

C[^]C* Cyclometalated Platinum(II) N-Heterocyclic Carbene Complexes with a
Sterically Demanding β-Diketonato Ligand – Synthesis, Characterization and
Photophysical Properties

Xyz-Coordinates of DFT-Calculations

Mario Tenne[†], Stefan Metz[‡], Gerhard Wagenblast[‡], Ingo Muenster[‡] and Thomas Strassner[†]

[†] Physikalische Organische Chemie, Technische Universität Dresden, 01069 Dresden,
Germany

[‡] BASF SE, 67056 Ludwigshafen, Germany

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Cartesian Coordinates of DFT-optimized ground states (BP86/6-31G(d))

Cartesian coordinates of **4**

Pt	-0.90008900	0.28598900	-0.16664500
C	-2.09508000	-1.28317100	0.23744600
C	-3.41946500	-1.26434000	0.67959000
C	-1.51030600	-2.55161200	0.05097200
C	-4.10740600	-2.46266500	0.91822300
H	-3.91312500	-0.31034900	0.83832100
C	-2.16238200	-3.75544100	0.27776600
C	-3.48778000	-3.69889300	0.72030600
H	-1.65308500	-4.70007300	0.11514100
H	-4.03119500	-4.62050400	0.90892900
C	0.31999400	-1.18897700	-0.57016500
N	-0.16699800	-2.43810400	-0.39590700
N	1.59734700	-1.40312300	-0.99606700
O	-2.36654400	1.68265800	0.32885200
O	0.44835800	1.91002700	-0.60828200
C	-2.23425700	2.95319000	0.28877300
C	0.14490600	3.14809400	-0.50741300
C	-1.08886100	3.67543900	-0.09179100
H	-1.16874200	4.75581400	-0.06326900
C	-3.47620400	3.71426900	0.70650700
H	-3.34449300	4.79763900	0.65338900
H	-4.31417700	3.42218900	0.06351400
H	-3.74530200	3.43566500	1.73183200
C	1.25932300	4.10237800	-0.89075100
H	2.15781300	3.86891900	-0.30838700
H	1.51406800	3.95921900	-1.94777500
H	0.99110800	5.14969400	-0.73201700
C	2.59881200	-0.36242800	-1.29695600
H	3.06707800	-0.62405500	-2.25107600
H	2.03660600	0.56500100	-1.42153100
H	-5.13835100	-2.42853200	1.26245000
C	3.64020000	-0.22224400	-0.20518500
C	4.92225500	-0.76006700	-0.36290200
C	3.31993100	0.44885400	0.98366800
C	5.87238600	-0.63938600	0.65397700
H	5.18421200	-1.26930800	-1.28848800
C	4.26726700	0.56635000	2.00028900
H	2.32947800	0.88096700	1.10024500
C	5.54438800	0.02152400	1.83834700
H	6.86571000	-1.05879400	0.51904900
H	4.01045800	1.08766400	2.91847200
H	6.28162900	0.11636600	2.63099500
N	1.79362300	-2.76732900	-1.03901500
C	0.72522300	-3.42908900	-0.68112100

H 0.67440102 -4.49706135 -0.63926181

Cartesian coordinates of **5**

Pt -1.36019500 -0.29984700 -0.01050800
C -3.09833400 0.70372900 -0.06645800
C -3.28499500 2.08751800 -0.13057500
C -4.26109700 -0.09198200 -0.04475700
C -4.57458400 2.63321000 -0.16861900
H -2.41608400 2.73825000 -0.15351800
C -5.55209100 0.42155300 -0.08149600
C -5.70272300 1.80998200 -0.14393500
H -6.42304400 -0.22880600 -0.06323000
H -6.69896600 2.24175900 -0.17384000
C -2.61389600 -1.80059000 0.04084600
N -3.95007700 -1.48238500 0.01671600
N -2.60800700 -3.14237500 0.10540300
O -0.22417700 1.44987700 -0.05299000
O 0.45814100 -1.44480700 0.03506600
C 1.05496300 1.51239300 -0.04257700
C 1.63251000 -0.93849000 0.02904500
C 1.95272000 0.43054900 -0.00608200
H 3.00793200 0.68007900 -0.00028600
C -1.45179600 -4.02547800 0.16135800
H -1.46539300 -4.69417100 -0.70338800
H -0.55296800 -3.40817800 0.15218300
H -1.49742000 -4.62040000 1.07724200
H -4.69888300 3.71215600 -0.21869200
C 1.61874000 2.90927700 -0.04460700
C 1.52239900 3.68556100 1.12842300
C 2.20122300 3.44298800 -1.20971600
C 2.03790200 4.98441800 1.11945900
C 2.69395100 4.75275900 -1.17499800
C 2.63071300 5.53705700 -0.02061400
H 1.96986800 5.58167700 2.02692000
H 3.13426800 5.17075600 -2.07833500
C 2.76232400 -1.93697200 0.04790400
C 3.44067900 -2.21758400 1.24867300
C 3.10068200 -2.61384900 -1.14122800
C 4.46311100 -3.17364000 1.23549600
C 4.13274600 -3.55584600 -1.10882700
C 4.82974500 -3.84862300 0.06831400
H 4.98278400 -3.39787100 2.16513800
H 4.39729600 -4.07595700 -2.02777900
C 0.87867200 3.13439600 2.38183300
H -0.18753300 2.93633200 2.22785100
H 1.33603600 2.18397600 2.68328700
H 0.98097500 3.83692200 3.21455400

C	2.28398600	2.64551400	-2.49415400
H	3.00365300	1.82162200	-2.41724600
H	1.31716300	2.20144500	-2.75693300
H	2.59811400	3.28439000	-3.32548100
C	3.20352200	6.93544500	0.00410400
H	4.23023300	6.93818300	0.39467300
H	3.23608200	7.37316700	-0.99927400
H	2.61307300	7.59981100	0.64481300
C	2.37250600	-2.32830400	-2.43646400
H	1.30128100	-2.53991200	-2.34871200
H	2.46220000	-1.27279700	-2.72200700
H	2.77586700	-2.93325300	-3.25421200
C	3.07458900	-1.52295000	2.54289300
H	3.31244900	-0.45305200	2.51056400
H	2.00182500	-1.60337600	2.75346000
H	3.61769100	-1.96097300	3.38605200
C	5.96069200	-4.85124500	0.07038500
H	5.75802600	-5.68731600	-0.60836800
H	6.90205200	-4.39014100	-0.25787600
H	6.13112200	-5.26136000	1.07141000
C	-4.66553200	-2.64606200	0.06769200
H	-5.74325900	-2.70360800	0.06337600
N	-3.87375900	-3.68527900	0.12256000

Cartesian coordinates of **6**

Pt	0.16106500	-1.24646100	-0.31780500
C	-0.14846400	-3.23053200	-0.29880700
C	-1.35873000	-3.90481000	-0.11357500
C	0.99481000	-4.02642000	-0.51098900
H	-2.26580700	-3.33023700	0.04773400
C	0.97619800	-5.41586200	-0.54090600
C	-0.25047600	-6.05848200	-0.34955300
H	1.88259400	-5.99262400	-0.70689400
H	-0.29732500	-7.14353600	-0.36704300
C	1.98994700	-1.87311500	-0.62582900
N	2.16645000	-3.23363600	-0.68802200
N	3.22717100	-1.38314100	-0.81100800
O	-1.85250600	-0.82408000	0.03209200
O	0.56609200	0.86507900	-0.39313300
C	-2.36909500	0.34597500	0.09545900
C	-0.32765100	1.77425900	-0.28911200
C	-1.70021400	1.57448000	-0.05335600
H	-2.31004600	2.46771000	0.02482700
C	3.65184000	0.02243200	-0.74855400
H	4.32718500	0.18467400	-1.59239900
H	2.74691000	0.61734000	-0.88653400
C	-3.84866100	0.37039400	0.37824400

C	-4.30295200	0.05199000	1.67457200
C	-4.76500300	0.67568300	-0.64570100
C	-5.67686700	0.07111600	1.92890000
C	-6.13256200	0.67103500	-0.34718200
C	-6.60947900	0.38138400	0.93351500
H	-6.02778900	-0.16732600	2.93132300
H	-6.84256600	0.89548700	-1.14099400
C	0.16464500	3.18993200	-0.46041800
C	0.49387500	3.97437500	0.66015000
C	0.31200300	3.70664400	-1.76392400
C	0.95393900	5.28078100	0.45512700
C	0.77465400	5.01584200	-1.92087500
C	1.09697000	5.82263900	-0.82422700
H	1.20924100	5.88796300	1.32158800
H	0.88493300	5.41609100	-2.92717600
C	-3.33314200	-0.30270300	2.78018400
H	-2.80550100	-1.23758300	2.56264500
H	-2.56568900	0.47116600	2.90600700
H	-3.85522400	-0.41743900	3.73503000
C	-4.30870500	0.98503700	-2.05595400
H	-3.82612800	1.96790600	-2.12209500
H	-3.58356000	0.24751500	-2.41759500
H	-5.15923800	0.98695300	-2.74484400
C	-8.08851500	0.42026400	1.24176500
H	-8.38191300	1.39143400	1.66300300
H	-8.69024500	0.26157500	0.34059800
H	-8.36626700	-0.34590900	1.97416400
C	-0.02222000	2.86888300	-2.97878700
H	0.60658500	1.97280100	-3.03246000
H	-1.06261700	2.52241500	-2.95502400
H	0.12196900	3.44094700	-3.90036300
C	0.39796600	3.42451400	2.06646600
H	-0.54337400	2.89064500	2.23395600
H	1.21096400	2.71494400	2.26709800
H	0.47135000	4.22793100	2.80604200
C	1.56328000	7.24673700	-1.02118500
H	2.20544300	7.34004800	-1.90420200
H	0.71366000	7.92757000	-1.16657900
H	2.12575400	7.60799500	-0.15385700
C	-1.40712700	-5.30457900	-0.13828600
H	-2.35810200	-5.81080000	0.00831500
C	4.32998600	0.35828300	0.56464000
C	3.55749000	0.57895000	1.71330100
C	5.72323700	0.44183600	0.65113100
C	4.17300300	0.87541600	2.92940800
H	2.47431000	0.51745200	1.64566700
C	6.33995200	0.74451100	1.86712300

H	6.32748700	0.26644700	-0.23555900
C	5.56582900	0.96068600	3.00811600
H	3.56588500	1.04426100	3.81488600
H	7.42337300	0.80938500	1.92211800
H	6.04468700	1.19576400	3.95498700
N	4.17475900	-2.36743700	-0.98143600
C	3.49409600	-3.48068000	-0.90438100
H	3.92547400	-4.46488000	-1.00496400

Cartesian coordinates of **16**

Pt	-0.90008900	0.28598900	-0.16664500
C	-2.09508000	-1.28317100	0.23744600
C	-3.41946500	-1.26434000	0.67959000
C	-1.51030600	-2.55161200	0.05097200
C	-4.10740600	-2.46266500	0.91822300
H	-3.91312500	-0.31034900	0.83832100
C	-2.16238200	-3.75544100	0.27776600
C	-3.48778000	-3.69889300	0.72030600
H	-1.65308500	-4.70007300	0.11514100
H	-4.03119500	-4.62050400	0.90892900
C	0.31999400	-1.18897700	-0.57016500
N	-0.16699800	-2.43810400	-0.39590700
N	1.59734700	-1.40312300	-0.99606700
O	-2.36654400	1.68265800	0.32885200
O	0.44835800	1.91002700	-0.60828200
C	-2.23425700	2.95319000	0.28877300
C	0.14490600	3.14809400	-0.50741300
C	-1.08886100	3.67543900	-0.09179100
H	-1.16874200	4.75581400	-0.06326900
C	-3.47620400	3.71426900	0.70650700
H	-3.34449300	4.79763900	0.65338900
H	-4.31417700	3.42218900	0.06351400
H	-3.74530200	3.43566500	1.73183200
C	1.25932300	4.10237800	-0.89075100
H	2.15781300	3.86891900	-0.30838700
H	1.51406800	3.95921900	-1.94777500
H	0.99110800	5.14969400	-0.73201700
C	2.59881200	-0.36242800	-1.29695600
H	3.06707800	-0.62405500	-2.25107600
H	2.03660600	0.56500100	-1.42153100
H	-5.13835100	-2.42853200	1.26245000
N	0.72522300	-3.42908900	-0.68112100
C	1.79362300	-2.76732900	-1.03901500
H	2.72563200	-3.22520100	-1.33450500
C	3.64020000	-0.22224400	-0.20518500
C	4.92225500	-0.76006700	-0.36290200
C	3.31993100	0.44885400	0.98366800

C	5.87238600	-0.63938600	0.65397700
H	5.18421200	-1.26930800	-1.28848800
C	4.26726700	0.56635000	2.00028900
H	2.32947800	0.88096700	1.10024500
C	5.54438800	0.02152400	1.83834700
H	6.86571000	-1.05879400	0.51904900
H	4.01045800	1.08766400	2.91847200
H	6.28162900	0.11636600	2.63099500

Cartesian coordinates of **17**

Pt	-1.35764900	-0.30268600	-0.01590800
C	-3.10447100	0.69726900	-0.06906700
C	-3.30351800	2.07809400	-0.13122500
C	-4.26113800	-0.10678600	-0.04562000
C	-4.60103500	2.60873300	-0.16535900
H	-2.44267600	2.73954000	-0.15569300
C	-5.55811700	0.38583300	-0.07800600
C	-5.72049800	1.77357700	-0.13852500
H	-6.40786000	-0.28922600	-0.05700900
H	-6.72064000	2.19687500	-0.16529300
C	-2.61290200	-1.80206800	0.03449500
N	-3.92770400	-1.48682000	0.01311200
N	-2.61428500	-3.16411800	0.09863000
O	-0.22626200	1.44836800	-0.05683700
O	0.46540100	-1.44775400	0.02993100
C	1.05217500	1.51365200	-0.04391700
C	1.63801800	-0.93629300	0.02692600
C	1.95312500	0.43332000	-0.00639600
H	3.00754600	0.68622800	0.00310600
C	-1.43432500	-4.02579600	0.14877300
H	-1.41825800	-4.68592700	-0.72338300
H	-0.54857200	-3.38924000	0.14596400
H	-1.45420400	-4.62867000	1.06123400
H	-4.73679200	3.68649900	-0.21396000
C	-3.93106700	-3.57375800	0.11096800
H	-4.23166100	-4.61013000	0.15774000
N	-4.76011200	-2.56491000	0.05959900
C	1.61315900	2.91160900	-0.04242500
C	1.50365700	3.68889900	1.12885600
C	2.20564300	3.44554800	-1.20242300
C	2.01665000	4.98875000	1.12355200
C	2.69501900	4.75647100	-1.16429700
C	2.61902100	5.54168700	-0.01133200
H	1.93853100	5.58676300	2.02969800
H	3.14256900	5.17479300	-2.06392000
C	2.77164500	-1.93075400	0.04970700
C	3.43209200	-2.22413200	1.25731500

C	3.13095100	-2.59157400	-1.14217300
C	4.45797700	-3.17657100	1.24849900
C	4.16526400	-3.53106400	-1.10527300
C	4.84504700	-3.83590800	0.07890000
H	4.96447700	-3.40994900	2.18317600
H	4.44599100	-4.03885500	-2.02635000
C	0.84836500	3.13833800	2.37653600
H	-0.21765600	2.94582100	2.21462600
H	1.29891300	2.18514000	2.67945400
H	0.94814300	3.83888000	3.21124100
C	2.30167300	2.64785300	-2.48584200
H	3.02324800	1.82618100	-2.40284500
H	1.33841800	2.20093800	-2.75672600
H	2.62085300	3.28754400	-3.31461300
C	3.18805500	6.94153500	0.01740700
H	4.21054200	6.94748200	0.41889600
H	3.23011800	7.37787000	-0.98621700
H	2.58909800	7.60531500	0.65077600
C	2.42225600	-2.29117600	-2.44487000
H	1.34794800	-2.49300700	-2.37234700
H	2.52508000	-1.23471300	-2.72217200
H	2.83061000	-2.89432000	-3.26150900
C	3.04413700	-1.54427500	2.55295000
H	3.28257400	-0.47412800	2.53601200
H	1.96784000	-1.62618400	2.74394400
H	3.57285600	-1.99146000	3.40044800
C	5.97972700	-4.83433600	0.08614100
H	5.79100700	-5.66272300	-0.60597000
H	6.92420800	-4.36571400	-0.22180300
H	6.13644100	-5.25613500	1.08456500

Cartesian coordinates of **18**

Pt	-0.76207500	-0.94808700	-0.02895100
C	-2.77205000	-0.82851800	-0.04519800
C	-3.55599500	0.31725100	-0.08147900
C	-3.44738800	-2.06897500	-0.01488400
C	-4.96213500	0.22394800	-0.08405700
H	-3.10191600	1.30230000	-0.11158400
C	-4.82499900	-2.19128000	-0.01722600
C	-5.59814500	-1.02352900	-0.05164400
H	-5.29562900	-3.16914400	0.00718600
H	-6.67850500	-1.10395600	-0.05335100
C	-1.21611700	-2.85214800	0.01231100
N	-2.53359800	-3.15500600	0.01639200
N	-0.60952100	-4.07399900	0.04683800
O	-0.53078800	1.12358400	-0.05849500
O	1.37770500	-1.16126500	-0.00690500

C	0.58356500	1.75254000	-0.04209200
C	2.19876300	-0.18017800	0.01268300
C	1.87165400	1.18621600	-0.00483200
H	2.70309000	1.88179800	0.01944800
C	0.83093600	-4.32274100	0.05850500
H	1.11504400	-4.90399900	-0.82362900
H	1.34341400	-3.36006200	0.04639400
H	1.10480100	-4.87525500	0.96199900
C	-1.60518000	-5.02650900	0.06941200
H	-1.41240400	-6.08881700	0.09837300
N	-2.79799900	-4.49111200	0.05151100
C	0.46402100	3.25358300	-0.03041200
C	-0.02988100	3.88876900	1.12858600
C	0.81120300	4.00884100	-1.16647600
C	-0.14337200	5.28100200	1.13516700
C	0.66760000	5.40079400	-1.11782000
C	0.20151600	6.05722300	0.02329300
H	-0.51651000	5.77200700	2.03217500
H	0.92325700	5.98473400	-1.99996200
C	3.65675600	-0.56489400	0.05097700
C	4.34254500	-0.60283500	1.27922100
C	4.30894000	-0.92272400	-1.14527600
C	5.68702800	-0.99174000	1.28707500
C	5.65387500	-1.30044400	-1.09122900
C	6.36322700	-1.33753800	0.11387500
H	6.21714000	-1.02709500	2.23704600
H	6.15969700	-1.57473700	-2.01536500
C	-0.42775300	3.09208700	2.35178000
H	-1.30727200	2.47046300	2.15347900
H	0.37390100	2.41327400	2.66784600
H	-0.65824300	3.75614000	3.19052700
C	1.30953600	3.35511300	-2.43836300
H	2.32918900	2.96706000	-2.32564900
H	0.67757000	2.51051800	-2.73474600
H	1.31847800	4.07483000	-3.26299500
C	0.08631400	7.56355400	0.06587200
H	0.92907900	8.01266200	0.60857700
H	0.07945900	7.99340300	-0.94116900
H	-0.83028700	7.88156600	0.57577300
C	3.57651200	-0.89845900	-2.46899200
H	2.70576100	-1.56358200	-2.45670000
H	3.20129300	0.10593100	-2.70113400
H	4.23370900	-1.20971400	-3.28674200
C	3.65053600	-0.24239900	2.57625500
H	3.38110400	0.82017600	2.60847700
H	2.72118000	-0.80872100	2.70704900
H	4.29749700	-0.44996000	3.43423000

C	7.82531500	-1.71988900	0.14074200
H	8.05616900	-2.47779500	-0.61613600
H	8.46746600	-0.85258500	-0.06427100
H	8.11855200	-2.11694800	1.11844200
O	-5.62278600	1.42080300	-0.11960400
C	-7.03849600	1.40784500	-0.12929700
H	-7.34883100	2.45428800	-0.16103700
H	-7.43376700	0.88675800	-1.01211500
H	-7.44686300	0.93730800	0.77575600

Cartesian coordinates of **19**

Pt	-1.04231800	-0.79048700	-0.01622800
C	-3.02168500	-0.41723100	-0.05083700
C	-3.66058200	0.82024200	-0.09808400
C	-3.84927400	-1.55792700	-0.02952300
C	-5.06558300	0.92256700	-0.12118500
H	-3.05806500	1.72480500	-0.12112600
C	-5.23357100	-1.50796700	-0.05258000
C	-5.83593300	-0.24624400	-0.09908200
H	-5.82358600	-2.41899400	-0.03715900
H	-6.92053900	-0.17486200	-0.11923500
C	-1.73673500	-2.61908900	0.02595700
N	-3.08219400	-2.75241300	0.01390800
N	-1.29060900	-3.90699600	0.07403600
O	-0.54523500	1.23517100	-0.04986500
O	1.05586700	-1.27654900	0.01464500
C	0.64157800	1.71473600	-0.03885500
C	1.99625700	-0.40945800	0.02151800
C	1.84634200	0.98800900	-0.00414200
H	2.76062000	1.57088500	0.00987800
C	0.10703900	-4.33378800	0.10961900
H	0.32858100	-4.95496300	-0.76314300
H	0.73454000	-3.44173200	0.09700300
H	0.29696400	-4.90671200	1.02188200
C	-2.39981000	-4.72592100	0.08745900
H	-2.34347600	-5.80392700	0.12354200
N	-3.51441500	-4.04422600	0.05138600
C	0.71508500	3.21907500	-0.03502100
C	0.33360900	3.91723000	1.12959100
C	1.12634900	3.91857100	-1.18529600
C	0.39605200	5.31301600	1.12750400
C	1.16076200	5.31753900	-1.14476900
C	0.80903600	6.03364400	0.00173800
H	0.10962300	5.85182300	2.02893300
H	1.46625100	5.85997200	-2.03752900
C	3.39232600	-0.97957400	0.04889600
C	4.09675200	-1.06714900	1.26422700

C	3.96205500	-1.46285200	-1.14565500
C	5.37618800	-1.63474900	1.26037500
C	5.24472600	-2.01718000	-1.10358700
C	5.97114500	-2.10948900	0.08827300
H	5.91899400	-1.70986300	2.20080000
H	5.68645700	-2.38846200	-2.02663600
C	-0.13154100	3.18261100	2.36777400
H	-1.07935100	2.66312600	2.19063000
H	0.59274700	2.41938400	2.67800200
H	-0.26992600	3.87573600	3.20320700
C	1.50648800	3.19925300	-2.46250700
H	2.46917700	2.68219700	-2.36855800
H	0.76314400	2.44279500	-2.73775700
H	1.59033700	3.90719000	-3.29305800
C	0.88878100	7.54256500	0.03413800
H	1.82805200	7.88211000	0.49144600
H	0.84481400	7.96791000	-0.97401100
H	0.07041300	7.97530400	0.62048200
C	3.21069100	-1.38118600	-2.45644600
H	2.24735200	-1.89955700	-2.39858900
H	2.99212800	-0.34089500	-2.72806000
H	3.79180200	-1.82559500	-3.27025100
C	3.49207500	-0.57450700	2.56146700
H	3.36424400	0.51458900	2.56015100
H	2.50079900	-1.00945200	2.73463400
H	4.12936200	-0.83579700	3.41198800
C	7.36819000	-2.68620800	0.10248300
H	7.47939100	-3.48821000	-0.63574600
H	8.11771200	-1.91994900	-0.13759200
H	7.62416100	-3.09340400	1.08647100
C	-5.72410400	2.28340300	-0.15952000
H	-5.56285400	2.83211100	0.77775100
H	-5.31465900	2.90321200	-0.96635100
H	-6.80520900	2.20207400	-0.31337000

Cartesian coordinates of **20**

Pt	0.05322100	-1.25564300	-0.31503600
C	-0.34609700	-3.22952100	-0.28478300
C	-1.58186800	-3.85405000	-0.10337200
C	0.76537800	-4.07288500	-0.48077900
H	-2.46886200	-3.24596700	0.04703200
C	0.70213800	-5.45906800	-0.50053400
C	-0.55099300	-6.05117000	-0.31346700
H	1.59790200	-6.05204700	-0.65582500
H	-0.64040300	-7.13382900	-0.32240100
C	1.84943700	-1.97420000	-0.61006000
N	1.95812400	-3.32107200	-0.65386400

N	3.13132400	-1.54615600	-0.78931200
O	-1.93838300	-0.73714500	0.02507700
O	0.56202500	0.83648000	-0.38866800
C	-2.39664000	0.45663300	0.09140100
C	-0.28781300	1.78652700	-0.28386500
C	-1.66924400	1.65205800	-0.05638200
H	-2.23464400	2.57323100	0.03094000
C	3.59072600	-0.14627300	-0.77908800
H	4.13598000	0.03714500	-1.71043600
H	2.68553500	0.46630100	-0.78330300
C	3.92493100	-2.66665100	-0.92172800
H	4.99433200	-2.62368900	-1.06357300
N	3.23088900	-3.77110200	-0.84702000
C	-3.87122000	0.55230500	0.38608300
C	-4.32714000	0.26525900	1.68910700
C	-4.78239600	0.89158200	-0.63150200
C	-5.69620700	0.34963400	1.95597400
C	-6.14584800	0.95247000	-0.32048300
C	-6.62319800	0.69464600	0.96682000
H	-6.04802200	0.13519500	2.96350000
H	-6.85234400	1.20299600	-1.10962700
C	0.28205200	3.17743400	-0.41155000
C	0.87699400	3.79328200	0.70644600
C	0.24919400	3.83339900	-1.65667200
C	1.41455400	5.07603800	0.56123300
C	0.80537600	5.11335100	-1.75781600
C	1.38575100	5.75580900	-0.66044700
H	1.87074000	5.55440800	1.42612200
H	0.78499100	5.61942600	-2.72129100
C	-3.36392000	-0.12589500	2.78805200
H	-2.88240100	-1.08576500	2.57219100
H	-2.56065600	0.61292800	2.90021800
H	-3.88118300	-0.20978000	3.74871700
C	-4.32521500	1.16887600	-2.04789800
H	-3.80013900	2.12902500	-2.12606100
H	-3.63636700	0.39756300	-2.40969700
H	-5.18059900	1.20368700	-2.72988600
C	-8.09595500	0.80274300	1.28834300
H	-8.34201200	1.79033000	1.70168400
H	-8.71286500	0.66148200	0.39454800
H	-8.40025500	0.05730200	2.03149300
C	-0.36439200	3.17680600	-2.87447700
H	0.03959600	2.17096400	-3.03652700
H	-1.45116400	3.06865400	-2.77187800
H	-0.17190100	3.76857200	-3.77477700
C	0.95611000	3.08410000	2.04012800
H	-0.01259300	2.66221900	2.33163500

H	1.66971800	2.25220300	2.00366800
H	1.28017500	3.76947500	2.82934600
C	1.94695800	7.15381500	-0.78348500
H	2.25261700	7.37431500	-1.81185500
H	1.20242700	7.90866500	-0.49628100
H	2.81730100	7.29557700	-0.13324000
C	-1.68037300	-5.25278500	-0.11749000
H	-2.65082600	-5.72195800	0.02567000
C	4.46384400	0.16503900	0.42026200
C	3.94226200	0.06618200	1.71873900
C	5.79260700	0.56588800	0.24910700
C	4.74144300	0.35963000	2.82266700
H	2.90965300	-0.24407300	1.86039900
C	6.59282700	0.86541000	1.35499200
H	6.20433000	0.65139400	-0.75440400
C	6.06901400	0.76051900	2.64327800
H	4.32768700	0.27855300	3.82409700
H	7.62316400	1.17739000	1.20731400
H	6.68985700	0.99027700	3.50489800

Cartesian coordinates of **21**

Pt	-0.31245200	-0.94209300	-0.32266600
C	-1.61093900	-2.48064200	-0.28940200
C	-2.98629600	-2.42857900	-0.10373300
C	-1.03606900	-3.75574200	-0.48779000
H	-3.49209800	-1.48085300	0.04987400
C	-1.76587500	-4.93049000	-0.50320900
C	-3.15183900	-4.85724000	-0.31206000
H	-1.27590300	-5.88646600	-0.65921600
H	-3.73602100	-5.76956900	-0.32142200
C	0.92087000	-2.43471900	-0.61917300
N	0.36951800	-3.66792300	-0.66380100
N	2.25161900	-2.67489300	-0.80125100
O	-1.80901000	0.46882800	0.01559600
O	1.13427900	0.64580500	-0.39452900
C	-1.64049900	1.73577600	0.08318800
C	0.84859900	1.88724100	-0.27822000
C	-0.42681300	2.43498800	-0.05458200
H	-0.47878500	3.51400600	0.03912300
C	3.32795700	-1.66949500	-0.79381900
H	3.88501400	-1.76260600	-1.73167800
H	2.83060600	-0.69617900	-0.78595700
C	2.40893000	-4.03766400	-0.93767000
H	3.36679000	-4.51399200	-1.08314900
N	1.26904900	-4.67315900	-0.86133400
C	-2.89152200	2.52434500	0.36970600
C	-3.45049900	2.47080400	1.66302300

C	-3.51365400	3.27231400	-0.64756400
C	-4.61780000	3.19420200	1.92125800
C	-4.68829600	3.97127900	-0.34563900
C	-5.25226200	3.95305600	0.93220900
H	-5.04608500	3.15830300	2.92132500
H	-5.17718300	4.53949000	-1.13477900
C	2.02046600	2.83111600	-0.38495700
C	2.82644000	3.07184800	0.74431000
C	2.32056700	3.43590200	-1.62043600
C	3.91571500	3.94027100	0.62071700
C	3.42411000	4.29193000	-1.70006600
C	4.22952200	4.56459100	-0.59038700
H	4.53694700	4.12980600	1.49422800
H	3.66017500	4.75600900	-2.65599800
C	-2.81031700	1.64984500	2.76071800
H	-2.86760100	0.57819800	2.54102600
H	-1.74688500	1.89295000	2.87618800
H	-3.30404800	1.82994300	3.72060500
C	-2.95839100	3.31667800	-2.05543800
H	-2.02969500	3.89800600	-2.10976000
H	-2.72969100	2.31360500	-2.43244600
H	-3.67766800	3.77768200	-2.73964000
C	-6.50219900	4.74345600	1.24407000
H	-6.25752800	5.71626500	1.69187300
H	-7.08814200	4.93932700	0.33983600
H	-7.14482800	4.21339400	1.95587100
C	1.48002900	3.16728100	-2.85001000
H	1.34882800	2.09273600	-3.02105400
H	0.47543800	3.59760000	-2.75563300
H	1.94498800	3.59855300	-3.74202400
C	2.54035000	2.39598500	2.06702400
H	1.49087700	2.51238300	2.36149300
H	2.73919200	1.31893400	2.01177400
H	3.16516000	2.81279400	2.86295100
C	5.39346700	5.52355000	-0.69156200
H	5.81548100	5.53711200	-1.70235100
H	5.08484700	6.55091400	-0.45494000
H	6.19459700	5.25765500	0.00670300
C	-3.75581300	-3.60917400	-0.11390400
C	4.25658800	-1.82603100	0.39427500
C	3.75888000	-1.71497000	1.70105900
C	5.62104300	-2.06576400	0.20397900
C	4.61431600	-1.84529800	2.79402900
H	2.69899000	-1.52966200	1.85797000
C	6.48032100	-2.19125700	1.29899200
H	6.01738300	-2.14894900	-0.80585300
C	5.97782400	-2.08339500	2.59554200

H	4.21762800	-1.75854000	3.80188400
H	7.53872000	-2.37595700	1.13635200
H	6.64327100	-2.18359800	3.44864400
O	-5.09750600	-3.42918600	0.08125400
C	-5.93512200	-4.57045100	0.08366700
H	-5.66668900	-5.26946500	0.88775900
H	-6.94826600	-4.20006300	0.25319200
H	-5.90073100	-5.10155400	-0.87756100

Cartesian coordinates of **22**

Pt	-0.13677300	-1.13118200	-0.33067400
C	-0.96751700	-2.96649100	-0.28882400
C	-2.30953000	-3.29777900	-0.11326200
C	-0.06791000	-4.03694800	-0.46807700
H	-3.03635000	-2.50124100	0.02473400
C	-0.44607400	-5.36968600	-0.47489500
C	-1.80266300	-5.65982600	-0.29368000
H	0.28916000	-6.15579300	-0.61546500
H	-2.12968200	-6.69664900	-0.29379200
C	1.45640500	-2.23411300	-0.60700100
N	1.26293100	-3.57173700	-0.63738100
N	2.80232000	-2.10372400	-0.78393300
O	-1.96138200	-0.17417700	-0.00857900
O	0.82762100	0.79073700	-0.41487500
C	-2.13775800	1.09134900	0.07280400
C	0.21987800	1.90820500	-0.28391100
C	-1.15505200	2.09097000	-0.05181200
H	-1.49357000	3.11569900	0.05361300
C	3.56195700	-0.84201600	-0.79243200
H	4.13583700	-0.79911400	-1.72369900
H	2.81710700	-0.04228300	-0.81091200
C	3.32688900	-3.37393100	-0.90221600
H	4.37928000	-3.57156400	-1.04025100
N	2.40407700	-4.29547300	-0.82022700
C	-3.55463400	1.51346500	0.36105300
C	-4.09792800	1.25236100	1.63627200
C	-4.33613800	2.12836900	-0.63576800
C	-5.41562500	1.63692000	1.89771400
C	-5.65567700	2.48361100	-0.33207200
C	-6.21219900	2.25585400	0.92870000
H	-5.83212900	1.44268300	2.88443800
H	-6.26474200	2.94667400	-1.10620500
C	1.09466700	3.13283200	-0.38757200
C	1.76206500	3.61426900	0.75439300
C	1.26576800	3.76218700	-1.63565600
C	2.58021500	4.74224100	0.62955600
C	2.09790200	4.88333500	-1.71545900

C	2.75829400	5.39455500	-0.59382300
H	3.09413100	5.11751000	1.51262600
H	2.23361300	5.36854200	-2.68039900
C	-3.28213100	0.57356300	2.71470800
H	-3.06667400	-0.46838900	2.45515300
H	-2.31434100	1.06924000	2.85934200
H	-3.81397700	0.58636000	3.67104900
C	-3.79454500	2.39249000	-2.02499000
H	-3.07943700	3.22440600	-2.03137000
H	-3.27220500	1.51919600	-2.43069000
H	-4.60643600	2.64997400	-2.71249100
C	-7.62713100	2.68246200	1.24497600
H	-7.64778000	3.67250900	1.72054000
H	-8.23929600	2.74435700	0.33894400
H	-8.11246000	1.98318400	1.93487100
C	0.57436900	3.23969400	-2.87629100
H	0.79107700	2.17757100	-3.03912700
H	-0.51602500	3.33145200	-2.80043400
H	0.89593100	3.79186100	-3.76478100
C	1.62511700	2.92109700	2.09209800
H	0.57527500	2.73614500	2.34654100
H	2.12940900	1.94690000	2.08557800
H	2.06873700	3.52222000	2.89182700
C	3.62196700	6.63072400	-0.69755300
H	4.09841700	6.70611200	-1.68120700
H	3.02897300	7.54422500	-0.55417000
H	4.41075500	6.63381500	0.06239900
C	-2.74294900	-4.63850200	-0.11369400
C	4.48084600	-0.71086400	0.40625300
C	3.95413800	-0.72700900	1.70626600
C	5.85903500	-0.55171300	0.23166600
C	4.79633400	-0.59000900	2.80867100
H	2.88319000	-0.84978300	1.84998100
C	6.70323500	-0.40790900	1.33610200
H	6.27593000	-0.53353300	-0.77311500
C	6.17336700	-0.42929500	2.62603300
H	4.37818800	-0.60552100	3.81144600
H	7.77222100	-0.28334600	1.18606200
H	6.82803600	-0.32113100	3.48647200
C	-4.20901200	-4.95918200	0.07307100
H	-4.60027000	-4.51935300	0.99888200
H	-4.81387500	-4.55863300	-0.75064400
H	-4.38078700	-6.03969900	0.11716300

Cartesian Coordinates of DFT-optimized triplet states T₁ (BP86/6-31G(d))

Cartesian coordinates of **4**

Pt	-0.86091500	0.25987300	0.00950700
C	-1.94871400	-1.41038300	0.27523800
C	-3.25249800	-1.51041200	0.77021700
C	-1.31341300	-2.61541100	-0.08738900
C	-3.87868400	-2.75828800	0.88813000
H	-3.77322200	-0.60624700	1.07046100
C	-1.90859900	-3.86555100	0.01893500
C	-3.21521600	-3.92887800	0.51585900
H	-1.38417600	-4.77235300	-0.27145000
H	-3.70691400	-4.89277100	0.61036900
C	0.43081500	-1.08849900	-0.61377800
N	0.01007700	-2.39445000	-0.57526700
N	1.67569200	-1.16906800	-1.10700100
O	-2.33539800	1.51263800	0.75052600
O	0.32977100	1.99289300	-0.33835900
C	-2.56001400	2.71913500	0.27489800
C	-0.20604200	3.14285000	-0.69649800
C	-1.55208200	3.48694000	-0.37981600
H	-1.84401500	4.50200600	-0.64228600
C	-3.92068600	3.29315400	0.56282200
H	-4.03319300	4.30380600	0.15697900
H	-4.70934600	2.66196100	0.13004400
H	-4.10941100	3.33593100	1.64525500
C	0.70237900	4.10988200	-1.40700900
H	1.58939900	4.33925000	-0.79881400
H	1.06993400	3.68475500	-2.35252100
H	0.19632700	5.05303100	-1.63761500
C	2.63163900	-0.06845500	-1.30688300
H	3.10672200	-0.24980000	-2.27467600
H	2.03169200	0.84150900	-1.35731100
H	-4.89272900	-2.81616000	1.27575400
C	3.65813400	0.02424200	-0.19604500
C	4.80935300	-0.77309600	-0.21607600
C	3.45406500	0.91258000	0.86756800
C	5.74443900	-0.68589000	0.81582800
H	4.96804500	-1.46639000	-1.03815000
C	4.39111700	0.99928800	1.89903400
H	2.56156100	1.53304900	0.87798200
C	5.53650000	0.20100100	1.87504200
H	6.63595500	-1.30700800	0.79161700
H	4.22655600	1.69214200	2.71994300
H	6.26644900	0.27075700	2.67730000
N	2.06489600	-2.46190700	-1.37469400
C	1.02517500	-3.18209800	-1.04191300
H	0.97609300	-4.25646200	-1.13199500

Cartesian coordinates of **5**

Pt	-1.35690000	-0.35420600	-0.16734400
C	-3.12884300	0.58697800	-0.17476800
C	-3.37294100	1.94348900	-0.40901900
C	-4.25503500	-0.23111900	0.04832100
C	-4.68111900	2.44612200	-0.40221000
H	-2.53451100	2.60348200	-0.60856400
C	-5.56165300	0.23882800	0.06126500
C	-5.76907300	1.60417500	-0.16536100
H	-6.40389600	-0.42550000	0.23708700
H	-6.78006800	2.00110300	-0.16054600
C	-2.54702100	-1.87859200	0.17084100
N	-3.88882700	-1.59680700	0.24601600
N	-2.48561300	-3.19904700	0.40279400
O	-0.28936100	1.40680600	-0.46417800
O	0.47919200	-1.43552900	-0.24266300
C	0.99317700	1.57444700	-0.24334600
C	1.67190200	-0.92634300	-0.03860800
C	1.90431800	0.48547100	-0.05756100
H	2.94135700	0.77935500	0.06394300
C	-1.29573500	-4.03686400	0.46020300
H	-1.36858700	-4.81987200	-0.29894700
H	-0.42866200	-3.40160200	0.27526600
H	-1.22807400	-4.49768400	1.44900000
H	-4.85082400	3.50404300	-0.58577300
C	1.48965400	2.96679600	-0.11745300
C	0.88125500	3.84794800	0.81736100
C	2.55374500	3.44283600	-0.92655400
C	1.35937000	5.15370300	0.93274400
C	2.99283900	4.76137200	-0.77339400
C	2.41711600	5.63469900	0.15235200
H	0.89785200	5.81515900	1.66409600
H	3.79762100	5.12185000	-1.41179100
C	2.81943900	-1.86202200	0.05427000
C	3.74853000	-1.77839700	1.12331100
C	2.98690200	-2.87473600	-0.92975700
C	4.81301900	-2.68410000	1.17892900
C	4.06716400	-3.75204600	-0.82843100
C	4.99793400	-3.67671600	0.21443600
H	5.50819800	-2.62135900	2.01449000
H	4.19410600	-4.51295600	-1.59690300
C	-0.23907600	3.39775100	1.72812000
H	-1.19363100	3.31723800	1.19866200
H	-0.03958400	2.40827300	2.15493900
H	-0.36779200	4.10525900	2.55376900
C	3.20201600	2.58632600	-1.99457200
H	3.98243000	1.92640700	-1.59124500
H	2.47221400	1.94738300	-2.50247400
H	3.68310000	3.21677300	-2.74966700
C	2.93011700	7.04514000	0.32267100
H	3.63808800	7.11438900	1.16017400
H	3.45361300	7.39243500	-0.57450800

H	2.11495800	7.74692600	0.53242000
C	2.05572000	-3.00235600	-2.11583100
H	1.09289100	-3.44443100	-1.83924100
H	1.82897000	-2.02606000	-2.55824900
H	2.50804000	-3.63151000	-2.88943300
C	3.60294800	-0.77054800	2.24485100
H	4.01723000	0.21331000	1.98506200
H	2.55415300	-0.61363200	2.51825600
H	4.13860300	-1.11167900	3.13696800
C	6.17214900	-4.62488400	0.27886200
H	5.88972400	-5.63709700	-0.03267400
H	6.98570600	-4.29994200	-0.38429700
H	6.58335700	-4.68530200	1.29213900
C	-4.55323900	-2.76014200	0.51529300
H	-5.62321800	-2.84313600	0.62976600
N	-3.72231600	-3.76515100	0.61748300

Cartesian coordinates of **6**

Pt	-0.35214400	-1.17473400	-0.26841300
C	-0.26956200	-3.16783900	-0.47823300
C	0.85898300	-3.98773400	-0.38337400
C	-1.49308600	-3.80080200	-0.77826700
C	0.75374800	-5.37134000	-0.57848800
H	1.82080100	-3.53836600	-0.15630600
C	-1.62670500	-5.16854200	-0.97608100
C	-0.47747300	-5.96046300	-0.87174900
H	-2.58885100	-5.61938200	-1.20530300
H	-0.55077600	-7.03383600	-1.02089200
C	-2.24475600	-1.55122400	-0.63219700
N	-2.57030500	-2.86750200	-0.84923000
N	-3.42169300	-0.91274100	-0.72179900
O	1.66382600	-1.02595100	0.20584600
O	-0.49515000	0.95323100	-0.15446100
C	2.42288300	0.04169200	0.11607800
C	0.52290400	1.78287100	-0.20012200
C	1.87686600	1.35551600	-0.05680400
H	2.60615900	2.15851000	-0.05374400
C	-3.68890400	0.51379200	-0.47742300
H	-2.72923400	1.02155800	-0.58230200
H	-4.36624800	0.83992100	-1.27124200
H	1.64155200	-5.99373800	-0.50024400
C	3.87105500	-0.12378700	0.37738700
C	4.84291700	0.44216300	-0.48959900
C	4.30522200	-0.87278100	1.50753700
C	6.20071400	0.26947300	-0.20347800
C	5.67222800	-1.01256400	1.74684500
C	6.64226100	-0.45225100	0.90711500
H	6.93563500	0.69730000	-0.88329100

H	5.99283000	-1.56833200	2.62653700
C	0.23891700	3.21536300	-0.48454800
C	-0.42921900	3.57721800	-1.68267800
C	0.61507300	4.22930000	0.43193700
C	-0.69202400	4.92466300	-1.93779800
C	0.32712200	5.56431000	0.13217500
C	-0.32145400	5.93825200	-1.04762000
H	-1.19167900	5.19296100	-2.86716200
H	0.60457700	6.33331200	0.85115900
C	-4.28153400	0.76898700	0.89368400
C	-5.65803700	0.64021500	1.11648100
C	-3.44412100	1.13564300	1.95465800
C	-6.19080900	0.87235100	2.38495800
H	-6.30990400	0.35229700	0.29575900
C	-3.97806300	1.36798300	3.22344300
H	-2.37714800	1.24259400	1.77671900
C	-5.35119200	1.23650200	3.44047500
H	-7.26055400	0.77255600	2.54865900
H	-3.32182200	1.65543800	4.04052900
H	-5.76681800	1.42041100	4.42773100
C	4.46842200	1.18835900	-1.75396800
H	3.59598800	0.74444300	-2.24491500
H	4.23154000	2.24536900	-1.56961600
H	5.30070600	1.17282600	-2.46542200
C	3.33083700	-1.48291900	2.49114200
H	2.52376000	-0.78725900	2.74630100
H	2.84664300	-2.37730200	2.08615300
H	3.84803200	-1.76151200	3.41525700
C	8.11450000	-0.65069400	1.18010100
H	8.72256300	0.10531300	0.67203100
H	8.33431000	-0.59689100	2.25271700
H	8.45763000	-1.63453600	0.83134200
C	1.28499900	3.90811900	1.75157400
H	0.86693400	3.00628200	2.21095100
H	2.36533900	3.74007600	1.64453700
H	1.16235400	4.73706500	2.45638700
C	-0.82487500	2.54643700	-2.71691700
H	-0.03708600	1.79979600	-2.86558500
H	-1.72576600	1.99472600	-2.42680200
H	-1.02537000	3.02695800	-3.68004600
C	-0.59109000	7.39052000	-1.36439900
H	-0.70616000	7.98560800	-0.45189700
H	0.23406700	7.83395100	-1.93871500
H	-1.50096800	7.50893000	-1.96303300
C	-3.91947800	-2.94334900	-1.05518600
H	-4.45855300	-3.85607200	-1.25805300
N	-4.47375500	-1.76127500	-0.98225800

Cartesian coordinates of **16**

Pt	-0.86091500	0.25987300	0.00950700
C	-1.94871400	-1.41038300	0.27523800
C	-3.25249800	-1.51041200	0.77021700
C	-1.31341300	-2.61541100	-0.08738900
C	-3.87868400	-2.75828800	0.88813000
H	-3.77322200	-0.60624700	1.07046100
C	-1.90859900	-3.86555100	0.01893500
C	-3.21521600	-3.92887800	0.51585900
H	-1.38417600	-4.77235300	-0.27145000
H	-3.70691400	-4.89277100	0.61036900
C	0.43081500	-1.08849900	-0.61377800
N	0.01007700	-2.39445000	-0.57526700
N	1.67569200	-1.16906800	-1.10700100
O	-2.33539800	1.51263800	0.75052600
O	0.32977100	1.99289300	-0.33835900
C	-2.56001400	2.71913500	0.27489800
C	-0.20604200	3.14285000	-0.69649800
C	-1.55208200	3.48694000	-0.37981600
H	-1.84401500	4.50200600	-0.64228600
C	-3.92068600	3.29315400	0.56282200
H	-4.03319300	4.30380600	0.15697900
H	-4.70934600	2.66196100	0.13004400
H	-4.10941100	3.33593100	1.64525500
C	0.70237900	4.10988200	-1.40700900
H	1.58939900	4.33925000	-0.79881400
H	1.06993400	3.68475500	-2.35252100
H	0.19632700	5.05303100	-1.63761500
C	2.63163900	-0.06845500	-1.30688300
H	3.10672200	-0.24980000	-2.27467600
H	2.03169200	0.84150900	-1.35731100
H	-4.89272900	-2.81616000	1.27575400
C	3.65813400	0.02424200	-0.19604500
C	4.80935300	-0.77309600	-0.21607600
C	3.45406500	0.91258000	0.86756800
C	5.74443900	-0.68589000	0.81582800
H	4.96804500	-1.46639000	-1.03815000
C	4.39111700	0.99928800	1.89903400
H	2.56156100	1.53304900	0.87798200
C	5.53650000	0.20100100	1.87504200
H	6.63595500	-1.30700800	0.79161700
H	4.22655600	1.69214200	2.71994300
H	6.26644900	0.27075700	2.67730000
N	2.06489600	-2.46190700	-1.37469400
C	1.02517500	-3.18209800	-1.04191300
H	0.97609300	-4.25646200	-1.13199500

Cartesian coordinates of **17**

Pt	-1.34980800	-0.35939500	-0.18393600
C	-3.13438500	0.57041500	-0.15700100
C	-3.40041000	1.92472300	-0.37178900
C	-4.24737200	-0.26322800	0.07286300
C	-4.71795500	2.40602100	-0.33797900
H	-2.57671200	2.60123900	-0.57768700
C	-5.56047200	0.17912700	0.11339500
C	-5.78918400	1.54510500	-0.09380300
H	-6.37472900	-0.51489600	0.29604600
H	-6.80524700	1.92846500	-0.06831500
C	-2.53115000	-1.89238500	0.15027200
N	-3.85113400	-1.61894700	0.24491700
N	-2.46801200	-3.23524800	0.36919400
O	-0.29510600	1.40757700	-0.47758800
O	0.49323200	-1.43062500	-0.28652100
C	0.98457400	1.58086500	-0.24602400
C	1.67914800	-0.91607100	-0.05132300
C	1.90069000	0.49802700	-0.05641600
H	2.93436000	0.79901600	0.07670600
C	-1.25170700	-4.04687900	0.39353400
H	-1.29992200	-4.81255600	-0.38601400
H	-0.40289200	-3.38554400	0.21295500
H	-1.14642000	-4.52656400	1.37074400
H	-4.90620600	3.46346600	-0.50623600
C	-3.75700700	-3.67888800	0.57751800
H	-4.00712500	-4.71088400	0.77485700
N	-4.62784800	-2.70647400	0.50733400
C	1.47266800	2.97706700	-0.12149000
C	0.85944800	3.85397500	0.81501700
C	2.53258400	3.45864700	-0.93034600
C	1.32830600	5.16223200	0.92950500
C	2.96329400	4.78117000	-0.77792800
C	2.38087400	5.65105100	0.14525100
H	0.86452600	5.82005200	1.66287400
H	3.76719300	5.14587100	-1.41482800
C	2.82952700	-1.84566900	0.05945200
C	3.73796800	-1.76172300	1.14645200
C	3.02129100	-2.85422400	-0.92447300
C	4.80468600	-2.66337300	1.22016200
C	4.10260900	-3.72814200	-0.80432800
C	5.01240600	-3.65266400	0.25669800
H	5.48334200	-2.59999600	2.06920000
H	4.24828900	-4.48555700	-1.57298000
C	-0.25438400	3.39358700	1.72865000
H	-1.20712600	3.29397500	1.19947200

H	-0.03948400	2.41050100	2.16299400
H	-0.39433000	4.10493400	2.54909000
C	3.18917100	2.60466700	-1.99532100
H	3.97426400	1.95214800	-1.58898600
H	2.46520800	1.95859600	-2.50249400
H	3.66613900	3.23694800	-2.75151500
C	2.86650200	7.07277800	0.30244100
H	3.31789000	7.23485800	1.29024000
H	3.62010100	7.32388700	-0.45092500
H	2.04318900	7.79149500	0.20648900
C	2.11670100	-2.97959500	-2.13133700
H	1.14943000	-3.42686800	-1.87931600
H	1.89542500	-2.00181400	-2.57312800
H	2.58870500	-3.60244700	-2.89829200
C	3.56697300	-0.75738700	2.26754500
H	3.98022400	0.22927300	2.01718000
H	2.51253600	-0.60656200	2.52217200
H	4.08852600	-1.09756500	3.16836300
C	6.19012100	-4.59498000	0.34115700
H	5.92853800	-5.59906500	-0.01179400
H	7.02796700	-4.24484100	-0.27750200
H	6.56025600	-4.68318600	1.36826000

Cartesian coordinates of **18**

Pt	-0.76815300	-0.94591600	-0.17729200
C	-2.77672000	-0.82472400	-0.09239800
C	-3.56894100	0.29814900	-0.29243500
C	-3.44270600	-2.04293300	0.16950000
C	-4.97494000	0.20858200	-0.21563000
H	-3.12232600	1.25959400	-0.52245000
C	-4.81710300	-2.16160400	0.25096200
C	-5.59925200	-1.01349300	0.05907800
H	-5.28102700	-3.12142300	0.45532300
H	-6.67786600	-1.09213500	0.12160100
C	-1.21027800	-2.82695900	0.17961900
N	-2.52255200	-3.11569700	0.31933800
N	-0.59615100	-4.02616400	0.38731700
O	-0.52800600	1.09591800	-0.47661700
O	1.34947200	-1.17069600	-0.34077700
C	0.56855300	1.77425800	-0.23520200
C	2.22210200	-0.22407500	-0.07928300
C	1.84621000	1.15843600	-0.05576700
H	2.66639400	1.85357300	0.08880500
C	0.84556500	-4.26960100	0.36512600
H	1.08825900	-4.99620300	-0.41559000
H	1.34365200	-3.32115700	0.15791600
H	1.17125500	-4.65424900	1.33579800

C	-1.58293000	-4.95533700	0.63404200
H	-1.38377000	-5.99821900	0.83197800
N	-2.77767900	-4.42348100	0.59919800
C	0.44284300	3.24654100	-0.08960700
C	-0.46673500	3.78093000	0.86293200
C	1.20567700	4.13044900	-0.89310500
C	-0.57252000	5.16500100	0.99897800
C	1.05882900	5.51088100	-0.72000300
C	0.18044000	6.05250500	0.22026400
H	-1.25863400	5.56504100	1.74377600
H	1.63681300	6.18195100	-1.35291100
C	3.65247700	-0.60186900	0.02150500
C	4.44767300	-0.17271000	1.11596500
C	4.24176900	-1.42245300	-0.97966100
C	5.79206100	-0.55342800	1.17855200
C	5.58794100	-1.77309300	-0.86967000
C	6.38799800	-1.34879500	0.19771700
H	6.38584200	-0.23188300	2.03260800
H	6.03174400	-2.38767000	-1.65139900
C	-1.29023200	2.89080000	1.76664800
H	-2.13837300	2.44292400	1.23948100
H	-0.69842100	2.05743100	2.16193000
H	-1.68210100	3.46369800	2.61342000
C	2.14421300	3.63195600	-1.97258200
H	3.12471100	3.33404700	-1.57618900
H	1.73365800	2.76346300	-2.49799900
H	2.32923900	4.41844600	-2.71170500
C	0.04706200	7.54625200	0.40204700
H	0.44677600	7.86873600	1.37278300
H	0.58866200	8.09393600	-0.37609200
H	-1.00253300	7.86308100	0.36785800
C	3.46634400	-1.88898700	-2.19266600
H	2.77714500	-2.70583100	-1.95369900
H	2.85289200	-1.08497100	-2.61355500
H	4.15156300	-2.24043800	-2.97110000
C	3.87855700	0.64551000	2.25680800
H	3.84020100	1.71955700	2.02919500
H	2.85884600	0.33638200	2.51032500
H	4.49896100	0.53573400	3.15248900
C	7.84986800	-1.72240200	0.27168200
H	8.02128200	-2.74854700	-0.07355800
H	8.46374100	-1.06465200	-0.35905500
H	8.23278800	-1.64135100	1.29461800
O	-5.64185200	1.38193700	-0.42626600
C	-7.05748100	1.37018200	-0.37805900
H	-7.37353400	2.39574600	-0.57885900
H	-7.48295300	0.70431500	-1.14116300

H -7.42726100 1.06485400 0.61038100

Cartesian coordinates of **19**

Pt -1.04350000 -0.79734000 -0.17415700
C -3.02272200 -0.43202800 -0.11883200
C -3.67441700 0.78265000 -0.32384000
C -3.83745900 -1.55699400 0.12362700
C -5.08011000 0.88271300 -0.27453000
H -3.08139500 1.66794600 -0.53774500
C -5.21922400 -1.50923900 0.18186500
C -5.83480300 -0.26681800 -0.01820700
H -5.80043200 -2.40614800 0.37136400
H -6.91901000 -0.19926300 0.02174000
C -1.71844500 -2.60973400 0.17167900
N -3.05897200 -2.73618100 0.28537500
N -1.25993100 -3.87391500 0.38983400
O -0.55546000 1.20225400 -0.46769100
O 1.03259900 -1.28067400 -0.30549600
C 0.62013900 1.74191300 -0.24804800
C 2.01797300 -0.44171800 -0.07876700
C 1.81630500 0.97501200 -0.08023200
H 2.71842600 1.56517700 0.04153600
C 0.14160900 -4.29078900 0.39853000
H 0.31163500 -5.04111100 -0.37891600
H 0.75498400 -3.40943900 0.20510900
H 0.39638600 -4.71237800 1.37502400
C -2.35810100 -4.67602000 0.61658200
H -2.29106700 -5.73510900 0.81742600
N -3.47752800 -4.00283600 0.55904200
C 0.67622600 3.21803400 -0.10371500
C -0.15366000 3.85953000 0.85514700
C 1.53221500 4.00435200 -0.91640700
C -0.09167300 5.24704200 0.98893500
C 1.55372900 5.39190800 -0.74481200
C 0.75642200 6.03666300 0.20351000
H -0.71909100 5.72760000 1.73781000
H 2.20031800 5.98800600 -1.38652000
C 3.39040600 -0.99517400 0.02781800
C 4.23433100 -0.65380500 1.11579200
C 3.86802200 -1.89975800 -0.95999400
C 5.51883900 -1.20383200 1.18623100
C 5.15767700 -2.41920100 -0.84315500
C 6.00602800 -2.08492400 0.21923900
H 6.15066000 -0.94789600 2.03516200
H 5.51836700 -3.09825300 -1.61429800
C -1.06891400 3.07492100 1.76831900
H -1.96092100 2.71471600 1.24630600

H	-0.57044600	2.18599100	2.17143200
H	-1.39424300	3.69514100	2.60999500
C	2.39136900	3.39829700	-2.00672000
H	3.33072100	2.97891900	-1.62091300
H	1.87157700	2.59029500	-2.53230300
H	2.66597000	4.15982400	-2.74399200
C	0.81885300	7.53423300	0.39091500
H	1.46438600	7.80476000	1.23793900
H	1.22184500	8.03261600	-0.49718800
H	-0.17202100	7.95565400	0.59533600
C	3.03682200	-2.28089600	-2.16597900
H	2.24739200	-2.99725200	-1.91483500
H	2.53297800	-1.41054200	-2.60032200
H	3.66935500	-2.73117600	-2.93806800
C	3.77695200	0.25141200	2.24097800
H	3.88235100	1.31695800	1.99534500
H	2.72480100	0.08509900	2.49539200
H	4.37558400	0.07526900	3.14088400
C	7.40608100	-2.64649800	0.30217700
H	7.42944100	-3.71106300	0.04101700
H	8.08588600	-2.13174500	-0.39055600
H	7.82221300	-2.53690700	1.30918000
C	-5.75114400	2.21988300	-0.49323100
H	-5.48911900	2.93279500	0.29914300
H	-5.44085700	2.67086500	-1.44372400
H	-6.84173400	2.12425800	-0.50700600

Cartesian coordinates of **20**

Pt	0.22912500	-1.20423400	-0.27296300
C	0.05104500	-3.19787500	-0.46531300
C	-1.11395500	-3.96576200	-0.39641300
C	1.25249700	-3.88938400	-0.72235800
H	-2.06319200	-3.47508600	-0.20424400
C	1.34052700	-5.26085500	-0.90141700
C	0.15348700	-6.00018900	-0.82290000
H	2.29744000	-5.73530300	-1.09421200
H	0.18365300	-7.07770400	-0.95759000
C	2.10719500	-1.68486400	-0.58897000
N	2.36088400	-2.99950500	-0.77330100
N	3.34063300	-1.11114900	-0.64867300
O	-1.78478000	-0.94694200	0.15616900
O	0.49393400	0.90815400	-0.17273400
C	-2.47033100	0.17134300	0.10708000
C	-0.47053200	1.80172500	-0.18357800
C	-1.84629100	1.45279800	-0.03978100
H	-2.52724500	2.29690800	-0.01863200
C	3.64924500	0.31993300	-0.45478500

H	4.18847200	0.66813500	-1.34159800
H	2.68359800	0.82907100	-0.41183600
C	4.25492600	-2.12234100	-0.85972800
H	5.31855500	-1.95522700	-0.93747700
N	3.68064300	-3.29326400	-0.94379700
C	-3.92564800	0.09077500	0.37176700
C	-4.40145100	-0.65350300	1.48761100
C	-4.86388700	0.72611600	-0.48396500
C	-5.77403700	-0.71707200	1.72809600
C	-6.22906900	0.62806400	-0.19792200
C	-6.71037800	-0.08082800	0.90455300
H	-6.12526500	-1.27588600	2.59399700
H	-6.93892200	1.10354500	-0.87274900
C	-0.09842100	3.21881300	-0.43711800
C	-0.42394300	4.23832600	0.49250500
C	0.60571900	3.56109400	-1.62124800
C	-0.05366700	5.55895300	0.21855000
C	0.95225400	4.89382500	-1.84944800
C	0.63109700	5.91336400	-0.94616000
H	-0.29398700	6.33106600	0.94751200
H	1.47840600	5.14719300	-2.76845400
C	-3.46340900	-1.34657100	2.45124000
H	-3.02959100	-2.25374600	2.01888100
H	-2.61908600	-0.70442500	2.72632600
H	-3.99558400	-1.62302100	3.36744100
C	-4.44842100	1.46260100	-1.74115300
H	-4.15451700	2.50325900	-1.54630900
H	-3.60132500	0.97679500	-2.23661400
H	-5.28018800	1.49943200	-2.45244600
C	-8.18803600	-0.14823700	1.20991700
H	-8.47233800	0.58536300	1.97706900
H	-8.79114300	0.06183800	0.32010700
H	-8.47586400	-1.13574400	1.58848300
C	0.94756700	2.52586100	-2.67004400
H	1.78694600	1.89113800	-2.36623300
H	0.10452800	1.85232300	-2.86087300
H	1.21760400	3.01008400	-3.61411800
C	-1.12507200	3.93717200	1.80059900
H	-2.21304200	3.84128100	1.68243800
H	-0.76937100	3.00214500	2.24590600
H	-0.95547600	4.74362400	2.52163700
C	0.99240600	7.35150100	-1.23512300
H	1.94792600	7.42717100	-1.76630500
H	0.23387800	7.83551500	-1.86577800
H	1.07007900	7.93838300	-0.31356200
C	-1.05990900	-5.35627500	-0.57432800
H	-1.97552600	-5.93963800	-0.51721000

C	4.46192900	0.56912300	0.79878100
C	3.85995300	0.45527300	2.05997000
C	5.81458200	0.91696000	0.71646200
C	4.60485100	0.67774000	3.21711500
H	2.80571900	0.19784000	2.12899200
C	6.56089500	1.14360800	1.87554500
H	6.28588000	1.02185600	-0.25880900
C	5.95711700	1.02142100	3.12719700
H	4.12904600	0.58938700	4.18988600
H	7.60973700	1.41691900	1.79874200
H	6.53511300	1.19773500	4.03023700

Cartesian coordinates of **21**

Pt	-0.11204500	-0.96269800	-0.22345600
C	-1.13841300	-2.68390200	-0.39466100
C	-2.51324600	-2.86127300	-0.30961300
C	-0.35373500	-3.82934900	-0.65755500
H	-3.17067200	-2.02107300	-0.11242000
C	-0.88297800	-5.09397600	-0.82862600
C	-2.27369300	-5.25382600	-0.73740400
H	-0.23820800	-5.94424700	-1.02730700
H	-2.70134600	-6.24049100	-0.86870100
C	1.37058300	-2.21330800	-0.53826100
N	1.02894500	-3.50787800	-0.71885800
N	2.73187100	-2.23118800	-0.60003500
O	-1.81572300	0.14486300	0.20108600
O	1.04283200	0.83425000	-0.16339500
C	-1.94907000	1.44898100	0.14333900
C	0.55654200	2.05429200	-0.18888000
C	-0.83500400	2.33313600	-0.02905100
H	-1.08631500	3.38812800	-0.01801800
C	3.62808400	-1.07401400	-0.40894800
H	4.22894400	-0.95985000	-1.31701200
H	2.97292600	-0.20429800	-0.31623700
C	3.11674500	-3.53775200	-0.81060900
H	4.14735000	-3.84901900	-0.88872400
N	2.09040300	-4.34446400	-0.89032200
C	-3.29094700	2.01178200	0.42197900
C	-4.02855100	1.55572800	1.55150500
C	-3.86828400	2.99029800	-0.42872600
C	-5.28481100	2.10249500	1.80961000
C	-5.13362300	3.50350700	-0.12424900
C	-5.85995200	3.08211900	0.99027500
H	-5.83184200	1.75785800	2.68569600
H	-5.57208600	4.24127100	-0.79411800
C	1.49709400	3.16643900	-0.48245100
C	1.64544200	4.25709000	0.41090600

C	2.27619500	3.13266500	-1.66955900
C	2.54831400	5.27918600	0.09968800
C	3.16168900	4.17769000	-1.93561400
C	3.31494300	5.26525200	-1.06745600
H	2.66748400	6.10298500	0.80147300
H	3.74197100	4.14959400	-2.85663900
C	-3.47603500	0.52388000	2.50996500
H	-3.48277200	-0.48088700	2.07616100
H	-2.43452200	0.73607700	2.77704100
H	-4.06839100	0.50509000	3.43074000
C	-3.19226900	3.46673400	-1.69844000
H	-2.48484400	4.28864000	-1.52075800
H	-2.63512300	2.66263800	-2.19010900
H	-3.93768700	3.84282600	-2.40712200
C	-7.21766200	3.66099900	1.31103900
H	-7.18056600	4.29879500	2.20457800
H	-7.59708500	4.27255300	0.48584300
H	-7.95355800	2.87293000	1.51224700
C	2.13371200	2.01672000	-2.68117800
H	2.60878300	1.08969600	-2.34320700
H	1.08130700	1.77281200	-2.86568600
H	2.59036800	2.30181800	-3.63455100
C	0.88883800	4.33152900	1.72063600
H	-0.13544500	4.70826100	1.59442700
H	0.81050000	3.35019800	2.20039000
H	1.39199700	5.01118200	2.41628000
C	4.26266400	6.39483700	-1.39635500
H	5.18858000	6.02418300	-1.85106800
H	3.81371400	7.09914500	-2.11024700
H	4.53091600	6.96572900	-0.50108800
C	-3.08225800	-4.14083900	-0.47970100
C	4.52003200	-1.23329300	0.80475200
C	3.97395900	-1.15755900	2.09405700
C	5.89362700	-1.45447300	0.65771500
C	4.78998200	-1.30952400	3.21387800
H	2.90876700	-0.97555300	2.21540600
C	6.71310200	-1.60303700	1.77960800
H	6.32808700	-1.50165300	-0.33884600
C	6.16143300	-1.53341300	3.05895600
H	4.35735200	-1.24740700	4.20860400
H	7.77902000	-1.77112200	1.65207500
H	6.79639100	-1.64866900	3.93312900
O	-4.44331900	-4.18847000	-0.37201800
C	-5.08826200	-5.43891300	-0.53436400
H	-4.76234900	-6.16469600	0.22328200
H	-6.15554100	-5.24499700	-0.41065100
H	-4.91056700	-5.85991200	-1.53341800

Cartesian coordinates of **22**

Pt	0.05940100	-1.10509300	0.02655300
C	0.74852500	-2.99592000	-0.08479200
C	2.02394300	-3.46291300	0.22694900
C	-0.19431400	-3.95698600	-0.50344400
H	2.77165000	-2.75746400	0.57977500
C	0.08681300	-5.30569500	-0.63560700
C	1.38476700	-5.73189400	-0.32621300
H	-0.67671800	-6.00410300	-0.96329400
H	1.63452600	-6.78556700	-0.42147900
C	-1.57530500	-2.03542900	-0.54632600
N	-1.46259400	-3.36565100	-0.75383500
N	-2.87355200	-1.77226600	-0.86352800
O	1.90870600	-0.31678600	0.55539400
O	-0.75876600	0.86569800	0.17879800
C	2.28011300	0.92351600	0.34315700
C	-0.06694300	1.95458000	-0.07638700
C	1.35986000	1.97647600	0.04666500
H	1.81502000	2.95526900	-0.06603500
C	-3.53430300	-0.45526100	-0.80952600
H	-2.75593900	0.25530100	-0.51666600
H	-3.86410600	-0.20040200	-1.82195500
C	-3.45707000	-2.96587500	-1.23329300
H	-4.49322400	-3.05631300	-1.52226800
N	-2.61204400	-3.96187600	-1.17827200
C	3.73685400	1.21670800	0.37859300
C	4.61405900	0.52200300	-0.49486500
C	4.26722400	2.16898600	1.28373600
C	5.98014000	0.80372400	-0.45218300
C	5.64444700	2.41371500	1.28921300
C	6.52040300	1.74724100	0.42966200
H	6.64362800	0.27703900	-1.13619600
H	6.04529400	3.13451200	1.99967700
C	-0.80442900	3.21577600	-0.33256300
C	-0.49461400	4.02146900	-1.45883500
C	-1.84544400	3.62457300	0.54468800
C	-1.20979200	5.20416700	-1.67344800
C	-2.52692000	4.81493400	0.28610800
C	-2.22669500	5.62581400	-0.81434800
H	-0.97487600	5.80468500	-2.55075800
H	-3.31112400	5.12618600	0.97447600
C	4.09945000	-0.48014600	-1.50365400
H	3.79238100	-1.41908700	-1.03263700
H	3.21814600	-0.09928700	-2.03297300
H	4.87052000	-0.70805500	-2.24674700
C	3.39418900	2.89829900	2.28380600

H	2.83932300	3.73156100	1.83160100
H	2.65368100	2.23063900	2.73720800
H	4.00462000	3.32296800	3.08745200
C	8.00148100	2.04516000	0.43479400
H	8.28141300	2.69659000	-0.40443300
H	8.30477300	2.55224700	1.35679600
H	8.59612600	1.12902100	0.34137700
C	-2.21070200	2.83203200	1.78072300
H	-2.82945800	1.95976200	1.54366400
H	-1.32182900	2.45159700	2.29507300
H	-2.77179900	3.45843400	2.48214400
C	0.55469300	3.62011100	-2.47536400
H	1.57330500	3.88135500	-2.15804300
H	0.54657300	2.54131700	-2.66469600
H	0.38023700	4.13281000	-3.42720700
C	-2.96495500	6.92275800	-1.04962300
H	-4.03136400	6.82770900	-0.81456500
H	-2.56779900	7.72975500	-0.41856100
H	-2.87622700	7.25077900	-2.09079800
C	2.35886900	-4.82779000	0.10972800
C	-4.70525100	-0.43864300	0.15163700
C	-6.00112400	-0.18678600	-0.31097700
C	-4.50085600	-0.66482900	1.52095800
C	-7.07969400	-0.15900500	0.57693200
H	-6.16830900	-0.00413100	-1.37037400
C	-5.57712100	-0.64228900	2.40670600
H	-3.49638100	-0.85886200	1.88964500
C	-6.86935100	-0.38920700	1.93649800
H	-8.08081300	0.04021300	0.20448400
H	-5.40734200	-0.81818800	3.46533500
H	-7.70665100	-0.37024800	2.62868700
C	3.75441300	-5.29625900	0.45493600
H	4.50853900	-4.80277100	-0.17101000
H	4.00590000	-5.06642200	1.49798800
H	3.86063600	-6.37704400	0.31584800

Geometries of DFT-optimized triplet states T_1 (BP86/6-31G(d))

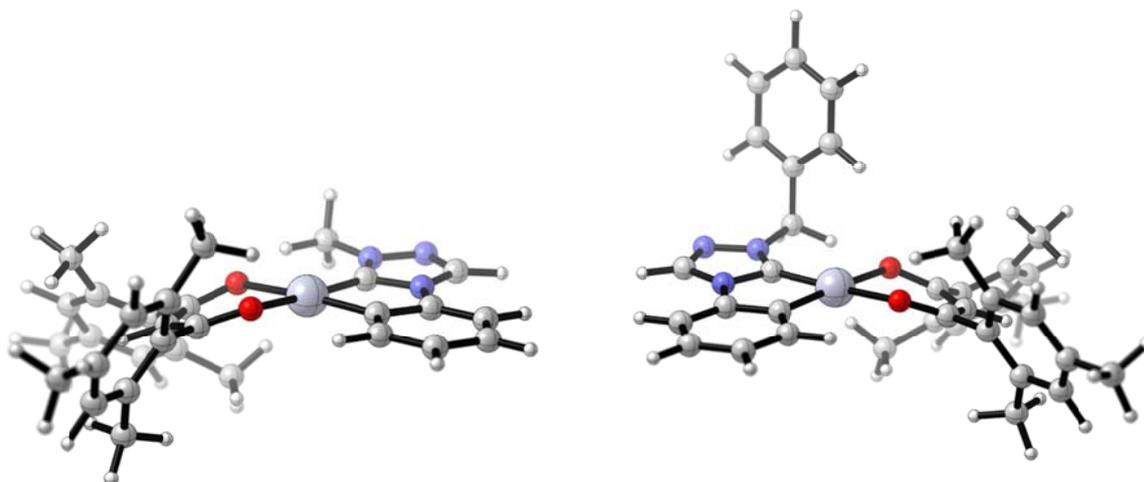


Figure S1. Optimized triplet geometries of **5** (left) and **6** (right), BP86/6-31G(d).

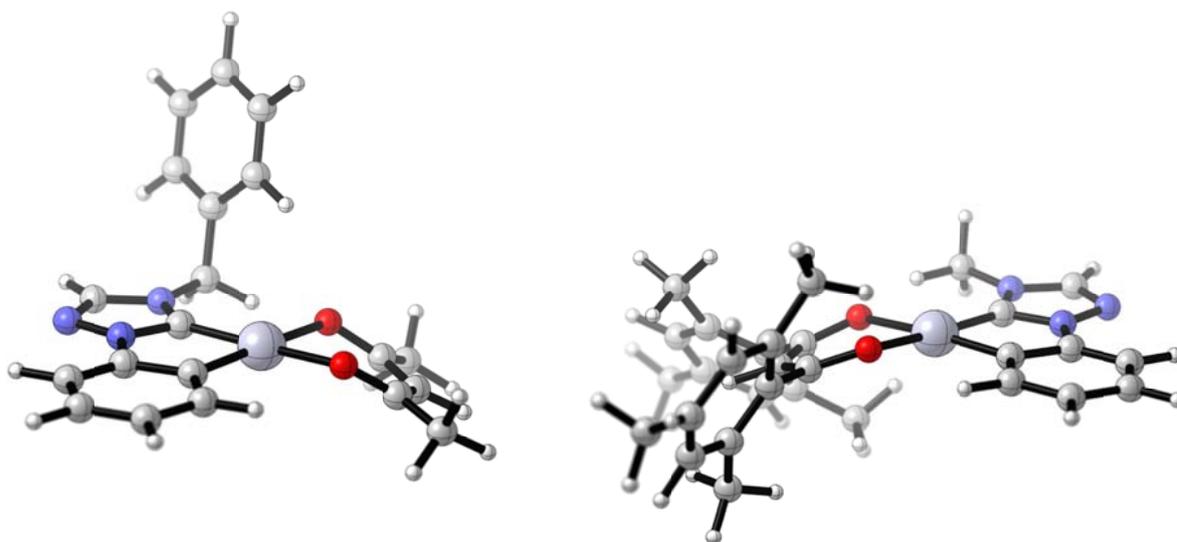


Figure S2. Optimized triplet geometries of **16** (left) and **17** (right), BP86/6-31G(d).

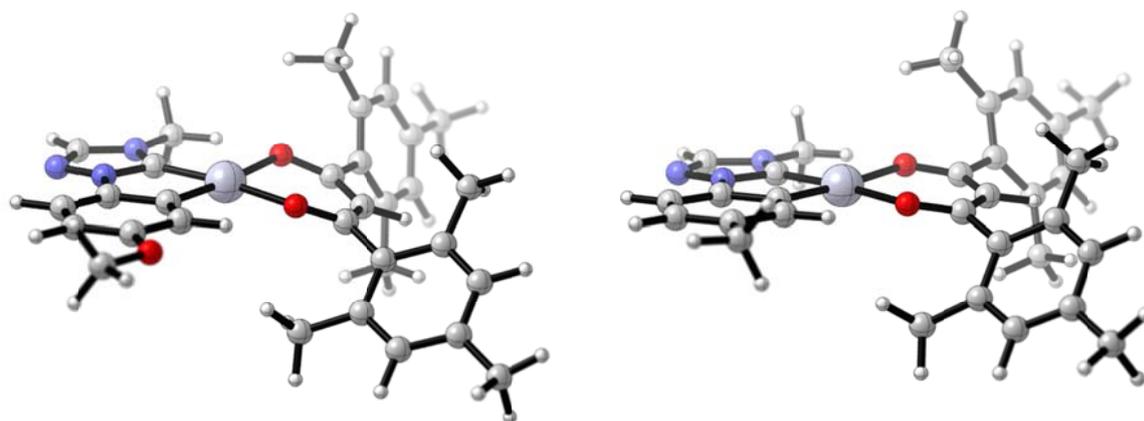


Figure S3. Optimized triplet geometries of **18** (left) and **19** (right), BP86/6-31G(d).

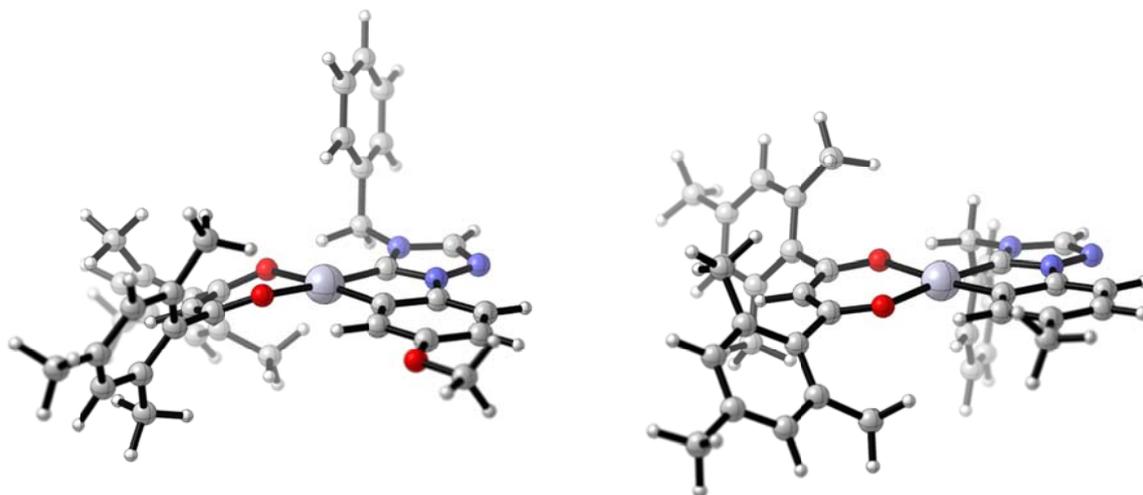


Figure S4. Optimized triplet geometries of **21** (left) and **22** (right), BP86/6-31G(d).