Supporting Information for:

Excited State Absorption Properties of Pt(II) Terpyridyl Complexes Bearing π-Conjugated Arylacetylides

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Complete Reference (84).

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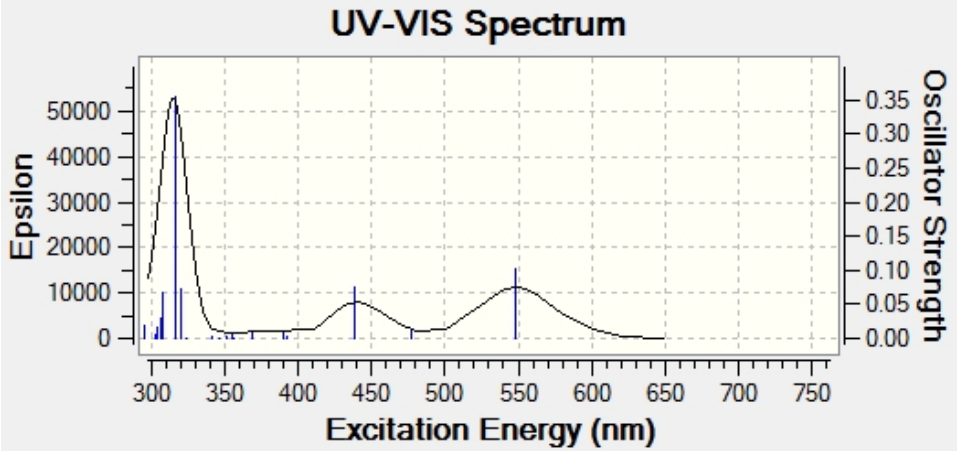
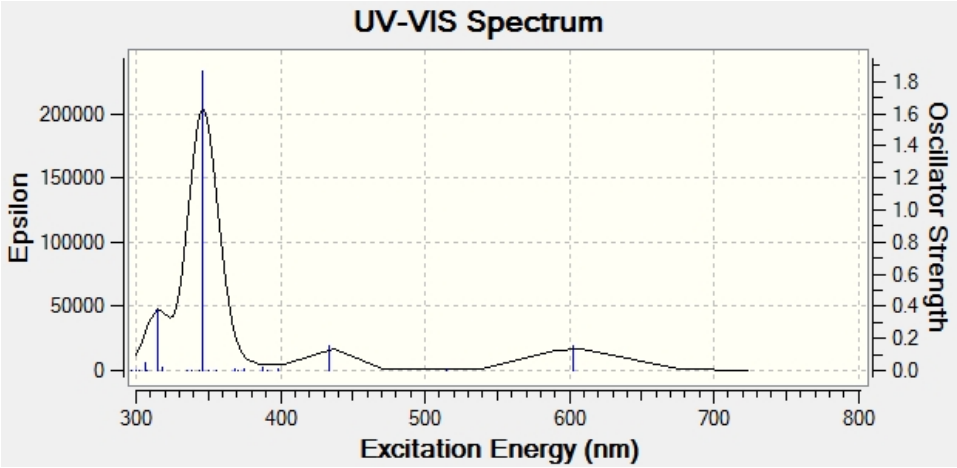
Compound 1



Compound 2



Compound 3

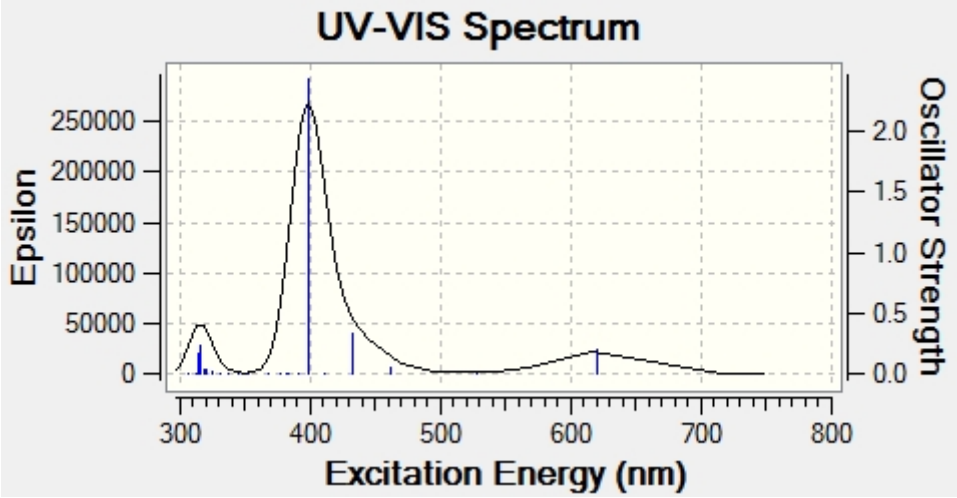


Figure S1. Simulated ground-state absorption spectra of **1-3** in a CH_2Cl_2 continuum (PCM) as generated in Gaussian '03.

Cartesian Coordinates (Å) and absolute energies of optimized singlet, doublet and triplet geometric structures.

1 Singlet, E = -1641.2025919 Hatree

Pt	0.27366300	-0.00723200	-0.00116100
C	1.97231900	-2.35232200	0.00480800
C	-0.26944300	-3.02380900	-0.00565400
C	2.37929600	-3.67843400	0.00703700
C	0.09739100	-4.36683000	-0.00386600
H	-1.30795900	-2.71418700	-0.01376200
C	1.44718200	-4.73296100	0.00335300
H	3.44067700	-3.89457400	0.01151300
H	-0.69665000	-5.10414700	-0.00877300
C	2.90472800	-1.19848400	0.00345700
C	4.29975700	-1.22412400	0.00231100
C	5.02592500	-0.02273800	-0.00593500
H	4.81847000	-2.17233500	0.00567800
C	2.91253700	1.17341600	-0.00624900
C	4.30373600	1.18756800	-0.00985400
H	4.83293300	2.13229200	-0.01545700
C	1.98369500	2.33108800	-0.00544100
C	2.39430600	3.65627600	-0.00378900
C	-0.25653600	3.00934500	0.00210500
C	1.46470600	4.71322400	0.00035600
H	3.45636600	3.87014900	-0.00450300
C	0.11384700	4.35100200	0.00312800
H	-1.29578700	2.70222600	0.00800500
H	-0.67805200	5.09057300	0.00766300
N	0.63361700	-2.03439200	-0.00000500
N	2.27226700	-0.01254400	-0.00095800
N	0.64399800	2.01749700	-0.00288900
C	-1.71013700	-0.00216000	-0.00173900
C	-2.93701800	0.00147800	-0.00196100
C	-4.36742000	0.00584300	-0.00201500
C	-5.09228000	-0.84350000	0.86094300
C	-5.08699500	0.85991800	-0.86471700
C	-6.48598200	-0.83478100	0.85957300
H	-4.55006700	-1.50539200	1.53246800
C	-6.48071700	0.86060900	-0.86261000
H	-4.54069400	1.51821700	-1.53645900
C	-7.18673500	0.01531400	-0.00130600
H	-7.02791500	-1.49556100	1.53369600
H	-7.01853200	1.52502400	-1.53645900
H	-8.27485900	0.01901000	-0.00100300
C	6.56244400	0.00779300	-0.01094300
C	7.04751000	0.75322700	-1.27824100

C	7.05543200	0.75144200	1.25440200
C	7.17450000	-1.40540100	-0.01454000
H	6.70883900	0.24724400	-2.18804100
H	6.69128000	1.78721600	-1.31231400
H	8.14168000	0.78107600	-1.29163100
H	6.72412500	0.24305100	2.16557100
H	8.14963600	0.78126900	1.26003900
H	6.69722400	1.78462300	1.29294000
H	8.26512100	-1.32376000	-0.02102800
H	6.89542100	-1.97692700	0.87722300
H	6.88445900	-1.97681500	-0.90287100
C	1.94672600	6.16885600	0.00550100
C	2.79280200	6.41407200	1.27879800
C	2.81348400	6.41877500	-1.25286600
C	0.77279900	7.16451400	-0.00224700
H	2.20178100	6.24362100	2.18440000
H	3.67397300	5.76651600	1.32173000
H	3.14421700	7.45079200	1.29192200
H	2.23734600	6.25174700	-2.16863900
H	3.16476700	7.45560000	-1.25634200
H	3.69568100	5.77204300	-1.28414700
H	1.16516400	8.18555000	0.00188400
H	0.14965600	7.05405300	-0.89579000
H	0.13622700	7.05245300	0.88153600
C	1.92698400	-6.18935500	0.00746400
C	2.79961500	-6.43740900	-1.24725800
C	2.76733800	-6.43905200	1.28372700
C	0.75155800	-7.18308200	-0.00857400
H	2.22803800	-6.26803500	-2.16545900
H	3.68240500	-5.79124900	-1.27340400
H	3.15006400	-7.47450100	-1.25112200
H	2.17215500	-6.27203100	2.18725600
H	3.11888700	-7.47573400	1.29463400
H	3.64807400	-5.79145400	1.33344400
H	1.14206800	-8.20483400	-0.00546200
H	0.11095000	-7.07225300	0.87247200
H	0.13288300	-7.06895600	-0.90474200

1 oxidative doublet, E = -1640.9870854 Hatree

Pt	0.25801800	-0.00650900	-0.00652100
C	1.95804600	-2.35531300	0.02495200
C	-0.28003300	-3.03479000	0.03057300
C	2.37008000	-3.67832300	0.04204400
C	0.09122100	-4.37637500	0.04792900
H	-1.32141600	-2.73855600	0.02559100
C	1.44175700	-4.73785500	0.05450400
H	3.43199100	-3.89063200	0.04593100
H	-0.70109000	-5.11556300	0.05631300
C	2.88635900	-1.19970900	0.01181500
C	4.27957400	-1.22502200	0.01647700
C	5.00628500	-0.02298400	0.00222000
H	4.79897900	-2.17240900	0.03169000
C	2.89506700	1.17559100	-0.01924000
C	4.28471200	1.18857900	-0.01681800
H	4.81499000	2.13227500	-0.02873700
C	1.97055900	2.33513300	-0.03434300
C	2.38603600	3.65738500	-0.04958800
C	-0.26616300	3.02136800	-0.04528900
C	1.46013000	4.71914700	-0.06349200
H	3.44861300	3.86764500	-0.05076400
C	0.10850900	4.36147200	-0.06108800
H	-1.30820400	2.72755700	-0.04317300
H	-0.68163500	5.10288500	-0.07132900
N	0.61862300	-2.04228700	0.01932600
N	2.25517800	-0.01184200	-0.00539900
N	0.63005400	2.02642500	-0.03190000
C	-1.68648100	-0.00126500	-0.00380700
C	-2.93503200	0.00201900	-0.00042800
C	-4.32500800	0.00567900	0.00368200
C	-5.05136000	-1.22744200	-0.00666600
C	-5.04486300	1.24256400	0.01853000
C	-6.43196500	-1.21410100	-0.00237300
H	-4.50476300	-2.16618400	-0.01850600
C	-6.42552200	1.23637800	0.02284600
H	-4.49335300	2.17847200	0.02700500
C	-7.12214600	0.01293900	0.01238300
H	-6.98818000	-2.14884100	-0.01045200
H	-6.97681900	2.17399100	0.03441000
H	-8.21119600	0.01577100	0.01576400
C	6.54107300	0.00588000	0.00537400
C	7.02956600	0.71749900	-1.28072800
C	7.02607100	0.78536900	1.25272500
C	7.15230400	-1.40688400	0.04425000
H	6.69519000	0.18694900	-2.17792100

H	6.67485900	1.75063300	-1.34354300
H	8.12361500	0.74349400	-1.28874300
H	6.68651600	0.30578000	2.17628600
H	8.12009300	0.80879800	1.26394200
H	6.67514700	1.82173000	1.25766900
H	8.24262800	-1.32418900	0.04821100
H	6.86362800	-1.95552000	0.94728700
H	6.87441900	-2.00050100	-0.83335000
C	1.94692200	6.17177600	-0.08049600
C	2.80312700	6.42949800	1.18390700
C	2.80567500	6.39886700	-1.34902100
C	0.77631800	7.17105500	-0.09382000
H	2.21874000	6.27262700	2.09616800
H	3.68417300	5.78192200	1.22828900
H	3.15615100	7.46550600	1.18005000
H	2.22316000	6.21961400	-2.25834200
H	3.15822100	7.43483000	-1.36964400
H	3.68716900	5.75087100	-1.37606000
H	1.17310100	8.19010000	-0.10618200
H	0.14720400	7.05189300	-0.98206800
H	0.14559800	7.07420400	0.79602400
C	1.92683100	-6.19102400	0.07564200
C	2.79259400	-6.45109500	-1.18175000
C	2.77661400	-6.41772100	1.35038000
C	0.75498600	-7.18881100	0.08130800
H	2.21517300	-6.29593300	-2.09873700
H	3.67407900	-5.80382600	-1.22132500
H	3.14540400	-7.48712300	-1.17320000
H	2.18734400	-6.23923600	2.25550100
H	3.12996700	-7.45335100	1.37322700
H	3.65708500	-5.76869600	1.38441100
H	1.15015900	-8.20844300	0.09632100
H	0.12017900	-7.06872200	0.96537100
H	0.13031700	-7.09085300	-0.81267800

1 reductive doublet, E = -1641.3205485 Hatree

Pt	0.27500600	-0.01084500	-0.00033700
C	1.99615900	-2.34933700	0.02775600
C	-0.26576300	-3.03113900	0.03695600
C	2.38432700	-3.69953300	0.04467000
C	0.09119300	-4.36503700	0.05370500
H	-1.30308600	-2.71664400	0.03340700
C	1.45906400	-4.73784000	0.05823000
H	3.44638700	-3.91898800	0.04727300
H	-0.70156700	-5.10277100	0.06333500
C	2.90497800	-1.22263700	0.01371700
C	4.30360700	-1.22500100	0.01424200
C	5.02827200	-0.02494900	-0.00081500
H	4.82703000	-2.17214000	0.02679000
C	2.91466100	1.18662500	-0.01603900
C	4.29952800	1.19378500	-0.01665800
H	4.83042700	2.13846600	-0.02903600
C	2.00028700	2.33009700	-0.02924600
C	2.39926000	3.66924100	-0.04508400
C	-0.25050000	3.01511600	-0.03729600
C	1.47556800	4.71703200	-0.05769400
H	3.46219300	3.88269000	-0.04742900
C	0.11350900	4.35008500	-0.05345000
H	-1.28871800	2.70407900	-0.03364100
H	-0.67726500	5.09039500	-0.06250800
N	0.63684000	-2.02694900	0.02408600
N	2.25898900	-0.01182500	-0.00129300
N	0.64975400	2.01144900	-0.02509200
C	-1.71865300	-0.00626500	-0.00133000
C	-2.94849200	-0.00035600	-0.00124600
C	-4.37691300	0.00477200	-0.00090400
C	-5.10979900	-1.20328200	0.01481700
C	-5.10164400	1.21770700	-0.01625900
C	-6.50339900	-1.19514900	0.01513000
H	-4.57177700	-2.14771300	0.02679000
C	-6.49527700	1.21901900	-0.01584500
H	-4.55732200	2.15853400	-0.02856100
C	-7.20499900	0.01432000	-0.00017000
H	-7.04533900	-2.13923400	0.02742400
H	-7.03086200	2.16673000	-0.02788200
H	-8.29310300	0.01799100	0.00011000
C	6.56592300	0.01557500	-0.00183900
C	7.06038300	0.73433300	-1.28067800
C	7.06196600	0.78663000	1.24552100
C	7.18810200	-1.39334000	0.02697700
H	6.73315100	0.20256000	-2.18023200

H	6.68776600	1.76134300	-1.34395600
H	8.15506700	0.77847400	-1.29040700
H	6.73477900	0.29354900	2.16687300
H	8.15667700	0.82970500	1.25256000
H	6.69122200	1.81607800	1.26606300
H	8.27934300	-1.30967100	0.02736500
H	6.90063900	-1.94908400	0.92602100
H	6.90452300	-1.98408300	-0.85070900
C	1.95234600	6.17717500	-0.07506300
C	2.80581800	6.45084400	1.18687500
C	2.80954700	6.41984800	-1.34081100
C	0.77428100	7.16875400	-0.08917900
H	2.22157100	6.29081500	2.09900800
H	3.68761100	5.80464200	1.23407300
H	3.15523300	7.48906000	1.18441900
H	2.22823300	6.23637700	-2.25039300
H	3.15780400	7.45820800	-1.36333700
H	3.69231400	5.77385100	-1.36938200
H	1.15984000	8.19283700	-0.10307800
H	0.14458900	7.04049600	-0.97573900
H	0.14356800	7.06521500	0.79989600
C	1.92755400	-6.20201900	0.07855000
C	2.78674700	-6.48417900	-1.17742800
C	2.77590500	-6.45136200	1.34881900
C	0.74372100	-7.18715300	0.08629600
H	2.20897900	-6.32096000	-2.09321000
H	3.67241300	-5.84307100	-1.22039800
H	3.12986600	-7.52471900	-1.17273400
H	2.19010000	-6.26482600	2.25499000
H	3.11929400	-7.49152800	1.37399000
H	3.66093400	-5.80878000	1.38300200
H	1.12257500	-8.21389200	0.10058600
H	0.11069800	-7.05588600	0.97001700
H	0.11730500	-7.07807000	-0.80514700

1 Triplet, E = -1641.1283675 Hatree

Pt	0.26845100	-0.00698200	-0.00484600
C	1.98113900	-2.35318300	0.02565100
C	-0.27808900	-3.03487700	0.03064600
C	2.37196400	-3.69986500	0.04322000
C	0.08090300	-4.36867200	0.04790700
H	-1.31738100	-2.72985500	0.02528100
C	1.44587700	-4.74035700	0.05506600
H	3.43372300	-3.91811900	0.04771500
H	-0.71233900	-5.10586500	0.05588200
C	2.88795000	-1.22437500	0.01296100
C	4.28203000	-1.22705100	0.01538100
C	5.00895800	-0.02535300	0.00119800
H	4.80556400	-2.17362900	0.02855800
C	2.89888400	1.19446900	-0.01685400
C	4.28080400	1.19495800	-0.01559800
H	4.81448700	2.13772800	-0.02725900
C	1.99031800	2.33812200	-0.03115400
C	2.39167800	3.67607200	-0.04616900
C	-0.25967600	3.02690600	-0.04216000
C	1.46880700	4.72519300	-0.05990400
H	3.45454100	3.88828100	-0.04701800
C	0.10683300	4.36075000	-0.05755400
H	-1.30027800	2.72664200	-0.04003300
H	-0.68335200	5.10150300	-0.06754100
N	0.62616900	-2.03332700	0.01963800
N	2.23820500	-0.00983400	-0.00302800
N	0.64059200	2.02394800	-0.02897100
C	-1.67082800	-0.00446300	-0.00365500
C	-2.92293500	-0.00218100	-0.00146000
C	-4.31609600	-0.00112900	0.00133100
C	-5.04217300	-1.23080700	0.02668100
C	-5.04079100	1.22939400	-0.02081400
C	-6.42557300	-1.22078100	0.02968200
H	-4.49492400	-2.16906100	0.04378400
C	-6.42418600	1.22107600	-0.01747900
H	-4.49247200	2.16699200	-0.04038600
C	-7.12068000	0.00056100	0.00770300
H	-6.97657100	-2.15850100	0.04917200
H	-6.97415100	2.15945000	-0.03444300
H	-8.20927600	0.00122800	0.01021100
C	6.54498900	0.01279500	0.00188600
C	7.03890300	0.73172800	-1.27758900
C	7.03802100	0.78449200	1.25055400
C	7.16461400	-1.39707600	0.03153700
H	6.71149800	0.20089500	-2.17749200

H	6.67043300	1.76025000	-1.34026500
H	8.13337000	0.77222800	-1.28535500
H	6.70849800	0.29297400	2.17177100
H	8.13250100	0.82350800	1.25814700
H	6.67177200	1.81557900	1.26910600
H	8.25553900	-1.31353900	0.03322400
H	6.87690500	-1.95229100	0.93085100
H	6.88290600	-1.98744300	-0.84703300
C	1.94676900	6.18407800	-0.07650400
C	2.79990000	6.45394800	1.18671300
C	2.80482400	6.42362600	-1.34249200
C	0.76964400	7.17654900	-0.09083200
H	2.21548500	6.29345100	2.09857200
H	3.68253000	5.80884400	1.23307600
H	3.14852700	7.49208900	1.18454500
H	2.22415200	6.24048100	-2.25246600
H	3.15258500	7.46182400	-1.36424100
H	3.68827700	5.77850400	-1.36987700
H	1.15739900	8.19954200	-0.10309000
H	0.14120000	7.05123500	-0.97872800
H	0.13814000	7.07382300	0.79781400
C	1.91525000	-6.20301100	0.07593900
C	2.77531600	-6.48128300	-1.18058400
C	2.76348100	-6.44803800	1.34738100
C	0.73207500	-7.18856500	0.08348000
H	2.19806000	-6.31876600	-2.09670400
H	3.66156500	-5.84090300	-1.22250900
H	3.11817800	-7.52146300	-1.17482300
H	2.17759600	-6.26157800	2.25340300
H	3.10624500	-7.48797500	1.37219400
H	3.64934900	-5.80658300	1.38091900
H	1.11296700	-8.21418500	0.09892400
H	0.09862600	-7.05839400	0.96710100
H	0.10675200	-7.08211400	-0.80908400

2 Singlet, E = -1948.4205256

Pt	0.23849900	-0.03139200	-0.01950700
C	1.95531500	-2.36289700	0.02163400
C	-0.28064500	-3.05272400	0.00176200
C	2.37300000	-3.68547600	0.03974200
C	0.09696500	-4.39266400	0.01931500
H	-1.32177600	-2.75255800	-0.01684600
C	1.44958700	-4.74763700	0.04006500
H	3.43600600	-3.89286300	0.05350200
H	-0.69105700	-5.13644300	0.01591100
C	2.87845300	-1.20176500	0.01653600
C	4.27355100	-1.21653200	0.03053500
C	4.99042000	-0.00961000	0.01946300
H	4.79943300	-2.16055800	0.05019200
C	2.86796600	1.16987400	-0.01666900
C	4.25895100	1.19482100	-0.00579700
H	4.78099800	2.14345000	-0.01552200
C	1.93043300	2.32023500	-0.03566000
C	2.33089100	3.64843500	-0.04700500
C	-0.31482000	2.98129400	-0.04939900
C	1.39327200	4.69826000	-0.06073500
H	3.39128300	3.87045400	-0.04449200
C	0.04529300	4.32568600	-0.06111800
H	-1.35187200	2.66696400	-0.04674300
H	-0.75235300	5.05896700	-0.06994200
N	0.61419600	-2.05583400	0.00424400
N	2.23687600	-0.02096200	-0.00578900
N	0.59317800	1.99634300	-0.03811000
C	-1.74443800	-0.04003100	-0.03005200
C	-2.97172100	-0.04148200	-0.03270300
C	-4.39867700	-0.04114400	-0.03386000
C	-5.12540600	-0.86481900	0.85408300
C	-5.12362000	0.78434300	-0.92157900
C	-6.51358700	-0.86247900	0.85680700
H	-4.58496800	-1.50598500	1.54653000
C	-6.51180300	0.78691000	-0.92255000
H	-4.58181400	1.42381000	-1.61453100
C	-7.23459600	-0.03618600	-0.03211200
H	-7.05687100	-1.50165900	1.54909700
H	-7.05369700	1.42817400	-1.61400100
C	6.52658500	0.03309500	0.03213400
C	7.01965200	0.74375500	-1.25206700
C	6.99957600	0.81908100	1.27938000
C	7.14949200	-1.37452700	0.07916200
H	6.69656200	0.20651900	-2.14954000
H	6.65338100	1.77242400	-1.32202800

H	8.11362600	0.78193800	-1.25376000
H	6.65827000	0.33891100	2.20210900
H	8.09343600	0.85361500	1.29835100
H	6.63774300	1.85174500	1.28018500
H	8.23940000	-1.28429400	0.09065800
H	6.85740800	-1.92319600	0.98106300
H	6.88132200	-1.97280300	-0.79828200
C	1.86411400	6.15752100	-0.07281400
C	2.71131400	6.42399400	1.19550700
C	2.72598800	6.39893600	-1.33617500
C	0.68243900	7.14387700	-0.08970200
H	2.12392400	6.25930400	2.10452600
H	3.59769800	5.78406000	1.24344700
H	3.05455000	7.46352300	1.19587400
H	2.14943400	6.21541200	-2.24851700
H	3.06833900	7.43860400	-1.35352200
H	3.61360700	5.75933300	-1.36116700
H	1.06685300	8.16788900	-0.09868800
H	0.05834700	7.01788000	-0.98049900
H	0.04858200	7.03743200	0.79674900
C	1.94150200	-6.19977900	0.06234200
C	2.81888600	-6.45509700	-1.18757700
C	2.78091100	-6.42752400	1.34335900
C	0.77441000	-7.20334700	0.05556900
H	2.24833900	-6.30002900	-2.10894100
H	3.69703000	-5.80280100	-1.21875300
H	3.17690200	-7.48957400	-1.17923200
H	2.18265800	-6.25345000	2.24351800
H	3.13949300	-7.46154400	1.36790200
H	3.65722200	-5.77350100	1.38700600
H	1.17343800	-8.22166600	0.07269900
H	0.13034800	-7.08677100	0.93336100
H	0.15732000	-7.10602400	-0.84367400
C	-8.65834200	-0.03230700	-0.02989300
C	-9.87641800	-0.02803400	-0.02703700
C	-11.30242100	-0.02238700	-0.02280300
C	-12.01948300	-0.86596400	0.85196200
C	-12.01803000	0.82727600	-0.89285000
C	-13.41251900	-0.85606000	0.85249200
H	-11.47321700	-1.52302400	1.52487900
C	-13.41107200	0.82943400	-0.88398700
H	-11.47064400	1.47972300	-1.56933600
C	-14.11296500	-0.01028100	-0.01338800
H	-13.95438000	-1.51126100	1.53179000
H	-13.95180400	1.48936900	-1.55959100
H	-15.20110200	-0.00553900	-0.00969200

2 Triplet, E =-1948.3526039 Hatree

Pt	0.24852600	-0.01089600	-0.00084300
C	1.96534500	-2.35374300	-0.00002000
C	-0.29174500	-3.03826000	0.00065700
C	2.35868200	-3.69915900	0.00091700
C	0.06914700	-4.37185600	0.00152500
H	-1.33116400	-2.73321700	0.00052400
C	1.43438700	-4.74170700	0.00170400
H	3.42086500	-3.91560900	0.00108700
H	-0.72287900	-5.11047200	0.00210000
C	2.87270800	-1.22225200	-0.00079400
C	4.26754200	-1.22596900	-0.00158600
C	4.99357700	-0.02390500	-0.00274800
H	4.79093900	-2.17273600	-0.00143500
C	2.88068700	1.19002200	-0.00164400
C	4.26472200	1.19335300	-0.00290400
H	4.79626500	2.13750000	-0.00407300
C	1.97018500	2.33324100	-0.00102200
C	2.37091400	3.67153400	0.00044300
C	-0.27967000	3.02077800	-0.00112400
C	1.44787600	4.72041300	0.00112100
H	3.43375300	3.88417200	0.00145300
C	0.08597600	4.35498800	-0.00005500
H	-1.31979200	2.71844900	-0.00161400
H	-0.70447500	5.09555400	0.00010700
N	0.61036300	-2.03464400	-0.00014800
N	2.22319000	-0.01238100	-0.00079700
N	0.62035300	2.01729100	-0.00139300
C	-1.70157500	-0.00878200	-0.00098400
C	-2.94944200	-0.00597200	-0.00121800
C	-4.33841100	-0.00384200	-0.00140500
C	-5.07496900	-1.23283000	-0.00238700
C	-5.07134000	1.22729300	-0.00055600
C	-6.44787300	-1.23078700	-0.00240700
H	-4.53105000	-2.17302200	-0.00314400
C	-6.44422100	1.22932200	-0.00057100
H	-4.52467400	2.16589200	0.00017600
C	-7.17045700	0.00033900	-0.00144800
H	-7.00075000	-2.16721700	-0.00314700
H	-6.99434200	2.16737300	0.00011600
C	6.53029300	0.01515200	-0.00512400
C	7.02140500	0.75291300	-1.27466100
C	7.02613900	0.76796600	1.25364100
C	7.15048300	-1.39482300	0.00226500
H	6.69161000	0.23573800	-2.18165000
H	6.65242100	1.78214500	-1.32096100

H	8.11587700	0.79388500	-1.28494900
H	6.69877300	0.26243900	2.16805100
H	8.12066400	0.80773500	1.25981900
H	6.65889000	1.79825500	1.28854500
H	8.24144800	-1.31112800	0.00160600
H	6.86578200	-1.96311200	0.89434900
H	6.86578000	-1.97264800	-0.88365600
C	1.92528500	6.17975600	0.00478200
C	2.77228300	6.43413000	1.27531900
C	2.78921300	6.43678500	-1.25366500
C	0.74774300	7.17184800	-0.00229600
H	2.18342500	6.26193000	2.18219200
H	3.65448600	5.78815200	1.31786300
H	3.12101000	7.47223100	1.28825800
H	2.21304800	6.26518200	-2.16876200
H	3.13666300	7.47535400	-1.26032700
H	3.67305400	5.79243200	-1.28531600
H	1.13476200	8.19523900	-0.00043900
H	0.12287700	7.05681800	-0.89411600
H	0.11266500	7.05775300	0.88238900
C	1.90651000	-6.20368700	0.00285900
C	2.76177600	-6.46511700	-1.26052600
C	2.76050600	-6.46342300	1.26746000
C	0.72517900	-7.19149300	0.00291600
H	2.18028800	-6.29234000	-2.17209300
H	3.64651300	-5.82237100	-1.29843000
H	3.10675700	-7.50463200	-1.26923000
H	2.17806300	-6.28951800	2.17820200
H	3.10557100	-7.50289700	1.27785300
H	3.64512700	-5.82052000	1.30543700
H	1.10778900	-8.21663500	0.00360200
H	0.09516900	-7.07364600	0.89072700
H	0.09585900	-7.07456000	-0.88550800
C	-8.56887800	0.00255300	-0.00130900
C	-9.79496600	0.00473000	-0.00119800
C	-11.20634000	0.00725800	-0.00095600
C	-11.92191200	-1.21471200	-0.00103300
C	-11.91750700	1.23180200	-0.00057800
C	-13.31137900	-1.20414500	-0.00068200
H	-11.37313200	-2.15363300	-0.00134000
C	-13.30700200	1.22624400	-0.00026500
H	-11.36535200	2.16874200	-0.00052100
C	-14.00583800	0.01230300	-0.00030600
H	-13.85903900	-2.14414400	-0.00071600
H	-13.85127500	2.16820800	0.00002300
H	-15.09419100	0.01426400	-0.00004400

3 Singlet, E = -2255.6381158 Hatree

Pt	0.24051800	-0.03751900	-0.02149200
C	1.96043600	-2.36670600	0.02166000
C	-0.27456400	-3.05956600	0.00027000
C	2.37989100	-3.68871700	0.04011500
C	0.10480000	-4.39897400	0.01825400
H	-1.31606300	-2.76079800	-0.01890900
C	1.45791500	-4.75211500	0.03985900
H	3.44316500	-3.89466600	0.05451700
H	-0.68214100	-5.14389900	0.01444800
C	2.88201100	-1.20434700	0.01669800
C	4.27709700	-1.21723400	0.03218600
C	4.99236000	-0.00936600	0.02051700
H	4.80421700	-2.16053600	0.05344900
C	2.86837400	1.16727400	-0.01855900
C	4.25929700	1.19406300	-0.00661100
H	4.78012000	2.14335700	-0.01680600
C	1.92932900	2.31637400	-0.03861900
C	2.32799200	3.64511700	-0.05011700
C	-0.31680000	2.97442500	-0.05391900
C	1.38895800	4.69367200	-0.06460900
H	3.38808900	3.86857000	-0.04711100
C	0.04147800	4.31926700	-0.06585800
H	-1.35336800	2.65860400	-0.05190300
H	-0.75709900	5.05151300	-0.07535000
N	0.61893900	-2.06145000	0.00329600
N	2.23886900	-0.02442100	-0.00727800
N	0.59252200	1.99069000	-0.04168600
C	-1.74226600	-0.04803600	-0.03225600
C	-2.96960300	-0.04883400	-0.03459200
C	-4.39624100	-0.04664500	-0.03539000
C	-5.12398500	-0.89243100	0.83098100
C	-5.11998100	0.80361800	-0.90074900
C	-6.51193300	-0.88720300	0.83509300
H	-4.58433900	-1.55272500	1.50579700
C	-6.50789600	0.80927100	-0.90069100
H	-4.57724100	1.45989200	-1.57700400
C	-7.23152900	-0.03562400	-0.03120000
H	-7.05625200	-1.54322700	1.51061100
H	-7.04909900	1.46972200	-1.57439300
C	6.52844300	0.03542700	0.03494300
C	7.02205200	0.74828000	-1.24781500
C	6.99885000	0.82061500	1.28369300
C	7.15321000	-1.37138800	0.08102600
H	6.70019200	0.21206500	-2.14634300
H	6.65507300	1.77677300	-1.31666500

H	8.11599400	0.78731000	-1.24848100
H	6.65802100	0.33829600	2.20547900
H	8.09261600	0.85757200	1.30343200
H	6.63467800	1.85245800	1.28580900
H	8.24301300	-1.27977200	0.09190400
H	6.86238300	-1.92080500	0.98288200
H	6.88531000	-1.96965400	-0.79650700
C	1.85776100	6.15359000	-0.07674900
C	2.70465500	6.42137000	1.19149000
C	2.71926200	6.39600800	-1.34019000
C	0.67471500	7.13829600	-0.09359900
H	2.11777500	6.25524400	2.10057800
H	3.59236100	5.78325600	1.23909100
H	3.04578600	7.46159100	1.19209300
H	2.14269300	6.21239600	-2.25250800
H	3.06093700	7.43590300	-1.35726100
H	3.60726000	5.75694700	-1.36548600
H	1.05769200	8.16285200	-0.10178300
H	0.05121800	7.01203000	-0.98477300
H	0.04061800	7.03036300	0.79250300
C	1.95180700	-6.20357800	0.06224400
C	2.82893700	-6.45783900	-1.18808900
C	2.79213800	-6.43002700	1.34286700
C	0.78610700	-7.20875400	0.05617700
H	2.25778100	-6.30349900	-2.10919800
H	3.70626500	-5.80445800	-1.21967700
H	3.18822300	-7.49187800	-1.17988700
H	2.19414300	-6.25654200	2.24331100
H	3.15199900	-7.46360100	1.36740500
H	3.66770200	-5.77496300	1.38597700
H	1.18656800	-8.22651400	0.07326500
H	0.14230100	-7.09296600	0.93426500
H	0.16845500	-7.11249100	-0.84279600
C	-8.65427900	-0.02762500	-0.02703500
C	-9.87282400	-0.01873500	-0.02231200
C	-11.29542800	-0.00673300	-0.01541600
C	-12.01891400	-0.84982200	0.85656100
C	-12.01287100	0.84949500	-0.87954900
C	-13.40637500	-0.83677000	0.86432900
H	-11.47794400	-1.51378700	1.52676400
C	-13.40032200	0.86259300	-0.87139700
H	-11.46720900	1.50337100	-1.55584000
C	-14.12378500	0.01985300	0.00075400
H	-13.95223700	-1.49052900	1.54057500
H	-13.94149000	1.52668100	-1.54132100
C	-15.54690400	0.03393900	0.00949400

C	-16.76485200	0.04663500	0.01737700
C	-18.19052700	0.06183500	0.02718000
C	-18.90320600	0.92373500	-0.83314100
C	-18.90942700	-0.78452700	0.89770100
C	-20.29609400	0.93494900	-0.81898000
H	-18.35378800	1.57812300	-1.50609400
C	-20.30228300	-0.76532200	0.90357400
H	-18.36481100	-1.45079600	1.56285300
C	-21.00002900	0.09247300	0.04734400
H	-20.83509700	1.60402400	-1.48689900
H	-20.84611100	-1.42252300	1.57932600
H	-22.08810600	0.10438700	0.05518900

3 Triplet, E = -2255.571657 Hatree

Pt	0.21328600	-0.01559500	-0.00299500
C	1.93436500	-2.35501700	-0.00075600
C	-0.32149800	-3.04305700	-0.00284900
C	2.32991200	-3.69977200	0.00032400
C	0.04147500	-4.37616600	-0.00192900
H	-1.36122500	-2.73883300	-0.00411900
C	1.40734500	-4.74384300	-0.00022700
H	3.39246900	-3.91450800	0.00166300
H	-0.74929700	-5.11614500	-0.00253900
C	2.84040600	-1.22185300	-0.00034300
C	4.23555000	-1.22375100	0.00042700
C	4.95957500	-0.02062600	0.00021300
H	4.76031300	-2.16978700	0.00105800
C	2.84431700	1.18891900	-0.00095700
C	4.22880300	1.19502100	-0.00064500
H	4.75856100	2.14020200	-0.00110300
C	1.93142800	2.33069800	-0.00128400
C	2.32988700	3.66969000	0.00044200
C	-0.31949700	3.01431200	-0.00364500
C	1.40512000	4.71702500	0.00012900
H	3.39239100	3.88413400	0.00241300
C	0.04382900	4.34922900	-0.00231100
H	-1.35890700	2.70933200	-0.00517300
H	-0.74783100	5.08850500	-0.00302900
N	0.57880600	-2.03783900	-0.00231500
N	2.18934400	-0.01387500	-0.00092700
N	0.58205100	2.01219500	-0.00298200
C	-1.74235700	-0.01615900	-0.00446700
C	-2.98762400	-0.01444500	-0.00506900
C	-4.37951200	-0.01306100	-0.00543000
C	-5.11574200	-1.24094800	-0.00418000
C	-5.11319200	1.21633700	-0.00680500
C	-6.48898400	-1.24034900	-0.00410900
H	-4.57165900	-2.18103600	-0.00319700
C	-6.48639300	1.21863800	-0.00673600
H	-4.56718900	2.15530100	-0.00783800
C	-7.21324700	-0.01009900	-0.00530900
H	-7.04064900	-2.17755200	-0.00305100
H	-7.03611100	2.15698200	-0.00772200
C	6.49640500	0.02094100	-0.00024800
C	6.98816500	0.76005800	-1.26868100
C	6.98958700	0.77379100	1.25948000
C	7.11884900	-1.38805200	0.00719800
H	6.66026500	0.24287100	-2.17636300
H	6.61752600	1.78870000	-1.31492700

H	8.08260400	0.80281200	-1.27768900
H	6.66198200	0.26712000	2.17318300
H	8.08405300	0.81563500	1.26712300
H	6.62025400	1.80333300	1.29459500
H	8.20971600	-1.30275600	0.00775400
H	6.83398100	-1.95718000	0.89869200
H	6.83588700	-1.96595400	-0.87923400
C	1.88014100	6.17723400	0.00389600
C	2.72650100	6.43326600	1.27450300
C	2.74386600	6.43584300	-1.25434400
C	0.70096700	7.16740200	-0.00343400
H	2.13774500	6.26016400	2.18127900
H	3.60964100	5.78859400	1.31727400
H	3.07366100	7.47191700	1.28750200
H	2.16807500	6.26342600	-2.16953100
H	3.08988800	7.47491900	-1.26096000
H	3.62855700	5.79265700	-1.28594400
H	1.08618100	8.19149700	-0.00165900
H	0.07637800	7.05110400	-0.89528000
H	0.06594700	7.05222600	0.88115500
C	1.88193000	-6.20509000	0.00105000
C	2.73892800	-6.46498200	-1.26145400
C	2.73501100	-6.46398500	1.26641600
C	0.70225900	-7.19489700	-0.00039800
H	2.15806100	-6.29297000	-2.17357100
H	3.62254300	-5.82062800	-1.29837900
H	3.08576800	-7.50390900	-1.27010400
H	2.15127600	-6.29134200	2.17658000
H	3.08190700	-7.50287800	1.27691200
H	3.61843300	-5.81950600	1.30560500
H	1.08649400	-8.21945700	0.00068200
H	0.07093200	-7.07807800	0.88661600
H	0.07380200	-7.07887200	-0.88955000
C	-8.60923200	-0.00828800	-0.00489400
C	-9.83717900	-0.00591000	-0.00443900
C	-11.24074800	-0.00270800	-0.00373100
C	-11.96401700	-1.22483800	-0.00187200
C	-11.95811000	1.22291300	-0.00470400
C	-13.34518200	-1.21991300	-0.00096300
H	-11.41862500	-2.16565800	-0.00113100
C	-13.33926500	1.22466400	-0.00379200
H	-11.40818600	2.16108800	-0.00612800
C	-14.06150000	0.00411700	-0.00187700
H	-13.89563200	-2.15758000	0.00052000
H	-13.88518300	2.16497700	-0.00451100
C	-15.47474300	0.00766300	-0.00077100

C	-16.69528700	0.01104700	0.00025300
C	-18.11568800	0.01497800	0.00150400
C	-18.83266600	-1.20210800	0.00419600
C	-18.82590500	1.23602800	0.00015800
C	-20.22429000	-1.19156600	0.00553700
H	-18.28656300	-2.14262400	0.00524400
C	-20.21756600	1.23320000	0.00150400
H	-18.27460300	2.17350500	-0.00191100
C	-20.91953300	0.02275500	0.00419500
H	-20.77044000	-2.13261600	0.00763800
H	-20.75849600	2.17726300	0.00046200
H	-22.00778500	0.02577700	0.00524900

[Pt(ᵗBu₃tpy)Cl]⁺, Triplet, E =-1793.5212609 Hatree

Pt	0.31402700	-0.01715300	-0.00944100
C	2.00599700	-2.35600300	-0.00087800
C	-0.25709300	-3.03524400	-0.01357900
C	2.40072200	-3.71371000	-0.00046200
C	0.10813400	-4.37592200	-0.01338000
H	-1.30041100	-2.73744500	-0.01860800
C	1.47250100	-4.74863900	-0.00678200
H	3.46203500	-3.93195400	0.00425200
H	-0.68659600	-5.11134200	-0.01842800
C	2.89229200	-1.24663300	0.00496600
C	4.29988900	-1.21983500	0.01763100
C	5.00434100	-0.02802100	0.02247900
H	4.83186300	-2.16174700	0.02457400
C	2.88409200	1.21832600	0.00333100
C	4.25010000	1.22186200	0.01380900
H	4.78418500	2.16337800	0.01682800
C	1.95966100	2.36416000	-0.00266200
C	2.34516700	3.69959100	-0.00065700
C	-0.29828400	3.00131000	-0.01776600
C	1.39595000	4.73415400	-0.00737200
H	3.40352700	3.93197000	0.00614200
C	0.04793900	4.34586800	-0.01701200
H	-1.33503800	2.68204700	-0.02414100
H	-0.75680600	5.07096300	-0.02333000
N	0.64364900	-2.04321900	-0.00770700
N	2.22443800	0.00834800	-0.00169500
N	0.62628700	2.02816000	-0.01031700
Cl	-2.04803500	-0.05091100	-0.01983600
C	1.84645100	6.20033700	-0.00394200
C	2.68864100	6.46585700	1.26793900
C	2.70641600	6.46686700	-1.26361100
C	0.65153900	7.17097400	-0.01186500
H	2.10258300	6.28407200	2.17459800
H	3.58339100	5.83735400	1.31031300
H	3.01768300	7.50994200	1.27928200
H	2.13342700	6.28527300	-2.17861900
H	3.03507700	7.51112000	-1.26974000
H	3.60207800	5.83890100	-1.29369700
H	1.02229100	8.20005400	-0.00838000
H	0.03067700	7.04711500	-0.90521800
H	0.01769100	7.04576700	0.87213700
C	6.53095600	0.04330400	0.03598900
C	7.01438500	0.78917600	-1.23444700
C	6.99271900	0.81748700	1.29755700
C	7.18109600	-1.35190300	0.05744500

H	6.71229600	0.25616300	-2.14150100
H	6.62242500	1.80923100	-1.29397600
H	8.10706400	0.85768700	-1.22592200
H	6.67227300	0.30679000	2.21115200
H	8.08553500	0.88269700	1.30777100
H	6.60362000	1.83994000	1.32613300
H	8.26950800	-1.24360700	0.06772800
H	6.89948700	-1.92053600	0.95017800
H	6.91890100	-1.93936900	-0.82895900
C	1.93667000	-6.21330400	-0.00788600
C	2.78948600	-6.47387700	-1.27314900
C	2.78976700	-6.47699100	1.25647000
C	0.74975100	-7.19424100	-0.00885900
H	2.20849900	-6.29563700	-2.18388600
H	3.67868500	-5.83710800	-1.30937900
H	3.12744300	-7.51536200	-1.28390700
H	2.20920800	-6.30037300	2.16779300
H	3.12706400	-7.51869700	1.26484800
H	3.67951600	-5.84112000	1.29385100
H	1.12837600	-8.22061200	-0.00822000
H	0.12008500	-7.07438400	0.87891300
H	0.12202400	-7.07498600	-0.89806500

Excitation energies and oscillator strengths:

1 oxidative doublet

Excited State 1:	0.9675 eV	1281.49 nm	f=0.0000
142B ->144B	1.01155		
Excited State 2:	1.3081 eV	947.79 nm	f=0.0004
141B ->144B	0.99897		
Excited State 3:	1.4330 eV	865.20 nm	f=0.0008
139A ->147A	-0.11189		
140B ->144B	1.01181		
Excited State 4:	1.4887 eV	832.81 nm	f=0.0003
134B ->144B	0.11606		
139B ->144B	0.52587		
143B ->144B	0.83680		
Excited State 5:	1.8213 eV	680.76 nm	f=0.0101
139B ->144B	0.83069		
143B ->144B	-0.54140		
Excited State 6:	2.0034 eV	618.88 nm	f=0.4200
144A ->147A	-0.16476		
138B ->144B	0.95607		
Excited State 7:	2.5368 eV	488.74 nm	f=0.0263
144A ->147A	0.11591		
135B ->144B	0.16901		
137B ->144B	0.96671		
Excited State 8:	2.7791 eV	446.14 nm	f=0.0001
144A ->147A	0.14005		
129B ->144B	0.15941		
135B ->144B	0.30295		
136B ->144B	0.90702		
137B ->144B	-0.14358		
Excited State 9:	2.8960 eV	428.13 nm	f=0.0042
144A ->147A	0.22683		
123B ->144B	0.10090		
129B ->144B	0.24456		
135B ->144B	0.82422		
136B ->144B	-0.39028		
137B ->144B	-0.15316		
Excited State 10:	2.9346 eV	422.49 nm	f=0.0294
137A ->151A	0.14061		
138A ->145A	0.29941		
140A ->146A	-0.11548		
140A ->150A	-0.10436		
143A ->145A	-0.17008		
143A ->146A	0.57867		
144A ->145A	0.42235		
137B ->145B	-0.15709		
137B ->151B	0.11341		

138B ->145B -0.24537
139B ->146B 0.13272
139B ->148B 0.10533
143B ->145B 0.17049
143B ->146B -0.55636
Excited State 11: 3.0359 eV 408.40 nm f=0.0022
136A ->150A -0.10401
137A ->146A -0.14199
138A ->146A 0.15261
140A ->148A -0.12363
143A ->145A 0.67829
143A ->146A 0.15550
137B ->146B -0.19528
139B ->147B 0.12487
143B ->145B -0.64003
143B ->146B -0.15124
Excited State 12: 3.1401 eV 394.84 nm f=0.0001
112B ->144B 0.10417
122B ->144B 0.45889
130B ->144B -0.56819
131B ->144B 0.32617
133B ->144B 0.56959
Excited State 13: 3.1793 eV 389.98 nm f=0.1825
137A ->145A 0.12553
143A ->146A -0.30704
144A ->145A 0.83292
144A ->147A -0.11099
129B ->144B -0.10282
135B ->144B 0.13764
137B ->145B 0.10839
143B ->146B 0.34247
Excited State 14: 3.2099 eV 386.25 nm f=0.0024
124B ->144B 0.18016
134B ->144B 0.94676
139B ->144B -0.15171
Excited State 15: 3.4777 eV 356.51 nm f=0.0006
144A ->145A 0.17748
144A ->147A 0.11339
123B ->144B 0.35842
129B ->144B 0.80309
135B ->144B -0.32976
141B ->149B -0.12072
Excited State 16: 3.4827 eV 356.00 nm f=0.0000
117B ->144B -0.10247
132B ->144B 0.97113
133B ->144B 0.16149

Excited State 17: 3.4999 eV 354.25 nm f=0.0000
122B ->144B -0.19539
130B ->144B 0.36814
131B ->144B -0.42851
132B ->144B -0.15547
133B ->144B 0.78028
Excited State 18: 3.5071 eV 353.52 nm f=0.0027
136A ->146A -0.14792
136A ->150A 0.10269
140A ->145A -0.65038
140A ->148A 0.10416
143A ->145A 0.13671
144A ->146A 0.14275
134B ->144B -0.14322
136B ->146B 0.13129
136B ->148B -0.10235
139B ->145B 0.67302
139B ->147B -0.11200
Excited State 19: 3.5457 eV 349.68 nm f=0.0000
142A ->145A -0.65060
141B ->145B 0.75773
Excited State 20: 3.5635 eV 347.93 nm f=0.0203
140A ->145A 0.21900
143A ->145A 0.63464
144A ->146A -0.17946
139B ->145B 0.10859
143B ->145B 0.66715
Excited State 21: 3.6048 eV 343.94 nm f=0.0001
142A ->145A 0.10182
117B ->144B -0.17591
122B ->144B -0.11209
126B ->144B 0.16471
128B ->144B 0.13579
130B ->144B 0.50605
131B ->144B 0.77713
132B ->144B -0.11138
133B ->144B 0.14350
Excited State 22: 3.6261 eV 341.92 nm f=0.0005
142A ->149A 0.72353
129B ->144B -0.12639
141B ->149B -0.72027
Excited State 23: 3.6533 eV 339.38 nm f=0.0050
142A ->145A 0.74687
141B ->145B 0.64212
Excited State 24: 3.7023 eV 334.88 nm f=0.0069
138A ->146A 0.16149

140A ->145A	0.20664
144A ->146A	0.93233
138B ->146B	-0.10907
143B ->145B	0.15198

1 reductive doublet

Excited State 1:	0.5724 eV	2166.10 nm	f=0.0495
145A ->146A	0.95069		
Excited State 2:	1.5058 eV	823.35 nm	f=0.0158
145A ->147A	0.95008		
145A ->148A	0.29826		
Excited State 3:	1.5820 eV	783.72 nm	f=0.0613
145A ->147A	-0.29835		
145A ->148A	0.94716		
Excited State 4:	2.0227 eV	612.95 nm	f=0.0001
145A ->150A	0.99605		
Excited State 5:	2.3096 eV	536.81 nm	f=0.0039
145A ->149A	0.71947		
145A ->151A	-0.65731		
Excited State 6:	2.3719 eV	522.72 nm	f=0.0661
144A ->149A	0.11959		
145A ->149A	0.61402		
145A ->151A	0.70878		
144B ->145B	0.28584		
144B ->149B	-0.14398		
Excited State 7:	2.5736 eV	481.76 nm	f=0.1790
144A ->149A	0.10051		
145A ->149A	-0.26545		
145A ->151A	-0.14512		
138B ->145B	0.11632		
142B ->146B	0.12313		
144B ->145B	0.91200		
Excited State 8:	2.7585 eV	449.47 nm	f=0.0061
138A ->146A	0.12136		
144A ->146A	0.95302		
144B ->146B	-0.23253		
Excited State 9:	2.8803 eV	430.46 nm	f=0.0038
139A ->146A	-0.22101		
139A ->148A	0.10508		
142A ->146A	0.65659		
144A ->146A	0.14983		
137B ->145B	0.13625		
138B ->145B	-0.13190		
138B ->146B	-0.13391		
140B ->146B	0.19360		
142B ->146B	-0.57664		
144B ->145B	0.13339		
144B ->146B	0.32874		
Excited State 10:	2.9343 eV	422.54 nm	f=0.0243
142A ->146A	-0.25352		
144A ->146A	0.18628		

138B ->146B	0.16114		
142B ->146B	0.20838		
144B ->146B	0.89597		
Excited State 11:	3.0586 eV	405.37 nm	f=0.0005
145A ->152A	0.99515		
Excited State 12:	3.1366 eV	395.29 nm	f=0.0105
137A ->146A	0.12420		
144A ->149A	0.22834		
145A ->154A	-0.21896		
137B ->146B	-0.12286		
142B ->145B	0.87224		
142B ->146B	-0.12099		
144B ->149B	-0.21674		
Excited State 13:	3.1741 eV	390.62 nm	f=0.0015
138A ->149A	-0.17589		
140A ->152A	0.24604		
142A ->146A	-0.10342		
144A ->149A	0.62471		
145A ->149A	-0.11110		
145A ->153A	0.15026		
138B ->145B	-0.11004		
138B ->149B	0.14765		
139B ->152B	0.24736		
140B ->145B	-0.11465		
140B ->149B	0.10387		
142B ->145B	-0.28488		
144B ->145B	-0.16031		
144B ->149B	-0.61432		
Excited State 14:	3.1884 eV	388.86 nm	f=0.0000
143B ->145B	0.99278		
Excited State 15:	3.3188 eV	373.58 nm	f=0.1451
145A ->154A	0.93918		
137B ->146B	-0.11062		
142B ->145B	0.19892		
Excited State 16:	3.3574 eV	369.29 nm	f=0.0000
143A ->146A	0.98212		
141B ->145B	-0.14506		
Excited State 17:	3.3666 eV	368.28 nm	f=0.0029
143A ->146A	0.14732		
141B ->145B	0.98311		
Excited State 18:	3.4464 eV	359.75 nm	f=0.0022
144A ->149A	-0.12082		
145A ->149A	0.11392		
145A ->153A	0.97300		
Excited State 19:	3.5456 eV	349.68 nm	f=0.0001
141A ->146A	0.99231		

Excited State 20:	3.5927 eV	345.10 nm	f=0.0000
143B ->146B	0.99146		
Excited State 21:	3.6669 eV	338.11 nm	f=0.0148
138A ->147A	0.11293		
139A ->146A	-0.39501		
142A ->146A	-0.36477		
144A ->147A	0.53231		
138B ->145B	-0.25403		
138B ->146B	-0.16666		
138B ->147B	-0.12485		
140B ->145B	-0.12588		
140B ->146B	0.22015		
144B ->147B	-0.40763		
Excited State 22:	3.6741 eV	337.46 nm	f=0.0177
139A ->146A	0.49701		
139A ->147A	-0.11867		
142A ->146A	0.25274		
142A ->147A	-0.11352		
144A ->147A	0.53783		
138B ->145B	0.16424		
140B ->145B	-0.31016		
140B ->146B	-0.25872		
142B ->145B	0.13182		
142B ->146B	0.11786		
144B ->147B	-0.21635		
Excited State 23:	3.7150 eV	333.74 nm	f=0.0000
131A ->150A	0.11291		
138A ->150A	0.21941		
144A ->150A	0.56592		
145A ->155A	-0.11559		
132B ->150B	-0.13167		
137B ->150B	-0.10519		
138B ->150B	-0.20415		
140B ->150B	-0.11140		
144B ->150B	-0.73545		
Excited State 24:	3.7500 eV	330.63 nm	f=0.0988
142A ->146A	0.13293		
144A ->147A	0.55535		
140B ->145B	0.59417		
142B ->146B	0.14387		
144B ->147B	0.47770		

1 Triplet

Excited State 1:	0.7104 eV	1745.33 nm f=0.0601
145A ->146A	0.95663	
145A ->149A	-0.10513	
143B ->144B	-0.14419	
Excited State 2:	0.8610 eV	1439.99 nm f=0.0000
140B ->144B	-0.47307	
141B ->144B	0.89297	
Excited State 3:	1.0764 eV	1151.84 nm f=0.0041
140B ->144B	0.34224	
141B ->144B	0.18526	
142B ->144B	0.10611	
143B ->144B	0.89889	
Excited State 4:	1.1592 eV	1069.58 nm f=0.0002
139B ->144B	1.00035	
Excited State 5:	1.3711 eV	904.30 nm f=0.0062
145A ->147A	0.78050	
145A ->148A	0.17465	
142B ->144B	-0.65596	
Excited State 6:	1.4929 eV	830.50 nm f=0.0124
145A ->147A	0.20385	
145A ->149A	0.10980	
134B ->144B	0.10981	
140B ->144B	0.75894	
141B ->144B	0.41100	
143B ->144B	-0.40483	
Excited State 7:	1.6140 eV	768.17 nm f=0.0001
145A ->150A	0.99851	
Excited State 8:	1.6250 eV	762.97 nm f=0.0039
145A ->147A	-0.30227	
145A ->148A	0.86518	
145A ->149A	0.35256	
142B ->144B	-0.14218	
Excited State 9:	1.6557 eV	748.84 nm f=0.0005
139A ->147A	-0.10775	
138B ->144B	1.00426	
Excited State 10:	1.6987 eV	729.86 nm f=0.0649
145A ->148A	-0.38061	
145A ->149A	0.91063	
Excited State 11:	1.7930 eV	691.47 nm f=0.4225
145A ->147A	0.48978	
145A ->148A	0.25485	
145A ->149A	0.13260	
145A ->152A	-0.14918	
137B ->144B	-0.10290	
140B ->144B	-0.21009	

142B ->144B 0.68844
Excited State 12: 2.1896 eV 566.25 nm f=0.0778
145A ->152A -0.26232
137B ->144B 0.94987
Excited State 13: 2.4380 eV 508.54 nm f=0.1840
144A ->147A -0.13534
145A ->152A 0.71019
135B ->144B 0.24035
136B ->144B 0.62222
Excited State 14: 2.5489 eV 486.42 nm f=0.0142
145A ->152A -0.59184
136B ->144B 0.73490
137B ->144B -0.21522
Excited State 15: 2.6359 eV 470.36 nm f=0.0005
145A ->151A 0.99695
Excited State 16: 2.7520 eV 450.52 nm f=0.0002
143A ->146A 0.10493
144A ->147A -0.22257
145A ->152A -0.13280
145A ->153A -0.10226
128B ->144B -0.15522
135B ->144B 0.90417
136B ->144B -0.20809
137B ->144B -0.11334
Excited State 17: 2.9067 eV 426.54 nm f=0.0000
116B ->144B 0.12737
122B ->144B 0.37832
129B ->144B -0.27489
133B ->144B 0.85211
Excited State 18: 2.9825 eV 415.70 nm f=0.0001
137A ->152A -0.13190
143A ->146A 0.72366
144A ->146A -0.13260
137B ->145B 0.11285
137B ->152B -0.11290
142B ->145B -0.20215
143B ->146B -0.68974
Excited State 19: 3.0595 eV 405.25 nm f=0.0025
123B ->144B -0.13193
131B ->144B 0.26158
134B ->144B 0.92582
140B ->144B -0.14213
Excited State 20: 3.2531 eV 381.13 nm f=0.0432
138A ->146A -0.12005
145A ->154A -0.29303
131B ->144B 0.52060

134B ->144B -0.21459
137B ->146B -0.11263
140B ->145B 0.11329
143B ->145B 0.71994
Excited State 21: 3.3133 eV 374.20 nm f=0.0041
138A ->147A 0.11429
144A ->147A -0.15254
123B ->144B -0.11201
124B ->144B -0.28278
125B ->144B 0.12884
128B ->144B -0.66197
131B ->144B 0.43798
135B ->144B -0.18514
143B ->145B -0.30380
Excited State 22: 3.3169 eV 373.79 nm f=0.0047
138A ->146A 0.12374
145A ->154A -0.13599
124B ->144B 0.22473
128B ->144B 0.45917
131B ->144B 0.58161
134B ->144B -0.17665
135B ->144B 0.10865
137B ->146B 0.10933
143B ->145B -0.46437
Excited State 23: 3.3208 eV 373.36 nm f=0.0002
121B ->144B 0.48499
127B ->144B 0.56808
128B ->144B -0.16097
129B ->144B -0.28642
132B ->144B -0.54574
Excited State 24: 3.4652 eV 357.80 nm f=0.1239
145A ->154A -0.91462
131B ->144B -0.28352
134B ->144B 0.10806
143B ->145B -0.10272

2 Triplet

Excited State 1:	0.6877 eV	1802.97 nm	f=0.0596
171A ->172A	-0.22278		
171A ->173A	0.93092		
171A ->175A	-0.10451		
Excited State 2:	0.8581 eV	1444.85 nm	f=0.0344
171A ->172A	0.92291		
171A ->173A	0.22715		
163B ->170B	-0.13802		
169B ->170B	-0.37159		
Excited State 3:	1.0765 eV	1151.70 nm	f=0.0000
167B ->170B	1.00198		
167B ->173B	0.10669		
Excited State 4:	1.3001 eV	953.66 nm	f=0.2003
171A ->172A	0.13492		
165B ->170B	0.28348		
168B ->170B	0.77721		
169B ->170B	0.50338		
Excited State 5:	1.3429 eV	923.27 nm	f=0.8879
170A ->172A	-0.18778		
171A ->172A	0.21839		
165B ->170B	-0.14640		
168B ->170B	-0.52771		
169B ->170B	0.71015		
Excited State 6:	1.4018 eV	884.44 nm	f=0.0003
166B ->170B	0.99536		
Excited State 7:	1.6038 eV	773.06 nm	f=0.0403
171A ->174A	0.93648		
171A ->175A	0.31092		
163B ->170B	-0.10869		
Excited State 8:	1.6588 eV	747.41 nm	f=0.0390
171A ->174A	-0.28617		
171A ->175A	0.90459		
165B ->170B	-0.28735		
168B ->170B	0.12028		
Excited State 9:	1.7218 eV	720.10 nm	f=0.0314
171A ->174A	-0.14359		
171A ->175A	0.26752		
165B ->170B	0.88709		
168B ->170B	-0.29876		
Excited State 10:	1.7395 eV	712.75 nm	f=0.0001
171A ->176A	0.99979		
Excited State 11:	1.9198 eV	645.83 nm	f=0.0008
164B ->170B	0.99750		
Excited State 12:	1.9764 eV	627.31 nm	f=0.0002
171A ->178A	0.15733		

162B ->170B 0.99696
Excited State 13: 1.9846 eV 624.74 nm f=0.0195
170A ->172A 0.14723
171A ->177A -0.17867
171A ->179A -0.13862
163B ->170B 0.94631
Excited State 14: 2.2246 eV 557.32 nm f=0.0000
160B ->170B 0.99680
Excited State 15: 2.3920 eV 518.33 nm f=0.0043
171A ->179A -0.67286
161B ->170B 0.72575
163B ->170B -0.10922
Excited State 16: 2.4548 eV 505.07 nm f=0.0500
170A ->172A 0.10474
171A ->177A 0.60382
171A ->179A -0.54095
158B ->170B -0.10573
159B ->170B -0.19507
161B ->170B -0.49666
Excited State 17: 2.4851 eV 498.91 nm f=0.0004
171A ->178A 0.98795
162B ->170B -0.13227
Excited State 18: 2.5694 eV 482.54 nm f=0.0593
170A ->172A 0.17947
171A ->177A 0.73964
171A ->179A 0.42645
171A ->181A -0.10222
161B ->170B 0.41669
163B ->170B 0.12303
Excited State 19: 2.7233 eV 455.28 nm f=0.0431
170A ->172A -0.17677
171A ->177A 0.11924
171A ->179A -0.11764
158B ->170B 0.33762
159B ->170B 0.87016
161B ->170B -0.14125
Excited State 20: 2.8020 eV 442.49 nm f=0.5761
170A ->172A 0.70228
155B ->170B 0.12525
158B ->170B -0.47660
159B ->170B 0.35847
163B ->170B -0.12790
169B ->171B -0.20937
169B ->173B 0.16514
Excited State 21: 2.9132 eV 425.59 nm f=0.1114
168A ->172A -0.18130

168A ->177A 0.12087
169A ->173A -0.33782
170A ->172A 0.35141
170A ->177A -0.14657
158B ->170B 0.67547
159B ->170B -0.21710
168B ->172B 0.27733
169B ->171B -0.24269
169B ->173B 0.13981
Excited State 22: 2.9675 eV 417.81 nm f=0.0731
161A ->179A 0.11760
168A ->172A -0.13806
169A ->172A -0.13431
169A ->173A 0.62335
170A ->172A 0.25863
158B ->170B 0.25319
163B ->171B 0.15383
168B ->172B -0.61051
169B ->172B -0.13158
169B ->173B 0.16486
Excited State 23: 3.0034 eV 412.82 nm f=0.0002
171A ->180A 0.99856
Excited State 24: 3.1121 eV 398.40 nm f=0.0000
145B ->170B 0.28495
151B ->170B 0.18811
156B ->170B 0.91723

3 Triplet

Excited State 1:	0.6735 eV	1840.93 nm f=0.0588
197A -> 198A	-0.26066	
197A -> 199A	0.91918	
197A -> 202A	-0.10200	
Excited State 2:	0.7215 eV	1718.50 nm f=0.0192
197A -> 198A	0.89638	
197A -> 199A	0.26704	
193B -> 196B	-0.22387	
195B -> 196B	-0.34185	
Excited State 3:	0.9762 eV	1270.09 nm f=1.4628
196A -> 198A	-0.16123	
197A -> 198A	0.27729	
197A -> 200A	0.13313	
195B -> 196B	0.85661	
Excited State 4:	1.1261 eV	1101.04 nm f=0.0000
192B -> 196B	0.99909	
Excited State 5:	1.3548 eV	915.18 nm f=0.0011
190B -> 196B	0.27170	
194B -> 196B	0.95262	
Excited State 6:	1.4578 eV	850.49 nm f=0.0003
191B -> 196B	0.99512	
Excited State 7:	1.5806 eV	784.41 nm f=0.0011
197A -> 200A	0.11204	
197A -> 201A	0.86374	
197A -> 202A	0.28646	
193B -> 196B	-0.38471	
Excited State 8:	1.6472 eV	752.70 nm f=0.1637
195A -> 198A	-0.11638	
196A -> 200A	-0.10195	
197A -> 198A	0.12942	
197A -> 200A	-0.35778	
197A -> 201A	0.35722	
197A -> 202A	0.18972	
190B -> 196B	-0.11040	
193B -> 196B	0.78315	
Excited State 9:	1.6505 eV	751.20 nm f=0.0511
197A -> 201A	-0.33565	
197A -> 202A	0.92374	
190B -> 196B	-0.13098	
Excited State 10:	1.7710 eV	700.08 nm f=0.0193
197A -> 202A	0.12982	
190B -> 196B	0.93415	
193B -> 196B	0.11124	
194B -> 196B	-0.26275	
Excited State 11:	1.7862 eV	694.14 nm f=0.0001

197A -> 203A 0.99959
Excited State 12: 1.8416 eV 673.25 nm f=0.0022
197A -> 200A 0.88507
188B -> 196B -0.18074
193B -> 196B 0.34649
Excited State 13: 1.9839 eV 624.95 nm f=0.0004
189B -> 196B 0.99816
Excited State 14: 2.0095 eV 617.00 nm f=0.0001
197A -> 204A -0.15730
185B -> 196B 0.99617
Excited State 15: 2.1281 eV 582.59 nm f=0.0380
195A -> 198A 0.11886
196A -> 198A 0.23009
197A -> 200A 0.16230
197A -> 206A -0.11697
188B -> 196B 0.93119
Excited State 16: 2.1329 eV 581.29 nm f=0.0004
187B -> 196B 0.99817
Excited State 17: 2.2774 eV 544.40 nm f=0.0000
183B -> 196B 0.93707
186B -> 196B 0.34368
Excited State 18: 2.3844 eV 519.97 nm f=0.0000
183B -> 196B -0.34414
186B -> 196B 0.93345
Excited State 19: 2.3993 eV 516.75 nm f=0.1964
195A -> 200A -0.11970
196A -> 198A -0.53259
196A -> 200A 0.13967
197A -> 206A 0.59500
184B -> 196B -0.42300
188B -> 196B 0.18696
195B -> 197B 0.25545
195B -> 198B -0.18763
195B -> 200B 0.10205
Excited State 20: 2.4242 eV 511.44 nm f=0.5744
195A -> 198A -0.12948
195A -> 200A 0.13602
196A -> 198A 0.57967
196A -> 200A -0.18435
197A -> 206A 0.64097
197A -> 207A 0.12353
184B -> 196B -0.16942
195B -> 197B -0.26911
195B -> 198B 0.22268
195B -> 200B -0.12384
Excited State 21: 2.4998 eV 495.99 nm f=0.0002

197A -> 204A 0.98783
185B -> 196B 0.13359
Excited State 22: 2.5377 eV 488.57 nm f=0.0255
197A -> 206A 0.39326
182B -> 196B -0.10578
184B -> 196B 0.85959
195B -> 197B 0.14435
Excited State 23: 2.7739 eV 446.97 nm f=0.2176
195A -> 198A 0.27894
195A -> 200A 0.11305
196A -> 198A 0.27114
196A -> 200A 0.16875
172B -> 196B 0.10764
181B -> 196B 0.34703
182B -> 196B 0.73412
188B -> 196B -0.10599
195B -> 197B 0.21825
195B -> 198B -0.17691
Excited State 24: 2.8000 eV 442.79 nm f=0.0002
197A -> 205A 0.99805

[Pt(^{t}Bu$_3$tpy)Cl]$^+$, Triplet

Excited State 1:	0.4892 eV	2534.28 nm	f=0.0016
127A ->128A	-0.32460		
117B ->126B	-0.13820		
124B ->126B	-0.38195		
125B ->126B	0.88629		
Excited State 2:	0.5309 eV	2335.39 nm	f=0.0000
122B ->126B	0.94954		
123B ->126B	0.39002		
Excited State 3:	0.8307 eV	1492.52 nm	f=0.0016
127A ->128A	-0.58235		
112B ->126B	0.11183		
117B ->126B	0.12439		
124B ->126B	0.78609		
125B ->126B	0.28203		
Excited State 4:	0.9325 eV	1329.56 nm	f=0.0000
122B ->126B	-0.38597		
123B ->126B	0.90547		
Excited State 5:	1.0730 eV	1155.52 nm	f=0.0643
127A ->128A	0.76888		
124B ->126B	0.39197		
125B ->126B	0.33810		
Excited State 6:	1.4094 eV	879.68 nm	f=0.0000
127A ->129A	0.99705		
Excited State 7:	1.5708 eV	789.30 nm	f=0.0146
127A ->130A	-0.14741		
127A ->131A	-0.16889		
127A ->132A	-0.24597		
120B ->126B	-0.37677		
121B ->126B	0.89295		
Excited State 8:	1.6527 eV	750.18 nm	f=0.0630
127A ->130A	0.31531		
127A ->131A	0.16536		
127A ->132A	0.17918		
120B ->126B	0.81957		
121B ->126B	0.40376		
Excited State 9:	1.9387 eV	639.52 nm	f=0.0158
127A ->130A	0.47401		
127A ->131A	0.59188		
127A ->132A	-0.11335		
117B ->126B	-0.15030		
119B ->126B	0.54695		
120B ->126B	-0.28632		
Excited State 10:	2.1486 eV	577.06 nm	f=0.0688
127A ->130A	-0.43280		
127A ->131A	-0.28878		

127A ->132A 0.20307
119B ->126B 0.76644
120B ->126B 0.10620
124B ->126B 0.10780
Excited State 11: 2.1856 eV 567.28 nm f=0.0218
127A ->130A -0.67690
127A ->131A 0.70284
119B ->126B -0.11487
Excited State 12: 2.4688 eV 502.20 nm f=0.0000
105B ->126B -0.36080
113B ->126B 0.10744
114B ->126B -0.24875
115B ->126B 0.25741
116B ->126B -0.34734
118B ->126B 0.75639
Excited State 13: 2.5377 eV 488.56 nm f=0.0093
127A ->132A -0.21951
107B ->126B 0.21484
113B ->126B -0.14862
117B ->126B 0.86833
119B ->126B 0.22630
124B ->126B -0.19585
Excited State 14: 2.6030 eV 476.31 nm f=0.0007
106B ->126B 0.43771
109B ->126B -0.20130
111B ->126B 0.79959
114B ->126B 0.24772
116B ->126B -0.23128
Excited State 15: 2.6255 eV 472.23 nm f=0.0515
127A ->132A 0.61286
107B ->126B 0.23068
110B ->126B 0.15451
112B ->126B 0.67005
120B ->126B -0.17524
124B ->126B -0.12229
125B ->128B 0.11759
Excited State 16: 2.7258 eV 454.86 nm f=0.0159
127A ->132A 0.27183
107B ->126B -0.17249
108B ->126B 0.30540
112B ->126B -0.28146
113B ->126B 0.68598
114B ->126B 0.30572
117B ->126B 0.29522
Excited State 17: 2.8680 eV 432.29 nm f=0.0893
126A ->128A -0.21624

127A ->132A 0.55241
107B ->126B -0.11030
112B ->126B -0.51463
113B ->126B -0.44709
114B ->126B -0.19836
120B ->126B -0.10107
125B ->127B -0.16940
Excited State 18: 2.8974 eV 427.91 nm f=0.0000
101B ->126B 0.12191
105B ->126B 0.17888
106B ->126B 0.10218
111B ->126B 0.15561
115B ->126B -0.35590
116B ->126B 0.67250
118B ->126B 0.56849
Excited State 19: 2.9613 eV 418.69 nm f=0.0000
105B ->126B 0.13787
109B ->126B 0.11044
111B ->126B -0.19423
113B ->126B -0.33091
114B ->126B 0.71351
115B ->126B 0.50176
118B ->126B 0.20365
Excited State 20: 3.0833 eV 402.12 nm f=0.0000
101B ->126B -0.10277
105B ->126B -0.16423
106B ->126B 0.18148
111B ->126B 0.11652
113B ->126B 0.14071
114B ->126B -0.31804
115B ->126B 0.67580
116B ->126B 0.54034
118B ->126B -0.18359
Excited State 21: 3.1700 eV 391.11 nm f=0.0101
121A ->128A 0.16843
121A ->132A -0.12232
125A ->128A -0.16300
126A ->128A 0.63039
108B ->126B 0.11435
112B ->126B -0.12981
113B ->126B -0.13006
121B ->127B -0.20002
121B ->128B -0.21395
124B ->130B 0.10444
125B ->127B 0.20804
125B ->128B 0.63828

Excited State 22: 3.1715 eV 390.93 nm f=0.0002
99B ->126B 0.10131
100B ->126B 0.13912
101B ->126B 0.21612
105B ->126B 0.39412
106B ->126B -0.40499
109B ->126B 0.51211
111B ->126B 0.40589
113B ->126B 0.10140
114B ->126B -0.22840
115B ->126B 0.24274
116B ->126B -0.16089
Excited State 23: 3.2006 eV 387.38 nm f=0.0002
100B ->126B 0.11242
101B ->126B 0.17642
105B ->126B 0.37853
106B ->126B 0.73855
109B ->126B 0.19928
111B ->126B -0.32729
114B ->126B -0.17217
116B ->126B -0.20551
Excited State 24: 3.2795 eV 378.06 nm f=0.0022
108B ->126B 0.49885
110B ->126B 0.78928
112B ->126B -0.18912
113B ->126B -0.11829
117B ->126B -0.13141
125B ->127B 0.11725
125B ->128B -0.10817

1 Ground State Singlet

Excited State	1:	Singlet-A	2.2624 eV	548.03 nm	f=0.1031
144 ->145		0.69132			
Excited State	2:	Singlet-A	2.6023 eV	476.43 nm	f=0.0110
144 ->146		0.70193			
Excited State	3:	Singlet-A	2.8246 eV	438.95 nm	f=0.0748
143 ->145		0.68934			
Excited State	4:	Singlet-A	3.1598 eV	392.38 nm	f=0.0035
141 ->145		0.68753			
143 ->146		-0.12909			
Excited State	5:	Singlet-A	3.1794 eV	389.96 nm	f=0.0100
141 ->145		0.12859			
143 ->146		0.68852			
Excited State	6:	Singlet-A	3.3587 eV	369.15 nm	f=0.0094
140 ->145		0.68867			
Excited State	7:	Singlet-A	3.4771 eV	356.57 nm	f=0.0003
142 ->145		0.70517			
Excited State	8:	Singlet-A	3.4926 eV	354.99 nm	f=0.0046
144 ->147		0.70159			
Excited State	9:	Singlet-A	3.5256 eV	351.67 nm	f=0.0025
144 ->148		0.69812			
Excited State	10:	Singlet-A	3.5884 eV	345.51 nm	f=0.0000
141 ->146		0.70338			
Excited State	11:	Singlet-A	3.6286 eV	341.69 nm	f=0.0017
138 ->149		0.13205			
144 ->149		0.67192			
Excited State	12:	Singlet-A	3.8347 eV	323.32 nm	f=0.0000
142 ->146		0.70690			
Excited State	13:	Singlet-A	3.8749 eV	319.97 nm	f=0.0739
138 ->145		0.23315			
139 ->146		0.18532			
140 ->146		0.59232			
141 ->149		-0.14830			
Excited State	14:	Singlet-A	3.9292 eV	315.55 nm	f=0.3551
139 ->145		0.63574			
140 ->147		0.11398			
143 ->149		-0.18333			
Excited State	15:	Singlet-A	4.0325 eV	307.46 nm	f=0.0671
139 ->145		0.16767			
143 ->148		-0.12392			
143 ->149		0.63982			
Excited State	16:	Singlet-A	4.0569 eV	305.62 nm	f=0.0306
138 ->145		0.61179			
139 ->146		-0.14772			
140 ->146		-0.18449			
140 ->148		-0.10617			

143 ->147 -0.12941
Excited State 17: Singlet-A 4.0764 eV 304.15 nm f=0.0175
143 ->147 0.68362
Excited State 18: Singlet-A 4.1045 eV 302.07 nm f=0.0044
143 ->148 0.69068
143 ->149 0.12108
Excited State 19: Singlet-A 4.1997 eV 295.22 nm f=0.0189
138 ->145 0.12520
141 ->149 0.64880
Excited State 20: Singlet-A 4.3744 eV 283.43 nm f=0.0101
138 ->146 -0.27444
139 ->146 -0.27136
144 ->150 0.56693
Excited State 21: Singlet-A 4.3785 eV 283.16 nm f=0.0519
138 ->146 0.59825
140 ->147 -0.12778
144 ->150 0.29997
Excited State 22: Singlet-A 4.4730 eV 277.18 nm f=0.2957
136 ->145 -0.15828
137 ->145 -0.10224
139 ->146 0.51006
140 ->146 -0.18937
140 ->148 0.13147
144 ->150 0.27143
Excited State 23: Singlet-A 4.5220 eV 274.18 nm f=0.0497
139 ->149 -0.15685
140 ->149 -0.44192
141 ->147 -0.13863
141 ->148 0.43876
144 ->151 0.13550
Excited State 24: Singlet-A 4.5384 eV 273.19 nm f=0.0055
140 ->149 -0.11090
141 ->147 0.68970

2 Ground State Singlet

Excited State	1:	Singlet-A	2.0587 eV	602.26 nm	f=0.1573
170 ->171		0.69201			
Excited State	2:	Singlet-A	2.4087 eV	514.73 nm	f=0.0066
170 ->172		0.69852			
Excited State	3:	Singlet-A	2.8584 eV	433.76 nm	f=0.1536
168 ->171		0.39986			
169 ->171		0.56008			
Excited State	4:	Singlet-A	3.1136 eV	398.21 nm	f=0.0133
168 ->171		0.56538			
169 ->171		-0.38847			
170 ->171		0.10792			
Excited State	5:	Singlet-A	3.1703 eV	391.08 nm	f=0.0034
165 ->171		0.69619			
Excited State	6:	Singlet-A	3.1997 eV	387.49 nm	f=0.0149
168 ->172		0.30420			
169 ->172		0.62474			
Excited State	7:	Singlet-A	3.3058 eV	375.05 nm	f=0.0136
170 ->173		0.69686			
Excited State	8:	Singlet-A	3.3411 eV	371.09 nm	f=0.0006
164 ->171		0.11084			
170 ->174		0.68298			
Excited State	9:	Singlet-A	3.3647 eV	368.48 nm	f=0.0106
164 ->171		0.67845			
170 ->174		-0.11462			
Excited State	10:	Singlet-A	3.4863 eV	355.63 nm	f=0.0005
168 ->172		0.61890			
169 ->172		-0.29331			
Excited State	11:	Singlet-A	3.5382 eV	350.42 nm	f=0.0031
168 ->176		-0.13578			
169 ->176		0.17643			
170 ->176		0.64294			
Excited State	12:	Singlet-A	3.5807 eV	346.26 nm	f=1.8603
170 ->175		0.64426			
Excited State	13:	Singlet-A	3.6019 eV	344.22 nm	f=0.0043
165 ->172		0.70266			
Excited State	14:	Singlet-A	3.6643 eV	338.36 nm	f=0.0005
166 ->171		0.70453			
Excited State	15:	Singlet-A	3.6957 eV	335.48 nm	f=0.0001
167 ->171		0.70624			
Excited State	16:	Singlet-A	3.9014 eV	317.80 nm	f=0.0211
161 ->171		-0.11342			
162 ->171		-0.13388			
162 ->172		0.19946			
164 ->172		0.59377			
165 ->176		-0.14117			

Excited State	17:	Singlet-A	3.9327 eV	315.27 nm	f=0.3778
162 ->171	0.63354				
164 ->172	0.11633				
164 ->173	0.11570				
169 ->176	-0.11545				
Excited State	18:	Singlet-A	4.0289 eV	307.74 nm	f=0.0000
166 ->172	0.69638				
167 ->172	-0.12024				
Excited State	19:	Singlet-A	4.0331 eV	307.42 nm	f=0.0004
163 ->171	0.70087				
Excited State	20:	Singlet-A	4.0346 eV	307.30 nm	f=0.0000
166 ->172	0.12036				
167 ->172	0.69669				
Excited State	21:	Singlet-A	4.0451 eV	306.51 nm	f=0.0516
162 ->171	0.13590				
168 ->176	0.39953				
169 ->176	0.51649				
Excited State	22:	Singlet-A	4.1054 eV	302.00 nm	f=0.0034
168 ->173	0.33006				
169 ->173	0.60655				
Excited State	23:	Singlet-A	4.1323 eV	300.04 nm	f=0.0044
168 ->174	0.33440				
169 ->174	0.61006				
Excited State	24:	Singlet-A	4.1720 eV	297.18 nm	f=0.0004
160 ->171	0.12548				
161 ->171	0.28604				
162 ->172	0.12873				
164 ->172	0.13161				
164 ->174	0.13740				
165 ->176	0.52346				
168 ->175	-0.11471				
169 ->175	-0.13450				
170 ->177	-0.10119				

3 Ground State Singlet

Excited State 1: Singlet-A 2.0017 eV 619.41 nm f=0.2049
195 -> 197 -0.14157
196 -> 197 0.68392
Excited State 2: Singlet-A 2.3512 eV 527.33 nm f=0.0056
195 -> 198 -0.14139
196 -> 198 0.69012
Excited State 3: Singlet-A 2.6853 eV 461.71 nm f=0.0572
193 -> 197 0.10308
195 -> 197 0.67323
196 -> 197 0.15757
Excited State 4: Singlet-A 2.8633 eV 433.01 nm f=0.3301
194 -> 197 0.67337
196 -> 199 -0.13638
Excited State 5: Singlet-A 3.0182 eV 410.79 nm f=0.0084
194 -> 198 0.13686
195 -> 198 0.66804
196 -> 198 0.14817
Excited State 6: Singlet-A 3.1152 eV 398.00 nm f=2.4313
194 -> 197 0.12289
196 -> 199 0.64701
Excited State 7: Singlet-A 3.1721 eV 390.86 nm f=0.0034
189 -> 197 0.69766
Excited State 8: Singlet-A 3.2424 eV 382.39 nm f=0.0079
194 -> 198 0.68182
195 -> 198 -0.12906
Excited State 9: Singlet-A 3.2539 eV 381.04 nm f=0.0025
195 -> 200 -0.15383
196 -> 200 0.68656
Excited State 10: Singlet-A 3.2935 eV 376.46 nm f=0.0015
195 -> 201 -0.16113
196 -> 201 0.68160
Excited State 11: Singlet-A 3.3650 eV 368.46 nm f=0.0085
188 -> 197 0.68642
Excited State 12: Singlet-A 3.5225 eV 351.98 nm f=0.0015
193 -> 202 -0.12441
195 -> 202 -0.29194
196 -> 202 0.60675
Excited State 13: Singlet-A 3.5248 eV 351.75 nm f=0.0035
184 -> 197 0.11107
193 -> 197 0.66637
195 -> 197 -0.12161
Excited State 14: Singlet-A 3.6046 eV 343.96 nm f=0.0000
189 -> 198 0.70267
Excited State 15: Singlet-A 3.6826 eV 336.67 nm f=0.0005
191 -> 197 0.70432

Excited State 16: Singlet-A 3.7470 eV 330.89 nm f=0.0000
192 -> 197 0.70691
Excited State 17: Singlet-A 3.8119 eV 325.25 nm f=0.0124
188 -> 198 0.10441
195 -> 199 0.65003
196 -> 203 0.13467
196 -> 204 -0.14736
Excited State 18: Singlet-A 3.8692 eV 320.44 nm f=0.0270
184 -> 198 0.11686
185 -> 197 -0.24768
193 -> 198 0.62834
195 -> 198 -0.10935
Excited State 19: Singlet-A 3.8799 eV 319.55 nm f=0.0003
190 -> 197 0.70530
Excited State 20: Singlet-A 3.8973 eV 318.13 nm f=0.0393
185 -> 198 0.18063
188 -> 198 0.53954
189 -> 202 0.12937
194 -> 200 -0.11774
195 -> 200 -0.28676
Excited State 21: Singlet-A 3.9389 eV 314.77 nm f=0.2319
185 -> 197 -0.47444
188 -> 198 0.10600
193 -> 198 -0.20302
195 -> 200 0.39570
Excited State 22: Singlet-A 3.9456 eV 314.24 nm f=0.1644
185 -> 197 0.36570
185 -> 198 0.11941
188 -> 198 0.23997
193 -> 198 0.14752
195 -> 200 0.45447
196 -> 200 0.10202
Excited State 23: Singlet-A 3.9767 eV 311.78 nm f=0.0004
194 -> 201 0.14457
195 -> 201 0.65891
196 -> 201 0.16480
Excited State 24: Singlet-A 4.0495 eV 306.17 nm f=0.0000
191 -> 198 0.70637