

Electronic Supplementary Information for

Activation of Carboplatin by Carbonate: A Theoretical Investigation

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Cartesian Coordinates of the calculated structures

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RA1-3H2O

O	6.74240	0.57540	3.33810
Pt	5.60730	1.19340	1.74190
O	6.53370	-0.13750	0.47670
C	7.08760	-1.23980	0.90310
C	6.82170	-1.66790	2.36500
C	7.24950	-0.62340	3.43010
C	5.34810	-2.15410	2.64880
C	7.30540	-3.09480	2.72800
C	5.93640	-3.37810	3.39820
H	5.46740	-4.35280	3.21200
H	5.97400	-3.20790	4.47900
N	4.67850	2.59260	2.94340
H	3.69000	2.35420	3.05030
H	4.58860	3.54910	2.42440
H	5.13480	2.64820	3.85150
N	4.46570	1.92890	0.17450
H	3.55830	2.30610	0.55610
H	4.30620	1.20910	-0.52630
H	4.94560	2.72990	-0.26590
H	7.46630	-3.67210	1.81500
H	8.18880	-3.13290	3.36810
H	4.70360	-1.46580	3.20180
H	4.84040	-2.43430	1.72000
O	7.75890	-1.96850	0.16950
O	7.99870	-0.95210	4.35310
C	2.83080	4.47400	1.20310
O	2.37150	3.27370	1.42850
O	2.13340	5.39440	0.67580
O	4.10330	4.71280	1.52560

H	4.98080	4.72720	0.26550
O	5.56500	4.58090	-0.56710
H	6.46300	4.60730	-0.21350
H	0.32570	4.67500	0.46360
O	-0.24650	3.89500	0.61500
H	0.47910	3.34180	0.96980
H	3.16770	6.61030	-0.27850
O	3.79030	7.07700	-0.88360
H	4.48020	6.40400	-0.98650

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TS1-3H2O

O	-1.73650	-2.40150	4.89090
Pt	-3.14660	-1.38280	3.10900
O	-2.34490	-2.74410	1.80970
C	-1.86760	-3.91510	2.18170
C	-2.11600	-4.43560	3.60990
C	-1.39620	-3.61950	4.76940
C	-3.61600	-4.66970	4.01990
C	-1.89130	-5.96170	3.77340
C	-3.19450	-6.04190	4.60920
H	-3.86740	-6.89490	4.44150
H	-2.98100	-5.96410	5.67980
N	-3.88140	0.06070	4.41050
H	-4.84320	-0.03150	4.72500
H	-3.25990	0.04770	5.21690
N	-4.98980	-2.00310	2.22030
H	-5.24390	-1.15940	1.67870
H	-5.74930	-2.33510	2.80870
H	-4.68890	-2.74830	1.59240
H	-1.96990	-6.47200	2.80960
H	-0.96200	-6.22680	4.27970
H	-4.05490	-3.92580	4.69150
H	-4.26880	-4.79060	3.14390
O	-1.27930	-4.63590	1.37190
O	-0.61550	-4.25440	5.50490
C	-1.90070	1.38740	2.52670
O	-1.53620	0.20900	2.96530
O	-3.18760	1.74260	2.57820
O	-1.03860	2.20360	2.08720
H	-4.23780	0.98200	1.48930
O	-4.79110	0.49270	0.80480
H	-4.08580	0.05360	0.30860
H	0.63990	1.52810	2.38380
O	1.38030	0.94930	2.67250
H	0.84510	0.19820	2.96990
H	-1.86240	3.95470	1.92620
O	-2.68580	4.47830	2.01130
H	-3.24320	3.70980	2.23690
H	-3.70990	0.92880	3.78950

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P1-3H2O

O	-5.32720	-4.56900	5.16090
Pt	-3.22380	-1.39690	3.86270
O	-2.66660	-3.37680	3.95800
C	-2.66510	-3.99070	5.11030
C	-3.04260	-5.45790	5.01160
C	-4.61280	-5.62090	5.14380
C	-2.49090	-6.27580	3.79960

C	-2.28180	-6.43100	5.96360
C	-2.08180	-7.41010	4.77650
H	-1.08370	-7.85200	4.64670
H	-2.83560	-8.19980	4.79620
N	-3.89730	0.56570	3.67540
H	-3.25900	0.90550	2.83660
H	-3.72040	1.12720	4.50540
H	-4.88620	0.63270	3.44470
N	-4.61150	-1.94870	5.32890
H	-4.07030	-2.01130	6.19310
H	-4.93410	-2.94860	5.15790
H	-5.41150	-1.33420	5.45410
H	-1.34910	-5.98510	6.32540
H	-2.85460	-6.81280	6.81330
H	-3.21580	-6.53640	3.02310
H	-1.63870	-5.77170	3.33430
O	-2.46620	-3.47240	6.22160
O	-5.02180	-6.79940	5.21290
C	-1.52330	-0.04240	1.69250
O	-1.75490	-1.09040	2.45740
O	-2.26660	1.03680	1.80700
O	-0.57710	-0.11300	0.86370
H	-0.20920	1.08720	-0.15080
O	-0.06310	1.72360	-0.92690
H	-0.63510	1.32140	-1.59330
H	-2.47610	2.32590	0.53040
O	-2.32420	3.11340	-0.04140
H	-1.43410	2.88210	-0.38340
H	-1.91520	3.86220	1.73670
O	-1.71700	3.73280	2.68450
H	-1.63940	2.76220	2.67980
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RA2-3H2O			
O	6.71880	0.04440	0.20620
Pt	5.96700	1.26310	1.63320
O	6.63110	0.13880	3.17930
C	7.60100	-0.74280	3.04560
C	8.46770	-0.68220	1.77100
C	7.69990	-0.80490	0.43280
C	9.43660	0.56500	1.71450
C	9.72470	-1.58930	1.79410
C	10.58700	-0.39380	1.31290
H	11.55590	-0.23810	1.80050
H	10.73740	-0.41260	0.22950
N	5.18930	2.34380	0.02380
H	4.17380	2.39640	0.09990
H	5.45210	1.82150	-0.81180
H	5.50320	3.33260	-0.04380
N	5.10000	2.47350	3.10460
H	4.28580	3.01040	2.74750
H	5.78820	3.13330	3.46260
H	4.82940	1.86480	3.87550
H	9.94340	-1.89240	2.81960
H	9.67660	-2.46110	1.14030
H	9.16370	1.36630	1.02230
H	9.57770	0.99630	2.71070
O	7.86400	-1.54140	3.93720
O	8.04260	-1.62040	-0.41610

C	2.12470	4.42260	1.61610
O	3.32040	4.02950	1.64270
O	1.58690	5.12460	0.70190
O	1.35270	4.05080	2.67280
H	0.45180	4.41610	2.52480
H	4.71870	4.96110	0.82800
O	5.37370	5.16860	0.13050
H	4.77070	5.46300	-0.58560
H	-0.06610	5.45110	1.10520
O	-0.84450	5.47590	1.72090
H	-0.73560	6.31930	2.17890
H	2.56710	5.53820	-0.66460
O	3.13590	5.67650	-1.46610
H	3.01090	4.86200	-1.96820

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TS2-3H2O

O	-1.89080	-2.30300	4.95970
Pt	-3.25250	-1.20460	3.20160
O	-2.35350	-2.44220	1.87090
C	-1.50100	-3.34230	2.35050
C	-1.93240	-4.25220	3.48760
C	-1.82020	-3.57460	4.91990
C	-3.33940	-4.93700	3.35060
C	-1.29400	-5.67180	3.46990
C	-2.68880	-6.28570	3.75450
H	-2.98280	-7.17120	3.17790
H	-2.81550	-6.47870	4.82080
N	-3.91310	0.18480	4.62290
H	-4.90040	0.24560	4.85660
H	-3.38080	-0.07460	5.45510
N	-5.02340	-1.98860	2.40550
H	-5.45940	-1.22230	1.86670
H	-5.67970	-2.40090	3.06410
H	-4.68640	-2.71520	1.77260
H	-0.90370	-5.92270	2.47950
H	-0.52810	-5.84250	4.22800
H	-4.13790	-4.55430	3.99640
H	-3.69000	-4.93960	2.31070
O	-0.38940	-3.47300	1.82810
O	-1.72030	-4.35420	5.88150
C	-1.79220	1.11860	2.52600
O	-1.50130	0.15210	3.34070
O	-2.67590	1.99070	2.73080
O	-1.08670	1.18990	1.38370
H	-0.46250	0.39830	1.35630
H	-3.56410	1.08530	4.25160
H	-4.81360	0.67780	2.14750
O	-5.50990	0.65380	1.46920
H	-5.02020	1.09160	0.73540
H	0.17200	-0.75970	2.63340
O	0.54610	-0.85330	1.73750
H	0.22870	-1.75030	1.48910
H	-2.88150	1.60860	-0.15580
O	-3.63070	2.15280	0.12710
H	-3.33590	2.38380	1.03740

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P2/R3-3H2O

O	-4.04380	-2.17850	9.19980
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Pt	-2.02950	1.07460	9.01360
O	-1.29750	-0.81850	8.94620
C	-1.52770	-1.64030	9.96970
C	-1.77360	-3.06370	9.54010
C	-3.29430	-3.21010	9.11490
C	-0.82540	-3.70630	8.47630
C	-1.34710	-4.17760	10.54320
C	-0.72190	-4.97280	9.36690
H	0.27970	-5.39100	9.52260
H	-1.39790	-5.75350	9.01540
N	-2.70640	3.05600	8.80790
H	-2.13910	3.40430	8.00490
H	-2.50560	3.62070	9.63070
H	-3.69470	3.14940	8.58460
N	-3.66930	0.27970	9.97980
H	-3.41680	0.18280	10.96350
H	-3.81210	-0.74820	9.61780
H	-4.54120	0.79790	9.89970
H	-0.60930	-3.80550	11.26100
H	-2.15890	-4.66790	11.08620
H	-1.26390	-3.85220	7.48510
H	0.12230	-3.16730	8.37830
O	-1.63680	-1.27200	11.13700
O	-3.63190	-4.33990	8.73390
C	-0.32890	2.23170	6.90040
O	-0.28670	1.62430	8.03990
O	-0.95480	3.28550	6.65360
O	0.40970	1.65670	5.93640
H	0.60220	0.72000	6.24400
H	0.58520	2.17680	3.96630
O	0.49460	2.57310	3.08550
H	-0.31590	3.09850	3.18680
H	-1.01680	4.20260	5.07980
O	-0.97000	4.70990	4.24110
H	-0.01850	4.75970	4.07940
H	-0.01320	-1.42610	6.25240
O	0.54450	-0.86800	6.80990
H	0.02350	-0.79100	7.64180
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TS3a-3H2O			
H	2.93210	3.73260	7.81470
O	3.52510	4.50660	7.76250
H	3.07820	5.06790	7.11430
H	0.73900	5.63000	8.13080
O	1.39920	6.34090	8.20280
H	2.17110	5.86790	8.55200
H	0.88700	-0.90030	6.84940
O	1.18740	-0.67800	7.73970
H	0.36800	-0.77110	8.26850
O	-4.01190	-2.17110	9.54120
Pt	-2.08710	1.06640	8.91330
O	-1.32230	-0.81200	8.97740
C	-1.46850	-1.51510	10.10590
C	-1.70790	-2.97870	9.84480
C	-3.23670	-3.19150	9.50170
C	-0.77990	-3.71110	8.82190
C	-1.22040	-3.96900	10.94580
C	-0.61020	-4.86990	9.84000

H	0.40770	-5.24140	10.00610
H	-1.27190	-5.70370	9.59920
N	-2.85270	3.02400	8.72500
H	-2.03520	3.61130	8.46470
H	-3.25170	3.38120	9.59030
H	-3.55710	3.09360	7.99270
N	-3.63440	0.32570	10.04160
H	-3.32650	0.34180	11.01420
H	-3.77130	-0.75760	9.79430
H	-4.52370	0.81320	9.95460
H	-0.47220	-3.50350	11.59470
H	-2.00150	-4.41680	11.56560
H	-1.24900	-3.97040	7.86980
H	0.14580	-3.15850	8.63170
O	-1.50130	-1.02010	11.22870
O	-3.56930	-4.35220	9.23120
C	0.21810	2.89340	7.87590
O	-0.43880	1.67460	7.76740
O	-0.32750	3.98750	8.04060
O	1.45130	2.53040	7.74160
H	0.74930	1.42380	7.72410
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TS3b-3H2O			
H	2.03870	2.99990	5.13340
O	2.59440	3.66190	4.69420
H	2.97020	4.11310	5.46990
H	2.71340	3.52320	7.49790
O	3.52750	4.06810	7.40410
H	4.18350	3.40170	7.16260
H	-1.07150	-1.47180	6.04290
O	-0.28150	-1.17580	6.51420
H	-0.55760	-1.21110	7.46040
O	-3.93620	-2.14580	9.12980
Pt	-2.01870	1.09340	9.03780
O	-1.23260	-0.78560	9.05220
C	-1.47950	-1.59290	10.08510
C	-1.70710	-3.02300	9.66070
C	-3.12580	-3.12870	8.97530
C	-0.59430	-3.74120	8.83150
C	-1.53040	-4.10960	10.76500
C	-0.74480	-4.98130	9.75080
H	0.17640	-5.45590	10.10770
H	-1.38960	-5.72980	9.28730
N	-2.71170	3.06510	8.89080
H	-1.79050	3.50420	8.72950
H	-3.13720	3.44690	9.73180
H	-3.32380	3.23390	8.09550
N	-3.61060	0.25080	10.00770
H	-3.34660	0.15890	10.98940
H	-3.73600	-0.79160	9.61890
H	-4.48300	0.76780	9.92530
H	-0.91380	-3.73120	11.58580
H	-2.44870	-4.53460	11.18040
H	-0.81620	-3.88870	7.77290
H	0.37900	-3.24980	8.93480
O	-1.61170	-1.20800	11.24350
O	-3.36170	-4.17930	8.36560
C	0.35480	2.19430	7.58720

O	-0.06350	2.71720	8.66450
O	-0.63120	1.40470	6.99220
O	1.45650	2.30270	7.02830
H	-0.28390	0.56720	6.58420

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PI3-3H2O			
O	-3.99580	-2.08810	9.00740
Pt	-1.97860	1.18110	8.85830
O	-1.24760	-0.72340	8.85760
C	-1.51680	-1.51750	9.89130
C	-1.74390	-2.95360	9.49040
C	-3.24010	-3.12100	9.00150
C	-0.74260	-3.62240	8.49360
C	-1.36250	-4.03700	10.54430
C	-0.68870	-4.86640	9.41970
H	0.30120	-5.28780	9.63250
H	-1.35500	-5.65080	9.05760
N	-2.68250	3.14660	8.64920
H	-1.82170	3.71120	8.82980
H	-3.44170	3.42660	9.26380
H	-2.95090	3.29600	7.67520
N	-3.64840	0.36870	9.73330
H	-3.45700	0.30000	10.73330
H	-3.76550	-0.68010	9.38660
H	-4.51630	0.87840	9.58280
H	-0.65490	-3.64230	11.28010
H	-2.19710	-4.51020	11.06790
H	-1.11830	-3.78460	7.48050
H	0.21030	-3.08490	8.44340
O	-1.67210	-1.12120	11.04430
O	-3.56420	-4.26490	8.65350
C	0.62750	3.15680	8.50520
O	-0.24860	1.94880	7.90820
O	-0.12570	4.07250	8.85140
O	1.81060	2.92570	8.43000
H	0.31470	1.17120	7.58560
H	0.34290	1.03330	4.17580
O	-0.52350	0.68930	4.42730
H	-1.00010	1.47510	4.77140
H	-1.03310	2.58970	6.53860
O	-1.52830	2.95890	5.76130
H	-1.04840	3.76730	5.53930
H	0.08560	-0.15160	6.02000
O	0.57220	-0.27650	6.86120
H	-0.04620	-0.74140	7.46340

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TS3'-3H2O			
O	-3.99070	-2.10270	9.04650
Pt	-1.98180	1.19020	8.80980
O	-1.25740	-0.71460	8.82850
C	-1.50530	-1.48930	9.88110
C	-1.72400	-2.93580	9.51320
C	-3.23080	-3.13070	9.06510
C	-0.74180	-3.61170	8.50200
C	-1.30090	-3.99470	10.57580
C	-0.65140	-4.83880	9.44780
H	0.34750	-5.24890	9.63970
H	-1.32170	-5.63420	9.11880

N	-2.66990	3.16320	8.57240
H	-1.88270	3.74170	8.90270
H	-3.52980	3.41630	9.05080
H	-2.76190	3.33200	7.56640
N	-3.65290	0.38650	9.71270
H	-3.45370	0.33670	10.71210
H	-3.76670	-0.66180	9.39030
H	-4.52690	0.88500	9.56060
H	-0.57590	-3.57980	11.28320
H	-2.11520	-4.46640	11.13170
H	-1.14080	-3.79500	7.50140
H	0.20380	-3.06580	8.41790
O	-1.64780	-1.07210	11.02880
O	-3.55320	-4.29000	8.76770
C	0.72550	3.19410	8.74420
O	-0.26820	1.95940	7.87630
O	-0.04430	4.09090	9.01980
O	1.85670	2.81350	8.76550
H	0.27330	1.17950	7.56030
H	0.25450	1.07050	4.15490
O	-0.63230	0.77340	4.39460
H	-1.04740	1.56890	4.79250
H	-0.93840	2.64850	6.58440
O	-1.45230	3.05990	5.82100
H	-0.94170	3.84220	5.57650
H	-0.00020	-0.15860	5.96320
O	0.52830	-0.31880	6.77080
H	-0.08120	-0.75820	7.39910
39			
PA3-3H2O			
O	-3.75010	-1.78940	9.52410
Pt	-1.68920	1.41270	8.57970
O	-1.06880	-0.52490	8.67990
C	-1.15390	-1.17850	9.82640
C	-1.45500	-2.64670	9.66370
C	-3.02250	-2.83620	9.51740
C	-0.67780	-3.45400	8.57440
C	-0.86080	-3.60130	10.74300
C	-0.43830	-4.57950	9.61550
H	0.57210	-5.00360	9.67060
H	-1.17070	-5.37950	9.49830
N	-2.35250	3.38520	8.25120
H	-1.92440	4.02270	8.91970
H	-3.36190	3.49660	8.30750
H	-2.03310	3.62960	7.29090
N	-3.29700	0.80320	9.76730
H	-3.04410	0.94770	10.74460
H	-3.44350	-0.26280	9.63750
H	-4.18360	1.26860	9.58470
H	-0.01320	-3.13980	11.25990
H	-1.56770	-3.98480	11.48330
H	-1.24940	-3.72540	7.68340
H	0.24510	-2.94940	8.26930
O	-1.08670	-0.65200	10.94030
O	-3.40800	-4.01180	9.41280
C	-0.49310	1.54490	12.19320
O	-0.06490	1.94030	7.42170
O	-1.61450	1.87270	12.31400

O	0.65390	1.33030	12.16460
H	0.21030	1.09740	6.99610
H	-0.30510	1.12630	3.84180
O	-1.23340	1.14990	4.10640
H	-1.29930	1.97850	4.63760
H	-0.56110	2.71960	6.45660
O	-1.11410	3.37400	5.75010
H	-0.48360	4.03800	5.44480
H	-0.65790	-0.14150	5.50880
O	0.03330	-0.50630	6.09320
H	-0.43360	-0.80790	6.89610

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P3-3H2O

O	-3.75360	-1.77510	9.44140
Pt	-1.67960	1.41500	8.58660
O	-1.04690	-0.51820	8.68460
C	-1.15560	-1.17160	9.83400
C	-1.46310	-2.63870	9.65800
C	-3.02430	-2.82170	9.45090
C	-0.64820	-3.45160	8.60060
C	-0.91820	-3.59690	10.76010
C	-0.45280	-4.57670	9.65120
H	0.55370	-5.00310	9.74720
H	-1.18120	-5.37560	9.50510
N	-2.36290	3.38180	8.25010
H	-1.93860	4.02900	8.91180
H	-3.37340	3.48280	8.30680
H	-2.04890	3.62220	7.28610
N	-3.25170	0.78570	9.80690
H	-2.90650	0.80450	10.76650
H	-3.44660	-0.26440	9.60230
H	-4.12470	1.30490	9.74720
H	-0.09230	-3.13770	11.31280
H	-1.65640	-3.97870	11.47030
H	-1.18660	-3.72270	7.68910
H	0.28700	-2.95040	8.32990
O	-1.10840	-0.63990	10.94380
O	-3.40850	-3.99550	9.32080
O	-0.07180	1.94770	7.40630
H	0.19850	1.10430	6.97810
H	-0.33020	1.12670	3.84700
O	-1.26120	1.15010	4.10180
H	-1.33080	1.97650	4.63610
H	-0.57780	2.71700	6.45260
O	-1.14320	3.37160	5.74570
H	-0.51920	4.03840	5.43330
H	-0.68170	-0.14440	5.51090
O	0.01820	-0.50390	6.08810
H	-0.43660	-0.80020	6.90080

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RA1-6H2O

H	-5.84980	3.68780	5.45780
O	-6.72550	3.39330	5.74310
H	-6.98080	2.84060	4.94460
H	-5.69040	-1.08820	4.46440
O	-5.28080	-1.39170	5.30310
H	-5.32440	-0.58570	5.86070
H	-8.72320	0.31370	3.42900

O	-8.73130	-0.45550	2.83500
H	-7.75250	-0.50180	2.70420
H	-5.81850	1.83770	6.50880
O	-5.05260	1.23220	6.43800
H	-4.78370	1.44250	5.51590
O	-0.46040	-1.52790	3.26550
Pt	-2.15570	-0.97990	2.25820
O	-1.39390	-1.59080	0.46070
C	-0.48520	-2.52830	0.36840
C	-0.13660	-3.33060	1.64220
C	0.34610	-2.46250	2.83380
C	-1.26350	-4.32800	2.11790
C	0.78030	-4.55870	1.41350
C	-0.17470	-5.42080	2.27900
H	-0.42000	-6.42790	1.91960
H	0.17220	-5.49350	3.31470
N	-2.93890	-0.31310	4.05660
H	-3.59470	-0.97880	4.50560
H	-3.52460	0.54020	3.92370
H	-2.17680	-0.13010	4.70730
N	-3.84120	-0.30500	1.24670
H	-4.70820	-0.34010	1.83790
H	-3.95650	-0.82740	0.38120
H	-3.69690	0.69180	1.03030
H	0.77090	-4.83440	0.35690
H	1.80490	-4.44050	1.77060
H	-1.83830	-4.03360	2.99970
H	-1.96240	-4.54940	1.30460
O	0.04740	-2.81890	-0.70270
O	1.42710	-2.69590	3.37560
C	-6.01430	1.18300	3.42280
O	-6.02700	-0.01900	2.92100
O	-7.11090	1.80390	3.65860
O	-4.85940	1.74200	3.72280
H	-3.87450	2.35470	2.41220
O	-3.23130	2.51040	1.67240
H	-2.42280	2.08220	1.98710
H	-8.21340	2.22080	2.02380
O	-8.87010	1.98750	1.34300
H	-8.97510	1.04150	1.55500
47			
TS1-6H2O			
H	-3.90550	2.30670	5.85030
O	-3.22770	2.93520	6.12690
H	-2.37920	2.45760	5.89660
H	-1.24730	4.00900	2.20280
O	-1.26830	4.90180	2.62140
H	-2.15280	4.87770	3.04640
H	-0.02870	4.04510	3.76740
O	0.55480	3.29070	4.00790
H	0.31540	2.68620	3.26980
H	-3.53750	3.93890	4.54870
O	-3.78700	4.20700	3.64070
H	-3.58550	3.38880	3.12270
H	-4.34610	0.96820	1.53260
O	-5.21170	0.67370	1.12870
H	-5.83530	1.29330	1.52710
H	-1.06150	0.90800	4.79610

O	-0.98820	1.59080	5.49460
H	-0.38390	2.25890	5.08070
O	-1.73650	-2.40150	4.89090
Pt	-3.14660	-1.38280	3.10900
O	-2.34490	-2.74410	1.80970
C	-1.86760	-3.91510	2.18170
C	-2.11600	-4.43560	3.60990
C	-1.39620	-3.61950	4.76940
C	-3.61600	-4.66970	4.01990
C	-1.89130	-5.96170	3.77340
C	-3.19450	-6.04190	4.60920
H	-3.86740	-6.89490	4.44150
H	-2.98100	-5.96410	5.67980
N	-3.88140	0.06070	4.41050
H	-4.84320	-0.03150	4.72500
H	-3.25990	0.04770	5.21690
N	-4.98980	-2.00310	2.22030
H	-5.24390	-1.15940	1.67870
H	-5.74930	-2.33510	2.80870
H	-4.68890	-2.74830	1.59240
H	-1.96990	-6.47200	2.80960
H	-0.96200	-6.22680	4.27970
H	-4.05550	-3.92680	4.69230
H	-4.26880	-4.79060	3.14390
O	-1.27930	-4.63590	1.37190
O	-0.61550	-4.25440	5.50490
C	-1.90070	1.38740	2.52670
O	-1.53620	0.20900	2.96530
O	-3.18760	1.74260	2.57820
O	-1.03860	2.20360	2.08720
H	-3.70990	0.92880	3.78950
47			
PA1-6H2O			
O	-2.21210	1.25760	5.01590
Pt	-0.41740	1.31920	8.61410
O	0.42810	1.20310	6.74020
C	0.11960	0.20650	5.95510
C	0.08950	0.58480	4.48510
C	-1.35720	1.09410	4.08870
C	1.19370	1.55620	3.95650
C	0.61360	-0.49130	3.48550
C	1.41900	0.61040	2.74700
H	2.45850	0.38070	2.47310
H	0.87500	0.96290	1.86840
N	-1.33140	1.56680	10.46980
H	-0.50490	2.05210	11.02450
H	-1.58310	0.68420	10.90940
H	-2.15860	2.15860	10.43650
N	-2.11760	0.57330	7.64820
H	-1.93270	-0.42350	7.52240
H	-2.15920	0.95170	6.65410
H	-3.00770	0.71320	8.11870
H	1.24440	-1.23020	3.99130
H	-0.14940	-1.00820	2.89690
H	0.87020	2.57560	3.72700
H	2.04580	1.60030	4.64110
O	-0.20790	-0.93790	6.31030
O	-1.53250	1.30360	2.86960

C	1.67600	2.51030	10.52070
O	1.38050	2.00100	9.34150
O	0.75370	2.59330	11.45490
O	2.85650	2.90510	10.71500
H	3.39210	3.39630	8.94020
O	3.22440	3.86900	8.09890
H	2.43110	3.39300	7.80620
H	0.32700	4.50200	11.78600
O	0.19170	5.46440	11.72860
H	0.89740	5.72430	11.10700
H	0.87210	1.26270	12.62660
O	1.10220	0.43700	13.11080
H	2.07610	0.49890	13.09030
H	2.69710	5.31370	9.30880
O	2.64090	5.68990	10.21140
H	2.81920	4.88490	10.73090
H	3.44190	2.20370	12.21290
O	3.58710	1.81860	13.11470
H	2.97500	2.34670	13.64370
H	-0.13970	-0.92940	10.52940
O	-0.50830	-1.10800	11.40790
H	0.12770	-0.67160	12.02060
59			
RA1-10H2O			
H	-6.38790	3.44130	5.64420
O	-7.16990	2.91540	5.85930
H	-7.27270	2.39720	5.00380
H	-5.27270	-1.16340	4.30200
O	-4.82020	-1.41510	5.13540
H	-5.03050	-0.65940	5.72870
H	-8.52080	-0.37420	3.39910
O	-8.35960	-1.07130	2.74370
H	-7.40290	-0.87060	2.58810
H	-5.96660	1.53540	6.49200
O	-5.09700	1.09400	6.40090
H	-4.85290	1.41730	5.50420
O	-0.39460	-1.56660	3.21750
Pt	-1.98830	-0.76960	2.17650
O	-1.22160	-1.62640	0.44860
C	-0.64920	-2.78940	0.42460
C	-0.34990	-3.52130	1.74730
C	0.21310	-2.66620	2.89990
C	-1.59630	-4.33940	2.28520
C	0.39710	-4.87600	1.61080
C	-0.65190	-5.54160	2.53800
H	-1.02390	-6.53270	2.25530
H	-0.31010	-5.57480	3.57630
N	-2.71340	0.03560	3.92540
H	-3.27020	-0.67470	4.44250
H	-3.40940	0.79750	3.77410
H	-1.92660	0.35490	4.50470
N	-3.54340	0.11460	1.15210
H	-4.44750	-0.08580	1.64260
H	-3.54790	-0.16640	0.16380
H	-3.43360	1.14140	1.19450
H	0.33370	-5.22570	0.57930
H	1.43260	-4.87140	1.95460
H	-2.13920	-3.90570	3.12860

H	-2.30670	-4.53180	1.47560
O	-0.39910	-3.37240	-0.64540
O	1.17950	-3.08090	3.56320
C	-5.99530	1.06250	3.37030
O	-5.80470	-0.08070	2.77900
O	-7.17830	1.46970	3.64670
O	-4.94820	1.78330	3.72500
H	-4.07570	2.64290	2.55280
O	-3.40320	2.95240	1.88450
H	-2.56960	2.89280	2.36820
H	-8.48670	1.70190	2.15860
O	-9.15850	1.39510	1.52210
H	-9.03200	0.43400	1.62240
O	0.11600	0.64500	4.95660
H	0.16950	0.18850	4.10190
H	0.40770	-0.07800	5.54840
O	-2.61520	-0.37310	-1.66040
H	-2.71310	-1.21940	-2.13810
H	-1.89700	-0.60030	-1.04420
O	0.79750	-1.87830	6.09080
H	1.07580	-2.23800	5.21630
H	-0.14940	-2.07140	6.09380
O	-2.43480	-3.08840	-2.48410
H	-3.11570	-3.37420	-1.86140
H	-1.61320	-3.13540	-1.93850
59			
TS1-10H2O			
O	1.89210	6.51800	10.03830
H	2.55980	7.13190	10.40330
H	2.44770	5.71760	9.82790
O	4.90010	2.96570	4.07290
H	4.92540	2.00420	4.25250
H	5.28420	3.33450	4.89330
H	1.34200	8.93830	9.18320
O	1.95560	9.68360	9.19430
H	2.79400	9.25180	9.51100
H	5.87290	10.49400	7.36320
O	5.58160	11.37320	7.69930
H	4.62910	11.35610	7.46130
H	5.93120	10.52960	9.36580
O	6.26040	9.77100	9.89900
H	6.46290	9.15500	9.15740
H	2.54040	10.43650	7.59580
O	2.98230	10.74470	6.77720
H	3.47530	9.94110	6.48700
H	3.79320	7.59660	4.79420
O	3.28020	7.32420	3.97880
H	2.64450	8.04470	3.89080
H	4.35840	7.64020	9.38450
O	4.04330	8.24590	10.10490
H	4.82610	8.83830	10.25080
O	3.48600	4.53310	9.21920
Pt	3.53190	5.22740	6.86860
O	4.96600	3.74410	6.75190
C	4.95340	2.63940	7.43400
C	3.76210	2.28350	8.33780
C	3.37480	3.28870	9.47280
C	2.45160	1.94530	7.51820

C	3.74620	0.81180	8.84460
C	2.27110	0.67680	8.39000
H	1.97590	-0.24710	7.87490
H	1.58560	0.86260	9.21940
N	2.18360	6.77030	7.08740
H	1.33350	6.71630	6.53250
H	1.94410	6.82670	8.08980
N	2.78490	4.67310	4.97600
H	2.81880	5.54570	4.42200
H	1.83800	4.30180	4.99770
H	3.41660	3.96560	4.55850
H	4.43580	0.19790	8.26120
H	3.93930	0.69100	9.91130
H	1.66160	2.70140	7.53360
H	2.68930	1.71280	6.47230
O	5.85900	1.79340	7.27230
O	2.91140	2.79660	10.52240
C	5.07770	7.95890	7.17660
O	4.86030	6.87630	7.89210
O	4.18970	8.32350	6.26830
O	6.09780	8.67370	7.40260
H	2.79120	7.58150	6.78870
O	0.97920	4.43230	11.95650
H	1.12500	5.25540	11.46100
H	1.66460	3.84840	11.57700
O	5.13270	0.32660	5.11830
H	4.26850	0.09810	5.48290
H	5.56820	0.78430	5.88040
59			
PA1-10H2O			
O	-6.94670	5.46700	14.45250
H	-6.59370	6.26810	14.02360
H	-6.27970	4.78190	14.25390
O	-7.78750	1.29830	13.10480
Pt	-6.55530	4.64170	11.02490
O	-5.72170	2.77680	11.35070
C	-5.40900	2.48640	12.57410
C	-5.38160	1.00130	12.88420
C	-6.80630	0.51390	13.30870
C	-4.76410	0.05280	11.80150
C	-4.27330	0.52760	13.87270
C	-3.93790	-0.64530	12.91400
H	-2.87790	-0.83110	12.70170
H	-4.41290	-1.57170	13.24290
N	-7.38660	6.52580	10.82160
H	-6.90910	6.90540	9.97210
H	-7.02700	7.04650	11.63890
H	-8.39960	6.57670	10.76020
N	-8.08990	3.98460	12.26350
H	-8.00190	4.53310	13.13490
H	-7.94930	2.97780	12.50140
H	-9.02480	4.08860	11.87580
H	-3.47350	1.26970	13.95110
H	-4.61630	0.25640	14.87360
H	-5.47010	-0.56850	11.24410
H	-4.15010	0.61280	11.09090
O	-5.17230	3.31080	13.48670
O	-6.86150	-0.63600	13.80210

C	-4.61670	6.31270	9.28690
O	-4.86400	5.19510	9.95880
O	-5.53380	7.18270	9.05060
O	-3.40870	6.46790	8.89090
H	-2.78360	4.67060	8.67320
O	-2.93980	3.75200	8.36730
H	-3.75830	3.56830	8.85520
H	-6.08760	6.99340	7.13330
O	-6.22390	6.69760	6.21710
H	-5.43010	6.15030	6.06560
H	-5.34180	8.63540	10.14470
O	-5.01400	9.29370	10.79490
H	-4.08370	9.36170	10.49580
H	-3.49120	4.66460	6.73310
O	-3.60710	5.48960	6.21870
H	-3.45670	6.14190	6.92750
H	-2.92480	8.11820	9.01070
O	-2.82160	9.10580	9.05470
H	-3.49920	9.38880	8.42650
H	-4.92340	6.90460	12.78780
O	-5.63710	7.58330	12.89370
H	-5.36400	8.31450	12.29190
O	-3.74550	5.58940	12.57830
H	-3.85040	5.43980	11.61940
H	-4.20010	4.80560	12.95470
O	-10.33160	0.60070	13.89490
H	-10.10010	0.13800	14.71250
H	-9.43530	0.84730	13.55620
O	-9.22340	-1.94840	14.49210
H	-9.78770	-1.46540	13.86980
H	-8.34990	-1.53160	14.30760