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Complex 2a, ground state, CH₂Cl₂

C	2.08858300	1.20211800	-0.04180000
C	2.21569300	2.62124000	0.00972600
C	3.23852900	0.42248500	-0.18988900
C	3.50100500	3.17571500	-0.08358400
C	0.97487500	3.39551400	0.14780700
C	4.48716300	1.03392000	-0.27498700
C	4.65014500	2.41035200	-0.22256400
C	0.86925900	4.78863200	0.27081900
C	-1.36403700	3.21015800	0.31850800
C	-0.38073900	5.38203600	0.41692700
C	-1.52311200	4.58340400	0.44649700
N	-0.15901800	2.63261100	0.16422600
H	3.19986600	-0.65890000	-0.25284300
H	5.62532600	2.87640100	-0.29232700
H	1.76115600	5.39592700	0.25678800
H	-2.21630200	2.54317700	0.34529000
H	-0.45756900	6.46059800	0.51227500
H	-2.51491200	5.00381200	0.56608300
P	0.44222000	-1.75173400	0.05968800
Pt	0.15720100	0.54304500	0.02496000
P	-2.06455400	-0.46019400	-0.10300300
C	1.06141100	-2.47215400	1.61826600
C	1.83368000	-1.69175400	2.49244900
C	0.75784700	-3.80247100	1.95956900
C	2.30460600	-2.23896500	3.68776000
H	2.06017000	-0.66069100	2.24145600
C	1.23128000	-4.34226300	3.15533600
H	0.15493400	-4.41973100	1.29929500
C	2.00535800	-3.56180300	4.01919600
H	2.90025400	-1.62849600	4.35989800
H	0.99306200	-5.36999100	3.41255400
H	2.37002700	-3.98434600	4.95091500
C	1.32982500	-2.52944600	-1.33905200
C	2.18509900	-3.62912200	-1.17453100
C	1.13149300	-1.99025400	-2.62269500
C	2.82246200	-4.18932200	-2.28422700
H	2.36063000	-4.04791900	-0.18954000
C	1.76408200	-2.55996000	-3.72645500
H	0.49103300	-1.12233800	-2.75566100
C	2.61082700	-3.65998900	-3.55838600
H	3.48548600	-5.03862700	-2.14844700
H	1.60343800	-2.13959100	-4.71480700
H	3.10876100	-4.09811500	-4.41846500
C	-3.23973200	-0.29242500	1.29454200
C	-4.63231300	-0.37603500	1.14359900
C	-2.69563700	-0.05557700	2.56959100
C	-5.46504200	-0.24159000	2.25646700
H	-5.07060700	-0.53955500	0.16480500
C	-3.53239600	0.06864800	3.67860600
H	-1.61909600	0.03637300	2.69034800
C	-4.91827600	-0.02371500	3.52309900
H	-6.54193400	-0.30583900	2.13062100

H	-3.10268800	0.24760000	4.65989500
H	-5.56999000	0.08133700	4.38565600
C	-3.00702600	-0.33113300	-1.66357700
C	-3.86644500	-1.35846500	-2.09158100
C	-2.85616600	0.81631800	-2.45810100
C	-4.57039600	-1.22980700	-3.28908900
H	-3.98893200	-2.25937100	-1.49674700
C	-3.56401500	0.94078500	-3.65535800
H	-2.18017300	1.60752300	-2.14809700
C	-4.42128100	-0.08014400	-4.07046600
H	-5.23224000	-2.02791000	-3.61209800
H	-3.43933100	1.83134100	-4.26418300
H	-4.96853000	0.01562400	-5.00372600
C	-1.36780000	-2.20680300	-0.06351400
H	-1.71222600	-2.77963300	0.80115800
H	-1.59340500	-2.76565900	-0.97534000
F	5.58231400	0.26145400	-0.41489300
F	3.67628500	4.51759000	-0.04565900

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Complex 2b, ground state, CH2C12

C	0.06874700	3.31028700	-0.59714800
C	2.23195700	2.54624100	-0.09628000
C	0.57580600	4.60652800	-0.77787000
C	-1.33815600	2.90804000	-0.70856000
C	2.78345800	3.80888900	-0.26125800
C	1.93365300	4.85563700	-0.61322500
C	-2.37963300	3.76567700	-1.09832700
C	-2.98814600	1.14146300	-0.49357000
C	-3.70303100	3.36321400	-1.19484400
C	-3.97624900	2.04013400	-0.88501800
H	2.85359100	1.70966400	0.19030000
H	-0.09441200	5.41024100	-1.03890900
H	3.84722000	3.95536000	-0.11383000
H	2.31947000	5.86055100	-0.75325500
H	-3.30277800	0.13160600	-0.26483300
H	-4.47690500	4.05664600	-1.50013100
P	1.98743400	-0.97010500	0.29929400
Pt	-0.00902000	0.39122800	0.02522500
P	-1.11923700	-1.57702300	0.51225400
C	3.07722400	-0.45521300	1.68924500
C	2.46056600	0.08638200	2.83163300
C	4.47447000	-0.58894300	1.66490600
C	3.22501900	0.46087300	3.93697600
H	1.38343600	0.22929000	2.84834700
C	5.23613500	-0.20312000	2.77014300
H	4.97393000	-0.98433500	0.78695800
C	4.61453200	0.31643800	3.90773200
H	2.73624600	0.87452000	4.81428800
H	6.31678800	-0.30760600	2.73828900
H	5.21080500	0.61566000	4.76487100
C	3.03521500	-1.19057500	-1.18699000
C	2.89253100	-0.30962100	-2.27103300
C	3.95184400	-2.25354800	-1.28459400
C	3.66483800	-0.47626400	-3.42268700

H	2.16810000	0.49744600	-2.22389000
C	4.72056000	-2.41656400	-2.43738600
H	4.06688300	-2.96034200	-0.46810100
C	4.58074500	-1.52654800	-3.50597600
H	3.54389600	0.21097800	-4.25488700
H	5.42490900	-3.24074500	-2.50123900
H	5.17918200	-1.65703600	-4.40294900
C	-2.55468100	-1.44164400	1.64457600
C	-3.75129000	-2.14386300	1.44015600
C	-2.42317200	-0.61460800	2.77380500
C	-4.79760100	-2.02598500	2.35888300
H	-3.87639200	-2.77662600	0.56805400
C	-3.46789100	-0.50621000	3.69028000
H	-1.51032200	-0.04563300	2.92897900
C	-4.65747400	-1.21163600	3.48352600
H	-5.72174900	-2.57089500	2.19013600
H	-3.35630100	0.13418000	4.56030700
H	-5.47310600	-1.12147100	4.19504700
C	-1.61933900	-2.55534100	-0.95188300
C	-1.92262300	-3.92518700	-0.84791300
C	-1.67960000	-1.93315900	-2.20957000
C	-2.28486000	-4.65247000	-1.98192700
H	-1.88150500	-4.43173200	0.11161600
C	-2.04390600	-2.66560100	-3.34101000
H	-1.43760900	-0.87905000	-2.30061900
C	-2.34652800	-4.02397100	-3.22875800
H	-2.51603100	-5.70955000	-1.89049200
H	-2.08653100	-2.17417500	-4.30848400
H	-2.62677700	-4.59367400	-4.10999100
C	0.07667900	-2.65325000	1.44814300
H	-0.34050500	-3.65654600	1.58005100
H	0.17725000	-2.21149200	2.44540200
C	1.42564500	-2.70238700	0.72548400
H	2.17820500	-3.20844500	1.33732000
H	1.33449500	-3.25045600	-0.21802900
F	-2.12888400	5.05933600	-1.41178700
F	-5.25086000	1.60906500	-0.96776100
C	-1.65509400	1.55173500	-0.39818600
N	0.92038500	2.29345700	-0.26628600

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Complex 2c, ground state, CH2Cl2

Pt	0.20977800	0.64337100	-0.03486100
P	-2.02930700	-0.28804800	-0.17780600
P	0.81959800	-1.58110600	-0.23455300
F	3.39370700	4.88501200	0.51045400
F	5.67148600	0.80791900	0.34661300
N	-0.27110500	2.71562100	0.14918600
C	-1.51914500	3.22026700	0.15584200
H	-2.32893800	2.51341200	0.05229300
C	-1.78480500	4.57722100	0.27335600
H	-2.81117900	4.92564500	0.27434000
C	-0.70550600	5.45111300	0.38188900
H	-0.86350100	6.52130700	0.47108300
C	0.58724400	4.94004400	0.37497500

H	1.43249000	5.60443600	0.45895200
C	0.80022500	3.55741900	0.26197700
C	2.10103500	2.88092900	0.26137000
C	2.09542500	1.45990500	0.13505400
C	3.33556400	3.53664700	0.39703400
C	4.55260900	2.87314300	0.42719200
H	5.48300900	3.41693900	0.53443900
C	4.51084200	1.49273700	0.31547000
C	3.32004300	0.78686500	0.16976300
H	3.39477200	-0.28794300	0.07728700
C	-3.25960500	0.58087100	-1.22777700
C	-2.84310600	1.00563500	-2.50262500
H	-1.82227300	0.82431100	-2.82973500
C	-3.73464600	1.66321500	-3.34811900
H	-3.40619800	1.98457600	-4.33218500
C	-5.04490100	1.91396200	-2.92686700
H	-5.73710100	2.43104800	-3.58499100
C	-5.46058200	1.50359000	-1.65940300
H	-6.47613500	1.69881200	-1.32759200
C	-4.57310100	0.83801700	-0.80870700
H	-4.90660100	0.52250400	0.17449200
C	-2.81792300	-0.56960400	1.45692800
C	-2.46888300	0.28153500	2.51923100
H	-1.73893200	1.07069400	2.36712800
C	-3.04765700	0.11257800	3.77814200
H	-2.77000100	0.77704700	4.59106000
C	-3.97186900	-0.91236600	3.99166200
H	-4.41792100	-1.04709700	4.97278800
C	-4.31654900	-1.76953500	2.94346300
H	-5.02892200	-2.57291600	3.10652000
C	-3.74366800	-1.60205800	1.68189500
H	-4.01437000	-2.28343900	0.88214600
C	-1.85811400	-1.93409600	-0.97409200
C	-2.93204100	-2.60042300	-1.57985300
H	-3.91690900	-2.14389400	-1.59663600
C	-2.73570500	-3.83968300	-2.19081400
H	-3.57273600	-4.34797600	-2.65960000
C	-1.46222300	-4.41175300	-2.21793600
H	-1.30305600	-5.36717000	-2.70838700
C	-0.38247600	-3.74553600	-1.63622600
H	0.60999300	-4.18063200	-1.69762900
C	-0.57437100	-2.50896200	-1.00402700
C	2.23494300	-1.97455100	-1.33060000
C	2.29168500	-1.34136500	-2.58424700
H	1.53140300	-0.61577200	-2.86129000
C	3.32710900	-1.63529800	-3.46919900
H	3.36511000	-1.14296600	-4.43645500
C	4.31737600	-2.55549800	-3.10888600
H	5.12674500	-2.77901100	-3.79778100
C	4.26768400	-3.18282300	-1.86332500
H	5.03632200	-3.89529100	-1.57882700
C	3.22923500	-2.89606700	-0.97248800
H	3.20068300	-3.38749600	-0.00542400
C	1.13659600	-2.37172800	1.39213800

C	1.62937200	-1.58319000	2.44587500
H	1.80367400	-0.52315300	2.29427200
C	1.89069000	-2.15724500	3.69090100
H	2.27128800	-1.53805700	4.49786500
C	1.65693300	-3.51825800	3.89901600
H	1.85615800	-3.96264000	4.86985000
C	1.15930200	-4.30655700	2.85856600
H	0.96868800	-5.36389800	3.01682600
C	0.89779400	-3.73898100	1.61073200
H	0.49941800	-4.36341900	0.81811000

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Complex 3a, ground state, CH2Cl2

Pt	3.15962300	0.48642300	0.23242600
Pt	-3.23720100	-0.37099600	0.41996800
Cl	2.47575700	2.34661700	1.78044800
Cl	-2.81203200	-1.70816600	2.52941500
P	1.34542700	-0.80760100	0.89720500
P	-1.44937300	1.01918100	0.98121900
F	4.57093600	-4.52580100	-1.30887200
F	7.16072200	-0.97544300	-2.91329200
F	-6.64400200	0.03273200	-3.60979100
F	-4.23723700	3.94403700	-2.71820700
N	4.73485900	1.64320700	-0.59214400
N	-4.71312300	-1.73478000	-0.25261200
C	4.87230200	2.96850400	-0.41223900
H	4.18311900	3.41745700	0.29206000
C	5.83716600	3.71126400	-1.08086900
H	5.91512900	4.77774100	-0.90203600
C	6.67934900	3.05070500	-1.97403300
H	7.44154900	3.59529000	-2.52294300
C	6.53843600	1.67965600	-2.16309900
H	7.18062700	1.15576200	-2.85416300
C	5.55345200	0.97463400	-1.45573800
C	5.28696800	-0.46443100	-1.51689600
C	4.16635500	-0.94704200	-0.77167700
C	3.96031200	-2.32991900	-0.70840800
H	3.15486500	-2.76889200	-0.13611000
C	4.80511900	-3.19936600	-1.38914900
C	5.87743400	-2.76272700	-2.15313600
H	6.52689600	-3.44844300	-2.68293500
C	6.09406400	-1.39416500	-2.19001300
C	-0.03958900	0.08392000	1.79431500
H	0.48125400	0.78782200	2.44567000
H	-0.54061100	-0.66248600	2.41674000
C	1.89384200	-1.94332000	2.24741400
C	1.78298200	-3.33978200	2.19490700
H	1.33794600	-3.82678500	1.33437700
C	2.25024500	-4.12419400	3.25389900
H	2.16028300	-5.20524600	3.19748200
C	2.82606100	-3.52455300	4.37393500
H	3.18573600	-4.13651700	5.19618500
C	2.94405100	-2.13245900	4.43153500
H	3.39720100	-1.65774500	5.29715000
C	2.48943100	-1.34596900	3.37393600

H	2.60700900	-0.26660200	3.41905200
C	0.54962100	-1.83336000	-0.40227100
C	-0.48852000	-2.72497400	-0.07908400
H	-0.84750100	-2.80974400	0.94079800
C	-1.08961000	-3.49748200	-1.07523800
H	-1.88639800	-4.18616000	-0.80975300
C	-0.67619400	-3.37790600	-2.40394800
H	-1.14591600	-3.97995900	-3.17669500
C	0.33922300	-2.47824000	-2.73673400
H	0.65998100	-2.37251000	-3.76904600
C	0.95015300	-1.71187200	-1.74286800
H	1.73744000	-1.01525000	-2.00699000
C	-0.71201800	1.99617800	-0.39507000
C	-0.53581000	1.36822700	-1.63911000
H	-0.85607600	0.34156100	-1.77740500
C	0.02373200	2.06377000	-2.71094500
H	0.15486500	1.56353400	-3.66624000
C	0.39150400	3.40392000	-2.56098500
H	0.81386400	3.95057200	-3.39945400
C	0.19822300	4.04184000	-1.33427000
H	0.46944600	5.08669000	-1.21296700
C	-0.34699200	3.34303100	-0.25436200
H	-0.48997600	3.85552800	0.68949900
C	-1.93487500	2.22571200	2.28562600
C	-3.30405400	2.45279300	2.50515200
H	-4.03850000	1.90762600	1.92037600
C	-3.72547000	3.36401800	3.47545700
H	-4.78770900	3.52596300	3.63452700
C	-2.78572400	4.05644700	4.24105500
H	-3.11315000	4.76208800	4.99939800
C	-1.42208700	3.83739500	4.03045000
H	-0.68513400	4.37338800	4.62173400
C	-0.99514600	2.92910500	3.06029700
H	0.06971600	2.78717700	2.90414500
C	-4.93249100	-2.94221200	0.29672300
H	-4.37979200	-3.14816800	1.20503800
C	-5.80990700	-3.86245600	-0.26290700
H	-5.95987100	-4.82355100	0.21590600
C	-6.47145600	-3.51472300	-1.43994100
H	-7.15848000	-4.20852900	-1.91478700
C	-6.24686000	-2.26565500	-2.00974500
H	-6.75013700	-1.98375400	-2.92173300
C	-5.35892700	-1.36825800	-1.39775800
C	-5.03278000	-0.01110000	-1.84201000
C	-4.02630100	0.68750800	-1.10375500
C	-3.79078900	2.03134000	-1.41512600
H	-3.06374300	2.62873900	-0.88315500
C	-4.49315700	2.64733800	-2.44501300
C	-5.44362300	1.98727600	-3.21001300
H	-5.97886300	2.47550100	-4.01492100
C	-5.69332700	0.66467100	-2.87909600

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Complex 3b, ground state, CH2Cl2

Pt	4.29075100	-0.55318500	-0.47972200
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C1	4.81429000	-2.70692600	-1.64207300
C	4.24582800	1.19500600	0.52268300
C	5.11958500	2.19611300	-0.00579900
C	3.55241100	1.48114000	1.70589000
C	5.16756700	3.44589200	0.62910600
C	5.98994100	1.79450100	-1.11605200
C	3.65557000	2.73750100	2.29428900
H	2.95030300	0.73965700	2.21530400
C	4.43865600	3.75344300	1.76830000
C	6.89102400	2.60959300	-1.81637100
H	4.50478900	4.73065600	2.23016600
C	7.69305700	2.05902400	-2.81148700
H	6.95889100	3.66056200	-1.58086900
C	6.67113700	-0.06014900	-2.39136700
C	7.59193900	0.69958800	-3.10263500
H	8.39085500	2.69089900	-3.35249400
H	6.52562700	-1.11781800	-2.57574500
H	8.20239700	0.23052000	-3.86605700
N	5.89470500	0.46958000	-1.43116700
C	1.59025000	-2.78727100	-0.66813500
C	1.39153200	-2.55197800	-2.03921100
C	1.15832000	-3.99661900	-0.10926300
C	0.76529700	-3.51067200	-2.83371400
H	1.73698000	-1.62490700	-2.48782400
C	0.54139700	-4.96086400	-0.91238600
H	1.29862500	-4.19354500	0.94819600
C	0.34187600	-4.71986800	-2.27196900
H	0.61689500	-3.31856700	-3.89253500
H	0.21530400	-5.89750600	-0.46935400
H	-0.13997500	-5.46924400	-2.89355600
C	2.49875900	-2.10019400	2.04584200
C	1.70050800	-1.69716400	3.12682200
C	3.53677400	-3.02446600	2.26702600
C	1.93137600	-2.21507700	4.40461900
H	0.90048200	-0.97748800	2.99235600
C	3.75490700	-3.54698700	3.54087300
H	4.17301200	-3.32953500	1.44051200
C	2.95337800	-3.14166000	4.61282700
H	1.30814900	-1.89200500	5.23329000
H	4.55588800	-4.26353500	3.69803700
H	3.12906700	-3.54421300	5.60626200
P	2.31530900	-1.43743900	0.34672300
C	0.93299600	-0.17639000	0.34993200
H	1.04893100	0.34812800	-0.60400000
H	1.16307400	0.54979500	1.12899000
C	-0.48971300	-0.73045400	0.49124600
H	-0.64933200	-1.24880900	1.43839000
H	-0.69723200	-1.46760200	-0.28806300
C	-1.44181300	1.41950300	-1.19256500
C	-1.45584600	0.66819400	-2.38195100
C	-1.11483900	2.78146500	-1.25395600
C	-1.13471000	1.26509500	-3.60051700
H	-1.72813100	-0.38384300	-2.35967300
C	-0.79980100	3.37809000	-2.47836300

H	-1.11230600	3.38968100	-0.35619500
C	-0.80519700	2.62298300	-3.65139200
H	-1.14868500	0.67124700	-4.50983700
H	-0.55260600	4.43531000	-2.50936400
H	-0.55928000	3.08870100	-4.60136200
C	-1.67967300	1.65193200	1.78840100
C	-0.52904200	2.43654000	1.99776900
C	-2.69375300	1.67092800	2.76155900
C	-0.39439000	3.20608800	3.15410700
H	0.26605600	2.46286000	1.26161000
C	-2.55995500	2.44889000	3.91320200
H	-3.58755100	1.07217000	2.61570300
C	-1.40979500	3.21408000	4.11341700
H	0.51114300	3.78467700	3.30528900
H	-3.35468500	2.45163400	4.65353800
H	-1.30357400	3.81386000	5.01286000
P	-1.87605000	0.51775300	0.35524600
Pt	-3.95802900	-0.50403100	0.21767100
Cl	-3.03715400	-2.62455600	1.19600300
C	-4.98668200	1.10451000	-0.43389600
C	-6.32655000	0.81722100	-0.84336100
C	-4.56039900	2.43689200	-0.45480700
C	-7.13196800	1.87683800	-1.28754100
C	-6.77894900	-0.57048300	-0.71012200
C	-5.41251500	3.44284900	-0.89656800
H	-3.57214600	2.73323900	-0.13269100
C	-6.70591500	3.19529000	-1.33169600
C	-8.02896800	-1.08676100	-1.08311100
H	-7.36052300	3.98505000	-1.67875100
C	-8.31722700	-2.43023600	-0.86543000
H	-8.76210100	-0.43963000	-1.53900300
C	-6.13288200	-2.69383700	0.06645500
C	-7.35796400	-3.25212800	-0.27621800
H	-9.28505700	-2.82780700	-1.15560700
H	-5.33876300	-3.27449100	0.51961700
H	-7.54272100	-4.30348400	-0.08651200
N	-5.85132500	-1.39640500	-0.14410600
F	2.95706900	2.98519100	3.42540900
F	5.96518700	4.42843700	0.14591200
F	-8.40403900	1.64633300	-1.69472400
F	-4.96391100	4.71569700	-0.90403700

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Complex 2a, ground state, gas phase

C	2.07066400	1.23550000	-0.02666300
C	2.17312100	2.65525000	0.04145200
C	3.22977400	0.47514500	-0.17983800
C	3.45026000	3.23220100	-0.03931000
C	0.92149700	3.40619300	0.17903500
C	4.47135100	1.10668600	-0.25316200
C	4.61042300	2.48535100	-0.18220100
C	0.79089100	4.79728000	0.31625000
C	-1.41743600	3.18258400	0.33104200
C	-0.46881300	5.36753400	0.45990500
C	-1.59984600	4.55049100	0.47267900

N	-0.20181500	2.62610300	0.17864900
H	3.20977000	-0.60554500	-0.26150300
H	5.57881900	2.96672000	-0.24212000
H	1.67453900	5.41708100	0.31466800
H	-2.25758100	2.49887200	0.34513400
H	-0.56408100	6.44388300	0.56721900
H	-2.59867500	4.95505100	0.59169200
P	0.47706700	-1.74049600	0.04274900
Pt	0.15103600	0.54928100	0.03225600
P	-2.05637800	-0.47761900	-0.09426500
C	1.10595000	-2.46762300	1.59276200
C	1.83937000	-1.67946100	2.49306700
C	0.84738900	-3.81585000	1.90128900
C	2.31375200	-2.23669400	3.68249600
H	2.03577100	-0.63692000	2.26434100
C	1.32347900	-4.36475400	3.09084800
H	0.27959300	-4.43993700	1.21577300
C	2.05742600	-3.57549100	3.98149300
H	2.88098400	-1.62175900	4.37484600
H	1.12116600	-5.40615200	3.32302500
H	2.42592600	-4.00546200	4.90824700
C	1.35644100	-2.50218800	-1.36570600
C	2.30787000	-3.51963200	-1.20132800
C	1.06284700	-2.02599700	-2.65600700
C	2.94680300	-4.06230700	-2.31854900
H	2.55649800	-3.88627700	-0.21102500
C	1.69785600	-2.57897500	-3.76568900
H	0.34939300	-1.21652400	-2.78924700
C	2.64105100	-3.59741400	-3.59792800
H	3.68560700	-4.84686200	-2.18468200
H	1.46587000	-2.20815100	-4.75968500
H	3.14127900	-4.02131700	-4.46367400
C	-3.24514800	-0.35888900	1.29434300
C	-4.61956200	-0.14873500	1.10905400
C	-2.72741100	-0.43704300	2.60018900
C	-5.46489800	-0.03885300	2.21587200
H	-5.03386300	-0.07089900	0.10935400
C	-3.57814400	-0.33691700	3.69910200
H	-1.65904700	-0.56734700	2.75726100
C	-4.94875300	-0.13760700	3.50827500
H	-6.52810600	0.12265100	2.06367800
H	-3.17086700	-0.40468200	4.70364500
H	-5.60978700	-0.05329200	4.36583000
C	-2.98768800	-0.34814300	-1.65976700
C	-3.93505500	-1.31880100	-2.03284900
C	-2.73106800	0.73039700	-2.52073000
C	-4.61717900	-1.20325200	-3.24306700
H	-4.14436000	-2.16229800	-1.37986000
C	-3.41826400	0.84215300	-3.73150000
H	-1.98743800	1.47462400	-2.25014500
C	-4.36023200	-0.12217200	-4.09205400
H	-5.34750000	-1.95613500	-3.52462600
H	-3.21271300	1.67869900	-4.39281800
H	-4.89215200	-0.03618800	-5.03502700

C	-1.33234100	-2.21542400	-0.06870100
H	-1.66145400	-2.79500100	0.79840500
H	-1.56334600	-2.77199500	-0.98142400
F	5.57244800	0.35460300	-0.39705000
F	3.59967000	4.57351300	0.01642100

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Complex 2b, ground state, gas phase

C	0.04452100	3.31267300	-0.59107200
C	2.21507700	2.56164200	-0.09282800
C	0.54468600	4.61409300	-0.76511000
C	-1.35733500	2.90426200	-0.70105000
C	2.75729600	3.82827900	-0.24941700
C	1.89949500	4.87106000	-0.59787700
C	-2.40550400	3.75998000	-1.08010300
C	-2.99513600	1.12698700	-0.48890600
C	-3.72605900	3.34933600	-1.17243300
C	-3.99256000	2.02280500	-0.87025000
H	2.84113900	1.72724000	0.19182900
H	-0.13311500	5.41289600	-1.02241900
H	3.81964700	3.98306800	-0.09786600
H	2.27858700	5.87972900	-0.73211900
H	-3.30603500	0.11575000	-0.26212800
H	-4.50575700	4.04001200	-1.46908300
P	1.99664900	-0.94896300	0.28986400
Pt	-0.01192500	0.39673700	0.01484400
P	-1.11932100	-1.57639800	0.49663900
C	3.07209000	-0.44750300	1.69531700
C	2.44894900	0.10188300	2.83053600
C	4.46747800	-0.60377100	1.69101100
C	3.20320400	0.45989300	3.94781700
H	1.37425700	0.26664200	2.83006400
C	5.21892400	-0.23492500	2.80843300
H	4.97279000	-1.00182600	0.81730100
C	4.58970100	0.29072100	3.93852900
H	2.71015400	0.88059100	4.81941600
H	6.29808600	-0.35711100	2.79271300
H	5.17830000	0.57612900	4.80550000
C	3.06042600	-1.16444900	-1.18441600
C	2.94094100	-0.27081000	-2.26049500
C	3.96960100	-2.23393900	-1.28143900
C	3.72808500	-0.43171700	-3.40237800
H	2.22196000	0.54126000	-2.21336100
C	4.75300300	-2.39148500	-2.42438200
H	4.06706200	-2.95002300	-0.47007300
C	4.63569000	-1.48858500	-3.48439600
H	3.62515300	0.26458900	-4.22949700
H	5.45113900	-3.22097100	-2.48858800
H	5.24537500	-1.61462400	-4.37429900
C	-2.55102100	-1.45926200	1.63168000
C	-3.72939300	-2.19558200	1.44073400
C	-2.43701900	-0.61462000	2.74939600
C	-4.77313200	-2.09515700	2.36353400
H	-3.84288900	-2.83777800	0.57369100
C	-3.47902300	-0.52425600	3.66983900

H	-1.54210800	-0.01304800	2.88731300
C	-4.64890400	-1.26487600	3.47779300
H	-5.68445700	-2.66425500	2.20556600
H	-3.38332500	0.13162000	4.53017100
H	-5.46358700	-1.18777000	4.19177900
C	-1.60519100	-2.56000000	-0.96665400
C	-1.87893000	-3.93656400	-0.86640000
C	-1.69442000	-1.93292400	-2.22008600
C	-2.23916600	-4.66610500	-1.99890300
H	-1.81967600	-4.44553100	0.09156300
C	-2.05739000	-2.66796800	-3.34990100
H	-1.47968600	-0.87250600	-2.30773900
C	-2.32931600	-4.03250700	-3.24118900
H	-2.44851200	-5.72812800	-1.91095500
H	-2.12496700	-2.17300500	-4.31412700
H	-2.60965200	-4.60337000	-4.12158400
C	0.09036300	-2.64299400	1.43100100
H	-0.32149600	-3.64777300	1.57232000
H	0.19390900	-2.19640100	2.42635300
C	1.43621500	-2.68698700	0.70182200
H	2.19318500	-3.19882200	1.30452100
H	1.33843200	-3.22540600	-0.24710300
F	-2.16017800	5.05373700	-1.38438500
F	-5.25816300	1.58464100	-0.94904300
C	-1.66692300	1.54529600	-0.39788600
N	0.90506300	2.29954500	-0.26755300

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Complex 2c, ground state, gas phase

Pt	0.20618300	0.65101000	-0.05039900
P	-2.02699300	-0.29613600	-0.17815100
P	0.83359500	-1.57126100	-0.23770000
F	3.35342400	4.90820900	0.52080500
F	5.66215900	0.85380300	0.31664700
N	-0.28982800	2.71574600	0.13620300
C	-1.54156600	3.21268400	0.14013000
H	-2.34537200	2.49951400	0.03003300
C	-1.81618600	4.56661300	0.26166500
H	-2.84465300	4.90978600	0.25923200
C	-0.74176300	5.44695800	0.37817400
H	-0.90695200	6.51617100	0.47118400
C	0.55333900	4.94516700	0.37402900
H	1.39556000	5.61290500	0.46377600
C	0.77714600	3.56319200	0.25582100
C	2.08020500	2.89742400	0.25476100
C	2.08679800	1.47768300	0.11843900
C	3.30980400	3.56313500	0.39530400
C	4.53118400	2.90851700	0.41850500
H	5.45743800	3.45856300	0.52993700
C	4.50249100	1.52867200	0.29389900
C	3.31476100	0.81466700	0.14424200
H	3.40138100	-0.25776000	0.03823500
C	-3.28503900	0.55807700	-1.20793400
C	-2.89997400	0.98207700	-2.49294400
H	-1.88499000	0.80691100	-2.84128300

C	-3.81361000	1.63029800	-3.32118800
H	-3.50923400	1.95066700	-4.31333600
C	-5.11621300	1.87300400	-2.87331700
H	-5.82611100	2.38204400	-3.51871700
C	-5.50154600	1.46438200	-1.59621600
H	-6.51163100	1.65305500	-1.24419100
C	-4.59141800	0.80821200	-0.76229300
H	-4.90129800	0.49383600	0.22921400
C	-2.79193300	-0.59197300	1.46291000
C	-2.40380700	0.22851300	2.53500400
H	-1.64867600	0.99482400	2.38525900
C	-2.97168700	0.05367400	3.79781000
H	-2.66392300	0.69317400	4.61993300
C	-3.92348400	-0.94620500	4.00433500
H	-4.36144400	-1.08547800	4.98844600
C	-4.30620500	-1.77465300	2.94629200
H	-5.03940100	-2.55988100	3.10607300
C	-3.74436000	-1.60136300	1.68147100
H	-4.04140800	-2.26106900	0.87234700
C	-1.84368500	-1.93724400	-0.98411300
C	-2.91088900	-2.60753500	-1.59749500
H	-3.89742900	-2.15398900	-1.61724200
C	-2.70496200	-3.84167000	-2.21506800
H	-3.53640100	-4.35223600	-2.69187800
C	-1.42796600	-4.40578800	-2.24017900
H	-1.26156000	-5.35713000	-2.73667700
C	-0.35509600	-3.73582900	-1.65055700
H	0.64202700	-4.16118600	-1.70994900
C	-0.55601400	-2.50333200	-1.01315300
C	2.25710900	-1.97147100	-1.31825100
C	2.34572500	-1.33041400	-2.56561600
H	1.60726300	-0.58401800	-2.84612900
C	3.38884300	-1.63778800	-3.43618400
H	3.45378900	-1.13730900	-4.39783600
C	4.35499400	-2.57933200	-3.06788600
H	5.17163700	-2.81184000	-3.74505500
C	4.27452600	-3.21440400	-1.82818700
H	5.02715900	-3.94106500	-1.53678000
C	3.22847300	-2.91441800	-0.95150200
H	3.17734900	-3.40801100	0.01385200
C	1.13956900	-2.35473500	1.39284700
C	1.71818100	-1.58650700	2.41770000
H	1.95669900	-0.54212700	2.24532500
C	1.98549000	-2.16211700	3.65994500
H	2.43497600	-1.56038400	4.44443900
C	1.67195000	-3.50220100	3.89548700
H	1.87734200	-3.94695300	4.86487600
C	1.08815900	-4.26868200	2.88486300
H	0.83532900	-5.30940100	3.06547900
C	0.82104800	-3.70054800	1.63872500
H	0.35542200	-4.30616100	0.86817700

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Complex 3a, ground state, gas phase

Pt	3.23431600	0.49204400	0.27460400
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Pt	-3.28058100	-0.41317700	0.44417200
Cl	2.48534400	2.29614900	1.80950200
Cl	-2.67584400	-1.89324700	2.35554300
P	1.38271900	-0.80638400	0.79977100
P	-1.44748300	0.94273300	0.92065300
F	4.65599800	-4.45660900	-1.46887200
F	7.35489000	-0.86420500	-2.76717300
F	-6.98454500	0.22299500	-3.29048800
F	-4.40383100	4.03671500	-2.47696900
N	4.86503300	1.65991800	-0.40596800
N	-4.85716000	-1.70076600	-0.14122800
C	5.01925300	2.96666400	-0.13511300
H	4.29947100	3.38331200	0.55950100
C	6.03545800	3.72466400	-0.70347800
H	6.12645300	4.77614900	-0.45346100
C	6.91171800	3.09934600	-1.58899900
H	7.71530400	3.65792200	-2.06091300
C	6.75449800	1.74682200	-1.86960100
H	7.42366200	1.24674900	-2.55276600
C	5.71666800	1.02326700	-1.26095400
C	5.43042500	-0.40324500	-1.41909500
C	4.27092800	-0.90736900	-0.74998500
C	4.04642600	-2.28866100	-0.77291100
H	3.21441100	-2.74600700	-0.25538800
C	4.90749900	-3.13293000	-1.46398300
C	6.01673300	-2.66977500	-2.15836500
H	6.67866900	-3.33549200	-2.69793900
C	6.25320100	-1.30578700	-2.10995600
C	-0.01578700	0.03518800	1.72410200
H	0.49375200	0.74457500	2.37902400
H	-0.49561600	-0.73136600	2.33961500
C	1.88921700	-2.04096000	2.07608700
C	1.67156700	-3.42093900	1.97172700
H	1.17365700	-3.83551300	1.10210900
C	2.10041100	-4.27944800	2.98742900
H	1.92892500	-5.34810200	2.89190300
C	2.74165400	-3.76958800	4.11563100
H	3.07145200	-4.43961600	4.90495000
C	2.96397800	-2.39439000	4.22496800
H	3.46945800	-1.98989300	5.09752700
C	2.54919600	-1.53400900	3.21009000
H	2.74872500	-0.46852200	3.29013000
C	0.61612500	-1.72155000	-0.59701900
C	-0.48157200	-2.57354900	-0.38375600
H	-0.90585500	-2.69530500	0.60752700
C	-1.06309300	-3.25189300	-1.45712400
H	-1.91203000	-3.90506500	-1.27623900
C	-0.56627800	-3.08225100	-2.75050400
H	-1.02096000	-3.61253400	-3.58317900
C	0.51142400	-2.22228500	-2.97196700
H	0.89764600	-2.07670500	-3.97712900
C	1.09782500	-1.54292300	-1.90357500
H	1.92643300	-0.86739700	-2.08050200
C	-0.74973000	1.84739600	-0.52603300

C	-0.79278500	1.22314500	-1.78334900
H	-1.25558000	0.24739100	-1.88424600
C	-0.27056700	1.86167500	-2.90747200
H	-0.31218700	1.36589600	-3.87340100
C	0.28443700	3.13803400	-2.79405700
H	0.67942500	3.64122200	-3.67269900
C	0.31791100	3.77057700	-1.55076600
H	0.74135300	4.76642600	-1.45447600
C	-0.19250500	3.13005200	-0.42040500
H	-0.15585800	3.63699500	0.53566900
C	-1.89605300	2.19985200	2.19264200
C	-3.25776800	2.40921100	2.46749400
H	-4.00603200	1.82071300	1.94621400
C	-3.65227400	3.35245800	3.41734700
H	-4.70958700	3.49861300	3.62033600
C	-2.69402300	4.09395700	4.10903800
H	-3.00129000	4.82522900	4.85202900
C	-1.33803600	3.88692900	3.84877500
H	-0.58415100	4.45504100	4.38684100
C	-0.93666300	2.94589100	2.89976000
H	0.12379900	2.80543200	2.71508300
C	-5.08611800	-2.90802700	0.40276800
H	-4.46302400	-3.15646500	1.25424700
C	-6.05485200	-3.77116600	-0.09399600
H	-6.20999000	-4.73511400	0.37844700
C	-6.80120300	-3.36277100	-1.19853100
H	-7.56265400	-4.01106300	-1.62331100
C	-6.56980100	-2.11182400	-1.75887300
H	-7.14062400	-1.77900900	-2.61202700
C	-5.58714600	-1.27109400	-1.21102200
C	-5.24870900	0.08464100	-1.64591300
C	-4.16608000	0.73061400	-0.96817000
C	-3.91610300	2.07602900	-1.26268500
H	-3.13198000	2.63773500	-0.77403400
C	-4.67426100	2.74258400	-2.21850400
C	-5.69917700	2.12994200	-2.92653100
H	-6.27766700	2.65616800	-3.67547300
C	-5.96373400	0.80703700	-2.61328600

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Complex 3b, ground state, gas phase

Pt	4.31396500	-0.54299300	-0.41512100
Cl	4.89851000	-2.71627400	-1.42024500
C	4.23010300	1.24531300	0.51660200
C	5.13046900	2.22331300	-0.01283300
C	3.50475900	1.57855000	1.66909000
C	5.16735500	3.49473200	0.57683500
C	6.04630100	1.77139300	-1.06513100
C	3.60111900	2.85183700	2.21851500
H	2.89141500	0.85308200	2.18862200
C	4.40495300	3.84607800	1.68057000
C	6.98394800	2.55059000	-1.75962600
H	4.46520100	4.83739800	2.11193700
C	7.82785600	1.95022600	-2.68844800
H	7.04540600	3.61089600	-1.56719400

C	6.77629200	-0.14489600	-2.21913000
C	7.73354600	0.57912200	-2.92031600
H	8.55445100	2.55396600	-3.22514700
H	6.62830400	-1.21080200	-2.35503900
H	8.37742700	0.07268600	-3.63120100
N	5.96043000	0.43456300	-1.32420600
C	1.60023400	-2.72339200	-0.78551500
C	1.63017500	-2.51840200	-2.17394300
C	0.93250500	-3.84127900	-0.26869000
C	0.99531400	-3.41742100	-3.02858000
H	2.17272300	-1.67192600	-2.58315800
C	0.30507800	-4.74409800	-1.13026300
H	0.89296400	-4.01053000	0.80221500
C	0.33382300	-4.53335400	-2.50854500
H	1.03176700	-3.25524000	-4.10240200
H	-0.21114100	-5.60624400	-0.71814700
H	-0.15544400	-5.23663600	-3.17707200
C	2.44646600	-2.18583100	1.97825000
C	1.67074800	-1.78225700	3.07441000
C	3.42786200	-3.17818300	2.15671400
C	1.86510200	-2.36788000	4.32830100
H	0.91228000	-1.01376200	2.96741500
C	3.60968600	-3.76447000	3.40773400
H	4.04909000	-3.47751900	1.31621700
C	2.83007700	-3.36048800	4.49565400
H	1.25663900	-2.04742700	5.16928200
H	4.36804900	-4.53203700	3.53470900
H	2.97808800	-3.81632500	5.47087600
P	2.31329500	-1.43484900	0.31178600
C	0.93065400	-0.17371400	0.35651200
H	1.05855500	0.38971800	-0.57390700
H	1.15084100	0.51910600	1.16789000
C	-0.49212900	-0.73285500	0.46501600
H	-0.66335800	-1.28550700	1.39081700
H	-0.69575800	-1.44821700	-0.33575600
C	-1.43433200	1.45732200	-1.16237100
C	-1.45870300	0.74331400	-2.37352800
C	-1.08401800	2.81414800	-1.18297200
C	-1.12279500	1.37055700	-3.57197200
H	-1.75490300	-0.30242100	-2.38122300
C	-0.75522500	3.44190200	-2.38751400
H	-1.07801100	3.39361900	-0.26607100
C	-0.76912900	2.72252700	-3.58185500
H	-1.14587200	0.80486500	-4.49923100
H	-0.49168800	4.49592000	-2.38695500
H	-0.51231000	3.21214800	-4.51712200
C	-1.70105100	1.61630200	1.81558600
C	-0.55150700	2.38804600	2.07197400
C	-2.74236300	1.62577100	2.75878000
C	-0.44582200	3.13960400	3.24286700
H	0.26668800	2.41657800	1.36102700
C	-2.63714700	2.38492900	3.92543900
H	-3.63107200	1.02985400	2.57331400
C	-1.48978800	3.14006600	4.17050000

H	0.45962200	3.70795700	3.42853300
H	-3.45294100	2.38034400	4.64287800
H	-1.40628700	3.72585900	5.08193000
P	-1.88191300	0.51191100	0.35648300
Pt	-3.95577500	-0.50110800	0.20028300
Cl	-3.02677700	-2.58613300	1.15579100
C	-5.00126000	1.09798900	-0.45797000
C	-6.34553500	0.79678300	-0.84467300
C	-4.58638500	2.43305100	-0.50786200
C	-7.16628000	1.84307800	-1.29154100
C	-6.78203500	-0.59284900	-0.69330800
C	-5.45112000	3.42700000	-0.95070200
H	-3.59285100	2.73956300	-0.21210900
C	-6.75044700	3.16299600	-1.36056700
C	-8.03600400	-1.12366800	-1.03524800
H	-7.41561000	3.94327000	-1.70866100
C	-8.30420700	-2.46840300	-0.80498100
H	-8.78437200	-0.48290200	-1.47542700
C	-6.09653900	-2.70760700	0.07871000
C	-7.32369900	-3.27868200	-0.23508100
H	-9.27531900	-2.87699600	-1.07057200
H	-5.28211000	-3.27224100	0.51846700
H	-7.49361000	-4.33134700	-0.03663100
N	-5.83605600	-1.40892500	-0.14456300
F	2.87502200	3.14390200	3.32328300
F	5.98728900	4.45624100	0.08489900
F	-8.44372300	1.59757800	-1.67764200
F	-5.01390800	4.70180900	-0.98632300

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Complex 2a, excited state, gas phase

C	1.69311400	1.37198400	0.51713200
C	1.48301800	2.72989100	0.89594200
C	2.94391600	0.79839100	0.74674400
C	2.55659900	3.43789000	1.46222000
C	0.14186500	3.28067600	0.70257200
C	3.96825500	1.55024500	1.31981800
C	3.80513200	2.87823800	1.68220000
C	-0.24239300	4.61712900	0.89941700
C	-2.04985400	2.75805400	0.04132900
C	-1.55412100	5.00825200	0.66214400
C	-2.48062700	4.06409000	0.22191000
N	-0.78348600	2.36768600	0.28104300
H	3.17777600	-0.22386000	0.48412200
H	4.60649300	3.45692100	2.12481100
H	0.49049500	5.33745300	1.22789200
H	-2.73001200	1.99635300	-0.31304200
H	-1.84571400	6.04306600	0.81434100
H	-3.51325800	4.32373400	0.01737600
P	1.03821900	-1.53686500	-0.89216300
Pt	-0.00175000	0.41723100	-0.12959400
P	-2.18791000	-0.67197200	-0.29385500
C	1.23060900	-2.82940200	0.38662200
C	1.32795100	-2.46532500	1.73912300
C	1.29422400	-4.18723500	0.02792700

C	1.49700000	-3.44658800	2.71651800
H	1.27156700	-1.41901900	2.02365100
C	1.45815200	-5.16313000	1.01071900
H	1.21578400	-4.48123400	-1.01503300
C	1.56117500	-4.79365600	2.35420400
H	1.57501900	-3.15846700	3.76070300
H	1.50464300	-6.21046600	0.72720200
H	1.68939300	-5.55569100	3.11743300
C	2.65382100	-1.28555300	-1.72687700
C	3.73255800	-2.15909300	-1.53132700
C	2.77637200	-0.22017800	-2.63358300
C	4.92176500	-1.96626800	-2.23841400
H	3.65344200	-2.98304100	-0.82950800
C	3.96279900	-0.03956800	-3.34249200
H	1.95268500	0.47536400	-2.77265900
C	5.03759000	-0.91098600	-3.14377800
H	5.75640400	-2.64229800	-2.07798200
H	4.05215400	0.78664500	-4.04176300
H	5.96404400	-0.76368700	-3.69100200
C	-2.96859700	-1.20401800	1.24338800
C	-4.07018700	-2.08742900	1.25720500
C	-2.39754600	-0.80699500	2.47070900
C	-4.60060300	-2.52991700	2.46613100
H	-4.49929900	-2.43872500	0.32385600
C	-2.93709200	-1.25221800	3.67555200
H	-1.53819700	-0.14222700	2.47344400
C	-4.04014600	-2.11035900	3.67679600
H	-5.44718500	-3.21022500	2.46457800
H	-2.49829300	-0.92766400	4.61457800
H	-4.45753600	-2.45796000	4.61720700
C	-3.44053300	-0.21765300	-1.50837900
C	-2.98987800	0.01694400	-2.82887000
C	-4.81403100	-0.05156900	-1.22134400
C	-3.88473900	0.38540900	-3.82784800
H	-1.93409000	-0.09226400	-3.06296300
C	-5.70163500	0.32019700	-2.22816000
H	-5.18118900	-0.19837500	-0.21143700
C	-5.24413200	0.53431400	-3.53218300
H	-3.52500100	0.55714300	-4.83808900
H	-6.75419900	0.44945400	-1.99326700
H	-5.94203400	0.82199900	-4.31281700
C	0.07838200	-2.28819900	-2.20412600
H	-0.82427800	-2.85094700	-1.98912300
H	0.35369500	-2.12001800	-3.24024200
F	5.15742500	0.96560000	1.52595700
F	2.40300400	4.72601600	1.83797700

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Complex 2b, excited state, gas phase

C	0.01016200	3.31865200	-0.64656500
C	2.19338700	2.54849600	-0.11619000
C	0.55693700	4.62601600	-0.89518700
C	-1.33125100	2.94079400	-0.70643600
C	2.73981800	3.81234100	-0.32636600
C	1.89475400	4.87592500	-0.74464000

C	-2.43883900	3.82582800	-1.03208000
C	-2.97950500	1.11634600	-0.53213200
C	-3.72369100	3.39731300	-1.13034600
C	-3.98130500	2.02337300	-0.88308600
H	2.83393200	1.73787200	0.20663400
H	-0.11490500	5.41366000	-1.20127400
H	3.80208700	3.95985300	-0.16717700
H	2.29929600	5.86413400	-0.93346500
H	-3.29356200	0.09862800	-0.33871200
H	-4.52638100	4.08038300	-1.38156800
P	1.99183000	-0.93559200	0.31630500
Pt	-0.01494900	0.39655600	0.00472500
P	-1.11768000	-1.58455100	0.49321900
C	3.05491000	-0.40999600	1.72416200
C	2.42102200	0.15103700	2.84748700
C	4.45094500	-0.56063300	1.73279100
C	3.16527500	0.52661200	3.96573700
H	1.34580200	0.31174100	2.83517300
C	5.19233400	-0.17478800	2.85120600
H	4.96481000	-0.96731900	0.86813800
C	4.55240700	0.36284500	3.96956800
H	2.66381300	0.95679400	4.82789400
H	6.27208300	-0.29275800	2.84521500
H	5.13315600	0.66177200	4.83730500
C	3.07600400	-1.16705900	-1.14205900
C	2.97049000	-0.28652500	-2.23011200
C	3.98860800	-2.23557200	-1.21309600
C	3.77469900	-0.45928100	-3.35829500
H	2.24811000	0.52349800	-2.20214600
C	4.78834900	-2.40568200	-2.34294800
H	4.07637800	-2.94125800	-0.39156600
C	4.68489900	-1.51562300	-3.41511200
H	3.68295900	0.22741200	-4.19476200
H	5.48844900	-3.23484500	-2.38730400
H	5.30743600	-1.65116100	-4.29469200
C	-2.57245700	-1.47227200	1.60279600
C	-3.75536300	-2.19199700	1.37890900
C	-2.47373100	-0.64251100	2.73325700
C	-4.81770100	-2.09046800	2.28052300
H	-3.85737700	-2.82425200	0.50325000
C	-3.53353400	-0.55172000	3.63315700
H	-1.57512700	-0.05325900	2.89761900
C	-4.70780600	-1.27596500	3.40767900
H	-5.73153100	-2.64770300	2.09650400
H	-3.44765800	0.09114400	4.50435100
H	-5.53602400	-1.19892700	4.10597300
C	-1.57844700	-2.59879300	-0.95979500
C	-1.86821200	-3.97016200	-0.83515000
C	-1.62689800	-2.00172000	-2.22964300
C	-2.20370100	-4.72347400	-1.95966600
H	-1.84082300	-4.45636200	0.13605100
C	-1.96629300	-2.75983600	-3.35170300
H	-1.39420400	-0.94645900	-2.33526400
C	-2.25396700	-4.11892700	-3.21865500

H	-2.42482700	-5.78138300	-1.85263900
H	-2.00168700	-2.28764700	-4.32905400
H	-2.51483600	-4.70829400	-4.09285100
C	0.08471800	-2.63264900	1.45712700
H	-0.32067900	-3.63985000	1.59999900
H	0.17107400	-2.17658100	2.44964700
C	1.44029000	-2.67223600	0.74642000
H	2.19471000	-3.16705300	1.36634000
H	1.36066200	-3.22569500	-0.19547300
F	-2.19039900	5.13237100	-1.25073700
F	-5.24480200	1.60070000	-0.98946900
C	-1.65567100	1.51592100	-0.42406200
N	0.89651500	2.25791100	-0.27952900

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Complex 2c, excited state, gas phase

Pt	0.21863700	0.64521300	-0.01703300
P	-2.02433000	-0.25713900	-0.19978900
P	0.80534600	-1.58869000	-0.24798800
F	3.45842100	4.90044000	0.38553300
F	5.66128700	0.77511600	0.45035100
N	-0.24876700	2.67379000	0.20485900
C	-1.47231100	3.21180300	0.25735100
H	-2.30601200	2.52960600	0.16237800
C	-1.71971300	4.57481100	0.40975000
H	-2.74614800	4.92259200	0.43957800
C	-0.62464300	5.47391000	0.51637200
H	-0.79037700	6.53888200	0.63604000
C	0.64451200	4.96373100	0.46546800
H	1.49997600	5.61706300	0.54680700
C	0.87530900	3.55099000	0.31337800
C	2.10656700	2.89983200	0.27958900
C	2.09336000	1.41546600	0.17665800
C	3.40451200	3.55379700	0.36237100
C	4.57526700	2.86870400	0.42437800
H	5.52555000	3.38414200	0.49688300
C	4.51046300	1.45211400	0.38049300
C	3.30828600	0.75168600	0.24969700
H	3.38258400	-0.32597900	0.18859100
C	-3.24442900	0.66010000	-1.22203100
C	-2.82037600	1.13821300	-2.47519300
H	-1.79726500	0.96962200	-2.80209200
C	-3.70503900	1.83309100	-3.29719700
H	-3.37036300	2.19568300	-4.26477500
C	-5.01719900	2.06852700	-2.87435800
H	-5.70429700	2.61410800	-3.51459200
C	-5.44125900	1.60599000	-1.62828800
H	-6.45876300	1.78922500	-1.29522000
C	-4.56035800	0.90316900	-0.80110100
H	-4.90032600	0.54797900	0.16645900
C	-2.83220800	-0.59150700	1.41427400
C	-2.45728200	0.19011600	2.51950500
H	-1.68546000	0.94676800	2.41039200
C	-3.05864800	-0.01239700	3.76245700
H	-2.76131100	0.59773400	4.61039000

C	-4.03028600	-1.00271500	3.91661500
H	-4.49392600	-1.16399400	4.88550500
C	-4.39956500	-1.79340900	2.82559100
H	-5.14790500	-2.57162700	2.94432500
C	-3.80503200	-1.59135600	1.57996300
H	-4.09281600	-2.22199200	0.74476000
C	-1.86060800	-1.87497100	-1.05663400
C	-2.92972100	-2.50070900	-1.71171800
H	-3.90622500	-2.02599400	-1.73318800
C	-2.73758800	-3.71671200	-2.36914000
H	-3.57030000	-4.19226300	-2.87881400
C	-1.47239600	-4.30631500	-2.39155300
H	-1.31618200	-5.24269600	-2.91888400
C	-0.39713400	-3.68047400	-1.75871100
H	0.59205600	-4.12443700	-1.81551300
C	-0.58464300	-2.46724900	-1.08222200
C	2.25050300	-1.99052900	-1.30221000
C	2.37736800	-1.32631800	-2.53425400
H	1.65317700	-0.56720700	-2.81757400
C	3.43799200	-1.62814900	-3.38550500
H	3.53044100	-1.11090500	-4.33604300
C	4.38553000	-2.58679500	-3.01273700
H	5.21555500	-2.81554200	-3.67481000
C	4.26804500	-3.24453200	-1.78804500
H	5.00531600	-3.98535000	-1.49285400
C	3.20337200	-2.95071800	-0.93155200
H	3.12312700	-3.46436100	0.02118900
C	1.05724000	-2.43475700	1.36223000
C	1.56920700	-1.69808400	2.44347500
H	1.78312600	-0.64062300	2.32490900
C	1.79524800	-2.31904500	3.67223500
H	2.19280500	-1.74067800	4.50115700
C	1.50493000	-3.67460000	3.83782200
H	1.67687400	-4.15503200	4.79665300
C	0.98580300	-4.41081900	2.77074300
H	0.75009600	-5.46352500	2.89699800
C	0.76138700	-3.79677200	1.53815300
H	0.34528900	-4.37962200	0.72289200

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Complex 3a, excited state, gas phase

Pt	3.19742700	0.45459500	0.28988400
Pt	-3.27453400	-0.35645800	0.43898800
Cl	2.54217100	2.20012400	1.92799400
Cl	-2.78753800	-1.78099800	2.42569300
P	1.35510100	-0.85728700	0.87643900
P	-1.42187200	0.95775700	0.94741900
F	4.69109600	-4.46192000	-1.47400100
F	6.81571200	-0.73956200	-3.39497100
F	-6.80793300	0.24762100	-3.46174600
F	-4.18243000	4.03037700	-2.64594200
N	4.78071700	1.63359100	-0.40728100
N	-4.85686100	-1.62456300	-0.17096800
C	5.02841200	2.90182900	-0.07079600
H	4.35741000	3.32707200	0.66674900

C	6.07260500	3.64317200	-0.62153500
H	6.21533500	4.67139700	-0.30828500
C	6.92081300	3.03514100	-1.58637300
H	7.74160300	3.59147100	-2.02795500
C	6.69203000	1.73187500	-1.94521200
H	7.32360800	1.23733200	-2.66942300
C	5.61433300	0.99170200	-1.35566600
C	5.27970900	-0.34672900	-1.57514200
C	4.18858100	-0.92504500	-0.73926400
C	4.04974300	-2.31580700	-0.70160800
H	3.32885300	-2.79776700	-0.05331400
C	4.82291200	-3.12196400	-1.51922800
C	5.75438400	-2.59241700	-2.45969500
H	6.29497400	-3.24818900	-3.13240100
C	5.94342300	-1.24690500	-2.48972600
C	-0.03402600	0.01211900	1.78379700
H	0.48162200	0.70720300	2.44933400
H	-0.54468900	-0.74125300	2.39084500
C	1.88332500	-2.04926400	2.18480800
C	1.68756800	-3.43492800	2.11216800
H	1.19065200	-3.87619700	1.25518900
C	2.13588500	-4.26392900	3.14412300
H	1.98127300	-5.33707800	3.07313600
C	2.77476800	-3.71884400	4.25698800
H	3.11955600	-4.36569700	5.05912300
C	2.97583800	-2.33809800	4.33418800
H	3.47969600	-1.90632100	5.19450800
C	2.54250400	-1.50688900	3.30295000
H	2.72752900	-0.43728200	3.35760800
C	0.56747700	-1.83379300	-0.46740300
C	-0.53141200	-2.66729900	-0.19372700
H	-0.94331500	-2.73392900	0.80787800
C	-1.13085800	-3.39997000	-1.22020900
H	-1.98018400	-4.03763600	-0.99213500
C	-0.65220600	-3.30304400	-2.52778400
H	-1.12136900	-3.87477700	-3.32417800
C	0.42573700	-2.46178100	-2.81028200
H	0.79768200	-2.37194800	-3.82730600
C	1.03102500	-1.72949000	-1.78817400
H	1.85993300	-1.06936500	-2.01360500
C	-0.65805000	1.83348100	-0.48334700
C	-0.66138000	1.19215300	-1.73288800
H	-1.13769600	0.22356500	-1.83937600
C	-0.08325000	1.80575300	-2.84338500
H	-0.09501600	1.29770300	-3.80378200
C	0.48829300	3.07446700	-2.72499600
H	0.92749900	3.55821700	-3.59340100
C	0.48120100	3.72462700	-1.49044600
H	0.91662400	4.71495700	-1.39113900
C	-0.08533900	3.10882600	-0.37303500
H	-0.08041800	3.62928100	0.57669400
C	-1.86317800	2.23455400	2.20078100
C	-3.22451800	2.48968300	2.43549700
H	-3.97640000	1.92203800	1.89642000

C	-3.61444800	3.45110700	3.36882600
H	-4.67164700	3.63286500	3.54122700
C	-2.65217000	4.16513800	4.08351000
H	-2.95610700	4.91042300	4.81380300
C	-1.29679300	3.91295200	3.86269200
H	-0.54032700	4.45991400	4.41870900
C	-0.90005700	2.95361000	2.93022000
H	0.16001900	2.77860500	2.77516500
C	-5.13606200	-2.80876300	0.39950700
H	-4.55637300	-3.04285100	1.28508700
C	-6.10133100	-3.66673900	-0.11274200
H	-6.29871200	-4.61158800	0.38200600
C	-6.78939800	-3.27821900	-1.26149100
H	-7.54573800	-3.92374400	-1.69940600
C	-6.50614000	-2.05077500	-1.84933500
H	-7.03156900	-1.73331700	-2.73684400
C	-5.52996500	-1.21375500	-1.28453900
C	-5.14332300	0.12058800	-1.74456200
C	-4.07512700	0.76311400	-1.04128300
C	-3.78524000	2.09466900	-1.36074000
H	-3.00988500	2.65376000	-0.85532000
C	-4.49006500	2.74950100	-2.36438900
C	-5.49786300	2.13788400	-3.09748200
H	-6.03421600	2.65464900	-3.88346100
C	-5.80303900	0.82979600	-2.75974300

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Complex 3b, excited state, gas phase

Pt	4.20213100	-0.62900300	-0.62963900
Cl	4.53278600	-2.59765800	-2.07524600
C	4.31893500	0.94035000	0.63438000
C	5.29455100	1.91872200	0.26245900
C	3.65783600	1.10612000	1.85921700
C	5.46883500	3.04207300	1.08308100
C	6.13157900	1.60330700	-0.89934200
C	3.88939800	2.23450300	2.63755900
H	2.98895300	0.35233800	2.25490200
C	4.77213200	3.23797500	2.26579200
C	7.12319900	2.41544900	-1.47033600
H	4.93801700	4.11692800	2.87599900
C	7.87653500	1.93796400	-2.53788900
H	7.29620900	3.40510600	-1.07579700
C	6.63398400	-0.10209800	-2.44105700
C	7.63889700	0.65597600	-3.03056000
H	8.64494700	2.56701000	-2.97873100
H	6.37669600	-1.10097000	-2.77656800
H	8.20881900	0.24492200	-3.85677700
N	5.90526000	0.35933500	-1.41224100
C	1.28618700	-2.45789200	-1.26470800
C	1.25883900	-1.97447900	-2.58246200
C	0.56420500	-3.61366200	-0.94093300
C	0.51016400	-2.63342400	-3.55587600
H	1.84562200	-1.10066900	-2.84876600
C	-0.17622600	-4.27695600	-1.92280300
H	0.57424400	-3.99960300	0.07313500

C	-0.20765500	-3.78719900	-3.22831700
H	0.50225300	-2.25649100	-4.57498700
H	-0.72912700	-5.17483900	-1.66143900
H	-0.78455000	-4.30417800	-3.99039100
C	2.26558700	-2.54008300	1.50410100
C	1.48965600	-2.35201400	2.65723500
C	3.21798700	-3.57553900	1.47460800
C	1.65874200	-3.19021900	3.76255600
H	0.74845600	-1.56179800	2.71064100
C	3.37462900	-4.41277600	2.57758800
H	3.83405100	-3.71436900	0.58970800
C	2.59729000	-4.22094200	3.72359900
H	1.04981800	-3.03528400	4.64861700
H	4.11112200	-5.21084100	2.54441400
H	2.72564200	-4.87230900	4.58387900
P	2.15415100	-1.47092000	0.01987300
C	0.89669700	-0.12879400	0.37473800
H	1.08466000	0.62713600	-0.39482600
H	1.16949700	0.32544200	1.32698700
C	-0.57244200	-0.56313300	0.37133700
H	-0.79479200	-1.31709100	1.12891900
H	-0.84249000	-1.01852100	-0.58593700
C	-1.36637300	2.04245000	-0.60177100
C	-1.22817300	1.63418500	-1.94017400
C	-1.17688100	3.39563200	-0.28495600
C	-0.89134200	2.55486900	-2.93088100
H	-1.39408000	0.59627500	-2.21527800
C	-0.84623400	4.31741300	-1.28197100
H	-1.29308300	3.73766000	0.73788800
C	-0.69921700	3.90002400	-2.60423600
H	-0.78558300	2.22245200	-3.95979000
H	-0.70598900	5.36240400	-1.01983600
H	-0.44156700	4.61761600	-3.37813100
C	-1.52911500	1.51903300	2.29312600
C	-0.31570200	2.15713900	2.61306900
C	-2.51842200	1.41113700	3.28315000
C	-0.09269700	2.65709100	3.89627300
H	0.45715200	2.28261700	1.86220200
C	-2.29708600	1.92440700	4.56239000
H	-3.45141000	0.90871900	3.05172700
C	-1.08504600	2.54197600	4.87247000
H	0.86034300	3.12142100	4.12779600
H	-3.07288500	1.83174200	5.31720700
H	-0.91149200	2.93232300	5.87172800
P	-1.85232500	0.77441300	0.64428100
Pt	-3.94612100	-0.23590600	0.43127400
Cl	-3.11362300	-1.90892400	2.06955500
C	-4.90915500	1.07392100	-0.71562300
C	-6.18376500	0.52640600	-1.27158200
C	-4.59329600	2.40480500	-0.98966700
C	-6.90079200	1.36037400	-2.21044600
C	-6.60670700	-0.71774300	-0.80275200
C	-5.39304300	3.16805300	-1.82627400
H	-3.70980400	2.87390200	-0.58095400

C	-6.54571500	2.64504200	-2.47552800
C	-7.82225900	-1.41373800	-1.12214900
H	-7.12040400	3.25345900	-3.16409000
C	-8.10787600	-2.62227200	-0.54410800
H	-8.50865900	-0.96003600	-1.82226700
C	-6.00450100	-2.48867200	0.66710300
C	-7.18002400	-3.18167600	0.37852300
H	-9.02949800	-3.14310900	-0.78355300
H	-5.26803100	-2.88144100	1.35942600
H	-7.36296200	-4.13632400	0.85895500
N	-5.70201400	-1.31116500	0.11700800
F	3.22229800	2.37041600	3.80705600
F	6.36424600	4.00418100	0.74904600
F	-7.98995200	0.85605600	-2.84037800
F	-5.07564700	4.45324500	-2.07686400