

Supporting Information (SI)

Study on the Mechanism of Platinum(II)-Catalyzed Asymmetric Ring-opening

Addition of Oxabicyclic Alkenes with Arylboronic Acids

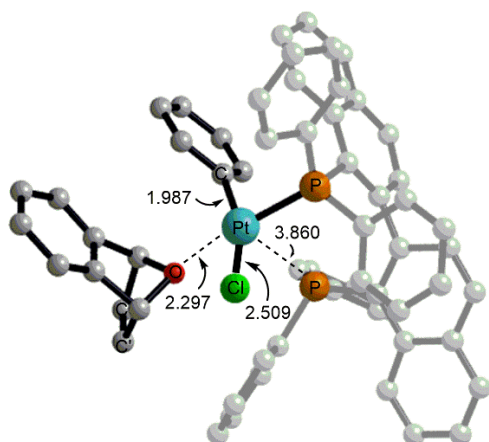
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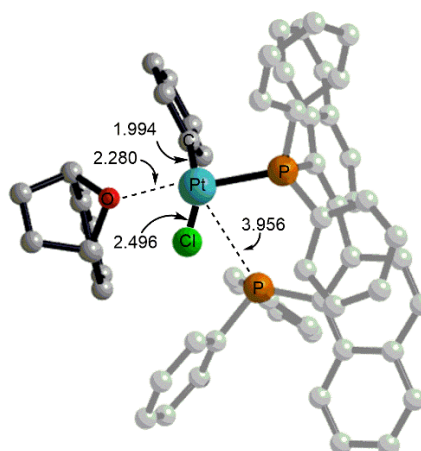
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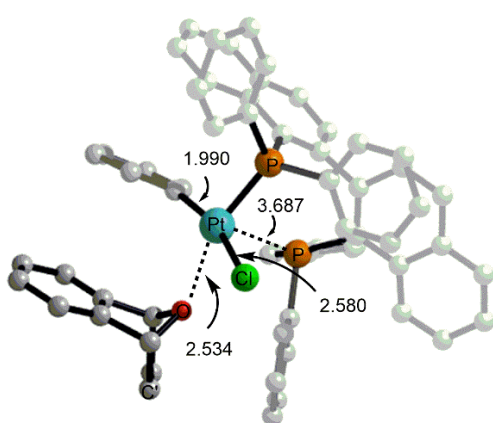
$$\Delta G=0.0$$

CIA10-1



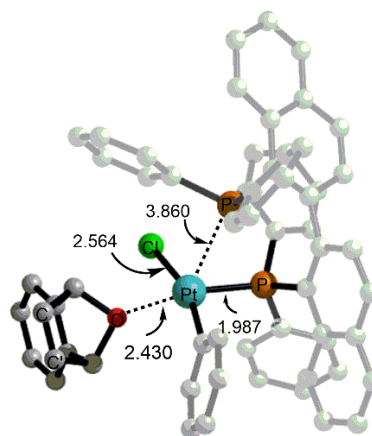
$$\Delta G=1.3$$

CIA10-2



$$\Delta G=28.8$$

CIA10-3



$$\Delta G=21.4$$

CIA10-4

Figure S1. Four low-energy isomers **CIA10-*n*** (*n*=1, 2, 3, 4) for the first step of carboplatinum in solvent when the bridging oxygen atom coordinated with platinum(II) center through *exo*-coordination from different orientations with respect to the formal Pt–O single bond axis (bond length in Å and Gibbs free energy in kcal/mol). For clarity, the H atoms are not shown and benzene are blurring.

Table S1. Free energies (G), total electronic energies (E) and the imaginary frequencies in solvent (dichloromethane/water 10:1, v/v) for the optimized species.

species	G (hartree)	E (hartree)	imaginary frequency (cm ⁻¹)
H ₂ O	-76.415489	-76.4199628	-
OA	-460.858929	-460.9797207	-
PRE	-3417.41011	-3417.5385032	-
PhBF ₃	-556.254892	-556.400214	-
TTS1	-3973.673752	-3974.3021523	-32.52
TIA1	-3973.67678	-3974.3225077	-
TTS2	-3513.270129	-3513.9180623	-46.01
TIA2	-3513.295766	-3513.9399354	-
TTS3	-3513.257964	-3513.9064733	-143.53
TIA3	-3513.288028	-3513.9322876	-
CIA1O-1	-3649.572157	-3650.351137	-
CTS1-1	-3649.55863	-3650.3418584	-75.50
CIA1C-1	-3649.56378	-3650.3447707	-
CTS2-1	-3649.536382	-3650.319211	-336.50
CIA2-1	-3649.566618	-3650.3526965	-
CIA1O-2	-3649.571574	-3650.3553094	-
CTS1-2	-3649.560465	-3650.341861	-78.86
CIA1C-2	-3649.56184	-3650.3450024	-
CTS2-2	-3649.529725	-3650.3159156	-351.71
CIA2-2	-3649.57134	-3650.355793	-
UTS	-3649.543098	-3650.3230731	-482.24
UIA	-3649.606215	-3650.4009586	-
RTS	-3726.0147	-3726.8221364	-141.83
RIA	-3726.061117	-3726.8727305	-

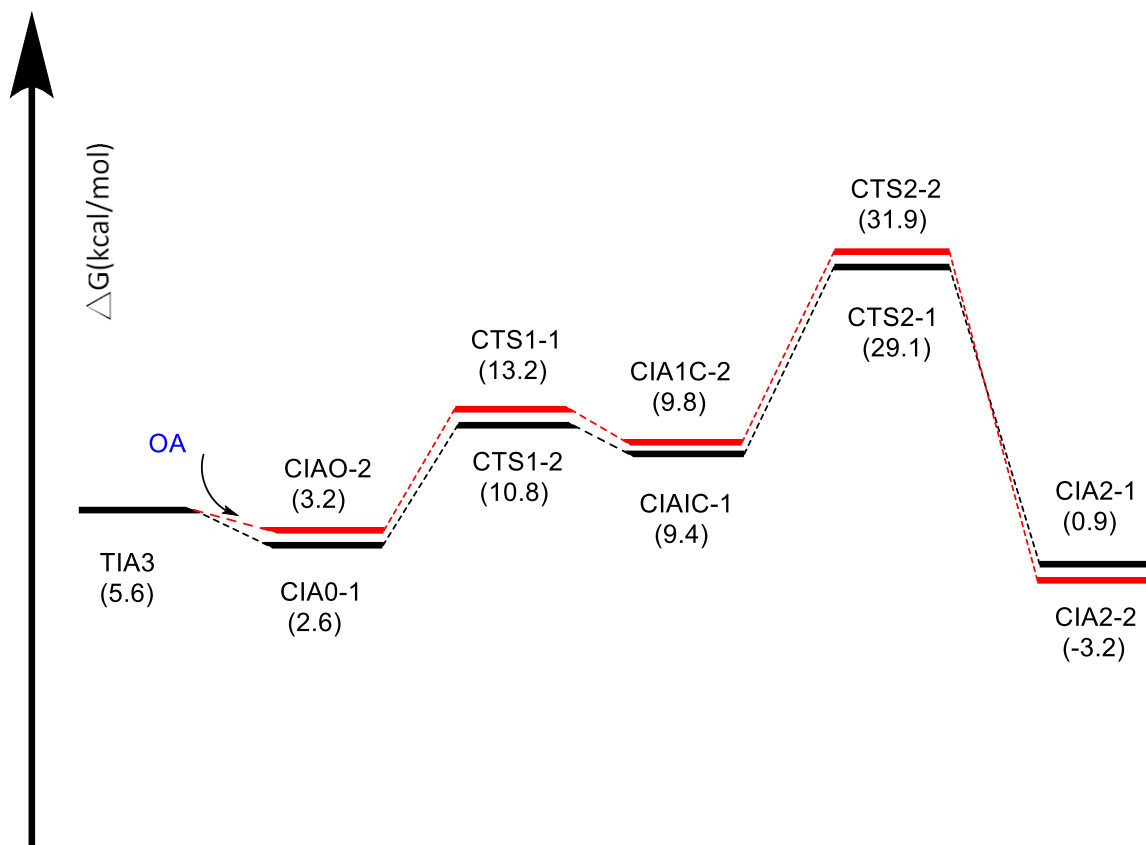
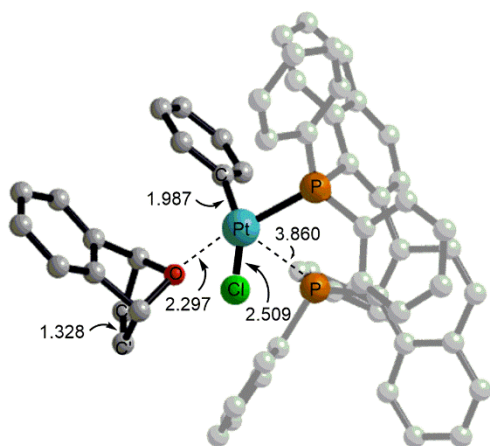
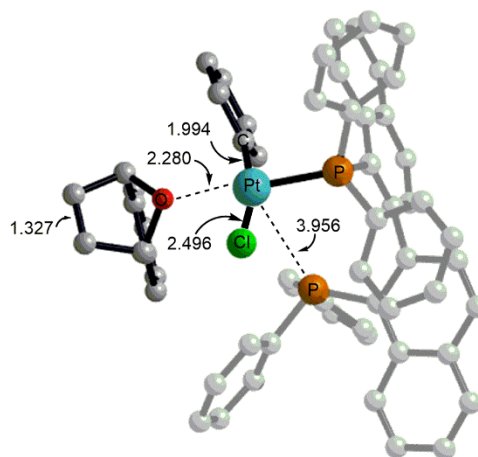


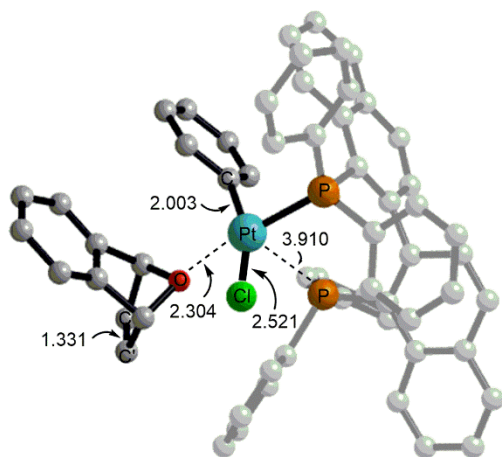
Figure S2. Gibbs free energy profile of carboplatinum process in the Pt(II)-catalyzed ARO reaction calculate by B3LYP. The results of reaction path is similar to that of M06-2X, but the performance of M06-2X functional for free energies is better.



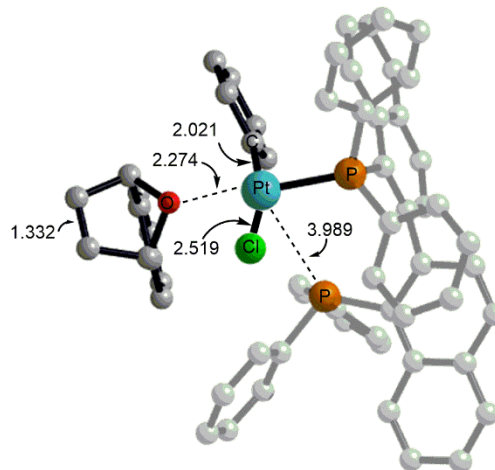
M06-2X-CIA10-1



M06-2X-CIA10-1



B3LYP-CIA10-1



B3LYP-CIA10-2

Figure S3. The geometries of isomers **CIA10- n ($n=1,2$)** optimization by M06-2X and B3LYP functional are similar (bond length in Å). For clarity, the H atoms are not shown and benzene are blurring.

Coordinates of DFT-Computed Stationary Points

TIA1

Pt	-0.62527100	0.00153500	-0.60118000
P	0.17382200	1.11798900	1.18057300
P	1.11861400	-1.33657100	-0.93342100
Cl	-1.54896900	-0.41757400	-2.85867000
B	-3.62646800	-0.17360800	0.60748500
C	-5.08777800	-0.17912400	-0.04950800
C	-6.23125500	0.15603100	0.68187900
C	-5.25509500	-0.53204200	-1.39552900
C	-7.49759300	0.14037900	0.09827300
H	-6.12970600	0.43751700	1.72573800
C	-6.51395800	-0.55050400	-1.98865800
H	-4.38127300	-0.79101400	-1.98861000
C	-7.64124300	-0.21417600	-1.24003700
H	-8.37067500	0.40539200	0.68545800
H	-6.61961300	-0.82413400	-3.03316900
H	-8.62382800	-0.22608700	-1.69914800
Cl	0.71280900	3.78354200	-3.14852100
F	-2.75375500	0.74652200	-0.14617400
F	-3.61043400	0.25907100	1.94156400
C	0.37305100	-2.77696700	-1.75780400
C	0.91738400	-3.31276100	-2.92164900
C	-0.78389200	-3.32828900	-1.19775100
C	0.31788200	-4.42436600	-3.51025600
H	1.79684000	-2.87386300	-3.37653000
C	-1.37107500	-4.43778100	-1.78654800
H	-1.22853200	-2.88241600	-0.31347600
C	-0.81682500	-4.99067900	-2.94108900
H	0.73925900	-4.84117400	-4.41751200
H	-2.26593400	-4.86675900	-1.35122000
H	-1.27932000	-5.85584600	-3.40214200
C	2.40037300	-0.65799500	-2.01612300
C	3.60350300	-1.35455100	-2.17057800
C	2.19590500	0.55912200	-2.66352100
C	4.59786400	-0.83104200	-2.98691700
H	3.76722000	-2.29281600	-1.64859300
C	3.20374100	1.08286000	-3.46795000
H	1.27492200	1.11764000	-2.53080900
C	4.39873800	0.38990300	-3.63130400

H	5.53076400	-1.36813200	-3.11255700
H	3.04224900	2.04074900	-3.94916100
H	5.18187700	0.80241900	-4.25740600
C	-0.95123600	2.54469700	1.20652800
C	-1.64716800	2.91260000	2.35640700
C	-1.15756400	3.23122900	0.00364700
C	-2.53272100	3.98677700	2.30821800
H	-1.51166900	2.36956200	3.28400300
C	-2.03822600	4.30243000	-0.03288800
H	-0.61438400	2.95802100	-0.89864500
C	-2.72624000	4.68156300	1.11920900
H	-3.07527400	4.27283200	3.20166700
H	-2.18796200	4.83808900	-0.96319600
H	-3.41690500	5.51652200	1.08691200
C	0.10213700	0.32403400	2.80623200
C	0.72727400	0.92993700	3.89939000
C	-0.57813000	-0.88361700	2.95607300
C	0.67102100	0.32053800	5.14618000
H	1.26215300	1.86692700	3.77504500
C	-0.62065800	-1.49330900	4.20708200
H	-1.06913000	-1.33863700	2.10113000
C	0.00272700	-0.89336100	5.29775400
H	1.15312200	0.78805600	5.99672200
H	-1.13937400	-2.43728200	4.32738700
H	-0.03177000	-1.37259800	6.26958300
F	-2.98379900	-1.43601500	0.53383100
C	1.97874800	-1.84022400	0.62178900
C	1.97707900	-3.16847400	1.19699300
C	2.56113500	-0.80110300	1.32817100
C	1.68499100	-4.36916200	0.49032200
C	2.38036600	-3.31430200	2.55899100
C	3.04778900	-1.00061200	2.64689800
C	1.67907500	-5.58975100	1.11759200
H	1.50573100	-4.34726300	-0.57055800
C	2.33200400	-4.58361100	3.19090300
C	2.90025900	-2.20318800	3.26787600
H	3.49979900	-0.16057600	3.16141500
C	1.96915900	-5.70305900	2.49328800
H	1.45987500	-6.47993100	0.53905400
H	2.61754500	-4.64420300	4.23575800
H	3.21704600	-2.33989500	4.29655500

H	1.93969500	-6.67158500	2.97838700
C	1.92138700	1.62953200	0.89366600
C	2.36274100	2.96824500	0.58860400
C	2.81963500	0.58073700	0.79816900
C	1.65008600	4.15492000	0.91648700
C	3.63955800	3.13039000	-0.02818900
C	4.12889800	0.78967900	0.29248500
C	2.10939800	5.39038400	0.53673200
H	0.74910100	4.10116200	1.50506800
C	4.07435600	4.41761200	-0.43676000
C	4.50133300	2.01504200	-0.17455200
H	4.80614800	-0.05534700	0.24234300
C	3.31505500	5.52717700	-0.18417100
H	1.54044000	6.27315600	0.80500400
H	5.03403100	4.49941800	-0.93586000
H	5.47674700	2.16287600	-0.62646800
H	3.65036600	6.50795900	-0.49993900

TIA2

Pt	0.63654900	-0.47567300	-0.76959000
P	-0.72093000	-1.11239500	0.89952900
P	-0.20027600	1.55485100	-0.98823400
Cl	1.80471200	-0.56197400	-2.91635300
B	3.38601600	-0.69265200	1.55226700
C	3.99347200	-1.50057000	0.29924100
C	5.01653900	-0.95953500	-0.49111100
C	3.55162700	-2.79191900	-0.01268700
C	5.57486600	-1.67278300	-1.54874800
H	5.38415800	0.04083100	-0.27538400
C	4.09908700	-3.51574300	-1.07230200
H	2.76549500	-3.24047800	0.58975300
C	5.11333300	-2.95564100	-1.84423700
H	6.36604900	-1.23219600	-2.14648800
H	3.73760200	-4.51507200	-1.29394700
H	5.54530000	-3.51285800	-2.66844400
F	4.32236300	-0.58024200	2.61229700
F	2.23105200	-1.34982600	2.05853900
C	1.10604400	2.66477400	-1.61619900
C	0.76012800	3.85385700	-2.26219000
C	2.45165800	2.33290800	-1.43174700
C	1.76016200	4.71080100	-2.71050700

H	-0.27534800	4.12658900	-2.41915700
C	3.44217400	3.19392100	-1.88593800
H	2.72724700	1.42541700	-0.90871900
C	3.09892000	4.38263700	-2.52452600
H	1.48790400	5.63202900	-3.21166700
H	4.48351500	2.93197700	-1.73935500
H	3.87460800	5.05135000	-2.87960400
C	-1.52996500	1.60110800	-2.23374600
C	-2.37896800	2.71217000	-2.26734700
C	-1.69791100	0.56265100	-3.15095200
C	-3.38419000	2.78706600	-3.22290100
H	-2.27386800	3.50879200	-1.53808000
C	-2.71731200	0.63939100	-4.09518100
H	-1.04883700	-0.30482000	-3.12164300
C	-3.55784200	1.74814100	-4.13328800
H	-4.03946300	3.64996000	-3.24353700
H	-2.85445000	-0.17158500	-4.80072200
H	-4.35119000	1.80202800	-4.87006400
C	-0.17657400	-2.84526800	0.86909600
C	0.22478100	-3.51191600	2.02804700
C	-0.07862400	-3.47609500	-0.38003500
C	0.69260500	-4.81712300	1.93714500
H	0.17309900	-3.01787500	2.99068900
C	0.40340700	-4.77802900	-0.46063800
H	-0.40902600	-2.96982300	-1.28412000
C	0.78099700	-5.44977300	0.69769000
H	0.99320000	-5.34161300	2.83651400
H	0.47537400	-5.26495800	-1.42590300
H	1.14910100	-6.46745700	0.63692400
C	-0.70274500	-0.49560000	2.60087700
C	-1.71053300	-0.94038600	3.46210800
C	0.24863400	0.42688600	3.03145500
C	-1.75353100	-0.46696400	4.76768100
H	-2.45785800	-1.64851300	3.11533800
C	0.18531300	0.90984400	4.33488300
H	1.02843500	0.75660600	2.35520700
C	-0.81043600	0.46332800	5.19986500
H	-2.52696600	-0.81553000	5.44185300
H	0.91512700	1.63708300	4.67269200
H	-0.85360500	0.84198400	6.21475800
F	3.00540600	0.64118300	1.19622200

C	-1.00067200	2.17124900	0.54660300
C	-0.45372900	3.18867700	1.41188600
C	-2.20943400	1.56988700	0.86979800
C	0.85497500	3.73469800	1.29772200
C	-1.24291700	3.63988200	2.51158800
C	-2.95353100	2.02366000	1.99106900
C	1.31253400	4.68944300	2.17052000
H	1.53243100	3.37848800	0.54136900
C	-0.75308900	4.64439200	3.38498800
C	-2.49979600	3.04457600	2.77042700
H	-3.89436100	1.53475400	2.21584400
C	0.49828900	5.17039800	3.21758200
H	2.32139800	5.06891700	2.05681800
H	-1.39148400	4.96710500	4.20046900
H	-3.08125700	3.39304000	3.61738800
H	0.87272000	5.93117400	3.89218100
C	-2.46027200	-0.90079900	0.31364700
C	-3.33131200	-1.97127900	-0.09949500
C	-2.88015000	0.41422600	0.17509100
C	-3.15849400	-3.33632800	0.26403500
C	-4.50296000	-1.64235500	-0.84444200
C	-4.10208000	0.70924200	-0.48405600
C	-4.02389200	-4.30677700	-0.17257200
H	-2.36199200	-3.62410300	0.93123900
C	-5.36262100	-2.67086600	-1.30987500
C	-4.85167000	-0.28291200	-1.04228400
H	-4.41204400	1.74444400	-0.56137000
C	-5.12279600	-3.98131000	-0.99710600
H	-3.86831700	-5.33435400	0.13523800
H	-6.23091600	-2.38722500	-1.89523800
H	-5.75493700	-0.04894100	-1.59573200
H	-5.78811600	-4.76177900	-1.34697200

TTS3

Pt	-0.27276300	-0.96244200	-0.64045900
P	-1.32883800	0.46256900	0.75898900
P	1.70153000	0.25804400	-0.85425300
Cl	0.25443200	-1.83557000	-2.98408500
B	-1.19719200	-3.16956700	1.42986300
C	-1.46169400	-2.78399700	-0.44357300
C	-0.69324700	-3.88668200	-0.91153800

C	-2.86505200	-2.95464800	-0.51493900
C	-1.26613000	-5.05184800	-1.39655600
H	0.38914400	-3.82846300	-0.85770500
C	-3.45336900	-4.11002300	-1.00974400
H	-3.51737200	-2.18489800	-0.12855800
C	-2.65277900	-5.15871800	-1.45568900
H	-0.63826500	-5.87164900	-1.72620900
H	-4.53360500	-4.19898900	-1.03624900
H	-3.11001000	-6.06537900	-1.83770400
F	-1.68960200	-4.42941100	1.65713600
F	-1.91343000	-2.21413700	2.10472600
C	2.87111500	-1.08977100	-1.24067600
C	3.74857000	-1.02515900	-2.31990000
C	2.82991600	-2.23514300	-0.43827700
C	4.60086400	-2.09539200	-2.58238500
H	3.77055100	-0.15137700	-2.96037000
C	3.68706000	-3.29545700	-0.70039100
H	2.12967300	-2.29832800	0.39044900
C	4.57683900	-3.22527200	-1.77158900
H	5.28145200	-2.04372500	-3.42430900
H	3.65849300	-4.17868400	-0.07253600
H	5.24310700	-4.05490100	-1.97841100
C	1.89304900	1.52347700	-2.14746900
C	3.02644900	2.34083300	-2.15882000
C	0.88273100	1.70812500	-3.09102500
C	3.14727400	3.34217300	-3.11488100
H	3.80544600	2.20486100	-1.41429500
C	1.00835200	2.71404600	-4.04506900
H	0.00199100	1.07517400	-3.07035000
C	2.13580900	3.53088800	-4.05506000
H	4.02519900	3.97770500	-3.12185100
H	0.22207800	2.86335000	-4.77599400
H	2.22812400	4.31679700	-4.79610000
C	-3.09661100	0.13562800	0.49438600
C	-3.97913200	-0.16428200	1.52813200
C	-3.55094500	0.17997600	-0.82863400
C	-5.32246900	-0.40036100	1.23788800
H	-3.62838400	-0.22461700	2.55140200
C	-4.88988400	-0.04628000	-1.11053800
H	-2.85628600	0.39306200	-1.63612300
C	-5.77858600	-0.33503500	-0.07488600

H	-6.00897200	-0.63888800	2.04181600
H	-5.23945000	-0.00526200	-2.13541700
H	-6.82440000	-0.51770600	-0.29402500
C	-0.97394700	0.52315400	2.54239300
C	-1.62306700	1.47621900	3.33035900
C	0.00187300	-0.30216700	3.09590700
C	-1.30714000	1.58456300	4.68047100
H	-2.36609900	2.13697800	2.89270400
C	0.32162800	-0.18280700	4.44377600
H	0.51124100	-1.02365600	2.46851700
C	-0.33474700	0.75602600	5.23580300
H	-1.81480000	2.31909100	5.29460200
H	1.08742500	-0.81908900	4.87266800
H	-0.08375400	0.84747900	6.28658000
F	0.16246400	-3.10045700	1.64248600
C	2.22945500	1.09735800	0.70753000
C	3.36882400	0.77270600	1.53453200
C	1.34318000	2.06724600	1.13628300
C	4.48997200	0.00125900	1.11558200
C	3.42888300	1.32589400	2.84991900
C	1.47664600	2.67169900	2.41487300
C	5.52674000	-0.28191800	1.96884900
H	4.56171300	-0.34381200	0.09835200
C	4.49803300	0.98929600	3.72078200
C	2.45620500	2.26740200	3.27019400
H	0.76372000	3.43513200	2.70574200
C	5.52238300	0.18584500	3.29984400
H	6.36598900	-0.86506200	1.60697500
H	4.49264300	1.40759700	4.72172100
H	2.53257800	2.68767600	4.26767600
H	6.33982100	-0.06314400	3.96624800
C	-1.04435600	2.23527600	0.22994600
C	-2.04466600	3.13879000	-0.30393400
C	0.26563200	2.67931200	0.28946700
C	-3.44386000	3.05617400	-0.04907300
C	-1.60503200	4.28202500	-1.03840100
C	0.66520400	3.88156200	-0.35481900
C	-4.33160800	3.94568100	-0.60079100
H	-3.82723700	2.31566300	0.63323700
C	-2.54703500	5.15578700	-1.64147000
C	-0.22727400	4.61252900	-1.07724900

H	1.70554100	4.17861400	-0.28943400
C	-3.89028200	4.98255100	-1.44932000
H	-5.38578600	3.85539900	-0.36447000
H	-2.16919400	5.98812900	-2.22588900
H	0.08561000	5.49273800	-1.62898700
H	-4.60575300	5.66083100	-1.89928400

TIA3

Pt	-0.23540100	0.15036600	-1.35391500
P	-1.30736900	0.22802400	0.62873100
P	2.08242200	0.32089200	-0.57637600
Cl	0.76290300	0.42312400	-3.63049700
B	-3.39598200	-3.97646600	0.72353000
C	-1.96472100	-0.28979900	-2.32087500
C	-2.64051900	-1.49067600	-2.08259600
C	-2.47448600	0.55661700	-3.31331300
C	-3.78979500	-1.83196000	-2.79794300
H	-2.27955500	-2.16870900	-1.31322800
C	-3.62575800	0.22769400	-4.02375800
H	-1.96706400	1.48936900	-3.53320600
C	-4.29090600	-0.97032300	-3.76877000
H	-4.29542100	-2.76855700	-2.58871400
H	-4.00331700	0.90824700	-4.78021500
H	-5.18720600	-1.22851100	-4.32188000
F	-4.32813900	-3.44104000	-0.03435700
F	-3.46430700	-3.84444700	2.02938200
C	2.98036400	-0.85181200	-1.65511300
C	3.99039900	-0.44809000	-2.52452700
C	2.57417900	-2.18810600	-1.63269600
C	4.60766700	-1.38295000	-3.35161600
H	4.29771600	0.59087300	-2.56271700
C	3.19578900	-3.11934700	-2.45526800
H	1.77677100	-2.50263100	-0.96602100
C	4.21654600	-2.71773500	-3.31482100
H	5.39330600	-1.06433400	-4.02717600
H	2.88204700	-4.15664300	-2.42857300
H	4.69963800	-3.44319800	-3.95938700
C	2.91642500	1.93563000	-0.74876800
C	4.17957200	2.15541600	-0.19107900
C	2.25136600	2.97580900	-1.39935400
C	4.77215100	3.40910400	-0.28712200

H	4.69312100	1.35045300	0.32630900
C	2.84852100	4.23041500	-1.49285500
H	1.26677800	2.80423100	-1.82225900
C	4.10511500	4.44746300	-0.93606400
H	5.75044800	3.57755200	0.14844400
H	2.32832200	5.03803200	-1.99492400
H	4.56622600	5.42620300	-1.00570700
C	-3.11939100	0.40661200	0.43232800
C	-4.02205400	-0.44312500	1.06604700
C	-3.59715900	1.39902400	-0.43154400
C	-5.39243700	-0.29536500	0.84873000
H	-3.67631100	-1.22901600	1.72505600
C	-4.95905900	1.55124500	-0.63691200
H	-2.89760600	2.05488100	-0.93859400
C	-5.86180600	0.70037400	0.00329100
H	-6.08554300	-0.96927500	1.33904900
H	-5.31835600	2.32542700	-1.30504500
H	-6.92648400	0.81261300	-0.16715000
C	-1.10023100	-1.20839400	1.73181400
C	-1.52297900	-1.12623800	3.06247100
C	-0.49271300	-2.37188000	1.26367500
C	-1.33333600	-2.20322900	3.91798100
H	-1.98460000	-0.21529400	3.43263500
C	-0.28406900	-3.44220300	2.13194300
H	-0.16789800	-2.43015900	0.22932700
C	-0.70272900	-3.35692700	3.45552400
H	-1.66220400	-2.13696800	4.94860800
H	0.20152000	-4.34078000	1.76933900
H	-0.54072100	-4.19074700	4.12898700
F	-2.41652100	-4.65846100	0.17254000
C	2.41235400	-0.19474100	1.16554900
C	3.38248600	-1.16945700	1.60161700
C	1.53852100	0.34561100	2.09040100
C	4.51526600	-1.57309000	0.83953600
C	3.26284500	-1.71057400	2.91518900
C	1.48855800	-0.15568500	3.41867400
C	5.39690800	-2.51331900	1.30951600
H	4.71666500	-1.10714100	-0.11224500
C	4.16742900	-2.70872200	3.36191100
C	2.27904900	-1.19942800	3.79854800
H	0.78782000	0.28912500	4.11596600

C	5.20727100	-3.11814600	2.57183700
H	6.25662300	-2.78453300	0.70716200
H	4.02925000	-3.11787200	4.35735100
H	2.20130800	-1.61897500	4.79623500
H	5.90084700	-3.87364400	2.92219500
C	-0.62200700	1.67007800	1.58687300
C	-1.31578600	2.91411700	1.82775700
C	0.73342100	1.60068200	1.87892700
C	-2.72776500	3.03429400	1.96831900
C	-0.54759800	4.09367700	2.06469100
C	1.46549800	2.78125900	2.18277900
C	-3.32616300	4.24771300	2.19476600
H	-3.34624400	2.15212100	1.95724400
C	-1.19410700	5.34329600	2.25362400
C	0.85920700	4.00246500	2.19407100
H	2.52766700	2.68921300	2.38039000
C	-2.55879300	5.42850200	2.29687800
H	-4.40264900	4.29366800	2.31494700
H	-0.57497600	6.22242500	2.39774200
H	1.43154600	4.90757000	2.36796200
H	-3.04799200	6.38282900	2.45325200

CIA1O-1

Pt	1.37760300	-0.24005800	-0.51301800
P	0.51748600	1.79060100	-0.76445900
P	-2.13252700	-0.88502200	0.95914900
Cl	1.46502400	-0.99855500	-2.96120100
C	1.93561800	0.13820300	1.35619400
C	1.13562300	-0.00288400	2.49058200
C	3.30720700	0.36705900	1.53137600
C	1.69376100	0.05607300	3.76801200
H	0.06860200	-0.15828300	2.37838800
C	3.86607700	0.42566200	2.80670200
H	3.95183300	0.49382200	0.66616200
C	3.06030300	0.26664400	3.93216400
H	1.05323000	-0.06008900	4.63650300
H	4.93129200	0.59983600	2.91843500
H	3.49223200	0.31327000	4.92560700
C	2.22673000	-4.32692300	1.21670700
C	2.74006500	-2.88710300	1.11429000
C	4.07796700	-2.93372800	0.37432200

C	3.74511700	-3.32032200	-0.93033300
C	2.22392200	-3.48352400	-0.90893100
C	1.91061400	-4.69137600	-0.02136200
H	5.64561600	-2.39729200	1.75062300
H	2.20852000	-4.90301600	2.13066600
H	2.66338300	-2.25695800	1.99307500
C	5.38389900	-2.70033700	0.74271100
C	4.70976300	-3.48270500	-1.89926300
H	1.68875500	-3.37166600	-1.84374500
H	1.56490600	-5.64691700	-0.38949700
C	6.04572900	-3.24547900	-1.53341100
C	6.37586100	-2.86163900	-0.24046000
H	4.45413200	-3.77524700	-2.91173000
H	6.82853600	-3.35837200	-2.27490300
H	7.41356200	-2.67903500	0.01469400
O	1.89647500	-2.41283300	0.02287700
C	-0.56296100	1.92579900	-2.25434600
C	-0.73014400	3.15440400	-2.90000000
C	-1.18155100	0.79355000	-2.78501400
C	-1.50125100	3.24254800	-4.05533300
H	-0.26443000	4.05318600	-2.51871500
C	-1.94506900	0.88049900	-3.94143100
H	-1.06574000	-0.16070300	-2.29559900
C	-2.10423000	2.10575900	-4.58273100
H	-1.61974500	4.20212800	-4.54528500
H	-2.41306700	-0.01245600	-4.34083200
H	-2.69544800	2.17270700	-5.48924900
C	-2.06724400	-2.59009700	0.24865900
C	-1.33635200	-2.77663500	-0.92950500
C	-2.61914800	-3.71026400	0.87843400
C	-1.21134800	-4.03966600	-1.49817500
H	-0.85273600	-1.93326500	-1.41042500
C	-2.47093900	-4.97870600	0.32186600
H	-3.18616800	-3.59993200	1.79586900
C	-1.77993100	-5.14742700	-0.87395800
H	-0.65881000	-4.15683300	-2.42455600
H	-2.91061900	-5.83495200	0.82123100
H	-1.67743100	-6.13391300	-1.31194300
C	-3.28434000	-1.08071000	2.38285600
C	-2.73370100	-1.59220200	3.56532700
C	-4.62802400	-0.69831400	2.37302800

C	-3.51793700	-1.74710800	4.70302200
H	-1.68476100	-1.87513900	3.59171200
C	-5.40854500	-0.83933500	3.51847100
H	-5.07044300	-0.28371300	1.47395100
C	-4.85841900	-1.36843000	4.68185400
H	-3.08066000	-2.15222700	5.60859600
H	-6.44965200	-0.53688400	3.49823900
H	-5.46841000	-1.47875000	5.57126100
C	1.78717000	3.05456100	-1.15070000
C	2.98334100	2.63012700	-1.72964100
C	1.56722100	4.41828900	-0.93168200
C	3.95437300	3.56357600	-2.08463900
H	3.15751400	1.57276500	-1.89956800
C	2.53853300	5.34469900	-1.28815000
H	0.64431100	4.75807200	-0.47264500
C	3.73486400	4.91818000	-1.86249700
H	4.88306700	3.22597300	-2.52989400
H	2.36383500	6.39953300	-1.11099600
H	4.49414100	5.64259100	-2.13411200
C	-0.44070800	2.37674100	0.71498900
C	0.24216800	2.99777600	1.83331900
C	-1.80174100	2.11512700	0.82105400
C	1.65014800	3.19997600	1.90765500
C	-0.51272300	3.40150100	2.97326300
C	-2.51697300	2.50858100	1.98905100
C	2.24163000	3.79098900	2.99434200
H	2.29569500	2.85575800	1.11773200
C	0.12109400	4.02274400	4.08199100
C	-1.90234300	3.14379900	3.02323000
H	-3.57917300	2.29559000	2.03121400
C	1.47297900	4.22458600	4.09651200
H	3.31894800	3.91279900	3.00806200
H	-0.49830900	4.31936400	4.92186500
H	-2.46311800	3.44484000	3.90187000
H	1.95427300	4.69429400	4.94628100
C	-3.09284100	0.18133500	-0.21654200
C	-4.15372900	-0.24295000	-1.09684700
C	-2.72570800	1.51795200	-0.20803400
C	-4.69055300	-1.55927100	-1.09898900
C	-4.74676500	0.70398600	-1.98090900
C	-3.38410800	2.46186500	-1.04366600

C	-5.69288500	-1.92287100	-1.96324600
H	-4.32066100	-2.28762500	-0.39366400
C	-5.76806100	0.29798600	-2.87776100
C	-4.33994700	2.06270400	-1.92778700
H	-3.09323900	3.50451600	-0.98030700
C	-6.22757400	-0.99243800	-2.88128100
H	-6.08162800	-2.93438800	-1.93470000
H	-6.18424500	1.03885100	-3.55278900
H	-4.81586600	2.77842500	-2.59044000
H	-7.01057000	-1.29672000	-3.56612700

CTS1-*I*

Pt	1.53636800	0.60695200	-0.68049200
P	-0.18123300	2.01005900	-0.72624800
P	-1.64875600	-1.61090400	0.90152100
Cl	1.83089600	0.41129800	-3.22355500
C	1.90399100	0.92721600	1.24749300
C	3.07196500	1.65836600	1.50502300
C	1.20704100	0.38887700	2.32835200
C	3.54402800	1.81882500	2.80546500
H	3.62690000	2.09882800	0.68213200
C	1.67822600	0.54930000	3.63191800
H	0.28590900	-0.15666200	2.15515500
C	2.84904200	1.26132300	3.87689500
H	4.45370800	2.38359400	2.98111800
H	1.12210400	0.11728800	4.45812300
H	3.21283300	1.38576100	4.89073300
C	2.53849500	-1.95452900	0.13825300
C	3.87935100	-1.39950300	0.64815300
C	4.92870700	-2.48095300	0.38303500
C	5.05016900	-2.51177800	-1.01126700
C	4.06381600	-1.45015400	-1.49894600
C	2.65806200	-1.99038200	-1.19510200
H	5.56558800	-3.31058000	2.26610100
H	1.74152000	-2.33793500	0.76227700
H	3.89055400	-0.90695800	1.61502300
C	5.65677200	-3.33009400	1.18579100
C	5.90290700	-3.39122900	-1.63888000
H	4.22344000	-0.99751700	-2.47126000
H	1.98276800	-2.40342700	-1.92978000
C	6.65637200	-4.25764100	-0.82778700

C	6.53517000	-4.22800600	0.55497600
H	5.99972000	-3.41821200	-2.71853000
H	7.34436900	-4.95711900	-1.28905400
H	7.12982100	-4.90434900	1.15854800
O	4.18688900	-0.48696900	-0.43015600
C	-1.22434100	1.62030200	-2.18894600
C	-1.83591600	2.62900300	-2.93480200
C	-1.34407700	0.29414400	-2.60616900
C	-2.57021200	2.30690800	-4.07463900
H	-1.74399700	3.66901800	-2.64974100
C	-2.08385300	-0.02747600	-3.73387100
H	-0.84615600	-0.48250200	-2.04224800
C	-2.69824300	0.98179100	-4.47358900
H	-3.03743200	3.09876500	-4.64857200
H	-2.17217500	-1.06401100	-4.04072700
H	-3.26975100	0.73330900	-5.36108800
C	-1.17424600	-3.26428800	0.23848400
C	-0.60990700	-3.33359700	-1.04065400
C	-1.22367500	-4.42612200	1.01497800
C	-0.13988700	-4.54088400	-1.54519500
H	-0.53938200	-2.44121200	-1.65353700
C	-0.73598900	-5.63145200	0.51422700
H	-1.65313700	-4.40062600	2.01008100
C	-0.19839800	-5.69508400	-0.76684400
H	0.28187500	-4.57737900	-2.54352500
H	-0.78175700	-6.52324500	1.12934700
H	0.17652900	-6.63487500	-1.15573400
C	-2.51480500	-2.03346000	2.47030800
C	-1.73528800	-2.06720100	3.63184800
C	-3.88858100	-2.27091600	2.56648400
C	-2.31600900	-2.34324000	4.86619800
H	-0.66857100	-1.87230400	3.56871500
C	-4.47043300	-2.53672100	3.80291500
H	-4.50986400	-2.23992700	1.67766200
C	-3.68618600	-2.57305300	4.95359600
H	-1.70134700	-2.36536400	5.75903700
H	-5.53788700	-2.71522400	3.86733200
H	-4.14356400	-2.77556900	5.91547600
C	0.29318000	3.74379800	-1.07362200
C	1.49224100	3.98872300	-1.74249500
C	-0.55143500	4.80649500	-0.74017700

C	1.84548200	5.29406300	-2.07580500
H	2.14602300	3.16155000	-1.99967400
C	-0.19030700	6.10714500	-1.07030100
H	-1.48557100	4.62216900	-0.21910000
C	1.00848400	6.35202700	-1.73696400
H	2.77810900	5.48088700	-2.59537300
H	-0.84387700	6.92990800	-0.80492300
H	1.28857700	7.36806500	-1.99088400
C	-3.01029600	-0.91961200	-0.15216300
C	-3.91312100	-1.65302100	-1.00184600
C	-3.09422300	0.46416200	-0.11922600
C	-4.01259800	-3.07222100	-1.00707100
C	-4.79930900	-0.93449500	-1.85658300
C	-4.03766300	1.15756200	-0.92256300
C	-4.87567900	-3.72617700	-1.84983000
H	-3.41642100	-3.65198800	-0.31865200
C	-5.66596500	-1.63631900	-2.73401600
C	-4.83741100	0.48213300	-1.79566800
H	-4.09113500	2.23814300	-0.84768300
C	-5.69838600	-3.00528300	-2.74349900
H	-4.93073700	-4.80849000	-1.82332000
H	-6.31243200	-1.05919800	-3.38740100
H	-5.52971000	1.01538300	-2.43927400
H	-6.36482500	-3.53577700	-3.41372300
C	-1.22952800	2.05358900	0.80234100
C	-0.77860100	2.82890500	1.94179900
C	-2.38839200	1.29512800	0.92139800
C	0.43536700	3.57252700	1.97642100
C	-1.56217300	2.84259200	3.13200500
C	-3.13038100	1.31471800	2.13868500
C	0.81003200	4.29526200	3.07993600
H	1.11027600	3.56160600	1.13625600
C	-1.15884500	3.60757000	4.25840100
C	-2.74193200	2.06626900	3.20391200
H	-4.03147800	0.71457900	2.19246700
C	0.00176600	4.32900100	4.23760700
H	1.74852800	4.83776800	3.06292700
H	-1.79361200	3.59506600	5.13799200
H	-3.32542400	2.07544500	4.11844000
H	0.30764200	4.91040600	5.09954600

CIAC1-*I*

Pt	1.51446800	0.37594000	-0.65347300
P	-0.07763400	2.00638800	-0.71181900
P	-1.74299000	-1.51009900	0.96428000
Cl	1.77911000	0.38233900	-3.23446300
C	1.90576100	0.78150300	1.27450200
C	3.07087500	1.52945900	1.48933100
C	1.20004900	0.32466800	2.38685800
C	3.52918000	1.78806500	2.77912800
H	3.64000500	1.89826900	0.64234700
C	1.65898900	0.58144000	3.67953300
H	0.28179600	-0.23487400	2.24836300
C	2.82811300	1.30810700	3.88348900
H	4.43799400	2.36431600	2.91900600
H	1.09372200	0.21047400	4.52893100
H	3.18453800	1.50462000	4.88858200
C	2.55244800	-1.68235100	0.18677800
C	3.95002400	-1.42725100	0.77732000
C	4.73700200	-2.70881700	0.47765800
C	4.92853300	-2.68113400	-0.90993100
C	4.23724700	-1.38591700	-1.35343500
C	2.73923100	-1.66034000	-1.15862000
H	5.04949300	-3.77945700	2.31955100
H	1.72252500	-2.10768700	0.73600900
H	4.01503500	-1.00845800	1.77603200
C	5.19891300	-3.75318600	1.24602200
C	5.58493500	-3.69948700	-1.56386700
H	4.54811800	-0.92250100	-2.28405200
H	2.09541600	-2.06646600	-1.92442300
C	6.06915000	-4.76580700	-0.78644700
C	5.88073800	-4.79221800	0.58879500
H	5.73238100	-3.68519100	-2.63793800
H	6.59836500	-5.57927800	-1.26972300
H	6.26513000	-5.62569800	1.16564900
O	4.50624100	-0.55585900	-0.21619000
C	-1.16094400	1.78196300	-2.18790200
C	-1.74130300	2.87943300	-2.82658400
C	-1.34946400	0.50657400	-2.72338800
C	-2.50355200	2.69832500	-3.97827400
H	-1.60436700	3.88333600	-2.44683000
C	-2.11285500	0.32572400	-3.86716200

H	-0.88452200	-0.34560700	-2.24900300
C	-2.69015900	1.42400200	-4.50092200
H	-2.94494400	3.55994300	-4.46576200
H	-2.24853900	-0.67234500	-4.26900500
H	-3.27774200	1.28484500	-5.40170000
C	-1.18747100	-3.12431000	0.26966400
C	-0.47017900	-3.10214500	-0.93117300
C	-1.34382100	-4.34209700	0.93790700
C	0.04151300	-4.27433600	-1.47651000
H	-0.30581100	-2.15769900	-1.44003900
C	-0.81487500	-5.51314600	0.39988900
H	-1.89303100	-4.38754900	1.87168700
C	-0.13065100	-5.48624200	-0.81121800
H	0.58257600	-4.23904900	-2.41567700
H	-0.94768800	-6.45080100	0.92793700
H	0.27295500	-6.40079000	-1.23035600
C	-2.78039900	-2.01663800	2.39948900
C	-2.11983300	-2.20306000	3.61982300
C	-4.16799000	-2.17469400	2.34938600
C	-2.82940600	-2.56334100	4.76140000
H	-1.04352600	-2.06580900	3.67579500
C	-4.87854100	-2.52298400	3.49540200
H	-4.70221800	-2.01805600	1.41885300
C	-4.21140500	-2.72267400	4.70061000
H	-2.30499100	-2.70886600	5.69900100
H	-5.95532200	-2.63970900	3.44459400
H	-4.76751200	-2.99298000	5.59112500
C	0.59420400	3.68326600	-1.01568300
C	1.85592800	3.79371800	-1.60067200
C	-0.13731500	4.83682100	-0.71518700
C	2.38339700	5.05199300	-1.88187300
H	2.42431800	2.89997900	-1.83656900
C	0.39445200	6.08881900	-0.99632500
H	-1.11500000	4.75786500	-0.25044600
C	1.65635300	6.19758400	-1.57884000
H	3.36493600	5.13285400	-2.33451500
H	-0.17372700	6.97993400	-0.75609900
H	2.07137900	7.17613900	-1.79202400
C	-2.98131100	-0.77804100	-0.20474200
C	-3.85840400	-1.48859600	-1.10220300
C	-3.04565700	0.60587600	-0.16027600

C	-3.94975400	-2.90676600	-1.15545700
C	-4.72604200	-0.74815200	-1.95709800
C	-3.97147700	1.32079400	-0.96800800
C	-4.78900300	-3.53802700	-2.03897200
H	-3.36355300	-3.50620200	-0.47605300
C	-5.57207200	-1.42539200	-2.87230700
C	-4.76565000	0.66710600	-1.86069800
H	-4.01831200	2.39997300	-0.87508300
C	-5.59794600	-2.79374200	-2.92535800
H	-4.83508300	-4.62103800	-2.05056300
H	-6.20565400	-0.83038400	-3.52232200
H	-5.45017000	1.21641100	-2.49903000
H	-6.24715000	-3.30546600	-3.62634600
C	-1.15055800	2.12545000	0.80169900
C	-0.69962500	2.88872800	1.94966600
C	-2.34599200	1.42240200	0.89485800
C	0.54974900	3.56711500	2.02496800
C	-1.52556100	2.95977200	3.11003500
C	-3.12632900	1.48882100	2.08582700
C	0.91383500	4.29592100	3.12783900
H	1.26129200	3.49296000	1.21985500
C	-1.12977200	3.72673200	4.23780600
C	-2.74158400	2.23984200	3.15254100
H	-4.05466200	0.92978000	2.11614000
C	0.06249400	4.39508300	4.24958700
H	1.88038800	4.78705600	3.14039000
H	-1.79732600	3.75863500	5.09222000
H	-3.35390600	2.28932700	4.04670200
H	0.36113300	4.97944400	5.11210100

CTS2-I

Pt	-0.18534100	-1.44683000	-0.94358200
P	2.06658900	-0.64215600	-0.67048100
P	-0.82211500	1.83472400	0.95621200
Cl	-0.05282500	-1.33185100	-3.41312400
C	-0.52024100	-2.24363800	1.03050300
C	-0.39615900	-1.55940800	2.24993000
C	-0.26975600	-3.63252500	1.02851800
C	-0.08877700	-2.23232400	3.42619000
H	-0.57882100	-0.49121300	2.27410900
C	0.06977400	-4.29805800	2.19853400

H	-0.38226900	-4.19242100	0.10878100
C	0.13588300	-3.60581500	3.40721700
H	-0.02509000	-1.67975700	4.35762400
H	0.26213100	-5.36496700	2.17070800
H	0.36980400	-4.13331200	4.32543400
C	-2.24777100	-1.75319300	0.29621200
C	-3.04255100	-3.06508400	0.47377100
C	-4.47001600	-2.70912800	0.06679400
C	-4.42065100	-2.58465100	-1.32723200
C	-2.95329900	-2.82748200	-1.66808000
C	-2.23389100	-1.57703700	-1.13998300
H	-5.67269000	-2.57386000	1.85065100
H	-2.45628800	-0.91223000	0.94598300
H	-2.89627900	-3.61429200	1.39859400
C	-5.63471900	-2.48539200	0.77059200
C	-5.54030800	-2.23510700	-2.05294300
H	-2.70504900	-3.17173300	-2.66720400
H	-2.52686000	-0.61812400	-1.56159600
C	-6.73679600	-2.03029700	-1.34771100
C	-6.78387300	-2.15245100	0.03661400
H	-5.50688300	-2.12463100	-3.13106800
H	-7.63877300	-1.77349800	-1.89163000
H	-7.72118800	-1.99025100	0.55631600
O	-2.60898500	-3.80277300	-0.67119200
C	3.44147900	-1.79655300	-1.05874900
C	3.16248400	-2.85149800	-1.92862500
C	4.73644900	-1.63724400	-0.55643800
C	4.17249700	-3.73709000	-2.29898500
H	2.15589600	-2.97999000	-2.31409700
C	5.73990000	-2.52535500	-0.92505700
H	4.95932500	-0.82641600	0.12965200
C	5.45928300	-3.57622700	-1.79698000
H	3.94866700	-4.55412700	-2.97508800
H	6.74105600	-2.39929000	-0.52925400
H	6.24354800	-4.26878600	-2.08025300
C	2.43761500	0.70440600	-1.87554900
C	3.73543500	0.98853800	-2.30664300
C	1.37256700	1.42202300	-2.41932900
C	3.95788700	1.98416600	-3.25480800
H	4.58301800	0.43961900	-1.91676800
C	1.59224800	2.42296900	-3.35648800

H	0.36710900	1.17991100	-2.10555900
C	2.88963300	2.70468200	-3.77908200
H	4.96976400	2.19223400	-3.58320000
H	0.75102500	2.97518900	-3.76210600
H	3.06520300	3.47904400	-4.51751500
C	-1.39553800	2.65195300	2.51110300
C	-1.05192000	3.95449800	2.88838300
C	-2.12781500	1.86504000	3.41074600
C	-1.46240900	4.46661500	4.11641200
H	-0.45577900	4.57594600	2.23075300
C	-2.55135400	2.38321700	4.63070300
H	-2.36269400	0.83461200	3.16088300
C	-2.22033700	3.68757700	4.98579400
H	-1.18782400	5.47854300	4.39208100
H	-3.12526100	1.76178900	5.30860900
H	-2.54030200	4.09025800	5.93994000
C	-2.27026100	1.95315400	-0.18653800
C	-3.53808200	1.60060100	0.29130600
C	-2.11762900	2.17415100	-1.56083500
C	-4.61777400	1.47022000	-0.57793500
H	-3.69506100	1.42109900	1.34925200
C	-3.19599800	2.03702700	-2.42999500
H	-1.16031300	2.48428800	-1.96026900
C	-4.45033800	1.67831200	-1.94420300
H	-5.59119200	1.20236900	-0.18214400
H	-3.05153900	2.21672700	-3.48952100
H	-5.28951700	1.56773700	-2.62135500
C	2.39348900	0.01861300	1.02918900
C	2.76560000	-0.91525000	2.06967900
C	2.14745300	1.34230300	1.37161000
C	2.88637900	-2.31944400	1.86944700
C	3.00560400	-0.43617200	3.39023400
C	2.32552500	1.77279800	2.71952000
C	3.31174400	-3.15490600	2.86904600
H	2.60475000	-2.76559200	0.92749600
C	3.44393700	-1.32226200	4.40935400
C	2.76555500	0.92531100	3.69107200
H	2.12618700	2.81305000	2.95228000
C	3.61919700	-2.65457400	4.15310400
H	3.38301300	-4.21940200	2.67609000
H	3.63028800	-0.91361600	5.39701400

H	2.92578300	1.27796600	4.70436900
H	3.96029000	-3.32701500	4.93163800
C	0.48918600	2.96211800	0.31502700
C	0.26925500	4.22902600	-0.33404700
C	1.78687800	2.49794900	0.47172200
C	-1.00470100	4.85865800	-0.40548600
C	1.37690700	4.92384900	-0.89617500
C	2.88521700	3.24062500	-0.04101400
C	-1.17084300	6.05953900	-1.04732600
H	-1.85736300	4.39213700	0.06947100
C	1.17418700	6.15470700	-1.57337300
C	2.68433300	4.39459500	-0.73845700
H	3.88780600	2.85849200	0.11475700
C	-0.07476100	6.70948100	-1.65909100
H	-2.15269000	6.51757300	-1.08041000
H	2.03551000	6.65067000	-2.00869900
H	3.52273100	4.93839200	-1.16169800
H	-0.22392200	7.65142800	-2.17395000

CIA2-I

Pt	-1.34813300	0.36552200	0.26988600
P	0.48705500	2.03800200	0.57636700
P	2.35023500	-1.73610100	-1.12401600
Cl	-1.19098500	-0.58326600	2.45700900
C	-2.78798200	0.53028200	-1.99739400
C	-1.41055300	0.29189600	-2.17511000
C	-3.32402400	1.74072500	-2.46463700
C	-0.59498500	1.24516000	-2.81598900
H	-1.01825400	-0.70619700	-2.00251000
C	-2.51962300	2.65101300	-3.12827300
H	-4.37473200	1.96330300	-2.32981300
C	-1.14998700	2.41294600	-3.30059800
H	0.46218700	1.03557300	-2.94896200
H	-2.95466100	3.56746000	-3.51196400
H	-0.53458000	3.14112400	-3.81639100
C	-3.60428100	-0.57742300	-1.35463100
C	-5.05228500	-0.17040500	-0.99129100
C	-5.73199100	-1.39725700	-0.41561800
C	-5.17947600	-1.53916400	0.86087800
C	-4.17948800	-0.40135400	0.96424500
C	-2.99386500	-0.82099400	0.05443900

H	-7.06454700	-2.20849900	-1.90573600
H	-3.58011600	-1.46229300	-1.99484100
H	-5.61171900	0.38147500	-1.74166500
C	-6.64167200	-2.31121000	-0.91201800
C	-5.51891100	-2.60650700	1.67217000
H	-3.92932000	-0.03855000	1.95589300
H	-2.70259700	-1.85383800	0.23596400
C	-6.46076500	-3.52277900	1.18633700
C	-7.01373300	-3.37787600	-0.08366700
H	-5.07917800	-2.73242000	2.65596700
H	-6.76468600	-4.35736400	1.80833400
H	-7.74214900	-4.09952600	-0.43605300
O	-4.83283100	0.61771900	0.18721200
C	-0.14629800	3.71525400	0.12216000
C	-1.48421900	3.83827500	-0.24348100
C	0.63301500	4.87058500	0.26452700
C	-2.03580800	5.09651000	-0.49205000
H	-2.10564400	2.95341400	-0.33407200
C	0.08764800	6.11897300	0.00685500
H	1.67214200	4.79351000	0.56579800
C	-1.25065700	6.23478400	-0.37505000
H	-3.07921600	5.17647700	-0.77622800
H	0.70234700	7.00602900	0.10840700
H	-1.67640300	7.21284400	-0.56906900
C	0.93766300	2.51830500	2.30500500
C	2.17331000	3.08586300	2.63039300
C	-0.06157600	2.45470100	3.27658300
C	2.41657300	3.54128800	3.92184800
H	2.95740200	3.16272000	1.88429200
C	0.18720200	2.90429400	4.57063000
H	-1.03231000	2.04470800	3.02524000
C	1.42860200	3.43902900	4.89863100
H	3.38077900	3.97334200	4.16501100
H	-0.59198700	2.83329600	5.32125400
H	1.62323400	3.78469800	5.90756600
C	0.79161900	-2.49117500	-1.75213400
C	0.66655700	-2.52151600	-3.14895600
C	-0.28153400	-2.93367000	-0.97375900
C	-0.47591600	-3.03558800	-3.75286200
H	1.47040500	-2.13706600	-3.77040600
C	-1.42719900	-3.44523500	-1.58024800

H	-0.23957300	-2.86840700	0.10696000
C	-1.52546200	-3.50497900	-2.96700300
H	-0.54939500	-3.05811400	-4.83419200
H	-2.24999500	-3.79005800	-0.96325200
H	-2.41952900	-3.90523300	-3.43158600
C	3.57336000	-3.12233400	-1.28848200
C	3.44643800	-4.13108200	-2.24743500
C	4.72311200	-3.09847200	-0.48904300
C	4.43762500	-5.09853300	-2.39469500
H	2.56684600	-4.18177300	-2.87826600
C	5.70995700	-4.06811200	-0.63548000
H	4.84469900	-2.32926300	0.26716500
C	5.57097800	-5.07374100	-1.58878700
H	4.31521800	-5.87681900	-3.13978100
H	6.58751500	-4.03994700	0.00091400
H	6.33878800	-5.83051000	-1.70195900
C	2.21089200	-1.60369000	0.72283100
C	2.01052500	-2.72802900	1.60131900
C	2.48918200	-0.35415800	1.26844700
C	1.79000700	-4.05652700	1.13932100
C	2.06883000	-2.53053400	3.00985300
C	2.58744800	-0.19438600	2.67685400
C	1.60887500	-5.09673900	2.01450900
H	1.76081600	-4.25877400	0.07780900
C	1.86818700	-3.62290500	3.89432000
C	2.36655400	-1.24391700	3.51959300
H	2.86722800	0.76854100	3.08017200
C	1.63841200	-4.88227600	3.41114800
H	1.44254200	-6.09606700	1.62871200
H	1.90726600	-3.43291800	4.96187500
H	2.44282400	-1.11109900	4.59403100
H	1.48747400	-5.71321700	4.09027700
C	2.16861000	1.77705700	-0.17710300
C	2.73507400	2.58845000	-1.22853200
C	2.95137700	0.77289400	0.37900800
C	1.96710500	3.42926200	-2.08289300
C	4.13220900	2.50047200	-1.50361300
C	4.34438500	0.71876500	0.09692100
C	2.54899100	4.16718600	-3.08177100
H	0.89572200	3.46682400	-1.97335700
C	4.71448700	3.29831800	-2.52336600

C	4.92977900	1.58253700	-0.77937900
H	4.93800600	-0.03489300	0.60163900
C	3.94468300	4.12500700	-3.29474400
H	1.92591100	4.78390300	-3.72010100
H	5.78374600	3.21672200	-2.68847300
H	5.99665700	1.54398100	-0.97152500
H	4.39337000	4.72386000	-4.07869600

CIA1O-2

Pt	-1.86047800	0.48093300	-1.07381100
P	-1.44452600	-1.57092800	-0.31032600
P	2.30476600	0.37758300	0.60085600
Cl	-1.91133500	-0.20730800	-3.53736700
C	-2.15019900	1.29147500	0.71856100
C	-1.16664900	1.49790200	1.68841300
C	-3.43748300	1.78515300	0.96998600
C	-1.45899600	2.16853400	2.87515700
H	-0.16308400	1.12301300	1.52305000
C	-3.73146300	2.46418300	2.15096700
H	-4.22884600	1.63052500	0.24102000
C	-2.74218000	2.65345700	3.11396100
H	-0.67697700	2.30839600	3.61560700
H	-4.73755600	2.83267100	2.32267400
H	-2.96974900	3.17288900	4.03827000
C	-1.55196100	4.18359500	-3.46559100
C	-0.90663200	3.06849000	-2.63732600
C	-0.26039500	3.73098000	-1.41754500
C	-1.33848400	4.20656300	-0.66002300
C	-2.57716300	3.79467800	-1.45399900
C	-2.57498800	4.62680000	-2.74267300
H	1.88212400	3.56777200	-1.59729300
H	-1.17247300	4.54142400	-4.41191000
H	-0.35606200	2.28981600	-3.15541600
C	1.04112500	3.92797300	-1.01424600
C	-1.14505300	4.89316300	0.51653100
H	-3.51387300	3.67974800	-0.92064000
H	-3.25425000	5.44372300	-2.93957900
C	0.17968200	5.08876500	0.94334700
C	1.24925100	4.61582900	0.19438200
H	-1.97831300	5.25830100	1.10685300
H	0.36830200	5.61346900	1.87332700

H	2.26290600	4.77695300	0.54535900
O	-2.10429100	2.53000000	-2.00021800
C	-0.35837700	-2.43190000	-1.51050000
C	-0.58086300	-3.75904800	-1.87739000
C	0.65974300	-1.70799200	-2.13326900
C	0.22549600	-4.36105700	-2.84070800
H	-1.38090700	-4.33413500	-1.42911900
C	1.47608700	-2.31459000	-3.07644400
H	0.79365400	-0.66234100	-1.87967300
C	1.25836900	-3.64508400	-3.43377100
H	0.04089400	-5.39107800	-3.12322400
H	2.27345700	-1.74754100	-3.54513500
H	1.88797600	-4.11537000	-4.18086500
C	3.34514100	1.35671400	-0.56195900
C	3.23720800	1.10258100	-1.93458400
C	4.11962400	2.43895500	-0.13717300
C	3.90386400	1.89808200	-2.85866900
H	2.64042600	0.26827500	-2.28551100
C	4.77615300	3.24464100	-1.06602800
H	4.22091500	2.65892500	0.91986600
C	4.67366700	2.97718500	-2.42731800
H	3.81818300	1.67748400	-3.91685000
H	5.37440100	4.08059600	-0.72051500
H	5.18916800	3.60224300	-3.14734500
C	3.01317100	0.79782000	2.24547200
C	2.41058100	1.85867200	2.93029700
C	4.06626300	0.10734900	2.85141500
C	2.86130300	2.23410100	4.19244600
H	1.58208100	2.39195100	2.47283900
C	4.50986000	0.47703000	4.11843800
H	4.53483100	-0.72756500	2.34057900
C	3.91023100	1.54099600	4.78926800
H	2.38532600	3.05925100	4.71046600
H	5.32511300	-0.06585800	4.58360900
H	4.25652000	1.82569200	5.77630000
C	-2.92304100	-2.65090600	-0.28716500
C	-4.00117500	-2.34680700	-1.11845800
C	-2.95939900	-3.79682000	0.51199000
C	-5.11281000	-3.18546000	-1.14573700
H	-3.97283900	-1.45687400	-1.73826800
C	-4.07116100	-4.63037000	0.47996700

H	-2.12493500	-4.03797400	1.16238900
C	-5.15025500	-4.32297100	-0.34582100
H	-5.95090700	-2.94372100	-1.78900700
H	-4.09599000	-5.51626500	1.10377900
H	-6.01942400	-4.97043100	-0.36420900
C	-0.73242200	-1.69863200	1.39444000
C	-1.62792700	-1.48088500	2.51304300
C	0.61703500	-1.91795700	1.64089100
C	-3.01179000	-1.17119400	2.37862600
C	-1.11962400	-1.54653600	3.84130200
C	1.09551300	-1.92856800	2.98574800
C	-3.82005100	-0.99119600	3.47142200
H	-3.45555800	-1.04411800	1.40327300
C	-1.97876700	-1.36867200	4.95740200
C	0.26216500	-1.76310100	4.04843900
H	2.15344700	-2.09926000	3.14679300
C	-3.30851500	-1.10399800	4.78316900
H	-4.86559300	-0.74664100	3.32132300
H	-1.54705400	-1.43930200	5.95014000
H	0.64554200	-1.79329900	5.06287300
H	-3.96275900	-0.96469000	5.63567500
C	2.73890700	-1.40725200	0.34612600
C	3.93747200	-1.92162600	-0.26321900
C	1.72678600	-2.29194300	0.69002100
C	5.11442900	-1.14638300	-0.46319600
C	3.99215800	-3.29712700	-0.63363300
C	1.82752200	-3.67062300	0.37039900
C	6.23289500	-1.68344000	-1.04900100
H	5.14366100	-0.12316000	-0.11803800
C	5.15187100	-3.81942500	-1.26339500
C	2.90278800	-4.14934900	-0.31955000
H	1.02104500	-4.33325300	0.66455500
C	6.24879100	-3.02929300	-1.47975600
H	7.11778100	-1.06979100	-1.17468000
H	5.15386300	-4.86589200	-1.55100200
H	2.95753900	-5.19540100	-0.60363200
H	7.13472100	-3.43625600	-1.95324500
CTS1-2			
Pt	-2.17614800	-0.31763600	-0.28050800
P	-0.71822700	-1.95904200	-0.55323600

P	2.78091200	1.01112100	0.99106300
Cl	-2.95581400	-0.35816900	-2.71111900
C	-1.87495900	-0.17212300	1.67608900
C	-0.69475900	0.32007400	2.23499100
C	-2.93533500	-0.47434500	2.53928400
C	-0.57432500	0.52299000	3.60867700
H	0.15793100	0.53166200	1.60180600
C	-2.82247100	-0.27027400	3.91323900
H	-3.85909900	-0.88193600	2.14023000
C	-1.63934700	0.22680600	4.45575200
H	0.35864100	0.90522800	4.01188500
H	-3.65750700	-0.51559700	4.56128300
H	-1.54853500	0.37707800	5.52577500
C	-4.47145800	1.69034900	-0.65058600
C	-3.41868800	2.63647400	-1.24860000
C	-3.81770200	4.05369900	-0.83239600
C	-3.60103400	4.08374500	0.55096600
C	-3.08848700	2.68204500	0.88394400
C	-4.26842400	1.72019200	0.66942900
H	-4.48076200	5.13087500	-2.57557700
H	-5.25599500	1.20318700	-1.21107200
H	-3.11348500	2.46541700	-2.27482500
C	-4.30968800	5.14942200	-1.50507000
C	-3.86703900	5.21042400	1.29560400
H	-2.48540900	2.55611700	1.77776700
H	-4.85170600	1.27071100	1.45943400
C	-4.36471600	6.33612300	0.61690400
C	-4.58180800	6.30607300	-0.75401600
H	-3.69795800	5.23770700	2.36620600
H	-4.57898800	7.24211800	1.17239100
H	-4.96479200	7.18842800	-1.25399500
O	-2.33449000	2.40766100	-0.31940900
C	-1.45645500	-3.60937800	-0.83903000
C	-2.77980500	-3.72338200	-1.26379100
C	-0.66919800	-4.75397200	-0.69020500
C	-3.31315700	-4.97992400	-1.53656000
H	-3.38907600	-2.83408700	-1.37867000
C	-1.20722100	-6.00574200	-0.96627800
H	0.36064700	-4.67331200	-0.35712900
C	-2.52959000	-6.11982800	-1.38827900
H	-4.34337700	-5.06503500	-1.86214600

H	-0.59460000	-6.89182900	-0.84749200
H	-2.94878000	-7.09747200	-1.59732600
C	0.10032300	-1.60069500	-2.15500900
C	0.16322900	-2.55728200	-3.16712200
C	0.55442200	-0.30335800	-2.40299700
C	0.69927500	-2.22082900	-4.40830600
H	-0.20572200	-3.56246700	-3.00844500
C	1.10902500	0.02250800	-3.63089900
H	0.47212800	0.45295400	-1.63185100
C	1.17953400	-0.93790500	-4.64000000
H	0.73991800	-2.96867500	-5.19209400
H	1.47636000	1.02842200	-3.80350900
H	1.60228600	-0.68010500	-5.60473600
C	2.31479900	2.65716500	0.27349700
C	3.13680300	3.78995800	0.26603000
C	0.99229400	2.79222400	-0.16802000
C	2.66308400	5.00933200	-0.20790600
H	4.15750200	3.72713000	0.62804300
C	0.52297400	4.00846200	-0.65775600
H	0.30241700	1.95458100	-0.11688500
C	1.35845500	5.12051000	-0.68067100
H	3.31795500	5.87342700	-0.20777600
H	-0.50512200	4.07974400	-0.99265000
H	0.99191400	6.07115500	-1.05118000
C	4.42702700	1.30468800	1.76026500
C	4.48955200	2.21287700	2.82648600
C	5.56929700	0.56510400	1.44137000
C	5.67468100	2.40646100	3.52558100
H	3.60528900	2.77792000	3.10764500
C	6.75367300	0.75202100	2.15163500
H	5.54474400	-0.16007400	0.63557300
C	6.81262300	1.67452400	3.19000300
H	5.70765400	3.12125000	4.34013900
H	7.63118600	0.17216100	1.88800700
H	7.73646700	1.82117400	3.73763000
C	3.16709900	-0.11721000	-0.43426100
C	4.00841800	0.22060300	-1.55471700
C	2.60123300	-1.38240100	-0.38155100
C	4.66845000	1.47186200	-1.68229100
C	4.22793600	-0.73980200	-2.58221600
C	2.87878000	-2.34563100	-1.39042100

C	5.44116800	1.76707500	-2.77716300
H	4.57437700	2.20462300	-0.89687600
C	5.02579200	-0.40953800	-3.70786500
C	3.65245200	-2.03077400	-2.46579900
H	2.44542700	-3.33497400	-1.29243000
C	5.61499300	0.82229800	-3.81271100
H	5.92913200	2.73282100	-2.84405900
H	5.15986600	-1.15930400	-4.48099700
H	3.84178200	-2.76251400	-3.24441000
H	6.22085800	1.07101000	-4.67635300
C	0.48565600	-2.25408300	0.82990800
C	-0.05289300	-2.86324700	2.03282700
C	1.82551700	-1.89331900	0.79829400
C	-1.41476900	-3.24050100	2.19687000
C	0.80965500	-3.10518000	3.13907300
C	2.64991800	-2.11960100	1.94077000
C	-1.86310600	-3.84788900	3.34288600
H	-2.14183900	-3.03420900	1.42634200
C	0.32133300	-3.72561100	4.31704400
C	2.16665900	-2.70492900	3.06842900
H	3.69319300	-1.82837700	1.88054500
C	-0.98964100	-4.10382200	4.41981600
H	-2.91063000	-4.11539700	3.42438000
H	1.01721600	-3.88961100	5.13278200
H	2.81247400	-2.88102900	3.92212700
H	-1.36025300	-4.58001300	5.31991500

CIAC1-2

Pt	-0.48039700	-1.15867100	-1.09908900
P	1.71505100	-1.25906100	-0.63335000
P	-0.17512300	1.84448000	0.82792400
Cl	-0.22550200	-0.38950000	-3.48126700
C	-0.88503300	-2.19019100	0.57068300
C	-1.01065400	-1.63179400	1.84160300
C	-1.19022700	-3.54927900	0.41737000
C	-1.44739300	-2.39439300	2.92138700
H	-0.76076100	-0.58813200	1.98896900
C	-1.63652500	-4.31438400	1.49184900
H	-1.07911300	-4.01970200	-0.55603000
C	-1.76970200	-3.73701100	2.75140500
H	-1.53195300	-1.93309000	3.89984100

H	-1.87058100	-5.36335900	1.34464900
H	-2.10952700	-4.32966100	3.59292900
C	-2.93713800	-0.29736600	-1.75347000
C	-3.70164000	0.50916500	-0.69185500
C	-5.16575600	0.09178300	-0.87104000
C	-5.20342900	-1.22619500	-0.40423200
C	-3.75536700	-1.51641300	0.01059200
C	-2.97313300	-1.57413400	-1.31972100
H	-6.25789300	1.73319400	-1.72958100
H	-2.63567000	0.06706800	-2.72506700
H	-3.49140900	1.56688600	-0.59381300
C	-6.28842400	0.71236000	-1.36596000
C	-6.36950900	-1.95506100	-0.41930500
H	-3.57195500	-2.29171600	0.74786000
H	-2.77793800	-2.47097900	-1.89305800
C	-7.52473900	-1.32745000	-0.91270200
C	-7.48545300	-0.02134000	-1.37688200
H	-6.40720300	-2.97662200	-0.05892200
H	-8.46136400	-1.87186600	-0.92864600
H	-8.39172300	0.43973400	-1.75107300
O	-3.36996400	-0.22276200	0.49079300
C	2.79751300	-0.10061400	-1.58026800
C	4.15204500	-0.40066500	-1.74289300
C	2.29083500	1.06390400	-2.15083100
C	4.97988800	0.45425200	-2.46107600
H	4.57366700	-1.30447100	-1.32367200
C	3.11665500	1.91820900	-2.86747900
H	1.24829300	1.30583200	-2.03099100
C	4.46330300	1.61280500	-3.02820100
H	6.02693400	0.20461100	-2.58492100
H	2.70168000	2.82247700	-3.29671800
H	5.10675700	2.27475100	-3.59645500
C	-1.30785200	2.85023100	-0.22652800
C	-1.27406300	2.63195500	-1.60703300
C	-2.29205100	3.69793600	0.29388700
C	-2.18093300	3.26170300	-2.45109600
H	-0.57256100	1.92964900	-2.04013500
C	-3.21046100	4.31485100	-0.55034500
H	-2.34460700	3.88000500	1.36117100
C	-3.15742900	4.10220600	-1.92501300
H	-2.13119500	3.07153100	-3.51716600

H	-3.96893900	4.96512200	-0.12994700
H	-3.87300100	4.58537300	-2.57987300
C	-0.61840600	2.42524300	2.51284300
C	-1.74758300	1.83714300	3.09607600
C	0.10576600	3.37741000	3.23120000
C	-2.14973100	2.21054800	4.37320100
H	-2.31720400	1.09655700	2.53825100
C	-0.29310900	3.73819500	4.51500300
H	0.98002900	3.84028400	2.78474900
C	-1.42027600	3.15780300	5.08615400
H	-3.02916300	1.75606700	4.81405500
H	0.27418100	4.47922300	5.06614600
H	-1.73011800	3.44294800	6.08462600
C	2.43759000	-2.84838900	-1.20182300
C	1.88429800	-3.41424500	-2.35064600
C	3.56282300	-3.43150500	-0.61344000
C	2.45132600	-4.56087600	-2.89938800
H	1.02657600	-2.94593700	-2.82394700
C	4.12028400	-4.57770300	-1.16357600
H	3.98944800	-3.00293500	0.28744300
C	3.56390600	-5.14430800	-2.30727700
H	2.01984600	-4.99268500	-3.79421000
H	4.98622800	-5.03094200	-0.69633800
H	4.00007800	-6.03937000	-2.73467700
C	1.54669600	2.49401600	0.58475500
C	1.92825400	3.78823900	0.07904600
C	2.53872500	1.56663800	0.85973200
C	1.01792400	4.86632500	-0.08609000
C	3.29588800	4.03973600	-0.22996000
C	3.90566500	1.86536300	0.61461100
C	1.42368300	6.07535900	-0.58971000
H	-0.01218500	4.74410000	0.20748300
C	3.68365700	5.29101200	-0.76978300
C	4.26863700	3.04631400	0.04398400
H	4.64872900	1.11381900	0.85490200
C	2.76763700	6.28932800	-0.95999500
H	0.70148500	6.87565300	-0.69886600
H	4.72937600	5.44405800	-1.01465200
H	5.30791000	3.24940500	-0.19193200
H	3.07300200	7.24470100	-1.36952300
C	2.09737500	-0.99639500	1.16452500

C	1.99787100	-2.07976800	2.12056500
C	2.30496800	0.29604400	1.63569400
C	1.67358100	-3.42222200	1.78069600
C	2.18030100	-1.80887400	3.50714900
C	2.43675400	0.53301200	3.03322400
C	1.58354800	-4.40782000	2.72593900
H	1.44655800	-3.68585100	0.76272900
C	2.09621700	-2.85063500	4.46638300
C	2.39119000	-0.48104300	3.93782500
H	2.58170900	1.55567000	3.36061000
C	1.81038400	-4.13128000	4.08990800
H	1.30838400	-5.40909300	2.41642300
H	2.25068700	-2.59790300	5.50973200
H	2.49888400	-0.28045200	4.99823600
H	1.73592400	-4.92174700	4.82690000

CTS2-2

Pt	0.47751300	-1.57900900	-1.11510300
P	2.14092700	0.13788200	-0.73924600
P	-1.49303400	1.27552500	0.83482500
Cl	0.29235700	-1.01784800	-3.53933300
C	0.61551300	-2.60917400	0.74907300
C	0.22006100	-1.92731700	1.91227400
C	1.54552100	-3.66187500	0.89004700
C	0.71866800	-2.28308500	3.16042100
H	-0.50139300	-1.12320600	1.82325200
C	2.01523800	-4.04186300	2.13657100
H	1.84624100	-4.22152900	0.00923900
C	1.59634600	-3.35715200	3.27893600
H	0.40411600	-1.73274100	4.04105800
H	2.70569400	-4.87348800	2.22288300
H	1.95698200	-3.66025900	4.25576200
C	-1.15522800	-2.80750600	-1.42080600
C	-2.49556500	-2.08929100	-1.13398500
C	-3.53573600	-3.20361600	-1.12505000
C	-3.25783600	-3.92050100	0.04440900
C	-2.10227100	-3.16404400	0.69483600
C	-0.88142800	-3.48337600	-0.18049800
H	-4.75249000	-3.05648600	-2.89766500
H	-1.04974800	-3.34063800	-2.35973000
H	-2.71751300	-1.18154300	-1.68876600

C	-4.53406800	-3.60526500	-1.98807400
C	-3.96111700	-5.05833500	0.37967400
H	-1.98477500	-3.24932100	1.77062800
H	-0.47075300	-4.48300800	-0.17240300
C	-4.98918600	-5.46348900	-0.48453700
C	-5.27068000	-4.74959900	-1.64414000
H	-3.74045100	-5.61747100	1.28226800
H	-5.57395800	-6.34357600	-0.24221000
H	-6.07338300	-5.08138700	-2.29295200
O	-2.38275800	-1.82801000	0.27903600
C	1.90816100	1.61486600	-1.82078600
C	2.97766500	2.41928100	-2.22199100
C	0.62933300	1.90536200	-2.29295600
C	2.76499400	3.49976000	-3.07377200
H	3.98420900	2.21397900	-1.88134100
C	0.41291300	2.98771800	-3.13700700
H	-0.19259800	1.26260900	-2.00753300
C	1.48355300	3.78708300	-3.53184100
H	3.60507100	4.11331000	-3.37884400
H	-0.58782000	3.20064700	-3.49853300
H	1.31835300	4.62546000	-4.19932600
C	-2.96690100	1.24771000	-0.28355500
C	-2.86064900	1.71967700	-1.59774000
C	-4.14412500	0.59385300	0.09176700
C	-3.88984500	1.52928700	-2.51361600
H	-1.98126900	2.27168300	-1.90393600
C	-5.17577600	0.40483200	-0.82460800
H	-4.26435700	0.21287400	1.09809300
C	-5.05065800	0.86041500	-2.13370700
H	-3.78276500	1.90973500	-3.52345800
H	-6.07868300	-0.10810800	-0.51181700
H	-5.85231300	0.70727500	-2.84702000
C	-2.22622600	1.43801200	2.51958900
C	-2.69871100	0.26791100	3.12958400
C	-2.23947900	2.62985200	3.25075600
C	-3.20533700	0.29656000	4.42508800
H	-2.67197500	-0.67037900	2.58255600
C	-2.73165600	2.65369300	4.55349700
H	-1.86056400	3.54522900	2.80922400
C	-3.22146100	1.49083900	5.14071600
H	-3.57697800	-0.61597400	4.87746600

H	-2.73441300	3.58543000	5.10796100
H	-3.60594400	1.51330800	6.15396500
C	3.86082600	-0.31609600	-1.20922900
C	4.01447100	-1.31229200	-2.17443700
C	4.99194800	0.30841200	-0.67559200
C	5.28800100	-1.68054600	-2.60391100
H	3.13782000	-1.80050400	-2.58879100
C	6.26069400	-0.06646800	-1.10103300
H	4.88361600	1.08046500	0.07951800
C	6.41086500	-1.06333100	-2.06405000
H	5.39873500	-2.45450300	-3.35475200
H	7.13369000	0.41636200	-0.67710500
H	7.40208000	-1.35649300	-2.39055500
C	-0.67077300	2.90427900	0.53841400
C	-1.32858100	4.11545400	0.12224000
C	0.71138400	2.89234900	0.65056900
C	-2.73895900	4.29431600	0.18409400
C	-0.54495900	5.22203800	-0.31124900
C	1.47502700	4.02508200	0.25815300
C	-3.32597500	5.46752700	-0.21696700
H	-3.35947500	3.50001000	0.57669900
C	-1.17944800	6.41489900	-0.74657200
C	0.87013300	5.13517500	-0.25500600
H	2.55399700	3.98443600	0.35843200
C	-2.54294400	6.53557800	-0.71078600
H	-4.40213300	5.57928000	-0.14788800
H	-0.55623500	7.23490500	-1.08815700
H	1.46136900	5.98201900	-0.58905100
H	-3.02236800	7.45116800	-1.03740800
C	2.20882500	0.75843400	1.00852500
C	2.95816100	-0.00738900	1.98336500
C	1.46741800	1.85066500	1.44180200
C	3.66528700	-1.20258500	1.67778500
C	3.01197900	0.43283600	3.33783800
C	1.46438100	2.20030100	2.82683300
C	4.45227100	-1.83291500	2.60729100
H	3.57445800	-1.65848400	0.70388200
C	3.82070700	-0.24467300	4.28617300
C	2.22581000	1.53791700	3.74019800
H	0.86131000	3.04780600	3.13283300
C	4.55475500	-1.34188100	3.92564300

H	4.97775200	-2.73997100	2.33032000
H	3.84180100	0.13245700	5.30327300
H	2.23939400	1.84672400	4.78010700
H	5.18328600	-1.84882600	4.64859000

CIA2-2

Pt	-1.18957000	-0.85521700	0.19870200
P	1.13286400	-1.86061300	0.21380800
P	1.73306400	2.54714000	0.42607400
Cl	-0.88456800	-0.02883900	2.40478000
C	-3.08083500	-1.71401700	-1.53505900
C	-3.44475100	-3.06998400	-1.56965900
C	-1.88357300	-1.32043600	-2.16135800
C	-2.68283300	-3.98115600	-2.27913000
H	-4.33713000	-3.40659300	-1.05839500
C	-1.11154300	-2.26432300	-2.86597500
H	-1.66124700	-0.25959600	-2.26494600
C	-1.51676400	-3.58041900	-2.94133300
H	-2.99408800	-5.01953500	-2.31965600
H	-0.21139400	-1.94840200	-3.37578900
H	-0.92948100	-4.30344100	-3.49473600
C	-3.08738700	-0.10808400	0.32040900
C	-3.96785700	-0.58264100	1.51086700
C	-5.13838900	0.38271700	1.53678900
C	-5.91258900	0.01917800	0.43027700
C	-5.18349400	-1.16753700	-0.17011700
C	-3.91955300	-0.63282200	-0.88093800
H	-4.87058900	1.76392200	3.17161300
H	-2.98362200	0.97891700	0.32060100
H	-3.45980000	-0.78555800	2.44683900
C	-5.47441200	1.47234100	2.31873900
C	-7.04023300	0.73515300	0.07588800
H	-5.78969000	-1.88035100	-0.72364100
H	-4.15477000	0.14168800	-1.61371400
C	-7.40010600	1.82644500	0.87780200
C	-6.63077700	2.18769800	1.98096500
H	-7.63693300	0.46268600	-0.78816800
H	-8.29159100	2.39521100	0.63835300
H	-6.93249000	3.03363300	2.58854300
O	-4.60043000	-1.76654700	0.99695800
C	1.02096800	-3.53386100	-0.53307300

C	-0.01430600	-4.37227400	-0.10584100
C	1.86690400	-3.96365300	-1.55845900
C	-0.15399400	-5.64757400	-0.64357200
H	-0.72370200	-4.02346600	0.63907400
C	1.70563200	-5.22953200	-2.11537100
H	2.65953800	-3.31830100	-1.92144400
C	0.70808400	-6.08017500	-1.64707800
H	-0.95096500	-6.29312800	-0.29211600
H	2.36817600	-5.55295400	-2.91009600
H	0.59384900	-7.07042900	-2.07341500
C	1.58655900	-2.12721700	1.99041900
C	2.21989700	-1.06702600	2.64628100
C	1.28487800	-3.28402600	2.70692900
C	2.56329800	-1.17172300	3.98798600
H	2.44821400	-0.15260800	2.10778000
C	1.62493300	-3.38440600	4.05519300
H	0.80635400	-4.12809500	2.22718300
C	2.26576900	-2.33195800	4.69884500
H	3.05977700	-0.34257200	4.47952300
H	1.39164100	-4.29407800	4.59699000
H	2.53336400	-2.41406800	5.74618400
C	0.39558200	3.60712600	1.12646800
C	-0.91423100	3.11782700	1.12994200
C	0.66076400	4.83550300	1.73679600
C	-1.94288700	3.85355200	1.70508400
H	-1.12894500	2.15815500	0.67383900
C	-0.37061800	5.56660500	2.32332200
H	1.66797300	5.23714700	1.74713000
C	-1.67459100	5.08242100	2.30517200
H	-2.95596300	3.46640000	1.68398000
H	-0.15148800	6.51999900	2.79120800
H	-2.47620400	5.65595300	2.75646600
C	3.04770000	3.78140400	0.03158600
C	4.02355500	3.98442700	1.01353800
C	3.14189000	4.48544500	-1.17236600
C	5.05377000	4.89892600	0.81167000
H	3.97508900	3.42349100	1.94209500
C	4.17903400	5.39068500	-1.37847900
H	2.41309500	4.32536300	-1.95884000
C	5.13304500	5.60277100	-0.38616200
H	5.79955700	5.05010800	1.58385700

H	4.24208400	5.92941600	-2.31726000
H	5.93807200	6.31017700	-0.54919000
C	1.10572400	2.01080800	-1.24112900
C	0.17722400	2.72419300	-2.08058700
C	1.57984300	0.77506300	-1.66605800
C	-0.25074200	4.06007200	-1.83181800
C	-0.30515900	2.10313400	-3.27109900
C	1.13750600	0.20682800	-2.88734500
C	-1.14165000	4.69315800	-2.65952200
H	0.15112300	4.60239100	-0.98911400
C	-1.24782400	2.77264900	-4.09725000
C	0.19828300	0.83578400	-3.65273700
H	1.57416700	-0.73314000	-3.20696400
C	-1.67116200	4.03768000	-3.79459400
H	-1.43634500	5.71365000	-2.44280600
H	-1.60789500	2.26036600	-4.98352800
H	-0.16057300	0.38508700	-4.57288800
H	-2.38640400	4.54707700	-4.42982100
C	2.73744900	-1.13611200	-0.38333100
C	3.99595300	-1.75041000	-0.01075300
C	2.75442100	0.08567300	-1.03588000
C	4.10417300	-3.03403300	0.59633400
C	5.21383800	-1.05695100	-0.26221100
C	3.99186900	0.74656500	-1.29200900
C	5.32015400	-3.56630700	0.94151100
H	3.22074900	-3.62214200	0.78924600
C	6.45943900	-1.62659000	0.11074000
C	5.17865500	0.20809500	-0.89916400
H	3.96975500	1.69666200	-1.81322300
C	6.51775000	-2.85631100	0.70701400
H	5.35938600	-4.54835200	1.39884200
H	7.36267600	-1.06134700	-0.09357700
H	6.11165100	0.73007700	-1.08492800
H	7.46995000	-3.28799800	0.99238500
UTS			
Pt	2.20160700	0.22913900	-0.86551300
P	-1.87441600	-0.88232600	0.43518900
P	0.81068000	1.89022200	0.08278400
Cl	3.57989500	1.75709900	-2.12164900
C	1.21614600	-1.70400600	-3.20170700

C	-0.09588200	-2.07308600	-3.51469600
C	1.85133000	-0.76225900	-4.01616800
C	-0.75669900	-1.49940700	-4.59920700
H	-0.61609200	-2.81463600	-2.91429300
C	1.19067600	-0.18334500	-5.09546600
H	2.86740800	-0.45851300	-3.79812600
C	-0.11970300	-0.54746300	-5.38963000
H	-1.77432300	-1.79808900	-4.82369400
H	1.70296500	0.55514600	-5.70235600
H	-0.63865400	-0.09548200	-6.22749900
C	1.95681600	-2.35983600	-2.04818500
C	1.12831500	-2.53421700	-0.73090100
C	1.74693400	-3.69792300	0.00499400
C	3.03477300	-3.30247600	0.38179500
C	3.38162900	-1.96107700	-0.12469900
C	3.14397000	-1.56392500	-1.50103700
H	0.25330000	-5.24324200	0.08706500
H	2.26582400	-3.35770800	-2.38498500
H	0.05063100	-2.60487900	-0.88288000
C	1.25597600	-4.93704000	0.36527000
C	3.85161600	-4.13109900	1.13708900
H	4.12123300	-1.39998700	0.44429900
H	4.02795100	-1.36861500	-2.10282800
C	3.36026400	-5.38820600	1.49727200
C	2.08119900	-5.78466000	1.11606500
H	4.84480500	-3.81321500	1.43477100
H	3.97568400	-6.05471400	2.09015300
H	1.71266700	-6.75797900	1.41967300
O	1.44984200	-1.43255300	0.13219600
C	1.45626200	3.60199800	0.30139700
C	1.78185000	4.31962600	-0.85547600
C	1.56785600	4.22580100	1.54507100
C	2.22202400	5.63423200	-0.76560300
H	1.67931700	3.85141700	-1.82747300
C	2.01201600	5.54416500	1.63114100
H	1.30091000	3.69993900	2.45400700
C	2.34121800	6.24900800	0.47925900
H	2.46821800	6.18048600	-1.66896000
H	2.09189200	6.01826300	2.60274400
H	2.68317600	7.27541200	0.54815600
C	-0.65233500	2.24970600	-0.96248600

C	-1.42067300	3.39734400	-0.74415000
C	-0.89860800	1.46137000	-2.08912800
C	-2.45515300	3.72575300	-1.60932200
H	-1.20858600	4.03833800	0.10391000
C	-1.92563500	1.80641600	-2.96721500
H	-0.28767700	0.58551000	-2.29251100
C	-2.71157400	2.92709800	-2.72248800
H	-3.05396200	4.60934500	-1.41863400
H	-2.10752100	1.19283100	-3.84289000
H	-3.51233400	3.18969600	-3.40459000
C	-2.79561700	-1.89504200	-0.79575300
C	-2.83198600	-3.28975100	-0.69057200
C	-3.29791800	-1.29718800	-1.95894700
C	-3.36724600	-4.06471700	-1.71833300
H	-2.44803100	-3.77979600	0.19738100
C	-3.85222600	-2.06997000	-2.97151200
H	-3.27779800	-0.21776600	-2.06024600
C	-3.88366900	-3.45935100	-2.85912900
H	-3.38725600	-5.14429800	-1.61786600
H	-4.25590600	-1.58669400	-3.85462200
H	-4.30930100	-4.06253100	-3.65291100
C	-1.93106800	-1.95458000	1.93423400
C	-3.11274500	-2.21171200	2.63671700
C	-0.73047400	-2.50509800	2.38745100
C	-3.09205800	-3.01032900	3.77503600
H	-4.04967000	-1.78282100	2.29484300
C	-0.71178300	-3.31106300	3.52570000
H	0.19060000	-2.28224500	1.85652700
C	-1.89029800	-3.56060500	4.22128500
H	-4.01166600	-3.20224400	4.31661500
H	0.22636600	-3.73160800	3.87186800
H	-1.87641000	-4.18023500	5.11104800
C	-2.92684800	0.55883600	0.96576700
C	-4.31362200	0.81731200	0.67873100
C	-2.20497000	1.51734100	1.66465600
C	-5.22161600	-0.17274200	0.20510400
C	-4.85173400	2.11025300	0.95684100
C	-2.78611600	2.76305800	2.01354600
C	-6.53193500	0.12787600	-0.06683500
H	-4.88420800	-1.19142600	0.08865700
C	-6.20401200	2.40226700	0.63331700

C	-4.05456700	3.07610500	1.61933400
H	-2.18930700	3.47523500	2.57405700
C	-7.02696900	1.43884300	0.11647900
H	-7.19796400	-0.65322100	-0.41573200
H	-6.57442100	3.40290100	0.83066900
H	-4.48301200	4.04855300	1.83917600
H	-8.05986300	1.66653500	-0.12080600
C	0.39218100	1.37716100	1.81057800
C	1.53168900	1.07717200	2.65490400
C	-0.88364200	1.21438400	2.31821000
C	2.88670800	1.26903900	2.25446800
C	1.31715800	0.59543000	3.97714200
C	-1.06248500	0.74809800	3.65622100
C	3.93307900	0.96161600	3.08760200
H	3.12552300	1.67542900	1.28102000
C	2.41749500	0.27769400	4.81552200
C	-0.00650400	0.43940900	4.45620900
H	-2.07667000	0.62741600	4.02064200
C	3.70394400	0.44863900	4.38250100
H	4.94878600	1.12282800	2.74459000
H	2.20963900	-0.09654100	5.81247800
H	-0.16214700	0.07120100	5.46477400
H	4.54114100	0.20518900	5.02613300

UIA

Pt	-2.28624100	1.05753700	-0.39976800
P	2.69515400	-0.15413000	1.13861600
P	-1.79471100	-1.14301700	-0.80201400
Cl	-4.62019700	0.99171500	-0.92545900
C	-0.03804900	3.98191300	-1.17695500
C	0.71992200	5.15184500	-1.24756900
C	-0.18184400	3.21284900	-2.33642300
C	1.30419000	5.56050800	-2.44181600
H	0.84323800	5.75788900	-0.35590200
C	0.41174000	3.61261400	-3.52913800
H	-0.77520300	2.30555200	-2.31239900
C	1.14844500	4.79269200	-3.58969600
H	1.87673900	6.48014600	-2.47377100
H	0.28411000	3.00374400	-4.41684400
H	1.59511700	5.11032500	-4.52466800

C	-0.68478000	3.59531300	0.13271700
C	-0.04595800	2.35658900	0.80170900
C	-0.64845100	2.17576100	2.18350600
C	-2.04033200	2.31823700	2.29966400
C	-2.80150800	2.71510500	1.10243000
C	-2.17291400	3.31269600	0.03027500
H	1.16123300	1.63831700	3.18315600
H	-0.57431100	4.44123300	0.82602200
H	1.03773100	2.49981900	0.89046600
C	0.09142300	1.78157500	3.28727900
C	-2.67162800	2.05991600	3.51350000
H	-3.88523600	2.68620200	1.14797100
H	-2.76092700	3.78947900	-0.74759700
C	-1.91778700	1.68911000	4.62188700
C	-0.53936800	1.55139900	4.50903200
H	-3.75062900	2.14615000	3.58647200
H	-2.40972400	1.49090000	5.56662900
H	0.04697000	1.24888600	5.36944300
O	-0.28777300	1.22611800	0.01023000
C	-3.11507200	-2.35309000	-1.13546600
C	-4.08060500	-2.05807100	-2.10017600
C	-3.11757800	-3.59666800	-0.50240200
C	-5.04119600	-3.00772000	-2.42594400
H	-4.08734200	-1.08695300	-2.58066200
C	-4.08110100	-4.54174800	-0.83447000
H	-2.37879700	-3.82216200	0.25918600
C	-5.04216500	-4.24771500	-1.79527200
H	-5.79497900	-2.77321300	-3.16758000
H	-4.08331000	-5.50375500	-0.33658300
H	-5.79683200	-4.98314700	-2.04808200
C	-0.69548200	-1.32334200	-2.25535900
C	-0.94876600	-2.26599300	-3.25350900
C	0.38859300	-0.45270800	-2.38050400
C	-0.10022200	-2.34712800	-4.35357500
H	-1.78906300	-2.94440100	-3.17553400
C	1.24760800	-0.56003100	-3.46429500
H	0.54710800	0.28693800	-1.60673500
C	1.00374600	-1.50898000	-4.45390500
H	-0.29986200	-3.07853200	-5.12797700
H	2.10922500	0.09634700	-3.52737400
H	1.67478000	-1.59264400	-5.30086300

C	3.61786400	1.15227900	0.21284400
C	4.89483100	1.60295300	0.55925000
C	2.93608900	1.79900700	-0.82266400
C	5.48357100	2.65511700	-0.13384000
H	5.44578800	1.11888400	1.35794500
C	3.53309200	2.83805800	-1.52651900
H	1.91789100	1.51294400	-1.06278500
C	4.81008300	3.26976200	-1.18382000
H	6.47597600	2.98919000	0.14644400
H	2.98494200	3.31938300	-2.32777000
H	5.27329400	4.08660600	-1.72474700
C	3.98794100	-0.82697800	2.27231100
C	4.58545500	-2.08185100	2.13517400
C	4.30012400	-0.05847300	3.40142700
C	5.48476700	-2.54647400	3.09140400
H	4.34985200	-2.70482200	1.28025100
C	5.21025500	-0.51451200	4.34612600
H	3.82792700	0.91082900	3.53537500
C	5.80486300	-1.76424100	4.19369000
H	5.93803300	-3.52328300	2.96805900
H	5.44711900	0.09905400	5.20756500
H	6.50778700	-2.12729100	4.93408000
C	-1.08576100	-1.63744600	0.83928400
C	-2.00470800	-1.50497000	1.95355700
C	0.23534000	-1.97077000	1.07762800
C	-3.38679200	-1.18624100	1.81978000
C	-1.52234100	-1.72154700	3.27407600
C	0.68093800	-2.17967900	2.41426100
C	-4.21269200	-1.10481800	2.91172500
H	-3.83573300	-1.00422900	0.85414000
C	-2.39922100	-1.63043500	4.38309800
C	-0.15987800	-2.04969100	3.47398900
H	1.71441300	-2.46774400	2.57082400
C	-3.72271700	-1.33289000	4.21293600
H	-5.25783500	-0.86233900	2.75903500
H	-1.98966200	-1.80214700	5.37312100
H	0.19949500	-2.21140700	4.48456100
H	-4.38856300	-1.26889400	5.06544000
C	2.46231600	-1.55613700	-0.06615500
C	3.41419600	-1.95640300	-1.07156100
C	1.25618200	-2.24003100	0.01994200

C	4.70860400	-1.38193200	-1.20028800
C	3.07808900	-3.00103500	-1.97874900
C	0.97347500	-3.32323300	-0.85301700
C	5.56971900	-1.77135800	-2.19283500
H	5.03231200	-0.63275400	-0.49598900
C	3.98335700	-3.37806300	-3.00231900
C	1.84278100	-3.67652700	-1.83846600
H	0.03094400	-3.84774500	-0.73717300
C	5.20191400	-2.76986900	-3.12023300
H	6.54747900	-1.30929700	-2.26083000
H	3.68612700	-4.16626600	-3.68592600
H	1.60356400	-4.48215200	-2.52434800
H	5.88893600	-3.06142500	-3.90555000

RTS

Pt	0.07410700	-0.68311100	-0.66050200
P	0.11150100	1.57828200	-0.61356600
P	-1.85184700	-0.98611100	0.41786700
Cl	0.36401300	-2.99736900	-1.54973300
C	5.08532300	-1.55866600	-1.26063500
C	5.54547100	-2.54194000	-2.13909600
C	5.00912400	-0.23854100	-1.71535700
C	5.93275500	-2.21545700	-3.43744900
H	5.60432700	-3.57239700	-1.80102100
C	5.40057300	0.09231700	-3.00812400
H	4.61295000	0.51911900	-1.04830400
C	5.86499900	-0.89578600	-3.87481200
H	6.29124900	-2.99160900	-4.10483000
H	5.33338400	1.12196000	-3.34383800
H	6.16931400	-0.63839500	-4.88322400
C	4.62809900	-1.91349500	0.13126100
C	3.07317100	-2.00024700	0.19381700
C	2.65571500	-2.29536100	1.63174400
C	3.35141000	-1.68192200	2.68988000
C	4.55526800	-0.89513200	2.38881100
C	5.15079000	-0.98071700	1.19562900
H	1.00092900	-3.54468500	1.09546400
H	5.00429000	-2.92090400	0.36477700
H	2.78783500	-2.86675600	-0.42322800
C	1.54245000	-3.08360600	1.91665600
C	2.90845900	-1.86128100	4.00494700

H	4.96267500	-0.26675700	3.17588600
H	6.05246100	-0.40958400	0.98827300
C	1.80367600	-2.66237200	4.27817400
C	1.12361800	-3.28152100	3.23235900
H	3.44740600	-1.38069100	4.81635700
H	1.47530700	-2.80211600	5.30229500
H	0.26458600	-3.91124600	3.43965100
O	2.47670400	-0.83149800	-0.23253300
O	1.68064100	-0.24097100	-2.45814500
H	2.28129000	-0.51646400	-1.64698900
H	1.56865900	-1.05098500	-2.96963200
C	-1.73329100	-0.60856800	2.19664900
C	-2.89422100	-0.66570300	2.97339300
C	-0.51801900	-0.24829300	2.77470900
C	-2.83576900	-0.36738500	4.32844100
H	-3.84249500	-0.93776900	2.51809800
C	-0.47010300	0.07579400	4.12869100
H	0.38334500	-0.21827500	2.16771600
C	-1.62429000	0.01331300	4.90398600
H	-3.73524500	-0.41588300	4.93119900
H	0.47308400	0.36952000	4.57524100
H	-1.58196000	0.26364300	5.95805800
C	-2.31110700	-2.75002300	0.32210400
C	-2.28844600	-3.55772900	1.45860000
C	-2.61244200	-3.31226500	-0.92297300
C	-2.59223600	-4.91476100	1.35241900
H	-2.03354100	-3.14511700	2.42699000
C	-2.93624400	-4.65601400	-1.02016200
H	-2.59942400	-2.69435500	-1.81372100
C	-2.92470400	-5.46101400	0.11920400
H	-2.57081200	-5.53735300	2.23933000
H	-3.18158900	-5.08090700	-1.98647600
H	-3.16836800	-6.51446600	0.04050700
C	1.85710300	2.07991000	-0.57001200
C	2.43384800	2.79921200	-1.61577400
C	2.58894800	1.81401600	0.58980400
C	3.71946300	3.31609200	-1.47029300
H	1.88337500	2.97837300	-2.53157100
C	3.85884300	2.35615900	0.74001300
H	2.15273600	1.21352500	1.37982200
C	4.41986100	3.11689900	-0.28390700

H	4.16532800	3.88314800	-2.27936400
H	4.41267200	2.18034900	1.65466500
H	5.41064100	3.54092600	-0.16284600
C	-0.62919300	2.24630300	-2.13868500
C	-0.81583700	3.62845800	-2.23449900
C	-1.05990400	1.40812800	-3.16614500
C	-1.43220700	4.16848500	-3.35642900
H	-0.49064100	4.28154900	-1.42956500
C	-1.68740700	1.95409500	-4.28237200
H	-0.91479300	0.33683400	-3.08726600
C	-1.87565100	3.32975500	-4.37701900
H	-1.57533200	5.24030500	-3.42902600
H	-2.03134700	1.30134700	-5.07631300
H	-2.36655000	3.75099400	-5.24694700
C	-0.77109900	2.48736200	0.72626400
C	-0.18996500	3.45510400	1.63132100
C	-2.08668600	2.10921500	0.91151700
C	0.96354700	4.23977400	1.34782800
C	-0.88387400	3.75109800	2.84145300
C	-2.78522800	2.47345100	2.09497700
C	1.44851900	5.15265300	2.25090300
H	1.44778600	4.16335000	0.38729800
C	-0.33421200	4.66455900	3.77783700
C	-2.17119900	3.20141600	3.06863800
H	-3.80620900	2.13078300	2.21728300
C	0.82151300	5.34337800	3.50042300
H	2.31903600	5.74382200	1.98965700
H	-0.87519000	4.83849900	4.70186000
H	-2.68272300	3.42837700	3.99820200
H	1.22977700	6.05193600	4.21162500
C	-3.22488200	0.09331800	-0.19842300
C	-4.39589800	-0.34319700	-0.92071300
C	-2.96701500	1.45021800	-0.11458200
C	-5.02598300	-1.60478200	-0.73608200
C	-5.05103300	0.58689800	-1.78038600
C	-3.69106100	2.37529000	-0.91462700
C	-6.13899000	-1.95941500	-1.45611800
H	-4.66055600	-2.27915900	0.02201700
C	-6.17150600	0.17756800	-2.54877300
C	-4.64246200	1.94445800	-1.79065700
H	-3.44620600	3.42826500	-0.83518700

C	-6.69641400	-1.07869800	-2.40861600
H	-6.60571300	-2.92137200	-1.27682000
H	-6.62222400	0.89995400	-3.22110500
H	-5.14826200	2.64172400	-2.45016400
H	-7.56118400	-1.38080700	-2.98770700

RIA

Pt	0.21179300	-0.76666600	-0.81182000
P	0.44009300	-0.53350700	1.43657000
P	1.87669600	0.79070800	-1.05016600
Cl	0.00697100	-1.34161800	-3.20290700
C	-4.39938300	-2.60824100	-1.64386300
C	-3.78928600	-2.99029700	-2.84070400
C	-4.33172600	-3.47525600	-0.55167400
C	-3.12672100	-4.21042600	-2.94615600
H	-3.82727700	-2.32045300	-3.69505100
C	-3.67851600	-4.69997800	-0.65534500
H	-4.78596300	-3.18354800	0.38939900
C	-3.07183900	-5.07094500	-1.85201100
H	-2.65625200	-4.48968800	-3.88250300
H	-3.63722700	-5.36206800	0.20283000
H	-2.56067500	-6.02361400	-1.93317500
C	-5.02978200	-1.24035900	-1.52209200
C	-3.96023600	-0.19859700	-1.10964600
C	-4.60614700	1.15469000	-0.89041000
C	-5.86068500	1.20648700	-0.25919800
C	-6.58583900	-0.04549100	-0.00346200
C	-6.21049800	-1.18776600	-0.58378900
H	-2.98221900	2.28990800	-1.70362500
H	-5.38248400	-0.93991400	-2.51970500
H	-3.22692700	-0.12050500	-1.92393300
C	-3.94801800	2.33674800	-1.20858800
C	-6.41212800	2.44728800	0.07041000
H	-7.46629800	-0.00107100	0.63033800
H	-6.78347000	-2.09687500	-0.42624700
C	-5.74265800	3.62617000	-0.24537600
C	-4.51490700	3.57287500	-0.89886400
H	-7.37785100	2.48344500	0.56493700
H	-6.18410100	4.58344800	0.00850900
H	-3.99535500	4.48876400	-1.15767500
O	-3.31657100	-0.56307200	0.09047500

O	-1.31522100	-2.13129100	-0.57580000
H	-2.60297800	-1.21895200	-0.13815200
H	-1.48974600	-2.50081000	-1.44879200
C	1.26839100	2.51009500	-0.86003600
C	2.17200400	3.57463600	-0.80230100
C	-0.09971000	2.76099100	-0.94944700
C	1.70284400	4.88146100	-0.80601000
H	3.23980000	3.38187800	-0.75251000
C	-0.56547800	4.07448300	-0.95909600
H	-0.79844600	1.93177100	-1.00498800
C	0.33294400	5.13296600	-0.88337800
H	2.40609400	5.70455000	-0.75198300
H	-1.63138800	4.26434000	-1.01870000
H	-0.03017500	6.15433500	-0.88925400
C	2.71831900	1.05035300	-2.66794400
C	4.09703900	1.23406200	-2.79207900
C	1.89347300	1.27555400	-3.77415600
C	4.64456900	1.58617500	-4.02304400
H	4.75487200	1.11553900	-1.94104300
C	2.44582100	1.62510800	-5.00022500
H	0.81857900	1.18629400	-3.67769800
C	3.82411600	1.77176100	-5.12984500
H	5.71661300	1.72054300	-4.10915600
H	1.79581800	1.79002200	-5.85162400
H	4.25471500	2.04383300	-6.08673300
C	-0.84141300	-1.14669200	2.60540100
C	-0.95842600	-0.56642000	3.87347700
C	-1.55572100	-2.30767000	2.30370700
C	-1.81176000	-1.12568700	4.81688400
H	-0.39047400	0.31931100	4.13267300
C	-2.41006500	-2.85845400	3.25674500
H	-1.45866500	-2.75667900	1.32200700
C	-2.54418300	-2.26964800	4.50871700
H	-1.90302000	-0.66537100	5.79399800
H	-2.97078900	-3.75399000	3.01295600
H	-3.21286100	-2.70040100	5.24534500
C	1.82403100	-1.58670100	2.02582000
C	2.35918200	-1.41006400	3.30402300
C	2.21180400	-2.68513800	1.25617900
C	3.29892800	-2.30985000	3.79258800
H	2.05306400	-0.56455600	3.91303300

C	3.14847100	-3.58770400	1.75375700
H	1.78997600	-2.83542500	0.26835800
C	3.69609200	-3.39836100	3.01800000
H	3.72248000	-2.16059900	4.77929100
H	3.44646900	-4.43676000	1.14890800
H	4.42729500	-4.09970900	3.40378900
C	3.20484500	0.47111100	0.19102700
C	4.20899800	-0.51783900	-0.08871900
C	3.18759100	1.07480300	1.43956300
C	4.12572700	-1.42652300	-1.17995700
C	5.28910100	-0.67581900	0.82476400
C	4.30601400	0.95314400	2.30571500
C	5.06797400	-2.40750300	-1.35685800
H	3.28824200	-1.38138400	-1.86615800
C	6.26797700	-1.67633900	0.59627400
C	5.34676400	0.13196500	1.98889000
H	4.29433500	1.48846500	3.24856300
C	6.16226900	-2.52789200	-0.47070200
H	4.96607500	-3.10410600	-2.18077400
H	7.08706900	-1.76566900	1.30192700
H	6.19373200	0.02744100	2.65854400
H	6.90368500	-3.30210300	-0.62955200
C	0.72389500	1.23035800	1.90849900
C	-0.42122100	2.07006900	2.13937700
C	1.99244500	1.79069100	1.95319500
C	-1.75099200	1.68564700	1.81329000
C	-0.21587100	3.39229400	2.62549500
C	2.17421100	3.10466400	2.46089600
C	-2.80274900	2.54437800	2.01005600
H	-1.96682800	0.73268800	1.34464900
C	-1.32636800	4.24601200	2.84955000
C	1.10514200	3.87006500	2.81928200
H	3.18146800	3.50141400	2.52242400
C	-2.59831700	3.83131800	2.55630600
H	-3.80114100	2.23042000	1.72345300
H	-1.13934000	5.24254800	3.23581600
H	1.24676700	4.87534700	3.20195200
H	-3.44313000	4.49168000	2.71579300