

Supporting information for Visible-Light Radical-Radical Coupling Vs. Radical Addition: Disentangling a Mechanistic Knot

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HAT reaction

In order to verify the absence of energetic barrier during the HAT process and thus, to discard that this step could be the rate-determining step of the proposed mechanisms, we have performed a relaxed scan in the reaction coordinate. To do this, we have started with the optimized structure of molecule **I** and we placed the DABCO in close to the H atom that is transferred. Then, we have calculated the energy at different C-H distances (relaxing all the other coordinates). As can be seen in the following figure, there is a single minimum (green arrow), which corresponds with the H already transferred.

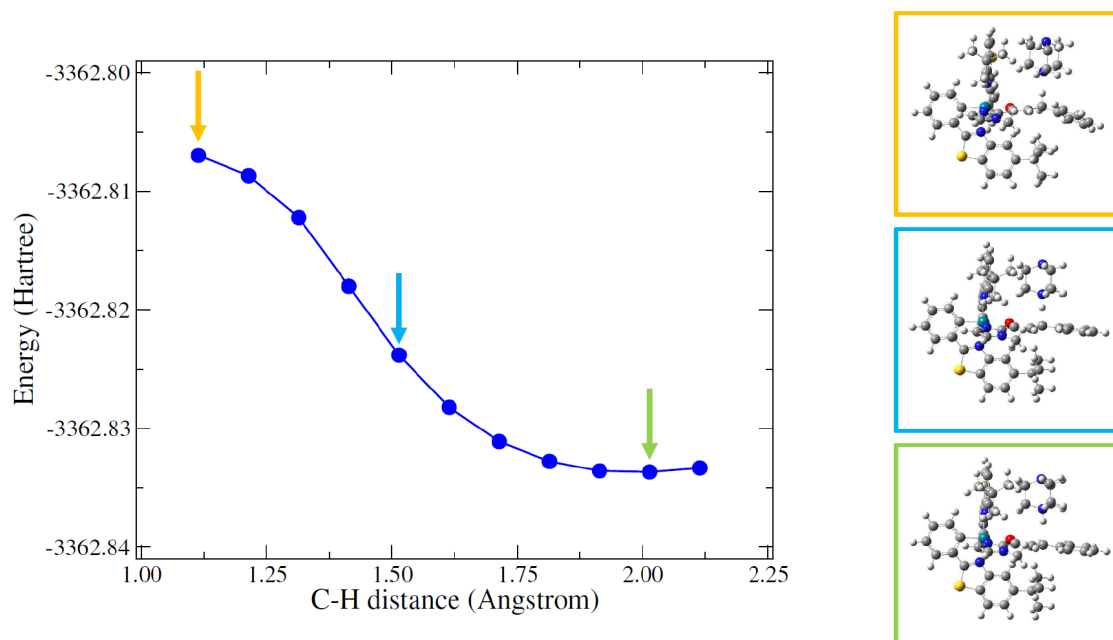


Figure S1. HAT reaction: Energy as a function of the C-H distance. Geometries at the points indicated with arrows are shown.

The critical points in the potential energy surface corresponding to the HAT reaction are given in the next figure. An intermediate is formed at $146.50 \text{ kJ}\cdot\text{mol}^{-1}$, and the final products lie $60.57 \text{ kJ}\cdot\text{mol}^{-1}$ below the reactants.

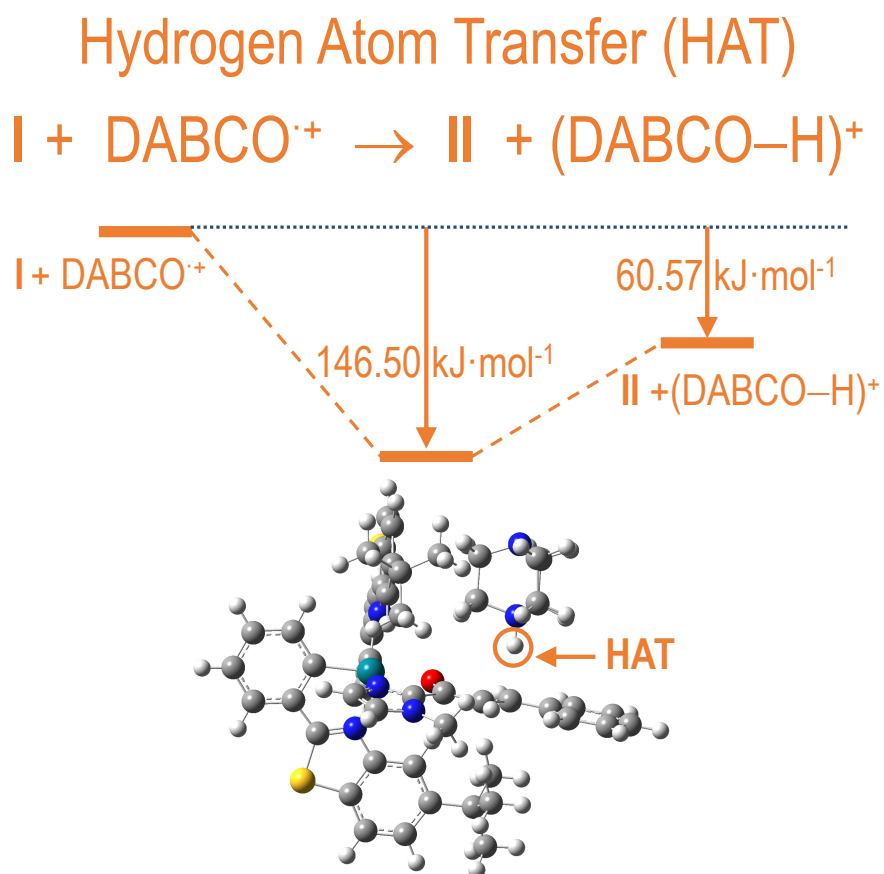


Figure S2. HAT reaction: Energy profile showing critical points. Geometry of the intermediate after hydrogen transfer is shown.

Enantioselective Addition

The radical-radical coupling is an enantioselective process. Fig.1 in the main article shows the energy profile to produce the favored enantiomer; it corresponds to the green path in the following figure. The energy profile of the addition through the opposite face is shown in pink. A relaxed scan elongating the C-C distance from the non-favored product demonstrates that the reaction occurs without transition state achieving the product at much higher energy, 53.48 kJ·mol⁻¹ with respect to the reactants.

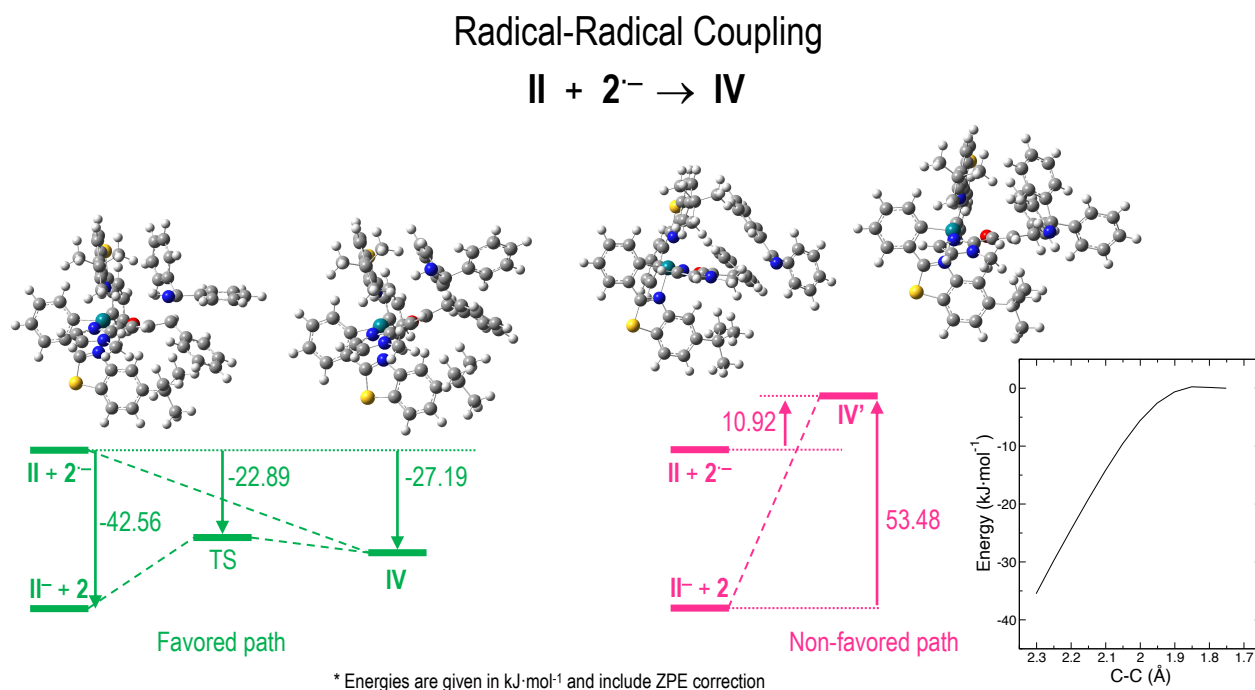
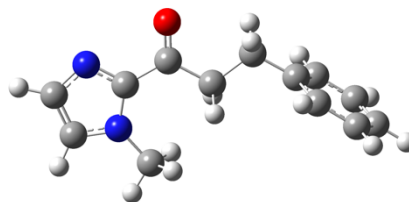


Figure S3. Enantioselective addition: Energy profile showing critical points of the favored and non-favored faces. Relaxed scan of the C-C bond which is being formed in the non-favored face is also given.

Optimized geometries – x y z coordinates in Å.

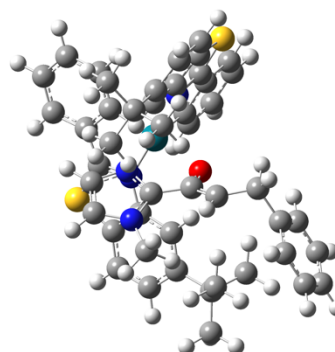
I)

C	-2.94792300	0.01502200	-0.51515300
C	-1.56773000	0.00633200	-0.62873400
C	-2.33286500	2.07621000	-0.62449500
N	-3.40412800	1.29075200	-0.51343500
H	-3.61276200	-0.84523200	-0.43623800
H	-0.84736300	-0.80784100	-0.66478200
C	0.21938400	1.72171500	-0.82144100
H	0.84244800	0.81991300	-0.83724400
H	0.38643100	2.27786100	-1.75278400
H	0.52490200	2.34146500	0.03119200
N	-1.17702500	1.31400800	-0.69802700
C	-2.47213700	3.55877500	-0.65836700
O	-3.58496000	4.05067300	-0.56948200
C	-1.24533700	4.44328700	-0.80525000
H	-0.54798300	4.23031600	0.02187500
H	-0.70725000	4.16092800	-1.72547200
C	-1.58554400	5.93813300	-0.83225400
H	-2.12547100	6.19609000	0.09175500
H	-2.28290300	6.12934000	-1.66224900
C	-0.34758400	6.79351200	-0.97571300
C	0.37344200	7.20987500	0.15585600
C	0.13761700	7.15098400	-2.24457100
C	1.54503400	7.96258100	0.02502800
H	0.00870600	6.94233000	1.15218900
C	1.30874900	7.90376300	-2.38066100
H	-0.41253500	6.83721100	-3.13681400
C	2.01749600	8.31190100	-1.24515800
H	2.08946100	8.28028100	0.91834600
H	1.66752900	8.17518600	-3.37713200
H	2.93150300	8.90225500	-1.34935600



II)

Rh	-0.89352600	1.52097800	0.36038600
C	-0.47973300	1.66907300	2.31689600
C	0.44093700	2.52104200	2.94759100
C	-1.20062700	0.76423900	3.14529700
C	0.63543800	2.47110000	4.33413700
H	1.01756600	3.23543200	2.35495000
C	-1.00794100	0.71084100	4.53759300
C	-0.08615100	1.56988500	5.13307900
H	1.35936600	3.14510500	4.80160400
H	-1.57351100	0.00160200	5.14903600
H	0.07359400	1.54071600	6.21336900
C	-2.17144200	3.04480600	0.56619500
C	-1.63955700	4.31862300	0.21422300
C	-3.51517900	3.00099000	0.97167400
C	-2.41587600	5.49056800	0.26229100
C	-4.29001100	4.16682600	1.02119600
H	-3.96846700	2.04792800	1.25444100
C	-3.74639900	5.41275600	0.66901600

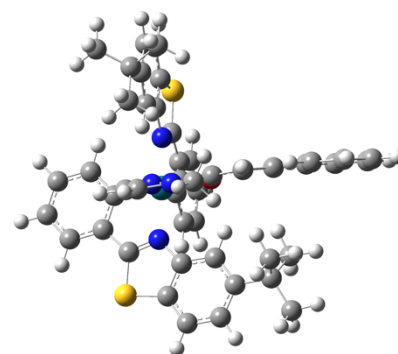


H	-1.98104400	6.45450300	-0.01777700
H	-5.33451900	4.10595100	1.34076900
H	-4.36118600	6.31464400	0.71284500
C	-2.11324100	-0.08013300	2.40133200
C	-3.68269300	-1.69928300	1.40639200
C	-3.07404100	-0.81140800	0.49228600
C	-4.57513000	-2.67938600	0.95900000
C	-3.36371300	-0.90175900	-0.87749200
C	-4.83105500	-2.76374200	-0.40727500
H	-5.05175900	-3.36827600	1.65900400
C	-4.23099500	-1.88818800	-1.34824200
H	-2.88258100	-0.19217400	-1.54040100
H	-5.51675100	-3.53952800	-0.75329100
C	-0.25532000	4.25449400	-0.20887600
C	2.05299200	4.41762300	-1.06440400
C	1.64767800	3.12147100	-0.66835400
C	3.33112400	4.62879100	-1.58274300
C	2.52177600	2.03555900	-0.78539900
C	4.18679800	3.53082100	-1.70507300
H	3.65684500	5.62367300	-1.89263200
C	3.80490300	2.22625100	-1.31367500
H	2.15776500	1.05958400	-0.46283800
H	5.17927200	3.70880200	-2.11778300
S	-3.12369300	-1.35894000	3.03474100
S	0.74300500	5.56089200	-0.80602300
N	0.34684400	3.07834300	-0.19293400
N	-2.20137300	0.08331500	1.09170300
C	4.75180000	1.01711400	-1.41591800
C	5.11799600	0.56519300	0.01608300
H	5.80704500	-0.29268300	-0.01716200
H	5.60534700	1.38283000	0.57142900
H	4.22590700	0.25001300	0.57758500
C	6.05098400	1.35194700	-2.16905300
H	6.67723900	0.44920700	-2.24278600
H	5.84886500	1.70404400	-3.19324500
H	6.64374100	2.12188500	-1.65069800
C	4.04589400	-0.14082200	-2.15693900
H	3.13336200	-0.47391800	-1.64346900
H	3.77121200	0.16171400	-3.18085400
H	4.71112100	-1.01559900	-2.22003500
C	-4.52285400	-2.06084000	-2.84926000
C	-3.76302700	-1.03280800	-3.70592000
H	-4.04220400	0.00175300	-3.45516100
H	-2.67299400	-1.12742200	-3.58640400
H	-3.99569000	-1.19133700	-4.77030300
C	-6.03665900	-1.89020700	-3.10507700
H	-6.63322000	-2.62891500	-2.54836900
H	-6.37338100	-0.88523500	-2.80410200
H	-6.25989100	-2.01955100	-4.17664100
C	-4.07676900	-3.47478100	-3.28743200
H	-2.99883100	-3.61542100	-3.10712900
H	-4.61806200	-4.26459300	-2.74472700
H	-4.26655100	-3.61810300	-4.36367600
C	0.25445700	-0.72867100	-1.23091100

C	0.48997400	-2.03631400	-1.54674400
H	0.29395900	-2.39146900	-2.55833800
O	0.43665700	-0.19143000	-0.04241800
C	1.00203700	-3.02839700	-0.53550300
C	-0.32637800	0.21332300	-2.22167800
N	-0.21572300	0.28118900	-3.58014800
C	-1.47150100	1.95953200	-2.87518500
C	-0.94300200	1.37982000	-4.00357400
H	-2.09250700	2.84718700	-2.77986200
H	-1.00892300	1.64847800	-5.05443000
N	-1.08085600	1.22521900	-1.78612400
C	0.56128500	-0.58616300	-4.45382700
H	1.47820300	-0.89737100	-3.93754900
H	-0.01377300	-1.48083800	-4.73634600
H	0.82614300	-0.03007800	-5.36204800
H	0.70652000	-2.69883300	0.47246300
H	0.52698100	-4.00938100	-0.71413600
C	2.51123700	-3.21268400	-0.57358400
C	3.12938200	-3.81613900	-1.68297000
C	3.32486200	-2.76819200	0.47851100
C	4.51645200	-3.97293800	-1.73781600
H	2.51066000	-4.16508900	-2.51529000
C	4.71489100	-2.92737700	0.43114200
H	2.86269100	-2.28857700	1.34581600
C	5.31707000	-3.52894700	-0.67734600
H	4.97669100	-4.44543700	-2.61007100
H	5.32931000	-2.57294300	1.26275100
H	6.40265500	-3.65028400	-0.71753000

II)

Rh	-0.96260000	1.59855900	0.34723400
C	-0.56671600	1.84470600	2.30318300
C	0.33823400	2.73412400	2.90497200
C	-1.29441500	0.97950300	3.16640900
C	0.51159900	2.75649800	4.29497500
H	0.92076700	3.42269600	2.28860700
C	-1.12420700	0.99898800	4.56276300
C	-0.21704400	1.89297200	5.12800900
H	1.22438900	3.45838100	4.73782300
H	-1.69530800	0.31860700	5.20118500
H	-0.07426500	1.92000900	6.21070100
C	-2.29060400	3.08388300	0.47000600
C	-1.78649600	4.35949600	0.08713300
C	-3.64693600	3.00912100	0.82515200
C	-2.60248800	5.50493800	0.05772900
C	-4.46105900	4.14856500	0.79624800
H	-4.08090000	2.05347500	1.12770600
C	-3.94512000	5.39732900	0.41443600
H	-2.18925100	6.47156400	-0.24470900
H	-5.51507800	4.06400600	1.07656800
H	-4.59066000	6.27832100	0.39626300
C	-2.19340400	0.09259600	2.45659200
C	-3.77565800	-1.56206900	1.55005600



C	-3.13166200	-0.75645500	0.58449100
C	-4.68853500	-2.54860400	1.16355800
C	-3.40330900	-0.94419300	-0.78025000
C	-4.93405200	-2.72257400	-0.19536400
H	-5.19169600	-3.17132500	1.90568500
C	-4.29776000	-1.93564900	-1.18894200
H	-2.89331700	-0.30171600	-1.48839800
H	-5.64199300	-3.49822100	-0.49312300
C	-0.38196200	4.33200200	-0.26680300
C	1.98335800	4.58832700	-0.91112100
C	1.59349100	3.27072500	-0.57316700
C	3.29793900	4.86316300	-1.28945500
C	2.52602800	2.22634600	-0.61388500
C	4.21138200	3.80772600	-1.32887200
H	3.60919300	5.87683500	-1.54895500
C	3.84944100	2.48084700	-0.99807100
H	2.18390000	1.22965600	-0.34258500
H	5.23327800	4.03626500	-1.62922200
S	-3.23787500	-1.11928700	3.15918400
S	0.61499500	5.67943600	-0.76254900
N	0.25523400	3.17449700	-0.21771700
N	-2.25293900	0.16567600	1.13623800
C	4.84497600	1.30865100	-1.09739300
C	4.77639700	0.44121500	0.17900700
H	5.49324900	-0.39249300	0.10815500
H	5.02598500	1.03481500	1.07317500
H	3.78098400	-0.00088000	0.32421900
C	6.29645700	1.78887700	-1.27408100
H	6.97218900	0.91982100	-1.29814700
H	6.43920900	2.33897200	-2.21702900
H	6.61372800	2.43972200	-0.44362800
C	4.45498100	0.44740200	-2.32156700
H	3.43333000	0.05378600	-2.22018800
H	4.50902700	1.03914700	-3.24959300
H	5.13832400	-0.41210700	-2.42084900
C	-4.60115400	-2.19867300	-2.67484900
C	-3.77995300	-1.28627600	-3.60141300
H	-3.99687300	-0.22116600	-3.43308800
H	-2.69775400	-1.43465300	-3.46608800
H	-4.01807500	-1.51150000	-4.65253100
C	-6.10199000	-1.94468500	-2.94155400
H	-6.74356300	-2.60032200	-2.33312700
H	-6.36860100	-0.90057400	-2.71207900
H	-6.33891100	-2.13376400	-4.00127200
C	-4.25512000	-3.66643700	-3.01455900
H	-3.18857700	-3.86972100	-2.82703800
H	-4.84634600	-4.37959700	-2.42055000
H	-4.46029300	-3.86846200	-4.07840500
C	0.49263000	-0.47480800	-1.26680800
C	1.35319600	-1.54213100	-1.62870300
H	1.37347300	-1.85539200	-2.66947200
O	0.42074300	-0.05514800	-0.03310000
C	2.18390300	-2.17565100	-0.71804400
C	-0.32510900	0.26779900	-2.22523500

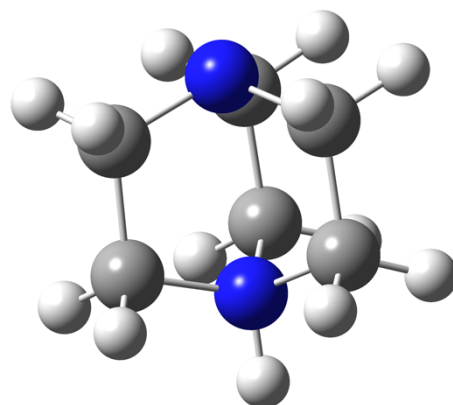
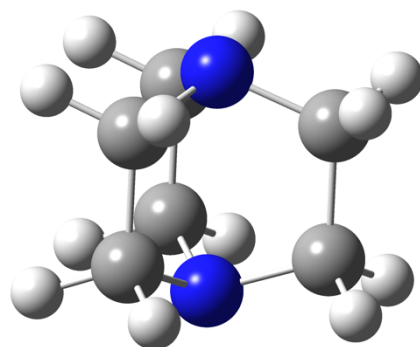
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C	-1.76160900	1.81556400	-2.83356000
C	-1.29745400	1.22436700	-3.98400500
H	-2.48283500	2.62045100	-2.71300000
H	-1.53130600	1.40173900	-5.03017100
N	-1.16407200	1.21315500	-1.76311500
C	0.34721400	-0.58398800	-4.53135500
H	1.42910600	-0.47171700	-4.37158600
H	0.07179300	-1.64253500	-4.41662400
H	0.10672000	-0.26809000	-5.55346700
H	2.11949100	-1.84324200	0.32144300
C	3.16923000	-3.19320000	-1.00815700
C	3.40803600	-3.70716000	-2.31129900
C	3.97358900	-3.70501600	0.04429300
C	4.38828400	-4.67092200	-2.53890800
H	2.81944100	-3.34096500	-3.15550500
C	4.95364200	-4.66845400	-0.18825400
H	3.81697800	-3.32528000	1.05818700
C	5.17078100	-5.16182200	-1.48265400
H	4.54844100	-5.04544800	-3.55398000
H	5.55616900	-5.03899500	0.64585200
H	5.93925500	-5.91653100	-1.66716600

DABCO)

C	-0.78298600	-1.34612200	-0.31974900
C	0.78300000	-1.34606100	-0.31997300
H	-1.18333800	-2.05310400	0.42520500
H	-1.18360800	-1.64272900	-1.30289700
H	1.18363300	-2.05324700	0.42463700
H	1.18335100	-1.64232400	-1.30333500
C	-0.78297800	0.39613600	1.32563800
H	-1.18329400	1.39477700	1.56545300
H	-1.18358700	-0.30698200	2.07407900
C	0.78297700	0.39592500	1.32570200
H	1.18355600	1.39437700	1.56586800
H	1.18332200	-0.30754300	2.07395400
C	0.78297200	0.95014000	-1.00573300
H	1.18328500	1.94989000	-0.77061600
H	1.18357800	0.65890900	-1.99048100
C	-0.78298400	0.94996500	-1.00588900
H	-1.18357900	1.94969700	-0.77117200
H	-1.18331700	0.65832800	-1.99062700
N	-1.27941900	-0.00000200	-0.00000100
N	1.27941900	0.00001100	-0.00000400

DABCO⁺H)

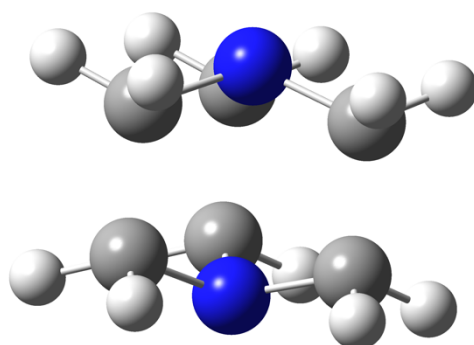
C	0.81753600	-1.38454400	0.06364900
C	-0.73887600	-1.42853400	0.09343100
H	1.19650200	-1.93241300	-0.81016000
H	1.22676500	-1.86430100	0.96355100
H	-1.17412500	-1.97493000	-0.75252100
H	-1.14377200	-1.84235300	1.02575600
C	0.81909300	0.63667000	-1.23015500



H	1.20001100	1.66657200	-1.26762800
H	1.22764900	0.09626200	-2.09522700
C	-0.73713500	0.63559900	-1.28387900
H	-1.17127200	1.64218800	-1.32879100
H	-1.14149600	0.03988500	-2.11184700
C	-0.73838800	0.79462900	1.19017900
H	-1.14205100	1.80963900	1.08472200
H	-1.17395400	0.33268600	2.08503500
C	0.81789900	0.74629400	1.16669900
H	1.22744000	1.76540100	1.13254600
H	1.19688900	0.26330600	2.07799600
N	1.29001300	-0.00078000	0.00021300
N	-1.22145300	0.00009700	-0.00133000
H	-2.24657400	-0.00065900	-0.00182800

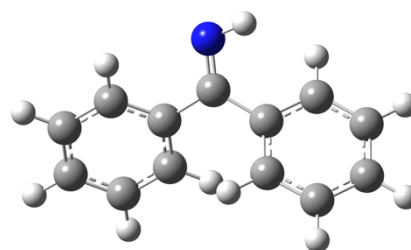
DABCO²⁺)

C	0.81847200	1.13579300	-0.77697900
C	-0.81839500	1.13590400	-0.77689800
H	1.18035700	2.06623400	-0.32342500
H	1.18056200	1.05103200	-1.80861500
H	-1.18011700	2.06634700	-0.32321800
H	-1.18058800	1.05129300	-1.80851000
C	0.81796800	0.10495600	1.37199300
H	1.17977100	-0.75260000	1.95182600
H	1.18059100	1.04043200	1.81413700
C	-0.81794200	0.10493000	1.37201000
H	-1.17971400	-0.75269300	1.95176600
H	-1.18057400	1.04035500	1.81425500
C	-0.81874800	-1.24075000	-0.59512100
H	-1.18187400	-2.09191100	-0.00660000
H	-1.18102900	-1.31350400	-1.62745400
C	0.81864400	-1.24084800	-0.59505400
H	1.18162800	-2.09199300	-0.00642200
H	1.18099200	-1.31374600	-1.62735400
N	1.22690500	0.00001400	-0.00001400
N	-1.22690600	0.00010700	0.00000200



2)

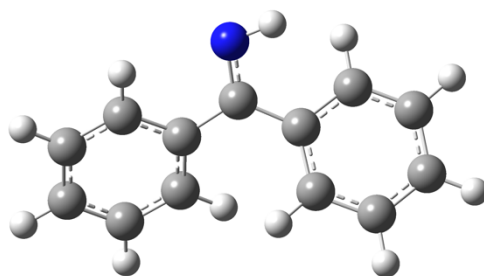
C	-0.86412600	0.94782200	0.06913500
N	-0.26568900	2.08254800	0.12736300
H	0.74735500	1.94836100	0.21910400
C	-0.13146400	-0.36020200	0.08901100
C	-0.55607300	-1.41902100	0.91201900
C	1.03446400	-0.52430200	-0.68018800
C	0.17755500	-2.60645400	0.97533300
H	-1.46031900	-1.30560400	1.51398200
C	1.75893900	-1.71765800	-0.62801200
H	1.36521400	0.28425100	-1.33717900
C	1.33447500	-2.76047000	0.20309400
H	-0.15646500	-3.41564700	1.62951700
H	2.65567800	-1.83531300	-1.24142400
H	1.90234700	-3.69321400	0.24621300



C	-2.35836600	0.93251000	-0.01450500
C	-3.05452700	-0.13044700	-0.61801600
C	-3.09265700	2.02599500	0.48239400
C	-4.44852700	-0.09984800	-0.72288200
H	-2.50364800	-0.98247900	-1.02068700
C	-4.48410700	2.05143400	0.38678000
H	-2.55051500	2.85131800	0.94713700
C	-5.16737600	0.98789800	-0.21753800
H	-4.97391000	-0.92983000	-1.20186000
H	-5.04107200	2.90262300	0.78674200
H	-6.25761500	1.00777200	-0.29248500

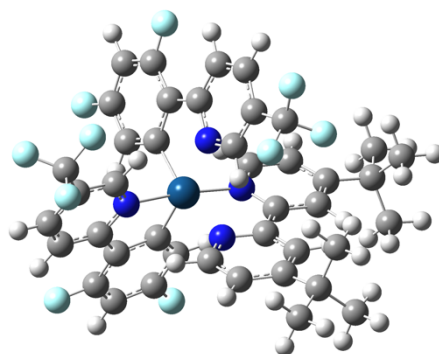
2⁻)

C	-0.91168800	0.87187000	0.03428100
N	-0.28624500	2.06377200	0.02345700
H	0.71437000	1.90497800	0.17845200
C	-0.15981600	-0.39449000	0.04657700
C	-0.61021300	-1.58511200	0.68828900
C	1.14966400	-0.45221600	-0.51937600
C	0.17432800	-2.73441100	0.74552700
H	-1.58287200	-1.58737000	1.18419000
C	1.93029500	-1.60543700	-0.46382100
H	1.53568600	0.42956200	-1.03793200
C	1.45661700	-2.76647400	0.16658400
H	-0.21029600	-3.61857400	1.26413600
H	2.92211000	-1.60392900	-0.92785500
H	2.07001300	-3.66992800	0.21312700
C	-2.37876300	0.88323700	0.00533100
C	-3.19263200	-0.21104600	-0.41399000
C	-3.07610300	2.09075700	0.32125100
C	-4.58134600	-0.11731300	-0.47132900
H	-2.72025300	-1.14297500	-0.72975900
C	-4.46424800	2.17772500	0.26291300
H	-2.47618400	2.95238100	0.61834200
C	-5.24435600	1.07524300	-0.12637400
H	-5.16062600	-0.98465100	-0.80495000
H	-4.95350000	3.12158000	0.52739600
H	-6.33437300	1.14486300	-0.17141800



Ir^{III})

Ir	0.65818600	-0.53749700	-0.16460900
C	1.63411900	-1.42180500	1.38773000
C	1.27376500	-0.92894300	2.68691200
C	2.58508200	-2.45135900	1.29676200
C	1.88193600	-1.51465300	3.81473400
C	0.30449600	0.17544900	2.74320100
C	3.15040600	-2.98638100	2.44916300
H	2.88875800	-2.85636000	0.33035900
C	2.81537400	-2.53828100	3.72606500
C	-0.24555300	0.75926400	3.90398100
H	3.26484900	-2.96424100	4.62248900
C	-0.92915600	1.66791500	1.41330100

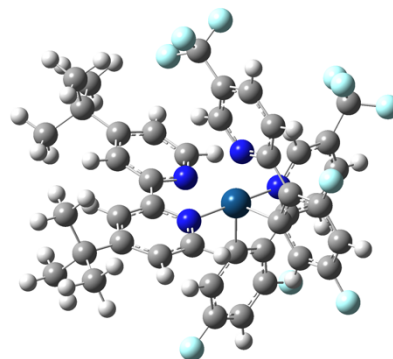


C	-1.16111200	1.80010600	3.79368400
H	0.03754200	0.38990000	4.88460300
C	-1.51161000	2.27161800	2.52410800
H	-1.15846300	2.01398100	0.40550500
H	-1.59632200	2.24710300	4.68902100
N	-0.06768100	0.65382500	1.52051900
F	4.05328400	-3.97476100	2.33961900
F	1.57746900	-1.08781800	5.05697200
C	-2.53470100	3.35236100	2.31114900
F	-2.72721800	4.09002800	3.41580500
F	-3.73409900	2.84082400	1.95974000
F	-2.17172700	4.18880000	1.31632300
C	1.42703700	-1.68160400	-1.62254200
C	2.65473000	-1.19515200	-2.17803300
C	0.88604300	-2.87814600	-2.12218400
C	3.27521700	-1.93647700	-3.20150400
C	3.15557800	0.05164400	-1.60629300
C	1.54690300	-3.56535200	-3.13301400
H	-0.04602200	-3.28783700	-1.73133200
C	2.74625800	-3.12022000	-3.69435600
C	4.32817600	0.74293800	-1.97206800
H	3.24989800	-3.67344500	-4.48629800
C	2.69085500	1.70180900	0.01033900
C	4.66823900	1.92503000	-1.33107700
H	4.96319400	0.34381400	-2.75734300
C	3.83343200	2.41881300	-0.31890800
H	2.01617600	2.04157400	0.79513800
H	5.57808000	2.45957800	-1.61097600
N	2.36052900	0.56026500	-0.61268000
C	4.15864600	3.71212300	0.37670100
F	5.43886200	3.73706300	0.79210600
F	3.99895600	4.76808800	-0.44549900
F	3.37804300	3.92118800	1.45032100
F	4.43149200	-1.51096800	-3.74730600
F	1.01993900	-4.70921700	-3.59956600
C	-1.99664000	0.15951200	-1.26801600
C	-0.39539200	1.61654700	-2.19847900
C	-3.02545800	1.01432000	-1.75763100
C	-2.21648100	-1.02293300	-0.49734500
C	-1.36679000	2.45988400	-2.71553500
H	0.66587200	1.83694400	-2.34306200
C	-2.74326200	2.17749200	-2.45306000
H	-4.05809300	0.76404200	-1.51692200
C	-3.48563000	-1.63273000	-0.29359400
H	-1.05136000	3.33381400	-3.28110600
C	-1.23527100	-2.75109700	0.78040300
C	-3.63910000	-2.79916500	0.43561800
H	-4.35498500	-1.16223700	-0.75243700
C	-2.45313200	-3.37700800	0.98279100
H	-0.31761300	-3.16892000	1.19838300
H	-2.46969200	-4.29593900	1.56438500
N	-0.67071800	0.52127600	-1.47411300
N	-1.09160500	-1.61060600	0.08090900
C	-5.03312600	-3.42344900	0.62141400

C	-4.98338400	-4.70601600	1.47061200
H	-5.99884100	-5.11698800	1.58283000
H	-4.36013700	-5.48294000	1.00105900
H	-4.58879300	-4.51201800	2.48020500
C	-5.95723300	-2.40672200	1.32963400
H	-5.55459800	-2.13328400	2.31810700
H	-6.07243700	-1.48223400	0.74366400
H	-6.96083100	-2.83885400	1.47604300
C	-5.62419300	-3.77866100	-0.76194400
H	-4.97868400	-4.49779200	-1.29116400
H	-6.62155900	-4.23406200	-0.64658800
H	-5.73387600	-2.88855600	-1.39995400
C	-3.87221500	3.15217400	-2.82868100
C	-4.39351600	3.80060800	-1.52351300
H	-5.19539400	4.52420500	-1.74609000
H	-4.79476300	3.04455600	-0.83132900
H	-3.58484800	4.33104200	-0.99672800
C	-5.02555100	2.40180100	-3.52882500
H	-5.46961000	1.62832000	-2.88464800
H	-5.82890500	3.10680400	-3.79735200
H	-4.67452200	1.91470700	-4.45262200
C	-3.38272500	4.26813800	-3.76927100
H	-2.61739100	4.89997300	-3.29319200
H	-2.96003700	3.85783900	-4.70007300
H	-4.22594900	4.92205500	-4.04131200

Ir^{III})

Ir	0.51134100	-0.57886100	-0.10663800
C	1.58613800	-1.46138700	1.37730800
C	1.57556000	-0.76747500	2.63069800
C	2.30075300	-2.66257700	1.26946600
C	2.28631800	-1.33150100	3.70884000
C	0.81863800	0.49069600	2.69625600
C	2.98229800	-3.16809100	2.37309100
H	2.33434900	-3.22285000	0.33462600
C	2.99209800	-2.52242600	3.60752200
C	0.63871000	1.30725900	3.83183100
H	3.53027500	-2.92701100	4.46407300
C	-0.46732000	1.98873000	1.42185200
C	-0.11056000	2.47341000	3.73861200
H	1.07948300	1.02141000	4.78154700
C	-0.67597100	2.82919900	2.50799600
H	-0.89147900	2.22752000	0.44736100
H	-0.25892200	3.10023800	4.62011700
N	0.24811600	0.86215300	1.51437800
F	3.65787100	-4.31915100	2.25177700
F	2.30939100	-0.71963100	4.90700100
C	-1.46875400	4.09934300	2.34930400
F	-0.66897900	5.18145700	2.30867800
F	-2.31709100	4.27839200	3.37629600
F	-2.19380900	4.09836800	1.21457800
C	0.90630700	-1.95226200	-1.53196200
C	2.10805400	-1.70685100	-2.26600400

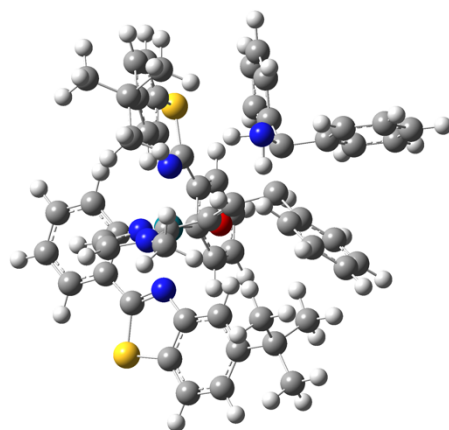


C	0.13431900	-3.07940900	-1.84568600
C	2.47591100	-2.61177300	-3.27970800
C	2.85625100	-0.51413800	-1.87681800
C	0.55054300	-3.93938400	-2.85773300
H	-0.78980500	-3.31232600	-1.31558800
C	1.71830900	-3.73146900	-3.59243600
C	4.06573200	-0.05445300	-2.43288800
H	2.02897000	-4.41541800	-4.38150600
C	2.85079800	1.31416300	-0.38814300
C	4.65851900	1.10372200	-1.95113600
H	4.53226000	-0.61380600	-3.23817800
C	4.04008400	1.80563600	-0.90842700
H	2.34248600	1.82306600	0.42920600
H	5.59900600	1.45764200	-2.37762400
N	2.27574400	0.19596900	-0.85809000
C	4.63751800	3.08251700	-0.37982800
F	5.96169700	2.95677800	-0.18307000
F	4.46677400	4.10052600	-1.24498800
F	4.08291600	3.45303800	0.78659000
F	3.59938300	-2.41623800	-3.99302600
F	-0.19526600	-5.01521100	-3.14598900
C	-2.15741800	0.28398300	-1.10825300
C	-0.52018700	1.45374400	-2.27221900
C	-3.15023600	1.09373400	-1.65781500
C	-2.42524200	-0.81108400	-0.14806800
C	-1.46818300	2.29026500	-2.85668000
H	0.54358800	1.57269500	-2.48573100
C	-2.82521700	2.14352400	-2.53341500
H	-4.18745000	0.92747300	-1.37380700
C	-3.70517300	-1.27364400	0.15041800
H	-1.11941200	3.06198700	-3.54008800
C	-1.50265600	-2.37402600	1.31247600
C	-3.91075900	-2.32169400	1.06213900
H	-4.55716500	-0.81414600	-0.34664400
C	-2.75940300	-2.86979900	1.64427200
H	-0.59822700	-2.79267500	1.75360400
H	-2.80939600	-3.68783900	2.36010700
N	-0.84900200	0.49211400	-1.40117800
N	-1.32903100	-1.36889200	0.43918700
C	-5.33060900	-2.80941700	1.36921300
C	-5.33551300	-3.95216200	2.39835900
H	-6.37188300	-4.26808400	2.59041500
H	-4.78216500	-4.83227900	2.03573000
H	-4.89997900	-3.63867100	3.35986300
C	-6.15318900	-1.62804200	1.93445000
H	-5.70280400	-1.24199900	2.86236500
H	-6.22824700	-0.79588300	1.21813700
H	-7.17666900	-1.96391100	2.16336900
C	-5.97815000	-3.31661000	0.05962800
H	-5.40077100	-4.15101400	-0.36834800
H	-6.99919000	-3.67468200	0.26455200
H	-6.04911300	-2.52402500	-0.70057100
C	-3.92194400	3.08470500	-3.04226300
C	-4.53330100	3.80832100	-1.81766700

H	-5.30097800	4.52385200	-2.15165900
H	-5.01249600	3.10284700	-1.12187400
H	-3.76202300	4.36230700	-1.25954200
C	-5.01326800	2.26373500	-3.76534800
H	-5.48222400	1.52043600	-3.10313100
H	-5.80804100	2.93645600	-4.12353900
H	-4.59533000	1.73267500	-4.63490100
C	-3.37003600	4.13915300	-4.01606400
H	-2.61898000	4.78613700	-3.53704400
H	-2.91501000	3.67555300	-4.90523000
H	-4.19135300	4.78528400	-4.36062300

IV)

Rh	-0.38328600	1.99292500	0.36946600
C	0.33486800	2.52413500	2.17302100
C	1.52172800	3.21160700	2.47348800
C	-0.51628400	2.19458800	3.26668100
C	1.84425800	3.55288000	3.79402200
H	2.20808700	3.49074500	1.66993300
C	-0.20140100	2.54295400	4.59200900
C	0.98507000	3.22633000	4.85501500
H	2.77802400	4.08414100	4.00109500
H	-0.87475000	2.27367700	5.41110900
H	1.24528400	3.50082300	5.87993500
C	-1.39778300	3.72542600	0.40049700
C	-0.72980000	4.81015000	-0.23577800
C	-2.67733100	3.98466300	0.91935700
C	-1.30466400	6.08995200	-0.33480400
C	-3.25414700	5.25748500	0.81980600
H	-3.24484800	3.19141400	1.40953100
C	-2.57182900	6.31493100	0.19900600
H	-0.76510400	6.90139600	-0.83188500
H	-4.25230300	5.42848200	1.23356400
H	-3.03076600	7.30378000	0.12963100
C	-1.68730800	1.44285800	2.86295000
C	-3.72716400	0.10819700	2.49429600
C	-2.90644200	0.28112700	1.35972200
C	-4.86651400	-0.70018800	2.43089300
C	-3.20956300	-0.38555900	0.16472000
C	-5.14520200	-1.35527400	1.23416000
H	-5.50580900	-0.84031900	3.30451400
C	-4.31531000	-1.23112700	0.09046800
H	-2.53766100	-0.24947200	-0.67154100
H	-6.02149900	-2.00526300	1.19661000
C	0.55581000	4.44089200	-0.79112400
C	2.72028300	4.09109400	-1.91806200
C	2.17433500	2.94511300	-1.29205100
C	3.93028100	4.01101700	-2.60795200
C	2.83821400	1.71626800	-1.36311000
C	4.57390900	2.77261100	-2.67736200
H	4.36289100	4.88932000	-3.09104800
C	4.04334500	1.61151700	-2.06960700
H	2.36965800	0.86734900	-0.86419200

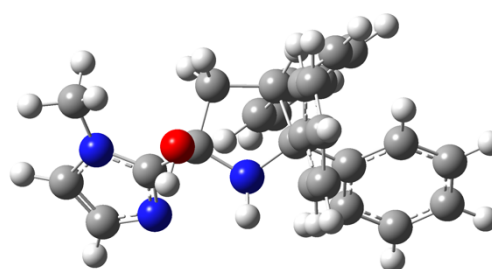


H	5.51265100	2.72200300	-3.22813300
S	-3.02558400	0.93918800	3.87159700
S	1.65449800	5.46776500	-1.68509800
N	0.96168100	3.19029800	-0.66301500
N	-1.79319100	1.07305200	1.59687000
C	4.71664700	0.23200500	-2.17502800
C	4.98107200	-0.31596000	-0.75474500
H	5.47871600	-1.29542100	-0.81250200
H	5.62656200	0.37160300	-0.18431400
H	4.04689800	-0.45910900	-0.19214900
C	6.05707800	0.28741600	-2.92756500
H	6.49643300	-0.72141400	-2.97036200
H	5.93218700	0.63710200	-3.96454100
H	6.78311400	0.94747200	-2.42633400
C	3.76699400	-0.72448200	-2.93337100
H	2.80540100	-0.84308000	-2.41316900
H	3.56517200	-0.34443800	-3.94854700
H	4.21282700	-1.72727600	-3.01684100
C	-4.61692200	-2.05089600	-1.17642300
C	-3.61133600	-1.75249500	-2.30342800
H	-3.63232200	-0.69435400	-2.60754900
H	-2.58318500	-2.00132900	-1.99980000
H	-3.85424100	-2.36006800	-3.18897200
C	-6.03774300	-1.71997800	-1.68274400
H	-6.80867400	-1.96419800	-0.93589600
H	-6.12787700	-0.64905500	-1.92667300
H	-6.26216800	-2.29843300	-2.59372100
C	-4.51748400	-3.55631100	-0.83634900
H	-3.49425300	-3.82239200	-0.52794000
H	-5.20585100	-3.84059000	-0.02559100
H	-4.77437300	-4.16078300	-1.72207100
C	0.24142600	-0.61872300	-0.99568000
C	0.40717600	-1.95314500	-1.23295400
H	-0.06878400	-2.36916000	-2.11648000
O	0.66535700	0.06080100	0.05889800
C	1.16826200	-2.95165700	-0.41975000
C	-0.51233100	0.20706300	-1.97325500
N	-0.77193600	0.03423500	-3.30680000
C	-1.68634400	1.93583100	-2.64068500
C	-1.52246000	1.11722400	-3.73124300
H	-2.20127600	2.89035100	-2.56075300
H	-1.85686300	1.20828800	-4.76121900
N	-1.05623600	1.35937400	-1.57039800
C	-0.33084400	-1.04115000	-4.18258500
H	0.69954300	-1.32518800	-3.93396100
H	-0.97701500	-1.92603400	-4.08066500
H	-0.37160800	-0.68746800	-5.22060600
H	1.61936900	-2.44564600	0.44235600
C	2.30811800	-3.54032700	-1.22555100
C	2.09319800	-4.11463300	-2.49333800
C	3.61683200	-3.54804900	-0.71780200
C	3.15152000	-4.66724000	-3.22223600
H	1.06945600	-4.16852800	-2.86269900
C	4.67994900	-4.09478800	-1.44327100

H	3.80500400	-3.11370100	0.26707000
C	4.45326600	-4.65516500	-2.70611600
H	2.95949600	-5.11188900	-4.20371600
H	5.68991900	-4.07711800	-1.02331300
H	5.28195300	-5.07761000	-3.28137200
C	0.16104000	-4.14644700	0.10205700
N	-0.62227200	-4.72338600	-0.93247200
H	-1.27642000	-3.99127500	-1.23137800
C	1.08346700	-5.22171900	0.72792200
C	1.89353000	-4.95586400	1.84497900
C	1.14557300	-6.50134000	0.16070000
C	2.74878400	-5.93045900	2.36932000
H	1.85502800	-3.96976900	2.31449700
C	1.99943400	-7.48295700	0.67836200
H	0.49229200	-6.67478400	-0.69543700
C	2.80914800	-7.20255300	1.78493000
H	3.37046100	-5.69738800	3.23914300
H	2.03331500	-8.47488300	0.21610900
H	3.47690600	-7.96712900	2.19249900
C	-0.68913700	-3.60078500	1.29459600
C	-1.76102600	-4.40293500	1.73207700
C	-0.44202500	-2.41452900	2.00478700
C	-2.52812200	-4.06356100	2.84700400
H	-1.97043700	-5.30229200	1.14953500
C	-1.20634600	-2.07032200	3.12782800
H	0.33167700	-1.72103800	1.67696000
C	-2.24937900	-2.88961100	3.56148400
H	-3.35082200	-4.71369500	3.16149000
H	-0.98206100	-1.14400500	3.66178900
H	-2.85080700	-2.60785900	4.43001000

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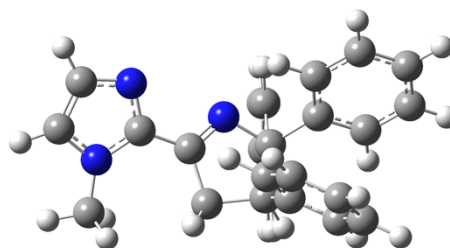
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N	2.88531100	-0.37019200	-1.82065600
H	4.55487800	-1.24362900	-2.87478600
H	6.04954600	-0.04466300	-0.85962100
C	4.44887300	1.31470200	0.99696900
H	5.47428600	1.69533100	0.90150500
H	3.76013100	2.15590100	1.13219500
H	4.39519900	0.65409400	1.87618100
N	4.09103500	0.59409300	-0.21788500
C	1.57342500	0.93206800	-0.09610000
O	1.71262200	2.36569300	0.00748700
C	1.27347400	0.42819300	1.34416900
H	2.02287800	-0.29179200	1.69564700
H	1.29830400	1.29657700	2.01404100
C	-0.13973200	-0.19592400	1.29502700
H	-0.71969100	0.08565200	2.18103300
C	-0.14679000	-1.71322000	1.23250700
C	0.76257800	-2.43680000	0.44222600
C	-1.11141000	-2.42933000	1.95876900



C	0.70400100	-3.83249200	0.38139700
H	1.50649200	-1.90748200	-0.15433700
C	-1.17468200	-3.82520100	1.89899500
H	-1.83161500	-1.88370900	2.57481100
C	-0.26495300	-4.53380700	1.10763200
H	1.41873000	-4.37532600	-0.24318000
H	-1.93639500	-4.35945800	2.47313500
H	-0.30972000	-5.62492600	1.05811500
H	1.89320000	2.71327800	-0.87843800
C	-0.76639100	0.47622200	0.01246100
C	-1.32101500	1.90037000	0.26861200
C	-1.71939600	2.65063700	-0.85270900
C	-1.44523100	2.49314300	1.53087800
C	-2.21077200	3.94930500	-0.72121300
H	-1.65045700	2.20624200	-1.84954100
C	-1.93961000	3.79746500	1.67089400
H	-1.15380400	1.95153200	2.43130100
C	-2.32199300	4.53272400	0.54780200
H	-2.51262500	4.50839700	-1.61086700
H	-2.02275100	4.23631600	2.66870100
H	-2.70686500	5.54982400	0.65683000
C	-1.87351700	-0.38397700	-0.60423500
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C	-3.16268100	-0.36490500	-0.04799000
C	-2.63141300	-2.06820900	-2.18924600
H	-0.61519500	-1.28754700	-2.10174600
C	-4.17159700	-1.19142300	-0.54813300
H	-3.37873000	0.30291600	0.78913500
C	-3.91039600	-2.04652800	-1.62539000
H	-2.41426600	-2.73341200	-3.02934400
H	-5.16697400	-1.16584300	-0.09680300
H	-4.69960500	-2.69060300	-2.02182100
N	0.42277600	0.50576300	-0.83561000
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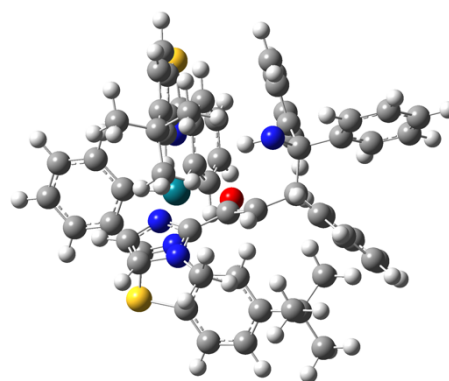
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C	2.94520800	0.60519400	0.67713200
N	3.10568500	0.82487800	1.97977100
H	4.81398000	1.47167800	3.11578100
H	6.07074100	1.47077300	0.63857200
C	4.39202400	0.69129700	-1.43444900
H	5.47659000	0.73901000	-1.58931400
H	4.03273600	-0.28161600	-1.79263100
H	3.91773600	1.49060500	-2.02025000
N	4.11663600	0.84663200	-0.01079000
C	1.67414800	0.18884400	0.07226300
C	1.28419100	0.41161700	-1.37978900
H	1.63082900	1.36942200	-1.79033100
H	1.70772700	-0.39133300	-2.00516000
C	-0.24937200	0.29514800	-1.30320200
H	-0.66394400	-0.16779400	-2.20474100



C	-0.95327200	1.62980000	-1.12627100
C	-0.41899200	2.67068900	-0.34749000
C	-2.20503400	1.83235700	-1.72990100
C	-1.11760400	3.86928600	-0.17277300
H	0.54909800	2.55197800	0.14284700
C	-2.90780700	3.02841500	-1.55797900
H	-2.64032900	1.03475200	-2.33785300
C	-2.36652700	4.05335400	-0.77510700
H	-0.68230700	4.66318400	0.43978000
H	-3.88102500	3.15955600	-2.03824200
H	-2.91239700	4.99027500	-0.63796400
C	-0.41327000	-0.67259400	-0.05762700
C	-0.29636900	-2.17139800	-0.41027800
C	-0.21949000	-3.08250400	0.66076200
C	-0.24738500	-2.67830900	-1.71513500
C	-0.09786200	-4.45301700	0.43405700
H	-0.25475000	-2.70053700	1.68286900
C	-0.12698000	-4.05627200	-1.94644300
H	-0.30795900	-2.01249300	-2.57634400
C	-0.05095700	-4.94833200	-0.87606200
H	-0.04133300	-5.14009500	1.28247700
H	-0.09411100	-4.42694100	-2.97422700
H	0.04219700	-6.02207000	-1.05746300
C	-1.71606100	-0.42862400	0.70235600
C	-1.73557200	0.32566800	1.88222000
C	-2.92910400	-0.91131200	0.18755900
C	-2.94437000	0.59848300	2.53257000
H	-0.79286500	0.69850700	2.28545300
C	-4.13759900	-0.63797400	0.83268900
H	-2.92711600	-1.50613000	-0.72927300
C	-4.14983400	0.12006900	2.00985100
H	-2.94238000	1.18939900	3.45246400
H	-5.07367500	-1.01923200	0.41616900
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N	0.76453000	-0.36742000	0.78481800

III-B)

Rh	-0.68814100	1.99335700	0.42760100
C	-0.07168700	2.44500300	2.28687200
C	1.07842500	3.14886600	2.67694200
C	-0.94700600	2.00899300	3.32108400
C	1.34307400	3.40481600	4.02926900
H	1.78336700	3.50530800	1.92190300
C	-0.69111700	2.27324500	4.67768400
C	0.45960700	2.97554300	5.03221700
H	2.25027700	3.94939600	4.30723700
H	-1.37908900	1.91881000	5.45060800
H	0.67445500	3.18402700	6.08279300
C	-1.74126200	3.69530300	0.49162600
C	-1.07828200	4.81780800	-0.08300100
C	-3.04310000	3.90014800	0.97511600
C	-1.68696600	6.08293100	-0.16374700
C	-3.65197100	5.15950100	0.89423000



H	-3.59935700	3.07388300	1.42254200
C	-2.97907400	6.25383000	0.32930500
H	-1.15323500	6.92531000	-0.61326600
H	-4.66763900	5.29099400	1.27862500
H	-3.46408700	7.23097300	0.27339500
C	-2.04797400	1.20793800	2.82982600
C	-3.89098700	-0.34573300	2.33209800
C	-3.10414100	0.02813900	1.22060900
C	-4.91973000	-1.28315000	2.19285300
C	-3.34389400	-0.55025200	-0.03485000
C	-5.13090900	-1.85226500	0.93943200
H	-5.53151800	-1.57668500	3.04794700
C	-4.34667300	-1.50857200	-0.19112800
H	-2.72035500	-0.23647800	-0.86131200
H	-5.92656100	-2.59272000	0.83960400
C	0.24554500	4.50452800	-0.58205400
C	2.49676400	4.24737500	-1.55765400
C	1.94140700	3.06904300	-1.00598300
C	3.76057800	4.22126600	-2.14945200
C	2.65132500	1.86430800	-1.04858200
C	4.44941200	3.00612700	-2.19360800
H	4.20216900	5.12458900	-2.57464200
C	3.91166100	1.81379800	-1.65531300
H	2.17637400	0.98769300	-0.61023100
H	5.43064000	2.99960600	-2.66712900
S	-3.32093800	0.47332200	3.77299200
S	1.37404900	5.58610400	-1.36707700
N	0.67821600	3.26170500	-0.46626800
N	-2.09840500	0.92985200	1.53575000
C	4.63059600	0.45526300	-1.75165200
C	4.70008700	-0.20197800	-0.35452200
H	5.23944600	-1.16091100	-0.41269700
H	5.23296900	0.44504600	0.36031200
H	3.69930500	-0.40801400	0.05378000
C	6.06387600	0.58973900	-2.29419100
H	6.54414900	-0.40073400	-2.32173000
H	6.07960400	0.99057000	-3.31959700
H	6.68063300	1.24473900	-1.65836400
C	3.82322900	-0.45604700	-2.70620000
H	2.80498900	-0.63701900	-2.32844900
H	3.74241900	0.00000800	-3.70616000
H	4.31542200	-1.43557300	-2.81326600
C	-4.61472400	-2.18501400	-1.54775500
C	-3.58170400	-1.76764000	-2.61074600
H	-3.60932800	-0.68605500	-2.81382400
H	-2.55741200	-2.03065500	-2.30533800
H	-3.79187300	-2.28705700	-3.55823400
C	-6.02135700	-1.77943600	-2.04228800
H	-6.80558400	-2.08498300	-1.33253900
H	-6.09000600	-0.68786900	-2.17540100
H	-6.23919500	-2.25761100	-3.01129600
C	-4.54528000	-3.72100100	-1.38561100
H	-3.55588100	-4.03526900	-1.01921400
H	-5.30394200	-4.09585800	-0.68208300

H	-4.72475000	-4.21094200	-2.35638400
C	0.08753800	-0.50601700	-1.05432900
C	0.33381000	-1.82060600	-1.33989600
H	-0.03963300	-2.22505400	-2.27679300
O	0.40703000	0.10755300	0.05512700
C	1.09307100	-2.78438600	-0.46378800
C	-0.63197800	0.35265600	-2.03425000
N	-0.80678600	0.25362100	-3.38669400
C	-1.83714100	2.07049700	-2.65715900
C	-1.57462800	1.33133800	-3.78633600
H	-2.39563100	2.99728700	-2.54958800
H	-1.85031900	1.47875800	-4.82712200
N	-1.24588100	1.45152100	-1.58995800
C	-0.26605000	-0.74687200	-4.29661300
H	0.76486900	-0.99042400	-4.01034600
H	-0.87132300	-1.66527700	-4.27916800
H	-0.27188700	-0.33643500	-5.31388500
H	1.83795800	-2.22093800	0.11053300
C	1.84326500	-3.76654400	-1.34946200
C	1.15937200	-4.66089400	-2.19051000
C	3.24489400	-3.77426100	-1.37152200
C	1.85640100	-5.53095800	-3.03205700
H	0.06679300	-4.68383000	-2.16718500
C	3.94919100	-4.64167400	-2.21425800
H	3.79339600	-3.08925000	-0.72137300
C	3.25702700	-5.52350400	-3.04974600
H	1.30457900	-6.22226400	-3.67471900
H	5.04239500	-4.62706400	-2.21534800
H	3.80350800	-6.20398500	-3.70787700
C	0.17257400	-3.54549900	0.63235000
N	-1.10199500	-3.80761800	0.01050300
H	-1.50384700	-2.87851900	-0.18502200
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C	0.90239100	-7.28558100	1.21458700
H	-0.69672300	-6.13872800	0.30911800
C	2.14012600	-7.23971600	1.86194600
H	3.70175400	-5.94496400	2.62273900
H	0.42628100	-8.24879700	1.01115800
H	2.63892800	-8.16285800	2.16836200
C	-0.05682800	-2.71531800	1.92045600
C	-1.17200900	-3.04732300	2.71318200
C	0.82891000	-1.74042800	2.39963800
C	-1.39158000	-2.42824200	3.94481200
H	-1.86862700	-3.81276300	2.36379800
C	0.61384000	-1.12387700	3.63622400
H	1.68408300	-1.42725500	1.80509600
C	-0.49253200	-1.46684100	4.41631200
H	-2.27157900	-2.69469400	4.53523600
H	1.30781000	-0.35362100	3.98121300
H	-0.66441200	-0.97201100	5.37496300