

**SUPPLEMENTARY MATERIAL**

**Functionalization of Imidazolin-2-imine to corresponding  
Phosphinamine, Chalcogenide (O, S, Se, Te) and Borane  
Compounds**

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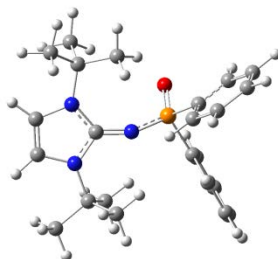
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## Optimized structures of ligand 3, 4 and 5

### Ligand 3

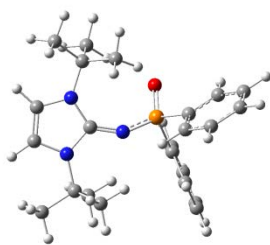
HF/3-21G(d)



C	1.77603900	0.41826900	0.24587500
C	4.03006600	0.30238800	0.12270200
C	3.72593200	1.56290300	0.38270600
H	4.98120900	-0.13751000	-0.02462500
H	4.36879400	2.39495400	0.50485600
N	2.33617000	1.65788200	0.47562400
N	2.83931000	-0.43885500	0.06103400
N	0.50635700	0.19189200	0.26448000
P	-0.82909200	-0.35836800	-0.40196600
C	-1.56271000	-1.47937600	0.82489900
C	-2.52843700	-2.39809600	0.43226100
C	-1.19830300	-1.41033300	2.16503100
C	-3.13421100	-3.21785900	1.36718200
H	-2.78010800	-2.47856200	-0.60572600
C	-1.80432000	-2.23199500	3.09917700
H	-0.43444600	-0.72335800	2.46745500
C	-2.77595400	-3.13372500	2.70152200
H	-3.87737100	-3.92367900	1.05346400
H	-1.51574300	-2.17205800	4.13015700
H	-3.24473900	-3.77154600	3.42472100
C	-2.04363400	1.00695300	-0.42945700
C	-2.45161900	1.56731900	-1.63294500
C	-2.56328900	1.51984600	0.75728500
C	-3.33714600	2.63203800	-1.65080600
H	-2.08150800	1.15398400	-2.54807900
C	-3.44942900	2.57978800	0.73936400
H	-2.29201200	1.08155400	1.69568600
C	-3.83470400	3.14189500	-0.46670900
H	-3.64079100	3.05313700	-2.58866300
H	-3.84460500	2.95963800	1.66081000
H	-4.52464600	3.96256200	-0.48076300
C	2.89192400	-1.91794900	-0.21457800
C	1.65924600	-2.66063300	0.32233700
C	3.02422600	-2.12383500	-1.73157000

C	4.12925900	-2.49560200	0.51034500
H	1.44331100	-2.37957800	1.34289400
H	0.79705300	-2.49849700	-0.29700500
H	1.87642600	-3.72176200	0.29684200
H	3.90001400	-1.60915300	-2.11092400
H	3.12349600	-3.18173600	-1.94798900
H	2.14157800	-1.74903300	-2.22890100
H	4.10537700	-3.57342600	0.41534700
H	5.06139400	-2.15770500	0.07833400
H	4.10890500	-2.23964700	1.56281000
C	1.59471400	2.92182400	0.76808100
C	2.60503500	4.05775800	1.01770600
C	0.72868600	3.30368200	-0.44207300
C	0.75560300	2.73867600	2.04348600
H	3.25159300	3.84042800	1.85951400
H	3.20657500	4.25916700	0.13957100
H	2.04474400	4.95491500	1.24886300
H	-0.01470200	2.55410900	-0.63935500
H	0.22354300	4.24189200	-0.24340700
H	1.35513400	3.42327500	-1.31852900
H	0.21769300	3.65513800	2.25560700
H	0.04903900	1.93821900	1.91635700
H	1.40545200	2.51259100	2.88160300
O	-0.74519335	-0.98630120	-1.76691433

B3LYP/6-311+G(2d,p)

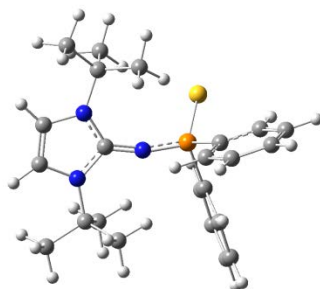


C	1.70113800	0.16380500	0.12570100
C	3.93606300	-0.07361000	-0.11925900
C	3.72825600	1.12295800	0.44948100
H	4.86639700	-0.52655800	-0.39562300
H	4.44850300	1.85986700	0.74455500
N	2.36333800	1.28473300	0.61964900
N	2.70794700	-0.69837700	-0.30619400
N	0.41050100	0.02650000	0.17968400
P	-0.87858600	-0.44805500	-0.67476500
C	-1.80763500	-1.54857900	0.45705900
C	-2.80764700	-2.35354900	-0.09593900

C	-1.56444100	-1.61837600	1.82936400
C	-3.55517700	-3.20438200	0.70998400
H	-2.98315800	-2.32012600	-1.16454800
C	-2.31301200	-2.46937600	2.63735600
H	-0.77590500	-1.01450600	2.26118700
C	-3.31135600	-3.26136300	2.07945600
H	-4.32467700	-3.82735700	0.26897300
H	-2.11363900	-2.51712700	3.70184600
H	-3.89327200	-3.92537300	2.70817400
C	-1.96442400	1.02322800	-0.84997600
C	-2.16851800	1.54083300	-2.13016600
C	-2.59623800	1.63376200	0.23586800
C	-2.97154800	2.66209300	-2.31871100
H	-1.69915700	1.04676900	-2.97200400
C	-3.40436700	2.74911300	0.04818300
H	-2.46757400	1.23313200	1.23460000
C	-3.58969500	3.26886900	-1.23041800
H	-3.12105600	3.05628700	-3.31738000
H	-3.89461600	3.21015500	0.89802100
H	-4.22066300	4.13790500	-1.37714900
C	2.60639900	-2.07975000	-0.90715100
C	1.54000200	-2.91490100	-0.18497200
C	2.31178100	-1.95740300	-2.40848200
C	3.95538200	-2.79790700	-0.71444800
H	1.66314400	-2.86025200	0.89831800
H	0.53197400	-2.61823500	-0.44712600
H	1.65646100	-3.95746300	-0.48671100
H	3.09351700	-1.37399700	-2.90210100
H	2.29826400	-2.95311000	-2.85935400
H	1.34068300	-1.49578900	-2.58156800
H	3.84218100	-3.82392600	-1.06450600
H	4.75971900	-2.35046800	-1.29993600
H	4.25452900	-2.83077900	0.33542700
C	1.71888700	2.51347100	1.18665300
C	2.81020000	3.47928700	1.67144300
C	0.90271500	3.21031500	0.08880500
C	0.84697800	2.13330500	2.39305000
H	3.43874300	3.03436400	2.44548100
H	3.44382300	3.83034100	0.85501000
H	2.32134600	4.35269600	2.10437600
H	0.10307100	2.57534800	-0.28028000
H	0.45604800	4.12427000	0.48621100
H	1.54885800	3.48296100	-0.74881700
H	0.39890000	3.03517900	2.81500400
H	0.05399000	1.45039100	2.10366000
H	1.45443600	1.65921100	3.16775400
O	-0.71213000	-1.07425500	-2.02241000

# Ligand 4

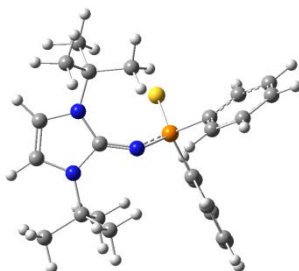
HF/3-21G(d)



C	-1.66452000	0.51083700	-0.09348400
C	-3.90548300	0.68939700	-0.36466400
C	-3.37683100	1.82743600	-0.78268400
H	-4.92230900	0.39886000	-0.33823800
H	-3.85928700	2.68310900	-1.17713600
N	-1.99028100	1.74329100	-0.62608100
N	-2.86685700	-0.15140900	0.06311100
N	-0.47017000	0.11536800	0.14556600
P	0.81985800	-0.58734100	0.73583000
C	1.35682000	-1.77543700	-0.53310900
C	2.31131000	-2.73611400	-0.21330500
C	0.85452600	-1.73029300	-1.82786400
C	2.76099200	-3.62330800	-1.17314900
H	2.68375700	-2.79325800	0.78933900
C	1.30452500	-2.62024900	-2.78877500
H	0.10819000	-1.00587400	-2.07972100
C	2.25963200	-3.56569600	-2.46288100
H	3.49508600	-4.36016800	-0.91432700
H	0.90754200	-2.57689100	-3.78385500
H	2.60742600	-4.25640400	-3.20553500
C	2.18011700	0.63107400	0.73272000
C	2.48629000	1.33141100	1.89568100
C	2.91310500	0.89962500	-0.41941600
C	3.47834500	2.29510900	1.89821400
H	1.95888800	1.10182200	2.79890500
C	3.90970900	1.85983700	-0.41500800
H	2.71929600	0.35038400	-1.31779700
C	4.19037100	2.56337700	0.74232300
H	3.70148700	2.82518600	2.80287700
H	4.46923400	2.04942800	-1.30973900
H	4.96473100	3.30501200	0.74678100
C	-3.12317100	-1.48667500	0.69990600
C	-2.18164800	-2.55858300	0.12819500
C	-2.97426700	-1.34679400	2.22274200
C	-4.56781300	-1.92346900	0.37866600

H	-2.23364700	-2.56592000	-0.95379700
H	-1.16539600	-2.40990200	0.43650100
H	-2.49582000	-3.52709700	0.49790300
H	-3.66352000	-0.59529800	2.59166300
H	-3.20377500	-2.29359000	2.69849700
H	-1.96529300	-1.07488600	2.48925200
H	-4.70712800	-2.92095200	0.77482500
H	-5.30236000	-1.28252000	0.84945000
H	-4.74236300	-1.95456200	-0.69043100
C	-1.03426100	2.83735800	-0.96993300
C	-1.81752700	4.04366300	-1.52168500
C	-0.28867200	3.28614500	0.29681100
C	-0.06891400	2.35118000	-2.06263400
H	-2.35632900	3.79181700	-2.42731900
H	-2.50725300	4.44150300	-0.78717500
H	-1.10346900	4.82078500	-1.76341500
H	0.29080900	2.48191700	0.71143900
H	0.38294100	4.10052400	0.05113900
H	-1.00063800	3.63200900	1.03749400
H	0.61271200	3.15131500	-2.32588800
H	0.50465300	1.51131100	-1.71469400
H	-0.62807800	2.06296300	-2.94589100
S	0.71421200	-1.42439100	2.50895400

B3LYP/6-311+G(2d,p)



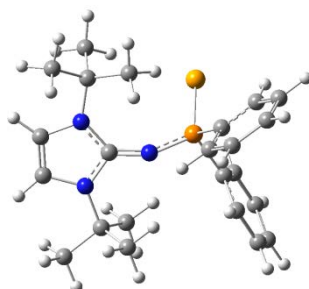
C	1.71446000	0.20596600	0.19925200
C	3.91438600	-0.05592900	-0.23499400
C	3.73018100	1.23036600	0.09571300
H	4.81796700	-0.55054100	-0.53377700
H	4.44981300	2.02348700	0.13577200
N	2.38905900	1.40813700	0.38547300
N	2.69699600	-0.71569400	-0.14236400
N	0.42960200	0.04376700	0.39356800
P	-0.82433800	-0.30210100	-0.58505000
C	-1.79812200	-1.57768200	0.31909900
C	-2.74259100	-2.33913400	-0.37057400
C	-1.64405600	-1.76754300	1.69352000
C	-3.52343900	-3.27076900	0.30451400
H	-2.84962400	-2.20882300	-1.44065000
C	-2.42588300	-2.69952300	2.36880700

H	-0.89860600	-1.19288600	2.22930800
C	-3.36860700	-3.45196000	1.67559100
H	-4.25011400	-3.86020000	-0.24244700
H	-2.29527600	-2.84099800	3.43562800
H	-3.97614500	-4.18012800	2.20033100
C	-1.99407500	1.13122800	-0.50883400
C	-2.41654200	1.76768600	-1.67473900
C	-2.48123500	1.58224500	0.72193500
C	-3.29834800	2.84356500	-1.61299700
H	-2.04831500	1.40932200	-2.62816000
C	-3.36266500	2.65424700	0.78435300
H	-2.18011100	1.09212100	1.63956900
C	-3.77252700	3.29013400	-0.38508600
H	-3.61710900	3.32910200	-2.52817200
H	-3.73524500	2.99018100	1.74528500
H	-4.46247300	4.12467900	-0.33705500
C	2.68074000	-2.21992600	-0.29536700
C	1.36122900	-2.85379300	0.13835500
C	2.95873700	-2.55325800	-1.76820900
C	3.78934100	-2.79201600	0.61199200
H	1.07912800	-2.56143300	1.14792100
H	0.55244100	-2.61902400	-0.54600500
H	1.49723100	-3.93722100	0.12525500
H	3.92201100	-2.15727800	-2.09766700
H	2.98032300	-3.63741000	-1.89899700
H	2.17315500	-2.14126600	-2.40176600
H	3.76333200	-3.88105500	0.55506000
H	4.79011200	-2.47580200	0.31819600
H	3.62814600	-2.50133000	1.65211300
C	1.79210000	2.71990200	0.80876800
C	2.92124200	3.72718900	1.07554600
C	0.91064900	3.26557700	-0.32130400
C	1.00857200	2.53154900	2.11639100
H	3.61287200	3.37714500	1.84450300
H	3.48403700	3.97103400	0.17268400
H	2.46749400	4.65156700	1.43423300
H	0.07781500	2.60491600	-0.53739300
H	0.50535700	4.23832400	-0.03460500
H	1.49759200	3.39398000	-1.23325400
H	0.57422700	3.48703500	2.41701400
H	0.21061000	1.80517700	1.99870900
H	1.67555900	2.19412600	2.91354500
S	-0.46325000	-0.79859300	-2.47728600



## Ligand 5

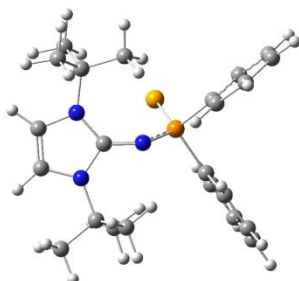
HF/3-21G(d)



C	1.77599100	0.41860600	0.24560700
C	3.72563900	1.56357300	0.38318400
C	4.03009300	0.30313400	0.12324200
H	4.36832100	2.39572200	0.50562700
H	4.98138000	-0.13656500	-0.02371100
N	2.33583300	1.65831300	0.47559500
N	2.83949500	-0.43833500	0.06105700
N	0.50635800	0.19206800	0.26379600
P	-0.82914300	-0.35874600	-0.40208300
C	-1.56225700	-1.47928300	0.82551200
C	-2.52800800	-2.39826400	0.43357600
C	-1.19742400	-1.40963300	2.16550400
C	-3.13339300	-3.21770800	1.36903700
H	-2.78002600	-2.47920000	-0.60429100
C	-1.80305900	-2.23095600	3.10018300
H	-0.43357700	-0.72241800	2.46739500
C	-2.77470800	-3.13297900	2.70321300
H	-3.87658100	-3.92373300	1.05584800
H	-1.51417300	-2.17054800	4.13104900
H	-3.24319200	-3.77054100	3.42683600
C	-2.04382200	1.00645200	-0.42995700
C	-2.56380000	1.51932500	0.75664000
C	-2.45139300	1.56687600	-1.63356500
C	-3.44986400	2.57934200	0.73847800
H	-2.29291000	1.08093100	1.69511000
C	-3.33683400	2.63164700	-1.65166300
H	-2.08107300	1.15349100	-2.54859400
C	-3.83471800	3.14150600	-0.46769100
H	-3.84531100	2.95916900	1.65982000
H	-3.64020200	3.05278000	-2.58959900
H	-4.52459200	3.96222800	-0.48194900
C	2.89228300	-1.91730700	-0.21517700
C	1.66017900	-2.66039200	0.32258800
C	3.02352000	-2.12270000	-1.73231900
C	4.13036500	-2.49495600	0.50853300

H	1.44491600	-2.37938500	1.34331000
H	0.79748500	-2.49847700	-0.29611000
H	1.87757800	-3.72147000	0.29691100
H	3.89878100	-1.60745200	-2.11212800
H	3.12317900	-3.18049200	-1.94911100
H	2.14033900	-1.74822200	-2.22891900
H	4.10636200	-3.57277500	0.41357800
H	5.06204700	-2.15711300	0.07548800
H	4.11112800	-2.23898400	1.56101700
C	1.59407900	2.92208300	0.76803700
C	0.72810700	3.30385100	-0.44217700
C	0.75481000	2.73860400	2.04330200
C	2.60416000	4.05817300	1.01789900
H	1.35460700	3.42361400	-1.31857100
H	-0.01513700	2.55416600	-0.63957500
H	0.22279600	4.24196800	-0.24350100
H	1.40458400	2.51262400	2.88150900
H	0.21661600	3.65490200	2.25540800
H	0.04849000	1.93795700	1.91599900
H	2.04367800	4.95524300	1.24892700
H	3.25055900	3.84095700	1.85986100
H	3.20586700	4.25965800	0.13989300
Se	-0.71136100	-1.24456300	-2.32533300

B3LYP/6-311+G(2d,p)

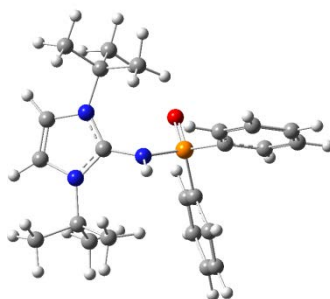


C	1.76230700	0.25304700	0.36311900
C	3.95373400	-0.06724200	-0.07006500
C	3.78626200	1.24328100	0.15949900
H	4.84968200	-0.59497100	-0.33360900
H	4.51413700	2.02934400	0.13214000
N	2.44999700	1.45843600	0.44487300
N	2.72990900	-0.70235700	0.08034200
N	0.47846400	0.11126200	0.59086400
P	-0.80161400	-0.22877600	-0.35382500
C	-1.77870500	-1.48008200	0.58296900
C	-2.74446400	-2.24158400	-0.07588500
C	-1.60726600	-1.64189300	1.95909900
C	-3.52815900	-3.14699600	0.63089400
H	-2.86569000	-2.13375200	-1.14707900
C	-2.39195900	-2.54776600	2.66571200

H	-0.84713900	-1.06569400	2.47211000
C	-3.35534000	-3.30141400	2.00299000
H	-4.27108100	-3.73718800	0.10715700
H	-2.24737200	-2.66763800	3.73336900
H	-3.96484500	-4.00959100	2.55220400
C	-1.96267200	1.21422900	-0.27191700
C	-2.43216200	1.83019300	-1.43064900
C	-2.39802500	1.68889300	0.96967400
C	-3.30953600	2.90856900	-1.35184400
H	-2.10401100	1.45564200	-2.39277300
C	-3.27379800	2.76432200	1.04884300
H	-2.06161600	1.21452700	1.88318000
C	-3.73161800	3.37898200	-0.11400200
H	-3.66532700	3.37739000	-2.26203000
H	-3.60484100	3.11881400	2.01825000
H	-4.41775200	4.21579800	-0.05285600
C	2.69898800	-2.21349200	0.04014900
C	1.35129800	-2.80088000	0.44765800
C	3.03817100	-2.65773700	-1.39031000
C	3.75576300	-2.72572700	1.03935800
H	1.03161800	-2.45223100	1.42693200
H	0.57811100	-2.58608700	-0.28416300
H	1.46730800	-3.88570200	0.49513600
H	4.02260600	-2.30573000	-1.70592900
H	3.04240800	-3.74862300	-1.43995100
H	2.28918300	-2.28044300	-2.08709400
H	3.73352500	-3.81648900	1.04934900
H	4.77025200	-2.42218700	0.78083800
H	3.53798700	-2.37113900	2.04897700
C	1.87454000	2.80784800	0.77110600
C	3.01937200	3.81896400	0.93982800
C	0.98251400	3.27327400	-0.38607100
C	1.11105500	2.73149600	2.10110100
H	3.71857000	3.52219500	1.72402300
H	3.57015400	3.98316400	0.01198100
H	2.58162400	4.77432600	1.23101800
H	0.13373200	2.61425200	-0.53272400
H	0.60047900	4.27443100	-0.17539400
H	1.55407800	3.31185400	-1.31563000
H	0.68816100	3.71128100	2.33115700
H	0.30668000	2.00450800	2.05319700
H	1.78839200	2.45216200	2.91186200
Se	-0.44809300	-0.79857900	-2.39783400

Ligand 3 protonated at N

HF/3-21G(d)

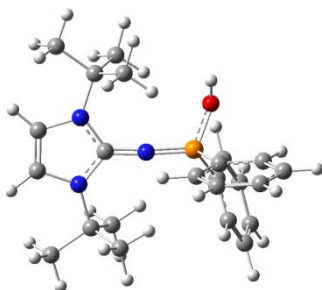


C	1.64756900	-0.21583500	0.32928100
C	3.69098500	-0.51775600	-0.45966000
C	3.65309600	0.69814400	0.08122000
H	4.48752800	-1.00892400	-0.95399600
H	4.41457900	1.43036100	0.14134900
N	2.37563700	0.89141700	0.59494100
N	2.44787000	-1.11248400	-0.26943500
N	0.30057300	-0.36165200	0.62512000
P	-0.94128700	-0.35270200	-0.55196700
C	-2.26258000	-1.22499100	0.27649400
C	-3.54843500	-1.08680300	-0.24969800
C	-2.06975300	-2.07851800	1.35912100
C	-4.60906600	-1.78083300	0.29689700
H	-3.71966300	-0.43746200	-1.08516700
C	-3.13503600	-2.76427000	1.91220200
H	-1.09271600	-2.22575300	1.76844700
C	-4.40381400	-2.61687800	1.38140900
H	-5.58935800	-1.66954900	-0.11958800
H	-2.97401700	-3.41482500	2.74784400
H	-5.22791800	-3.15236600	1.80781700
C	-1.51545700	1.32629800	-0.76980700
C	-1.21798800	1.94983200	-1.97800500
C	-2.24118700	2.01855200	0.19787900
C	-1.62186100	3.25393900	-2.20586000
H	-0.69024300	1.40092500	-2.73111200
C	-2.63668200	3.32203600	-0.02986200
H	-2.52120300	1.53636800	1.11473800
C	-2.32419200	3.94006300	-1.23137200
H	-1.39843000	3.72565400	-3.14129900
H	-3.19860200	3.84903600	0.71457700
H	-2.64090700	4.94802900	-1.41001600
C	2.26177400	-2.57808500	-0.69859600
C	1.02533600	-3.22284500	-0.06414400
C	2.16812000	-2.60676800	-2.23013800

C	3.50307100	-3.34778100	-0.19886000
H	1.02703500	-3.10784400	1.01161200
H	0.11924000	-2.83852500	-0.48953200
H	1.06911300	-4.28107800	-0.28689600
H	3.05996000	-2.18981200	-2.68281500
H	2.07723800	-3.63677000	-2.55371700
H	1.30019300	-2.05127700	-2.54697700
H	3.34761500	-4.39881500	-0.40340800
H	4.41074400	-3.05686400	-0.70759100
H	3.63503900	-3.22147700	0.86862600
C	2.00164900	2.20248100	1.27954900
C	3.25000900	2.71276800	2.02985200
C	1.58793400	3.20518900	0.19448800
C	0.88293900	2.01283000	2.31742600
H	3.63577600	1.95889500	2.70465200
H	4.03462000	3.03190200	1.35870100
H	2.96090700	3.57785800	2.61156800
H	0.71353100	2.86544600	-0.33795000
H	1.36189300	4.15743500	0.65859800
H	2.39454200	3.35320700	-0.51299400
H	0.80544100	2.92863500	2.88798000
H	-0.07309500	1.84438800	1.85353500
H	1.12236700	1.21372300	3.01052200
O	-0.39739000	-0.88439400	-1.81338300
H	0.06005400	-0.29042000	1.59577300

Ligand **3** protonated at O

HF/3-21G(d)

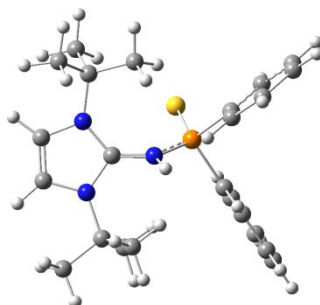


C	1.71692300	0.32297000	0.12036300
C	3.95382700	0.44081700	0.25472100
C	3.46283000	1.42901800	0.98981000
H	4.96215700	0.17330400	0.07752800
H	3.97451900	2.16138700	1.55690200
N	2.06589100	1.37067600	0.91402500
N	2.87457100	-0.26192100	-0.29830500
N	0.50548200	-0.05885200	-0.16464800
P	-0.87648800	-0.51812200	-0.62937100
C	-1.59380300	-1.67694000	0.51934800
C	-2.83321300	-2.24729800	0.22188700

C	-0.93366400	-2.04557900	1.68539000
C	-3.39673500	-3.16761500	1.08113200
H	-3.35332700	-1.96822900	-0.67374900
C	-1.50278900	-2.96805400	2.54557000
H	0.01856300	-1.61574700	1.91816200
C	-2.73115600	-3.52687900	2.24373600
H	-4.34781500	-3.60221500	0.84983800
H	-0.99062400	-3.24781200	3.44363800
H	-3.17151000	-4.24068100	2.91040900
C	-2.05792700	0.77175900	-0.97317000
C	-2.16357800	1.29640300	-2.25904400
C	-2.86008300	1.28366500	0.04376000
C	-3.04358700	2.33055100	-2.51532600
H	-1.57574900	0.88542700	-3.05324900
C	-3.74164300	2.31464500	-0.21896000
H	-2.81137600	0.87186500	1.03219100
C	-3.82989600	2.84075300	-1.49663000
H	-3.12226800	2.72860300	-3.50654000
H	-4.36120700	2.69918400	0.56558700
H	-4.51573500	3.63852700	-1.69937600
C	3.01881700	-1.42649300	-1.23647700
C	2.31610900	-2.66022500	-0.64457900
C	2.46483100	-1.03483500	-2.61741800
C	4.51253300	-1.76557400	-1.39660400
H	2.75550800	-2.91518700	0.31187700
H	1.26256000	-2.49313500	-0.49638700
H	2.44506600	-3.50056300	-1.31570000
H	2.99473400	-0.16817600	-2.99266500
H	2.62019900	-1.85441400	-3.30924400
H	1.41250300	-0.80878800	-2.58436400
H	4.59114200	-2.61726300	-2.05976600
H	5.06322000	-0.94813400	-1.84409700
H	4.96496300	-2.03742200	-0.45118600
C	1.14046100	2.36881300	1.55628200
C	1.97183800	3.37258400	2.37523200
C	0.39531800	3.13590600	0.45240000
C	0.18365900	1.64414300	2.51589600
H	2.52886200	2.88277200	3.16440500
H	2.64745700	3.94065600	1.74846500
H	1.28617900	4.07120500	2.83685700
H	-0.20171400	2.47846500	-0.15597000
H	-0.26082700	3.86896700	0.90533800
H	1.10634400	3.65377500	-0.17988900
H	-0.44641800	2.37497400	3.00728600
H	-0.44733700	0.94609300	1.99429900
H	0.74779400	1.11167900	3.27230600
O	-0.86493800	-1.26061500	-2.03905400
H	-0.52510000	-2.15689500	-2.16134300

Ligand 4 protonated at N

HF/3-21G(d)

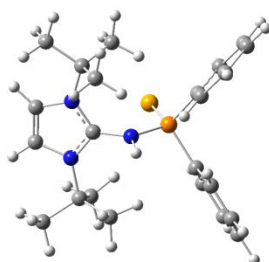


C	1.75131800	0.01522100	0.31481100
C	3.83736000	-0.46849800	-0.23544800
C	3.77203800	0.84950300	-0.05116900
H	4.66161300	-1.06840500	-0.52189500
H	4.53393400	1.57700800	-0.14504300
N	2.46882900	1.15868900	0.30910900
N	2.58134500	-0.99979700	0.02316300
N	0.39310300	-0.06182500	0.61119600
P	-0.89045900	-0.15693500	-0.52836700
C	-1.96873500	-1.46160000	0.09471700
C	-2.83915500	-2.06001500	-0.81091800
C	-2.02361800	-1.83581500	1.43546500
C	-3.74982400	-3.00858900	-0.38104400
H	-2.79646900	-1.79574500	-1.84830900
C	-2.93497800	-2.78230400	1.86136700
H	-1.35268000	-1.41120700	2.15522300
C	-3.80099100	-3.36814000	0.95291500
H	-4.41299000	-3.46431300	-1.08777300
H	-2.96724300	-3.06470300	2.89430100
H	-4.50681100	-4.10270200	1.28420600
C	-1.87059200	1.34252900	-0.30069600
C	-2.05403300	2.22226900	-1.36056900
C	-2.49252600	1.61170300	0.92043600
C	-2.82015300	3.36468100	-1.19584300
H	-1.60918800	2.00824500	-2.31079700
C	-3.24723300	2.75492600	1.08339700
H	-2.41943700	0.92008600	1.73667500
C	-3.40976500	3.63493000	0.02360500
H	-2.96027300	4.03181000	-2.02201700
H	-3.72216700	2.95153400	2.02327500
H	-4.00539400	4.51668200	0.14844100
C	2.42050700	-2.52255800	-0.02683400
C	1.04229600	-2.98915200	0.43647500
C	2.66188100	-2.96428500	-1.47855600
C	3.48098500	-3.11214100	0.92418400
H	0.82312700	-2.65978700	1.44134200

H	0.26365200	-2.67121200	-0.23103300
H	1.05510300	-4.07153400	0.43438800
H	3.65765100	-2.70855800	-1.81685200
H	2.55679700	-4.04058700	-1.53506500
H	1.93639400	-2.50475700	-2.13405100
H	3.35855800	-4.18728100	0.94541600
H	4.49142500	-2.90600300	0.60066300
H	3.34789100	-2.73079100	1.92894300
C	2.03090900	2.59621600	0.57342800
C	3.27769200	3.41456000	0.96527600
C	1.43231500	3.15676600	-0.72193400
C	1.03868200	2.66542400	1.74699400
H	3.79161700	2.97487600	1.81116500
H	3.96657700	3.53577100	0.14071900
H	2.94544000	4.40449200	1.24775600
H	0.56163600	2.59866000	-1.02161400
H	1.14085200	4.18759600	-0.56200100
H	2.16144000	3.12126800	-1.52135500
H	0.92680500	3.70389400	2.02946600
H	0.06199300	2.30364000	1.47882700
H	1.42263100	2.12707600	2.60667900
S	-0.18957900	-0.39595200	-2.31411100
H	0.16844300	0.10096200	1.57695700

Ligand 5 protonated at N:

HF/3-21G(d)



C	1.75059000	-0.20889600	0.45694100
C	3.84795800	0.25855500	-0.06305500
C	3.71088600	-1.06836800	-0.09799400
H	4.70168700	0.84867700	-0.26869400
H	4.42815400	-1.80704400	-0.33878300
N	2.62810200	0.80112500	0.31024200
N	2.40481600	-1.36720800	0.25651400
N	0.40258400	-0.08487700	0.79018000
P	-0.89036500	0.07648500	-0.33798600
C	-2.05119800	-1.24270900	0.07061800
C	-2.83888000	-1.75956300	-0.95225300
C	-2.22881600	-1.71545800	1.36966100
C	-3.79550100	-2.72098200	-0.67770800
H	-2.68897300	-1.42179400	-1.95744900
C	-3.18188500	-2.67738500	1.63922500
H	-1.62620000	-1.34920600	2.17657000



C	-3.96944900	-3.17833200	0.61498700
H	-4.39721000	-3.11116800	-1.47309400
H	-3.31057600	-3.03530800	2.64076700
H	-4.70985900	-3.92328900	0.82575800
C	-1.73493200	1.59728300	0.15329200
C	-2.28287000	1.74950200	1.42853700
C	-1.86401600	2.63059100	-0.76598000
C	-2.91696500	2.92278400	1.77957700
H	-2.24386300	0.95239300	2.14397400
C	-2.50897000	3.80428400	-0.41257300
H	-1.47312400	2.50427600	-1.75415200
C	-3.02857000	3.95398500	0.85805700
H	-3.33598100	3.03028100	2.75960300
H	-2.60888600	4.59079600	-1.13269600
H	-3.52967800	4.86095600	1.13025400
C	1.91612200	-2.80020500	0.46468100
C	1.39480000	-2.93355500	1.90362500
C	0.85220300	-3.15424200	-0.57905100
C	3.11194300	-3.75475300	0.29172200
H	2.16462600	-2.65642200	2.61389300
H	0.51838100	-2.32868600	2.06358200
H	1.12241700	-3.96645300	2.07918800
H	1.20862500	-2.93689200	-1.57603800
H	0.63634800	-4.21288000	-0.50318700
H	-0.06342200	-2.61857800	-0.41532700
H	2.75383100	-4.75740200	0.48379900
H	3.50023500	-3.73667600	-0.71861700
H	3.90521300	-3.54634600	0.99846200
C	2.46086800	2.31327900	0.46537500
C	2.14023200	2.89530300	-0.91766800
C	1.37627400	2.65224100	1.49852200
C	3.79482700	2.88421800	0.98922900
H	2.97731300	2.75388800	-1.59061700
H	1.27877000	2.41243300	-1.35053900
H	1.95189600	3.95750700	-0.82253700
H	1.57246700	2.15301600	2.44139300
H	1.41458900	3.71884100	1.67632300
H	0.38771100	2.41932200	1.15211300
H	3.64322400	3.93357300	1.20506000
H	4.10308300	2.38830700	1.90125000
H	4.58856000	2.82409500	0.25831500
Se	-0.16223200	0.07792100	-2.29234900
H	0.22559800	0.13444100	1.75592700