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Complex A, ground state, gas phase

Pt	0.67650500	-0.35659100	0.00001800
Cl	2.37246500	-2.19136800	0.00010100
N	-0.93753400	-1.65076600	-0.00019900
C	-0.82669300	0.98818400	0.00000200
C	-2.12433500	0.39533300	-0.00002500
C	-2.17202400	-1.06291700	-0.00003700
C	-0.81197100	-2.99025600	-0.00019700
H	0.20571200	-3.36144000	-0.00039400
C	-1.91704400	-3.83066000	0.00000700
H	-1.77270700	-4.90534600	0.00007500
C	-3.18809700	-3.25686700	0.00017500
H	-4.07694500	-3.88143500	0.00033100
C	-3.31778900	-1.87313800	0.00012200
H	-4.29312700	-1.41062300	0.00021900
C	-3.24266600	1.24143800	-0.00005600
C	-3.14386000	2.62289300	-0.00000400
H	-4.02829100	3.24779400	-0.00002600
C	-1.86229300	3.16052700	0.00005200
C	-0.71119700	2.37860200	0.00004200
H	0.25734300	2.86647800	0.00001700
F	-4.49452400	0.72046100	-0.00012300
F	-1.73835400	4.50050400	0.00008300
S	2.48368200	1.10926000	-0.00000600
O	2.30377100	2.59899200	-0.00012500
C	3.55037500	0.68352800	1.40635400
H	2.98838800	0.94294400	2.30581100
H	3.75885600	-0.38720200	1.37696200
H	4.45433900	1.29413600	1.33230600
C	3.55023000	0.68326100	-1.40645600
H	2.98798500	0.94235200	-2.30584900
H	4.45407000	1.29409100	-1.33276800
H	3.75887000	-0.38742300	-1.37684500

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Complex A, excited state, gas phase

Pt	-0.67079500	-0.36482200	0.00006700
Cl	-2.35003600	-2.20934100	-0.00002700
N	0.92045800	-1.63716600	-0.00000900
C	0.78474400	0.99124900	-0.00001600
C	2.14061500	0.37874500	-0.00013100
C	2.20530300	-1.01340000	-0.00010400
C	0.83938200	-2.97131500	0.00006500
H	-0.16513100	-3.37801300	0.00014300
C	1.96273400	-3.79598200	0.00003300
H	1.82439200	-4.87127400	0.00010900
C	3.26333200	-3.21218400	-0.00009900
H	4.14904500	-3.83871500	-0.00015000
C	3.37395500	-1.84782700	-0.00017000
H	4.34351600	-1.37096300	-0.00027200
C	3.26611100	1.28473100	-0.00026200
C	3.12145200	2.63662500	-0.00019100
H	3.98550700	3.29076100	-0.00028500
C	1.80345700	3.17149700	-0.00002400

C	0.66438500	2.37671200	0.00004300
H	-0.31093800	2.85259400	0.00011700
F	4.52013100	0.77377000	-0.00046700
F	1.68947700	4.51017500	0.00005000
S	-2.51173400	1.08470600	0.00011800
O	-2.34788700	2.57750400	0.00027200
C	-3.57588500	0.64904100	-1.40554300
H	-3.01921600	0.92024200	-2.30479500
H	-3.76833800	-0.42474000	-1.38030500
H	-4.48929200	1.24495900	-1.32765000
C	-3.57600200	0.64876000	1.40560500
H	-3.01940800	0.91979000	2.30495600
H	-4.48940400	1.24469000	1.32775000
H	-3.76844800	-0.42501700	1.38014600

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Complex A, ground state, CH<sub>2</sub>Cl<sub>2</sub> solution

Pt	-0.67007700	-0.36868100	0.00068400
Cl	-2.36685300	-2.23900200	-0.00013600
N	0.96561800	-1.64535100	0.00047700
C	0.81622100	0.98974800	0.00073900
C	2.12250600	0.41668800	-0.00002600
C	2.19256100	-1.04247900	-0.00016100
C	0.86208400	-2.98734300	0.00050200
H	-0.14699200	-3.37859700	0.00091900
C	1.97865000	-3.81238100	-0.00011400
H	1.84979400	-4.88864900	-0.00009500
C	3.24136400	-3.22098300	-0.00081100
H	4.13863300	-3.83206800	-0.00135600
C	3.34937100	-1.83436100	-0.00083000
H	4.31921500	-1.36079400	-0.00137800
C	3.22724700	1.28021200	-0.00058800
C	3.10955900	2.66149300	-0.00032600
H	3.98564500	3.29817500	-0.00080600
C	1.82067800	3.17753600	0.00059600
C	0.68146800	2.37900900	0.00114500
H	-0.29525900	2.84969200	0.00180400
F	4.48562100	0.77886700	-0.00145800
F	1.67174800	4.51874100	0.00091300
S	-2.50463300	1.09237900	-0.00072500
O	-2.31939500	2.58710800	0.00030600
C	-3.56441500	0.67646700	-1.41166900
H	-2.99604000	0.92415200	-2.31015700
H	-3.78992700	-0.39001300	-1.37917900
H	-4.46490000	1.29175200	-1.34286800
C	-3.56760400	0.67482200	1.40737000
H	-3.00140800	0.92202300	2.30736800
H	-4.46825300	1.28969400	1.33704500
H	-3.79247700	-0.39175100	1.37344400

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Complex 1a, ground state, gas phase

C	2.93123400	-2.88860300	-0.10365600
H	2.08716300	-3.56816800	-0.14589500
C	4.25045300	-3.32470200	-0.09682000
H	4.46601100	-4.38694500	-0.13611500

C	5.26284200	-2.36860900	-0.03877300
H	6.30752300	-2.66726400	-0.03102900
C	4.93191200	-1.01889900	0.00906900
H	5.70457100	-0.26710500	0.05338300
C	3.58294000	-0.62919000	-0.00156900
C	3.06428600	0.74088400	0.03720300
C	3.86619500	1.89110600	0.08985600
C	3.35457300	3.17845600	0.11523400
H	4.00798400	4.04096200	0.15550300
C	1.97232800	3.29845400	0.08220600
C	1.12403900	2.19864600	0.03073700
H	0.06116700	2.39901200	-0.00310100
C	1.64147200	0.89688400	0.01059800
C	-1.81013700	1.01609800	1.53486300
C	-0.89451100	0.96069300	2.59197100
H	0.02181700	0.39051700	2.48504300
C	-1.19127100	1.65144700	3.76867600
H	-0.50226800	1.62424200	4.60832700
C	-2.37963000	2.37321900	3.84397300
H	-2.65038400	2.92714000	4.73774500
C	-3.22888700	2.36827800	2.73436600
H	-4.16795300	2.91841000	2.75284400
C	-2.93681600	-1.11916800	-0.00967100
C	-3.30628000	-1.75413400	1.18467800
H	-2.75317900	-1.56318200	2.09917100
C	-4.37889400	-2.64264100	1.20540900
H	-4.65666000	-3.12790600	2.13705800
C	-5.08824000	-2.91398600	0.03312200
H	-5.92355000	-3.60893500	0.05024000
C	-4.71744100	-2.29415800	-1.15996600
H	-5.26046900	-2.50431200	-2.07741200
C	-3.64599800	-1.39962700	-1.18387400
H	-3.36748500	-0.92387800	-2.11818600
C	-1.83823700	1.14507200	-1.45506900
C	-2.95071700	2.00378400	-1.49751300
H	-3.61597400	2.05991000	-0.64381000
C	-3.18425600	2.78682600	-2.62798900
H	-4.04153200	3.45443700	-2.64933400
C	-2.32764800	2.71186800	-3.72919500
H	-2.51706600	3.32160000	-4.60876900
C	-1.23020500	1.85065700	-3.69832200
H	-0.56153100	1.78448800	-4.55209900
C	-0.98314000	1.07214400	-2.56614900
H	-0.12435700	0.40820000	-2.53703600
N	2.61092200	-1.58480600	-0.05719300
N	-2.96213900	1.70155900	1.60811500
Pt	0.62322500	-0.85502600	-0.05411500
Cl	-0.31265600	-3.11903700	-0.14587300
P	-1.50576100	0.03654100	-0.02324100
F	1.43594400	4.53495000	0.10241700
F	5.21905100	1.78663200	0.11936700

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Complex 1a, excited state, gas phase

C	2.93070800	-2.87554400	-0.10445900
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H	2.10292500	-3.57450100	-0.15360800
C	4.25682400	-3.30934500	-0.09146600
H	4.46624700	-4.37237400	-0.13255500
C	5.30152200	-2.34506200	-0.02356500
H	6.34096600	-2.65733400	-0.01312600
C	4.97546000	-1.01587000	0.02629400
H	5.74674500	-0.26148600	0.07568900
C	3.60094900	-0.59436800	0.00989300
C	3.10465400	0.71092900	0.04333500
C	3.90442600	1.91211800	0.11945600
C	3.37155200	3.16298900	0.10034600
H	4.00656900	4.03964900	0.15279600
C	1.95882200	3.28903200	0.00926600
C	1.11566600	2.19195200	-0.04341300
H	0.05362600	2.38948500	-0.11200800
C	1.62219700	0.88837400	-0.01580600
C	-1.81123200	1.06801100	1.51265200
C	-0.88709500	1.05768400	2.56359900
H	0.03540900	0.49566900	2.46937800
C	-1.18230800	1.78385000	3.71934500
H	-0.48632800	1.79163900	4.55364600
C	-2.37781500	2.49481100	3.78090800
H	-2.64757000	3.07501700	4.65813800
C	-3.23583500	2.44340300	2.67922800
H	-4.18104300	2.98316900	2.68725700
C	-2.92624700	-1.13689900	0.06403600
C	-3.26922000	-1.72885500	1.28797500
H	-2.70903300	-1.49053100	2.18700600
C	-4.32565800	-2.63421700	1.35898200
H	-4.58307200	-3.08575600	2.31315800
C	-5.04558100	-2.96416000	0.20846400
H	-5.86840800	-3.67176400	0.26482900
C	-4.70151900	-2.38624100	-1.01343000
H	-5.25287400	-2.64221400	-1.91408100
C	-3.64593600	-1.47598600	-1.08813300
H	-3.38720600	-1.03428500	-2.04456400
C	-1.89035300	1.09658200	-1.47724100
C	-3.02733300	1.92234600	-1.53281200
H	-3.68544900	1.98479700	-0.67422200
C	-3.29393300	2.66572800	-2.68242300
H	-4.17020300	3.30779100	-2.71373000
C	-2.44604300	2.58373300	-3.78994100
H	-2.66130600	3.16233100	-4.68446500
C	-1.32451600	1.75494100	-3.74607300
H	-0.66266100	1.68260300	-4.60463700
C	-1.04486700	1.01578700	-2.59512400
H	-0.16784400	0.37675900	-2.55791300
N	2.58642100	-1.58766500	-0.05650500
N	-2.97040400	1.74258400	1.57368700
Pt	0.63739500	-0.84552900	-0.05862300
Cl	-0.30420000	-3.10225000	-0.17483000
P	-1.51457000	0.03921900	-0.01656600
F	1.45009400	4.53681000	-0.01801000
F	5.25299100	1.80361300	0.21096200

Complex 1a, ground state, CH2Cl2 solution

C	2.93123400	-2.88860300	-0.10365600
H	2.08716300	-3.56816800	-0.14589500
C	4.25045300	-3.32470200	-0.09682000
H	4.46601100	-4.38694500	-0.13611500
C	5.26284200	-2.36860900	-0.03877300
H	6.30752300	-2.66726400	-0.03102900
C	4.93191200	-1.01889900	0.00906900
H	5.70457100	-0.26710500	0.05338300
C	3.58294000	-0.62919000	-0.00156900
C	3.06428600	0.74088400	0.03720300
C	3.86619500	1.89110600	0.08985600
C	3.35457300	3.17845600	0.11523400
H	4.00798400	4.04096200	0.15550300
C	1.97232800	3.29845400	0.08220600
C	1.12403900	2.19864600	0.03073700
H	0.06116700	2.39901200	-0.00310100
C	1.64147200	0.89688400	0.01059800
C	-1.81013700	1.01609800	1.53486300
C	-0.89451100	0.96069300	2.59197100
H	0.02181700	0.39051700	2.48504300
C	-1.19127100	1.65144700	3.76867600
H	-0.50226800	1.62424200	4.60832700
C	-2.37963000	2.37321900	3.84397300
H	-2.65038400	2.92714000	4.73774500
C	-3.22888700	2.36827800	2.73436600
H	-4.16795300	2.91841000	2.75284400
C	-2.93681600	-1.11916800	-0.00967100
C	-3.30628000	-1.75413400	1.18467800
H	-2.75317900	-1.56318200	2.09917100
C	-4.37889400	-2.64264100	1.20540900
H	-4.65666000	-3.12790600	2.13705800
C	-5.08824000	-2.91398600	0.03312200
H	-5.92355000	-3.60893500	0.05024000
C	-4.71744100	-2.29415800	-1.15996600
H	-5.26046900	-2.50431200	-2.07741200
C	-3.64599800	-1.39962700	-1.18387400
H	-3.36748500	-0.92387800	-2.11818600
C	-1.83823700	1.14507200	-1.45506900
C	-2.95071700	2.00378400	-1.49751300
H	-3.61597400	2.05991000	-0.64381000
C	-3.18425600	2.78682600	-2.62798900
H	-4.04153200	3.45443700	-2.64933400
C	-2.32764800	2.71186800	-3.72919500
H	-2.51706600	3.32160000	-4.60876900
C	-1.23020500	1.85065700	-3.69832200
H	-0.56153100	1.78448800	-4.55209900
C	-0.98314000	1.07214400	-2.56614900
H	-0.12435700	0.40820000	-2.53703600
N	2.61092200	-1.58480600	-0.05719300
N	-2.96213900	1.70155900	1.60811500
Pt	0.62322500	-0.85502600	-0.05411500
Cl	-0.31265600	-3.11903700	-0.14587300

P	-1.50576100	0.03654100	-0.02324100
F	1.43594400	4.53495000	0.10241700
F	5.21905100	1.78663200	0.11936700

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Complex 1b, ground state, gas phase

Pt	-0.62300400	-0.86277100	-0.00552500
Cl	0.31175500	-3.13318400	0.03539500
P	1.51199700	0.03358200	0.00674300
N	-2.60446000	-1.60874000	0.00219400
C	1.70916500	1.27544600	1.35785900
C	2.48701000	2.43541000	1.23249500
H	2.98090500	2.66492600	0.29421300
C	2.61687500	3.31655900	2.30808300
H	3.21348600	4.21760000	2.19449900
C	1.98105600	3.04467200	3.52035900
H	2.08321100	3.73239000	4.35544700
C	1.20589500	1.89048500	3.65388100
H	0.70179900	1.67593400	4.59213200
C	1.06310400	1.01439400	2.57774900
H	0.43995000	0.12958500	2.67491900
C	2.93810000	-1.10709000	0.26724700
C	3.68561700	-1.10010300	1.45140800
H	3.43065700	-0.42058700	2.25715500
C	4.77029800	-1.96796900	1.60525800
H	5.34148700	-1.95224200	2.52957900
C	5.11811400	-2.84464300	0.57905500
H	5.96262400	-3.51804700	0.69914100
C	4.37392200	-2.85797500	-0.60394000
H	4.63198200	-3.54597900	-1.40417900
C	3.28768000	-2.00080400	-0.75847800
H	2.70443600	-2.03441800	-1.67248700
C	1.97507000	0.86964500	-1.57125200
C	3.31202800	1.21695200	-1.83752500
H	4.08904500	0.97853100	-1.11757500
C	3.65480000	1.84507900	-3.03434300
H	4.69134600	2.10880500	-3.22610500
C	2.67145100	2.12092300	-3.98787500
H	2.94089300	2.60438100	-4.92306900
C	1.34627100	1.76173500	-3.74134400
H	0.57901900	1.95990300	-4.48459700
C	0.99807500	1.13797900	-2.54118200
H	-0.03137300	0.85017000	-2.35739000
C	-1.65910800	0.88192900	-0.03628400
C	-3.08097900	0.71274700	-0.03369400
C	-3.58617400	-0.66171000	-0.00966100
C	-2.91403400	-2.91610800	0.02143500
H	-2.06488000	-3.59001200	0.02999500
C	-4.22923700	-3.36371200	0.03073500
H	-4.43424000	-4.42865500	0.04638800
C	-5.25089700	-2.41606600	0.02025900
H	-6.29299800	-2.72360000	0.02771200
C	-4.93182300	-1.06307500	0.00003000
H	-5.71119200	-0.31713100	-0.00845300
C	-3.89581700	1.85485700	-0.05753700

C	-3.39916500	3.14782800	-0.08804600
H	-4.06249100	4.00346800	-0.10603200
C	-2.01817200	3.28092300	-0.09319800
C	-1.15801300	2.18954000	-0.06770300
H	-0.09778900	2.40152200	-0.06562200
F	-5.24793300	1.73671700	-0.05296200
F	-1.49393300	4.52262800	-0.12545000

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Complex 1b, excited state, gas phase

Pt	0.63660400	-0.85515500	-0.00174000
Cl	-0.30457200	-3.11874200	-0.05889800
P	-1.52175200	0.03589500	-0.00214600
N	2.57854100	-1.61263800	-0.00289500
C	-1.74500900	1.25978500	-1.36630100
C	-2.52036700	2.42160000	-1.24204200
H	-2.99811700	2.66289700	-0.29841000
C	-2.66879200	3.28931200	-2.32623200
H	-3.26314400	4.19193900	-2.21343300
C	-2.05455300	3.00194700	-3.54596900
H	-2.17125300	3.67909400	-4.38775000
C	-1.28220800	1.84571700	-3.67859100
H	-0.79501400	1.61888600	-4.62285100
C	-1.12038900	0.98332900	-2.59412900
H	-0.49906300	0.09734700	-2.69192700
C	-2.93660600	-1.12444200	-0.23333000
C	-3.69087300	-1.14718900	-1.41286000
H	-3.44819800	-0.47966600	-2.23230600
C	-4.76674500	-2.02960600	-1.54421900
H	-5.34341900	-2.03703500	-2.46520300
C	-5.09891300	-2.89116600	-0.50021200
H	-5.93655500	-3.57586800	-0.60298100
C	-4.34795200	-2.87455800	0.67848600
H	-4.59401300	-3.55027400	1.49283800
C	-3.27062000	-2.00262200	0.81081000
H	-2.68273500	-2.01209600	1.72259200
C	-1.98401100	0.89028100	1.56742500
C	-3.32412400	1.22435400	1.83578300
H	-4.10164900	0.96618800	1.12326600
C	-3.66900500	1.86534600	3.02509000
H	-4.70795100	2.11829100	3.21836100
C	-2.68452200	2.16813500	3.96928900
H	-2.95554200	2.66141000	4.89887200
C	-1.35605100	1.82322000	3.72055900
H	-0.58751900	2.04248400	4.45654900
C	-1.00591200	1.18617900	2.52787500
H	0.02659300	0.91002300	2.34293700
C	1.63842800	0.87203000	0.02387200
C	3.12101300	0.68120100	0.04098700
C	3.60393800	-0.62843600	0.02113000
C	2.91166400	-2.90439800	-0.02542400
H	2.07825500	-3.59759100	-0.04346700
C	4.23378600	-3.35009700	-0.02596800
H	4.43207200	-4.41591300	-0.04412800
C	5.28862500	-2.39507500	-0.00220200

H	6.32521900	-2.71681400	-0.00289800
C	4.97493300	-1.06249500	0.02075600
H	5.75332200	-0.31425100	0.03814700
C	3.93615200	1.87463500	0.07489600
C	3.41680400	3.13095500	0.08283800
H	4.06237100	4.00107400	0.10700500
C	2.00317400	3.26988800	0.05690800
C	1.14767200	2.18131700	0.02906100
H	0.08708400	2.39151400	0.00481000
F	5.28646700	1.75265900	0.10069500
F	1.50477100	4.52224900	0.06149600

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Complex 1b, ground state, CH2Cl2 solution

Pt	0.62127800	-0.86321200	-0.00622700
Cl	-0.32293200	-3.17324700	-0.09621300
P	-1.51734000	0.05585700	0.00457100
N	2.61243400	-1.60337800	0.00964300
C	-1.74304200	1.21299700	-1.41433800
C	-2.49072600	2.39736700	-1.33594200
H	-2.94574500	2.70111100	-0.39975700
C	-2.64164200	3.21075800	-2.46168400
H	-3.21579800	4.12965600	-2.38484900
C	-2.05748100	2.84761500	-3.67663900
H	-2.17760100	3.48198300	-4.55022400
C	-1.31156600	1.66925900	-3.76348300
H	-0.84874800	1.38253600	-4.70340700
C	-1.14765600	0.86066100	-2.63812200
H	-0.54882000	-0.04356400	-2.70526500
C	-2.94159300	-1.10829500	-0.14985800
C	-3.62838000	-1.27865000	-1.35915900
H	-3.33989600	-0.71395400	-2.23906500
C	-4.69806100	-2.17482100	-1.44234500
H	-5.22358200	-2.29437600	-2.38561200
C	-5.09215200	-2.90503300	-0.32088600
H	-5.92620400	-3.59814100	-0.38606400
C	-4.40999100	-2.74027100	0.88861400
H	-4.70945100	-3.30599700	1.76637500
C	-3.33980000	-1.85172200	0.97370900
H	-2.81590400	-1.73743800	1.91760000
C	-1.92979700	0.96327500	1.55372100
C	-3.24464700	1.39991300	1.80253400
H	-4.03378800	1.19856400	1.08479900
C	-3.55332500	2.07544800	2.98294100
H	-4.57130400	2.41059300	3.15946900
C	-2.55989200	2.30872600	3.93835900
H	-2.80359300	2.82996900	4.85978900
C	-1.25855300	1.85881000	3.71100900
H	-0.48527800	2.02325100	4.45587200
C	-0.94374800	1.18863700	2.52621800
H	0.06726200	0.83347600	2.35814800
C	1.64683000	0.88232700	0.01548400
C	3.06868100	0.72295900	0.03820500
C	3.58662100	-0.64820700	0.04200400
C	2.93871700	-2.90781800	0.00859600



H	2.10279000	-3.59567700	-0.01869100
C	4.25725100	-3.34364200	0.03940800
H	4.47303300	-4.40615000	0.03710100
C	5.26933600	-2.38609000	0.07340000
H	6.31348400	-2.68280800	0.09927200
C	4.93491100	-1.03593200	0.07448000
H	5.70862200	-0.28477200	0.10138200
C	3.87239900	1.87367100	0.04862500
C	3.36458500	3.16328000	0.03833300
H	4.02056700	4.02484800	0.04612500
C	1.98345700	3.28277300	0.01422900
C	1.13169600	2.18426600	0.00226000
H	0.07022800	2.38685600	-0.02293600
F	5.22374200	1.76706600	0.06820800
F	1.44496700	4.52049100	0.00258700

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Complex 2a, ground state, gas phase

C	-3.43573600	-2.31018800	0.10618000
H	-2.69391500	-3.09980100	0.15987700
C	-4.80349000	-2.55672400	0.09445300
H	-5.16629500	-3.57778400	0.14118100
C	-5.67537300	-1.46975900	0.02202200
H	-6.75112800	-1.62232400	0.01019600
C	-5.15493100	-0.18240000	-0.03446400
H	-5.81989100	0.67133200	-0.08993900
C	-3.76680000	0.01379000	-0.01858800
C	-3.08308700	1.30912900	-0.06585900
C	-3.78612200	2.52307000	-0.13031900
H	-4.87243600	2.52811200	-0.15416000
C	-3.10521500	3.73486900	-0.16191600
H	-3.65503300	4.67056600	-0.21103800
C	-1.70958400	3.72879200	-0.12479100
H	-1.16097400	4.66770000	-0.14249600
C	-1.00704200	2.52316800	-0.06219600
H	0.07520900	2.57427900	-0.02651400
C	-1.65894100	1.27976900	-0.03467500
C	1.78216200	0.96213300	-1.53470000
C	0.86749600	1.03504100	-2.59165200
H	-0.11743800	0.59372800	-2.48581200
C	1.25435400	1.68535500	-3.76514200
H	0.56782900	1.75490800	-4.60442700
C	2.52892400	2.24161600	-3.83781600
H	2.87187400	2.75794600	-4.72939800
C	3.36938600	2.11796100	-2.72847200
H	4.37388300	2.53724200	-2.74493700
C	2.61658700	-1.30429000	0.00889600
C	2.93211800	-1.95801400	-1.19051800
H	2.43780700	-1.67451000	-2.11462500
C	3.87574000	-2.98296200	-1.20567600
H	4.11258200	-3.48128700	-2.14179200
C	4.50842800	-3.37207000	-0.02302600
H	5.24300000	-4.17288400	-0.03584500
C	4.18997200	-2.73285600	1.17514200
H	4.67292900	-3.03389600	2.10085600

C	3.24791200	-1.70319900	1.19345900
H	3.00784100	-1.21493300	2.13206200
C	1.82927900	1.08627900	1.44930100
C	3.07034900	1.74481100	1.50632800
H	3.75263800	1.67382700	0.66735400
C	3.41058800	2.49577500	2.63132900
H	4.36895000	3.00735400	2.66442300
C	2.53072600	2.58635200	3.71311200
H	2.80335000	3.16902500	4.58927600
C	1.30341100	1.92430900	3.66747200
H	0.61534900	1.98735100	4.50599200
C	0.95130700	1.17907700	2.54042800
H	-0.00681200	0.66989900	2.49935200
N	-2.93721000	-1.06362100	0.05074500
N	3.01537900	1.48812100	-1.60499500
Pt	-0.86887300	-0.58928600	0.05143200
Cl	-0.24351600	-2.96518000	0.17496200
P	1.34738800	0.02813500	0.02095200

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Complex 2a, excited state, gas phase

C	3.44334700	-2.29429300	-0.08701300
H	2.72132200	-3.10085200	-0.14912100
C	4.81426800	-2.53553000	-0.05773400
H	5.17460800	-3.55731700	-0.09834500
C	5.71106700	-1.43385400	0.02606200
H	6.78415500	-1.59730000	0.04928500
C	5.19613000	-0.16449700	0.07378900
H	5.85744300	0.69316400	0.13329700
C	3.78229100	0.05337300	0.04076500
C	3.12992400	1.29003000	0.07268200
C	3.80740100	2.55581400	0.16263700
H	4.88951100	2.58436300	0.24312800
C	3.09848700	3.72360100	0.13675900
H	3.62333700	4.67398600	0.19730400
C	1.66820900	3.71948000	0.02533700
H	1.12819400	4.66085400	-0.00509900
C	0.98371400	2.51281700	-0.03875400
H	-0.09646400	2.54964400	-0.12245500
C	1.63867000	1.26964900	-0.00284600
C	-1.79170500	1.02974700	1.49764800
C	-0.87723900	1.15883100	2.54923200
H	0.11384300	0.72782000	2.46307800
C	-1.27122300	1.85324400	3.69495000
H	-0.58454100	1.96633200	4.52933400
C	-2.55236000	2.39617000	3.74641500
H	-2.90070700	2.94538300	4.61593900
C	-3.39251400	2.21460200	2.64481400
H	-4.40235200	2.62108600	2.64502500
C	-2.59756900	-1.32428500	0.08383900
C	-2.85945400	-1.93577900	1.31813600
H	-2.34062900	-1.60627000	2.21323900
C	-3.78137400	-2.97668600	1.40543700
H	-3.97667800	-3.44211900	2.36767200
C	-4.44627600	-3.42299200	0.26118300

H	-5.16398600	-4.23606200	0.33022500
C	-4.18192300	-2.82489900	-0.97084100
H	-4.69028300	-3.17050500	-1.86685900
C	-3.26108500	-1.77993000	-1.06189300
H	-3.06250700	-1.32475200	-2.02635300
C	-1.87748200	1.00924200	-1.48950100
C	-3.13089700	1.64314400	-1.56107100
H	-3.80040600	1.60200400	-0.71010200
C	-3.49921300	2.33229500	-2.71628100
H	-4.46678300	2.82531300	-2.76040900
C	-2.63565800	2.38511100	-3.81361200
H	-2.93024000	2.91966400	-4.71299300
C	-1.39658600	1.74675700	-3.75347300
H	-0.72115400	1.77970500	-4.60384200
C	-1.01652100	1.06304200	-2.59688600
H	-0.04935700	0.57221600	-2.54739200
N	2.92226800	-1.06326000	-0.03964100
N	-3.03166800	1.54189500	1.54882900
Pt	0.89073500	-0.57191700	-0.05594500
Cl	0.25360100	-2.93336000	-0.21441800
P	-1.35704600	0.03030800	-0.01858300

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Complex 2a, ground state, CH2Cl2 solution

C	3.43573600	-2.31018800	-0.10618000
H	2.69391500	-3.09980100	-0.15987700
C	4.80349000	-2.55672400	-0.09445300
H	5.16629500	-3.57778400	-0.14118100
C	5.67537300	-1.46975900	-0.02202200
H	6.75112800	-1.62232400	-0.01019600
C	5.15493100	-0.18240000	0.03446400
H	5.81989100	0.67133200	0.08993900
C	3.76680000	0.01379000	0.01858800
C	3.08308700	1.30912900	0.06585900
C	3.78612200	2.52307000	0.13031900
H	4.87243600	2.52811200	0.15416000
C	3.10521500	3.73486900	0.16191600
H	3.65503300	4.67056600	0.21103800
C	1.70958400	3.72879200	0.12479100
H	1.16097400	4.66770000	0.14249600
C	1.00704200	2.52316800	0.06219600
H	-0.07520900	2.57427900	0.02651400
C	1.65894100	1.27976900	0.03467500
C	-1.78216200	0.96213300	1.53470000
C	-0.86749600	1.03504100	2.59165200
H	0.11743800	0.59372800	2.48581200
C	-1.25435400	1.68535500	3.76514200
H	-0.56782900	1.75490800	4.60442700
C	-2.52892400	2.24161600	3.83781600
H	-2.87187400	2.75794600	4.72939800
C	-3.36938600	2.11796100	2.72847200
H	-4.37388300	2.53724200	2.74493700
C	-2.61658700	-1.30429000	-0.00889600
C	-2.93211800	-1.95801400	1.19051800
H	-2.43780700	-1.67451000	2.11462500

C	-3.87574000	-2.98296200	1.20567600
H	-4.11258200	-3.48128700	2.14179200
C	-4.50842800	-3.37207000	0.02302600
H	-5.24300000	-4.17288400	0.03584500
C	-4.18997200	-2.73285600	-1.17514200
H	-4.67292900	-3.03389600	-2.10085600
C	-3.24791200	-1.70319900	-1.19345900
H	-3.00784100	-1.21493300	-2.13206200
C	-1.82927900	1.08627900	-1.44930100
C	-3.07034900	1.74481100	-1.50632800
H	-3.75263800	1.67382700	-0.66735400
C	-3.41058800	2.49577500	-2.63132900
H	-4.36895000	3.00735400	-2.66442300
C	-2.53072600	2.58635200	-3.71311200
H	-2.80335000	3.16902500	-4.58927600
C	-1.30341100	1.92430900	-3.66747200
H	-0.61534900	1.98735100	-4.50599200
C	-0.95130700	1.17907700	-2.54042800
H	0.00681200	0.66989900	-2.49935200
N	2.93721000	-1.06362100	-0.05074500
N	-3.01537900	1.48812100	1.60499500
Pt	0.86887300	-0.58928600	-0.05143200
Cl	0.24351600	-2.96518000	-0.17496200
P	-1.34738800	0.02813500	-0.02095200