2.638260
H	0.686444	1.463053	3.121898
C	-1.132727	2.528336	1.383061
H	-1.060570	2.842115	0.336197
H	-2.182449	2.667882	1.673857

H	-0.517105	3.200518	1.988856

3

Atom	X	Y	Z
C	-0.478112	-1.826421	-0.654730
O	-1.309989	-2.847594	-0.890372
N	-0.958748	-0.635677	-0.701365
C	1.484686	-3.339755	-0.278798
C	2.825019	-3.468770	-0.004664
C	3.620258	-2.311649	0.157328
C	2.993399	-1.021453	0.041987
C	0.939317	-2.043923	-0.364594
H	5.476875	-3.362049	0.506457
H	0.836244	-4.195210	-0.427230
H	3.284488	-4.449954	0.079710
C	5.013881	-2.383096	0.414892
C	3.788668	0.146561	0.161934
C	5.139828	0.032733	0.403167
C	5.759726	-1.234022	0.537518
H	3.303174	1.110997	0.054036
H	5.741761	0.932555	0.491173
H	6.826580	-1.294418	0.732066
N	1.645701	-0.914797	-0.197527
C	-2.603029	-2.243223	-1.273996
H	-2.724052	-2.456289	-2.337996
C	-2.412759	-0.733347	-0.930823
H	-2.672887	-0.047655	-1.739788
C	-3.741531	-2.781845	-0.395449
H	-4.640605	-2.931517	-1.008142
H	-3.480210	-3.758288	0.027765
C	-3.949609	-1.700323	0.645249
C	-3.223338	-0.543511	0.338467
C	-4.753584	-1.740425	1.784440
C	-3.275581	0.584194	1.159451
C	-4.812872	-0.614706	2.609826
H	-5.322954	-2.633153	2.032062
C	-4.078666	0.536546	2.301506
H	-2.685773	1.465535	0.923661
H	-5.431740	-0.636018	3.502983
H	-4.127056	1.399548	2.959444
Pd	0.385391	0.855453	-0.359056
C	1.639205	2.825936	1.204751
O	1.023322	2.304271	2.129047
O	1.724098	2.340571	-0.018103
C	-1.524606	2.507336	-1.710917
O	-0.959394	2.350392	-0.539248
O	-1.441489	1.733054	-2.665104
C	-2.323311	3.804563	-1.812370
H	-1.678193	4.571870	-2.257489
H	-3.179772	3.660640	-2.477252
H	-2.653191	4.159784	-0.833252
C	2.399950	4.136066	1.372969
H	3.399015	4.071604	0.928956
H	1.862403	4.933327	0.846738
H	2.475185	4.390842	2.432269

cat1

Atom	X	Y	Z
Pd	-1.269824	0.059914	0.021532
C	-3.521474	-1.504476	-0.362147
O	-2.769312	-2.156215	-1.082765
O	-3.174971	-0.419374	0.299419
C	-1.309808	2.840004	0.235075
O	-1.899793	1.883178	-0.450907
O	-0.452012	2.672244	1.098022
C	-1.826199	4.219393	-0.154370
H	-2.880038	4.309233	0.130215
H	-1.242739	4.987389	0.357229
H	-1.766821	4.359732	-1.238192
C	-4.983190	-1.869907	-0.148525
H	-5.207549	-1.941583	0.920487
H	-5.622682	-1.084199	-0.564921
H	-5.200557	-2.819127	-0.642142
C	0.921547	-1.779070	0.473804
O	-0.302208	-1.814389	0.558215
C	1.599773	-0.488876	0.011040
O	0.788813	0.419615	-0.240218
C	3.040753	-0.263477	-0.091767
C	3.996695	-1.298465	-0.149466
C	3.464750	1.082993	-0.162264
C	5.346455	-0.985183	-0.279191
H	3.688930	-2.334855	-0.108535
C	4.815271	1.381988	-0.278350
H	2.719915	1.869748	-0.104789
C	5.757849	0.348995	-0.339648
H	6.079614	-1.784175	-0.333565
H	5.137106	2.418077	-0.318844
H	6.814210	0.585036	-0.433100
O	1.683191	-2.819389	0.788695
H	1.088325	-3.550181	1.056880

cat2

Atom	X	Y	Z
C	-0.457211	-1.602084	-0.740914
O	-1.272485	-2.607699	-1.003424
N	-0.925708	-0.402109	-0.845158
C	1.525738	-3.067257	-0.216302
C	2.847318	-3.134059	0.172487
C	3.568656	-1.949250	0.434287
C	2.898965	-0.680849	0.286647
C	0.935945	-1.801035	-0.338750
H	5.428625	-2.925455	0.945984
H	0.936707	-3.952312	-0.426653
H	3.342694	-4.094720	0.280027
C	4.930033	-1.966803	0.836868
C	3.612848	0.516612	0.546398
C	4.932532	0.452155	0.935071
C	5.598751	-0.790973	1.082382
H	3.116796	1.472138	0.437654
H	5.473660	1.372383	1.132604
H	6.639468	-0.808959	1.389944
N	1.585100	-0.646708	-0.101092
C	-2.569449	-2.012921	-1.416808
H	-2.692343	-2.295423	-2.462698
C	-2.369456	-0.477323	-1.174085
H	-2.561185	0.138154	-2.057834
C	-3.704654	-2.488189	-0.496822
H	-4.581296	-2.760520	-1.097463
H	-3.405807	-3.388909	0.050779
C	-3.989363	-1.297538	0.395431
C	-3.273291	-0.162583	-0.001237
C	-4.875075	-1.223814	1.470781
C	-3.432280	1.060798	0.652132
C	-5.029413	-0.005975	2.137357
H	-5.441268	-2.096390	1.785075
C	-4.316690	1.128670	1.730598
H	-2.882832	1.940982	0.329929
H	-5.715681	0.062806	2.976293
H	-4.456966	2.069475	2.254470
O	-0.619522	2.822568	-0.648731
Pd	0.392913	1.054160	-0.396621
C	0.427139	3.496202	-0.326667
O	1.464343	2.805245	-0.028257
C	0.437247	4.986925	-0.331900
H	1.123362	5.361804	0.431468
H	0.789107	5.336339	-1.310373
H	-0.571230	5.373825	-0.169337

cat3

Atom	X	Y	Z
C	-1.889354	1.561471	-0.865522
O	-2.243884	2.776932	-1.252260
N	-0.627713	1.302942	-0.771052
C	-4.253595	0.768688	-0.626669
C	-5.113347	-0.254152	-0.290381
C	-4.596638	-1.497961	0.126923
C	-3.164694	-1.677400	0.188436
C	-2.874297	0.530343	-0.542523
H	-6.521997	-2.428166	0.437478
H	-4.605337	1.741527	-0.949312
H	-6.189061	-0.112188	-0.341236
C	-5.447141	-2.575562	0.488366
C	-2.646998	-2.927520	0.611868
C	-3.510247	-3.944954	0.954325
C	-4.916214	-3.776331	0.894545
H	-1.576247	-3.075773	0.656890
H	-3.101027	-4.897544	1.276787
H	-5.569789	-4.597846	1.170548
N	-2.330400	-0.641131	-0.157466
C	-0.993055	3.511636	-1.555820
H	-1.006585	3.671867	-2.634697
C	0.130651	2.544382	-1.051820
H	0.895668	2.330272	-1.803817
C	-0.905719	4.801940	-0.727998
H	-0.529060	5.620116	-1.354574
H	-1.898205	5.104618	-0.376630
C	0.061746	4.465679	0.387519
C	0.669326	3.219901	0.193418
C	0.408456	5.249297	1.488533
C	1.633531	2.741156	1.081746
C	1.364439	4.769671	2.386782
H	-0.054474	6.219538	1.647015
C	1.975194	3.526024	2.184849
H	2.108713	1.777736	0.921043
H	1.639998	5.370235	3.248689
H	2.720833	3.170911	2.890032
C	4.644452	-2.749421	0.074102
C	6.029383	-2.725621	-0.051621
C	6.678384	-1.565516	-0.482281
C	5.943266	-0.411446	-0.792367
C	4.563970	-0.419947	-0.669977
C	3.892668	-1.590529	-0.234268
H	4.132550	-3.642961	0.405438
H	6.604638	-3.614705	0.186282

H	7.760370	-1.556146	-0.579270
H	6.454454	0.485080	-1.128998
H	3.985551	0.464972	-0.910802
C	2.449103	-1.560101	-0.120156
O	1.820514	-0.488576	-0.363135
C	1.564464	-2.770035	0.286548
O	2.020148	-3.855735	0.580387
O	0.283725	-2.481359	0.276306
Pd	-0.212492	-0.602967	-0.221978

C1

Atom	X	Y	Z
C	5.319118	-1.784695	1.046936
C	4.082330	-1.129087	0.943399
C	3.257238	-1.444297	-0.157728
C	3.652329	-2.422374	-1.078667
C	4.887492	-3.056499	-0.960072
C	5.727954	-2.726603	0.103374
H	5.954379	-1.557031	1.898061
H	2.983357	-2.671437	-1.897442
H	5.186959	-3.804803	-1.688531
H	6.693093	-3.214510	0.210814
C	1.912216	-0.808415	-0.375776
O	0.896785	-1.524623	-0.351255
N	1.803911	0.530898	-0.587617
H	0.829575	0.867259	-0.562618
C	2.775523	1.531737	-0.831922
C	2.447333	2.841839	-0.450393
C	3.988875	1.289752	-1.490025
C	3.332138	3.887578	-0.700315
H	1.493571	3.027015	0.035687
C	4.874208	2.343142	-1.719595
H	4.236809	0.291967	-1.830958
C	4.556231	3.643941	-1.326832
H	3.063205	4.896651	-0.399386
H	5.813756	2.141959	-2.227711
H	5.248266	4.459420	-1.517246
C	3.670478	-0.180449	2.024459
C	4.416696	0.893529	2.309390
H	5.300124	1.146436	1.730537
H	4.149413	1.569457	3.117785
C	2.438569	-0.540982	2.825926
H	2.595028	-1.485463	3.364192
H	2.206208	0.237711	3.558835
H	1.558590	-0.690636	2.191205
C	-5.319281	1.784443	1.046708
C	-4.082474	1.128875	0.943168
C	-3.257248	1.444354	-0.157779
C	-3.652228	2.422644	-1.078534
C	-4.887411	3.056735	-0.959939
C	-5.728004	2.726579	0.103322
H	-5.954655	1.556557	1.897690
H	-2.983164	2.671907	-1.897174
H	-5.186792	3.805210	-1.688257
H	-6.693160	3.214453	0.210757
C	-1.912193	0.808514	-0.375774
O	-0.896750	1.524695	-0.350821
N	-1.803862	-0.530720	-0.588055
H	-0.829527	-0.867058	-0.563024
C	-2.775406	-1.531517	-0.832786
C	-2.447155	-2.841736	-0.451704
C	-3.988739	-1.289377	-1.490869
C	-3.331880	-3.887441	-0.702042
H	-1.493405	-3.027024	0.034358
C	-4.873990	-2.342745	-1.720861
H	-4.236727	-0.291491	-1.831462
C	-4.555954	-3.643662	-1.328542
H	-3.062897	-4.896602	-0.401454
H	-5.813522	-2.141439	-2.228958
H	-5.247927	-4.459117	-1.519286
C	-3.670753	0.179951	2.024032
C	-4.416940	-0.894169	2.308504
H	-5.300245	-1.146969	1.729415
H	-4.149763	-1.570306	3.116759
C	-2.439036	0.540368	2.825845
H	-1.558958	0.690322	2.191333
H	-2.595702	1.484665	3.364374
H	-2.206728	-0.238527	3.558558

C2

Atom	X	Y	Z
C	4.981509	-1.047979	1.172197
C	3.613820	-0.760061	1.043825
C	2.920690	-1.326665	-0.047843
C	3.578059	-2.190866	-0.932610
C	4.938053	-2.457107	-0.789153
C	5.643284	-1.872658	0.263049
H	5.519981	-0.628524	2.016973
H	3.012197	-2.642193	-1.742366
H	5.439118	-3.119661	-1.489061
H	6.703698	-2.073488	0.389890
C	1.460820	-1.087221	-0.299751

O	0.684998	-2.062865	-0.285322
N	0.990519	0.164286	-0.533444
H	-0.035851	0.211113	-0.550701
C	1.660167	1.387200	-0.797721
C	1.008099	2.568262	-0.416353
C	2.882591	1.461190	-1.477280
C	1.583491	3.806590	-0.690284
H	0.050427	2.505564	0.093001
C	3.458129	2.706319	-1.730450
H	3.375511	0.557948	-1.815887
C	2.817120	3.882845	-1.339778
H	1.065986	4.713728	-0.390374
H	4.408374	2.752282	-2.255671
H	3.268062	4.848513	-1.549611
C	2.945488	0.069057	2.094401
C	3.371439	1.310846	2.355493
H	4.163137	1.778061	1.777176
H	2.922312	1.908379	3.144788
C	1.846209	-0.590912	2.898285
H	1.044180	-0.984593	2.264623
H	2.243339	-1.447187	3.459365
H	1.406303	0.112674	3.611677
C	-2.493016	-0.952959	-0.730166
O	-1.923875	0.117829	-0.534853
C	-4.002077	-1.012645	-1.033891
O	-4.355470	-1.624237	-2.027308
C	-4.951440	-0.294624	-0.142138
C	-4.547037	0.396795	1.011171
C	-6.317007	-0.355216	-0.469236
C	-5.497622	1.016518	1.821096
H	-3.495150	0.461858	1.263838
C	-7.260874	0.266873	0.339688
H	-6.609856	-0.898648	-1.361676
C	-6.851897	0.953666	1.487787
H	-5.180308	1.551525	2.711809
H	-8.314948	0.217240	0.081091
H	-7.589618	1.438762	2.121581
O	-1.922207	-2.133415	-0.775184
H	-0.926090	-2.055323	-0.607064

C3

Atom	X	Y	Z
C	-5.407687	1.734200	0.754488
C	-4.164588	1.085799	0.827616
C	-3.199994	1.394262	-0.155550
C	-3.474283	2.359873	-1.133602
C	-4.716297	2.988023	-1.189084
C	-5.690702	2.663551	-0.245175
H	-6.149789	1.512577	1.515823
H	-2.705390	2.603669	-1.860936
H	-4.918026	3.726524	-1.959873
H	-6.663804	3.146593	-0.273421
C	-1.860885	0.725400	-0.212349
O	-0.865141	1.593063	-0.078038
N	-1.611371	-0.532579	-0.374458
H	-0.040987	-1.137864	-0.210052
C	-2.574936	-1.518337	-0.686630
C	-2.456528	-2.766196	-0.053490
C	-3.560888	-1.349351	-1.672020
C	-3.328355	-3.805554	-0.368422
H	-1.675519	-2.905539	0.688347
C	-4.428499	-2.395743	-1.984311
H	-3.637405	-0.405056	-2.200214
C	-4.322922	-3.625627	-1.332644
H	-3.225708	-4.762014	0.137700
H	-5.185489	-2.248410	-2.750539
H	-4.998849	-4.438730	-1.582754
C	-3.900719	0.160053	1.971768
C	-4.696766	-0.893257	2.191440
H	-5.506783	-1.149085	1.514758
H	-4.542974	-1.550657	3.043406
C	-2.767731	0.519882	2.908054
H	-2.953090	1.493773	3.380157
H	-2.660383	-0.230080	3.697716
H	-1.808572	0.605138	2.386307
C	5.407686	-1.734232	0.754405
C	4.164591	-1.085825	0.827574
C	3.199989	-1.394234	-0.155601
C	3.474273	-2.359789	-1.133708
C	4.716283	-2.987940	-1.189233
C	5.690693	-2.663527	-0.245309
H	6.149789	-1.512661	1.515752
H	2.705375	-2.603542	-1.861049
H	4.918007	-3.726398	-1.960062
H	6.663791	-3.146574	-0.273585
C	1.860877	-0.725374	-0.212361
O	0.865135	-1.593045	-0.078088
N	1.611361	0.532606	-0.374454
H	0.040983	1.137889	-0.210023
C	2.574923	1.518364	-0.686621
C	2.456495	2.766234	-0.053505
C	3.560908	1.349359	-1.671975

C	3.328331	3.805588	-0.368428
H	1.675461	2.905591	0.688305
C	4.428528	2.395748	-1.984257
H	3.637445	0.405051	-2.200146
C	4.322928	3.625645	-1.332616
H	3.225666	4.762058	0.137675
H	5.185545	2.248400	-2.7504 56
H	4.998863	4.438744	-1.582717
C	3.900739	-0.160148	1.971783
C	4.696837	0.893106	2.191540
H	5.506880	1.148938	1.514892
H	4.543062	1.550460	3.043544
C	2.767710	-0.519965	2.908024
H	1.808542	-0.605054	2.386261
H	2.952963	-1.493930	3.380020
H	2.660440	0.229925	3.697767

C4

Atom	X	Y	Z
C	5.007699	-0.798114	1.141208
C	3.618990	-0.614852	1.049086
C	2.936659	-1.265766	-0.001042
C	3.630860	-2.107698	-0.880561
C	5.009698	-2.271713	-0.771462
C	5.701058	-1.603232	0.238832
H	5.538396	-0.312726	1.954866
H	3.079606	-2.622693	-1.661902
H	5.536519	-2.918946	-1.466743
H	6.776517	-1.722892	0.338474
C	1.467897	-1.099838	-0.233808
O	0.819313	-2.255889	-0.128965
N	0.831012	-0.010258	-0.514546
H	-0.782621	0.066320	-0.662147
C	1.447424	1.233144	-0.803907
C	0.866186	2.389295	-0.261555
C	2.526633	1.365176	-1.690778
C	1.377973	3.647911	-0.568280
H	0.014890	2.287503	0.405236
C	3.032648	2.628671	-1.994880
H	2.957554	0.482344	-2.150360
C	2.467171	3.774566	-1.433153
H	0.919789	4.532610	-0.134149
H	3.868097	2.715265	-2.684724
H	2.862143	4.756702	-1.677508
C	2.926820	0.194781	2.098402
C	3.284934	1.464655	2.323314
H	4.030848	1.965533	1.713231
H	2.821597	2.051799	3.112155
C	1.888373	-0.509570	2.944302
H	1.082198	-0.941412	2.341500
H	2.342538	-1.342779	3.496452
H	1.441628	0.178976	3.668080
C	-2.388581	-1.007923	-0.813979
O	-1.813545	0.171920	-0.771912
C	-3.895845	-0.952136	-1.123150
O	-4.268002	-1.467145	-2.163066
C	-4.820410	-0.312282	-0.151509
C	-4.372494	0.279469	1.039433
C	-6.195006	-0.334867	-0.440845
C	-5.289195	0.840043	1.927576
H	-3.311812	0.316692	1.264421
C	-7.105896	0.227396	0.446069
H	-6.520365	-0.801082	-1.365218
C	-6.653649	0.814828	1.632663
H	-4.938905	1.298507	2.848005
H	-8.168069	0.208457	0.218568
H	-7.366117	1.252999	2.326568
O	-1.821677	-2.088085	-0.680284
H	-0.149899	-2.157440	-0.361026

1a-2

Atom	X	Y	Z
C	-2.191734	-0.903805	1.487694
C	-1.389599	0.039123	0.825605
C	-1.420633	0.058042	-0.585741
C	-2.268173	-0.813869	-1.283558
C	-3.054153	-1.742505	-0.605217
C	-3.006046	-1.792754	0.787829
H	-2.183845	-0.914564	2.573593
H	-2.293997	-0.766305	-2.368297
H	-3.699122	-2.417664	-1.160507
H	-3.614472	-2.510273	1.331877
C	-0.550450	0.964714	-1.394872
O	-1.293771	1.788191	-2.182665
N	0.719223	1.063299	-1.459991
C	1.636241	0.204768	-0.827778
C	2.772430	0.784761	-0.240035
C	1.527351	-1.195943	-0.851667
C	3.751904	-0.011849	0.347104
H	2.865429	1.866671	-0.250763
C	2.518220	-1.988169	-0.272297
H	0.674529	-1.659526	-1.336878

C	3.630295	-1.403826	0.336416
H	4.619227	0.455833	0.806293
H	2.420406	-3.070564	-0.303011
H	4.400110	-2.025754	0.784980
C	-0.598655	1.011585	1.640520
C	0.285463	0.576636	2.546356
H	0.507818	-0.479443	2.667649
H	0.837885	1.269714	3.175632
C	-0.906999	2.481974	1.460882
H	-1.957000	2.689212	1.705904
H	-0.274741	3.095156	2.110278
H	-0.755163	2.813679	0.428197
H	-0.644217	2.291901	-2.711139

A1

Atom	X	Y	Z
Pd	-0.372060	-0.293048	0.400546
C	-0.158726	-1.592747	2.989705
O	-0.598477	-2.615646	2.460748
O	0.023899	-0.442050	2.398694
C	0.228271	-1.564409	4.467649
H	1.293602	-1.330113	4.574402
H	-0.328021	-0.778292	4.989614
H	0.021855	-2.532703	4.927683
C	-3.239925	0.675770	0.619467
O	-4.538740	0.430691	0.881984
N	-2.423001	-0.309457	0.757718
C	-3.988810	2.864593	-0.331301
C	-3.697826	4.149425	-0.720661
C	-2.379897	4.647559	-0.571059
C	-1.400911	3.762780	-0.008466
C	-2.939714	2.065881	0.202119
H	-2.737629	6.630047	-1.367369
H	-4.986701	2.453606	-0.424643
H	-4.469179	4.790723	-1.140270
C	-1.993401	5.962051	-0.940387
C	-0.069065	4.224378	0.171513
C	0.272072	5.505412	-0.197905
C	-0.694177	6.380455	-0.757422
H	0.654482	3.541229	0.602051
H	1.292909	5.850586	-0.061615
H	-0.403391	7.387922	-1.042266
N	-1.701209	2.490314	0.364922
C	-4.655836	-0.961816	1.298563
H	-5.037520	-0.940378	2.321290
C	-3.202957	-1.510045	1.171054
H	-2.768792	-1.891039	2.096393
C	-5.556842	-1.758218	0.331953
H	-6.324624	-2.311119	0.888070
H	-6.086065	-1.073938	-0.342005
C	-4.605747	-2.694453	-0.383513
C	-3.300172	-2.584313	0.108107
C	-4.904741	-3.627664	-1.376586
C	-2.282628	-3.418685	-0.353386
C	-3.882533	-4.446731	-1.863995
H	-5.917048	-3.723807	-1.762483
C	-2.583570	-4.347487	-1.352130
H	-1.287420	-3.345575	0.070764
H	-4.102062	-5.175644	-2.640001
H	-1.800493	-4.996215	-1.733497
C	6.186050	-1.572380	-0.364381
C	4.864907	-1.372516	-0.803512
C	3.836520	-1.501782	0.156830
C	4.140836	-1.834813	1.483694
C	5.457004	-2.047792	1.885811
C	6.483963	-1.915521	0.952142
H	6.998183	-1.474625	-1.078010
H	3.330243	-1.927943	2.200805
H	5.675061	-2.309904	2.917099
H	7.517610	-2.076965	1.246169
C	2.372690	-1.350642	-0.144361
O	1.804733	-2.444931	-0.586099
N	1.689463	-0.272499	0.120560
C	2.360113	0.960572	0.412420
C	2.425479	1.448968	1.723998
C	2.910869	1.705568	-0.638068
C	3.073097	2.658791	1.978507
H	1.952250	0.882619	2.517653
C	3.557079	2.914462	-0.373464
H	2.827873	1.328457	-1.652080
C	3.647028	3.392323	0.935980
H	3.128978	3.028806	2.998948
H	3.986696	3.483115	-1.194139
H	4.156270	4.329924	1.142770
C	4.626120	-0.991529	-2.229802
C	3.682962	-1.571343	-2.987119
H	3.038842	-2.360253	-2.618522
H	3.541012	-1.266732	-4.021252
C	5.532435	0.079596	-2.802296
H	6.576816	-0.252863	-2.856928
H	5.519629	0.982021	-2.178994
H	5.221075	0.349928	-3.815955

C	-0.607239	-0.905828	-2.455436
O	-0.801486	0.016750	-1.581886
O	-0.014086	-1.991403	-2.269533
C	-1.206007	-0.628507	-3.825089
H	-1.332970	0.443182	-3.992974
H	-0.578575	-1.068191	-4.604198
H	-2.190957	-1.108118	-3.875485
H	0.928687	-2.239474	-1.104865

A2

Atom	X	Y	Z
C	-3.354159	-1.033477	-2.598274
C	-2.242275	-1.505372	-1.886074
C	-2.400596	-2.565562	-0.973029
C	-3.670859	-3.124277	-0.793259
C	-4.775439	-2.641345	-1.492554
C	-4.616522	-1.595585	-2.403597
H	-3.222825	-0.226089	-3.313983
H	-3.762313	-3.952372	-0.098686
H	-5.754659	-3.084913	-1.333704
H	-5.467686	-1.220591	-2.966059
C	-1.256126	-3.211898	-0.222536
O	-1.369301	-4.409289	0.068576
C	1.036954	-3.008715	0.550093
C	2.267562	-2.439230	0.172816
C	1.054792	-4.088606	1.454518
C	3.472852	-2.923719	0.675849
H	2.267092	-1.595467	-0.511200
C	2.267424	-4.571771	1.946767
H	0.122612	-4.551539	1.743998
C	3.482626	-3.998541	1.566936
H	4.406132	-2.459932	0.364679
H	2.256625	-5.408900	2.641067
H	4.420893	-4.383752	1.957638
C	-0.903297	-0.887989	-2.141478
C	-0.714788	0.454827	-1.939303
H	-1.544774	1.093732	-1.657051
H	0.201129	0.942251	-2.259344
C	0.101240	-1.714689	-2.910555
H	0.218912	-2.714289	-2.490337
H	-0.269528	-1.822299	-3.939422
H	1.078655	-1.226083	-2.946598
Pd	-0.223757	-0.391940	0.144583
C	-0.781148	-0.836526	2.912349
O	-1.961470	-0.635906	2.612341
O	0.241987	-0.678743	2.112450
C	-0.372243	-1.314398	4.300731
H	-0.024717	-2.350951	4.229338
H	0.461515	-0.719148	4.686202
H	-1.223415	-1.261187	4.982597
N	-0.148140	-2.446902	0.007475
C	0.762367	2.491674	0.718237
O	0.531951	3.656657	1.361590
N	-0.221909	1.665161	0.642455
C	3.178821	3.087875	0.871850
C	4.474899	2.931099	0.445001
C	4.760827	2.041885	-0.619341
C	3.656346	1.340007	-1.205614
C	2.157389	2.331253	0.233478
H	6.902488	2.356763	-0.672392
H	2.924448	3.762826	1.679496
H	5.284673	3.483434	0.915108
C	6.069412	1.823378	-1.123314
C	3.903537	0.448473	-2.284856
C	5.184325	0.256956	-2.750238
C	6.276249	0.948372	-2.165769
H	3.057864	-0.072374	-2.721145
H	5.365416	-0.430402	-3.571536
H	7.280059	0.782789	-2.546258
N	2.377034	1.495291	-0.765549
C	-0.875719	3.683101	1.725370
H	-0.917262	3.927403	2.787633
C	-1.376508	2.252139	1.387759
H	-1.562254	1.605778	2.247724
C	-1.679343	4.676532	0.850314
H	-2.060703	5.516766	1.441868
H	-1.025431	5.103240	0.079017
C	-2.792960	3.831228	0.265407
C	-2.628927	2.475601	0.574256
C	-3.904616	4.251945	-0.464677
C	-3.576156	1.525237	0.192319
C	-4.844711	3.301279	-0.873685
H	-4.047439	5.302814	-0.704910
C	-4.685793	1.950188	-0.543694
H	-3.451804	0.484362	0.476468
H	-5.716236	3.618382	-1.440487
H	-5.431491	1.224281	-0.854052

A2-1

Atom	X	Y	Z
C	1.724664	-3.245297	2.583331
C	1.368903	-2.800666	1.300695

C	2.380804	-2.448106	0.390136
C	3.723116	-2.570272	0.774182
C	4.068293	-3.014399	2.048902
C	3.064614	-3.348034	2.958989
H	0.944410	-3.533290	3.282635
H	4.483966	-2.313304	0.044633
H	5.113847	-3.105063	2.327879
H	3.318800	-3.696033	3.955838
C	2.130911	-1.956299	-1.005787
O	3.006531	-2.084229	-1.860564
C	0.616161	-0.910798	-2.585010
C	-0.653113	-1.173462	-3.143942
C	1.526457	-0.111691	-3.312026
C	-1.021166	-0.623198	-4.372035
H	-1.329274	-1.842263	-2.618076
C	1.158494	0.411884	-4.546588
H	2.523437	0.048476	-2.921383
C	-0.116816	0.171760	-5.076636
H	-2.000936	-0.838778	-4.788292
H	1.873196	1.006612	-5.108626
H	-0.390421	0.584553	-6.043147
C	-0.085098	-2.819768	0.952386
C	-0.946861	-2.017568	1.656534
H	-0.572296	-1.380491	2.453950
H	-2.015388	-2.198107	1.640513
C	-0.557254	-3.939013	0.058549
H	-0.007388	-3.948891	-0.886330
H	-0.355633	-4.894007	0.561066
H	-1.629767	-3.878334	-0.149541
Pd	-0.534356	-0.566018	-0.126334
N	0.886475	-1.432384	-1.300029
C	-0.809768	2.317971	0.094937
O	-0.544440	3.622893	0.073350
N	0.071073	1.504703	-0.380167
C	-3.068236	2.767306	1.089600
C	-4.301824	2.281032	1.458745
C	-4.609992	0.917714	1.246278
C	-3.591434	0.063116	0.700666
C	-2.112458	1.860967	0.592228
H	-6.655817	1.032358	1.937461
H	-2.811491	3.816615	1.171018
H	-5.056880	2.942048	1.874678
C	-5.899192	0.381903	1.508160
C	-3.934137	-1.269279	0.353369
C	-5.204417	-1.745755	0.591973
C	-6.189809	-0.925439	1.196063
H	-3.195572	-1.886751	-0.144301
H	-5.459333	-2.761263	0.304173
H	-7.179645	-1.326983	1.388054
N	-2.326790	0.543845	0.468233
C	0.722283	3.779170	-0.669794
H	0.448696	4.206967	-1.636516
C	1.266869	2.318028	-0.724712
H	1.620381	2.017667	-1.714059
C	1.713932	4.622339	0.137628
H	2.307503	5.245756	-0.543533
H	1.188577	5.304234	0.815013
C	2.574249	3.595000	0.840486
C	2.349250	2.305531	0.341822
C	3.528296	3.808432	1.835074
C	3.079845	1.218513	0.820263
C	4.252671	2.718852	2.324660
H	3.709134	4.806818	2.224393
C	4.031637	1.432754	1.819384
H	2.916575	0.220484	0.430805
H	4.996967	2.873020	3.100543
H	4.603454	0.592936	2.202919

A3

Atom	X	Y	Z
C	-2.884015	-1.514600	-2.913799
C	-2.130201	-1.860593	-1.792953
C	-2.769688	-2.315158	-0.642253
C	-4.156777	-2.446517	-0.562650
C	-4.909559	-2.105767	-1.684785
C	-4.274198	-1.647402	-2.849953
H	-2.409181	-1.148207	-3.819872
H	-4.616756	-2.803811	0.353452
H	-5.991849	-2.195909	-1.661983
H	-4.874240	-1.391115	-3.719231
C	-1.777425	-2.679324	0.383569
O	-1.945245	-3.263017	1.428428
C	0.618029	-3.178179	0.232164
C	1.760600	-2.695466	0.872699
C	0.502419	-4.547144	-0.042302
C	2.796460	-3.573138	1.204833
H	1.820407	-1.643697	1.133070
C	1.536201	-5.418764	0.295396
H	-0.400532	-4.933414	-0.504950
C	2.690518	-4.933239	0.914249
H	3.678398	-3.187740	1.709011
H	1.434894	-6.478767	0.079565

H	3.493961	-5.614296	1.181333
C	-0.627059	-1.779097	-1.612984
C	-0.140278	-0.327260	-1.543304
H	-0.816320	0.381503	-2.027946
H	0.882363	-0.205627	-1.914063
C	0.128816	-2.645702	-2.622312
H	-0.215714	-3.684494	-2.628322
H	-0.034401	-2.225751	-3.621020
H	1.204273	-2.632943	-2.423085
Pd	-0.179925	-0.198774	0.480283
C	-1.291259	-0.318881	3.186809
O	-2.318933	0.143275	2.659213
O	-0.148576	-0.460714	2.596138
C	-1.318250	-0.797422	4.636510
H	-1.386744	-1.891808	4.641663
H	-0.395957	-0.522594	5.157670
H	-2.186479	-0.389155	5.159590
N	-0.468794	-2.277438	-0.128790
C	0.987075	2.665599	0.544250
O	0.769409	3.954880	0.892655
N	-0.008970	1.859432	0.660514
C	3.221802	3.505805	-0.186455
C	4.494015	3.267535	-0.644344
C	4.926602	1.935714	-0.856765
C	3.989625	0.888428	-0.571195
C	2.365224	2.394834	0.062250
H	6.927044	2.399943	-1.543878
H	2.861256	4.511623	-0.013586
H	5.174301	4.091358	-0.846359
C	6.221661	1.600513	-1.330233
C	4.385779	-0.462801	-0.771127
C	5.649172	-0.754407	-1.233134
C	6.574888	0.282624	-1.514883
H	3.668554	-1.244754	-0.545985
H	5.944751	-1.789001	-1.383569
H	7.567566	0.031191	-1.877716
N	2.731562	1.138112	-0.115399
C	-0.618285	4.078137	1.312562
H	-0.595772	4.448447	2.339082
C	-1.178558	2.633767	1.169295
H	-1.511255	2.155604	2.093086
C	-1.412558	4.997261	0.356362
H	-1.911179	5.800818	0.912711
H	-0.730763	5.480450	-0.354061
C	-2.413652	4.074772	-0.307858
C	-2.307145	2.764748	0.170240
C	-3.396515	4.401967	-1.243289
C	-3.196281	1.771516	-0.240875
C	-4.270282	3.404378	-1.683456
H	-3.490374	5.418405	-1.618768
C	-4.176734	2.101138	-1.179675
H	-3.128344	0.776478	0.187068
H	-5.040325	3.647706	-2.411297
H	-4.875867	1.339783	-1.514004

A4

Atom	X	Y	Z
C	-1.401920	-2.642432	-2.884495
C	-1.940551	-2.455912	-1.612849
C	-3.259340	-2.811762	-1.358751
C	-4.087646	-3.355302	-2.338967
C	-3.553701	-3.536970	-3.614235
C	-2.222999	-3.180121	-3.880946
H	-0.372186	-2.376199	-3.107992
H	-5.112754	-3.621818	-2.099409
H	-4.167082	-3.955437	-4.407303
H	-1.822238	-3.325289	-4.880859
C	-3.595922	-2.491601	0.043109
O	-4.677504	-2.658565	0.588131
C	-2.399690	-1.262775	1.842604
C	-1.163969	-0.961702	2.480034
C	-3.590040	-0.837129	2.466548
C	-1.154803	-0.298039	3.724878
H	-0.238372	-1.467451	2.199485
C	-3.544475	-0.155913	3.679435
H	-4.540832	-1.062095	2.007792
C	-2.333703	0.120079	4.324088
H	-0.194151	-0.146479	4.199291
H	-4.482036	0.159715	4.131086
H	-2.317858	0.636534	5.279005
C	-1.278745	-1.925191	-0.345667
C	-0.787524	-0.478681	-0.539035
H	-1.630641	0.143379	-0.864640
H	-0.038772	-0.476042	-1.341002
C	-0.158823	-2.923594	0.033439
H	-0.584049	-3.912168	0.236107
H	0.533723	-3.017583	-0.809460
H	0.431037	-2.608992	0.894521
Pd	0.095454	0.445272	1.060773
C	2.030715	0.707005	3.187429
O	2.018329	-0.537383	3.128520
O	1.203563	1.487963	2.573543

C	3.085456	1.425393	4.027235
H	3.851581	1.842921	3.362104
H	2.641731	2.260033	4.578897
H	3.564823	0.728963	4.719259
N	-2.432192	-1.945019	0.613973
C	1.852165	1.853316	-1.048108
O	2.149549	2.991323	-1.712652
N	0.843454	1.888031	-0.252254
C	3.491072	0.599202	-2.495246
C	4.329458	-0.480098	-2.652287
C	4.467382	-1.427160	-1.605434
C	3.703778	-1.205300	-0.411302
C	2.759896	0.707439	-1.281532
H	5.898382	-2.734022	-2.576908
H	3.377716	1.351428	-3.267622
H	4.898058	-0.610814	-3.569939
C	5.321118	-2.558668	-1.672219
C	3.833895	-2.094932	0.690993
C	4.676831	-3.178972	0.589661
C	5.417870	-3.415791	-0.597847
H	3.269299	-1.865404	1.592052
H	4.783948	-3.861431	1.428149
H	6.074562	-4.279769	-0.653482
N	2.856336	-0.151909	-0.284838
C	1.179973	4.000090	-1.304098
H	1.759704	4.834600	-0.907036
C	0.309314	3.269562	-0.235173
H	0.436181	3.649400	0.783832
C	0.250032	4.415171	-2.466996
H	0.331252	5.488900	-2.674776
H	0.544038	3.892152	-3.385327
C	-1.137595	4.030338	-1.995611
C	-1.108333	3.404660	-0.744764
C	-2.355163	4.248478	-2.641863
C	-2.285976	2.998656	-0.116222
C	-3.536216	3.833177	-2.021841
H	-2.388616	4.737397	-3.612548
C	-3.503295	3.214506	-0.766322
H	-2.253240	2.513960	0.855966
H	-4.489893	3.997982	-2.516111
H	-4.430042	2.902507	-0.293037

A5

Atom	X	Y	Z
C	4.030265	2.404507	0.771918
C	3.908143	1.055515	0.443283
C	5.017571	0.341799	0.006441
C	6.273083	0.930174	-0.128472
C	6.398181	2.281712	0.194234
C	5.284675	3.009538	0.640781
H	3.178004	2.983427	1.119471
H	7.115560	0.339181	-0.475594
H	7.361017	2.777057	0.101641
H	5.398955	4.061853	0.888836
C	4.624459	-1.058326	-0.278612
O	5.365768	-1.940136	-0.697774
C	2.429829	-2.252650	-0.318435
C	1.039045	-2.087629	-0.544280
C	3.027521	-3.522038	-0.451731
C	0.342730	-3.214655	-1.024679
C	2.289079	-4.615618	-0.895242
H	4.082381	-3.629227	-0.244994
C	0.941207	-4.462622	-1.210167
H	-0.712797	-3.114262	-1.265181
H	2.778913	-5.580216	-1.003241
H	0.356604	-5.298928	-1.587055
C	2.694130	0.141890	0.494327
C	1.595773	0.624594	-0.457686
H	1.984362	0.647324	-1.482943
H	1.303976	1.646063	-0.178411
C	2.213885	0.003728	1.954168
H	3.046007	-0.285107	2.605254
H	1.811171	0.958597	2.311853
H	1.421850	-0.746204	2.023479
Pd	-0.124649	-0.443747	-0.364340
N	3.262082	-1.146754	0.014019
C	-2.711958	0.863961	-0.941443
O	-3.526806	1.724676	-1.586956
N	-1.500075	1.230366	-0.709354
C	-4.636737	-0.699084	-0.557064
C	-5.095914	-1.879026	-0.022662
C	-4.189036	-2.763187	0.610194
C	-2.797530	-2.404888	0.624783
C	-3.250379	-0.425628	-0.491747
H	-5.654463	-4.233510	1.219561
H	-5.301107	0.022173	-1.018153
H	-6.152314	-2.132445	-0.059368
C	-4.601161	-3.965708	1.240276
C	-1.874801	-3.246378	1.301858
C	-2.314401	-4.397385	1.916765
C	-3.681956	-4.767189	1.878904
H	-0.831721	-2.955518	1.319453

H	-1.602740	-5.031979	2.436634
H	-4.003902	-5.683756	2.364875
N	-2.348755	-1.260133	0.028083
C	-2.695026	2.862369	-1.984951
H	-2.585267	2.799506	-3.070374
C	-1.378826	2.622807	-1.183016
H	-0.470566	2.720987	-1.785121
C	-3.306002	4.186618	-1.502558
H	-3.159311	4.964957	-2.263199
H	-4.386964	4.086778	-1.353996
C	-2.545177	4.502325	-0.231819
C	-1.454861	3.641949	-0.057705
C	-2.801975	5.509767	0.698604
C	-0.614321	3.770002	1.048205
C	-1.959448	5.643196	1.804697
H	-3.647521	6.181000	0.569317
C	-0.873192	4.778027	1.979508
H	0.218554	3.088051	1.190746
H	-2.151347	6.422522	2.537206
H	-0.229168	4.888550	2.847492

A6

Atom	X	Y	Z
C	4.165705	-2.878615	-1.891025
C	3.886782	-1.794830	-1.062479
C	4.896675	-0.883291	-0.736385
C	6.200786	-1.031768	-1.203382
C	6.483702	-2.126093	-2.022075
C	5.474874	-3.039866	-2.359121
H	3.393462	-3.592688	-2.165644
H	6.964169	-0.311281	-0.924589
H	7.490830	-2.274839	-2.401706
H	5.713988	-3.888973	-2.994072
C	4.364636	0.146776	0.196250
O	4.967755	1.045886	0.762522
C	2.252039	-0.046346	1.524757
C	1.393554	-1.191681	1.629716
C	2.375501	0.893618	2.529224
C	0.646763	-1.372135	2.827562
C	1.612470	0.704826	3.705187
H	3.068592	1.719703	2.428000
C	0.770721	-0.385373	3.855241
H	0.213888	-2.339226	3.073730
H	1.699258	1.430729	4.509266
H	0.215538	-0.521471	4.779413
C	2.575248	-1.336498	-0.457346
C	1.878733	-2.227546	0.610415
H	2.608348	-2.901157	1.082146
H	1.082389	-2.836564	0.176945
C	1.586428	-0.916552	-1.562547
H	2.039790	-0.166473	-2.218262
H	1.313325	-1.787746	-2.169327
H	0.673367	-0.503392	-1.118144
Pd	-0.681094	-0.536619	1.289062
N	3.007558	-0.149303	0.338203
C	-3.056861	1.103056	0.032968
O	-4.391215	1.198626	-0.204830
N	-2.636486	0.035243	0.618303
C	-2.907013	3.452935	-0.826544
C	-2.137383	4.528558	-1.198837
C	-0.724204	4.435081	-1.148669
C	-0.162869	3.189467	-0.709766
C	-2.250968	2.264399	-0.399794
H	-0.282925	6.440348	-1.838320
H	-3.989232	3.493030	-0.848365
H	-2.601421	5.455029	-1.528796
C	0.145545	5.497964	-1.505238
C	1.250787	3.051349	-0.640618
C	2.065939	4.104337	-0.988872
C	1.511047	5.334826	-1.425737
H	1.655842	2.104743	-0.301129
H	3.144713	3.993715	-0.924577
H	2.171979	6.153452	-1.697079
N	-0.936583	2.130799	-0.352308
C	-5.026060	0.033384	0.388697
H	-5.626211	0.395370	1.227743
C	-3.810333	-0.850124	0.798582
H	-3.837829	-1.181045	1.840469
C	-5.849148	-0.745875	-0.653984
H	-6.806718	-1.064029	-0.220903
H	-6.084974	-0.108699	-1.513911
C	-4.977951	-1.934261	-1.005075
C	-3.849929	-2.007762	-0.180967
C	-5.195900	-2.905045	-1.984007
C	-2.927224	-3.044963	-0.317485
C	-4.274083	-3.945062	-2.125579
H	-6.069303	-2.855163	-2.629923
C	-3.147226	-4.015541	-1.297382
H	-2.046720	-3.073791	0.319827
H	-4.433450	-4.705789	-2.885309
H	-2.438844	-4.830690	-1.419358

B1

Atom	X	Y	Z
Pd	-0.206164	-0.324578	0.150004
C	0.058826	-0.673542	3.044943
O	-0.279630	-1.856955	2.921322
O	0.234208	0.177700	2.076240
C	0.348297	-0.094872	4.428323
H	1.356834	-0.395524	4.735804
H	0.294438	0.996062	4.431747
H	-0.355452	-0.513001	5.153416
C	-3.150919	0.374090	0.718464
O	-4.350628	-0.065368	1.150737
N	-2.213110	-0.504102	0.637718
C	-4.305809	2.555420	0.310164
C	-4.236313	3.899567	0.035476
C	-2.973306	4.520427	-0.125932
C	-1.809353	3.690845	0.001156
C	-3.090391	1.822184	0.408159
H	-3.696595	6.528988	-0.492740
H	-5.254236	2.051769	0.450586
H	-5.141630	4.495237	-0.053615
C	-2.811991	5.904205	-0.395190
C	-0.520868	4.276590	-0.135663
C	-0.400969	5.622850	-0.394461
C	-1.551481	6.442313	-0.526767
H	0.346865	3.634299	-0.034088
H	0.584842	6.066614	-0.501023
H	-1.432736	7.502566	-0.732664
N	-1.893630	2.358459	0.257642
C	-4.206520	-1.469253	1.523197
H	-4.338564	-1.510399	2.606737
C	-2.770724	-1.824317	1.042455
H	-2.116200	-2.220344	1.822661
C	-5.204034	-2.354761	0.753966
H	-5.695173	-3.058230	1.438583
H	-5.995948	-1.741836	0.307587
C	-4.351833	-3.078678	-0.267057
C	-2.990764	-2.799272	-0.098836
C	-4.772063	-3.972045	-1.253356
C	-2.030492	-3.420657	-0.897938
C	-3.814147	-4.585725	-2.063484
H	-5.828308	-4.193724	-1.387434
C	-2.452585	-4.314967	-1.883497
H	-0.976177	-3.201775	-0.765667
H	-4.128498	-5.283948	-2.834955
H	-1.716420	-4.803407	-2.516046
C	6.223093	0.735810	0.194831
C	4.847505	0.577125	0.433616
C	3.956230	0.924430	-0.606849
C	4.450890	1.465359	-1.805380
C	5.818727	1.606380	-2.019678
C	6.709782	1.225853	-1.015620
H	6.912860	0.489996	0.996501
H	3.743854	1.756497	-2.576066
H	6.183164	2.012977	-2.958757
H	7.781276	1.331968	-1.163137
C	2.472525	0.752459	-0.542945
O	1.810950	1.854822	-0.836221
N	1.831987	-0.356749	-0.282890
C	2.445100	-1.647358	-0.334981
C	3.275006	-2.006210	-1.408134
C	2.131295	-2.603387	0.642825
C	3.819323	-3.288536	-1.476395
H	3.485542	-1.286627	-2.191759
C	2.677412	-3.883911	0.561599
H	1.450816	-2.353001	1.450596
C	3.528274	-4.232443	-0.490108
H	4.461193	-3.550628	-2.313435
H	2.429290	-4.613030	1.328286
H	3.947513	-5.233257	-0.548866
C	4.418065	0.147746	1.798683
C	4.893856	-0.985793	2.330975
H	5.523341	-1.665733	1.764112
H	4.639845	-1.282955	3.345266
C	3.523472	1.090615	2.573113
H	2.504473	1.119403	2.172078
H	3.921136	2.113277	2.548060
H	3.453008	0.775750	3.619176
H	0.926261	1.632484	-1.327143
C	-0.564310	0.235505	-2.679263
O	-0.681648	-0.701846	-1.806512
O	-0.040665	1.356395	-2.494627
C	-1.160843	-0.092075	-4.039255
H	-0.937632	-1.125748	-4.316550
H	-2.251403	0.005088	-3.982702
H	-0.783259	0.597720	-4.796482

B2

Atom	X	Y	Z
Pd	-0.461785	-0.261882	0.183344
C	-0.693782	0.203176	3.133984
O	-1.614460	1.015311	2.997787

O	-0.070842	-0.433459	2.183889
C	-0.189192	-0.188957	4.520426
H	-0.579927	-1.181921	4.770435
H	0.902566	-0.252017	4.536206
H	-0.541385	0.530184	5.263129
C	0.807091	2.587572	0.475247
O	0.575073	3.901335	0.683786
N	-0.225926	1.835694	0.310598
C	3.201042	3.159611	0.913978
C	4.520056	2.779121	0.968615
C	4.884742	1.454274	0.626303
C	3.833694	0.564292	0.222891
C	2.236032	2.197594	0.505463
H	7.013406	1.652650	0.973378
H	2.887234	4.162023	1.176588
H	5.288005	3.484031	1.277586
C	6.219755	0.975450	0.667446
C	4.153106	-0.777387	-0.118221
C	5.458080	-1.210291	-0.063333
C	6.498942	-0.329729	0.328690
H	3.344718	-1.439125	-0.405694
H	5.695095	-2.238621	-0.320303
H	7.522291	-0.692796	0.364914
N	2.533225	0.957349	0.161568
C	-0.856955	4.115683	0.565860
H	-1.162571	4.668522	1.454831
C	-1.447112	2.682004	0.490114
H	-1.909968	2.327240	1.414298
C	-1.228663	4.842791	-0.749821
H	-1.609941	5.852850	-0.561490
H	-0.335729	4.953147	-1.378658
C	-2.271009	3.941464	-1.380375
C	-2.399129	2.734402	-0.681824
C	-3.078758	4.201151	-2.488203
C	-3.355781	1.788386	-1.055604
C	-4.018746	3.244821	-2.882070
H	-2.989583	5.137875	-3.033113
C	-4.162381	2.049857	-2.166835
H	-3.476008	0.868801	-0.488553
H	-4.656156	3.438879	-3.740571
H	-4.915237	1.326771	-2.468411
C	1.734345	-1.972013	-3.023262
C	0.765885	-2.055092	-2.011105
C	0.915270	-3.009219	-0.986382
C	2.020869	-3.868804	-1.009589
C	2.977114	-3.783324	-2.019699
C	2.834154	-2.830062	-3.031076
H	1.611442	-1.239918	-3.817393
H	2.090796	-4.614039	-0.224127
H	3.826001	-4.462137	-2.023984
H	3.570829	-2.756255	-3.826493
C	-0.136013	-3.255709	0.071559
O	-0.173189	-4.374505	0.596298
N	-1.032045	-2.248786	0.297843
C	-2.331490	-2.521096	0.787344
C	-2.951524	-3.777785	0.590227
C	-3.099833	-1.505369	1.390768
C	-4.270670	-3.990778	0.980007
H	-2.384013	-4.590897	0.158697
C	-4.421940	-1.733621	1.777288
H	-2.661287	-0.534308	1.588632
C	-5.023354	-2.974632	1.574761
H	-4.712994	-4.970872	0.816174
H	-4.975326	-0.926352	2.251332
H	-6.050990	-3.151549	1.880523
C	-0.427402	-1.153162	-2.092339
C	-0.257425	0.209219	-2.042260
H	0.738104	0.637123	-1.980458
H	-1.070829	0.874248	-2.314949
C	-1.727416	-1.755510	-2.573107
H	-1.984638	-2.671648	-2.040010
H	-1.606535	-2.008354	-3.635899
H	-2.554305	-1.046192	-2.479799

B2-1

Atom	X	Y	Z
Pd	-0.891819	-0.355789	-0.327145
C	0.613942	2.518430	0.108816
O	1.320826	3.666546	0.260726
N	1.216829	1.469892	-0.304470
C	-1.319264	3.912184	0.818794
C	-2.663490	4.079041	1.045714
C	-3.548864	2.997298	0.842201
C	-2.995238	1.743759	0.420379
C	-0.835012	2.649608	0.400527
H	-5.353083	4.071204	1.355539
H	-0.615025	4.723339	0.946444
H	-3.054795	5.038799	1.371637
C	-4.950905	3.114924	1.033315
C	-3.878621	0.655601	0.193013
C	-5.235428	0.805556	0.381632
C	-5.780331	2.041182	0.808799

H	-3.470101	-0.294069	-0.138569
H	-5.896994	-0.035655	0.197743
H	-6.851816	2.136452	0.953333
N	-1.638467	1.593515	0.225875
C	2.707196	3.337649	-0.038453
H	3.040269	4.058254	-0.786282
C	2.626226	1.866619	-0.557164
H	2.800604	1.766237	-1.634404
C	3.594011	3.335913	1.228869
H	4.365018	4.112879	1.179460
H	2.982821	3.554661	2.113452
C	4.188624	1.942476	1.263951
C	3.659974	1.124138	0.259033
C	5.172427	1.449895	2.122718
C	4.118513	-0.181648	0.082472
C	5.620752	0.136648	1.960100
H	5.595607	2.079637	2.900992
C	5.102106	-0.674270	0.943194
H	3.725754	-0.802721	-0.718710
H	6.390779	-0.253863	2.619266
H	5.476069	-1.686082	0.815708
C	-1.150254	-3.916875	2.375139
C	-0.579968	-3.208470	1.307104
C	-0.222873	-3.904366	0.136400
C	-0.388059	-5.293567	0.075865
C	-0.940552	-5.989699	1.149089
C	-1.335114	-5.297903	2.295375
H	-1.411827	-3.387333	3.287332
H	-0.094590	-5.807729	-0.833267
H	-1.071069	-7.065814	1.087514
H	-1.772442	-5.831066	3.134331
C	0.237932	-3.230443	-1.115631
O	0.957666	-3.793627	-1.932266
N	-0.378522	-2.009891	-1.397284
C	-0.001394	-1.177109	-2.427992
C	1.273943	-1.089894	-3.051727
C	-0.997142	-0.185934	-2.718899
C	1.531536	-0.028520	-3.894611
H	2.005129	-1.866874	-2.872943
C	-0.679405	0.913108	-3.550813
H	-2.039693	-0.425870	-2.517614
C	0.572074	0.989762	-4.128593
H	2.495668	0.031859	-4.392409
H	-1.443130	1.650252	-3.780333
H	0.814349	1.806078	-4.802591
C	-0.221625	-1.778053	1.538653
C	-1.197558	-0.854892	1.860943
H	-2.236353	-1.163249	1.939341
H	-0.928696	0.082732	2.339206
C	1.246515	-1.494138	1.751942
H	1.863246	-1.914175	0.953480
H	1.555924	-1.990948	2.682055
H	1.457176	-0.426647	1.831508

B3

Atom	X	Y	Z
Pd	-0.474006	-0.114747	0.342930
C	-1.469477	0.407275	3.105003
O	-2.494094	0.888055	2.579620
O	-0.439699	-0.042934	2.473305
C	-1.377493	0.288421	4.625778
H	-1.481066	-0.765685	4.909162
H	-0.397181	0.622962	4.979935
H	-2.170489	0.865982	5.106743
C	0.765716	2.701346	0.424285
O	0.536613	4.019426	0.619976
N	-0.265784	1.950955	0.258075
C	3.125039	3.228019	1.050780
C	4.450419	2.871982	1.101949
C	4.863586	1.626686	0.568603
C	3.850858	0.789686	-0.006358
C	2.198357	2.318785	0.466997
H	6.974351	1.818819	1.013854
H	2.775355	4.173623	1.445653
H	5.187090	3.536281	1.547204
C	6.210909	1.181207	0.574650
C	4.224211	-0.464317	-0.560904
C	5.539882	-0.866830	-0.539248
C	6.541221	-0.040366	0.031960
H	3.445527	-1.082804	-0.992394
H	5.816490	-1.828945	-0.961012
H	7.574112	-0.377320	0.040303
N	2.539930	1.150493	-0.043727
C	-0.901122	4.233595	0.572393
H	-1.177896	4.684911	1.526854
C	-1.484814	2.806795	0.357066
H	-2.068113	2.412132	1.195488
C	-1.299432	5.103044	-0.642342
H	-1.840811	6.002227	-0.323932
H	-0.400101	5.444165	-1.169547
C	-2.169262	4.194238	-1.485462
C	-2.290149	2.920233	-0.919058

C	-2.849389	4.509097	-2.662740
C	-3.119593	1.959228	-1.498644
C	-3.658289	3.539526	-3.260253
H	-2.761310	5.498085	-3.106384
C	-3.799496	2.274715	-2.677377
H	-3.238087	0.986112	-1.032009
H	-4.194447	3.774765	-4.175936
H	-4.450233	1.537120	-3.139475
C	1.634536	-2.847564	-2.746328
C	0.816787	-2.704596	-1.624616
C	1.228633	-3.220752	-0.398499
C	2.435649	-3.905233	-0.245692
C	3.243589	-4.064220	-1.369924
C	2.843210	-3.536529	-2.608482
H	1.340693	-2.443245	-3.711090
H	2.715418	-4.301870	0.725541
H	4.185006	-4.600994	-1.292679
H	3.482276	-3.670229	-3.477410
C	0.183270	-3.015949	0.621068
O	0.137372	-3.449542	1.748018
N	-0.882041	-2.238793	-0.006696
C	-2.228629	-2.673136	0.360956
C	-2.562521	-4.029336	0.237825
C	-3.176166	-1.765050	0.835020
C	-3.845451	-4.466427	0.559450
H	-1.817503	-4.744475	-0.098199
C	-4.463335	-2.211063	1.151477
H	-2.907074	-0.726972	1.012371
C	-4.804363	-3.555225	1.009887
H	-4.092743	-5.519970	0.461597
H	-5.188464	-1.496719	1.530694
H	-5.804365	-3.896714	1.263372
C	-0.531892	-2.022155	-1.526469
C	-0.425995	-0.496860	-1.645613
H	0.518808	-0.153839	-2.073835
H	-1.273063	-0.054819	-2.178158
C	-1.561268	-2.639737	-2.475812
H	-1.649687	-3.723717	-2.358454
H	-1.243469	-2.429938	-3.503133
H	-2.547446	-2.190400	-2.328777

B4

Atom	X	Y	Z
Pd	0.477409	-0.209833	1.111294
C	2.156807	-0.346437	3.448137
O	1.468512	-1.201552	2.765429
O	2.190451	0.880624	3.227008
C	2.945392	-0.938115	4.615467
H	3.493858	-1.830574	4.296337
H	3.636414	-0.199041	5.026696
H	2.251291	-1.253894	5.403618
C	1.401826	-2.294709	-0.966682
O	2.436581	-2.941743	-1.549393
N	1.696619	-1.341044	-0.154588
C	-0.091313	-3.577022	-2.517823
C	-1.346269	-4.031305	-2.845591
C	-2.448866	-3.718590	-2.012129
C	-2.187233	-2.928735	-0.843534
C	0.057222	-2.792434	-1.340733
H	-3.972813	-4.744010	-3.160842
H	0.773291	-3.801808	-3.130553
H	-1.503307	-4.630321	-3.739280
C	-3.776457	-4.145392	-2.274680
C	-3.261536	-2.592356	0.025138
C	-4.537588	-3.020914	-0.261264
C	-4.797553	-3.802435	-1.416734
H	-3.039724	-1.992699	0.902187
H	-5.358042	-2.759482	0.400873
H	-5.812600	-4.130166	-1.623042
N	-0.940795	-2.485912	-0.532225
C	3.660481	-2.288919	-1.110001
H	4.303941	-3.077056	-0.716879
C	3.176024	-1.272749	-0.035151
H	3.421437	-1.548929	0.994317
C	4.329313	-1.481079	-2.248185
H	5.315765	-1.887514	-2.500902
H	3.718546	-1.545360	-3.157589
C	4.412681	-0.069698	-1.702797
C	3.783227	0.045328	-0.458106
C	5.037886	1.038377	-2.275695
C	3.780890	1.250339	0.246562
C	5.025475	2.253689	-1.585444
H	5.535413	0.959771	-3.239484
C	4.407194	2.357590	-0.333395
H	3.306631	1.317880	1.223847
H	5.513295	3.122684	-2.019528
H	4.423010	3.304708	0.199087
C	-0.337752	3.320229	-2.583765
C	-1.089568	3.021836	-1.448896
C	-2.407641	3.450651	-1.355496
C	-3.029016	4.177805	-2.369364
C	-2.282651	4.471083	-3.510048

C	-0.950177	4.042611	-3.612988
H	0.697350	3.002537	-2.676931
H	-4.061043	4.496616	-2.257411
H	-2.730632	5.033423	-4.324551
H	-0.382306	4.278137	-4.509399
C	-2.987471	2.991266	-0.077805
O	-4.130325	3.183220	0.312329
N	-1.970769	2.278913	0.586009
C	-2.188097	1.436408	1.689970
C	-1.099437	0.910364	2.438414
C	-3.493964	1.056468	2.063861
C	-1.340733	0.037302	3.519190
H	-0.104239	1.375942	2.397595
C	-3.698393	0.184358	3.129080
H	-4.337772	1.459701	1.525084
C	-2.630298	-0.341498	3.863713
H	-0.489004	-0.338916	4.071787
H	-4.719247	-0.087489	3.387391
H	-2.805648	-1.019406	4.693485
C	-0.675649	2.293521	-0.175439
C	-0.228082	0.850953	-0.483844
H	-1.062920	0.301080	-0.934071
H	0.591495	0.892603	-1.210275
C	0.405595	3.162557	0.511138
H	0.007727	4.161728	0.718242
H	1.259374	3.266869	-0.166317
H	0.786866	2.735129	1.439167

B5

Atom	X	Y	Z
Pd	-0.173039	-0.200805	0.015893
C	-2.722512	1.126243	-0.872233
O	-3.554381	2.147806	-1.167653
N	-1.474419	1.391732	-0.710883
C	-4.633394	-0.468783	-1.130181
C	-5.097831	-1.761044	-1.099961
C	-4.210594	-2.816117	-0.778971
C	-2.850167	-2.479654	-0.458518
C	-3.279820	-0.230162	-0.790657
H	-5.639449	-4.422404	-1.018768
H	-5.268527	0.365450	-1.403148
H	-6.133793	-1.986600	-1.339808
C	-4.606861	-4.178378	-0.782275
C	-1.927530	-3.527003	-0.195298
C	-2.345066	-4.839003	-0.221078
C	-3.693240	-5.170019	-0.505367
H	-0.898899	-3.266177	0.019575
H	-1.629588	-5.631482	-0.021827
H	-4.000676	-6.211832	-0.514706
N	-2.420837	-1.181521	-0.425056
C	-2.710608	3.329191	-1.356569
H	-2.711069	3.542328	-2.429014
C	-1.339321	2.861192	-0.784198
H	-0.485856	3.112955	-1.421297
C	-3.205922	4.497975	-0.493369
H	-3.071702	5.444009	-1.035038
H	-4.276573	4.401308	-0.281692
C	-2.332168	4.435437	0.741668
C	-1.273867	3.533463	0.578218
C	-2.464775	5.156657	1.928376
C	-0.339249	3.334362	1.594904
C	-1.529764	4.961911	2.947860
H	-3.285037	5.857748	2.062310
C	-0.475440	4.056357	2.782917
H	0.464942	2.616163	1.473930
H	-1.624516	5.515441	3.878171
H	0.240907	3.908376	3.586055
C	4.154142	1.413451	-2.286837
C	3.948631	0.462825	-1.288482
C	5.007242	0.053786	-0.486332
C	6.292590	0.570489	-0.633481
C	6.501268	1.526931	-1.627555
C	5.439556	1.941911	-2.445932
H	3.342597	1.743526	-2.930742
H	7.093804	0.227032	0.014318
H	7.489793	1.954192	-1.773365
H	5.619450	2.686739	-3.217176
C	4.528617	-0.954849	0.488376
O	5.209564	-1.501818	1.348750
N	3.168749	-1.131731	0.228295
C	2.268005	-1.855519	1.059449
C	0.885416	-1.546122	1.080393
C	2.782170	-2.871790	1.889634
C	0.099829	-2.217232	2.037729
C	1.960535	-3.530486	2.800749
H	3.835188	-3.108107	1.839849
C	0.612687	-3.191598	2.897356
H	-0.957843	-1.968964	2.114164
H	2.385513	-4.300897	3.439423
H	-0.035309	-3.678154	3.622953
C	2.683670	-0.282841	-0.894498
C	1.605254	0.687053	-0.399402

H	1.993636	1.243894	0.461479
H	1.368281	1.401928	-1.199766
C	2.216696	-1.162810	-2.072382
H	3.040753	-1.788368	-2.431980
H	1.873585	-0.531936	-2.900526
H	1.385227	-1.801346	-1.764068

B6

Atom	X	Y	Z
Pd	0.653103	-1.078958	0.011874
C	2.625038	1.135272	-1.056055
O	3.752560	1.424297	-1.757995
N	2.362077	-0.108629	-0.847555
C	2.380353	3.612988	-0.761888
C	1.644685	4.682574	-0.311877
C	0.382546	4.465075	0.295103
C	-0.068826	3.107544	0.404345
C	1.843963	2.304605	-0.600863
H	-0.096921	6.537303	0.704586
H	3.349321	3.744795	-1.227679
H	2.021497	5.697441	-0.414915
C	-0.441459	5.509301	0.788981
C	-1.329170	2.840766	1.006343
C	-2.102898	3.877283	1.477045
C	-1.657859	5.219999	1.367092
H	-1.648273	1.807475	1.083932
H	-3.063448	3.666029	1.938398
H	-2.284131	6.023745	1.744409
N	0.667550	2.059364	-0.049912
C	4.331013	0.163791	-2.193732
H	4.214655	0.124627	-3.280193
C	3.486168	-0.887992	-1.415665
H	3.076363	-1.680428	-2.048156
C	5.794517	0.030491	-1.735162
H	6.404623	-0.403640	-2.538433
H	6.220384	1.014705	-1.509125
C	5.725245	-0.887846	-0.532694
C	4.441909	-1.418439	-0.362596
C	6.753659	-1.244456	0.340819
C	4.164449	-2.306282	0.676758
C	6.480807	-2.133993	1.382759
H	7.753689	-0.835682	0.216605
C	5.194674	-2.661299	1.550220
H	3.156221	-2.689314	0.809987
H	7.273385	-2.416741	2.070604
H	4.995755	-3.347975	2.368591
C	-5.073417	-1.554630	-2.449346
C	-4.481569	-1.119190	-1.266600
C	-5.276498	-0.642821	-0.218545
C	-6.666145	-0.603853	-0.308174
C	-7.260190	-1.053634	-1.488328
C	-6.469481	-1.525768	-2.545734
H	-4.473913	-1.918899	-3.279758
H	-7.255431	-0.236570	0.526952
H	-8.341722	-1.040496	-1.591642
H	-6.949108	-1.876756	-3.455726
C	-4.418737	-0.290607	0.945291
O	-4.759763	0.069681	2.061845
N	-3.108044	-0.502987	0.514934
C	-2.053545	-1.031883	1.286461
C	-1.309455	-1.959703	0.482606
C	-1.813644	-0.846123	2.633961
C	-0.293708	-2.735757	1.107588
C	-0.786049	-1.612633	3.232021
H	-2.429185	-0.170099	3.214724
C	-0.045501	-2.526448	2.500545
H	0.088467	-3.636075	0.631322
H	-0.585780	-1.485390	4.292499
H	0.716847	-3.125157	2.991925
C	-3.018551	-0.982894	-0.895571
C	-2.144776	-2.263194	-0.765700
H	-2.779026	-3.142587	-0.584124
H	-1.552928	-2.448403	-1.664747
C	-2.331120	0.072989	-1.783294
H	-2.873298	1.022771	-1.739175
H	-2.314431	-0.269892	-2.824507
H	-1.298379	0.231817	-1.452294

C-TS1

Atom	X	Y	Z
C	2.425184	-0.062403	-1.573134
C	1.664538	0.354893	-0.471513
C	1.255089	-0.621750	0.466181
C	1.651841	-1.956574	0.300970
C	2.398118	-2.352285	-0.805666
C	2.776265	-1.400638	-1.752317
H	2.759696	0.686440	-2.285215
H	1.345698	-2.681487	1.048721
H	2.680350	-3.394130	-0.927701
H	3.357966	-1.693249	-2.622295
C	0.383770	-0.326746	1.655978
O	0.577113	-0.858822	2.726438

N	-0.746136	0.566115	1.477124
H	-0.467759	1.535036	1.363121
C	-1.765335	0.188479	0.579580
C	-2.467419	1.164869	-0.146003
C	-2.143029	-1.158062	0.446934
C	-3.517434	0.799489	-0.985653
H	-2.187701	2.210719	-0.045365
C	-3.184920	-1.512461	-0.407766
H	-1.635253	-1.920708	1.030067
C	-3.880571	-0.540984	-1.129938
H	-4.050929	1.571263	-1.534859
H	-3.461245	-2.559843	-0.498583
H	-4.696622	-0.822989	-1.788750
C	1.427203	1.821947	-0.288467
C	0.750833	2.534765	-1.198632
H	0.290777	2.065671	-2.063268
H	0.631019	3.611183	-1.100315
C	2.092419	2.468430	0.909787
H	1.806117	1.994318	1.857647
H	3.183045	2.365509	0.840569
H	1.851579	3.534210	0.972813

C-TS2

Atom	X	Y	Z
C	-5.308340	1.743651	0.798132
C	-4.080379	1.067106	0.871117
C	-3.082030	1.407276	-0.067008
C	-3.308567	2.430083	-0.997702
C	-4.536909	3.084333	-1.055489
C	-5.544781	2.729618	-0.158623
H	-6.076198	1.497653	1.525753
H	-2.512427	2.697772	-1.686292
H	-4.702136	3.866866	-1.790730
H	-6.507591	3.232770	-0.188811
C	-1.746760	0.727190	-0.114901
O	-0.741594	1.531188	0.078962
N	-1.547630	-0.549537	-0.325599
H	-0.271648	-1.053045	-0.113078
C	-2.519794	-1.493584	-0.731411
C	-2.433314	-2.785723	-0.188701
C	-3.483995	-1.233977	-1.717864
C	-3.314439	-3.784121	-0.597000
H	-1.670529	-2.993316	0.555942
C	-4.365242	-2.238046	-2.118113
H	-3.535093	-0.253207	-2.177657
C	-4.290206	-3.515065	-1.559382
H	-3.236053	-4.777111	-0.161956
H	-5.107051	-2.020492	-2.882389
H	-4.975821	-4.294864	-1.879340
C	-3.865660	0.078481	1.972240
C	-4.682241	-0.972768	2.111890
H	-5.474624	-1.180390	1.398776
H	-4.563835	-1.675856	2.932474
C	-2.758652	0.373303	2.960954
H	-2.953687	1.318124	3.485499
H	-2.677934	-0.423476	3.706706
H	-1.784272	0.485146	2.473575
C	5.308333	-1.743691	0.798118
C	4.080370	-1.067153	0.871137
C	3.082038	-1.407253	-0.067031
C	3.308589	-2.429994	-0.997795
C	4.536931	-3.084239	-1.055612
C	5.544790	-2.729586	-0.158705
H	6.076178	-1.497749	1.525773
H	2.512459	-2.697633	-1.686416
H	4.702170	-3.866719	-1.790907
H	6.507600	-3.232736	-0.188914
C	1.746775	-0.727160	-0.114920
O	0.741593	-1.531201	0.078866
N	1.547652	0.549580	-0.325542
H	0.271671	1.053073	-0.112975
C	2.519808	1.493633	-0.731372
C	2.433405	2.785744	-0.188584
C	3.483919	1.234050	-1.717917
C	3.314522	3.784139	-0.596908
H	1.670690	2.993318	0.556136
C	4.365161	2.238116	-2.118188
H	3.534955	0.253297	-2.177756
C	4.290201	3.515107	-1.559387
H	3.236199	4.777109	-0.161806
H	5.106903	2.020580	-2.882534
H	4.975808	4.294907	-1.879362
C	3.865642	-0.078605	1.972330
C	4.682255	0.972605	2.112087
H	5.474648	1.180272	1.398997
H	4.563857	1.675625	2.932730
C	2.758570	-0.373440	2.960969
H	1.784200	-0.485196	2.473555
H	2.953561	-1.318340	3.485391
H	2.677861	0.423243	3.706825

C-TS3

Atom	X	Y	Z
C	4.927303	-0.838893	1.161702
C	3.542229	-0.643207	1.047060
C	2.875712	-1.278078	-0.023436
C	3.577851	-2.117793	-0.899076
C	4.953239	-2.292327	-0.767225
C	5.630613	-1.639137	0.262425
H	5.446853	-0.367835	1.990726
H	3.036192	-2.620794	-1.694629
H	5.487837	-2.936335	-1.459352
H	6.703140	-1.767849	0.380096
C	1.414206	-1.106643	-0.279493
O	0.753733	-2.243424	-0.233865
N	0.800078	0.014086	-0.534146
H	-0.522043	0.051565	-0.600519
C	1.418202	1.268950	-0.786079
C	0.790751	2.410586	-0.267802
C	2.544572	1.414393	-1.607583
C	1.306342	3.676562	-0.536055
H	-0.099311	2.294759	0.342896
C	3.055774	2.685338	-1.867937
H	3.009276	0.540782	-2.050757
C	2.445033	3.820153	-1.331329
H	0.812936	4.553034	-0.125007
H	3.929344	2.786564	-2.506357
H	2.844313	4.808023	-1.543103
C	2.836878	0.157938	2.094143
C	3.199453	1.422637	2.340212
H	3.959298	1.925751	1.749438
H	2.726398	2.003282	3.127962
C	1.780365	-0.550121	2.914398
H	0.979150	-0.968078	2.295136
H	2.219898	-1.393824	3.462303
H	1.327572	0.132167	3.640124
C	-2.294407	-0.955484	-0.862600
O	-1.699984	0.174500	-0.671499
C	-3.796459	-0.854067	-1.184707
O	-4.169370	-1.250689	-2.275806
C	-4.728771	-0.296443	-0.165930
C	-4.290422	0.187702	1.075811
C	-6.100745	-0.289073	-0.466399
C	-5.213566	0.671129	2.002209
H	-3.230959	0.203314	1.307903
C	-7.018649	0.195103	0.459021
H	-6.418723	-0.671290	-1.431079
C	-6.575780	0.675202	1.696155
H	-4.869852	1.047103	2.961902
H	-8.079045	0.198282	0.221972
H	-7.293248	1.052374	2.420261
O	-1.761292	-2.075994	-0.855816
H	-0.232601	-2.151308	-0.499898

C-TS4

Atom	X	Y	Z
C	-2.492240	-1.585651	0.072556
C	-1.552056	-0.621162	0.465953
C	-1.515292	0.592905	-0.257043
C	-2.424012	0.828450	-1.298946
C	-3.343367	-0.148084	-1.673506
C	-3.368473	-1.363621	-0.989502
H	-2.542318	-2.514560	0.632747
H	-2.388982	1.781676	-1.817155
H	-4.036287	0.041930	-2.488029
H	-4.082948	-2.133569	-1.268141
C	-0.529446	1.661142	0.018095
O	-0.888968	2.890467	0.218049
N	0.790434	1.634024	0.104837
H	0.419208	2.917597	0.295472
C	1.755635	0.683840	-0.260296
C	3.000184	0.734843	0.386446
C	1.554030	-0.260568	-1.281334
C	4.014364	-0.152773	0.035045
H	3.153545	1.476302	1.165026
C	2.571856	-1.150336	-1.619516
H	0.607762	-0.287428	-1.811487
C	3.805215	-1.104243	-0.965749
H	4.971930	-0.101005	0.546676
H	2.402298	-1.876338	-2.410710
H	4.596859	-1.796024	-1.239494
C	-0.696227	-0.888012	1.662562
C	0.084492	-1.974360	1.708768
H	0.174697	-2.651845	0.864780
H	0.681571	-2.204186	2.587362
C	-0.826684	0.059109	2.835521
H	-0.593312	1.093789	2.563102
H	-1.855818	0.058645	3.217987
H	-0.157366	-0.235766	3.649293

HOAc

Atom	X	Y	Z
C	-0.092247	0.125912	0.000314
O	-0.645376	1.202172	-0.000084

O	-0.778837	-1.046773	-0.000050
H	-1.723458	-0.802526	-0.000131
C	1.397256	-0.110034	-0.000071
H	1.685315	-0.690820	0.882235
H	1.684698	-0.692973	-0.881142
H	1.917095	0.847863	-0.001347

PGA

Atom	X	Y	Z
C	-2.119453	-0.384948	-0.064965
O	-2.084659	-1.438981	-0.662526
C	-0.999834	0.676546	-0.081673
O	-1.332908	1.845693	-0.168920
C	0.417884	0.235545	-0.032621
C	0.809000	-1.107879	0.098088
C	1.401111	1.240028	-0.088408
C	2.162539	-1.433826	0.170082
H	0.061337	-1.890886	0.127061
C	2.748713	0.908474	-0.018997
H	1.080088	2.271980	-0.184773
C	3.131697	-0.430865	0.111267
H	2.460366	-2.473806	0.268872
H	3.502821	1.689183	-0.064087
H	4.185494	-0.690824	0.166793
O	-3.175406	0.035318	0.651402
H	-3.856259	-0.660334	0.569851

Qox

Atom	X	Y	Z
C	-0.227921	-0.655248	-0.674466
O	-0.884779	-1.814006	-0.334644
N	-0.873218	0.253416	-1.293595
C	1.777571	-1.735008	0.386532
C	3.098436	-1.674651	0.758328
C	3.850494	-0.504551	0.489055
C	3.170753	0.570798	-0.171488
C	1.198073	-0.609209	-0.264293
H	5.729093	-1.169981	1.337660
H	1.172877	-2.613282	0.576455
H	3.575003	-2.515197	1.257634
C	5.217929	-0.351200	0.836459
C	3.887157	1.764603	-0.461002
C	5.212387	1.882575	-0.111017
C	5.883774	0.817377	0.542603
H	3.349674	2.563839	-0.961301
H	5.754498	2.797351	-0.334597
H	6.930627	0.929019	0.811436
N	1.863013	0.500738	-0.534658
C	-2.227720	-1.699910	-0.868208
H	-2.333267	-2.472961	-1.634477
C	-2.255690	-0.237101	-1.417902
H	-2.567699	-0.169469	-2.466823
C	-3.294515	-1.808641	0.240802
H	-4.113859	-2.466386	-0.078531
H	-2.864448	-2.253578	1.145436
C	-3.774400	-0.386206	0.445896
C	-3.214485	0.487080	-0.492120
C	-4.670212	0.093474	1.402362
C	-3.531222	1.844657	-0.484407
C	-4.993892	1.452147	1.410419
H	-5.110670	-0.578287	2.135680
C	-4.427289	2.323646	0.473126
H	-3.074678	2.518604	-1.204055
H	-5.689371	1.835919	2.152359
H	-4.683471	3.379586	0.493983

R-2a

Atom	X	Y	Z
C	-2.781116	-1.415110	-0.213460
C	-1.694804	-0.584613	0.046669
C	-1.842854	0.804924	-0.014939
C	-3.055568	1.400714	-0.350903
C	-4.141950	0.568105	-0.623266
C	-4.002905	-0.824987	-0.556231
H	-2.690747	-2.497281	-0.162998
H	-3.135587	2.482717	-0.399301
H	-5.102926	0.998943	-0.890143
H	-4.858390	-1.458293	-0.775681
C	-0.534171	1.464741	0.250806
O	-0.246282	2.647186	0.177267
C	1.701021	0.341739	0.197362
C	1.953295	-0.906298	-0.395006
C	2.691876	1.306721	0.343981
C	3.237424	-1.215599	-0.824335
C	3.977623	0.984939	-0.105773
H	2.461492	2.271010	0.781409
C	4.253670	-0.261939	-0.672712
H	3.451649	-2.177095	-1.284801
H	4.773884	1.717303	-0.004146
H	5.262170	-0.493436	-1.003740
C	-0.283014	-0.925150	0.479967
C	0.654064	-1.686565	-0.509600

H	0.266871	-1.643462	-1.535970
H	0.751745	-2.742910	-0.238235
C	-0.268633	-1.600773	1.863718
H	-0.793015	-0.983883	2.599203
H	-0.760172	-2.579046	1.813667
H	0.762416	-1.749123	2.202387
N	0.342447	0.424568	0.568934

S-2a

Atom	X	Y	Z
C	2.781062	-1.415111	-0.213661
C	1.694789	-0.584620	0.046613
C	1.842844	0.804923	-0.014893
C	3.055556	1.400722	-0.350861
C	4.141909	0.568118	-0.623361
C	4.002843	-0.824975	-0.556452
H	2.690673	-2.497284	-0.163282
H	3.135591	2.482727	-0.399169
H	5.102873	0.998967	-0.890263
H	4.858302	-1.458273	-0.776028
C	0.534159	1.464737	0.250802
O	0.246282	2.647188	0.177437
N	-0.342456	0.424529	0.568919
C	-1.701015	0.341692	0.197428
C	-1.953356	-0.906408	-0.394773
C	-2.691822	1.306789	0.343797
C	-3.237452	-1.215625	-0.824275
C	-3.977554	0.985027	-0.105974
H	-2.461386	2.271127	0.781088
C	-4.253651	-0.261895	-0.672802
H	-3.451674	-2.177106	-1.284775
H	-4.773769	1.717462	-0.004484
H	-5.262134	-0.493366	-1.003897
C	0.283013	-0.925155	0.479996
C	-0.654160	-1.686743	-0.509344
H	-0.267094	-1.644019	-1.535770
H	-0.751877	-2.743001	-0.237624
C	0.268826	-1.600635	1.863856
H	0.793228	-0.983596	2.599200
H	0.760435	-2.578875	1.813872
H	-0.762184	-1.749016	2.202634

TS1'

Atom	X	Y	Z
Pd	-0.267554	-0.708250	0.912686
C	0.678538	-0.350872	-2.127199
O	1.771012	0.338891	-2.094014
O	0.107608	-0.912220	-1.162728
C	0.039623	-0.470732	-3.491903
H	0.792252	-0.433885	-4.282414
H	-0.549335	-1.387957	-3.552643
H	-0.643038	0.378438	-3.618955
C	-1.091510	-1.598578	3.491548
O	-1.439762	-2.653005	2.960314
O	-0.670977	-0.525075	2.865765
C	-1.097169	-1.420841	5.005768
H	-0.072841	-1.534303	5.379296
H	-1.442554	-0.421391	5.285309
H	-1.726812	-2.185139	5.466299
C	-2.919014	0.705558	0.270327
O	-4.260434	0.600997	0.334455
N	-2.250470	-0.374142	0.483406
C	-3.152635	3.181849	0.454735
C	-2.740580	4.444129	0.103860
C	-1.633538	4.603248	-0.765306
C	-0.976157	3.414055	-1.224197
C	-2.429261	2.068745	-0.053663
H	-1.668053	6.766884	-0.854057
H	-4.008371	3.020423	1.099672
H	-3.261449	5.322893	0.475990
C	-1.167249	5.868766	-1.207177
C	0.126172	3.533226	-2.114189
C	0.546254	4.775645	-2.531902
C	-0.102395	5.951797	-2.075825
H	0.626832	2.625972	-2.434600
H	1.387716	4.860993	-3.213792
H	0.247196	6.922653	-2.415874
N	-1.382321	2.167669	-0.853004
C	-4.586162	-0.765404	0.746611
H	-4.985261	-0.694056	1.761352
C	-3.221561	-1.495114	0.634997
H	-2.932953	-2.075498	1.514112
C	-5.554895	-1.415112	-0.254794
H	-6.297595	-2.019727	0.282239
H	-6.108403	-0.650840	-0.811969
C	-4.663784	-2.279473	-1.122275
C	-3.361664	-2.346116	-0.613666
C	-5.009817	-2.996385	-2.268350
C	-2.392028	-3.138724	-1.228861
C	-4.039285	-3.781986	-2.894226
H	-6.019610	-2.948773	-2.668966
C	-2.740568	-3.855564	-2.375926

H	-1.384559	-3.185587	-0.829170
H	-4.296233	-4.344990	-3.787648
H	-1.998103	-4.478286	-2.867771
C	5.177323	-2.922592	-1.346692
C	4.580152	-1.827682	-0.700227
C	3.334787	-2.038360	-0.050807
C	2.768291	-3.326249	-0.042140
C	3.385219	-4.396123	-0.681903
C	4.592976	-4.188646	-1.348659
H	6.134167	-2.768417	-1.836506
H	1.824383	-3.461687	0.473790
H	2.925437	-5.380426	-0.663129
H	5.089078	-5.010923	-1.858145
C	2.540100	-0.957647	0.605087
O	1.634914	-1.332749	1.445268
N	2.758075	0.294717	0.216177
H	2.310437	0.353429	-1.096565
C	2.373832	1.434986	0.952584
C	2.531328	2.671343	0.294545
C	1.970724	1.446201	2.304397
C	2.279177	3.873270	0.949892
H	2.878712	2.670531	-0.734228
C	1.734239	2.657241	2.955117
H	1.833831	0.515477	2.837757
C	1.877902	3.875588	2.288143
H	2.404672	4.810766	0.414200
H	1.426673	2.641060	3.997815
H	1.686254	4.812471	2.804572
C	5.354111	-0.544799	-0.696122
C	5.672051	0.057872	-1.848908
H	5.302618	-0.302620	-2.804994
H	6.291861	0.950982	-1.866377
C	5.888671	-0.064231	0.634351
H	5.082059	0.130807	1.346887
H	6.543848	-0.823919	1.081532
H	6.465563	0.857983	0.512631

TS2'

Atom	X	Y	Z
C	5.050786	-1.370084	-1.121428
C	4.118633	-1.766614	-0.151313
C	2.743259	-1.649709	-0.461103
C	2.348258	-1.167792	-1.718835
C	3.293345	-0.794182	-2.672623
C	4.651345	-0.888589	-2.367294
H	6.108980	-1.440038	-0.885649
H	1.292359	-1.110180	-1.970726
H	2.969900	-0.444146	-3.648713
H	5.398752	-0.594591	-3.098730
C	1.733807	-2.204560	0.505224
O	1.818914	-3.347534	0.908392
C	-0.243591	-1.733749	1.971358
C	-0.797783	-0.724858	2.788421
C	-0.677509	-3.060547	2.146583
C	-1.774645	-1.030660	3.733101
H	-0.434880	0.293112	2.711351
C	-1.649326	-3.352834	3.102893
H	-0.240429	-3.858763	1.569684
C	-2.209223	-2.347054	3.894019
H	-2.178831	-0.237691	4.355270
H	-1.961834	-4.384775	3.235806
H	-2.960554	-2.590243	4.639514
C	4.619228	-2.300742	1.156812
C	4.521456	-1.584450	2.281945
H	4.056558	-0.603864	2.310333
H	4.901709	-1.972042	3.223670
C	5.252436	-3.671465	1.107212
H	4.512318	-4.418664	0.795823
H	6.074392	-3.710078	0.380592
H	5.645918	-3.959085	2.086505
Pd	-0.501956	-0.108246	-0.314469
N	0.707255	-1.295375	0.966385
H	1.341957	-0.310961	1.447170
C	-3.061734	0.619272	-1.323860
O	-4.063446	1.389849	-1.723128
N	-1.936069	1.186362	-1.045019
C	-4.444116	-1.449042	-1.572396
C	-4.498458	-2.824525	-1.598503
C	-3.315801	-3.571769	-1.412831
C	-2.089669	-2.867057	-1.137272
C	-3.215648	-0.835145	-1.273100
H	-4.223824	-5.506700	-1.734470
H	-5.310452	-0.830166	-1.773380
H	-5.433291	-3.339906	-1.799471
C	-3.290570	-4.986114	-1.539937
C	-0.885010	-3.605340	-1.075549
C	-0.892061	-4.972539	-1.235219
C	-2.104089	-5.675071	-1.449799
H	0.044678	-3.080984	-0.923425
H	0.046493	-5.516541	-1.192769
H	-2.088347	-6.754718	-1.560137
N	-2.083912	-1.502645	-0.992870

C	-3.520213	2.760792	-1.849615
H	-3.471468	2.957907	-2.922166
C	-2.132753	2.659118	-1.135404
H	-1.307579	3.087703	-1.710314
C	-4.387436	3.746669	-1.061594
H	-4.460142	4.694692	-1.609891
H	-5.408390	3.365354	-0.951431
C	-3.646250	3.920063	0.245748
C	-2.367963	3.348247	0.199118
C	-4.072005	4.601850	1.385470
C	-1.492027	3.475951	1.277625
C	-3.203891	4.711021	2.474438
H	-5.061764	5.048840	1.425498
C	-1.919727	4.157859	2.418578
H	-0.487445	3.074150	1.247658
H	-3.524955	5.240190	3.366949
H	-1.241422	4.262316	3.259913
C	3.741039	3.598473	0.196163
C	4.666937	4.390653	-0.475312
C	4.655083	4.455849	-1.871253
C	3.714597	3.723254	-2.606672
C	2.788763	2.926977	-1.946981
C	2.789594	2.856933	-0.536599
H	3.730166	3.569213	1.278548
H	5.395274	4.962802	0.090780
H	5.379747	5.077552	-2.389479
H	3.712843	3.774651	-3.691334
H	2.065598	2.342928	-2.504818
C	1.824909	1.986070	0.133431
O	0.929639	1.420136	-0.543476
C	1.838865	1.813215	1.658112
O	1.781723	2.844471	2.316658
O	1.862162	0.601452	2.093728

TS3'

Atom	X	Y	Z
Pd	-0.323246	-0.508627	-0.341518
C	-2.393969	-2.432129	-0.428929
N	-2.270796	-1.148587	-0.419849
C	-1.322716	-4.694462	-0.510317
C	-0.177067	-5.438935	-0.679339
C	1.049250	-4.785603	-0.927275
C	1.078300	-3.345235	-0.935138
C	-1.213178	-3.294272	-0.505115
H	2.206194	-6.591358	-1.196070
H	-2.298220	-5.149022	-0.384481
H	-0.212832	-6.524469	-0.665034
C	2.237637	-5.505925	-1.219692
C	2.275990	-2.691182	-1.313191
C	3.398029	-3.425166	-1.625481
C	3.391498	-4.840599	-1.558940
H	2.275378	-1.613514	-1.382504
H	4.302434	-2.910723	-1.936274
H	4.293157	-5.395506	-1.798067
N	-0.053333	-2.626637	-0.640303
C	-4.547340	-1.792426	-0.579246
H	-4.941581	-1.861644	-1.594141
C	-3.628827	-0.555834	-0.320187
H	-3.723663	0.223407	-1.081033
C	-5.611993	-1.826195	0.522195
H	-6.576944	-1.502628	0.111539
H	-5.753759	-2.844855	0.899225
C	-5.097366	-0.852065	1.560332
C	-4.004197	-0.116875	1.085035
C	-5.605588	-0.611757	2.836904
C	-3.410771	0.871845	1.871976
C	-5.008246	0.370030	3.630516
H	-6.455227	-1.176969	3.210597
C	-3.920040	1.108129	3.150948
H	-2.568196	1.445318	1.498709
H	-5.395007	0.565223	4.626533
H	-3.471048	1.873760	3.777286
C	5.350173	2.546047	0.941259
C	3.993488	2.235506	0.742270
C	3.661671	1.439101	-0.376485
C	4.658183	1.051136	-1.287599
C	5.992933	1.380782	-1.072474
C	6.339328	2.124483	0.056584
H	5.630643	3.160772	1.790396
H	4.374291	0.483726	-2.169061
H	6.752424	1.065754	-1.781749
H	7.375618	2.394265	0.238443
C	2.281768	0.942487	-0.708375
O	1.869039	1.309611	-1.871757
N	1.600574	0.109798	0.065023
C	2.063224	-0.369776	1.331862
C	3.281450	-1.051193	1.473141
C	1.227474	-0.220181	2.450878
C	3.656725	-1.562187	2.715806
H	3.936896	-1.170701	0.618822
C	1.603134	-0.745633	3.686920
H	0.291815	0.320858	2.348104

C	2.819911	-1.417909	3.825051
H	4.606262	-2.080674	2.813355
H	0.947547	-0.620293	4.543894
H	3.114451	-1.824027	4.788152
C	2.973384	2.810355	1.664952
C	1.883812	3.422518	1.178176
H	1.710282	3.534767	0.112164
H	1.150285	3.869991	1.843845
C	3.252043	2.746912	3.149934
H	4.137470	3.336294	3.418666
H	3.439970	1.718411	3.477443
H	2.408608	3.145202	3.721316
C	-1.288031	1.212565	-2.601982
O	-0.183186	0.702580	-3.004053
O	-2.423401	1.041326	-3.041834
H	0.870819	0.979426	-2.340973
C	-1.220295	2.074207	-1.331466
O	-0.881649	1.506900	-0.254551
O	-3.617902	-2.939977	-0.437747
C	-1.610717	3.477529	-1.339356
C	-1.517532	4.241227	-0.156213
C	-2.052890	4.087213	-2.532403
C	-1.857523	5.587072	-0.169429
H	-1.168425	3.766823	0.754128
C	-2.389725	5.436774	-2.535531
H	-2.152664	3.497662	-3.436538
C	-2.292240	6.185586	-1.359107
H	-1.783251	6.175857	0.739733
H	-2.731954	5.904965	-3.453023
H	-2.555677	7.239418	-1.366942

TS1a

Atom	X	Y	Z
Pd	-0.366381	-0.260857	0.437616
C	-0.171991	-1.278490	3.145381
O	-0.567875	-2.366591	2.724484
O	-0.017115	-0.189781	2.438459
C	0.196508	-1.078001	4.614358
H	1.268497	-0.867777	4.704191
H	-0.338203	-0.216991	5.028842
H	-0.042868	-1.977062	5.185521
C	-3.312341	0.534385	0.576412
O	-4.599023	0.195980	0.799369
N	-2.430526	-0.386899	0.753849
C	-4.218025	2.715892	-0.254221
C	-4.002675	4.014189	-0.649252
C	-2.689729	4.546069	-0.634107
C	-1.633207	3.679849	-0.195480
C	-3.098640	1.938916	0.154334
H	-3.180766	6.528839	-1.355405
H	-5.209344	2.279769	-0.249675
H	-4.830897	4.640157	-0.972613
C	-2.378240	5.874680	-1.023141
C	-0.300474	4.172671	-0.156225
C	-0.033816	5.466689	-0.541065
C	-1.077040	6.323501	-0.977515
H	0.482842	3.504456	0.183414
H	0.987042	5.836237	-0.510369
H	-0.843801	7.341726	-1.276649
N	-1.860944	2.396243	0.188547
C	-4.631587	-1.215383	1.158402
H	-5.121742	-1.270318	2.131845
C	-3.130891	-1.631179	1.179378
H	-2.738596	-1.913902	2.157469
C	-5.345371	-2.058110	0.076286
H	-6.187053	-2.615848	0.505135
H	-5.763165	-1.399690	-0.695262
C	-4.267532	-2.982534	-0.451459
C	-3.039670	-2.766659	0.184022
C	-4.391421	-3.987157	-1.411892
C	-1.927936	-3.560417	-0.099150
C	-3.274276	-4.768876	-1.720669
H	-5.342133	-4.167961	-1.908281
C	-2.054493	-4.561639	-1.065457
H	-0.996402	-3.399748	0.434592
H	-3.358361	-5.554480	-2.467295
H	-1.198109	-5.184373	-1.307249
C	6.206719	-1.372772	-0.255982
C	4.883923	-1.247565	-0.718083
C	3.848508	-1.306912	0.241985
C	4.155499	-1.497602	1.596492
C	5.472774	-1.641085	2.024901
C	6.504241	-1.578842	1.088796
H	7.021206	-1.325943	-0.972560
H	3.342448	-1.535968	2.316001
H	5.688861	-1.795134	3.078434
H	7.539201	-1.687404	1.402251
C	2.374172	-1.238790	-0.076626
O	1.828569	-2.324725	-0.476708
N	1.673271	-0.145066	0.171850
C	2.300272	1.121077	0.375012
C	2.289735	1.741072	1.633534

C	2.888386	1.783113	-0.713248
C	2.888060	2.990871	1.798718
H	1.796699	1.238595	2.457418
C	3.488996	3.031023	-0.538701
H	2.868154	1.308715	-1.689310
C	3.495389	3.638862	0.719057
H	2.880611	3.459873	2.779383
H	3.947380	3.529387	-1.389272
H	3.966880	4.608422	0.856865
C	4.652744	-1.010668	-2.176862
C	3.750701	-1.702717	-2.888236
H	3.138190	-2.478903	-2.446704
H	3.614077	-1.506764	-3.949385
C	5.521853	0.041724	-2.835659
H	6.580800	-0.246285	-2.841353
H	5.458745	0.997414	-2.300934
H	5.219296	0.201264	-3.875369
C	-0.534255	-1.108609	-2.440269
O	-0.788285	-0.202558	-1.601494
O	0.228090	-2.119567	-2.261321
C	-1.213780	-1.031076	-3.788669
H	-1.624032	-0.034418	-3.958498
H	-0.511093	-1.299557	-4.581657
H	-2.029939	-1.763063	-3.804833
H	0.875095	-2.162874	-1.311666

TS1b

Atom	X	Y	Z
Pd	-0.215595	-0.350124	0.161475
C	-0.049586	-0.587147	3.070810
O	-0.468566	-1.747005	2.996081
O	0.203707	0.204596	2.066842
C	0.264484	0.046076	4.424137
H	1.336321	-0.059111	4.628627
H	0.028119	1.113491	4.426636
H	-0.288783	-0.470296	5.211947
C	-3.143270	0.471801	0.713363
O	-4.362017	0.082797	1.140554
N	-2.246555	-0.447414	0.618379
C	-4.155471	2.756171	0.561030
C	-4.012084	4.100854	0.318291
C	-2.743042	4.621710	-0.034476
C	-1.651869	3.693800	-0.130308
C	-3.010562	1.921205	0.434346
H	-3.334994	6.697579	-0.215257
H	-5.109120	2.327775	0.843119
H	-4.863050	4.772816	0.400405
C	-2.505913	5.997638	-0.286737
C	-0.355227	4.174114	-0.464187
C	-0.162063	5.516641	-0.698773
C	-1.241165	6.433750	-0.612811
H	0.457949	3.458198	-0.522078
H	0.828903	5.882051	-0.953021
H	-1.063768	7.488604	-0.804012
N	-1.813042	2.362974	0.096130
C	-4.292773	-1.337261	1.466204
H	-4.458245	-1.410642	2.543150
C	-2.860745	-1.745375	1.014418
H	-2.236088	-2.157972	1.810183
C	-5.308409	-2.149116	0.638626
H	-5.882118	-2.822178	1.288380
H	-6.031645	-1.479246	0.158649
C	-4.457668	-2.922250	-0.347121
C	-3.090949	-2.716529	-0.127074
C	-4.887306	-3.796811	-1.346308
C	-2.135909	-3.397777	-0.882702
C	-3.933808	-4.466965	-2.115998
H	-5.948013	-3.962027	-1.520418
C	-2.567215	-4.272838	-1.881755
H	-1.076849	-3.242300	-0.703981
H	-4.255897	-5.151985	-2.896048
H	-1.834952	-4.809100	-2.479199
C	6.183272	0.698375	0.171103
C	4.803366	0.560572	0.400722
C	3.927982	0.792166	-0.683960
C	4.444868	1.204238	-1.922920
C	5.815983	1.326076	-2.129053
C	6.691043	1.058244	-1.075678
H	6.859115	0.540775	1.006349
H	3.749562	1.413849	-2.730124
H	6.195704	1.632016	-3.099992
H	7.764852	1.151699	-1.215383
C	2.433858	0.641181	-0.628145
O	1.768770	1.665691	-1.042640
N	1.811076	-0.458320	-0.236589
C	2.421257	-1.744280	-0.170384
C	3.282062	-2.193642	-1.186251
C	2.081955	-2.624367	0.870399
C	3.829093	-3.475447	-1.133603
H	3.519737	-1.540829	-2.018911
C	2.625797	-3.907703	0.907713
H	1.379679	-2.313105	1.636060

C	3.508279	-4.339448	-0.085250
H	4.496942	-3.801393	-1.927021
H	2.353011	-4.572754	1.722978
H	3.928695	-5.340918	-0.050689
C	4.352996	0.273117	1.796359
C	4.819722	-0.798550	2.450918
H	5.456690	-1.533501	1.967161
H	4.551095	-0.988528	3.487111
C	3.446687	1.289369	2.455649
H	2.432712	1.266441	2.042500
H	3.839354	2.305671	2.323428
H	3.366875	1.089655	3.529277
H	0.816330	1.364271	-1.785049
C	-0.528657	0.057907	-2.763788
O	-0.690624	-0.757900	-1.814489
O	0.124520	1.154458	-2.716928
C	-1.167323	-0.280646	-4.093040
H	-1.694849	-1.233526	-4.037000
H	-1.865853	0.516359	-4.369300
H	-0.396852	-0.321048	-4.869734

TS2a

Atom	X	Y	Z
C	-2.857864	-1.418552	-2.940168
C	-2.002541	-1.783236	-1.894269
C	-2.519523	-2.443756	-0.773701
C	-3.879215	-2.753128	-0.694802
C	-4.729345	-2.392197	-1.738233
C	-4.216907	-1.730899	-2.860635
H	-2.466162	-0.898058	-3.810212
H	-4.240388	-3.276770	0.184606
H	-5.788731	-2.627120	-1.683565
H	-4.878161	-1.456309	-3.678295
C	-1.545091	-2.902869	0.258860
O	-1.826955	-3.770368	1.076017
C	0.863806	-3.093604	0.434241
C	2.010121	-2.482274	0.971093
C	0.910873	-4.477951	0.163597
C	3.164399	-3.227938	1.220007
H	1.979800	-1.427216	1.218657
C	2.061759	-5.214678	0.426527
H	0.031698	-4.977786	-0.227257
C	3.200760	-4.596190	0.950559
H	4.033771	-2.731073	1.643712
H	2.068116	-6.281494	0.217313
H	4.097017	-5.175615	1.154895
C	-0.542927	-1.458582	-1.918209
C	-0.178433	-0.102090	-1.725664
H	-0.968062	0.637863	-1.849825
H	0.813324	0.206607	-2.052775
C	0.385476	-2.411029	-2.619680
H	0.143399	-3.456204	-2.416414
H	0.284882	-2.241379	-3.702031
H	1.427294	-2.223785	-2.344218
Pd	-0.173947	-0.258116	0.410003
C	-1.285355	-0.575479	3.057409
O	-2.353768	-0.235861	2.528437
O	-0.121626	-0.558693	2.477940
C	-1.250244	-1.088539	4.493499
H	-1.220675	-2.184223	4.469558
H	-0.352370	-0.743780	5.014633
H	-2.148437	-0.774134	5.030210
N	-0.279932	-2.330663	0.097005
C	0.795138	2.678339	0.625447
O	0.502834	3.930926	1.037682
N	-0.147536	1.805321	0.711071
C	2.979056	3.678072	-0.064221
C	4.256072	3.530137	-0.547646
C	4.750838	2.236685	-0.844099
C	3.870385	1.127831	-0.614539
C	2.181157	2.513234	0.119698
H	6.718038	2.839541	-1.520056
H	2.572686	4.652598	0.174275
H	4.893151	4.397095	-0.704783
C	6.055382	1.994981	-1.347535
C	4.331043	-0.189025	-0.891093
C	5.602847	-0.388573	-1.378353
C	6.471105	0.708961	-1.610437
H	3.660868	-1.018801	-0.692460
H	5.950087	-1.397010	-1.584870
H	7.470998	0.528969	-1.995206
N	2.605030	1.289153	-0.139760
C	-0.887468	3.949713	1.467888
H	-0.881085	4.278921	2.508347
C	-1.356912	2.479514	1.268455
H	-1.641622	1.948185	2.178084
C	-1.743889	4.854433	0.552680
H	-2.280236	5.608958	1.141391
H	-1.098820	5.399588	-0.147096
C	-2.698770	3.899615	-0.133310
C	-2.509116	2.580578	0.292489
C	-3.713520	4.203559	-1.041896

C	-3.345830	1.552468	-0.143835
C	-4.534513	3.173512	-1.508490
H	-3.872659	5.226238	-1.375950
C	-4.358057	1.860040	-1.056585
H	-3.216285	0.547878	0.246354
H	-5.328710	3.398651	-2.215815
H	-5.016169	1.071800	-1.410483

TS2b

Atom	X	Y	Z
Pd	-0.472076	-0.175816	0.276044
C	-1.116825	0.308293	3.142894
O	-2.124207	0.949972	2.806874
O	-0.248223	-0.227334	2.343279
C	-0.818820	0.049729	4.618264
H	-1.072826	-0.990186	4.854298
H	0.246700	0.180906	4.829119
H	-1.416269	0.713143	5.247704
C	0.704562	2.670893	0.460406
O	0.452352	3.981962	0.663510
N	-0.312679	1.904397	0.274360
C	3.033078	3.181502	1.199495
C	4.360092	2.835057	1.272779
C	4.805513	1.632857	0.671199
C	3.824427	0.826756	0.003840
C	2.139792	2.304677	0.523546
H	6.896328	1.814792	1.205290
H	2.657999	4.094432	1.645218
H	5.073292	3.474053	1.787687
C	6.157022	1.201157	0.696355
C	4.231759	-0.383186	-0.619103
C	5.550506	-0.773722	-0.575397
C	6.520861	0.022053	0.085532
H	3.477546	-0.980936	-1.117297
H	5.852589	-1.703683	-1.048416
H	7.556556	-0.305243	0.109492
N	2.510884	1.178094	-0.056648
C	-0.982852	4.177873	0.539490
H	-1.306058	4.686910	1.448608
C	-1.548591	2.737037	0.393485
H	-2.075657	2.356871	1.273498
C	-1.342472	4.959596	-0.746918
H	-1.803188	5.926745	-0.514196
H	-0.430902	5.171981	-1.319627
C	-2.291659	4.038558	-1.485354
C	-2.415393	2.800613	-0.843460
C	-3.029468	4.310292	-2.638145
C	-3.301993	1.834411	-1.321817
C	-3.897202	3.334448	-3.135174
H	-2.941491	5.271229	-3.139479
C	-4.039029	2.107039	-2.477274
H	-3.421909	0.890373	-0.797487
H	-4.479626	3.537148	-4.030050
H	-4.736181	1.366603	-2.860156
C	1.695479	-2.468580	-2.939731
C	0.836542	-2.424507	-1.834100
C	1.194679	-3.082645	-0.651470
C	2.389168	-3.804202	-0.575824
C	3.234991	-3.860941	-1.681703
C	2.887178	-3.193235	-2.862268
H	1.427678	-1.953223	-3.858468
H	2.619888	-4.322002	0.349884
H	4.160678	-4.427931	-1.631173
H	3.543378	-3.239496	-3.727341
C	0.191795	-3.115241	0.456872
O	0.276496	-3.929239	1.368772
N	-0.874234	-2.240668	0.251607
C	-2.175158	-2.637967	0.644519
C	-2.578965	-3.986507	0.522543
C	-3.127921	-1.696177	1.072597
C	-3.883258	-4.367615	0.818518
H	-1.857501	-4.737314	0.220116
C	-4.438282	-2.088932	1.355712
H	-2.835180	-0.663886	1.235324
C	-4.827875	-3.421409	1.229117
H	-4.164401	-5.413627	0.724099
H	-5.148955	-1.340586	1.697132
H	-5.846291	-3.723723	1.457566
C	-0.468000	-1.697381	-1.889949
C	-0.443093	-0.284133	-1.866603
H	0.521119	0.198725	-2.019127
H	-1.306514	0.244562	-2.266431
C	-1.654123	-2.430917	-2.452846
H	-1.701205	-3.469154	-2.118581
H	-1.561639	-2.429008	-3.549030
H	-2.590379	-1.929838	-2.191054

TS3a

Atom	X	Y	Z
C	1.559649	-1.060582	3.552797
C	2.171074	-1.299956	2.323601
C	3.482317	-1.751450	2.275535

C	4.236578	-1.976332	3.425709
C	3.632023	-1.728726	4.657796
C	2.305605	-1.273761	4.716598
H	0.531835	-0.712855	3.616003
H	5.259850	-2.330931	3.345223
H	4.186755	-1.887150	5.578565
H	1.849526	-1.083746	5.684936
C	3.898323	-1.914752	0.867231
O	4.997154	-2.308160	0.495918
C	2.859290	-1.231356	-1.308018
C	1.723487	-0.734352	-2.023045
C	4.090408	-1.381217	-1.985357
C	1.944019	-0.313500	-3.362877
H	0.550129	-1.446728	-2.150550
C	4.237613	-0.972588	-3.305146
H	4.932236	-1.799944	-1.456369
C	3.168807	-0.411674	-4.006346
H	1.090106	0.069789	-3.913460
H	5.206295	-1.094425	-3.784209
H	3.283547	-0.083110	-5.035810
C	1.601685	-1.202841	0.916152
C	1.078992	0.210124	0.621407
H	1.906106	0.927109	0.676904
H	0.342238	0.481914	1.387243
C	0.537404	-2.312481	0.769101
H	0.962787	-3.280119	1.057443
H	-0.311124	-2.098891	1.426906
H	0.160781	-2.381956	-0.251033
Pd	0.104525	0.340072	-1.153087
C	-1.262485	-1.188034	-3.204297
O	-0.487204	-2.085309	-2.711186
O	-1.156485	0.047388	-2.972864
C	-2.383737	-1.673564	-4.101527
H	-3.207161	-2.029777	-3.470590
H	-2.754273	-0.858969	-4.727095
H	-2.047837	-2.510636	-4.718787
N	2.803869	-1.517380	0.076811
C	-2.439016	1.619693	0.190697
O	-3.155467	2.746904	0.413418
N	-1.315344	1.748747	-0.420628
C	-4.052767	0.451554	1.711498
C	-4.654373	-0.710122	2.132304
C	-4.311351	-1.942245	1.521492
C	-3.327298	-1.908150	0.478583
C	-3.080265	0.373462	0.676009
H	-5.638052	-3.209152	2.674185
H	-4.302649	1.411663	2.146940
H	-5.397654	-0.694135	2.925757
C	-4.893432	-3.185207	1.882198
C	-2.963306	-3.117024	-0.177061
C	-3.550081	-4.304813	0.197208
C	-4.519059	-4.340683	1.233072
H	-2.217772	-3.065451	-0.964837
H	-3.269671	-5.227652	-0.302589
H	-4.967799	-5.289746	1.512818
N	-2.728466	-0.752523	0.082787
C	-2.410246	3.860738	-0.150562
H	-3.064641	4.322299	-0.892084
C	-1.143028	3.184488	-0.757993
H	-1.083856	3.258970	-1.849005
C	-1.944388	4.853447	0.937768
H	-2.316082	5.864927	0.733342
H	-2.350845	4.558228	1.912798
C	-0.432087	4.785886	0.887295
C	0.018504	3.867565	-0.067131
C	0.483851	5.528344	1.634176
C	1.382293	3.687540	-0.301374
C	1.850167	5.341911	1.411805
H	0.142154	6.246241	2.375994
C	2.297267	4.430170	0.448021
H	1.723021	2.970763	-1.043398
H	2.572202	5.914844	1.987466
H	3.362678	4.299758	0.280332

TS3b

Atom	X	Y	Z
Pd	-0.351839	-0.107277	1.104666
C	-1.472319	-1.445277	3.467357
O	-1.530631	-0.263463	3.023554
O	-0.649782	-2.333867	3.048856
C	-2.407446	-1.863336	4.586091
H	-1.825662	-2.006251	5.503702
H	-3.172296	-1.104051	4.759428
H	-2.873202	-2.823715	4.345227
C	-1.937581	2.226338	-0.219248
O	-3.130603	2.804414	-0.487887
N	-1.956099	1.051216	0.304924
C	-0.850299	4.044800	-1.564676
C	0.269648	4.783514	-1.863439
C	1.480270	4.541863	-1.166528
C	1.467421	3.520194	-0.160010
C	-0.749993	3.044744	-0.558562

H	2.692357	6.027965	-2.174833
H	-1.792236	4.206336	-2.075584
H	0.237950	5.553696	-2.630279
C	2.683153	5.253590	-1.411594
C	2.655994	3.242842	0.569309
C	3.806455	3.949925	0.302982
C	3.820458	4.961842	-0.691662
H	2.620262	2.461593	1.322293
H	4.715950	3.733018	0.855817
H	4.739578	5.507827	-0.885216
N	0.351800	2.798374	0.125511
C	-4.171770	1.888945	-0.045611
H	-4.746115	2.423875	0.713034
C	-3.375594	0.666037	0.505004
H	-3.512798	0.484155	1.574803
C	-5.042620	1.401351	-1.224162
H	-6.105399	1.592637	-1.030886
H	-4.783333	1.951283	-2.136810
C	-4.749100	-0.081196	-1.322969
C	-3.836426	-0.497470	-0.347588
C	-5.297183	-1.006488	-2.212724
C	-3.472720	-1.839587	-0.233718
C	-4.925134	-2.349114	-2.110876
H	-6.008977	-0.691267	-2.971952
C	-4.021912	-2.764476	-1.125168
H	-2.767110	-2.156385	0.528405
H	-5.347310	-3.078404	-2.797118
H	-3.748784	-3.813391	-1.049688
C	0.820888	-2.164307	-3.438111
C	1.537669	-2.180145	-2.243058
C	2.873917	-2.554633	-2.237496
C	3.551122	-2.917973	-3.400133
C	2.840946	-2.893755	-4.600184
C	1.488569	-2.518637	-4.615064
H	-0.228507	-1.882594	-3.465546
H	4.597128	-3.206137	-3.353777
H	3.332945	-3.166065	-5.529937
H	0.949647	-2.504067	-5.559068
C	3.403961	-2.476976	-0.860274
O	4.550160	-2.750516	-0.526338
N	2.349026	-2.018957	-0.049807
C	2.490780	-1.511375	1.263497
C	1.381758	-0.966859	1.983124
C	3.776030	-1.484582	1.850883
C	1.669338	-0.326196	3.218233
H	0.266753	-1.714245	2.304545
C	3.992207	-0.860645	3.073357
H	4.601885	-1.939081	1.325994
C	2.942450	-0.251981	3.764682
H	0.834485	0.095960	3.770676
H	4.999068	-0.852100	3.484403
H	3.110398	0.242938	4.717538
C	1.071027	-1.893597	-0.823445
C	0.495962	-0.475177	-0.700596
H	1.280423	0.259869	-0.912717
H	-0.306844	-0.351811	-1.437261
C	0.086352	-3.017166	-0.426919
H	0.544854	-3.996102	-0.605381
H	-0.817905	-2.943895	-1.040257
H	-0.206513	-2.954063	0.621672

TS4a

Atom	X	Y	Z
C	3.950093	-2.990161	-0.310803
C	3.808046	-1.607035	-0.385248
C	4.900761	-0.808252	-0.723806
C	6.158801	-1.348385	-0.980820
C	6.306605	-2.733468	-0.892309
C	5.211758	-3.543593	-0.557891
H	3.109904	-3.631469	-0.056585
H	6.989771	-0.696640	-1.234329
H	7.274314	-3.190282	-1.080783
H	5.345918	-4.620012	-0.487618
C	4.504060	0.622582	-0.682423
O	5.221395	1.598511	-0.849651
C	2.538109	1.593365	0.481221
C	1.500181	1.099265	1.316291
C	3.023980	2.898565	0.618822
C	1.151416	1.884124	2.440145
C	2.553739	3.699368	1.664713
H	3.802245	3.245847	-0.048152
C	1.648024	3.183841	2.592782
H	0.467515	1.486569	3.185186
H	2.940566	4.708682	1.777916
H	1.325182	3.786273	3.438465
C	2.570652	-0.735047	-0.237199
C	1.832027	-0.805470	1.107651
H	2.512009	-0.849350	1.959931
H	1.209076	-1.710347	1.152225
C	1.632704	-1.009991	-1.433454
H	2.178867	-0.888612	-2.374602
H	1.242698	-2.032793	-1.386186

H	0.781965	-0.319770	-1.414495
Pd	-0.223178	0.111536	0.906129
N	3.143633	0.632208	-0.356228
C	-3.259221	-0.155190	0.372693
O	-4.483690	-0.726218	0.477800
N	-2.243077	-0.818939	0.795125
C	-4.363993	1.794978	-0.768892
C	-4.252332	3.052300	-1.313288
C	-3.000232	3.715507	-1.306363
C	-1.886837	3.026882	-0.716353
C	-3.202324	1.195573	-0.216639
H	-3.646231	5.531303	-2.294061
H	-5.305404	1.258700	-0.754828
H	-5.116633	3.546564	-1.750225
C	-2.801841	5.012436	-1.846751
C	-0.614716	3.659666	-0.681235
C	-0.459709	4.918465	-1.216061
C	-1.556994	5.599678	-1.802612
H	0.213785	3.126917	-0.228000
H	0.514897	5.396725	-1.186591
H	-1.410474	6.592755	-2.218304
N	-2.014612	1.780463	-0.185607
C	-4.302968	-1.997232	1.164405
H	-4.811774	-1.905490	2.127028
C	-2.749218	-2.126247	1.266370
H	-2.387918	-2.291416	2.286425
C	-4.824225	-3.171084	0.313928
H	-5.416205	-3.858468	0.932149
H	-5.487317	-2.805627	-0.478473
C	-3.571699	-3.840347	-0.211668
C	-2.414271	-3.279843	0.339663
C	-3.479055	-4.909843	-1.103657
C	-1.154602	-3.785724	0.018450
C	-2.218460	-5.411969	-1.434447
H	-4.374578	-5.349796	-1.535910
C	-1.062529	-4.855404	-0.874540
H	-0.260700	-3.347153	0.451368
H	-2.134750	-6.243511	-2.128993
H	-0.088169	-5.258572	-1.136790

TS4b

Atom	X	Y	Z
Pd	0.170485	-0.288798	0.240239
C	2.907951	0.046017	-1.182282
O	4.044279	-0.406487	-1.766485
N	2.068959	-0.823582	-0.744117
C	3.672800	2.388803	-1.691825
C	3.451799	3.742072	-1.591470
C	2.304944	4.221665	-0.911113
C	1.413105	3.248165	-0.346617
C	2.729415	1.507827	-1.101619
H	2.679161	6.336280	-1.193200
H	4.538182	1.986613	-2.205189
H	4.148708	4.451995	-2.030328
C	2.002985	5.600395	-0.764718
C	0.251398	3.684350	0.347093
C	-0.009666	5.030334	0.467993
C	0.869067	5.994436	-0.089766
H	-0.409364	2.934298	0.767751
H	-0.899322	5.358657	0.997367
H	0.642123	7.051436	0.018566
N	1.647478	1.913211	-0.454753
C	3.954574	-1.860911	-1.803223
H	3.874259	-2.141234	-2.856603
C	2.677041	-2.152163	-0.955906
H	1.950430	-2.795469	-1.462801
C	5.153388	-2.514549	-1.090926
H	5.520117	-3.370086	-1.673380
H	5.985662	-1.806411	-1.008261
C	4.599855	-2.952098	0.249691
C	3.214251	-2.772485	0.319821
C	5.291593	-3.498564	1.331682
C	2.500572	-3.129445	1.464173
C	4.581297	-3.858340	2.479568
H	6.368591	-3.641574	1.286413
C	3.194928	-3.674800	2.546382
H	1.427776	-2.963578	1.515434
H	5.110232	-4.282836	3.328730
H	2.655990	-3.955508	3.447132
C	-4.113598	-3.023285	-1.405670
C	-4.012629	-1.728614	-0.903168
C	-5.164330	-0.980680	-0.656756
C	-6.439769	-1.493263	-0.882752
C	-6.543725	-2.796252	-1.372169
C	-5.390358	-3.552119	-1.627888
H	-3.228514	-3.619354	-1.613293
H	-7.315702	-0.886361	-0.673070
H	-7.522171	-3.231668	-1.555809
H	-5.489847	-4.567114	-2.004016
C	-4.789762	0.335888	-0.080109
O	-5.540581	1.211777	0.324499
N	-3.390915	0.351633	-0.040652

C	-2.637667	0.934180	1.000981
C	-1.443011	0.245525	1.341894
C	-3.100097	2.009823	1.767084
C	-0.874101	0.527013	2.605594
C	-2.431403	2.349195	2.947932
H	-4.004005	2.523271	1.466484
C	-1.344161	1.591137	3.384635
H	-0.042758	-0.070355	2.970248
H	-2.799442	3.176764	3.548725
H	-0.858237	1.820625	4.329888
C	-2.785467	-0.873441	-0.627369
C	-1.777295	-1.421642	0.392834
H	-2.259967	-1.892074	1.250955
H	-1.142414	-2.186956	-0.077590
C	-2.117654	-0.528898	-1.977079
H	-2.852354	-0.089547	-2.659627
H	-1.710539	-1.435579	-2.439531
H	-1.294773	0.177682	-1.823052