

## **Enhancing the blue phosphorescence of iridium complexes of dicyclopentylphosphite ligand via aza-substitution: a density functional theory investigation**

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**Electronic Supporting information**

XYZ coordinates of the optimized T<sub>1</sub> structure for **1**

Ir	-0.45988100	-1.18505900	0.05866600	C	-6.93710500	2.15217400	-0.35751300
P	0.45819300	0.92053600	-0.13882000	H	-5.78936200	3.95946900	-0.11702900
P	-2.56976000	-0.67523100	0.09014900	H	-7.80852200	0.20279800	-0.63373500
O	-3.44238300	-2.03524200	-0.02322200	H	-7.89261400	2.64423700	-0.20867100
C	1.23973300	-2.16505700	-2.30358600	H	-1.29988600	-1.84623500	-5.16522000
C	1.65372400	-2.51136100	-3.64639100	C	4.96689800	-2.48245700	0.77524100
H	2.67515600	-2.85203900	-3.77980700	F	5.63002100	-1.33285300	0.55117800
C	0.77181000	-2.40702200	-4.67108100	F	4.92077900	-2.67283300	2.09317100
H	1.05377600	-2.66354800	-5.68553700	F	5.67750400	-3.46773600	0.22826900
C	-0.55578600	-1.94355900	-4.38502600	O	1.25991400	1.22876200	-1.52095900
C	-0.90260300	-1.59637800	-3.06113000	O	-0.61558500	2.13916500	-0.00721200
C	-1.27760700	-3.06611500	0.29741500	O	1.56239500	1.22210000	1.00388700
C	-0.56785400	-4.24488900	0.53091000	C	2.50687800	1.85298800	-1.56726700
H	0.51332300	-4.20268500	0.63668700	C	3.63223900	1.12404800	-1.19740300
C	-1.21615600	-5.47615600	0.64139500	C	2.59817400	3.16852900	-2.00370500
H	-0.63669300	-6.37610000	0.82333700	C	4.87953300	1.73669300	-1.24573400
C	-2.60073600	-5.55357600	0.52769500	H	3.52618500	0.09669400	-0.86411300
H	-3.10681400	-6.50959100	0.61684300	C	3.85547600	3.76821400	-2.05084900
C	-3.34558100	-4.39703100	0.30831600	H	1.70185700	3.70599900	-2.29676000
H	-4.42707000	-4.41893400	0.22670100	C	4.99337500	3.06126600	-1.66796900
C	-2.66773800	-3.19403300	0.20117400	H	5.75669800	1.17174300	-0.94760900
C	-0.70578600	-0.76552000	2.04970600	H	3.94046100	4.79634500	-2.38834900
C	0.26485500	-0.93966100	3.03992100	H	5.96745200	3.53825800	-1.70473300
C	-1.92380300	-0.21187300	2.46767700	C	-0.56860300	3.31894000	-0.74257700
C	0.02047700	-0.57207600	4.36444100	C	-1.02669700	3.29188100	-2.05656300
H	1.23172600	-1.35162000	2.76545200	C	-0.11727700	4.49186100	-0.14876300
C	-2.19537800	0.16878400	3.77264000	C	-1.00369100	4.46538700	-2.80434800
C	-1.20190800	-0.01569900	4.73205600	H	-1.38716400	2.35445100	-2.46967900
H	0.79578200	-0.71559300	5.11048000	C	-0.10117400	5.65839000	-0.91105300
H	-3.16333400	0.59217700	4.01844800	H	0.21251400	4.48666600	0.88497200
H	-1.38914600	0.27221800	5.76175500	C	-0.53366700	5.64856700	-2.23547300
H	-1.90221800	-1.22367700	-2.84519300	H	-1.35234500	4.45322400	-3.83196400
N	-0.08061400	-1.68395700	-2.04548300	H	0.25489600	6.57990900	-0.46159600
N	1.54993100	-1.89214300	0.06859200	H	-0.51381400	6.56181900	-2.82114800
C	2.04922600	-2.24557400	-1.19977300	C	1.63065900	2.37633900	1.77636900
C	3.59315500	-2.40006400	0.17890900	C	2.66368300	3.27943500	1.55681300
N	2.53299000	-1.98388700	0.93185300	C	0.67452400	2.57455000	2.76704100
N	3.37628100	-2.58140300	-1.10633200	C	2.72111500	4.42687500	2.34574800
O	-2.93913900	-0.01266400	1.51405000	H	3.39686500	3.08271300	0.78063500
C	-4.50983100	0.89967400	-0.73557500	C	0.74576200	3.72722200	3.54294700
C	-4.52779500	2.26584000	-0.49367500	H	-0.10815700	1.83598400	2.91199900
C	-5.67018900	0.13981900	-0.79232300	C	1.76302400	4.65752300	3.33144700
C	-5.75674700	2.89153700	-0.30693000	H	3.51984400	5.14388000	2.18446900
H	-3.58947900	2.81029500	-0.45393100	H	0.00208000	3.89359600	4.31574100
C	-6.89091400	0.78090200	-0.59657600	H	1.81309000	5.55546900	3.93891300
H	-5.60629800	-0.92646200	-0.98036500	O	-3.26613600	0.29950700	-0.97425000

XYZ coordinates of the optimized T<sub>1</sub> structure for **2a**

Ir	-0.15325600	0.19402000	0.22349200	C	4.22494900	0.21333800	-0.200367
P	0.42443200	-1.34277500	-1.51232000	C	4.79759700	2.88826200	-0.770031
P	1.81218500	0.77905400	1.02974200	H	2.96407400	3.34218800	0.271220
O	1.57523200	2.09685200	1.95637600	C	5.38575200	0.54831600	-0.891193
C	-1.91879900	1.74763400	-1.75914900	H	4.01163900	-0.82589800	0.036671
C	-2.36455100	2.71257800	-2.72035800	C	5.67019200	1.88131600	-1.178510
H	-3.40346200	2.66882100	-3.03110100	H	5.02708300	3.92785100	-0.981065
C	-1.48960900	3.63465800	-3.20940100	H	6.06839600	-0.23748400	-1.199859
H	-1.80425300	4.37450700	-3.93674300	H	6.57760000	2.13810600	-1.716471
C	-0.13937400	3.60908700	-2.73815000	C	2.05366900	-2.16585600	-1.435960
C	0.23647200	2.65680400	-1.78965200	C	3.04960600	-1.94268500	-2.390497
C	-0.75221600	1.52752800	1.67795400	C	2.32249600	-3.01482400	-0.352702
C	-2.06692100	1.76725300	2.08490100	C	4.29785200	-2.54999600	-2.263163
H	-2.87514700	1.18247900	1.65331500	H	2.86345200	-1.28600000	-3.234903
C	-2.37136500	2.73365200	3.04550900	C	3.57357000	-3.60903900	-0.221716
H	-3.40509100	2.89618700	3.33588300	H	1.55813600	-3.20651700	0.396270
C	-1.35871800	3.48351200	3.63470800	C	4.56506600	-3.37613200	-1.175284
H	-1.59175600	4.23375200	4.38385500	H	5.06224000	-2.37015700	-3.013214
C	-0.03347000	3.26241900	3.26802300	H	3.77218600	-4.25424300	0.628481
H	0.78533600	3.81552300	3.71613800	H	5.53997100	-3.84244400	-1.071198
C	0.23047500	2.29808300	2.30853600	C	0.34080700	-0.63419200	-3.200666
C	0.09644400	-1.28762300	1.60163300	H	0.54120100	-1.38780000	-3.967771
C	-0.83517200	-2.28609000	1.90540300	H	-0.66609300	-0.22756500	-3.339509
C	1.32132700	-1.37390400	2.28017900	H	1.04755700	0.19454100	-3.296869
C	-0.53797600	-3.31892200	2.79852400	C	-0.72746400	-2.76758400	-1.609553
H	-1.80994000	-2.25627300	1.42550200	H	-1.73564200	-2.39774900	-1.816106
C	1.64417000	-2.37858200	3.17938500	H	-0.41457500	-3.47018800	-2.386568
C	0.69930500	-3.37026900	3.43405300	H	-0.74927000	-3.27016500	-0.638300
H	-1.28327000	-4.08262300	3.00087200	H	0.59504900	4.31992000	-3.096454
H	2.61878200	-2.37690700	3.65646900	C	-6.00428400	-1.21113100	0.872240
H	0.92980900	-4.17015300	4.13075300	H	-6.19063800	-0.16187000	1.123124
H	1.26199700	2.62639200	-1.42690100	H	-6.93926400	-1.76712400	1.002488
N	-0.58229900	1.74475600	-1.28986500	H	-5.25954600	-1.60699600	1.568097
N	-2.17265500	-0.17354400	-0.31051300	C	-5.26841100	-2.82849200	-0.902107
C	-2.72035300	0.75198000	-1.23917300	H	-6.19947900	-3.39401600	-0.787001
C	-4.22877800	-0.60073100	-0.71580300	H	-4.91874400	-2.95163400	-1.932908
N	-3.12199100	-1.01600800	0.01452700	H	-4.51644300	-3.24778000	-0.228030
N	-4.03043800	0.45618800	-1.48186400	C	-6.56562600	-0.76685300	-1.541031
O	2.31394100	-0.42974400	1.99861900	H	-6.74053500	0.29219800	-1.333934
C	-5.52392000	-1.34566400	-0.58413600	H	-6.23367200	-0.85213400	-2.579746
C	3.34698500	1.22277600	0.20430700	H	-7.51009600	-1.30951400	-1.428177
C	3.63563200	2.56278200	-0.07716900				

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XYZ coordinates of the optimized T<sub>1</sub> structure for **2c**

Ir	-0.16035200	0.18981500	0.21743800	C	5.40638900	0.54927300	-0.83976400
P	0.42911500	-1.34012400	-1.52306000	H	4.02680700	-0.83254100	0.06891000
P	1.81289800	0.76418700	1.03790600	C	5.68878900	1.88416800	-1.12017000
O	1.56500900	2.06919700	1.98468300	H	5.03664900	3.92816400	-0.92491900
C	-1.91485900	1.74585700	-1.76192900	H	6.09603700	-0.23280500	-1.14191900
C	-2.35638600	2.71290200	-2.72208200	H	6.60160600	2.14557600	-1.64651400
H	-3.39541800	2.67366400	-3.03299500	C	2.06098000	-2.15594300	-1.44460000
C	-1.47772000	3.63234200	-3.21017300	C	3.06357100	-1.91177600	-2.38685200
H	-1.78953600	4.37412800	-3.93659000	C	2.32414000	-3.02426000	-0.37553300
C	-0.12804700	3.60186900	-2.73854700	C	4.31222000	-2.51852000	-2.26079900
C	0.24475700	2.64916300	-1.79071300	H	2.88238900	-1.24046000	-3.22073700
C	-0.76355600	1.52075200	1.66261200	C	3.57545700	-3.61794100	-0.24492300
C	-2.06775100	1.80342900	2.06841000	H	1.55335500	-3.23644200	0.36106100
H	-2.91062100	1.26161400	1.64823400	C	4.57322600	-3.36419300	-1.18649600
C	-2.30045700	2.78492300	3.03336000	H	5.08157100	-2.32360600	-3.00189600
H	-3.31852300	3.00873700	3.34571200	H	3.76819500	-4.28056500	0.59301400
C	-0.08358800	3.23027600	3.26559700	H	5.54809500	-3.83075900	-1.08412300
H	0.71238000	3.79212000	3.74921900	C	0.34584900	-0.61917600	-3.20524600
C	0.21934400	2.27365300	2.30968800	H	0.55605900	-1.36709400	-3.97519600
C	0.07123900	-1.29046200	1.58856700	H	-0.66384100	-0.22047200	-3.34639900
C	-0.84696900	-2.29220300	1.91483400	H	1.04622100	0.21577200	-3.29349300
C	1.29300200	-1.38792800	2.26742100	C	-0.72368000	-2.76277800	-1.62528600
C	-0.49183500	-3.29763300	2.81643800	H	-1.73154600	-2.39015400	-1.82837000
H	-1.83393600	-2.29489900	1.46026600	H	-0.41289100	-3.46111900	-2.40686200
C	1.57228300	-2.41166100	3.15909100	H	-0.74565500	-3.27255800	-0.65786800
H	-1.20319700	-4.08573600	3.05611300	H	0.60851900	4.31076200	-3.09618300
H	2.54000100	-2.45368100	3.65439900	C	-5.99812900	-1.18955300	0.89515900
H	1.26988400	2.61533600	-1.42697500	H	-6.17861000	-0.13841800	1.14238800
N	-0.57829000	1.73879400	-1.29181500	H	-6.93510900	-1.74024500	1.03207400
N	-2.17011400	-0.17281200	-0.31328800	H	-5.25278900	-1.58665700	1.58967500
C	-2.71927400	0.75229200	-1.24152600	C	-5.27830500	-2.81892000	-0.87552700
C	-4.22946200	-0.59446700	-0.70527700	H	-6.21166100	-3.37897400	-0.75378400
N	-3.11901200	-1.01109000	0.02213100	H	-4.93393500	-2.94880000	-1.90725900
N	-4.03049100	0.45870200	-1.47642000	H	-4.52621700	-3.23949600	-0.20239000
O	2.29894000	-0.46080400	1.99839700	C	-6.57070700	-0.75470300	-1.51750300
C	-5.52631300	-1.33339300	-0.56342300	H	-6.74030700	0.30601500	-1.31465500
C	3.35391800	1.21409400	0.23373300	H	-6.24539700	-0.84698000	-2.55771200
C	3.63957900	2.55637500	-0.04086200	H	-7.51660600	-1.29275700	-1.39627900
C	4.23910400	0.20793100	-0.16339300	N	0.69099500	-3.37637800	3.42890900
C	4.80809700	2.88735400	-0.71952800	N	-1.33998600	3.49412500	3.62639800
H	2.96221900	3.33325200	0.30202900				

XYZ coordinates of the optimized T<sub>1</sub> structure for **2d**

Ir	-0.15674000	0.17368200	0.20811300	C	5.41484800	0.59663600	-0.78277800
P	0.44817700	-1.33277500	-1.54243200	H	4.03905200	-0.80930200	0.09274000
P	1.79696300	0.75385400	1.05450000	C	5.68786000	1.93754400	-1.04274700
O	1.53439600	2.04392200	2.02545300	H	5.01421900	3.97258300	-0.82891300
C	-1.90834600	1.77362000	-1.73632500	H	6.11427700	-0.17522900	-1.08861800
C	-2.35101200	2.76938400	-2.66395300	H	6.60335400	2.21407800	-1.55663100
H	-3.39380100	2.74768300	-2.96389300	C	2.09459000	-2.12108300	-1.47195500
C	-1.46919300	3.69394500	-3.13756400	C	3.09423400	-1.85316000	-2.41055700
H	-1.78229500	4.45815600	-3.83974200	C	2.37139600	-2.99286900	-0.40909900
C	-0.11413600	3.63705500	-2.68352200	C	4.35258000	-2.44070900	-2.28795900
C	0.25863500	2.65801400	-1.76476500	H	2.90243600	-1.17917900	-3.23996900
C	-0.77864600	1.48448000	1.66944100	C	3.63147200	-3.56838800	-0.28263000
C	-2.09295800	1.74557300	2.06485600	H	1.60365700	-3.22084000	0.32597900
H	-2.91338800	1.18783700	1.61695900	C	4.62607900	-3.29165200	-1.22095100
C	-1.48675700	3.34330100	3.57957200	H	5.11952400	-2.22745100	-3.02656600
H	-1.80326100	4.06977900	4.32504300	H	3.83399400	-4.23516600	0.54971200
C	-0.13253500	3.17944600	3.30001100	H	5.60777400	-3.74454900	-1.12217400
H	0.63646700	3.74942700	3.80879400	C	0.34974800	-0.59831300	-3.21785400
C	0.18859200	2.23786500	2.33730500	H	0.57236800	-1.33367300	-3.99640100
C	0.08297000	-1.32595600	1.56816900	H	-0.66758700	-0.21702700	-3.35297000
C	-0.82778900	-2.34674100	1.86243500	H	1.03306300	0.25155800	-3.29797200
C	1.29321800	-1.41245700	2.26705700	C	-0.67773100	-2.77581400	-1.65438600
H	-1.80099800	-2.34657200	1.37573600	H	-1.69762100	-2.41855500	-1.82133600
C	1.56762700	-2.43185400	3.16318100	H	-0.37300600	-3.44580100	-2.46275900
C	0.57378600	-3.39203200	3.33808500	H	-0.66592900	-3.31455300	-0.70274000
H	2.51399000	-2.47459700	3.69043500	H	0.62601100	4.34667600	-3.03249500
H	0.73510100	-4.22236900	4.02246300	C	-5.29314000	-2.80282700	-0.91269200
H	1.28729100	2.60466700	-1.41319300	H	-4.53874900	-3.23774000	-0.25148100
N	-0.56900300	1.74362600	-1.27806000	H	-6.23083500	-3.35462200	-0.78671800
N	-2.15879100	-0.18737600	-0.34390000	H	-4.96126800	-2.92538000	-1.94950100
C	-2.71424600	0.76832200	-1.23830100	C	-5.97688000	-1.18546700	0.88373700
C	-4.22349500	-0.58834000	-0.72711900	H	-6.13837300	-0.13498500	1.14614100
N	-3.10665100	-1.03260800	-0.02596400	H	-6.92006100	-1.72471600	1.02387800
N	-4.02730200	0.48746200	-1.46843100	H	-5.22952600	-1.60206400	1.56447500
O	2.28597300	-0.47143000	2.02038800	C	-6.57319200	-0.71848900	-1.51776900
C	-5.52403800	-1.31865100	-0.58253900	H	-6.26088400	-0.80149400	-2.56289500
C	3.34540500	1.22857600	0.27819100	H	-7.52275000	-1.24903900	-1.39215700
C	3.62134200	2.57678700	0.02363900	H	-6.73020200	0.34118900	-1.29999500
C	4.24380300	0.23603500	-0.12325700	N	-2.45405700	2.64699800	2.98583700
C	4.79372700	2.92722300	-0.63841000	N	-0.59884400	-3.36316900	2.70702200
H	2.93250900	3.34304900	0.36749600				

XYZ coordinates of the optimized T<sub>1</sub> structure for **2b**

Ir	-0.16155400	0.19217100	0.22917900	C	5.37903200	0.55437100	-0.90721300
P	0.40737900	-1.35419900	-1.50506000	H	4.01859300	-0.83722400	0.01550100
P	1.81851100	0.75079600	1.03699900	C	5.65577200	1.89235000	-1.17840300
O	1.59119500	2.04442000	1.99510600	H	5.00845700	3.93398500	-0.94569700
C	-1.91810600	1.74050100	-1.76030000	H	6.06501400	-0.22371500	-1.22765900
C	-2.35710700	2.69895800	-2.73202800	H	6.55958800	2.16005300	-1.71707300
H	-3.39543900	2.65733300	-3.04495100	C	2.03962400	-2.17124100	-1.43819700
C	-1.47642600	3.61195900	-3.22736400	C	3.02621100	-1.94947000	-2.40289200
H	-1.78570300	4.34640200	-3.96239400	C	2.32356000	-3.01014800	-0.35129900
C	-0.12763200	3.58494800	-2.75288000	C	4.27876600	-2.54881800	-2.28063300
C	0.24302500	2.63932100	-1.79516800	H	2.82923500	-1.30102800	-3.25114200
C	-0.73851800	1.53398900	1.67350000	C	3.57982300	-3.59315800	-0.22223700
C	-2.03648800	1.83131500	2.07693400	H	1.56582800	-3.20663400	0.40277800
H	-2.87627800	1.28630700	1.65225800	C	4.56097400	-3.36220800	-1.18676200
C	-2.26903500	2.82472500	3.03352100	H	5.03587200	-2.37087000	-3.03839500
H	-3.27637900	3.06798200	3.35422000	H	3.79110300	-4.22241200	0.63636400
C	-1.18246400	3.49767000	3.56941900	H	5.54060300	-3.81880200	-1.08502200
H	-1.31617500	4.27964500	4.31243300	C	0.30371800	-0.65511000	-3.19554400
C	0.25107900	2.28998300	2.32545600	H	0.49808600	-1.41362100	-3.95923400
C	0.07801100	-1.28452200	1.60365500	H	-0.70513500	-0.25119100	-3.32751000
C	-0.85390500	-2.26040700	1.94979300	H	1.00866100	0.17355600	-3.30412300
C	1.31877600	-1.41804200	2.26017600	C	-0.74461700	-2.78030400	-1.57910500
C	-0.50865800	-3.28125900	2.84302200	H	-1.75724700	-2.41228600	-1.76659000
H	-1.84764700	-2.22794200	1.50908800	H	-0.44561000	-3.48311000	-2.36130400
C	0.76885300	-3.29327400	3.38134400	H	-0.74696100	-3.28464200	-0.60852100
H	-1.22348800	-4.05147800	3.11369600	H	0.61037000	4.28974300	-3.11548600
H	1.08268200	-4.07186600	4.07220000	C	-6.01795400	-1.18434700	0.89997000
H	1.26775000	2.60759100	-1.43017500	H	-6.20150200	-0.13376400	1.14745100
N	-0.58128000	1.73567600	-1.28931300	H	-6.95472700	-1.73671900	1.03181800
N	-2.18160200	-0.16302200	-0.29311700	H	-5.27529100	-1.58072800	1.59777300
C	-2.72459300	0.75353500	-1.23263800	C	-5.28694500	-2.81028500	-0.86875200
C	-4.24008500	-0.58589700	-0.69200700	H	-6.21989000	-3.37226000	-0.75217800
N	-3.13497800	-0.99676600	0.04492600	H	-4.93744000	-2.93795000	-1.89902000
N	-4.03630400	0.45998200	-1.47119300	H	-4.53683600	-3.23034900	-0.19302000
O	2.31638500	-0.48496000	1.97008400	C	-6.57794300	-0.74715200	-1.51479500
C	-5.53786200	-1.32544600	-0.55573000	H	-6.74954900	0.31330500	-1.31210100
C	3.34464500	1.20620300	0.20704500	H	-6.24662600	-0.83788600	-2.55318700
C	3.62603100	2.55181400	-0.05485800	H	-7.52406200	-1.28620800	-1.39929700
C	4.22380400	0.20498900	-0.21435300	N	1.68747400	-2.36020000	3.09567800
C	4.78248000	2.89065600	-0.75037700	N	0.08366000	3.23200100	3.22235700
H	2.95695400	3.32406100	0.31398600				

XYZ coordinates of the optimized T<sub>1</sub> structure for **2e**

Ir	-0.14263400	0.13661100	0.15919200	H	6.18626200	0.07750200	-0.78916600
P	0.58187900	-1.21910100	-1.66767700	H	6.58924900	2.49041600	-1.22212600
P	1.72755200	0.78414000	1.12086000	C	2.21309100	-2.02806800	-1.51781100
O	1.34999400	2.02469500	2.11873300	C	3.29887300	-1.67069600	-2.32195800
C	-1.97056500	1.82499100	-1.62230800	C	2.39425300	-2.99471100	-0.51718900
C	-2.46649200	2.88242800	-2.43644600	C	4.54700500	-2.25995600	-2.12646000
H	-3.52205900	2.86818600	-2.68950800	H	3.18186000	-0.92374000	-3.10105900
C	-1.62071300	3.85939100	-2.87642000	C	3.64463000	-3.57018500	-0.31508300
H	-1.97647400	4.67197000	-3.49930400	H	1.55665600	-3.30140200	0.10491900
C	-0.24209100	3.78600300	-2.49300000	C	4.72500200	-3.20204900	-1.11753800
C	0.18279200	2.74735300	-1.67725600	H	5.38095000	-1.97558800	-2.76124900
C	-0.91382800	1.35181700	1.62724900	H	3.77181100	-4.31070900	0.46849100
C	-2.66065800	2.34894300	2.75083100	H	5.69890100	-3.65562300	-0.96112000
H	-3.73983800	2.41225900	2.86917500	C	0.63479200	-0.34365600	-3.27536300
C	-1.82133600	3.13832600	3.52634100	H	0.92163300	-1.00974000	-4.09424800
H	-2.22969100	3.82300800	4.26148600	H	-0.36652200	0.05814600	-3.46014700
C	-0.01559600	2.13829600	2.37208100	H	1.32369600	0.50371500	-3.22110500
C	0.14548200	-1.45272900	1.38788500	C	-0.57087400	-2.61150100	-1.96885300
C	1.31267200	-1.48398300	2.18370400	H	-1.50556500	-2.20157800	-2.36231600
C	-0.39239100	-3.55054600	2.19827800	H	-0.15155800	-3.33386500	-2.67387600
C	0.72810300	-3.62248500	3.01591400	H	-0.80147900	-3.08353900	-1.00838900
H	-1.10467100	-4.37221700	2.16617500	H	0.47213100	4.53268300	-2.81895900
H	0.90753900	-4.49282000	3.63773400	C	-5.79815900	-1.41546000	1.00881200
H	1.22610500	2.68074400	-1.37263100	H	-5.91857200	-0.39738100	1.39254000
N	-0.61406700	1.77985600	-1.22767600	H	-6.73097400	-1.96433900	1.18065100
N	-2.11821700	-0.27857300	-0.42588700	H	-4.99166200	-1.89984800	1.56561700
C	-2.74172000	0.76239000	-1.16812900	C	-5.29269100	-2.83772400	-0.99677100
C	-4.19615300	-0.65077600	-0.68171700	H	-6.21514700	-3.40598400	-0.83365500
N	-3.02953400	-1.15440600	-0.11905400	H	-5.06572000	-2.85352500	-2.06825500
N	-4.06103200	0.49649300	-1.33138400	H	-4.47535700	-3.32760500	-0.46102100
O	2.22026100	-0.43854700	2.08969600	C	-6.60898600	-0.70592000	-1.26832200
C	-5.48331900	-1.39553600	-0.49882400	H	-6.73818400	0.32515900	-0.92866800
C	3.29590100	1.34970900	0.45096900	H	-6.39117100	-0.67777100	-2.33993800
C	3.52028400	2.70961600	0.21237500	H	-7.54731600	-1.24947600	-1.11435800
C	4.25636300	0.40108200	0.09020600	C	1.61907600	-2.54950600	3.00402700
C	4.70704400	3.11554100	-0.38997300	H	2.52732200	-2.53929100	3.59781500
H	2.77837700	3.44164800	0.51873900	C	-0.44509700	3.03333300	3.33060200
C	5.43980700	0.81583000	-0.51259900	H	0.26974100	3.62295800	3.89550800
H	4.08410900	-0.65276800	0.29364500	N	-0.67310300	-2.50600800	1.40794000
C	5.66368600	2.16945300	-0.75388500	N	-2.22450000	1.48148700	1.82938900
H	4.88895200	4.17053400	-0.56789900				

XYZ coordinates of the optimized S<sub>0</sub> structure for **1**

Ir	-0.436593	-1.185286	0.054547	C	-6.945530	2.114200	-0.331836
P	0.430593	0.936652	-0.117635	H	-5.872840	3.928173	-0.778547
P	-2.566359	-0.761692	0.080079	H	-7.738751	0.155050	0.077019
O	-3.378978	-2.151243	-0.113252	H	-7.895552	2.616530	-0.182725
C	1.222459	-2.105856	-2.331901	H	-1.312544	-1.837470	-5.171848
C	1.634235	-2.469510	-3.612457	C	5.011900	-2.391132	0.757661
H	2.652747	-2.813348	-3.752796	F	5.705220	-1.262325	0.497580
C	0.721757	-2.376810	-4.652050	F	4.991597	-2.546958	2.082178
H	1.010721	-2.654099	-5.660685	F	5.702610	-3.402406	0.225371
C	-0.570286	-1.924178	-4.387178	O	1.314689	1.212672	-1.454642
C	-0.902092	-1.579050	-3.085054	O	-0.671745	2.135872	-0.097984
C	-1.187121	-3.100866	0.265450	O	1.449379	1.294254	1.083123
C	-0.438924	-4.252600	0.515689	C	2.556251	1.853620	-1.440432
H	0.635341	-4.168161	0.659851	C	3.659428	1.159191	-0.956834
C	-1.042695	-5.508975	0.595264	C	2.659433	3.150599	-1.927018
H	-0.434799	-6.386768	0.792047	C	4.899749	1.787964	-0.950304
C	-2.418432	-5.639826	0.433055	H	3.539838	0.152260	-0.570117
H	-2.889085	-6.615734	0.497754	C	3.909804	3.766348	-1.916562
C	-3.200987	-4.511506	0.198737	H	1.777484	3.662052	-2.299518
H	-4.277510	-4.575317	0.080925	C	5.026588	3.093026	-1.426328
C	-2.567560	-3.282172	0.124363	H	5.760692	1.249926	-0.567552
C	-0.699897	-0.799323	2.043871	H	4.005929	4.779883	-2.292952
C	0.291501	-0.914950	3.020886	H	5.995375	3.582149	-1.418544
C	-1.948212	-0.331772	2.474324	C	-0.593370	3.295958	-0.859991
C	0.034961	-0.573776	4.350068	C	-0.933811	3.224153	-2.207751
H	1.279974	-1.260104	2.730049	C	-0.227756	4.495338	-0.260890
C	-2.232640	0.018908	3.785065	C	-0.879719	4.380288	-2.980936
C	-1.219499	-0.105640	4.733214	H	-1.226285	2.265999	-2.627322
H	0.825119	-0.670888	5.087926	C	-0.176785	5.643455	-1.048800
H	-3.224276	0.374240	4.043637	H	0.010648	4.521331	0.797176
H	-1.415958	0.160696	5.766973	C	-0.493225	5.589717	-2.404670
H	-1.893007	-1.215718	-2.827645	H	-1.137379	4.334117	-4.034208
N	-0.025221	-1.666896	-2.079011	H	0.114314	6.585148	-0.594380
N	1.599996	-1.829648	0.038307	H	-0.448698	6.489425	-3.009673
C	2.097356	-2.155619	-1.168905	C	1.448572	2.468001	1.827491
C	3.633942	-2.302330	0.188415	C	2.463095	3.396233	1.627652
N	2.591440	-1.915791	0.924073	C	0.447331	2.659026	2.773780
N	3.391014	-2.463407	-1.122883	C	2.453982	4.563681	2.388182
O	-2.982714	-0.191285	1.530058	H	3.234398	3.202669	0.888673
C	-4.529135	0.833095	-0.707827	C	0.452050	3.833022	3.521385
C	-4.588928	2.211708	-0.854341	H	-0.315215	1.897054	2.909400
C	-5.645637	0.075223	-0.378626	C	1.449038	4.788848	3.327266
C	-5.811099	2.850417	-0.667070	H	3.237956	5.299880	2.242003
H	-3.686246	2.759178	-1.106284	H	-0.325428	3.995524	4.260969
C	-6.858093	0.732070	-0.185685	H	1.448126	5.701644	3.914205

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H -5.559888 -1.001641 -0.276622 O -3.291693 0.226626 -0.951526

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XYZ coordinates of the optimized  $S_0$  structure for **2a**

Ir	-0.14003700	0.18233300	0.21158500	C	4.23127900	0.21049700	-0.23113700
P	0.40036300	-1.42668100	-1.45552300	C	4.80321400	2.88362900	-0.80798000
P	1.82456200	0.77965000	1.01141100	H	2.97984900	3.34079500	0.25026600
O	1.58513200	2.11327300	1.91685700	C	5.38733400	0.54301400	-0.93100400
C	-1.87310700	1.75022300	-1.75965100	H	4.01902400	-0.82750400	0.01068800
C	-2.34708700	2.69298200	-2.67355100	C	5.67123400	1.87525200	-1.22254400
H	-3.38794400	2.64315300	-2.97282600	H	5.03350400	3.92286100	-1.02021800
C	-1.47004700	3.64996000	-3.15699500	H	6.06668400	-0.24418200	-1.24332100
H	-1.81089300	4.39666100	-3.86723800	H	6.57490300	2.13038400	-1.76750900
C	-0.14438200	3.64101200	-2.72087500	C	2.05416600	-2.20131700	-1.40932500
C	0.24814800	2.67240300	-1.80886700	C	3.01477000	-1.98334100	-2.40036700
C	-0.74286300	1.54286800	1.64135000	C	2.37732400	-3.00954800	-0.30956400
C	-2.05925600	1.78181000	2.04463100	C	4.28116700	-2.55656800	-2.29375000
H	-2.86374600	1.18606800	1.62074100	H	2.78493100	-1.36076000	-3.25984800
C	-2.36426300	2.75953700	2.99381200	C	3.64524600	-3.57126400	-0.20067900
H	-3.39783200	2.92181900	3.28480000	H	1.64152100	-3.19391900	0.46931800
C	-1.35292900	3.51958600	3.57284700	C	4.60098500	-3.34457100	-1.19159000
H	-1.58791300	4.27828400	4.31292000	H	5.01828900	-2.38171100	-3.07174400
C	-0.02662500	3.29708400	3.21043100	H	3.88555400	-4.18593200	0.66116000
H	0.79065300	3.85650400	3.65357100	H	5.58894700	-3.78637800	-1.10517200
C	0.23921600	2.32047100	2.26373700	C	0.22367400	-0.80922500	-3.17243200
C	0.09810700	-1.25600700	1.62777700	H	0.42902300	-1.59098800	-3.90947100
C	-0.85640300	-2.21978700	1.96582600	H	-0.80942000	-0.46594300	-3.28930800
C	1.32212200	-1.33775000	2.30719700	H	0.88598300	0.04488100	-3.34009000
C	-0.57672700	-3.22515000	2.89491100	C	-0.71369000	-2.88145500	-1.43580000
H	-1.83045200	-2.18181800	1.48303400	H	-1.74678500	-2.53842500	-1.54044300
C	1.62655400	-2.31744600	3.23990000	H	-0.45294800	-3.57686800	-2.23830700
C	0.66153400	-3.27959000	3.52911800	H	-0.62723800	-3.38153800	-0.46736100
H	-1.33723300	-3.96506000	3.12659700	H	0.57440900	4.36920900	-3.07776700
H	2.60090100	-2.31765700	3.71752400	C	-5.45278900	-2.55066100	0.32913800
H	0.87641300	-4.05895200	4.25356500	H	-5.14004100	-2.26248100	1.33688700
H	1.27077800	2.61833100	-1.44600300	H	-6.43095200	-3.04030300	0.39199800
N	-0.59281200	1.74631600	-1.33507400	H	-4.72465100	-3.27399200	-0.05094700
N	-2.16586200	-0.17298900	-0.34139500	C	-6.57019100	-0.33187900	-0.03121100
C	-2.70557900	0.69208900	-1.21257700	H	-6.62115100	0.55805300	-0.66530600
C	-4.20582300	-0.64067500	-0.67840200	H	-7.56414800	-0.79202800	0.01157800
N	-3.12594600	-1.03484600	0.01077500	H	-6.29252700	-0.01725300	0.98045700
N	-3.99018300	0.43884600	-1.46068700	C	-5.97158500	-1.76298200	-1.99796100
O	2.32752600	-0.41407300	1.99760000	H	-5.26168100	-2.48677900	-2.41332200
C	-5.54407900	-1.32990500	-0.58840800	H	-6.96170600	-2.23204300	-1.96738400
C	3.35702400	1.22077200	0.17880100	H	-6.01168500	-0.89918800	-2.66770200
C	3.64614200	2.56019900	-0.10567200				

XYZ coordinates of the optimized  $S_0$  structure for **2c**

Ir	-0.15017800	0.18599000	0.20528300	C	5.40647700	0.49690900	-0.87377900
P	0.38811200	-1.43556800	-1.45332700	H	4.01529900	-0.86525400	0.04545100
P	1.82451800	0.76207300	1.02282700	C	5.70527500	1.82764400	-1.15725000
O	1.58187600	2.09428000	1.93474500	H	5.08294600	3.88033200	-0.95680800
C	-1.84166800	1.75167100	-1.78967700	H	6.08296400	-0.29508400	-1.17984900
C	-2.29476800	2.68904900	-2.71974500	H	6.61803300	2.07644900	-1.68971600
H	-3.33303300	2.64821300	-3.02926400	C	2.04078800	-2.21043600	-1.40435100
C	-1.40153900	3.62974700	-3.20503800	C	3.00430300	-1.98429800	-2.39073800
H	-1.72659900	4.37213400	-3.92706600	C	2.35934400	-3.03028500	-0.31212200
C	-0.08012900	3.61134100	-2.75542400	C	4.26853400	-2.56260800	-2.28673500
C	0.29227200	2.64991600	-1.82814000	H	2.77820200	-1.35313500	-3.24494200
C	-0.75036100	1.55957400	1.61401500	C	3.62467500	-3.59837000	-0.20600100
C	-2.05521000	1.85417000	2.01006000	H	1.62059600	-3.22330100	0.46172300
H	-2.89774000	1.30338300	1.60034400	C	4.58289300	-3.36404500	-1.19272500
C	-2.28353900	2.85752900	2.95377600	H	5.00782100	-2.38242200	-3.06136100
H	-3.30061000	3.09190100	3.26123800	H	3.86043000	-4.22496900	0.64833600
C	-0.06401900	3.29736600	3.18228300	H	5.56863300	-3.81119000	-1.10943600
H	0.73321400	3.86510300	3.65703100	C	0.20832300	-0.82064300	-3.16966900
C	0.23608900	2.31761500	2.24896500	H	0.41889200	-1.60402800	-3.90337300
C	0.05128300	-1.24176200	1.62682800	H	-0.82671500	-0.48420100	-3.28863100
C	-0.89887800	-2.19817100	1.99068400	H	0.86586600	0.03662900	-3.33923700
C	1.26796000	-1.33841200	2.31403200	C	-0.73487400	-2.88239900	-1.42108900
C	-0.57408600	-3.17072800	2.93846900	H	-1.76655500	-2.53403200	-1.52425900
H	-1.88257800	-2.18708200	1.52737300	H	-0.48110300	-3.58320100	-2.22103800
C	1.51496100	-2.32993700	3.25077900	H	-0.64921700	-3.38013100	-0.45147800
H	-1.30833400	-3.92600800	3.21201400	H	0.64995000	4.32763400	-3.11324600
H	2.47873600	-2.37648600	3.75331000	C	-6.07145500	-1.09560600	0.85167200
H	1.31045800	2.58868000	-1.45385000	H	-6.22399500	-0.02957300	1.05120100
N	-0.56490100	1.73905200	-1.35211000	H	-7.03146900	-1.60923700	0.97743600
N	-2.16641900	-0.14851100	-0.35021300	H	-5.36613900	-1.48504400	1.59177700
C	-2.68977600	0.71029400	-1.23770900	C	-5.33124800	-2.81119500	-0.81874000
C	-4.20635000	-0.60380400	-0.70004700	H	-6.28184600	-3.34527200	-0.70911300
N	-3.13268700	-0.99699600	0.00564800	H	-4.95250600	-2.99070200	-1.83126400
N	-3.97574500	0.46170100	-1.49264100	H	-4.61274800	-3.22564300	-0.10557300
O	2.29553000	-0.44239900	2.01532600	C	-6.52370000	-0.74112000	-1.59119800
C	-5.53467200	-1.30956400	-0.57228600	H	-6.67048600	0.33145800	-1.43697500
C	3.36989600	1.18947400	0.21324300	H	-6.15877300	-0.88238900	-2.61309600
C	3.67282200	2.52763000	-0.06365600	H	-7.49012200	-1.24714300	-1.49097700
C	4.23922000	0.17188900	-0.18947500	N	0.60504000	-3.25541300	3.55817800
C	4.84106400	2.84261800	-0.75070100	N	-1.32035100	3.57584500	3.53207600
H	3.00953700	3.31368300	0.28578700				

XYZ coordinates of the optimized  $S_0$  structure for **2d**

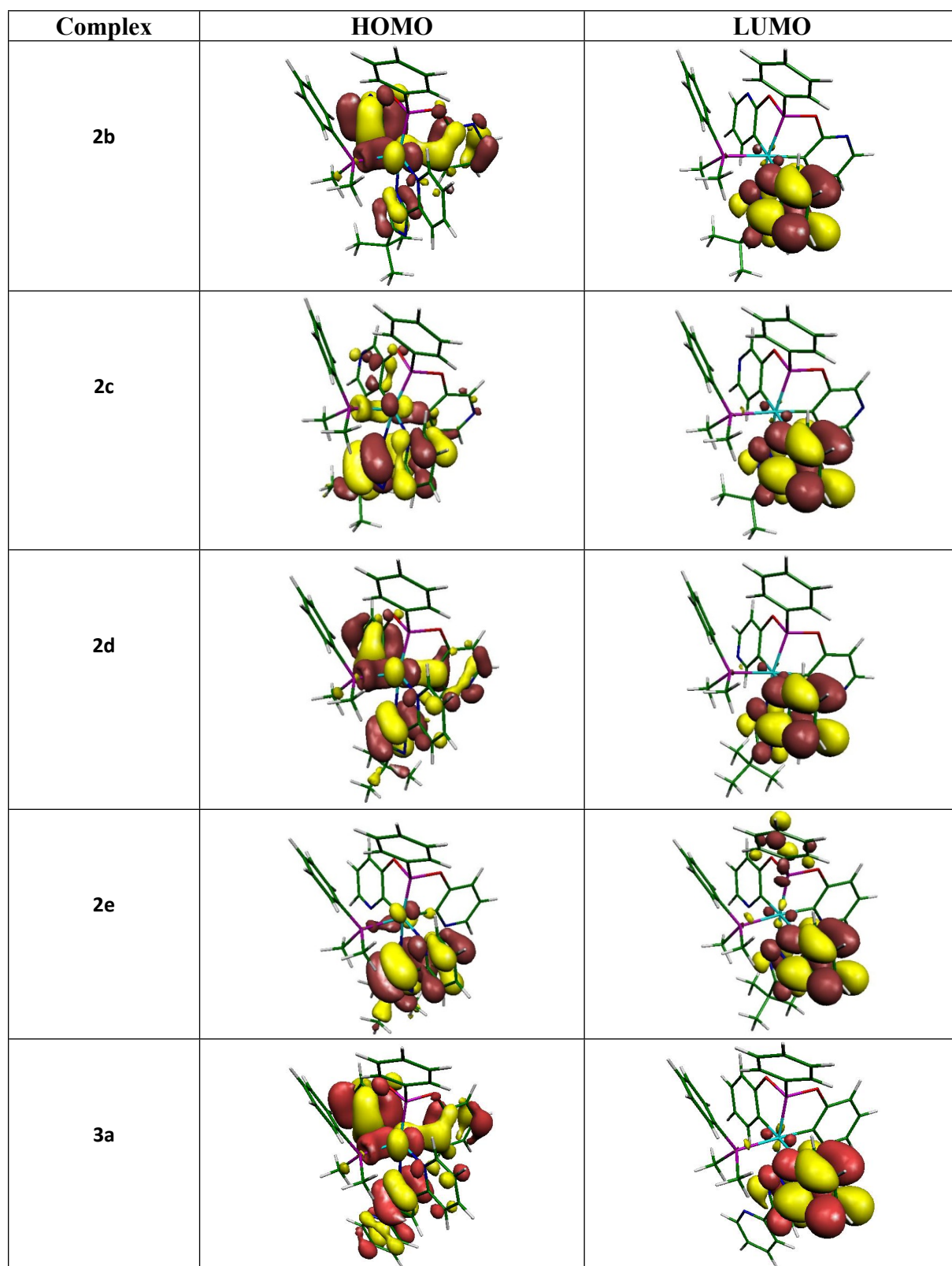
Ir	-0.14347300	0.17172600	0.20600900	C	5.40405400	0.54834100	-0.87131400
P	0.39757200	-1.44632700	-1.45040100	H	4.02465000	-0.83470100	0.03313900
P	1.81857600	0.76359000	1.02569000	C	5.69181800	1.88433100	-1.14114200
O	1.56848600	2.08766600	1.95506100	H	5.05194700	3.92946100	-0.92075300
C	-1.84772900	1.74464500	-1.77267900	H	6.08650300	-0.23487600	-1.18655600
C	-2.30899000	2.69126800	-2.68914000	H	6.60190700	2.14602300	-1.67200600
H	-3.35036100	2.65365700	-2.98845300	C	2.06509600	-2.19123100	-1.41977800
C	-1.41994500	3.63618000	-3.17362200	C	3.01505000	-1.94969900	-2.41552500
H	-1.75111400	4.38589200	-3.88520600	C	2.41005900	-3.00248900	-0.32902300
C	-0.09420700	3.61175200	-2.73693300	C	4.29063800	-2.50483600	-2.32300000
C	0.28577200	2.64174400	-1.82172800	H	2.76916000	-1.32524900	-3.26916500
C	-0.75159400	1.54030500	1.62192000	C	3.68601300	-3.54834900	-0.23496600
C	-2.06368600	1.81773500	2.01611900	H	1.68302600	-3.20510600	0.45351400
H	-2.88790000	1.24800500	1.59081000	C	4.63025600	-3.29925500	-1.23140800
C	-1.43712900	3.45782000	3.47871700	H	5.01889100	-2.31271500	-3.10524200
H	-1.74512800	4.20892100	4.20322200	H	3.94131300	-4.16936900	0.61784300
C	-0.08491400	3.27633800	3.19964700	H	5.62434900	-3.72935400	-1.15789200
H	0.68997100	3.85433000	3.69022700	C	0.18546300	-0.83996400	-3.16619400
C	0.22471300	2.30347600	2.26451300	H	0.40300000	-1.61982300	-3.90165200
C	0.08035300	-1.26152500	1.62879000	H	-0.85820000	-0.52626500	-3.27202100
C	-0.86141900	-2.23353300	1.98258500	H	0.82139700	0.03159900	-3.34538800
C	1.29383600	-1.34236900	2.32157700	C	-0.69797000	-2.91329700	-1.40115800
H	-1.83932400	-2.22257600	1.50377700	H	-1.73786000	-2.57989300	-1.46277000
C	1.54774900	-2.32424700	3.26484900	H	-0.46042600	-3.59690200	-2.22077000
C	0.52758300	-3.24386400	3.49553500	H	-0.57297300	-3.42704700	-0.44433000
H	2.49655800	-2.36706800	3.78763100	H	0.63357200	4.33005200	-3.09556800
H	0.67123600	-4.04302400	4.21965100	C	-5.45679800	-2.52242500	0.33347500
H	1.30762000	2.57633100	-1.45801900	H	-5.12713600	-2.24397800	1.33838600
N	-0.56784500	1.72774600	-1.34531600	H	-6.44038300	-2.99924800	0.40692300
N	-2.15557400	-0.17276900	-0.35390900	H	-4.74362400	-3.25403600	-0.05886700
C	-2.69081900	0.69665300	-1.22471700	C	-6.54855800	-0.28629000	0.00076000
C	-4.19976300	-0.62346600	-0.68103900	H	-6.59970800	0.60641800	-0.62948400
N	-3.12005900	-1.02598200	0.00415800	H	-7.54696400	-0.73479200	0.05839600
N	-3.97721000	0.45299100	-1.46677300	H	-6.25025400	0.02168200	1.00839000
O	2.30532700	-0.43321500	2.02673100	C	-5.99797000	-1.71507800	-1.98272400
C	-5.54514700	-1.29607700	-0.57696500	H	-5.30452500	-2.44664600	-2.41213700
C	3.36251400	1.21283100	0.22404500	H	-6.99369300	-2.17073200	-1.93943100
C	3.65396200	2.55611100	-0.03985700	H	-6.03673700	-0.84738500	-2.64756000
C	4.23978300	0.20677100	-0.19009600	N	-2.41220500	2.75021300	2.91174800
C	4.81928300	2.88780600	-0.72414100	N	-0.65162800	-3.21058800	2.87675500
H	2.98340200	3.33298500	0.31610000				

XYZ coordinates of the optimized  $S_0$  structure for **2b**

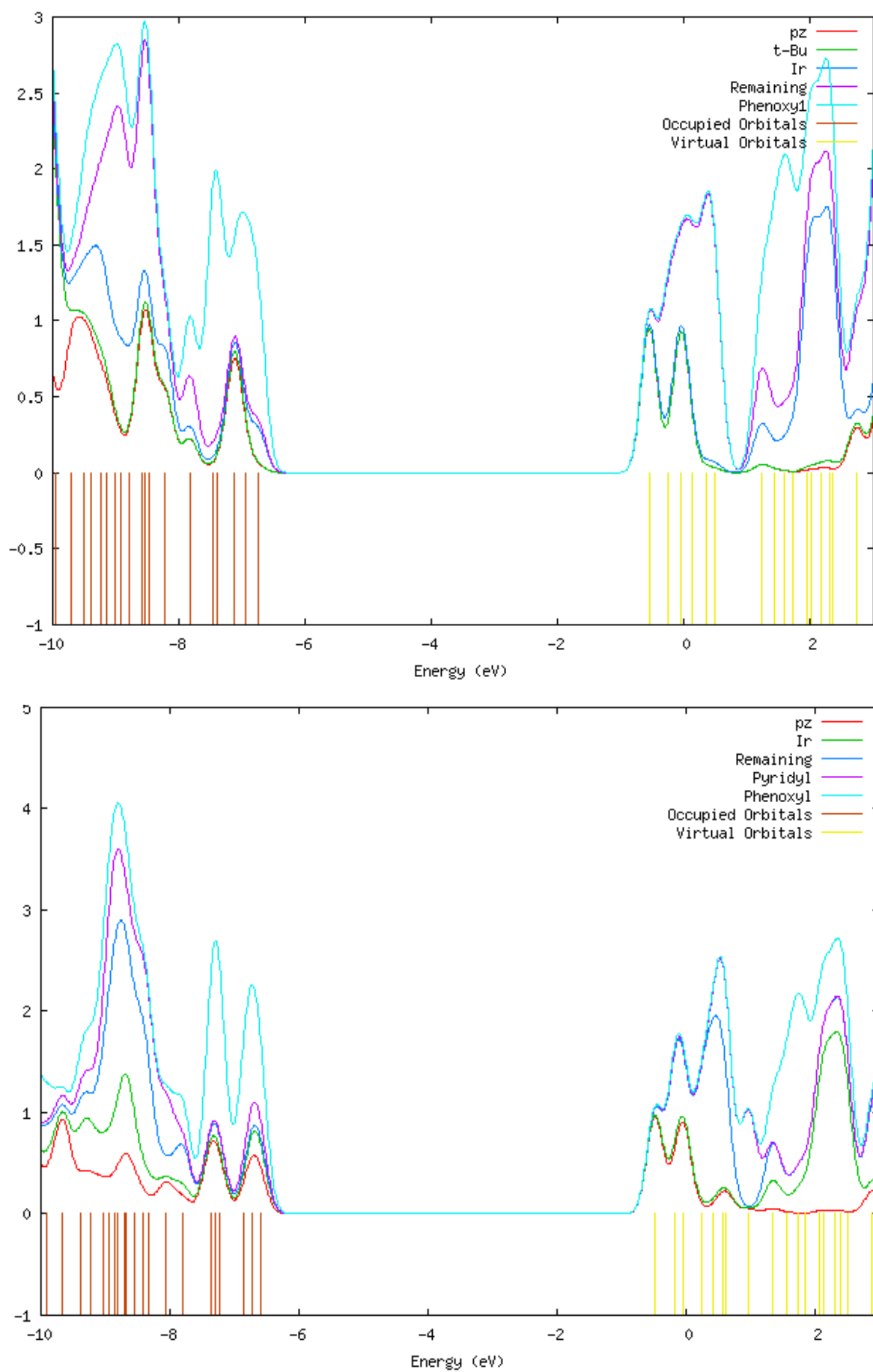
Ir	-0.15167800	0.18447400	0.21327600	C	5.38230400	0.53692900	-0.91087100
P	0.38243000	-1.42897600	-1.45575100	H	4.01501500	-0.85181400	0.00535800
P	1.82271600	0.74243600	1.03625300	C	5.66764200	1.87501300	-1.17276400
O	1.58981400	2.04826900	1.97835800	H	5.03595400	3.91911200	-0.92045700
C	-1.84355200	1.76082000	-1.77978200	H	6.06190700	-0.24358700	-1.23888400
C	-2.29303200	2.69758400	-2.71196500	H	6.57183300	2.14069500	-1.71177800
H	-3.33036300	2.65743300	-3.02478400	C	2.03630900	-2.20247800	-1.41665200
C	-1.39696800	3.63641300	-3.19633600	C	2.99235200	-1.98084100	-2.41142000
H	-1.71885200	4.37808500	-3.92058500	C	2.36766100	-3.00913000	-0.31850500
C	-0.07705600	3.61632000	-2.74320900	C	4.26071500	-2.55031200	-2.30930100
C	0.29166800	2.65494800	-1.81386000	H	2.75745200	-1.35899900	-3.27002400
C	-0.73882000	1.54431800	1.63861300	C	3.63834000	-3.56449200	-0.21143000
C	-2.04070100	1.83700400	2.03481900	H	1.63584400	-3.20187400	0.46178500
H	-2.87546200	1.28393200	1.61002300	C	4.58833300	-3.33525700	-1.20708000
C	-2.27792500	2.83400600	2.98673300	H	4.99414200	-2.37342100	-3.09025200
H	-3.28676200	3.07454100	3.30477300	H	3.88507100	-4.17109300	0.65387100
C	-1.19501300	3.51290800	3.52335400	H	5.57900800	-3.77117500	-1.12303500
H	-1.33412100	4.29845500	4.26165900	C	0.19094300	-0.81612800	-3.17199800
C	0.24688700	2.30063000	2.29486400	H	0.39771000	-1.59908300	-3.90724100
C	0.05880000	-1.25922800	1.61787400	H	-0.84511900	-0.48054600	-3.28470700
C	-0.90077800	-2.20078700	1.98035100	H	0.84666600	0.04172400	-3.34586800
C	1.29089100	-1.39750000	2.28707800	C	-0.73587300	-2.88059500	-1.41929800
C	-0.58357500	-3.20361500	2.90337800	H	-1.77085800	-2.53531000	-1.49814500
H	-1.88867500	-2.15274700	1.52602700	H	-0.49539000	-3.57196000	-2.23146300
C	0.69047200	-3.23030100	3.45051900	H	-0.62838200	-3.38998500	-0.45790100
H	-1.31751200	-3.94943500	3.19059100	H	0.65534400	4.33081500	-3.09994400
H	0.98170000	-3.99803600	4.16315400	C	-6.08779400	-1.07496900	0.85162100
H	1.30890300	2.59219700	-1.43724900	H	-6.23791300	-0.00850300	1.05087900
N	-0.56816400	1.74644700	-1.33870500	H	-7.04938200	-1.58610700	0.97594700
N	-2.17536700	-0.14197800	-0.34451900	H	-5.38450400	-1.46624900	1.59274600
C	-2.69533800	0.72057800	-1.22968300	C	-5.34981900	-2.79222100	-0.81769300
C	-4.21771800	-0.58857100	-0.69631100	H	-6.30216500	-3.32362200	-0.70966300
N	-3.14610900	-0.98754100	0.00895800	H	-4.96980500	-2.97252900	-1.82953300
N	-3.98274200	0.47793900	-1.48588600	H	-4.63327800	-3.20866900	-0.10373400
O	2.30711800	-0.48589900	1.98570700	C	-6.53416100	-0.71829100	-1.59182800
C	-5.54873900	-1.28997900	-0.57130000	H	-6.67773800	0.35473600	-1.43770500
C	3.35470900	1.19349000	0.21361100	H	-6.16737400	-0.86026500	-2.61292000
C	3.64555900	2.53923800	-0.03786800	H	-7.50241000	-1.22137400	-1.49386600
C	4.22637100	0.19026500	-0.21795600	N	1.63247000	-2.32608300	3.14890100
C	4.80254800	2.87572900	-0.73402500	N	0.07395500	3.24797100	3.18543500
H	2.98394800	3.31300200	0.34124100				

XYZ coordinates of the optimized  $S_0$  structure for **2e**

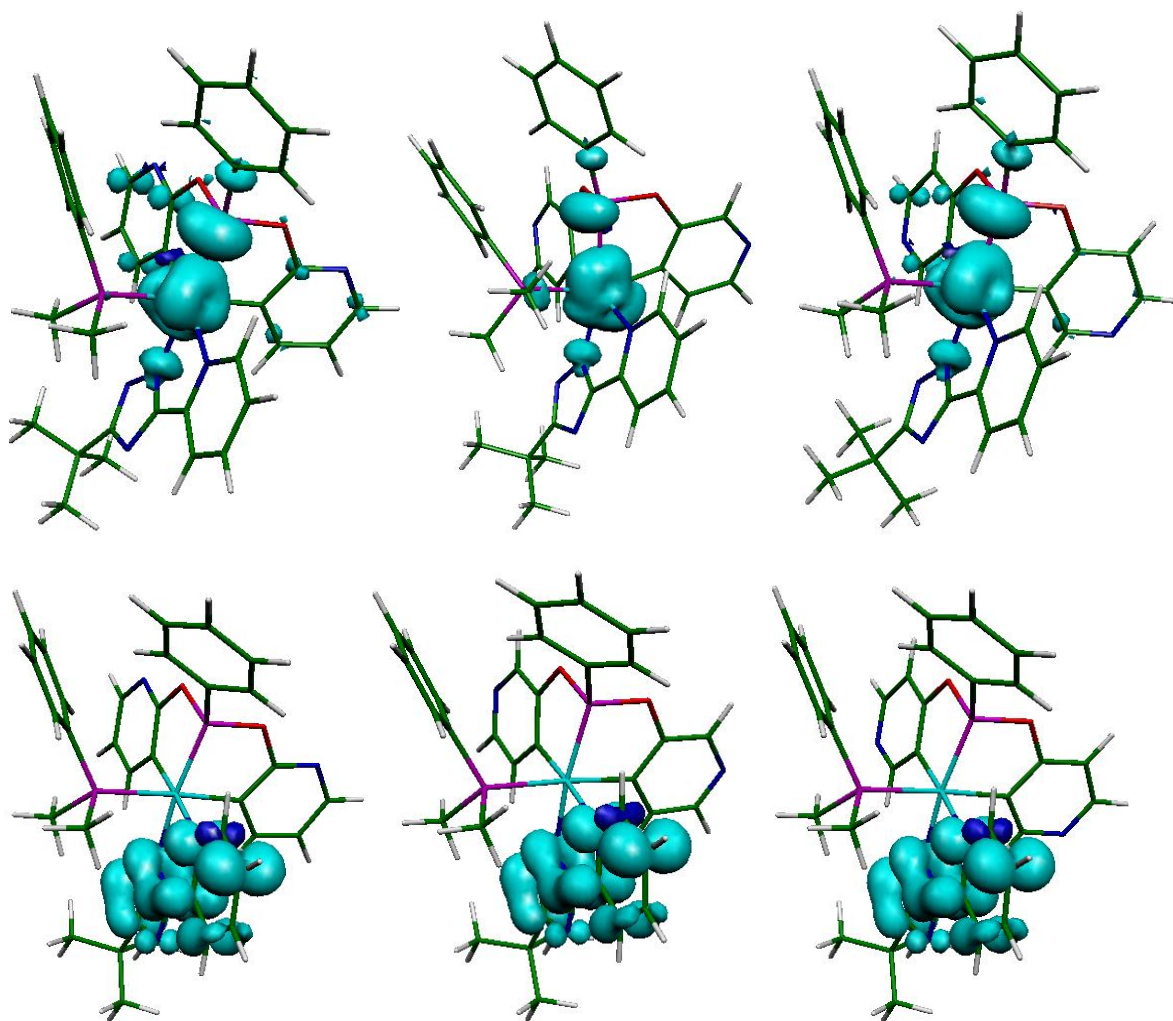
Ir	-0.13188200	0.19941400	0.21483200	C	5.38959600	0.44174000	-0.92703600
P	0.35774900	-1.41109200	-1.47205100	H	3.98335700	-0.85185500	0.06803700
P	1.83306200	0.83722100	0.98102500	C	5.70897000	1.75309600	-1.27265500
O	1.59472200	2.21336800	1.83451000	H	5.12580200	3.82363100	-1.15822600
C	-1.92356500	1.73652300	-1.70959000	H	6.04522400	-0.37648900	-1.20849000
C	-2.43230600	2.67603300	-2.61200900	H	6.61881600	1.96137000	-1.82714500
H	-3.47957400	2.61091900	-2.88456700	C	1.97083200	-2.26291400	-1.37227800
C	-1.58225500	3.64445500	-3.11601000	C	2.97882100	-2.06273900	-2.31952100
H	-1.95188100	4.38580000	-3.81753000	C	2.22271000	-3.09886600	-0.27455000
C	-0.24365400	3.65670000	-2.71517900	C	4.22096100	-2.67783500	-2.17122600
C	0.18467900	2.69436600	-1.81463300	H	2.80585000	-1.41911100	-3.17673300
C	-0.73147300	1.61007000	1.59587000	C	3.46795200	-3.70056300	-0.12215200
C	-2.33087900	2.80457700	2.74463600	H	1.44527100	-3.28212600	0.46376700
H	-3.39231400	2.93160400	2.94405400	C	4.47138400	-3.48904000	-1.06859100
C	-1.39655400	3.62789500	3.36095900	H	4.99291400	-2.51676400	-2.91783500
H	-1.71222300	4.40309800	4.05069800	H	3.65262600	-4.33827300	0.73690800
C	-0.04820000	3.43343600	3.06756400	H	5.44097600	-3.96243500	-0.94842500
H	0.73735000	4.03877700	3.50855100	C	0.28926700	-0.75177300	-3.18085500
C	0.25932000	2.42264400	2.17893700	H	0.47346700	-1.53284700	-3.92416000
C	0.15188300	-1.24288400	1.60389300	H	-0.71466500	-0.34195700	-3.32970000
C	1.35932300	-1.24991300	2.33753000	H	1.00969400	0.06112400	-3.30666700
C	-0.46598700	-3.18080800	2.69853400	C	-0.86132800	-2.77683000	-1.49782700
C	1.64487800	-2.22387800	3.27210000	H	-1.80863400	-2.38393600	-1.87813400
C	0.69204400	-3.22451200	3.46415300	H	-0.51161600	-3.60350700	-2.12169800
H	-1.22909300	-3.94819400	2.80559900	H	-1.04371800	-3.09952400	-0.46818500
H	2.58316100	-2.19987700	3.81688700	H	0.45450100	4.39519400	-3.09112700
H	0.85163500	-4.01842000	4.18547600	C	-5.34855000	-2.64576000	0.43797300
H	1.21745900	2.65329400	-1.47808700	H	-5.01331800	-2.35142400	1.43613700
N	-0.63101100	1.75555300	-1.32088300	H	-6.31377600	-3.15820800	0.52329700
N	-2.14822700	-0.18693200	-0.27996800	H	-4.61178100	-3.34926900	0.03810100
C	-2.71956200	0.66551500	-1.14673800	C	-6.53053900	-0.45617300	0.10817100
C	-4.17174900	-0.70217400	-0.58634700	H	-6.61653800	0.43369500	-0.52252800
N	-3.07341600	-1.06814200	0.08981200	H	-7.51189300	-0.94134600	0.17019400
N	-3.99940400	0.37851300	-1.37809100	H	-6.23759900	-0.13625400	1.11349400
O	2.32092100	-0.28659800	2.06387700	C	-5.93565400	-1.86506000	-1.87490600
C	-5.49029500	-1.42523500	-0.47307500	H	-5.21619500	-2.57052300	-2.30584800
C	3.38137900	1.22143600	0.15454000	H	-6.91355300	-2.35836100	-1.82757100
C	3.70316100	2.53894100	-0.18744900	H	-6.00872300	-1.00084000	-2.54152600
C	4.22631100	0.17028000	-0.21357800	N	-0.72382900	-2.22592800	1.79641600
C	4.86854800	2.80101300	-0.90126100	N	-2.01216200	1.82688600	1.88924100
H	3.05612500	3.35188700	0.12914300				



**Figure S1.** Frontier orbitals involved in the lower-lying electronic transitions for complexes **2b-e** and **3a**.



**Figure S2:** Partial density of state (PDOS) for complexes **2a** (top) and **3a** (bottom).



**Figure S3:** Spin density distribution (isocontour value of  $5 \cdot 10^{-3}$  au) for **2b-c** in both the optimized <sup>3</sup>MLCT and <sup>3</sup>MC structures.



**Table S1:** M062X ionization potentials (IPs), electron affinities (EAs), extraction potentials for hole (HEP) and electron (EEP), and inner reorganization energies for electron/hole ( $\lambda_e/\lambda_h$ ) for the studied molecules.\*

<b>Cplx</b>	<b>IP(v)</b>	<b>EA(v)</b>	<b>IP(a)</b>	<b>EA(a)</b>	<b>HEP</b>	<b>EEP</b>	$\lambda_h$	$\lambda_e$
<b>2a</b>	7.21	0.41	6.93	0.66	6.65	0.90	0.56	0.49
<b>4N1</b>	7.82	0.64	7.54	0.89	7.17	1.12	0.65	0.48
<b>4N2</b>	7.54	0.57	7.26	0.82	6.96	1.05	0.59	0.48
<b>4N3</b>	7.49	0.56	7.22	0.80	6.92	1.04	0.57	0.48
<b>4N4</b>	7.38	0.26	6.84	0.50	6.43	0.76	0.95	0.50
<b>5c</b>	7.07	0.36	6.81	0.59	6.51	0.83	0.56	0.47
<b>4c</b>	7.19	0.48	6.92	0.73	6.63	0.97	0.55	0.48

\*Cplx = Complex. (v) and (a) indicate vertical and adiabatic values, respectively. Values are in eV.