

Electronic Supplementary Information

Hydrolysis of cis- and transplatin: structure and reactivity of the aqua complexes in a solvent free environment

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Complete reference [32]

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, 2009.

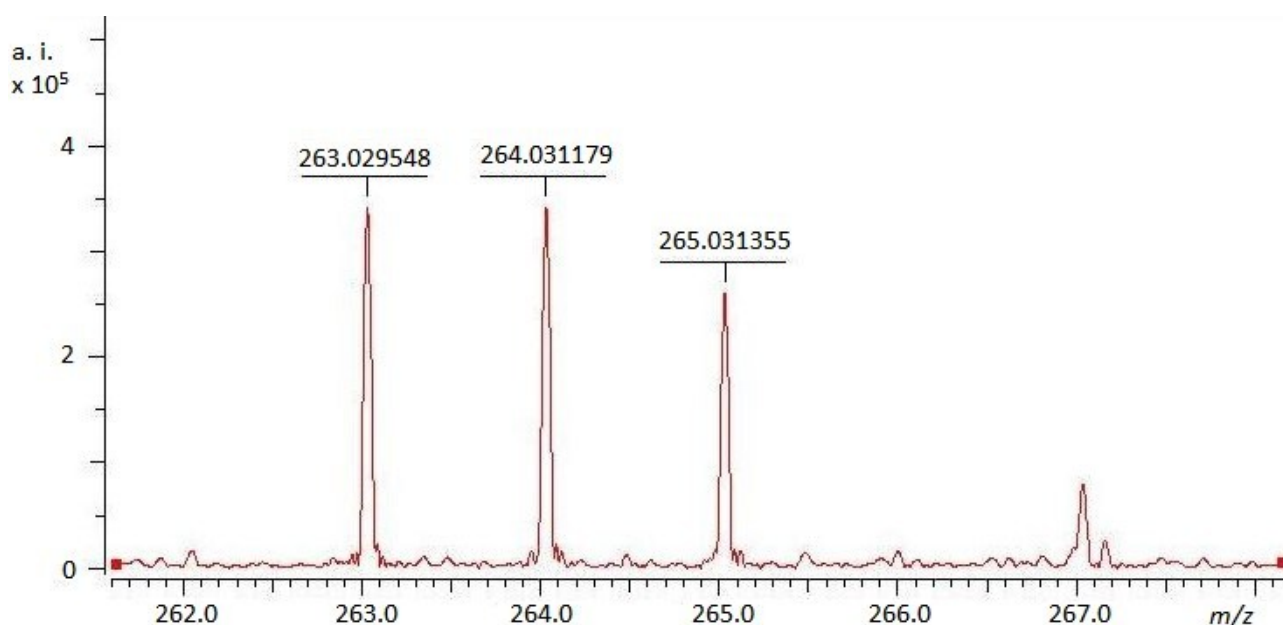


Figure S1. High resolution mass spectrum of *cis*-[Pt(OH)(NH₃)₂(H₂O)]⁺. Calculated m/z values are: 263.029082 Da (¹⁹⁴Pt¹⁴N₂¹H₉¹⁶O₂); 264.031194 Da (¹⁹⁵Pt¹⁴N₂¹H₉¹⁶O₂); 265.031354 Da (¹⁹⁶Pt¹⁴N₂¹H₉¹⁶O₂). The deviation between experimental and calculated values is always within 2 ppm.

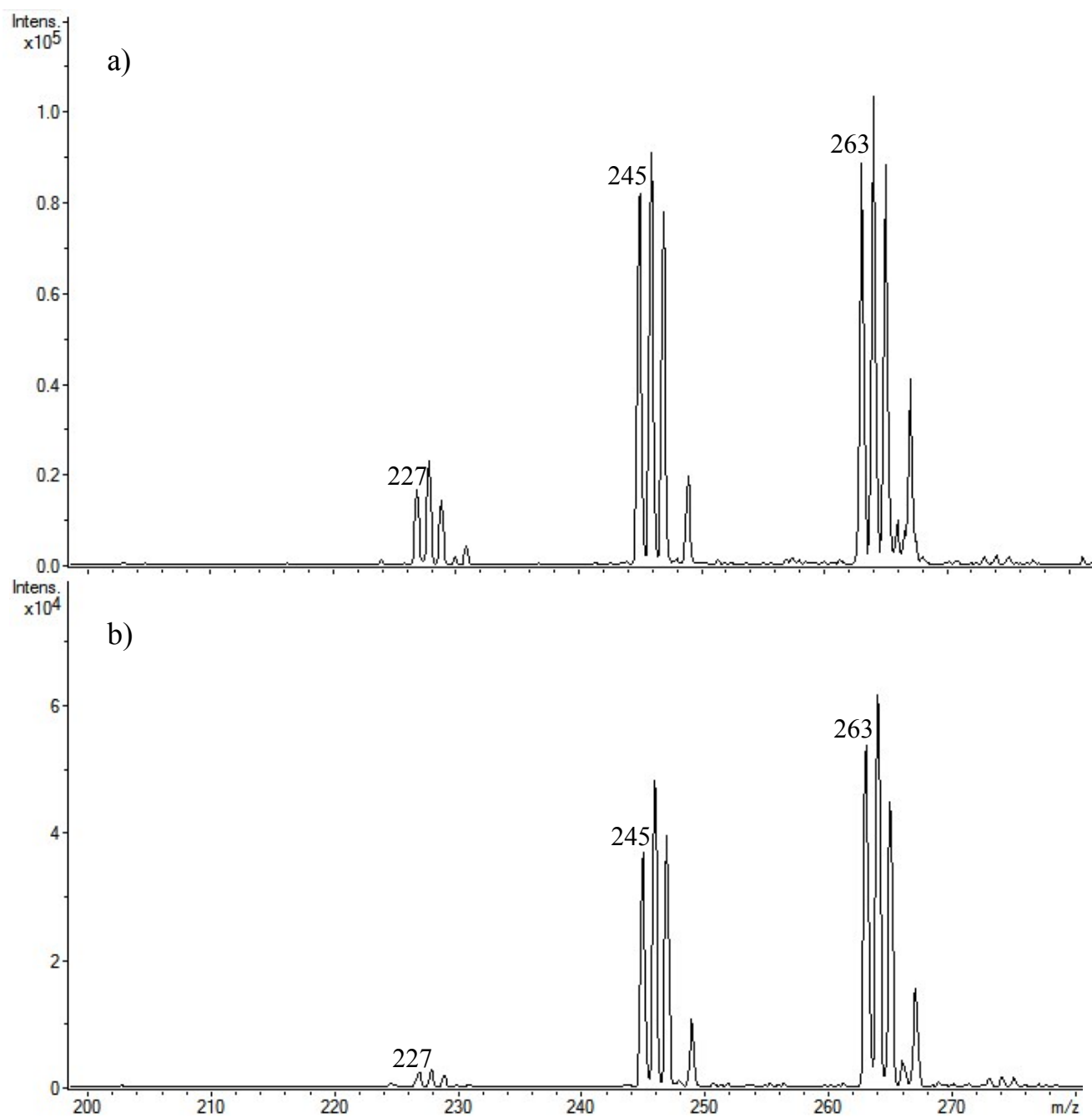
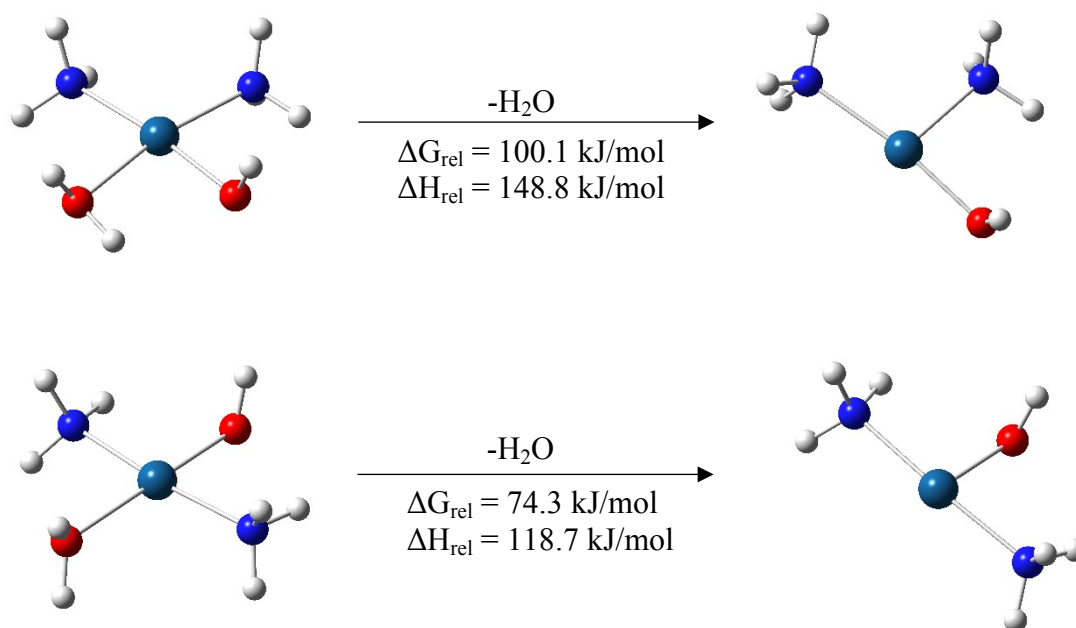


Figure S2. CID mass spectra of a) *cis*-[Pt(OH)(NH₃)₂(H₂O)]⁺ and b) *trans*-[Pt(OH)(NH₃)₂(H₂O)]⁺, recorded in a Paul ion trap (Esquire 6000+, Bruker Daltonics) upon mass selection of the isotopic cluster and activation with a radio frequency amplitude of 0.6.



Scheme S1. Optimized geometries and relative energies at 298K for the dissociation reaction of water from *cis* and *trans*-[Pt(OH)(NH₃)₂(H₂O)]⁺.

Table S1. Theoretically calculated thermodynamic parameters for the most stable structures of sampled Pt(II) complexes. Calculation performed at B3LYP/aug-cc-pVTZ(-PP) level.

B3LYP/aug-cc-pVTZ(-PP)								
Species	Energy ^a	Relative Energy ^b	Zero-point Energy ^b	Enthalpy Correction ^b	Relative Enthalpy ^b (298K)	Entropy ^c	H-TS ^b (298k)	Relative Free Energy ^b (298K)
H ₂ O	-76.466197	0.0	55.76	65.68	0.00	194.50	7.72	0.00
H ₂ ¹⁸ O	-76.466197	0.0	55.58	65.50	0.18	195.89	7.12	0.60
<i>cis</i> -[Pt(OH)(NH ₃) ₂ (H ₂ O)] ⁺	-384.855559	5.5	313.05	340.53	6.60	399.35	221.52	7.56
<i>cis</i> -[Pt(OH)(NH ₃) ₂ (H ₂ ¹⁸ O)] ⁺	-384.855559	0.0	312.64	340.19	6.26	400.45	220.86	6.89
<i>trans</i> -[Pt(OH)(NH ₃) ₂ (H ₂ O)] ⁺	-384.857664	0.0	311.09	339.46	0.00	402.57	219.49	0.00
<i>cis</i> -[Pt(OH)(NH ₃) ₂ (H ₂ O)] ⁺ ·H ₂ O	-461.351465	0.0	380.00	412.17	0.00	431.82	283.49	0.00
<i>cis</i> -[Pt(OH)(NH ₃) ₂ (H ₂ O)] ⁺ ·H ₂ ¹⁸ O	-461.351465	0.0	379.55	411.83	-0.34	432.93	282.82	-0.67
<i>cis</i> -[Pt(OH)(NH ₃) ₂ (H ₂ ¹⁸ O)] ⁺ ·H ₂ O	-461.351465	0.0	379.68	411.92	-0.25	433.09	282.86	-0.63
TS	-461.314935	95.9	375.68	408.85	92.59	436.49	278.77	91.19
TS-H ₂ ¹⁸ O	-461.314935	95.9	375.36	408.61	92.35	437.67	278.19	90.61
<i>cis</i> -[Pt(OH)(NH ₃) ₂] ⁺	-308.329253	37.03	243.60	265.85	36.75	368.50	156.04	33.27
<i>trans</i> -[Pt(OH)(NH ₃) ₂] ⁺	-308.343356	0.00	244.49	266.13	0.00	356.83	159.80	0.00

^a Electronic energy at 0K. In Hartree particle⁻¹. ^b In kJ mol⁻¹. ^c In J mol⁻¹K⁻¹.

Table S2. Theoretically calculated thermodynamic parameters for the structures of sampled Pt(II) complexes partaking the profile for the reaction of *cis*- and *trans*-[PtCl(NH₃)₂(H₂O)]⁺ with TA. Calculation performed at ω B97X-D/6-311++G** level employing the LanL2TZ PP for the platinum atom.

ω B97X-D/6-311++G**								
Species	Energy ^a	Relative Energy ^b	Zero-point Energy ^b	Enthalpy Correction ^b	Relative Enthalpy ^b (298K)	Entropy ^c	H-TS ^b (298k)	Relative Free Energy ^b (298K)
H ₂ O	-76.432249	-	56.91	66.83	-	188.62	10.62	-
TA	-669.726987	-	341.08	363.98	-	374.82	252.28	-
<i>cis</i> -[PtCl(NH ₃) ₂ (H ₂ O)] ⁺	-768.790763	5.24	284.99	312.61	6.40	407.87	191.06	9.22
<i>trans</i> -[PtCl(NH ₃) ₂ (H ₂ O)] ⁺	-768.792760	0.00	282.97	311.45	0.00	417.31	187.09	0.00
<i>cis</i> -[PtCl(NH ₃) ₂ (H ₂ O)] ⁺ ·TA	-1438.563406	56.95	632.30	681.67	57.43	580.21	508.77	65.49
<i>trans</i> -[PtCl(NH ₃) ₂ (H ₂ O)] ⁺ ·TA	-1438.562430	59.51	633.63	682.57	60.89	581.67	509.23	68.51
<i>cis</i> -TS	-1438.535468	130.30	625.50	677.01	126.12	603.26	497.24	127.31
<i>trans</i> -TS	-1438.540908	116.02	625.66	677.41	112.24	609.10	495.90	111.69
<i>cis</i> -[PtCl(NH ₃) ₂ (TA)] ⁺ ·H ₂ O	-1438.585098	0.00	629.25	681.19	0.00	607.25	500.23	0.00
<i>trans</i> -[PtCl(NH ₃) ₂ (TA)] ⁺ ·H ₂ O	-1438.582417	7.04	629.03	680.87	3.27	603.70	500.97	4.33
<i>cis</i> -[PtCl(NH ₃) ₂ (TA)] ⁺	-1362.125910	8.37	562.50	606.95	7.30	554.04	441.85	2.48
<i>trans</i> -[PtCl(NH ₃) ₂ (TA)] ⁺	-1362.129098	0.00	564.62	608.02	0.00	537.85	447.74	0.00

^a Electronic energy at 0K. In Hartree particle⁻¹. ^b In kJ mol⁻¹. ^c In J mol⁻¹K⁻¹.

Table S3. Cartesian coordinates of aqua complexes from hydrolysis of cis- and transplatin and related species.

cis-[Pt(OH)(NH₃)₂(H₂O)]⁺

Pt	0.01237900	0.00152800	0.01142100
N	0.26866600	2.10700600	-0.01843000
H	-0.56442000	2.55146400	-0.39831200
H	1.04202000	2.42581800	-0.59632200
H	0.41359100	2.49676600	0.90996100
N	1.98426500	-0.49634600	-0.01637600
H	2.52176600	-0.07655200	-0.77066400
H	1.96620800	-1.50662400	-0.17530200
H	2.47537800	-0.32316500	0.85718200
H	-2.27734900	-0.76403000	-0.35951700
O	-2.07410800	0.15381000	-0.09049600
H	-2.51928500	0.29306600	0.75739300
O	-0.35178500	-1.92353900	-0.11345800
H	-0.38680600	-2.33272500	0.76000100

trans-[Pt(OH)(NH₃)₂(H₂O)₂]⁺

Pt	-0.00853900	-0.00967400	0.00760000
N	1.81749000	-0.97056300	-0.02444200
H	2.46738000	-0.59795100	-0.71174600
H	1.61084000	-1.93716900	-0.27647900
H	2.29210300	-0.97678200	0.87489000
H	0.89561700	2.47993600	-0.77050600
O	1.00138700	1.90810900	-0.00003800
H	0.93316600	2.45997200	0.78882700
O	-0.84024200	-1.76573100	-0.10820400
H	-0.92600900	-2.14332700	0.77693000
N	-1.95418300	0.69149700	-0.01997000
H	-2.26789400	1.12619100	0.84374300
H	-2.17577300	1.32277100	-0.78517400
H	-2.49571000	-0.16466500	-0.15649100

cis-[Pt(OH)(NH₃)₂(H₂O)₂]⁺

Pt	0.26826200	0.00316900	-0.06146100
N	1.52890000	-1.63119200	0.32832500
H	0.95253000	-2.47048500	0.36071800
H	2.01037800	-1.57744600	1.22220100
H	2.23614700	-1.78186700	-0.38663400
N	1.58748600	1.51413600	0.30752100
H	2.02672300	1.48483500	1.22395800
H	0.99370700	2.34654900	0.26945300
H	2.32033300	1.61481200	-0.39004200

H	-2.07739600	-0.99508800	0.00988800
O	-1.22168400	-1.41188300	-0.37409900
H	-1.38538400	-1.58159100	-1.31055700
O	-1.01480300	1.50513900	-0.31203500
H	-1.10292500	1.72559100	-1.24660200
O	-3.03377800	0.01317800	0.64790800
H	-3.98243000	0.12329800	0.53500300
H	-2.56874400	0.83209400	0.36147400

TS

Pt	0.19193500	0.02569400	-0.00512800
N	2.21314900	-0.02344500	0.11392200
N	-0.07188900	2.06057900	-0.47228000
O	-1.83170400	-1.10284600	-0.95106400
H	2.68312200	0.29874200	-0.72771700
H	2.59975500	0.47431400	0.91157400
H	-0.97652000	2.31137800	-0.07434900
H	-0.11559800	2.24077800	-1.47207300
H	-1.95651500	-1.18837000	-1.90321300
H	2.40503900	-1.02221500	0.22907400
H	0.61397500	2.70132700	-0.08422900
H	-1.30479800	-1.87585500	-0.65558100
O	-2.13445200	0.68125200	0.98652500
H	-2.35845300	0.60257500	1.92061100
H	-2.66913100	0.03055100	0.50894900
O	0.33317600	-1.91818100	0.33781500
H	0.18322800	-2.11912400	1.26925000

cis-[Pt(OH)(NH₃)₂]⁺

Pt	0.01107800	-0.17513900	0.00339600
N	-2.11818700	-0.08023100	-0.00478600
H	-2.50848400	-0.80619400	0.59371200
H	-2.49197500	-0.24378200	-0.93791300
H	-2.52595700	0.79234400	0.32151900
N	0.36199400	1.79690100	0.00345500
H	-0.10601400	2.28601500	-0.75639100
H	1.37278000	1.86949600	-0.14220200
H	0.12860800	2.24659900	0.88626100
O	1.90594900	-0.48402000	-0.12065200
H	2.31269500	-0.62818000	0.74469700

trans-[Pt(OH)(NH₃)₂]⁺

Pt	0.00000000	-0.18300700	0.00868900
N	-2.06492900	-0.10083300	-0.02359100
H	-2.47950200	-0.64325700	-0.77878300

H	-2.31065000	0.87673500	-0.18308300
H	-2.50655500	-0.39440700	0.84496800
O	-0.00000400	1.74025500	-0.11332800
H	-0.00001000	2.08599300	0.79296900
N	2.06493000	-0.10082800	-0.02359000
H	2.50655800	-0.39441200	0.84496400
H	2.47950100	-0.64324600	-0.77878900
H	2.31065300	0.87674000	-0.18307500

Table S4. Cartesian coordinates of Pt^{II}-complexes and related species of species partaking the potential energy profile for the reaction of *cis*- and *trans*-[PtCl(NH₃)₂(H₂O)]⁺ with TA.

TA

C	-2.60851600	-0.04019600	0.23624800
C	-0.53711500	-1.18689800	-0.20931600
C	-0.58261300	1.21986700	-0.10026200
C	-1.94844100	1.18030600	0.15713000
C	-1.90151900	-1.22328900	0.05225500
H	0.01543700	-2.10650200	-0.36591700
H	-0.06376100	2.16929000	-0.16726900
H	-2.49580200	2.10614200	0.29447000
H	-2.41348200	-2.17751300	0.10650500
H	-3.67394700	-0.07009400	0.43499700
C	0.12962400	0.03548100	-0.28093600
S	1.88383700	0.08562800	-0.62533600
C	2.52666200	-0.12021800	1.06466500
H	2.20422600	-1.07193000	1.48833600
H	3.61505800	-0.11094600	0.99115600
H	2.20238700	0.70118100	1.70438800

cis-[PtCl(NH₃)₂(H₂O)]⁺

Pt	-0.15055800	-0.02333000	0.00000000
N	0.06338400	-2.05179100	0.00000100
N	-2.26837700	-0.02720600	-0.00000100
Cl	2.13768100	0.11405800	0.00000100
O	-0.25453100	2.09585000	-0.00000100
H	-0.32662000	-2.50282000	0.82546100
H	-0.32662000	-2.50282100	-0.82545900
H	-2.67779600	-0.46976700	-0.81999200
H	-2.59556900	0.93802200	-0.00000100
H	0.20446000	2.45582100	0.77066200
H	1.06959700	-2.23753100	0.00000100
H	-2.67779700	-0.46976700	0.81999100
H	0.20446000	2.45582000	-0.77066400

trans-[PtCl(NH₃)₂(H₂O)]⁺

Pt	0.13908100	0.01042600	0.00000600
N	-0.04452600	2.08297900	0.00001800
H	-1.04423900	2.29380800	-0.00003800
H	0.35383600	2.53030500	-0.82296400
H	0.35373700	2.53028100	0.82306200
Cl	-2.12543100	-0.09518000	-0.00009000
O	2.31363100	0.00813500	0.00009300
H	2.81393600	0.26107800	-0.78141500
H	2.81387400	0.26105900	0.78164600
N	0.18374000	-2.06057300	-0.00001000
H	1.12334500	-2.45173100	0.00000700
H	-0.30700600	-2.42094300	-0.81715600
H	-0.30703800	-2.42095500	0.81711200

cis-[PtCl(NH₃)₂(H₂O)]⁺·TA

Pt	1.14304300	-0.18241600	-0.20994100
O	0.64075200	1.19274600	-1.71868200
H	1.26045200	1.93236800	-1.73651000
S	-2.23049800	1.84478600	-0.69177600
H	-0.25374900	1.56656800	-1.49652800
C	-1.88850300	2.90626800	0.73570500
H	-0.90916500	2.69617900	1.16569200
H	-1.90265500	3.92475500	0.34756800
H	-2.67978300	2.80263900	1.47772000
C	-2.25399900	0.20171600	-0.00548100
C	-1.91404700	-0.09726600	1.31228500
C	-2.61866700	-0.83024100	-0.87556100
C	-1.93203500	-1.41961100	1.74910500
H	-1.63330700	0.68491500	2.00535500
C	-2.61518900	-2.14820100	-0.43656400
H	-2.92552500	-0.60000500	-1.89097500
C	-2.26517500	-2.45082700	0.87891800
H	-1.70709600	-1.63508700	2.78867000
H	-2.92881500	-2.93694600	-1.11205200
H	-2.30148800	-3.47541600	1.23094800
N	0.61220300	-1.68413700	-1.57823300
H	0.46893500	-1.25037800	-2.48870400
H	1.30494200	-2.41706700	-1.70720800
H	-0.27301400	-2.11934300	-1.31311100
Cl	1.68349200	1.54127800	1.22577700
N	1.56977500	-1.47714200	1.31034100
H	0.72997300	-1.97668100	1.60266600
H	2.29986700	-2.15496000	1.10371600
H	1.88752900	-0.91546300	2.10259600

trans-[PtCl(NH₃)₂(H₂O)]⁺·TA

Pt	1.26906500	0.02520300	-0.25935800
N	2.56567700	1.30532000	0.73352600
O	0.47336800	1.72782000	-1.28193400
H	2.39015600	2.28679500	0.52982700
H	3.52624400	1.09597200	0.46675700
H	2.50752900	1.16865000	1.74084700
H	0.56559400	1.80067300	-2.23598500
S	-2.33872600	2.06203400	-0.06105900
H	-0.46851000	1.92339100	-1.02952900
C	-1.70366600	2.59987800	1.54692600
H	-0.72366400	2.16934700	1.75686200
H	-1.61795600	3.68460300	1.48487500
H	-2.41081900	2.34367600	2.33517900
C	-2.55194300	0.30139400	0.14336200
C	-2.03366700	-0.42254200	1.21431500
C	-3.25670300	-0.35887800	-0.86762900
C	-2.22157800	-1.80055600	1.27243000
H	-1.48498500	0.06488800	2.00927000
C	-3.43291900	-1.73641800	-0.80308600
H	-3.68949100	0.20409400	-1.68803200
C	-2.91503700	-2.46205200	0.26659700
H	-1.81878100	-2.35343900	2.11288200
H	-3.99307200	-2.23888900	-1.58307300
H	-3.06778900	-3.53311000	0.32362100
Cl	2.10619500	-1.71230600	0.95487700
N	0.04937800	-1.33514000	-1.23051300
H	-0.91225000	-1.01601200	-1.35746800
H	0.42039400	-1.61038300	-2.13714900
H	0.00538700	-2.17823700	-0.65804100

cis-TS

Pt	-1.08307500	-0.44109800	0.01633800
O	-0.82432200	-0.07445100	2.38022000
H	-0.72233200	0.86792200	2.55262700
H	-1.64156600	-0.33264600	2.81853800
S	0.76966700	1.70212100	0.43306300
C	2.24290000	0.77602900	0.06959900
C	2.94923200	0.27432500	1.16426400
C	2.65106000	0.46047500	-1.22565000
C	4.04674900	-0.55326500	0.96057500
H	2.64978900	0.54068700	2.17249300
C	3.76125800	-0.35725100	-1.41816700
H	2.12518100	0.85594200	-2.08599800
C	4.45527100	-0.87370900	-0.32992900
H	4.59471100	-0.93244000	1.81526200
H	4.08647900	-0.58311400	-2.42720000

H	5.32059800	-1.50622400	-0.48640700
C	0.42997800	2.65977700	-1.06282900
H	0.21502300	2.01376000	-1.91211800
H	-0.46550300	3.23687300	-0.83403100
H	1.26343600	3.32900100	-1.27260700
N	0.47659000	-1.83289400	0.23158200
H	1.28596900	-1.57743900	-0.33619400
H	0.78810400	-1.79984700	1.20150700
H	0.24311800	-2.80078800	0.02806700
Cl	-2.78587400	1.11122400	-0.12085100
N	-1.96227500	-1.35244300	-1.61357800
H	-1.35847000	-1.41462900	-2.42928800
H	-2.32463600	-2.28064100	-1.40963100
H	-2.75916500	-0.76086200	-1.85890300

trans-TS

Pt	-1.13886900	-0.11908400	0.22033600
N	-2.62091700	1.11059800	-0.56595000
O	-0.69207200	1.19821300	2.27750400
H	-3.13226500	1.62403800	0.14802600
H	-3.28882400	0.51016600	-1.05144300
H	-0.33160000	2.08928000	2.26438500
H	-2.27502900	1.78482200	-1.24389500
H	-1.29189600	1.14388600	3.02603500
S	0.96562500	1.83908000	-0.32117400
C	2.25552900	0.61213800	-0.25638200
C	3.05087300	0.59160200	0.88787700
C	2.42951700	-0.35181400	-1.24892300
C	4.00898000	-0.40363300	1.04455100
H	2.93524900	1.35795600	1.64654300
C	3.40304700	-1.33290200	-1.08932900
H	1.81199700	-0.35348500	-2.13884800
C	4.18767600	-1.36733500	0.05853600
H	4.62976100	-0.41215300	1.93282000
H	3.54239900	-2.07471200	-1.86703200
H	4.94357700	-2.13413600	0.17683700
C	0.70842700	2.09349300	-2.09760200
H	0.20796800	1.24238400	-2.55873200
H	0.08846500	2.98566200	-2.19356500
H	1.66646600	2.28285800	-2.58063200
N	0.23733500	-1.44750400	0.99384100
H	1.01053500	-1.58988500	0.34271400
H	0.63403700	-1.10992000	1.86840500
Cl	-2.09496800	-1.84746100	-0.94031200
H	-0.19728400	-2.35332700	1.15859900

cis-[PtCl(NH₃)₂(TA)]⁺·H₂O

Pt	-0.95258100	0.08554600	-0.02893700
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N	-1.35149200	-1.98122100	0.10071800
N	-2.63097100	0.38928400	-1.24923700
H	-2.37866900	0.31090400	-2.23176200
H	-3.40481600	-0.24974400	-1.05545100
Cl	-0.63430800	2.37045700	-0.21969900
H	-2.94306100	1.34861800	-1.10448100
H	-1.03028900	-2.37508600	0.98200300
H	-2.35669600	-2.16476900	0.02994400
H	-0.88361400	-2.49613800	-0.64169400
S	0.90331400	-0.26208700	1.33479700
C	1.24483500	1.24353600	2.28992600
H	2.12993200	1.04347300	2.89217900
H	1.39633000	2.08232100	1.61538300
H	0.37776500	1.42466900	2.92341500
C	2.34120100	-0.35807900	0.26417100
C	3.23389500	-1.40033800	0.49115800
C	2.56530800	0.58672800	-0.73363000
C	4.37455100	-1.49630800	-0.29855500
H	3.04880100	-2.12272600	1.27807400
C	3.71069300	0.48103500	-1.50942000
H	1.85796900	1.39065000	-0.90118700
C	4.61210300	-0.55724300	-1.29409800
H	5.07926100	-2.30122800	-0.12766600
H	3.89881400	1.21305900	-2.28559900
H	5.50478400	-0.63233000	-1.90371700
O	-4.32162500	-1.87120000	-0.23061800
H	-4.86807000	-2.45849200	-0.75974000
H	-4.84217300	-1.67298600	0.55278000

trans-[PtCl(NH₃)₂(TA)]⁺·H₂O

Pt	1.08917700	-0.04348800	-0.10725600
N	0.04507600	-1.77596300	-0.57830100
H	-0.09460400	-1.87421000	-1.58187600
H	0.61955400	-2.56321100	-0.27551300
H	-0.86616400	-1.84746500	-0.12772900
S	-0.76141500	1.32550500	-0.57428200
C	-0.81032200	2.65630100	0.66438700
H	-1.76967000	3.16223800	0.56602500
H	-0.68800400	2.25916500	1.67041400
H	-0.01215900	3.35782600	0.42131600
C	-2.21722400	0.37900000	-0.12422500
C	-3.19257400	0.20296300	-1.09896100
C	-2.35858500	-0.17567900	1.14803200
C	-4.32796800	-0.54241000	-0.79307600
H	-3.07406000	0.64747500	-2.08038800
C	-3.49832000	-0.91057800	1.44202800
H	-1.58606700	-0.04439500	1.89831800
C	-4.48070800	-1.09485500	0.47138400
H	-5.09447600	-0.68202100	-1.54571400

H	-3.62023600	-1.34103700	2.42877500
H	-5.36906900	-1.66877000	0.70648400
N	2.35173000	1.54144200	0.38434900
H	3.25872800	1.11354500	0.58089700
H	2.48998900	2.20763500	-0.37229100
Cl	2.91139400	-1.41454100	0.30292500
H	2.07592200	2.05756300	1.21625500
O	0.25471147	-1.06730060	-2.83422777
H	0.94712240	-0.92846523	-3.48452912
H	0.10406951	-0.24736903	-2.35818237

cis-[PtCl(NH₃)₂(TA)]⁺

Pt	-1.15843300	-0.24105900	-0.04980100
N	-0.99613100	-2.34880100	0.13137900
N	-2.83473000	-0.34105700	-1.32468400
H	-2.66375500	-0.81845700	-2.20654700
H	-3.66121300	-0.74987400	-0.89496800
Cl	-1.37023300	2.04323400	-0.30066600
H	-3.05940600	0.63116600	-1.54520000
H	-0.82788900	-2.62013800	1.09835300
H	-1.82004700	-2.86079800	-0.17293800
H	-0.21109500	-2.69721800	-0.41618300
S	0.67784100	-0.10479700	1.37280200
C	0.71721700	1.50891400	2.20089200
H	1.59310300	1.50761600	2.84827300
H	0.76101900	2.30679000	1.46454900
H	-0.19765200	1.58940700	2.78595900
C	2.12168200	-0.03794900	0.30993100
C	3.13847900	-0.95252000	0.56289100
C	2.22087500	0.89556700	-0.71886400
C	4.27800800	-0.93226300	-0.23442600
H	3.05140900	-1.66338100	1.37689300
C	3.36825700	0.91045900	-1.49851400
H	1.41663500	1.59746900	-0.90870200
C	4.39199000	-0.00253200	-1.25985400
H	5.07732200	-1.63856800	-0.04527900
H	3.46105200	1.63645200	-2.29726300
H	5.28374900	0.01488500	-1.87518400

trans-[PtCl(NH₃)₂(TA)]⁺

Pt	1.08917700	-0.04348800	-0.10725600
N	0.04507600	-1.77596300	-0.57830100
H	-0.09460400	-1.87421000	-1.58187600
H	0.61955400	-2.56321100	-0.27551300
H	-0.86616400	-1.84746500	-0.12772900
S	-0.76141500	1.32550500	-0.57428200

C	-0.81032200	2.65630100	0.66438700
H	-1.76967000	3.16223800	0.56602500
H	-0.68800400	2.25916500	1.67041400
H	-0.01215900	3.35782600	0.42131600
C	-2.21722400	0.37900000	-0.12422500
C	-3.19257400	0.20296300	-1.09896100
C	-2.35858500	-0.17567900	1.14803200
C	-4.32796800	-0.54241000	-0.79307600
H	-3.07406000	0.64747500	-2.08038800
C	-3.49832000	-0.91057800	1.44202800
H	-1.58606700	-0.04439500	1.89831800
C	-4.48070800	-1.09485500	0.47138400
H	-5.09447600	-0.68202100	-1.54571400
H	-3.62023600	-1.34103700	2.42877500
H	-5.36906900	-1.66877000	0.70648400
N	2.35173000	1.54144200	0.38434900
H	3.25872800	1.11354500	0.58089700
H	2.48998900	2.20763500	-0.37229100
C1	2.91139400	-1.41454100	0.30292500
H	2.07592200	2.05756300	1.21625500