Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Supporting Information for

A Spectroscopic and Computational Study on the Effects of Methyl and Phenyl Substituted Phenanthroline Ligands on the Photochemical Properties of Re(I) Tricarbonyl Complexes Containing 2,6-Dimethylphenylisocyanide

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Table S1. Optimized geometries of complexes **8.1 – 8.6** in the singlet ground state.

1. Optimized geometry of $[Re(CO)_3(CNx)(phen)]^+$ (**8.1**) in the singlet ground state in the gas phase with E(RB+HF-LYP) = -1393.363920 au.

Atom	Coordinates		
	x	y	z
Re	0.67001100	-1.27246100	-0.26282700
C	2.49275300	-2.10339700	-0.36537100
C	0.02558100	-2.77880400	0.80416300
C	0.14083900	-2.18872300	-1.90804600
C	-1.23136100	-0.38110200	-0.14370700
N	1.44927900	0.59574800	-1.20885100
C	1.51829300	0.85730400	-2.51444000
C	2.04022000	2.05492500	-3.02079600
C	2.50505600	3.01372400	-2.14735900
C	2.44814500	2.77085200	-0.75967000
C	1.90876700	1.53596100	-0.33248800
H	1.15035400	0.09064300	-3.18369000
H	2.07145600	2.20470900	-4.09209000
H	2.91555600	3.94776100	-2.51335500
C	2.91155900	3.70844300	0.22113700
N	1.32371700	0.02669100	1.43441800
C	1.83973800	1.23567800	1.06748100
C	2.30673100	2.17839500	2.01144900
C	2.22296500	1.83319800	3.37586900
C	1.70066700	0.60918900	3.73223300
C	1.26142500	-0.26914500	2.73282200
C	2.84268700	3.42510200	1.54855500
H	2.57191400	2.52997100	4.12925000
H	1.62444000	0.30851000	4.76896900
H	0.85255200	-1.23710600	2.99136700
O	-0.16503600	-2.68846900	-2.89451400
N	-2.30501800	0.07254600	-0.08145000
O	3.52657500	-2.58399800	-0.42628900
O	-0.35020200	-3.63793700	1.46606300
C	-3.59901400	0.57078200	0.00361600
C	-4.49982400	-0.06002000	0.88337100
C	-5.79144400	0.46005500	0.94811100
C	-6.16417000	1.55393400	0.17272100
C	-5.25034000	2.15395100	-0.68891700
C	-3.94547700	1.67687900	-0.79532500
H	-6.51138500	-0.00193500	1.61331900
H	-7.17436800	1.94018400	0.23857700
H	-5.55184300	3.00299100	-1.29104800
C	-2.94829300	2.30989300	-1.72895200
H	-3.39653400	3.15239700	-2.25536600
H	-2.07112100	2.67761900	-1.18748500
H	-2.59465100	1.59452800	-2.47775700
C	-4.08488700	-1.24623400	1.71187500
H	-3.76471100	-2.08191900	1.08259000
H	-3.24975300	-0.99932500	2.37466700
H	-4.91301700	-1.59120700	2.33043200
H	3.19746200	4.13877200	2.28276700
H	3.32255900	4.65129600	-0.11999000

2. Optimized geometry of $[Re(CO)_3(CNx)(4\text{-methyl-phen})]^+$ (**8.2**) in the singlet ground state in the gas phase with E(RB+HF-LYP) = -1432.69477 au.

Atom	Coordinates		
	x	y	z
Re	-0.41987900	-1.46116400	-0.03169900
C	-2.13854800	-2.49431200	-0.06104600
C	0.23301500	-2.47208000	-1.57272500
C	0.36983600	-2.77523200	1.18304900
C	1.36925000	-0.35693800	-0.00113300
N	-1.25228400	-0.08788300	1.51868400
C	-1.19111500	-0.25839900	2.83947600
C	-1.76097400	0.64270700	3.74868300
C	-2.41519400	1.75767200	3.27378600
C	-2.49883900	1.96934900	1.88216600
C	-1.89870300	1.01280900	1.03284800
H	-0.67578200	-1.14237200	3.19122100
H	-1.67944200	0.44401400	4.80930200
H	-2.86774400	2.46996900	3.95404100
C	-3.16121600	3.09520900	1.29743100
N	-1.37676400	0.21275700	-1.15858700
C	-1.96523400	1.17635400	-0.39122500
C	-2.62820900	2.29624300	-0.94423800
C	-2.67970800	2.42110600	-2.36230000
C	-2.07144400	1.42511900	-3.10630800
C	-1.43709600	0.34748400	-2.48185000
C	-3.22147100	3.25064900	-0.05216400
H	-2.08024300	1.46379900	-4.18843100
H	-0.96853800	-0.42938500	-3.07186100
O	0.82751500	-3.51759500	1.92908800
N	2.38745000	0.21386600	0.01310000
O	-3.11252400	-3.09014700	-0.07786700
O	0.60757100	-3.03163000	-2.50248600
C	3.61835000	0.85768300	0.01278900
C	4.48856000	0.63417100	-1.07159300
C	5.71902700	1.28860700	-1.04232300
C	6.06275600	2.12351800	0.01663700
C	5.18025700	2.32313700	1.07443200
C	3.93681700	1.69478900	1.09893000
H	6.41424100	1.13720300	-1.85969200
H	7.02558900	2.62048100	0.01872300
H	5.45871300	2.97278700	1.89587600
C	2.97575600	1.89334500	2.24067800
H	3.38957600	2.58419500	2.97513600
H	2.02099300	2.30065700	1.89392100
H	2.76272700	0.94833400	2.74976000
C	4.10736400	-0.27677800	-2.20774700
H	3.93238900	-1.29914300	-1.85965400
H	3.19070200	0.06014300	-2.70127400
H	4.89893800	-0.30869600	-2.95591400
H	-3.72991300	4.11018600	-0.46818200
H	-3.61917600	3.82505300	1.95465000
C	-3.36549900	3.57835400	-3.03137600
H	-4.42547300	3.61749200	-2.76405600

H	-2.91760600	4.53034800	-2.73208700
H	-3.29478600	3.49859200	-4.11560600

3. Optimized geometry of $[Re(CO)_3(CNx)(4,7\text{-dimethyl-phen})]^+$ (**8.3**) in the singlet ground state in the gas phase with E(RB+HF-LYP) = -1472.02584 au.

Atom	Coordinates		
	x	y	z
Re	0.07894900	-1.56678200	-0.04400200
C	1.60682300	-2.86498200	-0.05784400
C	-0.84683900	-2.64106600	1.30176900
C	-0.80948300	-2.56483500	-1.47123000
C	-1.50655900	-0.18754300	-0.02514600
N	1.23781600	-0.16434900	-1.33617300
C	1.24860400	-0.14653400	-2.66738800
C	2.02382400	0.75007200	-3.40845500
C	2.83211700	1.67884100	-2.77754600
C	2.83297600	1.67841900	-1.35284600
C	2.02100300	0.73962700	-0.67652700
H	0.62214600	-0.87291000	-3.16848700
H	1.98162300	0.70011800	-4.48932000
C	3.62117200	2.58181800	-0.56939500
N	1.20094900	-0.23370100	1.35002700
C	2.00047900	0.70321200	0.75941400
C	2.79083400	1.60752500	1.50489500
C	2.74804400	1.53778400	2.92722800
C	1.92486200	0.57722800	3.48722600
C	1.17422400	-0.28267100	2.68027900
C	3.60060100	2.54842700	0.79077000
H	1.85134300	0.47336500	4.56257900
H	0.53627500	-1.03416000	3.12686800
O	-1.31959400	-3.11860700	-2.33797700
N	-2.42021900	0.53934600	-0.01458600
O	2.47275400	-3.60960300	-0.06539900
O	-1.38049900	-3.24155500	2.12212400
C	-3.55104800	1.34552300	0.00035600
C	-4.81079700	0.72362600	0.10283300
C	-5.92879200	1.55626500	0.11556500
C	-5.79561400	2.93878900	0.02955900
C	-4.53596000	3.52253200	-0.07171700
C	-3.38316700	2.74017800	-0.08888800
H	-6.91396100	1.11169900	0.19320000
H	-6.67934400	3.56565900	0.04107000
H	-4.44302200	4.60019500	-0.13868800
C	-2.01391700	3.35661200	-0.20021800
H	-2.08576300	4.44290500	-0.25387300
H	-1.38942100	3.10135200	0.66149900
H	-1.49153500	3.00789500	-1.09643900
C	-4.94058900	-0.77318300	0.19288200
H	-4.50957400	-1.26572100	-0.68388500
H	-4.42531800	-1.16800000	1.07369400
H	-5.98851900	-1.06459400	0.25906400
H	4.21094400	3.24532300	1.34960200
H	4.24825500	3.30457900	-1.07422700
C	3.56178300	2.46014600	3.79003800

H	4.63192600	2.33555200	3.60022600
H	3.31522600	3.50751900	3.59373000
H	3.38249200	2.26374700	4.84656400
C	3.67338400	2.63917800	-3.56964900
H	3.42033300	3.67677300	-3.33358400
H	4.73667600	2.50458000	-3.35061900
H	3.52918700	2.49190500	-4.63946500

4. Optimized geometry of $[Re(CO)_3(CNx)(3,4,7,8\text{-tetramethyl-phen})]^+$ (**8.4**) in the singlet ground state in the gas phase with E(RB+HF-LYP) = -1550.68093 au.

Atom	Coordinates		
	x	y	z
Re	0.04161100	-0.58965400	-1.49597000
C	1.60929800	-1.19340100	-2.58954900
C	-0.95358000	-2.19401200	-2.00058400
C	-0.68808500	0.37167400	-3.03432000
C	-1.58050400	0.04572200	-0.32211300
N	1.25737300	1.08043100	-0.65153800
C	1.39474300	2.29950100	-1.16749200
C	2.19127200	3.31355400	-0.60844000
C	2.88749300	3.03943100	0.56909400
C	2.75430500	1.74203500	1.13918100
C	1.93204300	0.79231900	0.49622400
H	0.84851700	2.49561300	-2.08174100
C	3.42320200	1.33944200	2.34261800
N	0.98844300	-1.40015700	0.35540500
C	1.78728800	-0.53068100	1.03429000
C	2.46236600	-0.90180000	2.21652000
C	2.30550200	-2.22556800	2.71536200
C	1.48496200	-3.10163100	2.00433000
C	0.85592700	-2.63305400	0.83813000
C	3.28421000	0.08632700	2.85360600
H	0.21811200	-3.30112400	0.27285700
O	-1.10215000	0.97545300	-3.91890800
N	-2.51071300	0.38135000	0.29888500
O	2.49819100	-1.53798500	-3.21878300
O	-1.52866000	-3.15519400	-2.25562300
C	-3.64958300	0.74217500	1.00722700
C	-4.74564100	-0.14213900	1.00313900
C	-5.87568100	0.24490000	1.72177000
C	-5.91012800	1.45465400	2.40869800
C	-4.81067100	2.30803800	2.39136700
C	-3.65411900	1.97314600	1.68987900
H	-6.73793300	-0.41124000	1.73844500
H	-6.80012500	1.73522300	2.95938900
H	-4.84820800	3.24942000	2.92695700
C	-2.45986200	2.88938900	1.65555900
H	-2.64255600	3.78006900	2.25667400
H	-1.56483500	2.39496300	2.04539900
H	-2.23557500	3.21165300	0.63405200
C	-4.69827400	-1.44474200	0.25034700
H	-4.53341400	-1.28322000	-0.81907200
H	-3.88834500	-2.08670800	0.60996200
H	-5.63474900	-1.98978800	0.36653900

H	3.81038600	-0.17397700	3.76194700
H	4.05733100	2.05030900	2.85467700
C	3.01844700	-2.64809000	3.97155900
H	4.10254300	-2.55908500	3.85352200
H	2.73117600	-2.01592400	4.81688900
H	2.79864800	-3.67840600	4.23907400
C	3.76457300	4.06753600	1.23148100
H	3.42535900	4.27307800	2.25110100
H	4.79754100	3.71353600	1.29879000
H	3.77253200	5.00939700	0.68897200
C	1.24285100	-4.53080300	2.42342000
H	2.17415800	-5.10248700	2.45071800
H	0.79270500	-4.58660100	3.41803100
H	0.56944500	-5.03137800	1.72685900
C	2.25528200	4.64543200	-1.31464100
H	1.89954000	5.45685000	-0.67421000
H	3.27735000	4.88874500	-1.61646500
H	1.63899300	4.63943800	-2.21435000

5. Optimized geometry of $[Re(CO)_3(CNx)(2,9\text{-dimethyl-phen})]^+$ (**8.5**) in the singlet ground state in the gas phase with E(RB+HF-LYP) = -1472.014595 au.

Atom	Coordinates		
	x	y	z
Re	0.62443800	-1.18841600	-0.44013600
C	2.46010800	-1.95744500	-0.66997300
C	-0.01283400	-2.88014900	0.29046400
C	0.08241500	-1.92793600	-2.16201300
C	-1.28197100	-0.33757300	-0.18418000
N	1.39684400	0.85846900	-1.09950800
C	1.47639100	1.36018800	-2.34584400
C	1.99426400	2.64131200	-2.60862900
C	2.43962200	3.43274400	-1.58394600
C	2.37384300	2.94393200	-0.26902900
C	1.84483100	1.64248300	-0.06307600
H	2.03403500	2.98515000	-3.63342500
H	2.84215400	4.42155800	-1.77317500
C	2.82957400	3.72809300	0.83442200
N	1.28644800	-0.14099700	1.47963600
C	1.78510400	1.12362000	1.27845100
C	2.25231400	1.93413400	2.34613900
C	2.19605400	1.41278800	3.64873300
C	1.69961000	0.15094800	3.83692900
C	1.25090600	-0.60848700	2.74128400
C	2.76988100	3.24151400	2.09562600
H	2.54656400	2.00775700	4.48429500
H	1.64595400	-0.28283900	4.82635200
O	-0.24181600	-2.35749400	-3.17673800
N	-2.35394300	0.10283300	-0.05370700
O	3.50441100	-2.40095400	-0.80504000
O	-0.39207200	-3.87271200	0.72617200
C	-3.64416600	0.59864800	0.09782600
C	-4.56315200	-0.14207600	0.86682500
C	-5.84874400	0.38249700	0.99719600
C	-6.19879400	1.58499600	0.38937300

C	-5.26783900	2.29227400	-0.36619900
C	-3.96839700	1.81637200	-0.53102200
H	-6.58220100	-0.16186500	1.58060300
H	-7.20454400	1.97248600	0.50348200
H	-5.55128500	3.22582300	-0.83828900
C	-2.95330700	2.56647500	-1.35190500
H	-3.38489500	3.48429300	-1.75094800
H	-2.07700800	2.83694800	-0.75487100
H	-2.60169300	1.96528800	-2.19574900
C	-4.17466900	-1.44417800	1.51414300
H	-3.85956400	-2.18274700	0.77115200
H	-3.34402300	-1.31065100	2.21379700
H	-5.01461900	-1.86341000	2.06750600
H	3.11716800	3.83113900	2.93567300
H	3.22639100	4.71709700	0.63860800
C	1.00781800	0.55511500	-3.53651400
H	1.58789500	-0.35646700	-3.62466000
H	-0.04163400	0.30813100	-3.43071600
H	1.13753800	1.13794300	-4.44191200
C	0.72352000	-1.99371700	3.04018100
H	-0.30719000	-2.07989200	2.71816200
H	1.32474200	-2.74071100	2.53445400
H	0.76940400	-2.17606800	4.10820400

6. Optimized geometry of $[Re(CO)_3(CNx)(2,9\text{-dimethyl-}4,7\text{-diphenyl-phen})]^+$ (**8.6**) in the singlet ground state in the gas phase with E(RB+HF-LYP) = -1934.23673 au.

Atom	Coordinates		
	x	y	z
Re	1.94925200	-0.30832800	-1.34644000
C	1.79168800	-0.43905000	-3.33759100
C	3.51604100	0.84337300	-1.49011300
C	3.25271800	-1.75857600	-1.29717300
C	2.06942100	-0.15726900	0.74731900
N	0.02324000	-1.46910600	-1.06352000
C	-0.15320700	-2.79798400	-1.13839100
C	-1.36021500	-3.39512100	-0.73523000
C	-2.42308500	-2.65625000	-0.25981700
C	-2.28210300	-1.23720100	-0.27485800
C	-1.04149000	-0.68802200	-0.68484800
H	-1.43294300	-4.47421700	-0.77210800
C	-3.36704600	-0.36089100	0.03245300
N	0.29753800	1.24114800	-1.24371900
C	-0.89457900	0.74496000	-0.77523800
C	-1.98994700	1.58056700	-0.44320100
C	-1.83786300	2.99049000	-0.59632500
C	-0.65840300	3.43427200	-1.15637000
C	0.39161800	2.55876000	-1.48331300
C	-3.22671500	0.98688000	-0.04609800
H	-0.51049100	4.49328300	-1.32305900
O	4.05257200	-2.58163500	-1.24747900
N	2.19627700	-0.07024000	1.90479700
O	1.70583800	-0.51481500	-4.47492500
O	4.46421000	1.48984600	-1.55022500
C	2.41850500	0.05081900	3.27045900

C	3.71025800	0.40454200	3.70680500
C	3.90412500	0.52223500	5.08237700
C	2.86198100	0.29696700	5.97657700
C	1.59703200	-0.05342200	5.51324000
C	1.34494800	-0.18543100	4.14927600
H	4.88576100	0.79294700	5.45304500
H	3.03702000	0.39372200	7.04151500
H	0.79229900	-0.22902000	6.21759600
C	-0.01646400	-0.56847900	3.63271300
H	-0.71798100	-0.69132900	4.45803300
H	-0.41708700	0.19315700	2.95686200
H	0.01935400	-1.51034100	3.07665700
C	4.83056500	0.64099600	2.72985700
H	5.03724500	-0.25337100	2.13438300
H	4.59106100	1.44792700	2.03098800
H	5.74629100	0.91279100	3.25428400
H	-4.07058700	1.63263600	0.15189900
H	-4.32318900	-0.79246900	0.29280400
C	0.93966700	-3.69423000	-1.64326900
H	1.41743700	-3.28140700	-2.53107000
H	1.71006200	-3.84917700	-0.88423800
H	0.53005900	-4.67151800	-1.89802100
C	1.63003200	3.14388300	-2.09681300
H	2.43080400	3.24204000	-1.36016700
H	1.99812100	2.52891600	-2.91722500
H	1.41734700	4.14033700	-2.48371900
C	-3.65131400	-3.34490200	0.20844600
C	-4.28781900	-4.27940200	-0.62027500
C	-4.16527400	-3.11624100	1.49334500
C	-5.41960500	-4.95815600	-0.17921900
H	-3.90891300	-4.45672300	-1.62043200
C	-5.28812500	-3.80819800	1.93613200
H	-3.66927300	-2.41667500	2.15657700
C	-5.92069100	-4.72617400	1.09979800
H	-5.90997800	-5.66751000	-0.83527100
H	-5.66671200	-3.63389400	2.93644100
H	-6.79853000	-5.25966300	1.44443300
C	-2.88748400	3.96556300	-0.21075000
C	-3.33157400	4.91990500	-1.13670400
C	-3.41340500	3.98584700	1.08955300
C	-4.28879900	5.86261400	-0.77457100
H	-2.94357500	4.90783000	-2.14897100
C	-4.35928000	4.93947500	1.45193300
H	-3.06092000	3.27263300	1.82594700
C	-4.80300500	5.87608600	0.52013700
H	-4.63317000	6.58573100	-1.50434600
H	-4.74636000	4.95447700	2.46398800
H	-5.54403200	6.61431500	0.80278200

Table S2. Molecular Orbital Energies and Percent Contributions for Complexes **8.1 - 8.6**. The contributions for Re are listed per s (Re_s), p (Re_p) and d (Re_d) orbitals. The contributions of all three CO ligands are listed together. The hydrogen atom contributions are included for CNx and diimine ligands. L = diimine ligand.

8.1	H-6	H-5	H-4	H-3	H-2	H-1	H	L	L+1	L+2	L+3	L+4	L+5	L+6	L+7	L+8
Energy	-63.0	-62.3	-59.8	-58.4	-57.9	-56.9	-54.9	-22.8	-20.8	-16.7	-14.0	-11.2	-8.0	-5.7	-5.4	-4.9
% Re_s	0.013	0.042	0.014	0.002	0.578	0.024	0.072	0.169	0.002	0.13	0.31	0.15	1.268	0.002	0.011	0.016
% Re_p	0.041	0.089	0.51	0.008	1.76	0.613	0.892	7.776	0.012	11.93	15.87	3.106	10.96	0.074	0.052	3.737
% Re_d	14.07	26.74	11.48	0.242	71.53	60.58	47.46	0.579	0.283	3.973	5.325	0.104	3.88	0.528	0.059	2.092
% CO	3.276	6.329	3.443	0.077	21.87	16.3	13.22	5.105	0.53	20.56	28.21	3.419	39.64	12.03	0.394	54.83
% CNx	11.78	28.43	23.66	99.62	0.354	6.715	29.78	5.171	0.435	49.61	31.87	3.53	28.49	1.26	99.02	14.17
% phen	70.83	38.37	60.89	0.056	3.905	15.77	8.578	81.2	98.74	13.8	18.42	89.69	15.77	86.11	0.466	25.16
% Total	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**
Type	L	Del	L, CNx	CNx	Re_d, CO	Re_d	Re_d, CNx	L	L	CNx, CO	Del	L	Del	L	CNx	CO, L

8.2	H-6	H-5	H-4	H-3	H-2	H-1	H	L	L+1	L+2	L+3	L+4	L+5	L+6	L+7	L+8
Energy	-62.9	-62.2	-59.4	-58.3	-57.7	-56.7	-54.7	-22.4	-20.9	-16.6	-13.9	-11.1	-7.8	-5.3	-5.2	-4.8
% Re_s	0.013	0.044	0.023	0.002	0.615	0.023	0.075	0.193	0.012	0.130	0.337	0.194	1.206	0.011	0.003	0.021
% Re_p	0.042	0.089	0.546	0.007	1.745	0.633	0.997	7.755	0.217	11.78	15.95	3.365	10.86	0.034	0.322	3.501
% Re_d	15.09	25.25	12.68	0.209	71.08	59.73	47.01	0.534	0.296	3.894	5.309	0.113	3.792	0.071	0.639	2.082
% CO	3.526	5.985	3.759	0.067	21.75	16.09	13.26	4.976	0.548	20.41	28.22	3.432	38.79	0.316	19.43	49.47
% CNx	12.80	27.13	25.68	99.64	0.446	6.839	27.79	5.205	0.435	49.42	31.88	3.627	28.07	97.24	2.829	14.21
% 4-Me-phen	68.52	41.50	57.31	0.076	4.361	16.68	10.87	81.34	98.49	14.38	18.30	89.27	17.28	2.324	76.77	30.72
% Total	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**
Type	L	Del	L, CNx	CNx	Re_d, CO	Re_d	Re_d, CNx	L	L	CNx, CO	Del	L	Del	CNx	L, CO	CO, L

8.3	H-6	H-5	H-4	H-3	H-2	H-1	H	L	L+1	L+2	L+3	L+4	L+5	L+6	L+7	L+8	L+9
Energy	-63.1	-61.3	-60.7	-58.3	-58.0	-56.3	-54.8	-22.1	-21.3	-17.3	-12.0	-11.2	-9.3	-5.3	-5.0	-4.1	-3.7
% Re_s	0.000	0.018	0.102	0.001	0.636	0.058	0.002	0.256	0.000	0.002	1.057	0.679	0.048	0.003	0.000	1.001	0.306
% Re_p	0.023	0.055	0.320	0.002	1.591	1.570	0.329	7.903	0.010	11.48	17.54	4.362	7.425	0.010	0.032	11.58	2.370
% Re_d	13.37	21.63	32.31	0.076	71.89	44.95	49.69	0.606	0.307	4.387	3.989	0.417	6.780	0.118	0.485	4.436	2.115
% CO	3.129	5.534	7.544	0.028	21.73	12.77	13.75	4.853	0.391	20.79	32.32	3.250	27.59	0.115	20.66	46.50	54.33
% CNx	10.50	42.50	8.979	99.87	0.428	6.446	31.10	5.104	0.076	46.79	29.83	3.709	32.13	98.04	1.500	26.40	9.706
% 4,7-Me_2-phen	72.98	30.26	50.75	0.020	3.724	34.20	5.135	81.28	99.22	16.55	15.27	87.58	26.03	1.709	77.33	10.08	31.17
% Total	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**
Type	L	Del	L, Re_d	CNx	Re_d, CO	Re_d, L	Re_d, CNx	L	L	CNx, CO	CO, CNx	L	Del	CNx	L, CO	CO, CNx	CO, L

8.4	H-6	H-5	H-4	H-3	H-2	H-1	H	L	L+1	L+2	L+3	L+4	L+5	L+6	L+7
Energy	-62.5	-60.7	-59.4	-58.3	-58.1	-56.5	-54.8	-21.8	-21.4	-16.9	-13.7	-10.8	-8.2	-5.3	-5.0
% Re_s	0.052	0.016	0.032	0.014	0.603	0.028	0.063	0.184	0.007	0.071	0.327	0.489	0.940	0.009	0.013
% Re_p	0.119	0.076	0.411	0.041	1.607	0.853	0.949	7.906	0.082	11.88	15.30	4.764	9.579	0.034	1.850
% Re_d	35.53	17.38	14.08	1.581	69.82	49.97	45.41	0.494	0.289	4.135	5.027	0.216	4.372	0.066	1.344
% CO	8.406	4.017	3.969	0.496	21.11	13.80	12.80	5.151	0.451	20.06	26.95	3.216	35.49	0.099	45.35
% CNx	36.70	2.150	23.63	97.72	1.309	7.228	27.98	5.223	0.315	45.69	31.61	3.871	27.69	99.57	6.518
% 3,4,7,6-Me_4-phen	19.19	76.36	57.88	0.147	5.550	28.13	12.8	81.04	98.86	18.16	20.79	87.44	21.93	0.223	44.93
% Total	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**
Type	CNx, Re_d	L	L, CNx	CNx	Re_d, CO	Re_d, L	Re_d, CNx	L	L	CNx, CO	Del	L	Del	CNx	CO, L

8.5	H-6	H-5	H-4	H-3	H-2	H-1	H	L	L+1	L+2	L+3	L+4	L+5	L+6
Energy	-63.0	-61.4	-59.1	-58.6	-58.5	-57.0	-55.3	-22.8	-19.3	-17.0	-14.3	-10.8	-7.9	-5.6
% Re_s	0.065	0.011	0.057	0.089	0.915	0.015	0.057	0.137	0.006	0.073	0.148	0.019	0.843	0.091
% Re_p	0.343	0.072	0.315	0.101	0.807	0.857	1.210	9.356	0.022	12.99	19.18	4.638	12.63	0.101
% Re_d	38.77	10.63	27.16	6.968	66.41	46.38	43.29	0.302	0.220	3.011	4.663	0.389	3.892	0.267
% CO	10.00	2.909	7.429	2.202	20.78	12.73	12.50	6.254	0.495	19.73	29.15	12.26	32.93	4.452
% CNx	37.40	2.232	21.82	89.91	4.546	6.372	28.44	6.585	0.262	52.44	29.22	6.923	28.50	64.08
% 2,9-Me_2-phen	13.42	84.14	43.22	0.729	6.547	33.64	14.51	77.37	98.99	11.76	17.63	75.77	21.20	31.01
% Total	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**
Type	Re_d, CNx	L	L, Re_d	CNx	Re_d, CO	Re_d, L	Re_d, CNx	L	L	CNx, CO	Del	L	Del	CNx, L

8.6	H-10	H-9	H-8	H-7	H-6	H-5	H-4	H-3	H-2	H-1	H
Energy	-62.6	-61.6	-61.1	-59.7	-59.6	-59.5	-58.6	-58.3	-58.2	-55.1	-54.5
% Re_s	0.005	0.009	0.104	0.072	0.017	0.067	6E-04	0.381	0.400	0.024	0.043
% Re_p	0.062	0.074	0.066	0.173	0.18	0.223	0.002	0.589	1.146	0.623	1.325
% Re_d	26.87	10.37	9.598	31.57	14.73	12.47	0.045	34.49	46.97	42.61	30.62
% CO	7.114	2.612	2.509	8.146	3.857	3.242	0.020	10.84	14.75	12.20	9.705
% CNx	32.63	14.85	4.189	4.435	2.248	1.622	99.62	6.884	5.820	18.38	11.22
% 29-dm-47-dph-phen	33.32	72.08	83.53	55.61	78.97	82.38	0.308	46.81	30.91	26.17	47.08
% Total	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**
Type	Del	L	L	L, Re_d	L	L	CNx	L, Re_d	Re_d, L	Re_d, L	L, Re_d

8.6 Continued	L	L+1	L+2	L+3	L+4	L+5	L+6	L+7	L+8	L+9	L+10	L+11
Energy	-23.0	-20.5	-17.4	-13.0	-11.4	-9.5	-8.5	-5.7	-5.6	-5.5	-5.2	-4.4
% Re_s	0.323	0.002	0.012	0.578	0.908	0.015	0.066	7.614	0.010	11.38	0.436	0.051
% Re_p	7.652	0.487	12.29	16.00	4.013	6.557	6.449	5.954	0.645	5.337	0.831	4.807
% Re_d	0.529	0.367	3.287	3.857	0.728	2.401	3.669	2.129	0.250	0.825	0.126	1.423
% CO	5.395	0.832	19.85	28.01	9.748	9.319	25.54	14.27	1.469	5.573	0.215	62.59
% CNx	5.289	0.335	49.69	26.19	5.585	11.37	22.61	11.36	92.76	5.882	1.276	2.796
% 2,9-dm-47-dph-phen	80.81	97.98	14.87	25.37	79.02	70.33	41.67	58.67	4.870	71.00	97.12	28.34
% Total	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**
Type	L	L	CNx, CO	Del	L	L	Del	L	CNx	L	L	CO, L

Table S3. Calculated singlet excited-states of **8.1** – **8**.**6** in ethanol with $f > 0.01$.

1. Singlet excited states of complex **8.1.**

Excited State 1: Singlet-A 3.3409 eV 371.12 nm f=0.0404
109 ->111 0.15500
110 ->111 0.67128
This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -1393.30860105
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.4992 eV 354.33 nm f=0.0509
108 ->111 0.11778
109 ->111 0.65504
109 ->112 -0.10100
110 ->111 -0.13001
110 ->112 -0.10320

Excited State 4: Singlet-A 3.6660 eV 338.20 nm f=0.0354
109 ->111 0.10008
110 ->112 0.66970

Excited State 5: Singlet-A 3.8229 eV 324.32 nm f=0.0306
104 ->111 -0.12895
106 ->111 0.26935
109 ->112 0.60875

Excited State 6: Singlet-A 3.8916 eV 318.59 nm f=0.0679
105 ->113 0.11178
109 ->113 -0.19595
109 ->114 0.16389
110 ->113 0.53179
110 ->114 -0.31887

Excited State 8: Singlet-A 3.9600 eV 313.09 nm f=0.0137
104 ->112 -0.14264
105 ->111 -0.15750
105 ->112 0.10417
106 ->111 0.57056
109 ->112 -0.27259

Excited State 9: Singlet-A 3.9978 eV 310.13 nm f=0.0002
107 ->111 0.70455

Excited State 10: Singlet-A 4.0306 eV 307.61 nm f=0.0138
106 ->113 0.10617
109 ->113 0.60958
109 ->116 0.11240
110 ->114 -0.27653

Excited State 11: Singlet-A 4.1490 eV 298.83 nm f=0.0741
108 ->113 -0.28944
109 ->113 0.16902
109 ->114 0.29082
110 ->113 0.22148
110 ->114 0.42847
110 ->116 0.10324

Excited State 13: Singlet-A 4.1915 eV 295.80 nm f=0.0283
106 ->112 0.22708
108 ->113 0.53266
108 ->114 -0.13618
109 ->114 0.15464
110 ->113 0.12883
110 ->114 0.21514

Excited State 15: Singlet-A 4.3333 eV 286.12 nm f=0.0249
104 ->111 0.31687
105 ->111 0.58467
106 ->111 0.15687

Excited State 16: Singlet-A 4.4481 eV 278.74 nm f=0.0738
108 ->113 0.18840
108 ->114 0.59698
108 ->116 0.11695
109 ->114 0.20117
110 ->113 -0.10745
110 ->114 -0.10405

Excited State 17: Singlet-A 4.5525 eV 272.35 nm f=0.0171
106 ->118 -0.10291
107 ->113 0.64409
110 ->118 0.18966

Excited State 18: Singlet-A 4.5596 eV 271.92 nm f=0.3293
105 ->112 0.35587
106 ->112 0.11637
108 ->114 -0.21096
109 ->114 0.37522
110 ->113 -0.19882
110 ->114 -0.13442

Excited State 19: Singlet-A 4.5919 eV 270.01 nm f=0.2124
105 ->112 0.48207
106 ->112 0.15331
106 ->115 0.10029
108 ->114 0.12892
109 ->114 -0.30091
110 ->113 0.16934
110 ->114 0.12284

Excited State 20: Singlet-A 4.6258 eV 268.03 nm f=0.4144
104 ->111 0.40573
104 ->112 -0.21817
105 ->111 -0.11264
106 ->112 -0.29386
106 ->115 0.12304
109 ->112 0.11305
109 ->115 0.10797
110 ->115 0.26070

Excited State 21: Singlet-A 4.6411 eV 267.14 nm f=0.1431
104 ->111 0.16381
104 ->112 0.53858
105 ->111 -0.10832
105 ->112 0.24179
106 ->115 -0.10738
109 ->115 0.20095

Excited State 22: Singlet-A 4.7568 eV 260.64 nm f=0.0460
105 ->113 -0.10220
106 ->113 0.65666
106 ->114 -0.13028
109 ->113 -0.14065

Excited State 23: Singlet-A 4.8624 eV 254.99 nm f=0.1239
104 ->111 -0.12322
104 ->112 0.14930
110 ->115 0.60294

Excited State 25: Singlet-A 4.9519 eV 250.37 nm f=0.0328
105 ->113 0.23186
105 ->114 -0.12793
106 ->114 -0.18363
108 ->116 -0.11172
109 ->116 0.18981
110 ->115 0.12028
110 ->116 0.43768
110 ->119 -0.21874

2. Singlet excited states of complex **8.2.**

Excited State 1: Singlet-A 3.3634 eV 368.62 nm f=0.0425
113 ->115 0.13164
114 ->115 0.67636
This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -1432.63588528
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.5436 eV 349.88 nm f=0.0418
113 ->115 0.63138
113 ->116 -0.15042
114 ->116 -0.20263

Excited State 4: Singlet-A 3.6359 eV 341.00 nm f=0.0723
112 ->115 -0.17010

113 ->115 0.20713
114 ->116 0.62483

Excited State 5: Singlet-A 3.8001 eV 326.27 nm f=0.0370
108 ->115 -0.12144
110 ->115 0.20798
113 ->115 0.10082
113 ->116 0.62936

Excited State 6: Singlet-A 3.8771 eV 319.78 nm f=0.0685
109 ->117 0.10499
112 ->116 0.10256
113 ->117 -0.17908
113 ->118 -0.15722
114 ->117 0.53479
114 ->118 0.32028

Excited State 9: Singlet-A 4.0242 eV 308.10 nm f=0.0124
110 ->117 0.11453
113 ->117 0.60818
113 ->120 0.11040
114 ->118 0.28016

Excited State 11: Singlet-A 4.1376 eV 299.65 nm f=0.0794
112 ->117 0.26720
113 ->117 -0.18604
113 ->118 0.28344
114 ->117 -0.22459
114 ->118 0.43316
114 ->120 -0.10192
Excited State 12: Singlet-A 4.1653 eV 297.66 nm f=0.0172
108 ->115 0.26999
109 ->115 -0.20613
109 ->116 -0.14606
110 ->116 0.55995
112 ->117 -0.10608

Excited State 13: Singlet-A 4.1800 eV 296.62 nm f=0.0284
112 ->117 0.58304
112 ->118 0.14337
113 ->118 -0.14425
114 ->117 0.12962
114 ->118 -0.21420

Excited State 15: Singlet-A 4.3791 eV 283.13 nm f=0.0294
108 ->115 0.31100
109 ->115 0.57957
110 ->115 0.16929

Excited State 16: Singlet-A 4.4449 eV 278.93 nm f=0.0708
112 ->117 -0.18493
112 ->118 0.60510
112 ->120 -0.11711
113 ->118 0.18432
114 ->117 0.10028

Excited State 17: Singlet-A 4.5397 eV 273.11 nm f=0.2106
109 ->115 0.15427
109 ->116 0.47862
110 ->116 0.18731
112 ->118 0.15259
113 ->118 -0.26206
114 ->117 -0.12620

Excited State 18: Singlet-A 4.5568 eV 272.08 nm f=0.0200
110 ->121 0.10978
111 ->117 0.64338
114 ->121 -0.18691

Excited State 19: Singlet-A 4.5752 eV 270.99 nm f=0.3176
109 ->116 0.33239
110 ->116 0.12544
112 ->118 -0.17255
113 ->118 0.41634
113 ->123 -0.10737
114 ->117 0.21948
114 ->118 -0.15912

Excited State 20: Singlet-A 4.6196 eV 268.39 nm f=0.1380
108 ->115 -0.25447
108 ->116 0.49461
110 ->116 0.16535
110 ->119 -0.15915
114 ->119 -0.28397

Excited State 21: Singlet-A 4.6310 eV 267.72 nm f=0.4048
108 ->115 0.39119
108 ->116 0.30571
109 ->115 -0.16753
109 ->116 0.24591
110 ->116 -0.14669
113 ->119 0.21895

Excited State 22: Singlet-A 4.7287 eV 262.20 nm f=0.0673
109 ->117 -0.10391
110 ->117 0.65263
110 ->118 0.12540
113 ->117 -0.15093

Excited State 23: Singlet-A 4.8511 eV 255.58 nm f=0.1373
108 ->115 -0.12169
108 ->116 0.16919
113 ->119 0.10426
114 ->119 0.59391

Excited State 24: Singlet-A 4.9412 eV 250.92 nm f=0.0298
109 ->117 0.18801
109 ->118 0.10284
110 ->118 0.18086
112 ->120 -0.10647
113 ->120 0.19297
114 ->119 0.11980
114 ->120 0.46470
114 ->123 -0.21196

3. Singlet excited states of complex **8.3.**

Excited State 2: Singlet-A 3.5130 eV 352.93 nm f=0.0176
113 ->120 0.10848
117 ->119 0.43309
118 ->120 0.54283

Excited State 3: Singlet-A 3.6266 eV 341.87 nm f=0.1342
116 ->119 -0.28519
117 ->119 0.46975
118 ->120 -0.40313

Excited State 4: Singlet-A 3.6493 eV 339.75 nm f=0.0309
116 ->119 0.64184
117 ->119 0.21578
118 ->120 -0.16950

Excited State 5: Singlet-A 3.7553 eV 330.15 nm f=0.0732
112 ->119 0.16040
114 ->120 0.11635
117 ->120 0.65816

Excited State 7: Singlet-A 3.8783 eV 319.69 nm f=0.0208
114 ->121 0.17248
117 ->121 0.61842
117 ->124 0.10708
118 ->121 0.21110

Excited State 8: Singlet-A 3.9120 eV 316.93 nm f=0.2335
117 ->121 -0.22176
117 ->122 -0.19253
118 ->121 0.58445
118 ->124 0.11329

Excited State 9: Singlet-A 4.0778 eV 304.05 nm f=0.0101
112 ->120 0.18073
113 ->119 0.12171
113 ->120 -0.16530
114 ->119 0.62536

Excited State 12: Singlet-A 4.2073 eV 294.69 nm f=0.0158
112 ->119 -0.24233
113 ->119 0.18178
113 ->120 0.12211
114 ->120 0.60047

Excited State 15: Singlet-A 4.3499 eV 285.03 nm f=0.0259
112 ->119 0.17707
113 ->119 0.63789
114 ->119 -0.12906
114 ->120 -0.12316
118 ->119 -0.10160

Excited State 16: Singlet-A 4.4799 eV 276.75 nm f=0.0790
113 ->120 0.63645
114 ->119 0.16104
114 ->120 -0.13226

Excited State 17: Singlet-A 4.5023 eV 275.38 nm f=0.0385
113 ->125 0.12806
115 ->121 0.65605
118 ->125 -0.18417

Excited State 18: Singlet-A 4.5991 eV 269.58 nm f=0.1037
112 ->120 0.51404
113 ->120 0.10317
114 ->119 -0.12058
114 ->123 0.12865
116 ->122 -0.31275
117 ->122 0.11922
117 ->123 -0.22544

Excited State 20: Singlet-A 4.6354 eV 267.47 nm f=0.3709
112 ->119 0.50202
113 ->123 0.11903
114 ->120 0.18641
117 ->120 -0.12825
118 ->123 0.34810

Excited State 22: Singlet-A 4.7508 eV 260.97 nm f=0.4986
112 ->121 -0.10323
113 ->121 -0.26148
114 ->121 0.10410
117 ->122 0.52138
118 ->121 0.19801
118 ->128 -0.14194

Excited State 23: Singlet-A 4.8015 eV 258.22 nm f=0.1328
113 ->124 0.11455
118 ->121 -0.11275
118 ->123 -0.13885
118 ->124 0.59864
118 ->128 -0.15804

Excited State 24: Singlet-A 4.8193 eV 257.27 nm f=0.2890
112 ->119 -0.24602
114 ->120 -0.10444
116 ->124 0.14159
118 ->123 0.55952
118 ->124 0.14993

Excited State 25: Singlet-A 4.9260 eV 251.69 nm f=0.0143
113 ->121 -0.22416
114 ->124 0.15683
116 ->124 -0.10266
117 ->124 0.60071

4. Singlet excited states of complex **8.4.**

Excited State 1: Singlet-A 3.4367 eV 360.76 nm f=0.0353
125 ->127 0.10081
126 ->127 0.67255
This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -1550.61029699
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 3: Singlet-A 3.6231 eV 342.20 nm f=0.0935
121 ->127 0.12508
125 ->127 0.44721
125 ->128 -0.15976
126 ->127 -0.10204
126 ->128 0.46221

Excited State 5: Singlet-A 3.7479 eV 330.81 nm f=0.0862
122 ->127 -0.17822
124 ->127 -0.10404
125 ->127 0.23583
125 ->128 0.58957
126 ->127 -0.10323

Excited State 6: Singlet-A 3.8553 eV 321.60 nm f=0.0704
120 ->129 0.11646
124 ->128 -0.12796
125 ->129 -0.23587
125 ->130 -0.14571
126 ->129 0.54067
126 ->130 0.25030

Excited State 8: Singlet-A 3.9852 eV 311.11 nm f=0.0443
121 ->129 0.10637
122 ->129 -0.12061
125 ->129 0.59613
125 ->132 -0.11625
126 ->129 0.15967
126 ->130 0.24098

Excited State 9: Singlet-A 4.0010 eV 309.88 nm f=0.0122
121 ->127 -0.25668
121 ->128 0.26040
122 ->127 0.53394
122 ->128 0.17174
125 ->128 0.11910

Excited State 11: Singlet-A 4.1364 eV 299.74 nm f=0.0304
124 ->129 0.50442
124 ->130 0.12680
125 ->130 0.19221
126 ->129 -0.11669
126 ->130 0.33153

Excited State 13: Singlet-A 4.1729 eV 297.12 nm f=0.0577
124 ->129 -0.41171
125 ->130 0.24114
126 ->129 -0.17698
126 ->130 0.41692

Excited State 15: Singlet-A 4.3680 eV 283.84 nm f=0.1997
120 ->127 0.14924
121 ->128 0.50760
122 ->127 -0.28872
122 ->128 0.14147
122 ->131 0.12407
126 ->131 -0.10762

Excited State 16: Singlet-A 4.4168 eV 280.71 nm f=0.2883
120 ->127 -0.35393
121 ->127 0.44740
122 ->127 0.12938
122 ->128 0.27679

Excited State 17: Singlet-A 4.4755 eV 277.03 nm f=0.0788
120 ->127 0.21048
124 ->129 -0.15535
124 ->130 0.56822
124 ->132 0.10233
125 ->130 0.17501
126 ->130 -0.10133

Excited State 18: Singlet-A 4.5243 eV 274.04 nm f=0.2950
120 ->127 0.48797
121 ->127 0.19057
121 ->128 -0.16481
122 ->128 0.12961
123 ->129 0.16879
124 ->130 -0.16250
125 ->130 -0.14617
126 ->131 0.10780

Excited State 19: Singlet-A 4.5387 eV 273.17 nm f=0.0954
120 ->127 -0.10155
120 ->133 -0.10966
122 ->133 0.10336
123 ->129 0.62541
126 ->133 0.17377

Excited State 20: Singlet-A 4.5538 eV 272.27 nm f=0.0414
120 ->128 0.66243

Excited State 21: Singlet-A 4.5710 eV 271.24 nm f=0.3090
120 ->127 0.10127
120 ->128 -0.10134
120 ->129 -0.12364
124 ->130 -0.27871
125 ->130 0.46752
126 ->129 0.21667
126 ->130 -0.17506

Excited State 22: Singlet-A 4.6667 eV 265.68 nm f=0.0885
121 ->129 -0.16471
122 ->129 0.63074
125 ->129 0.18001

Excited State 23: Singlet-A 4.8022 eV 258.18 nm f=0.0123
121 ->129 0.65983
122 ->129 0.19319

Excited State 24: Singlet-A 4.8596 eV 255.13 nm f=0.1056
124 ->132 0.11039
125 ->131 0.11450
126 ->131 0.60162
126 ->132 -0.19274

Excited State 25: Singlet-A 4.9050 eV 252.77 nm f=0.0592
120 ->129 -0.14286
120 ->132 0.10137
125 ->132 0.19605
126 ->131 0.25613
126 ->132 0.49464
126 ->134 -0.18200

5. Singlet excited states of complex **8.5.**

Excited State 1: Singlet-A 3.3926 eV 365.45 nm f=0.0282
117 ->119 0.15592
118 ->119 0.66977
This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -1471.95280497
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.5371 eV 350.52 nm f=0.0458
117 ->119 0.65600
118 ->119 -0.14205

Excited State 4: Singlet-A 3.8591 eV 321.28 nm f=0.0149
114 ->119 0.60195
117 ->120 0.16107
118 ->120 0.23274

Excited State 5: Singlet-A 3.8973 eV 318.13 nm f=0.0160
113 ->119 0.24155
114 ->119 -0.21557
117 ->120 -0.10238
118 ->120 0.59809

Excited State 6: Singlet-A 3.9684 eV 312.43 nm f=0.1017
112 ->121 0.11676
114 ->122 -0.10803
117 ->120 0.10566
117 ->121 -0.13842
117 ->122 0.16342
118 ->121 0.53645
118 ->122 -0.30692

Excited State 7: Singlet-A 4.0259 eV 307.96 nm f=0.0113
113 ->119 0.23894
114 ->119 0.10249
115 ->119 0.49581
117 ->120 -0.38074
118 ->120 -0.11081

Excited State 8: Singlet-A 4.0299 eV 307.66 nm f=0.0111
113 ->119 -0.23608
115 ->119 0.49924
117 ->120 0.38125
118 ->120 0.11602

Excited State 9: Singlet-A 4.0608 eV 305.32 nm f=0.0237
114 ->121 -0.22364
117 ->121 0.61127
117 ->124 0.10786
118 ->122 -0.14559

Excited State 10: Singlet-A 4.1267 eV 300.44 nm f=0.0515
112 ->122 0.10381
117 ->122 0.28500
118 ->121 0.23241
118 ->122 0.54043

Excited State 12: Singlet-A 4.2003 eV 295.18 nm f=0.0178
113 ->119 0.20401
114 ->120 -0.21044
116 ->121 0.54970
116 ->122 -0.18029
117 ->120 0.15317

Excited State 13: Singlet-A 4.2574 eV 291.22 nm f=0.0595
113 ->119 -0.24359
114 ->120 0.47921
116 ->121 0.31475
117 ->120 -0.18845
118 ->120 0.11529

Excited State 14: Singlet-A 4.3827 eV 282.89 nm f=0.0384
112 ->119 0.62506
113 ->119 0.17925
114 ->119 -0.10738
114 ->120 0.17640

Excited State 15: Singlet-A 4.4565 eV 278.21 nm f=0.0467
114 ->120 -0.14081
116 ->121 0.20922
116 ->122 0.59899

Excited State 17: Singlet-A 4.5184 eV 274.40 nm f=0.3992
112 ->119 -0.24587
113 ->119 0.29113
114 ->120 0.30886
115 ->121 0.22954
116 ->122 0.16200
117 ->120 0.19532
117 ->122 0.10297
117 ->123 -0.14249
118 ->123 -0.10032

Excited State 18: Singlet-A 4.5431 eV 272.90 nm f=0.1550
113 ->119 -0.11391
114 ->120 -0.11220
114 ->125 -0.10286
115 ->121 0.60389
118 ->125 -0.16467

Excited State 19: Singlet-A 4.5740 eV 271.07 nm f=0.1292
112 ->121 0.16770
113 ->120 -0.10995
114 ->121 0.39374
114 ->122 -0.12509
116 ->122 -0.12669
117 ->121 0.18521
117 ->122 0.34270
118 ->121 -0.21906
118 ->122 -0.10239

Excited State 20: Singlet-A 4.5829 eV 270.53 nm f=0.1172
113 ->120 0.52873
114 ->121 0.25588
114 ->123 0.13714
117 ->121 0.10840
117 ->123 0.18193
118 ->123 -0.19297

Excited State 21: Singlet-A 4.6229 eV 268.20 nm f=0.3721
113 ->120 -0.21418
114 ->121 0.38498
116 ->122 0.10165
117 ->121 0.15925
117 ->122 -0.37543
117 ->123 -0.10116
118 ->121 0.16259
118 ->122 0.13479
118 ->123 0.10103

Excited State 23: Singlet-A 4.8787 eV 254.13 nm f=0.1331
112 ->120 -0.15569
113 ->121 0.18949
114 ->122 0.58121
117 ->122 0.16165
118 ->123 0.13321

Excited State 24: Singlet-A 4.9022 eV 252.91 nm f=0.0478
113 ->121 0.64649
114 ->121 -0.16178
114 ->122 -0.12735

Excited State 25: Singlet-A 4.9274 eV 251.62 nm f=0.0935
112 ->120 -0.11197
114 ->122 -0.20109
116 ->123 -0.11465
117 ->123 0.24823
118 ->123 0.49645

6. Singlet excited states of complex **8.6.**

Excited State 1: Singlet-A 3.2927 eV 376.54 nm f=0.0557
157 -> 159 0.31246
158 -> 159 0.61141
This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -1934.17661572
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.3492 eV 370.20 nm f=0.0941
157 -> 159 0.60842
157 -> 160 0.10216
158 -> 159 -0.28072

Excited State 3: Singlet-A 3.6289 eV 341.66 nm f=0.0136
155 -> 159 0.42785
156 -> 159 0.53164
158 -> 160 -0.10968

Excited State 4: Singlet-A 3.6469 eV 339.97 nm f=0.2515
155 -> 159 0.21982
157 -> 160 -0.12304
158 -> 160 0.62179

Excited State 5: Singlet-A 3.7216 eV 333.15 nm f=0.1587
157 -> 160 0.64951
158 -> 160 0.16076

Excited State 6: Singlet-A 3.8628 eV 320.97 nm f=0.0194
151 -> 161 -0.15341
152 -> 161 -0.10085
155 -> 159 -0.19403
156 -> 159 0.15041
157 -> 161 -0.16180
158 -> 161 0.55258

Excited State 7: Singlet-A 3.8735 eV 320.08 nm f=0.0201
149 -> 159 0.14929
151 -> 159 0.20186
152 -> 159 0.23464
153 -> 159 0.12988
155 -> 159 0.38521
156 -> 159 -0.29929
158 -> 160 -0.10592
158 -> 161 0.25190

Excited State 8: Singlet-A 3.9258 eV 315.82 nm f=0.0407
150 -> 159 0.16216
151 -> 159 0.35488
152 -> 159 0.17617
153 -> 159 0.37134
155 -> 159 -0.18979
156 -> 159 0.22410
157 -> 161 0.16663

Excited State 9: Singlet-A 3.9472 eV 314.11 nm f=0.1682
151 -> 159 -0.13757
151 -> 162 -0.10204
153 -> 159 -0.11648
157 -> 161 0.56750
158 -> 161 0.14605
158 -> 162 0.16191

Excited State 10: Singlet-A 3.9869 eV 310.98 nm f=0.0374
152 -> 159 0.46048
153 -> 159 -0.39222
153 -> 160 -0.14394
154 -> 159 -0.26949

Excited State 12: Singlet-A 3.9937 eV 310.45 nm f=0.0109
151 -> 159 0.42777
152 -> 159 -0.36738
152 -> 160 0.15332
153 -> 159 -0.22823
154 -> 159 -0.29373

Excited State 14: Singlet-A 4.0612 eV 305.29 nm f=0.1625
149 -> 159 0.10652
150 -> 159 0.42376
155 -> 160 -0.42367
156 -> 160 0.23115

Excited State 16: Singlet-A 4.1759 eV 296.91 nm f=0.0175
150 -> 159 0.13115
151 -> 160 0.13590
152 -> 160 0.10411
155 -> 160 0.14617
155 -> 161 -0.15427
156 -> 161 -0.18452
157 -> 162 0.43599
158 -> 162 0.33634

Excited State 17: Singlet-A 4.1859 eV 296.20 nm f=0.3086
149 -> 159 0.55657
150 -> 160 -0.14969
151 -> 160 0.17943
152 -> 160 0.15891
153 -> 160 0.11553
155 -> 159 -0.11132
155 -> 160 0.11134
156 -> 159 0.10965

Excited State 18: Singlet-A 4.2061 eV 294.77 nm f=0.0243
149 -> 159 -0.11573
150 -> 159 0.38949
150 -> 160 0.13013
151 -> 160 0.16592
152 -> 160 0.15153
153 -> 160 0.10813
155 -> 160 0.23582
155 -> 161 0.14591
156 -> 160 -0.28291
156 -> 161 0.15665
157 -> 162 -0.13252

Excited State 19: Singlet-A 4.2461 eV 291.99 nm f=0.0221
149 -> 159 -0.16392
150 -> 159 -0.24523
150 -> 160 0.16978
151 -> 160 0.35803
152 -> 160 0.25416
153 -> 160 0.28067
155 -> 160 -0.19273
156 -> 160 0.18283

Excited State 23: Singlet-A 4.3487 eV 285.11 nm f=0.0769
148 -> 159 0.61077
149 -> 159 -0.15158
150 -> 160 -0.23130

Excited State 24: Singlet-A 4.4328 eV 279.69 nm f=0.0265
148 -> 160 0.13258
149 -> 160 0.23951
150 -> 160 -0.12232
151 -> 161 -0.16599
152 -> 161 -0.11429
153 -> 161 -0.10507
155 -> 161 -0.13711
155 -> 162 -0.17462
156 -> 162 -0.16312
157 -> 162 -0.25608
158 -> 161 -0.17794
158 -> 162 0.33608
158 -> 163 0.12203

Excited State 25: Singlet-A 4.4661 eV 277.61 nm f=0.0213
148 -> 160 0.12077
149 -> 160 0.41162
150 -> 160 0.11171
150 -> 161 0.12425
151 -> 161 0.21146
152 -> 161 0.15557
153 -> 161 0.13339
155 -> 161 0.15549
157 -> 161 -0.10486
158 -> 161 0.13819
158 -> 163 0.25082

Excited State 26: Singlet-A 4.4823 eV 276.61 nm f=0.0834
149 -> 160 -0.21719
150 -> 160 0.19433
150 -> 161 0.11190
151 -> 161 0.16470
152 -> 161 0.11778
153 -> 161 0.10345
155 -> 161 0.15670
155 -> 162 -0.21203
156 -> 162 -0.22530
157 -> 161 -0.12070
157 -> 162 -0.18616
157 -> 163 0.17108
158 -> 162 0.26096
158 -> 163 -0.16143

Excited State 27: Singlet-A 4.4984 eV 275.62 nm f=0.0389
154 -> 161 0.65026
157 -> 167 0.13259
158 -> 167 0.10162

Excited State 28: Singlet-A 4.5061 eV 275.15 nm f=0.1318
148 -> 159 0.20180
150 -> 160 0.47827
151 -> 161 -0.13713
155 -> 161 -0.17755
157 -> 163 0.16445
158 -> 164 0.12916

Excited State 29: Singlet-A 4.6424 eV 267.07 nm f=0.0428
148 -> 160 -0.11963
149 -> 161 0.16126
151 -> 161 0.16467
152 -> 161 0.15997
155 -> 161 -0.41268
156 -> 161 0.43481

Excited State 30: Singlet-A 4.6550 eV 266.34 nm f=0.0580
148 -> 160 0.45857
149 -> 160 -0.29993
155 -> 162 0.18419
156 -> 162 0.20615
158 -> 162 0.14016
158 -> 163 0.11472

Excited State 31: Singlet-A 4.7061 eV 263.45 nm f=0.1910
148 -> 160 -0.29546
148 -> 161 0.11526
149 -> 160 0.13134
155 -> 162 0.26962
156 -> 162 0.30462
157 -> 162 -0.18884
158 -> 162 0.20315
158 -> 163 -0.18621

Excited State 32: Singlet-A 4.7822 eV 259.26 nm f=0.1713
148 -> 160 -0.11969
150 -> 160 -0.11886
157 -> 162 0.14099
157 -> 163 0.47725
158 -> 163 0.34084
158 -> 165 0.12340

Excited State 33: Singlet-A 4.8632 eV 254.94 nm f=0.0245
148 -> 161 0.10717
152 -> 161 0.35943
153 -> 161 -0.49903
157 -> 164 0.13389
158 -> 163 -0.10314
158 -> 164 0.14206

Excited State 34: Singlet-A 4.8733 eV 254.41 nm f=0.0693
152 -> 161 -0.15900
153 -> 161 0.25417
157 -> 164 0.30007
157 -> 165 0.19228
157 -> 170 -0.12525
158 -> 163 -0.13331
158 -> 164 0.34907
158 -> 165 0.18266
158 -> 170 -0.10390

Excited State 36: Singlet-A 4.9067 eV 252.69 nm f=0.0383
148 -> 160 0.25372
149 -> 160 0.15542
150 -> 163 0.11811
155 -> 163 0.14207
157 -> 163 0.33395
158 -> 163 -0.30992
158 -> 164 -0.14572

Excited State 38: Singlet-A 4.9590 eV 250.02 nm f=0.0249
149 -> 161 0.19901
151 -> 165 -0.10677
157 -> 164 -0.35386
157 -> 165 -0.24143
158 -> 164 0.36524
158 -> 165 0.15860

Additional comments. Excited states 20 (ε = 29,100 $M^{-1}cm^{-1}$) at 37,300 cm^{-1} for complex **1**, 21 (ε = 37,400 $M^{-1}cm^{-1}$) at 37,400 cm^{-1} for complex **2**, 20 (ε = 26,000 $M^{-1}cm^{-1}$) at 37,400 cm^{-1} for complex **3**, and 16 (ε = 20,200 $M^{-1}cm^{-1}$) at 35,600 cm^{-1} for complex **4** were primarily based on phen ligand $\pi \rightarrow \pi^*$ transitions that occurred from HOMOs-6 for **1**, **2** and **3** and from HOMO-5 for **4** to the corresponding LUMOs. These excited states made large contributions to the most intense experimental peaks in the range 36,000 cm^{-1} to 37,000 cm^{-1} for complexes **1** – **4**. The calculated MCDCT states were 18 (ε = 23,100 $M^{-1}cm^{-1}$) at 36,800 cm^{-1} for complex **1** and 19 (ε = 22,300 $M^{-1}cm^{-1}$) at 36,900 cm^{-1} for complex **2**. The appropriate state listed above together with CDLCT state 19 (ε = 14,500 $M^{-1}cm^{-1}$) at 37,100 cm^{-1} made the largest contribution to the experimental absorption peak at 37,000 cm^{-1} for **1** and CDLCT state17 (ε = 14,800 $M^{-1}cm^{-1}$) at 36,700 cm^{-1} made the largest contribution to the experimental absorption peak at 36,800 cm^{-1} for **2**. However, only the assignment of the excited state nearest to the experimental peak, namely excited state 19 for **1** and excited state 18 for **2**, are listed in Table 1. For complex **3**, the MLLCT excited state 22 (ε = 35,000 $M^{-1}cm^{-1}$) at 38,300 cm^{-1} made a large contribution to the experimental absorption peak at 36,800 cm^{-1}. For complex **4**, excited states 18 (ε = 20,700 $M^{-1}cm^{-1}$) at 36,500 cm^{-1} and 21 (ε = 21,700 $M^{-1}cm^{-1}$) [1] at 36,900 cm^{-1} were assigned as LMLCT and MCDCT, respectively, and made large contributions to the experimental peak at 36,000 cm^{-1}. For complexes **3** and **4**, the assignments of excited states 18 and 17, respectively, are listed in Table 1 next to the experimental absorption maxima.