

Supporting Information for  
**MECHANISTIC STUDIES OF NICKEL(II)-CATALYZED DIRECT ALCOHOLYSIS  
OF 8-AMINOQUINOLINE AMIDES**

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## 1. Optimized Geometry and Energies for Each Structure (Schemes 3, 4 and 5)

### Detailed Information for Calculated Structures

#### 8-Aminoquinoline Amide 1b



B3LYP/6-31G(d) free energy: -609.803167 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.152461 (a.u.)

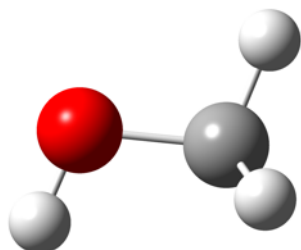
Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -609.6933463 (a.u.)

C	2.93496900	-0.25699900	-0.00000200
O	3.40963400	0.87106700	-0.00000400
C	3.82050800	-1.49506700	0.00000800
H	4.46875100	-1.46289800	-0.88128400
H	4.46859900	-1.46299500	0.88141600
H	3.26651400	-2.43853200	-0.00008500
N	1.58528900	-0.52364900	-0.00000700
C	0.51851600	0.37907100	-0.00000100
C	-0.78774900	-0.22045600	-0.00000200
C	0.63621600	1.75948100	-0.00000100
C	-1.94544600	0.61537000	0.00000000
C	-0.52424800	2.56821900	0.00000200
H	1.62144100	2.20418400	-0.00000200
C	-3.20488500	-0.03610200	0.00000200
C	-1.78932300	2.02536000	0.00000300
C	-2.05445400	-2.14327200	-0.00000300
H	-0.39979900	3.64769500	0.00000200
C	-3.26487500	-1.41088200	0.00000200
H	-4.11215800	0.56359300	0.00000500
H	-2.67227800	2.65901000	0.00000500
H	-2.07747900	-3.23218700	0.00000000

H	-4.21507200	-1.93607600	0.00000600
N	-0.86119000	-1.58055900	-0.00000300
H	1.27035100	-1.48921700	-0.00000900

### Methanol (2a)



B3LYP/6-31G(d) free energy: -115.685651 (a.u.)

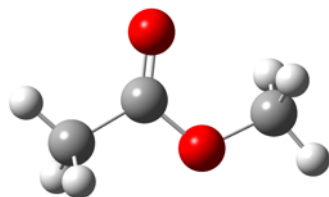
B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.028755 (a.u.)

Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -115.6970337 (a.u.)

C	0.66193200	-0.01951700	0.00000900
H	1.03668600	-0.54520800	-0.89236400
H	1.07993700	0.99092800	-0.00167000
H	1.03714500	-0.54248500	0.89380600
O	-0.74887000	0.12250300	0.00002000
H	-1.13439300	-0.76616200	0.00001500

### Methyl Acetate (3b)



B3LYP/6-31G(d) free energy: -268.328044 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.06044 (a.u.)

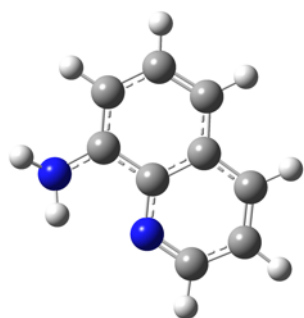
Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -268.3131699 (a.u.)

C	-0.46054500	0.17823200	-0.00004400
O	-0.28535100	1.37656000	-0.00000600
C	-1.80144200	-0.51808700	0.00001900

H	-1.89250400	-1.16110000	-0.88155300
H	-1.89289500	-1.15993600	0.88241600
H	-2.59713900	0.22744400	-0.00059600
O	0.54946100	-0.72395000	-0.00006500
C	1.87191000	-0.16317100	0.00004100
H	2.02927100	0.45330600	-0.88918900
H	2.02908600	0.45339900	0.88923800
H	2.55176200	-1.01583800	0.00015600

### 8-Aminoquinoline



B3LYP/6-31G(d) free energy: -457.169133 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.120416 (a.u.)

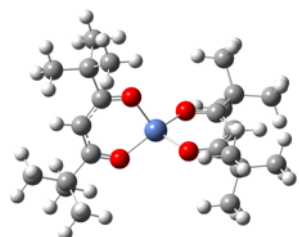
Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -457.0764285 (a.u.)

N	-1.66542200	-2.12126000	-0.08487900
C	-1.35110100	-0.77929200	-0.01339700
C	0.03983600	-0.40991400	-0.00603200
C	-2.30667800	0.22884700	0.00832500
C	0.40542700	0.97203200	-0.00839000
C	-1.92795900	1.58797100	0.01610900
H	-3.36150700	-0.03524600	0.00634100
C	1.79441500	1.26144400	-0.01129000
C	-0.60327100	1.96917900	0.00140800
C	2.23451100	-1.09953700	0.01710900
H	-2.70781800	2.34516100	0.02991400
C	2.70910800	0.23375800	-0.00269800
H	2.11951100	2.29945100	-0.01855000
H	-0.31971300	3.01806300	0.00094900

H	2.94170700	-1.92800600	0.03781100
H	3.77757900	0.42817300	-0.00476400
N	0.95440500	-1.41808100	0.01528900
H	-2.55323700	-2.40606900	0.30435300
H	-0.88513500	-2.73307200	0.12421000

### Ni(tmhd)<sub>2</sub>



B3LYP/6-31G(d) free energy: -2669.918063 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs the free energy: 0.50046 (a.u.)

Number of imaginary frequencies: 0

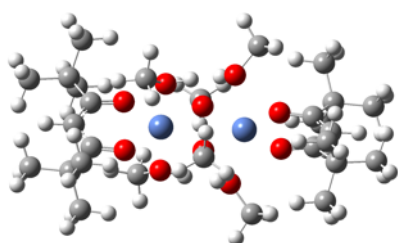
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2669.958852 (a.u.)

C	-2.40636500	1.09888500	0.76138200
C	-2.41802400	2.02237200	3.07713600
C	-2.64998400	3.55891700	1.08825400
C	-3.19558700	0.14016600	0.09812000
C	-2.69507400	-0.84326500	-0.77379300
C	-3.03535600	2.17787600	1.66772000
C	-3.62735000	-1.82436000	-1.51300400
C	-3.39544300	-1.63725400	-3.03057000
C	-5.11924500	-1.61903800	-1.20164600
C	-3.21594800	-3.25812800	-1.10431500
C	-4.56666600	2.08540000	1.77536800
Ni	0.00000300	-0.00013600	-0.31331200
O	-1.45044100	-1.00780100	-1.03235100
O	-1.13115200	1.17631300	0.67129200
O	1.45051700	1.00753400	-1.03221800
O	1.13117100	-1.17645700	0.67145500
C	2.69512700	0.84314500	-0.77348800
C	2.40635900	-1.09894300	0.76172100
C	3.19562100	-0.14021700	0.09850800

C	3.62740800	1.82435000	-1.51256100
C	3.03528600	-2.17773400	1.66833700
C	3.21602500	3.25801800	-1.10355000
C	5.11929500	1.61887900	-1.20128600
C	3.39547900	1.63760900	-3.03018300
C	2.64963900	-3.55895800	1.08949900
C	2.41811500	-2.02152700	3.07776100
C	4.56662300	-2.08547500	1.77576900
H	-2.68379600	1.05497700	3.52011500
H	-2.79230100	2.81140900	3.74007500
H	-1.32810900	2.09036500	3.03351900
H	-1.56457800	3.65704200	1.00638400
H	-3.08369200	3.70352000	0.09136300
H	-3.02619700	4.35723900	1.73886800
H	-3.99601500	-2.36091500	-3.59421100
H	-2.34266100	-1.78525600	-3.28430100
H	-3.68842800	-0.63104100	-3.35385600
H	-5.71298000	-2.35019800	-1.76217100
H	-5.33935100	-1.76322800	-0.13790300
H	-5.46530600	-0.62106100	-1.49332700
H	-3.81329700	-3.99240900	-1.65765800
H	-3.38157200	-3.42601700	-0.03335000
H	-2.15878400	-3.43481900	-1.31803900
H	-4.89078200	1.12840900	2.19952700
H	-4.93413500	2.87913600	2.43586900
H	-5.05483900	2.21491900	0.80289800
H	2.15887300	3.43477900	-1.31730300
H	3.38158000	3.42568300	-0.03253800
H	3.81340400	3.99242800	-1.65669400
H	5.46519700	0.62083100	-1.49290800
H	5.33951200	1.76313400	-0.13757500
H	5.71308200	2.34992100	-1.76191300
H	3.68848800	0.63148400	-3.35372000
H	2.34269400	1.78565200	-3.28384900
H	3.99605000	2.36142600	-3.59361900
H	3.02570000	-4.35705100	1.74048100

H	1.56421900	-3.65691700	1.00766700
H	3.08332900	-3.70409300	0.09267700
H	2.79240100	-2.81029300	3.74101900
H	1.32818700	-2.08947900	3.03428800
H	2.68399900	-1.05394400	3.52025000
H	4.93405800	-2.87918800	2.43631900
H	4.89094800	-1.12849200	2.19979400
H	5.05463700	-2.21516800	0.80324600
H	4.26185400	-0.18044400	0.24865900
H	-4.26183300	0.18043100	0.24816700

**[Ni(tmhd- $\kappa O, O'$ )( $\mu$ -OMe)(MeOH)<sub>2</sub>]<sub>2</sub> I**



B3LYP/6-31G(d) free energy: -4871.078764 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.77312 (a.u.)

Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -4871.295301 (a.u.)

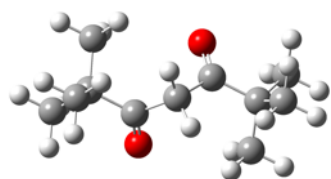
Ni	-1.54970000	0.00016700	0.00019600
Ni	1.62624700	0.00006600	-0.00051700
O	0.05566100	-1.28351800	-0.12633800
O	0.05573400	1.28379200	0.12622700
O	-2.94849700	1.41313000	0.13307900
O	-2.94831700	-1.41303100	-0.13248700
O	2.99927100	1.40636100	-0.15119200
O	2.99906800	-1.40639800	0.14935300
O	-1.47037500	0.17277000	-2.13568800
H	-0.52881900	0.21090600	-2.40541700
O	1.17877300	-0.49531900	-2.17697800
H	0.66434800	-1.16180300	-1.61308100
C	-5.02398500	-2.54163100	-0.38920000
C	-4.20868400	-1.24237400	-0.16106100

C	-4.85985200	-0.00006400	0.00018900
H	-5.93737300	-0.00010900	0.00010800
C	-4.20883600	1.24233300	0.16144400
C	-5.02433800	2.54152900	0.38931200
C	5.07295200	-2.53986900	0.39384900
C	4.26414000	-1.23912400	0.16719800
C	4.91421200	-0.00004500	0.00031600
H	5.99162200	-0.00002700	0.00097900
C	4.26432800	1.23903800	-0.16749600
C	5.07347100	2.53971600	-0.39352100
C	-2.27343900	1.02251400	-2.95146000
H	-2.04041800	2.08204200	-2.79285600
H	-2.14096000	0.77296900	-4.01184600
H	-3.31202400	0.84219200	-2.67188500
C	2.04760600	-1.13603600	-3.11124200
H	2.72005400	-1.83552100	-2.60408500
H	1.47063200	-1.67243400	-3.87535000
H	2.64219300	-0.35806100	-3.59624300
C	0.02198300	-2.56240400	0.46812600
H	0.89323900	-3.15833000	0.16310100
H	-0.89344800	-3.09333400	0.17696400
H	0.04312400	-2.49909700	1.56783300
C	0.02186600	2.56286900	-0.46776700
H	-0.89292300	3.09417000	-0.17524800
H	0.04146300	2.49991200	-1.56753400
H	0.89384700	3.15826500	-0.16377800
O	-1.46975600	-0.17256000	2.13622100
O	1.17965900	0.49522200	2.17621200
C	-2.27254400	-1.02260000	2.95196300
H	-2.14008800	-0.77311800	4.01236700
H	-2.03924900	-2.08204600	2.79323700
H	-3.31118200	-0.84250900	2.67243900
C	2.04859500	1.13579400	3.11040800
H	2.72010500	1.83635100	2.60347100
H	2.64423100	0.35790000	3.59425900
H	1.47175000	1.67099400	3.87546400

C	4.65322700	3.11064500	-1.76784000
H	3.57241500	3.26839200	-1.80800800
H	5.15503900	4.06869400	-1.94979200
H	4.93030600	2.42617400	-2.57902700
C	6.59882500	2.34250400	-0.37814800
H	6.95207200	1.95287900	0.58330300
H	6.93160300	1.66033700	-1.16831500
H	7.09452900	3.30603200	-0.54514300
C	4.68582100	3.54372300	0.71525300
H	4.98499800	3.17408600	1.70415600
H	5.18954900	4.50378500	0.55082400
H	3.60632800	3.71548100	0.72375800
C	6.59833400	-2.34273100	0.37993900
H	6.95249800	-1.95301800	-0.58113700
H	6.93039200	-1.66065700	1.17049100
H	7.09383700	-3.30629700	0.54730600
C	4.68629600	-3.54372400	-0.71541400
H	5.18983900	-4.50382200	-0.55063400
H	3.60680600	-3.71543500	-0.72494500
H	4.98640400	-3.17396600	-1.70399000
C	4.65137800	-3.11092800	1.76770400
H	3.57051800	-3.26861700	1.80684100
H	5.15295900	-4.06902800	1.95002300
H	4.92773500	-2.42656800	2.57923300
C	-4.65857500	3.53878500	-0.73248600
H	-5.15804200	4.50059100	-0.56376700
H	-3.57917800	3.70777100	-0.76409700
H	-4.97693000	3.16383200	-1.71328300
C	-6.54885100	2.33728800	0.39817500
H	-6.91512300	1.94187200	-0.55607800
H	-6.86579600	1.65615600	1.19577900
H	-7.04721500	3.29903600	0.56896800
C	-4.58755600	3.12559100	1.75237800
H	-5.08846200	4.08464100	1.93309600
H	-4.85165700	2.44738100	2.57306400
H	-3.50635300	3.28329700	1.77657800

C	-4.58697900	-3.12544000	-1.75230000
H	-3.50575500	-3.28302300	-1.77639400
H	-5.08775900	-4.08451900	-1.93322300
H	-4.85106000	-2.44713900	-2.57291900
C	-6.54852700	-2.33758800	-0.39818600
H	-6.91493200	-1.94233900	0.55608400
H	-6.86548600	-1.65639500	-1.19573300
H	-7.04675100	-3.29937800	-0.56915100
C	-4.65822800	-3.53902200	0.73249600
H	-5.15755700	-4.50085900	0.56355900
H	-3.57881400	-3.70786300	0.76421300
H	-4.97675600	-3.16425200	1.71330500
H	-0.52808600	-0.21086400	2.40548700
H	0.66486000	1.16171700	1.61261900

#### tmhd-H



B3LYP/6-31G(d) free energy: -581.423487 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.249055 (a.u.)

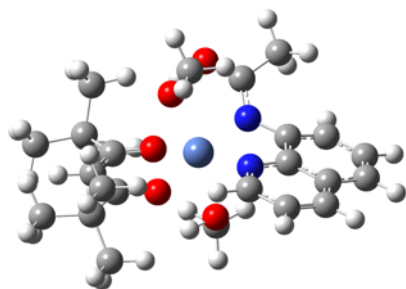
Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -581.4386049 (a.u.)

C	1.12771100	0.56651200	-0.01797800
C	-0.00000300	-0.00004100	0.86544700
H	-0.35003500	0.81345000	1.50644400
C	-1.12769100	-0.56647800	-0.01799700
C	-2.52240300	0.08074300	0.03572500
C	2.52239700	-0.08073600	0.03574000
O	-0.88563200	-1.52278600	-0.73056000
O	0.88562200	1.52283000	-0.73049500
C	-3.45444600	-0.64759500	-0.94575300
H	-3.54112800	-1.70982900	-0.69845900
H	-4.45436300	-0.20011800	-0.91263600

H	-3.07841500	-0.57893500	-1.97076200
C	-3.07708800	-0.05162700	1.47406300
H	-2.45692900	0.47034400	2.21096900
H	-4.08064200	0.38683200	1.52049600
H	-3.15674400	-1.10237500	1.77649400
C	-2.41832900	1.57379100	-0.35093600
H	-1.76667900	2.13842300	0.32240000
H	-2.02264900	1.69552100	-1.36389700
H	-3.41633000	2.02621600	-0.31338700
C	2.41823000	-1.57384300	-0.35069900
H	1.76744000	-2.13855900	0.32342000
H	2.02150000	-1.69578600	-1.36321900
H	3.41636300	-2.02606400	-0.31410500
C	3.07729300	0.05185300	1.47397100
H	4.08070300	-0.38692100	1.52040500
H	3.15729300	1.10266600	1.77607400
H	2.45704700	-0.46970100	2.21110300
C	3.45434100	0.64741400	-0.94598800
H	3.54087900	1.70973600	-0.69903000
H	4.45431200	0.20006800	-0.91276600
H	3.07830500	0.57836200	-1.97097500
H	0.35007000	-0.81362800	1.50630300

**[Ni(tmhd- $\kappa O, O'$ )(1b- $\kappa N, N'$ )(MeOH)<sub>2</sub>] II**



B3LYP/6-31G(d) free energy: -2929.644986 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.502812 (a.u.)

Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2929.640533 (a.u.)

N	1.70876600	-1.40420200	-0.29137800
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C	2.90923300	-0.84295700	0.12337300
C	2.95804500	0.59825400	0.02680400
C	4.03695400	-1.47130600	0.65031900
C	4.14456900	1.32261100	0.34041000
C	5.20356200	-0.74493100	0.98121400
H	4.02919600	-2.53960700	0.82325800
C	4.10895300	2.72983800	0.17107600
C	5.28133200	0.61940000	0.81500300
C	1.81069400	2.55147600	-0.49339900
H	6.05764600	-1.28977600	1.37553000
C	2.95310000	3.34410100	-0.25508200
H	5.00096500	3.31176400	0.39108200
H	6.18731200	1.16743600	1.05816900
H	0.86070300	2.99888900	-0.76901000
H	2.89920800	4.41987100	-0.38838600
Ni	0.18008100	-0.03838300	-0.12365200
N	1.81450600	1.23554000	-0.36260600
C	0.20754100	-0.08829700	-3.20944000
H	-0.17368200	-0.59589800	-4.10401000
H	0.02481900	0.98468300	-3.30994400
H	1.28892000	-0.25906200	-3.13206600
O	-0.48340500	-0.53846400	-2.04849800
H	-0.27770900	-1.51784700	-1.91462100
O	0.51564700	0.45201000	2.01279800
H	-0.28292800	1.00799100	2.01442700
C	0.42641400	-0.54024100	3.04186500
H	1.33150000	-1.14480500	2.96419800
H	0.39685500	-0.06666800	4.03080100
H	-0.44746500	-1.18251600	2.90022700
C	-2.37019800	1.43893200	0.06122100
C	-3.10197100	0.24994500	0.17572900
H	-4.17515100	0.31152300	0.10257800
C	-2.53222600	-1.02673800	0.40088300
C	-3.42291800	-2.28488000	0.53798300
C	-3.08190400	2.79850400	-0.14130800
O	-1.28686100	-1.24838000	0.50579200

O	-1.08895200	1.51782600	0.12803400
C	-3.09310900	-3.20275700	-0.66350500
H	-2.02309400	-3.42240100	-0.70676700
H	-3.64739100	-4.14582200	-0.57836400
H	-3.38069100	-2.72701000	-1.60894200
C	-3.03986800	-3.00543700	1.84948500
H	-3.26960400	-2.38464800	2.72516900
H	-3.60508100	-3.94025000	1.94500100
H	-1.97309700	-3.24141600	1.86263700
C	-4.93218700	-1.98846200	0.55194900
H	-5.21256800	-1.32506500	1.37853800
H	-5.26938700	-1.53134200	-0.38495900
H	-5.48814900	-2.92527800	0.67627900
C	-4.61761200	2.71099500	-0.12893600
H	-4.99817000	2.08306900	-0.94192100
H	-4.99557500	2.31164200	0.81879600
H	-5.04389800	3.71270700	-0.25984400
C	-2.62585700	3.36530400	-1.50555400
H	-3.06554100	4.35625100	-1.67217300
H	-1.53702100	3.45921700	-1.54527400
H	-2.94113600	2.71173900	-2.32744700
C	-2.62638500	3.75048300	0.98762400
H	-1.53687200	3.83651000	1.00937400
H	-3.05245800	4.74976500	0.83780600
H	-2.96167800	3.38756900	1.96734400
C	1.57949600	-2.57712000	-0.95002700
C	2.72353800	-3.56962700	-1.12141600
H	2.88804800	-4.14107700	-0.20027000
H	2.44094100	-4.26822200	-1.91056400
H	3.66709400	-3.07994600	-1.38105400
O	0.49167100	-2.88913400	-1.49601200

**II-TS**



B3LYP/6-31G(d) free energy: -2929.620075 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.496637 (a.u.)

Number of imaginary frequencies: 1 (-619.3423)

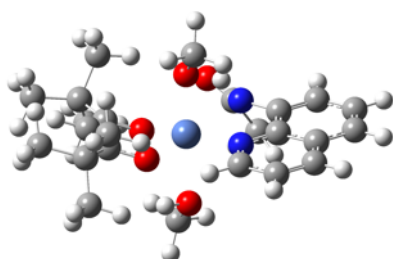
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2929.611178 (a.u.)

N	1.79313100	-1.46717000	-0.46136900
C	3.01502700	-0.78213900	-0.36682500
C	2.98359300	0.63372700	-0.12901900
C	4.25257200	-1.37953800	-0.56655400
C	4.19852900	1.38583900	-0.10810600
C	5.45215200	-0.63698200	-0.51687500
H	4.29491500	-2.44046900	-0.79038800
C	4.10057900	2.78228900	0.11468900
C	5.43649000	0.72212200	-0.30035300
C	1.72249400	2.54183300	0.29853200
H	6.39556700	-1.15223600	-0.67466400
C	2.86914200	3.36183400	0.31203400
H	5.00865500	3.38014300	0.12787400
H	6.35691200	1.29887300	-0.27851300
H	0.73122600	2.95207500	0.46578900
H	2.76456000	4.42814800	0.48339600
Ni	0.09545600	0.09324300	0.15578800
N	1.77465200	1.23567700	0.08929000
C	0.33109200	0.55111000	-2.83742800
H	0.43109400	0.01058200	-3.79212600
H	-0.49212000	1.27342500	-2.95695500
H	1.25846500	1.13646000	-2.69327600
O	0.06504800	-0.34175700	-1.79073000
H	1.07454900	-1.09584300	-1.32722500
O	0.17116700	0.40810600	2.36559300

H	-0.62744100	0.95944500	2.27120100
C	-0.07952200	-0.63883600	3.31149700
H	0.84397900	-1.21615600	3.38981600
H	-0.31762300	-0.21953500	4.29657700
H	-0.88551000	-1.29640700	2.97238300
C	-2.48221300	1.38632000	0.05500500
C	-3.09130100	0.14648700	-0.15602400
H	-4.11680200	0.14331900	-0.48736000
C	-2.47546300	-1.11449400	0.06790400
C	-3.23111600	-2.42899300	-0.21261900
C	-3.26887600	2.70619700	-0.11348500
O	-1.28569400	-1.25324000	0.48572600
O	-1.25255200	1.55006100	0.41902900
C	-2.72153100	-2.92722200	-1.59004900
H	-1.63721000	-3.06595100	-1.57374600
H	-3.19933700	-3.88453100	-1.83429900
H	-2.96542900	-2.21123500	-2.38316300
C	-2.85668800	-3.46806100	0.86494200
H	-3.18184800	-3.14403500	1.86219400
H	-3.35038600	-4.42205200	0.64567300
H	-1.77755000	-3.63186000	0.88449000
C	-4.76149200	-2.26746300	-0.25407900
H	-5.15200200	-1.83255100	0.67389200
H	-5.09110900	-1.64199000	-1.09076000
H	-5.22868400	-3.25059600	-0.38397800
C	-4.74487200	2.50966600	-0.49931600
H	-4.85050000	2.00129500	-1.46392300
H	-5.29088400	1.93236100	0.25492000
H	-5.23425100	3.48683200	-0.58705600
C	-2.57036200	3.53648400	-1.21489700
H	-3.06479800	4.50894700	-1.32775900
H	-1.51913900	3.70817900	-0.96872400
H	-2.61264500	3.02082700	-2.18149500
C	-3.20189000	3.47359600	1.22706200
H	-2.16498800	3.64245400	1.53001400
H	-3.69790500	4.44686300	1.13220000

H	-3.70735300	2.91621400	2.02547700
C	1.62447000	-2.79597600	-0.06512600
C	2.43571700	-3.31529500	1.12132400
H	3.00701800	-2.54508200	1.64419600
H	1.72981600	-3.78486700	1.81277800
H	3.12384400	-4.09985700	0.78821100
O	0.78683800	-3.51274200	-0.58919100

### III-H



B3LYP/6-31G(d) free energy: -2929.619138 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.498562 (a.u.)

Number of imaginary frequencies: 0

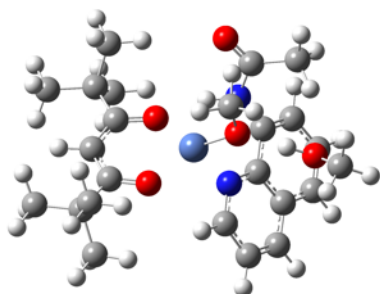
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2929.615274 (a.u.)

N	-1.91243900	1.51773900	-0.48248500
C	-3.09544800	0.75323200	-0.37910300
C	-2.99434600	-0.65761500	-0.14017400
C	-4.35397000	1.30470900	-0.55719400
C	-4.18295500	-1.45208400	-0.10031400
C	-5.52575100	0.52020300	-0.48589600
H	-4.43599600	2.36337100	-0.78061000
C	-4.03887200	-2.84441200	0.12253600
C	-5.44855100	-0.83593000	-0.27147800
C	-1.67010100	-2.52300700	0.27874300
H	-6.49080400	0.99830700	-0.62686800
C	-2.78757000	-3.38190600	0.30647200
H	-4.92754900	-3.47022200	0.14754100
H	-6.34414300	-1.44997100	-0.23377900
H	-0.66503300	-2.90187000	0.43765300
H	-2.64439600	-4.44357200	0.47836300

Ni	-0.06554000	-0.09427900	0.08125600
N	-1.76319300	-1.21946200	0.06633200
C	-0.24274900	-0.65172000	-2.82003000
H	-0.32314100	-0.16739400	-3.80844700
H	0.60577400	-1.35823000	-2.88347200
H	-1.15672000	-1.26870800	-2.69479500
O	-0.06260800	0.30034200	-1.81925600
H	-1.25985400	1.23539600	-1.28625900
O	-0.16117300	-0.38107000	2.33810400
H	0.63665300	-0.92985800	2.22234900
C	0.11336200	0.66238800	3.27901400
H	-0.80643300	1.24248400	3.38105600
H	0.37404700	0.24333100	4.25896600
H	0.91242400	1.32007800	2.92343600
C	2.52038600	-1.35816000	0.06864400
C	3.11884500	-0.11500800	-0.15360800
H	4.15034700	-0.10678500	-0.46512200
C	2.48563600	1.14301900	0.03641300
C	3.23244800	2.46445400	-0.23639000
C	3.32647300	-2.67083300	-0.05676000
O	1.28726100	1.27687700	0.43019400
O	1.28521200	-1.53073100	0.41105000
C	2.62810800	3.04001600	-1.54268700
H	1.55021200	3.18913300	-1.43923900
H	3.10082300	4.00301000	-1.77391900
H	2.79904200	2.36285400	-2.38714900
C	2.94819600	3.44319500	0.92330200
H	3.35374000	3.06705900	1.87168000
H	3.42073900	4.41084300	0.71760200
H	1.87368900	3.59960500	1.03956900
C	4.75321200	2.30000600	-0.40135100
H	5.21412900	1.83929100	0.48069100
H	5.01025900	1.69602300	-1.27847500
H	5.21380200	3.28497900	-0.54064600
C	4.80651700	-2.46343500	-0.42089600
H	4.92264300	-1.97406100	-1.39405600

H	5.33217300	-1.86373800	0.33035300
H	5.30929500	-3.43596700	-0.47948800
C	2.65889800	-3.53475500	-1.15145200
H	3.16966300	-4.50178300	-1.23456600
H	1.60628900	-3.71701200	-0.91939400
H	2.70903900	-3.03919500	-2.12794400
C	3.24559300	-3.40910900	1.29939300
H	2.20576500	-3.58583100	1.58758200
H	3.75629200	-4.37726100	1.23499300
H	3.72898300	-2.82734600	2.09408600
C	-1.76698000	2.82838300	-0.02077200
C	-2.59178800	3.25852600	1.18806000
H	-3.06801200	2.43020600	1.71751600
H	-1.91827000	3.79317400	1.86331800
H	-3.36708500	3.96871000	0.88012100
O	-0.95061800	3.58481700	-0.51778700

#### IV-H



B3LYP/6-31G(d) free energy: -2929.628806 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.498149 (a.u.)

Number of imaginary frequencies: 0

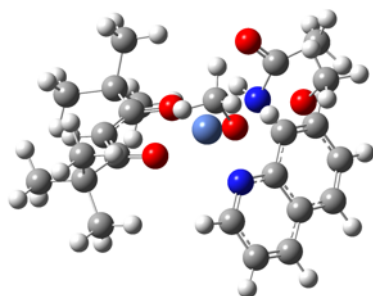
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2929.61216 (a.u.)

C	1.97975200	2.23106400	1.34163000
O	1.11575700	2.84802400	1.95155700
C	3.34799600	1.94756400	1.92850800
H	3.31987600	2.24940500	2.97670900
H	3.60136200	0.88395000	1.84752600
H	4.12911300	2.52542500	1.42291400
O	3.42184200	-1.41545100	1.54443800

N	1.70047200	1.74267200	0.07047900
C	2.55957200	1.02743700	-0.79093000
C	2.24253600	-0.30541200	-1.21752700
C	3.71780000	1.62236100	-1.26002600
C	3.14006300	-0.96844200	-2.11745900
C	4.61161300	0.95042300	-2.11952600
H	3.92574800	2.64483900	-0.96260800
C	2.81483000	-2.27670400	-2.54763800
C	4.32506000	-0.32179500	-2.55021500
C	0.84587300	-2.17075300	-1.20129200
H	5.51316200	1.45599000	-2.45266500
C	1.66640400	-2.87934500	-2.09653300
H	3.48674400	-2.78876900	-3.23184900
H	4.99336600	-0.85017300	-3.22463800
H	-0.06414800	-2.62146700	-0.81712100
H	1.38716900	-3.88139500	-2.40402800
Ni	-0.23994700	-0.37657500	0.64968500
C	3.92338500	-2.37186700	2.45112400
H	4.94890100	-2.61787100	2.15163300
H	3.95869100	-2.00209200	3.48988800
H	3.33946100	-3.30741500	2.44851800
N	1.10989800	-0.94138600	-0.77441800
H	0.72203700	1.85410700	-0.19355700
C	0.43676100	-0.51325000	3.38758500
H	0.60945100	0.53292000	3.68435300
H	-0.63932700	-0.72341300	3.51849900
H	0.97511300	-1.15908100	4.09928900
O	0.87448300	-0.75827300	2.07062700
H	2.48481400	-1.20173100	1.80141700
C	-3.27640900	0.35516300	-0.37207000
H	-4.29069600	0.60919700	-0.63175100
C	-3.00008600	-0.98275000	-0.03412100
C	-2.32263600	1.38810600	-0.37351600
C	-2.69204700	2.84593200	-0.70703000
C	-4.10507700	-2.06107700	-0.04580400
O	-1.84593900	-1.41757900	0.31372400

O	-1.08593600	1.20744300	-0.08923600
C	-4.20859700	-2.63934800	1.38489100
H	-4.94252100	-3.45352300	1.40949400
H	-3.24323900	-3.02911600	1.71796500
H	-4.53263200	-1.87168400	2.09774900
C	-5.48400500	-1.53447500	-0.47825500
H	-5.85662600	-0.75787400	0.19878100
H	-5.46670400	-1.12627100	-1.49504800
H	-6.20887600	-2.35644900	-0.46531800
C	-3.66565400	-3.17910800	-1.01914500
H	-4.40657800	-3.98708100	-1.02212300
H	-3.57673300	-2.79953600	-2.04434900
H	-2.70055800	-3.59770200	-0.72164500
C	-2.34622500	3.70571000	0.53378000
H	-1.30340000	3.57567800	0.83593100
H	-2.52040200	4.76519000	0.31085900
H	-2.98190700	3.43390100	1.38526100
C	-1.82679800	3.29908800	-1.90623600
H	-2.04449200	4.34593800	-2.14728600
H	-0.76057400	3.21736700	-1.67984400
H	-2.03663200	2.69635800	-2.79829600
C	-4.17599500	3.03963100	-1.06234300
H	-4.46586500	2.46276000	-1.94819500
H	-4.83480300	2.75552300	-0.23434100
H	-4.36270700	4.09695200	-1.28170700

#### IV-H-TS



B3LYP/6-31G(d) free energy: -2929.601558 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.499735 (a.u.)

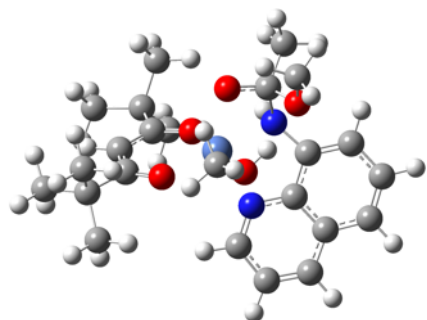
Number of imaginary frequencies: 1 (-473.4697)

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2929.592263 (a.u.)

C	2.24267100	1.19881700	1.86610700
O	1.36034700	1.33619500	2.70385400
C	3.60232800	1.85082500	2.03994800
H	3.87682100	1.78407200	3.09452700
H	4.38066600	1.38865000	1.43407000
H	3.52224500	2.91651200	1.78458000
O	2.91619500	-0.69140100	1.90619300
N	1.71253900	1.03171000	0.45885900
C	2.54464100	0.67631000	-0.66192500
C	2.16228100	-0.49455700	-1.38256300
C	3.62819700	1.40166400	-1.11457900
C	2.94763100	-0.95969400	-2.47753600
C	4.40057000	0.95543200	-2.21458500
H	3.90326500	2.32548300	-0.61789500
C	2.52563100	-2.14791900	-3.12587500
C	4.08488000	-0.21012500	-2.87338900
C	0.64094300	-2.23303300	-1.64034000
H	5.25548500	1.54579400	-2.53135100
C	1.38418200	-2.78980500	-2.70347300
H	3.11073600	-2.53653200	-3.95571300
H	4.68647200	-0.56050400	-3.70780100
H	-0.28074200	-2.68807800	-1.29141200
H	1.03864800	-3.70187300	-3.17860700
Ni	-0.01311400	-0.25678400	0.49600800
C	3.54688500	-1.00922000	3.12279400
H	4.61865700	-0.76341000	3.08384600
H	3.10151100	-0.46744500	3.97492500
H	3.46222800	-2.08676300	3.33247000
N	1.01133600	-1.13080900	-1.01262700
H	1.18718200	1.88669200	0.26373400
C	0.02096400	-1.63303600	3.04412700
H	0.13738100	-0.69974100	3.61154600
H	-1.04732000	-1.82114700	2.88543300
H	0.42277000	-2.46228800	3.64453600

O	0.68036900	-1.57179800	1.79000700
H	1.79773700	-1.19959600	1.90328000
C	-3.12874400	0.56794600	-0.34338000
H	-4.13901400	0.83445100	-0.60577300
C	-2.87722100	-0.77060400	0.02480600
C	-2.16031900	1.58405600	-0.35896900
C	-2.53022000	3.04413100	-0.70585600
C	-4.01983200	-1.81504200	0.05584400
O	-1.73937500	-1.22540900	0.37388800
O	-0.92198600	1.40445900	-0.08590300
C	-4.18656200	-2.27587700	1.52245900
H	-4.95637700	-3.05422500	1.58895100
H	-3.24829100	-2.68086100	1.91088900
H	-4.49303800	-1.44224800	2.16560000
C	-5.36788600	-1.28384500	-0.46101800
H	-5.74878300	-0.46196100	0.15516700
H	-5.29958300	-0.93369400	-1.49729300
H	-6.11333400	-2.08713500	-0.43160500
C	-3.59025100	-3.02046200	-0.80993900
H	-4.35538600	-3.80492900	-0.77201600
H	-3.46123600	-2.72797200	-1.85960100
H	-2.64771500	-3.43956100	-0.44815800
C	-2.19297800	3.91467600	0.52709800
H	-1.14582400	3.79546200	0.81703800
H	-2.37673000	4.97261300	0.30431500
H	-2.81447500	3.63694000	1.38651900
C	-1.65726800	3.48522200	-1.90272500
H	-1.84279400	4.54000800	-2.13782900
H	-0.59469400	3.36163400	-1.67790200
H	-1.88709900	2.89445200	-2.79783600
C	-4.01150600	3.24353000	-1.06925000
H	-4.30077500	2.65397100	-1.94657700
H	-4.67561800	2.97564700	-0.24014700
H	-4.19141900	4.29852300	-1.30675400

**V-H**



B3LYP/6-31G(d) free energy: -2929.613124 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.506006 (a.u.)

Number of imaginary frequencies: 0

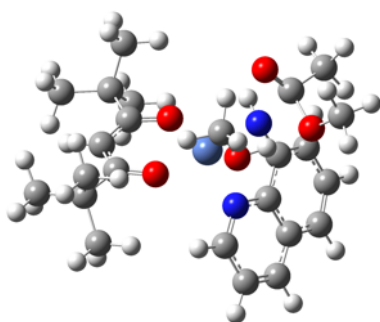
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2929.610005 (a.u.)

C	1.60681600	1.39496800	1.81606300
O	0.38911000	1.03888700	2.15006300
C	1.98628300	2.83521100	2.17745300
H	1.81895200	3.00805800	3.24437800
H	3.03026200	3.06561700	1.93658000
H	1.33181700	3.52330100	1.63251000
O	2.66249300	0.46711700	2.32401800
N	1.71375800	1.14795600	0.30051100
C	2.78699100	0.56347500	-0.43394200
C	2.40909600	-0.50616900	-1.30879800
C	4.10920200	0.95396100	-0.38331400
C	3.38417500	-1.11396300	-2.15395800
C	5.08041900	0.33019300	-1.20188200
H	4.40297400	1.74907100	0.29337400
C	2.94429400	-2.15248600	-3.01452700
C	4.72971600	-0.66985500	-2.08155800
C	0.74065200	-1.91290100	-2.08940500
H	6.11331000	0.66133400	-1.14095400
C	1.62693000	-2.54693200	-2.99067500
H	3.65949800	-2.63083900	-3.67942000
H	5.47534200	-1.13547200	-2.72082100
H	-0.29653000	-2.22882400	-2.01251700
H	1.26196500	-3.34143500	-3.63350200
Ni	0.06618200	-0.11217600	0.40816200

C	2.76003200	0.45155900	3.74380500
H	3.32041700	1.31959300	4.11604300
H	1.76528000	0.43779500	4.20412700
H	3.30536900	-0.45606800	4.01975700
N	1.10732700	-0.93318700	-1.28554000
H	1.28721300	1.93203400	-0.19062500
C	0.42574500	-2.20079600	2.59882300
H	-0.01664000	-1.40527900	3.20733500
H	-0.36881800	-2.81700800	2.17980400
H	1.08492700	-2.82551500	3.21545800
O	1.15302900	-1.64730400	1.49624000
H	1.83534600	-1.03512800	1.86826400
C	-3.10434300	0.34396700	-0.37280200
H	-4.15055500	0.51706700	-0.56202900
C	-2.74423900	-0.89185700	0.19624200
C	-2.20250600	1.36950100	-0.72458300
C	-2.70694000	2.69229700	-1.35388100
C	-3.82178000	-1.96006700	0.51270300
O	-1.55505000	-1.24593900	0.49671500
O	-0.94068200	1.30686700	-0.57450600
C	-3.82765300	-2.17615500	2.04352100
H	-4.53872900	-2.96677600	2.31310500
H	-2.83564100	-2.46387500	2.40095900
H	-4.12442600	-1.26022400	2.56820000
C	-5.24124400	-1.57778300	0.05926000
H	-5.60674400	-0.67960000	0.56907500
H	-5.29188800	-1.40376300	-1.02149000
H	-5.93418200	-2.39395400	0.29628600
C	-3.41118200	-3.27341900	-0.19005600
H	-4.10898700	-4.07851800	0.07021500
H	-3.42685000	-3.15642900	-1.28116400
H	-2.40364400	-3.57497800	0.10713700
C	-2.28637200	3.84384000	-0.41238400
H	-1.20576600	3.83545100	-0.24763500
H	-2.56768300	4.81128200	-0.84618500
H	-2.77662100	3.75328200	0.56400800

C	-2.00617100	2.86364900	-2.72035100
H	-2.28086700	3.82534700	-3.17057000
H	-0.91960100	2.82939000	-2.60634600
H	-2.30089100	2.06890100	-3.41667000
C	-4.22973400	2.75003000	-1.56302100
H	-4.58053300	1.96035900	-2.23702300
H	-4.77579500	2.66227100	-0.61723300
H	-4.50228600	3.71242400	-2.01242300

### V-H-TS



B3LYP/6-31G(d) free energy: -2929.604002 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.503988 (a.u.)

Number of imaginary frequencies: 1 (-144.0497)

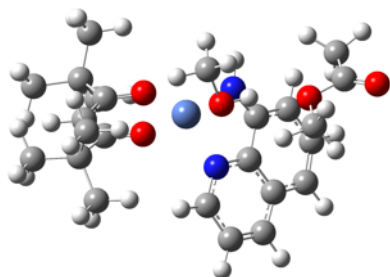
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2929.595216 (a.u.)

C	2.48915400	1.04790300	2.04404800
O	1.56925800	1.21983200	2.85151400
C	3.60735900	2.08007000	1.91428400
H	4.12052800	2.15843800	2.87962000
H	4.34060000	1.81822900	1.14909400
H	3.17583800	3.06214900	1.69904100
O	3.06074500	-0.32731900	1.95921100
N	1.70187000	1.01115800	0.35324600
C	2.45219500	0.67172000	-0.78936400
C	2.13614900	-0.58058100	-1.41052500
C	3.46523700	1.42724300	-1.36707000
C	2.91344100	-1.09459300	-2.48905400
C	4.22017300	0.93531100	-2.45593200
H	3.69230900	2.41069700	-0.96737700

C	2.53479000	-2.35680200	-3.01303300
C	3.98098500	-0.31085300	-2.99530100
C	0.67810100	-2.39170300	-1.48755500
H	5.01487600	1.55494300	-2.86309700
C	1.43263200	-3.00995500	-2.50749600
H	3.11707000	-2.79221000	-3.82167400
H	4.58049400	-0.69134700	-3.81765300
H	-0.22561200	-2.84496300	-1.09265200
H	1.12098500	-3.97467900	-2.89447900
Ni	0.00613300	-0.15201500	0.43171500
C	3.80633900	-0.68251900	3.12219300
H	4.78490200	-0.18443500	3.13658500
H	3.25815000	-0.42636200	4.03721800
H	3.96804600	-1.76365600	3.08294200
N	1.01705700	-1.22505800	-0.96549600
H	1.42733800	1.99233700	0.32076100
C	-0.00913900	-1.48783300	3.13178800
H	0.13228400	-0.52737800	3.63444300
H	-1.06610000	-1.66310100	2.92851100
H	0.37309400	-2.30233100	3.75975000
O	0.66702400	-1.48942000	1.86602800
H	1.59952900	-1.16655100	1.99913300
C	-3.16414700	0.51067600	-0.34091600
H	-4.18481000	0.71975000	-0.61502500
C	-2.85239900	-0.79224800	0.09294500
C	-2.23956800	1.56837600	-0.39917400
C	-2.67468200	2.99616100	-0.80106300
C	-3.94745300	-1.88371500	0.18292100
O	-1.69242200	-1.17522800	0.46249700
O	-0.99602900	1.45633700	-0.12498900
C	-4.09898000	-2.27318600	1.67141100
H	-4.84262100	-3.07198300	1.77991300
H	-3.14877000	-2.62924600	2.07872100
H	-4.43213400	-1.41813200	2.27171400
C	-5.31678800	-1.44037300	-0.36058400
H	-5.73494200	-0.60514200	0.21186600

H	-5.26106900	-1.14159900	-1.41341700
H	-6.02607900	-2.27329800	-0.28974700
C	-3.46609100	-3.11435500	-0.61744100
H	-4.19802400	-3.92705100	-0.53875000
H	-3.34542200	-2.87244200	-1.68065700
H	-2.50794700	-3.47452900	-0.23376500
C	-2.35853700	3.93011000	0.39017800
H	-1.30336800	3.86412800	0.66725200
H	-2.58834100	4.96949000	0.12640500
H	-2.95763800	3.66407800	1.26925100
C	-1.83006200	3.42007000	-2.02434300
H	-2.05678200	4.45714400	-2.29928400
H	-0.76238300	3.34230500	-1.80425200
H	-2.04685000	2.78582700	-2.89262300
C	-4.16647300	3.11978200	-1.15435000
H	-4.43992500	2.48520700	-2.00502900
H	-4.81079900	2.85729200	-0.30786700
H	-4.39267500	4.15629800	-1.43065900

## VI-H



B3LYP/6-31G(d) free energy: -2929.644748 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.494598 (a.u.)

Number of imaginary frequencies: 0

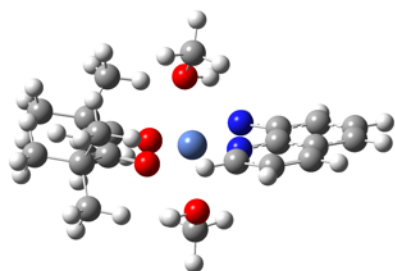
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2929.617013 (a.u.)

C	4.91537800	1.29196300	-1.64037500
O	6.00085500	1.81184100	-1.52817100
C	4.60992900	0.01999300	-2.38702500
H	4.49182800	-0.79835800	-1.66644600
H	3.67041200	0.10154000	-2.93983100

H	5.43576600	-0.20764300	-3.06237000
O	3.79402700	1.80299900	-1.05302000
N	1.23218100	-1.06310500	-1.08543900
C	1.98201000	-1.66485500	-0.13934300
C	1.75922800	-1.22377800	1.22472700
C	2.96863600	-2.65677900	-0.31136400
C	2.54689500	-1.70230100	2.31415500
C	3.72755900	-3.13032700	0.77251200
H	3.14012200	-3.06160700	-1.30650200
C	2.23790000	-1.17436900	3.59463400
C	3.55365600	-2.66654800	2.06679500
C	0.46364400	0.12211300	2.61839100
H	4.48324900	-3.88896600	0.57951600
C	1.21158900	-0.26609600	3.74732100
H	2.81827000	-1.50130000	4.45449700
H	4.15885900	-3.03939900	2.88754800
H	-0.36733300	0.81659300	2.69374600
H	0.96311700	0.14351900	4.72146400
Ni	-0.24864700	0.03036300	-0.33065200
C	3.99982400	2.97777300	-0.24248400
H	4.69667500	2.75871100	0.56985300
H	4.40289300	3.79228700	-0.84939400
H	3.01469400	3.23016500	0.14878700
N	0.73306800	-0.34549600	1.40583200
H	1.27053500	-1.54309800	-1.98052800
C	0.51339400	2.43814300	-1.99540000
H	0.43052600	1.75539000	-2.85187400
H	-0.46925700	2.85311000	-1.76918600
H	1.20317000	3.25123600	-2.24928900
O	0.95016400	1.75208900	-0.81951100
H	1.82460600	1.35324600	-1.00280900
C	-3.55546700	0.02712600	-0.11847700
H	-4.62666300	0.00558900	-0.00415900
C	-2.87121600	1.18237600	0.30120000
C	-2.93610100	-1.08275600	-0.72506600
C	-3.76212700	-2.28453500	-1.23751400

C	-3.63196200	2.39612300	0.88670100
O	-1.60551500	1.34333200	0.22276700
O	-1.67774900	-1.19328200	-0.91453900
C	-3.35987100	3.60898600	-0.03234700
H	-3.84480000	4.50621600	0.37061700
H	-2.28647400	3.80179000	-0.11111400
H	-3.75567000	3.43669900	-1.04072800
C	-5.15114600	2.18511700	1.00206400
H	-5.61619700	2.01268400	0.02510600
H	-5.39811400	1.33979900	1.65405600
H	-5.61397500	3.08047300	1.43329600
C	-3.05559400	2.68409700	2.29159800
H	-3.53053000	3.57413400	2.72144700
H	-3.23878400	1.84398500	2.97292100
H	-1.97745700	2.85787200	2.23875600
C	-3.48208600	-2.43295000	-2.75070100
H	-2.41055800	-2.54198800	-2.93631000
H	-3.99799400	-3.31647200	-3.14527400
H	-3.84026600	-1.55741400	-3.30618400
C	-3.25737600	-3.54527100	-0.49810300
H	-3.76758000	-4.43726700	-0.88110700
H	-2.18053800	-3.67000000	-0.63693400
H	-3.45819900	-3.47804100	0.57805400
C	-5.27759100	-2.14300800	-1.01741600
H	-5.53082100	-2.05668300	0.04529200
H	-5.68836900	-1.27220800	-1.54090100
H	-5.78864100	-3.03179900	-1.40561500

## VII-H



B3LYP/6-31G(d) free energy: -2777.012362 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.466162 (a.u.)

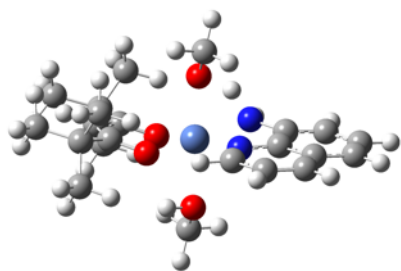
Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2777.014514 (a.u.)

N	1.57940200	-1.82055900	-0.24200800
C	2.88590800	-1.45983400	-0.16053000
C	3.14598100	-0.03779500	-0.07096400
C	4.01189500	-2.29860800	-0.17291000
C	4.47567700	0.48144700	-0.04902900
C	5.31656500	-1.77581200	-0.14171800
H	3.86529900	-3.37535200	-0.22144600
C	4.60306900	1.89219400	0.02970400
C	5.57061300	-0.41582900	-0.09198500
C	2.20794600	2.08375300	0.09623800
H	6.15256400	-2.47179000	-0.16280800
C	3.48101100	2.68961400	0.09859600
H	5.59745500	2.33307700	0.04137300
H	6.58564600	-0.02994900	-0.07461600
H	1.29638000	2.66817600	0.17695600
H	3.56115000	3.77039900	0.16407900
Ni	0.28674200	-0.31540900	0.15028800
N	2.05070500	0.77018200	0.01185800
H	1.43870300	-2.82247200	-0.13849500
C	0.54197900	0.35392000	-3.03709500
H	0.61214500	-0.14346200	-4.01309400
H	-0.18677400	1.16464000	-3.10952200
H	1.51927100	0.77816700	-2.77657500
O	0.06854900	-0.54999400	-2.04113700
H	0.74578900	-1.24982300	-1.86237400
O	0.40817600	-0.10919700	2.29001600
H	-0.29216900	0.56232500	2.35711100
C	0.10756100	-1.22091100	3.14283200
H	0.90994100	-1.94438200	2.99302300
H	0.09706500	-0.90647300	4.19306200
H	-0.84715100	-1.68320000	2.87346500
C	-2.12518400	1.37157200	0.11802300

C	-2.94333200	0.25311700	-0.10059500
H	-3.97656900	0.43259100	-0.34723500
C	-2.52376000	-1.09434100	0.00869800
C	-3.52341700	-2.25656600	-0.21157000
C	-2.70003600	2.80721600	0.04157700
O	-1.34384500	-1.46276300	0.30077600
O	-0.87494800	1.31785400	0.40268800
C	-2.99144700	-3.10302000	-1.39090800
H	-1.97839400	-3.45789600	-1.18537600
H	-3.64144600	-3.97076600	-1.55733300
H	-2.96302700	-2.51549600	-2.31594400
C	-3.53783700	-3.11859600	1.07079700
H	-3.92593400	-2.54982300	1.92519700
H	-4.18208700	-3.99503800	0.93138100
H	-2.53001100	-3.46352600	1.31621000
C	-4.95925900	-1.80353800	-0.52622400
H	-5.38902500	-1.20769400	0.28705300
H	-5.00962800	-1.21375600	-1.44829000
H	-5.59929700	-2.68308400	-0.66370100
C	-4.21588000	2.86528800	-0.21357800
H	-4.48704700	2.41612300	-1.17533800
H	-4.78215100	2.35653700	0.57449400
H	-4.54485900	3.91098400	-0.23527700
C	-1.97157400	3.54310100	-1.10661400
H	-2.30192200	4.58757800	-1.15957700
H	-0.88879600	3.52954400	-0.95532000
H	-2.18758600	3.07245500	-2.07355900
C	-2.39186300	3.51543700	1.38029900
H	-1.31967900	3.49988600	1.59260300
H	-2.72390800	4.55978400	1.34318700
H	-2.91462500	3.02774900	2.21266900

## VII-H-TS



B3LYP/6-31G(d) free energy: -2777.003683 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.463006 (a.u.)

Number of imaginary frequencies: 1 (-848.3130)

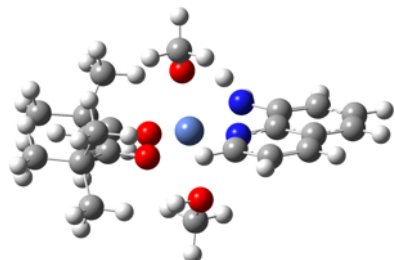
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2777.000033 (a.u.)

N	1.64584500	-1.86573200	-0.44107300
C	2.95917900	-1.44512800	-0.27244500
C	3.15844800	-0.03303500	-0.10047500
C	4.08319400	-2.26226500	-0.25902400
C	4.47191200	0.51228400	0.00397500
C	5.38037400	-1.72102600	-0.12603300
H	3.95889000	-3.33639400	-0.37321100
C	4.57339800	1.91998400	0.14166300
C	5.58841500	-0.36229400	-0.01471100
C	2.17440500	2.05645200	0.13069800
H	6.23106900	-2.39769700	-0.12904200
C	3.43363800	2.69037800	0.19479100
H	5.55810400	2.37629600	0.21089900
H	6.59063300	0.04857000	0.06791900
H	1.24960700	2.61952100	0.21244700
H	3.48574900	3.76919500	0.30186500
Ni	0.25420300	-0.29207600	0.08376100
N	2.04099100	0.74786100	-0.01044600
H	1.53354100	-2.87177600	-0.34481000
C	0.51489000	0.23324600	-2.93227300
H	0.56716100	-0.27657700	-3.90844800
H	-0.23000000	1.03914700	-3.02672900
H	1.49481500	0.71428200	-2.76039200
O	0.15085600	-0.66344100	-1.91794200
H	1.07855900	-1.44049100	-1.41883200

O	0.42128500	-0.01200100	2.26802600
H	-0.27159300	0.67199000	2.23664000
C	0.05187200	-1.03375700	3.20016600
H	0.85270600	-1.77520000	3.17977300
H	-0.02504100	-0.62234400	4.21410800
H	-0.88808100	-1.51534200	2.91348100
C	-2.14425000	1.36555200	0.06984500
C	-2.94160400	0.22903700	-0.11940100
H	-3.97197800	0.38548600	-0.39202300
C	-2.51169300	-1.10970800	0.05561500
C	-3.49941200	-2.28830400	-0.12190300
C	-2.73758000	2.78846700	-0.06158900
O	-1.33379400	-1.45296800	0.38252300
O	-0.89535300	1.34022000	0.37665200
C	-2.95189600	-3.17436800	-1.26476300
H	-1.93716600	-3.51141700	-1.03937700
H	-3.59433000	-4.05300100	-1.40179500
H	-2.91870900	-2.62168800	-2.21033000
C	-3.51338300	-3.09918700	1.19332600
H	-3.91215200	-2.50148100	2.02280100
H	-4.14839000	-3.98662900	1.08435300
H	-2.50389600	-3.42457100	1.45785600
C	-4.93757600	-1.86176300	-0.46190600
H	-5.37674500	-1.23559000	0.32319300
H	-4.98826000	-1.31280100	-1.40871500
H	-5.56896000	-2.75224900	-0.56482200
C	-4.24762600	2.81518000	-0.35365000
H	-4.48840100	2.33132400	-1.30653700
H	-4.82544400	2.32359000	0.43697700
H	-4.59080500	3.85459900	-0.41710400
C	-1.99337600	3.50225100	-1.21373800
H	-2.34220600	4.53795400	-1.30694700
H	-0.91481100	3.51394900	-1.03553800
H	-2.17307800	2.99684200	-2.16993600
C	-2.47265000	3.53948300	1.26314900
H	-1.40557700	3.54843900	1.50071200

H	-2.82010700	4.57674800	1.18772300
H	-3.00668400	3.06720500	2.09721200

### VIII-H



B3LYP/6-31G(d) free energy: -2777.002432 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.466036 (a.u.)

Number of imaginary frequencies: 0

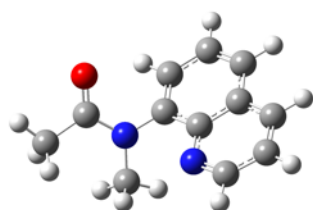
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2777.00714 (a.u.)

N	1.71992700	-1.92212400	-0.47897100
C	3.02791300	-1.45333900	-0.26643200
C	3.18360000	-0.03789700	-0.12173900
C	4.15164700	-2.25518800	-0.17402400
C	4.48275600	0.52942800	0.02984900
C	5.43502600	-1.69269600	0.01598100
H	4.04673000	-3.33291400	-0.27148000
C	4.56262200	1.94165100	0.13021500
C	5.61081200	-0.32908200	0.09512100
C	2.16473800	2.03959300	0.01168500
H	6.29435100	-2.35477300	0.07729900
C	3.41166400	2.69520000	0.10851600
H	5.53745000	2.41269400	0.23111300
H	6.60071000	0.10210400	0.21603100
H	1.23031100	2.59149800	0.04514900
H	3.44312500	3.77730200	0.18494600
Ni	0.25271600	-0.30300300	-0.03166200
N	2.05148600	0.72693900	-0.09764100
H	1.62360900	-2.92547700	-0.35004000
C	0.28784500	0.38473000	-2.92308100
H	0.30592400	-0.04125300	-3.94276300

H	-0.53887300	1.12069800	-2.90834100
H	1.22638900	0.96710300	-2.81068300
O	0.12779200	-0.61362500	-1.96888700
H	1.29028700	-1.60893700	-1.40469100
O	0.47786700	-0.01500200	2.20198200
H	-0.20201700	0.67929900	2.12239100
C	0.05831900	-0.98926100	3.16053600
H	0.84273600	-1.74811400	3.19806000
H	-0.04317000	-0.53879200	4.15618700
H	-0.88205100	-1.46460700	2.86399000
C	-2.14536000	1.34936700	0.09585500
C	-2.94320400	0.21178400	-0.07968200
H	-3.98468200	0.36745300	-0.30666800
C	-2.50278800	-1.12870700	0.05937700
C	-3.49389900	-2.30714400	-0.10138100
C	-2.75549600	2.76994100	0.03108600
O	-1.31443300	-1.47243300	0.34201600
O	-0.88192600	1.32730500	0.34108100
C	-2.98514100	-3.17160400	-1.27826200
H	-1.96210400	-3.50899300	-1.09497000
H	-3.63005900	-4.04965500	-1.40776900
H	-2.98603500	-2.60231800	-2.21440300
C	-3.45854100	-3.14019900	1.19937100
H	-3.83135000	-2.55883500	2.05225800
H	-4.09255100	-4.02923000	1.09729500
H	-2.43884300	-3.46406500	1.42351200
C	-4.94454800	-1.88009200	-0.38269200
H	-5.35755200	-1.26910500	0.42819700
H	-5.03036500	-1.31516300	-1.31746200
H	-5.57651600	-2.77100400	-0.47854400
C	-4.27719400	2.79018900	-0.19355700
H	-4.55537300	2.33133700	-1.14862100
H	-4.81541800	2.27060400	0.60703000
H	-4.63161200	3.82763900	-0.21189800
C	-2.07005600	3.52743000	-1.12917700
H	-2.43358300	4.56137200	-1.17390300

H	-0.98490600	3.54657700	-0.99825100
H	-2.28478700	3.04963600	-2.09201200
C	-2.43981900	3.48310900	1.36584300
H	-1.36322800	3.49833700	1.55570400
H	-2.80169800	4.51785200	1.33836800
H	-2.93057600	2.97889500	2.20779600

### ***N*-Me amide 1c**



B3LYP/6-31G(d) free energy: -649.06603 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.179308 (a.u.)

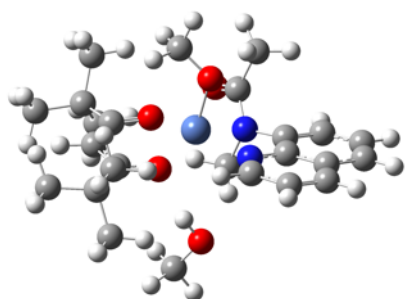
Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -648.9651836 (a.u.)

C	2.64739900	0.05498500	-0.47353400
O	2.59185000	0.96532400	-1.28852400
C	3.88374200	-0.82735500	-0.35971300
H	4.55429900	-0.55352000	-1.17487200
H	4.40360500	-0.66763200	0.59259100
H	3.64169200	-1.89325800	-0.42890100
N	1.60612300	-0.23236100	0.39858700
C	0.38727600	0.50125400	0.29613000
C	-0.84658200	-0.18727900	0.06181500
C	0.38690200	1.87855100	0.40785500
C	-2.05852900	0.57520800	-0.01640400
C	-0.81102300	2.62060400	0.31234400
H	1.32795500	2.39296200	0.56187300
C	-3.26325600	-0.13751200	-0.24564600
C	-2.01552300	1.98596600	0.11331800
C	-1.97604000	-2.15782300	-0.31307400
H	-0.77101500	3.70218000	0.40526800
C	-3.22912600	-1.50298800	-0.39527900

H	-4.20019700	0.41162800	-0.30586300
H	-2.94113200	2.55217100	0.04458000
H	-1.92535700	-3.23950100	-0.43705000
H	-4.13228500	-2.07802800	-0.57576900
N	-0.83152600	-1.54306800	-0.09282500
C	1.69110500	-1.32534000	1.37332600
H	0.88566800	-1.20659600	2.09859800
H	1.58031400	-2.30820000	0.90652500
H	2.64140800	-1.27643200	1.91404300

### III-Me



B3LYP/6-31G(d) free energy: -2968.898598 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.523924 (a.u.)

Number of imaginary frequencies: 0

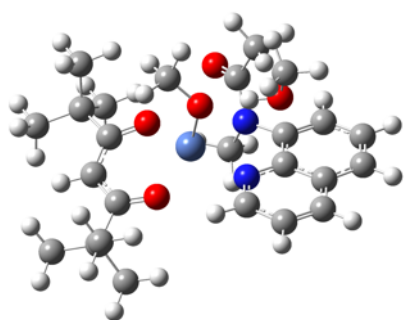
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2968.896516 (a.u.)

C	-1.59951600	-2.79659700	-0.03773200
O	-0.95382200	-3.65337000	-0.61434900
C	-2.15341300	-2.96608900	1.36000600
H	-1.80449400	-3.92655600	1.74260800
H	-1.78938900	-2.14204100	1.99082800
H	-3.24750100	-2.95336700	1.37377500
O	-0.25852200	2.01263700	-2.36247500
N	-1.77895100	-1.51701400	-0.63377900
C	-3.00960300	-0.80718200	-0.41325100
C	-2.96644900	0.54928800	0.02477500
C	-4.23069200	-1.38826800	-0.69528600
C	-4.18697400	1.27995900	0.15621400
C	-5.43984400	-0.67349000	-0.53758300
H	-4.25540500	-2.41457900	-1.05113800

C	-4.10283700	2.63305700	0.57020500
C	-5.42010500	0.63875400	-0.12589700
C	-1.72095900	2.38998600	0.68594500
H	-6.38217700	-1.16566500	-0.75893200
C	-2.87357300	3.19084400	0.82560400
H	-5.01619500	3.21268200	0.67791800
H	-6.34290100	1.20193600	-0.01479700
H	-0.73332700	2.78990800	0.88868300
H	-2.77281400	4.22390400	1.14085100
Ni	-0.10176900	-0.03980300	0.52446000
C	0.55283100	1.91516100	-3.52113800
H	-0.10574200	2.03088000	-4.38729400
H	1.31608600	2.70640900	-3.56578400
H	1.05866700	0.94091000	-3.60438700
N	-1.75910200	1.12504000	0.30256200
C	0.47473400	-0.82969300	3.19370600
H	0.88423700	-1.81879000	2.91172600
H	1.33759400	-0.13983900	3.27443100
H	0.06368100	-0.93418100	4.21311400
O	-0.51118300	-0.36694800	2.32068000
H	0.30562300	1.88942800	-1.57524100
C	3.12048800	0.10404000	0.06110000
H	4.19763000	0.13396700	0.06073700
C	2.43391100	1.31946600	0.14114300
C	2.49845100	-1.16305100	-0.06695600
C	3.31883300	-2.44872400	-0.30064900
C	3.18495200	2.66305300	0.26864300
O	1.14640900	1.43067600	0.10931400
O	1.24147400	-1.34098600	-0.00817300
C	2.74811300	3.30698200	1.60622400
H	3.23385200	4.28208400	1.73070100
H	1.66521400	3.45254600	1.63780300
H	3.02902800	2.67625700	2.45765900
C	4.71684400	2.52144200	0.26407700
H	5.07378500	1.91224100	1.10160400
H	5.08399000	2.07612500	-0.66734100

H	5.17557300	3.51242500	0.35884000
C	2.76608700	3.57905700	-0.90350600
H	3.20609000	4.57523800	-0.77784400
H	3.11898400	3.17693300	-1.86089200
H	1.67955400	3.68842600	-0.95776300
C	3.03055300	-3.40751500	0.87845500
H	1.96043800	-3.61679600	0.95109000
H	3.56245500	-4.35449300	0.72764800
H	3.36585400	-2.97880900	1.83048800
C	2.81117400	-3.09625600	-1.61075000
H	3.35398200	-4.03041300	-1.79765000
H	1.74423400	-3.32380600	-1.54348200
H	2.97728100	-2.43473300	-2.47042600
C	4.83423100	-2.20842000	-0.40522600
H	5.08730700	-1.53961300	-1.23588200
H	5.24792600	-1.78442000	0.51694200
H	5.34320000	-3.16257700	-0.58339300
C	-1.27080300	-1.38812800	-2.01821400
H	-0.26148400	-1.79430600	-2.05168700
H	-1.90287800	-1.94212100	-2.72325800
H	-1.25551300	-0.32901400	-2.28604300

#### IV-Me



B3LYP/6-31G(d) free energy: -2968.90916 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.523513 (a.u.)

Number of imaginary frequencies: 0

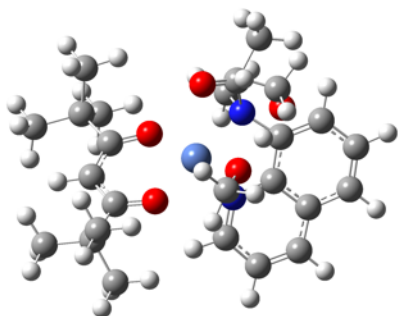
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2968.900856 (a.u.)

C	1.30367400	2.74113300	-0.36535600
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O	0.52832700	3.61522400	-0.71297000
C	2.19955100	2.87908300	0.85005500
H	1.64306500	3.45126900	1.59607900
H	2.52108600	1.92653900	1.27604700
H	3.08784700	3.46435700	0.58300500
O	3.19779100	-0.21827700	2.22557700
N	1.36844100	1.52246400	-1.08020900
C	2.61000300	0.80402600	-1.14537200
C	2.63670000	-0.58006700	-0.80359800
C	3.76282800	1.41359600	-1.59893900
C	3.85742400	-1.30739900	-0.94792300
C	4.97650200	0.69884700	-1.71510000
H	3.72881200	2.46312100	-1.87749700
C	3.84697300	-2.68515100	-0.62325000
C	5.02216600	-0.63922200	-1.40320900
C	1.52870300	-2.47715000	-0.05734100
H	5.86666300	1.21310800	-2.06477800
C	2.68346100	-3.27337100	-0.18880300
H	4.76404100	-3.26038000	-0.72257400
H	5.94660600	-1.20248500	-1.49878800
H	0.59302700	-2.90097000	0.29116100
H	2.64022400	-4.32632800	0.06862300
Ni	-0.13942200	-0.12007300	0.28006500
C	3.65416500	-0.29761500	3.55629700
H	4.74526700	-0.40690000	3.53621000
H	3.42121700	0.60547200	4.14573100
H	3.24158500	-1.16545900	4.09830100
N	1.49726400	-1.18546900	-0.35166700
C	-0.21568400	0.58348200	3.06280200
H	-0.83250600	1.45294800	2.78166600
H	-0.89897900	-0.19085300	3.45604600
H	0.42714800	0.89829700	3.90167200
O	0.56867500	0.11340300	2.00091000
H	2.20390100	-0.13271400	2.23324200
C	-3.37099000	-0.30616800	-0.13351100
H	-4.44331900	-0.37085700	-0.21532000

C	-2.63905100	-1.50390900	-0.17992000
C	-2.79841400	0.97850300	-0.02739300
C	-3.66320100	2.25665100	-0.05793200
C	-3.34346400	-2.86908800	-0.34864500
O	-1.36086300	-1.58128400	-0.10289300
O	-1.54535600	1.19308500	0.08531100
C	-3.01028600	-3.72388100	0.89631100
H	-3.44240400	-4.72644900	0.79337800
H	-1.92926000	-3.82308800	1.02588100
H	-3.42046200	-3.27064200	1.80655200
C	-4.87191500	-2.76998100	-0.49050400
H	-5.33745000	-2.32282900	0.39471500
H	-5.16395700	-2.18171700	-1.36753200
H	-5.29361100	-3.77456100	-0.61155800
C	-2.76580000	-3.54921000	-1.61091400
H	-3.19389700	-4.55172600	-1.72923900
H	-3.00419600	-2.97232800	-2.51272000
H	-1.67871800	-3.64007000	-1.54325100
C	-3.39824200	3.03300600	1.25294100
H	-2.33452600	3.26011000	1.35780800
H	-3.95779400	3.97598300	1.24877100
H	-3.71771500	2.45443800	2.12831000
C	-3.19406700	3.11504500	-1.25644400
H	-3.76748500	4.04915200	-1.29184300
H	-2.13317100	3.36387500	-1.16936100
H	-3.35588100	2.58844300	-2.20574300
C	-5.17090700	1.98278900	-0.18878900
H	-5.41337000	1.45678100	-1.11925100
H	-5.55536900	1.39263200	0.65095400
H	-5.71481100	2.93432200	-0.19798000
C	0.58260400	1.47982300	-2.32922500
H	-0.42830100	1.82368600	-2.12008000
H	1.02713000	2.12063600	-3.10078400
H	0.55845800	0.44843200	-2.68945500

#### IV-Me-TS



B3LYP/6-31G(d) free energy: -2968.872037 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.526415 (a.u.)

Number of imaginary frequencies: 1 (-266.9691)

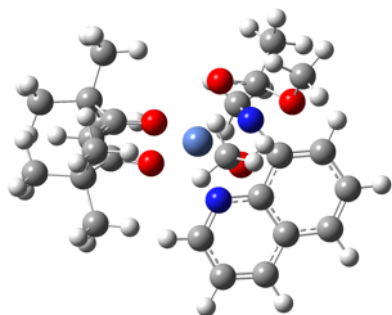
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2968.867714 (a.u.)

C	1.68418600	1.96603400	1.22149700
O	0.57441000	1.91415800	1.74390300
C	2.61642900	3.13327700	1.46861100
H	2.55498500	3.40851000	2.52297800
H	3.65345000	2.91511000	1.21438700
H	2.27737100	3.99464700	0.88027300
O	2.84525000	0.58311600	2.24949100
N	1.73362100	1.26393300	-0.11694500
C	2.78572500	0.37572700	-0.55474300
C	2.33768800	-0.82737700	-1.18497700
C	4.13758000	0.64063500	-0.51219500
C	3.27907100	-1.71047900	-1.79032700
C	5.07467600	-0.25412900	-1.08111900
H	4.49754600	1.54312100	-0.03493100
C	2.77173500	-2.87246400	-2.42594500
C	4.66078300	-1.39864400	-1.72192400
C	0.56226000	-2.20498400	-1.76950200
H	6.13278100	-0.01704100	-1.01837900
C	1.41838300	-3.11594100	-2.42745400
H	3.46484600	-3.56223100	-2.90132600
H	5.37968900	-2.07621900	-2.17488800
H	-0.50564100	-2.39026200	-1.70165600
H	1.00093900	-3.99782000	-2.90207600
Ni	0.01884400	-0.02503700	0.27939200

C	2.73122100	0.85248600	3.63208100
H	3.52549200	1.54406500	3.94198800
H	1.75556300	1.29931000	3.88101500
H	2.84230200	-0.07191000	4.21617900
N	0.99789800	-1.10854900	-1.17704900
C	0.61131500	-1.81349300	2.60184600
H	-0.04797000	-1.25598200	3.28974200
H	0.02244800	-2.63792500	2.17925100
H	1.42156900	-2.25750300	3.20333400
O	1.14753400	-1.00581300	1.58476600
H	2.09603700	-0.22043700	2.00162500
C	-3.27540700	0.13317500	-0.25636500
H	-4.34208700	0.20566900	-0.38837700
C	-2.76550800	-1.02299200	0.36319700
C	-2.48260800	1.20939900	-0.69753300
C	-3.13216900	2.47150200	-1.31819800
C	-3.70753900	-2.16000700	0.83073500
O	-1.53076400	-1.23370900	0.59978600
O	-1.21100000	1.25384300	-0.62304000
C	-3.57641500	-2.26902100	2.36734600
H	-4.18300900	-3.10291600	2.74150400
H	-2.53604700	-2.43516000	2.65791600
H	-3.92485900	-1.35169100	2.85699900
C	-5.18573500	-1.93879100	0.46732500
H	-5.59535700	-1.04217000	0.94547300
H	-5.33159500	-1.84764300	-0.61506500
H	-5.78000000	-2.79393300	0.81069400
C	-3.22314200	-3.47578100	0.18148200
H	-3.82072200	-4.32093300	0.54382200
H	-3.32667800	-3.43733400	-0.91068200
H	-2.17353000	-3.66263900	0.42221300
C	-2.80694700	3.66263000	-0.38738200
H	-1.72859400	3.76028900	-0.23723400
H	-3.18770700	4.59667200	-0.81858400
H	-3.27115200	3.52955000	0.59689400
C	-2.49395300	2.70878300	-2.70480200

H	-2.87910700	3.63591600	-3.14628500
H	-1.40684800	2.78574600	-2.62673000
H	-2.72811200	1.88628000	-3.39191100
C	-4.65844800	2.37416300	-1.48585500
H	-4.94582400	1.54014300	-2.13612600
H	-5.16944300	2.25231100	-0.52454200
H	-5.03647900	3.29597600	-1.94380700
C	1.45652200	2.25824700	-1.19057500
H	0.60033000	2.86442000	-0.89894200
H	2.33211900	2.89132200	-1.38613400
H	1.19336700	1.72155300	-2.10423200

### V-Me



B3LYP/6-31G(d) free energy: -2968.885244 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.533219 (a.u.)

Number of imaginary frequencies: 0

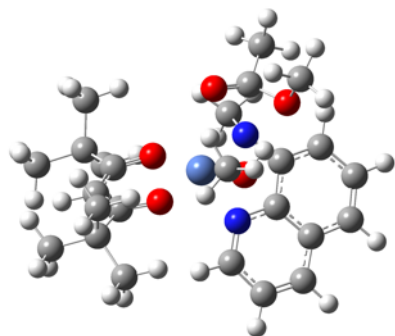
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2968.889963 (a.u.)

C	1.67701100	1.44365700	1.72873000
O	0.45158000	1.11676300	2.05821200
C	2.12419100	2.83641800	2.18997200
H	2.04108800	2.88714800	3.27866500
H	3.15817700	3.06154500	1.90503100
H	1.46250200	3.60429600	1.78532400
O	2.70813300	0.46406800	2.21557400
N	1.77729000	1.24181100	0.18078100
C	2.80451600	0.46550400	-0.45543300
C	2.34872700	-0.58611400	-1.31313300
C	4.15836600	0.71976200	-0.36963500

C	3.28674100	-1.32499100	-2.09422400
C	5.08965000	-0.03267800	-1.12271700
H	4.50945100	1.50502300	0.29098900
C	2.77402600	-2.34053800	-2.94188500
C	4.66812500	-1.02466300	-1.97999500
C	0.57194500	-1.83014200	-2.13262200
H	6.14878900	0.19026800	-1.02879500
C	1.42180800	-2.58829100	-2.97074700
H	3.46172900	-2.91698100	-3.55607700
H	5.38309800	-1.59164000	-2.57059300
H	-0.49541600	-2.03073300	-2.09479600
H	1.00043500	-3.36078200	-3.60581600
Ni	0.04212000	0.00181200	0.35013500
C	2.77206300	0.36340400	3.63498400
H	3.39093300	1.16178000	4.06481900
H	1.76872800	0.40136200	4.07417300
H	3.23873000	-0.59825700	3.87055500
N	1.00846000	-0.86965400	-1.34093800
C	0.56973600	-2.22308300	2.46454100
H	0.09425800	-1.48425000	3.11914500
H	-0.19613000	-2.88074200	2.05598900
H	1.29179300	-2.81941800	3.03844200
O	1.21591300	-1.58759100	1.35932500
H	1.90413300	-0.97873100	1.72636800
C	-3.22241000	0.17451500	-0.26405100
H	-4.28603700	0.25065900	-0.41616200
C	-2.72597600	-1.01243000	0.30319300
C	-2.42506800	1.27066900	-0.65225000
C	-3.07023800	2.54176000	-1.26221900
C	-3.68433500	-2.17058200	0.68176000
O	-1.49646700	-1.24503400	0.55201300
O	-1.15928200	1.32332100	-0.54627100
C	-3.60561800	-2.35872500	2.21415100
H	-4.22787200	-3.20676100	2.52580500
H	-2.57719000	-2.54608700	2.53275900
H	-3.96473300	-1.46482000	2.73788800

C	-5.15125100	-1.92786400	0.28643400
H	-5.57550600	-1.05797800	0.79974800
H	-5.26400900	-1.77790300	-0.79323800
H	-5.75531700	-2.79973600	0.56482500
C	-3.18546300	-3.45282700	-0.02095300
H	-3.79128000	-4.31469400	0.28414700
H	-3.26386500	-3.35843300	-1.11163700
H	-2.14090900	-3.65379700	0.22983100
C	-2.78575900	3.71428400	-0.29566200
H	-1.71171500	3.83125300	-0.12937800
H	-3.17938200	4.65124200	-0.70880000
H	-3.26109900	3.54616100	0.67789000
C	-2.38998000	2.81814900	-2.62119800
H	-2.76727200	3.75365900	-3.05193800
H	-1.30667900	2.89915300	-2.50374800
H	-2.59583600	2.01155300	-3.33579500
C	-4.58952600	2.43430500	-1.47950500
H	-4.84837400	1.61135500	-2.15534400
H	-5.12928000	2.28777600	-0.53743200
H	-4.96212800	3.36203100	-1.93010200
C	1.51748400	2.47113600	-0.59669600
H	0.62956600	2.96199500	-0.20236200
H	2.37608500	3.15650400	-0.57588400
H	1.30930700	2.19511100	-1.63303600

### V-Me-TS



B3LYP/6-31G(d) free energy: -2968.874897 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.52951 (a.u.)

Number of imaginary frequencies: 1 (-141.8427)

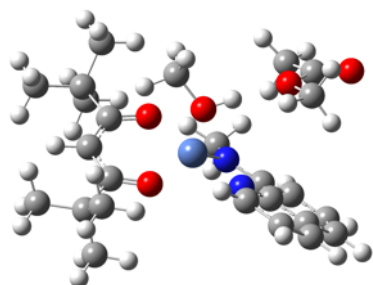
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2968.869973 (a.u.)

C	1.91772100	1.73075000	1.92880100
O	0.75933500	1.59228500	2.30982500
C	2.60939700	3.07552100	1.83885600
H	2.85976800	3.39779400	2.85805000
H	3.53308500	3.02599200	1.25916400
H	1.93900900	3.82387800	1.41653400
O	2.87397200	0.67896900	2.21681600
N	1.70033200	1.15885600	-0.12323300
C	2.66857900	0.37393700	-0.77416400
C	2.24830400	-0.89315400	-1.30552700
C	3.99704200	0.73329100	-0.97441700
C	3.15751700	-1.74755400	-1.99849600
C	4.90157500	-0.11447200	-1.64888200
H	4.34908900	1.68742600	-0.59469500
C	2.64299500	-2.96891000	-2.50395500
C	4.50366400	-1.33432800	-2.15535100
C	0.48688300	-2.37849700	-1.62565300
H	5.93309000	0.20727800	-1.76865300
C	1.31512200	-3.28334000	-2.32487000
H	3.30940700	-3.64677300	-3.03239300
H	5.20358200	-1.98145700	-2.67703200
H	-0.56028800	-2.60046600	-1.44288200
H	0.89701700	-4.21066400	-2.70310500
Ni	0.03994800	0.00708300	0.21119300
C	3.26250900	0.63620500	3.59435300
H	3.91866500	1.47894400	3.84641400
H	2.38726800	0.64722400	4.25443400
H	3.81810200	-0.29422700	3.73477500
N	0.93413200	-1.23462800	-1.13992000
C	0.46556500	-1.61585700	2.84685700
H	0.09910900	-0.73503400	3.38496900
H	-0.37362500	-2.25901400	2.58887600
H	1.16922500	-2.17277000	3.47956000
O	1.09901600	-1.23792700	1.62134500

H	1.85867700	-0.64937300	1.85108400
C	-3.25642000	0.17281600	-0.31754700
H	-4.31602000	0.21897700	-0.50607700
C	-2.76210300	-0.92725700	0.40360900
C	-2.45841700	1.23996800	-0.77385700
C	-3.08930600	2.45690000	-1.49335600
C	-3.71986200	-2.02513600	0.93098600
O	-1.53306300	-1.10619200	0.70170300
O	-1.19424200	1.30875800	-0.63493500
C	-3.71853000	-1.94033100	2.47504200
H	-4.35199500	-2.72918000	2.89893100
H	-2.70769100	-2.05664500	2.87452700
H	-4.10827300	-0.97366300	2.81530900
C	-5.16730200	-1.88520300	0.42765600
H	-5.63576500	-0.95806600	0.77535200
H	-5.22234000	-1.90814100	-0.66657200
H	-5.76986300	-2.71852100	0.80812200
C	-3.17139500	-3.40012400	0.49037600
H	-3.78202600	-4.20643400	0.91410200
H	-3.19734300	-3.50129900	-0.60224400
H	-2.13870800	-3.53395500	0.82167300
C	-2.77735100	3.71169700	-0.64604600
H	-1.70020500	3.82388300	-0.49967800
H	-3.15858600	4.61029600	-1.14632700
H	-3.24963600	3.64773300	0.34155800
C	-2.41454100	2.59022900	-2.87719500
H	-2.78361100	3.48432000	-3.39421200
H	-1.32957900	2.66919400	-2.77344300
H	-2.63518200	1.72081100	-3.50874100
C	-4.61163900	2.35046400	-1.68718100
H	-4.88744300	1.47923600	-2.29213900
H	-5.14305100	2.28742000	-0.73101000
H	-4.97772200	3.24281300	-2.20860700
C	1.46704500	2.42005400	-0.84132700
H	0.71460100	3.00057600	-0.30491300
H	2.38081300	3.02430700	-0.94076600

H 1.07619100 2.23649600 -1.85159000

### VI-Me



B3LYP/6-31G(d) free energy: -2968.931273 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.522679 (a.u.)

Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2968.911079 (a.u.)

C	-3.44300200	-2.24214500	1.64809800
O	-4.63915000	-2.33292400	1.77417000
C	-2.56244200	-3.06356300	0.74480100
H	-3.16755700	-3.82641700	0.25413200
H	-2.09136700	-2.42019900	-0.00872200
H	-1.76180900	-3.53971900	1.32095500
O	-2.70625400	-1.32236200	2.35454000
N	-0.92000400	-0.74867600	-1.66900300
C	-2.10458700	-0.11618900	-1.88330800
C	-2.41759400	0.96663000	-0.97428100
C	-3.05884900	-0.38749000	-2.87766300
C	-3.62529600	1.71718900	-1.07917100
C	-4.25120000	0.35842700	-2.96800500
H	-2.88057100	-1.18136800	-3.59424300
C	-3.80521600	2.75957800	-0.13594600
C	-4.55311000	1.39135000	-2.10099900
C	-1.67633800	2.21779300	0.84012700
H	-4.95673900	0.10529000	-3.75642200
C	-2.83828200	3.01332300	0.81630900
H	-4.71139900	3.35984200	-0.17748000
H	-5.47720300	1.95469400	-2.19077400
H	-0.88577100	2.38083400	1.56605300

H	-2.95657200	3.81514000	1.53876100
Ni	0.15366000	-0.01159100	-0.21526000
C	-3.46798600	-0.44252800	3.20739300
H	-4.16590800	0.14874700	2.61101000
H	-4.02157700	-1.02238800	3.94896600
H	-2.73365900	0.20381100	3.68849400
N	-1.48456200	1.22672200	-0.02051500
C	0.87318000	-1.13122000	2.66813300
H	0.93944900	-2.17727700	2.34911700
H	1.84303100	-0.65547200	2.51957900
H	0.60660400	-1.08415900	3.73093800
O	-0.07378300	-0.39666100	1.88633600
H	-0.96863100	-0.76899200	2.02502500
C	3.44075200	0.20495200	-0.02577100
H	4.51404000	0.28593000	0.01976900
C	2.69352900	1.39122100	0.12889900
C	2.89472100	-1.06891400	-0.28311200
C	3.81955300	-2.29298800	-0.50726600
C	3.39631200	2.75530800	0.33569900
O	1.42155700	1.45929000	0.10875700
O	1.64820900	-1.32154200	-0.37662600
C	2.87935900	3.35915200	1.66093000
H	3.30378400	4.35882900	1.81311500
H	1.78957600	3.44145500	1.64924000
H	3.16777600	2.73735000	2.51761600
C	4.93108500	2.67122100	0.38963100
H	5.27839600	2.04038300	1.21581900
H	5.35262500	2.27941700	-0.54268300
H	5.34772800	3.67369700	0.54289500
C	2.98158000	3.67082000	-0.83927200
H	3.40490000	4.67378000	-0.70580500
H	3.34660100	3.27469000	-1.79452600
H	1.89343500	3.75476300	-0.89939500
C	3.33059100	-3.44596500	0.39627500
H	2.27530200	-3.66188100	0.21283300
H	3.91305000	-4.35391500	0.19962100

H	3.45182300	-3.19484600	1.45754500
C	3.67881200	-2.71214900	-1.98924300
H	4.29319700	-3.59795200	-2.19188500
H	2.63980500	-2.95072700	-2.23214500
H	4.01046700	-1.90999800	-2.65906300
C	5.30381100	-2.02075000	-0.20553600
H	5.73050100	-1.27007400	-0.87959100
H	5.45502000	-1.68152900	0.82558100
H	5.87997400	-2.94391900	-0.33919200
C	-0.57278800	-1.82143900	-2.58044000
H	0.39149600	-2.23459900	-2.28051600
H	-1.31478700	-2.63871900	-2.57277100
H	-0.48975500	-1.47240500	-3.62306000

### VII-Me



B3LYP/6-31G(d) free energy: -2816.293076 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.492906 (a.u.)

Number of imaginary frequencies: 0

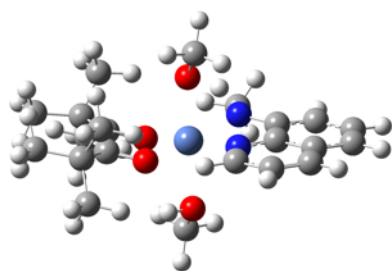
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2816.297965 (a.u.)

N	1.61232800	-1.69965200	-0.17489700
C	2.89843900	-1.26787500	-0.12621700
C	3.09392800	0.16882400	-0.06144400
C	4.06613400	-2.05344000	-0.13355000
C	4.39882500	0.74918900	-0.06523300
C	5.34443800	-1.46551000	-0.13198600
H	3.98510500	-3.13452400	-0.15516400
C	4.46521500	2.16430200	-0.00844200
C	5.53503300	-0.09617900	-0.10983500
C	2.06749000	2.25324400	0.08789000

H	6.21242300	-2.12147200	-0.15142300
C	3.31061600	2.91431200	0.06508800
H	5.43986400	2.64731900	-0.01676000
H	6.53044000	0.33825100	-0.11236900
H	1.13109900	2.79607100	0.17138000
H	3.34438000	3.99836500	0.11465600
Ni	0.26136200	-0.21234700	0.16642700
N	1.96878200	0.93147700	0.02338200
C	0.50564600	0.48214100	-3.02534300
H	0.61105200	-0.01171700	-3.99965000
H	-0.27879400	1.23869900	-3.09878800
H	1.45018400	0.97379400	-2.76362800
O	0.09420000	-0.45133700	-2.02772200
H	0.80880800	-1.10992300	-1.85652500
O	0.34139900	0.00835700	2.30622000
H	-0.37625600	0.66325500	2.35300400
C	0.05584100	-1.09906100	3.16998600
H	0.89197200	-1.79156100	3.06497500
H	-0.00590200	-0.76551000	4.21246600
H	-0.86890400	-1.60574000	2.87665100
C	-2.20617300	1.41379800	0.11621300
C	-2.99439500	0.27464700	-0.10584800
H	-4.03260700	0.42705000	-0.34950300
C	-2.53838700	-1.06089400	-0.00283500
C	-3.50747300	-2.24701400	-0.23414800
C	-2.81886600	2.83402800	0.04308000
O	-1.34791500	-1.39850100	0.28564500
O	-0.95551100	1.39077900	0.40112100
C	-2.99084800	-3.02907400	-1.46411900
H	-1.96083000	-3.36081000	-1.31048900
H	-3.61946700	-3.90997700	-1.64298600
H	-3.01407200	-2.40545400	-2.36539600
C	-3.45416400	-3.15812800	1.01244400
H	-3.83540800	-2.63648500	1.89940700
H	-4.07334900	-4.04962100	0.85661000
H	-2.42928700	-3.47795900	1.21659700

C	-4.96687300	-1.82953400	-0.48441700
H	-5.38212300	-1.26575300	0.35871300
H	-5.07013000	-1.22066600	-1.38944100
H	-5.58556600	-2.72450300	-0.61972100
C	-4.33641200	2.85198000	-0.20820300
H	-4.59808000	2.39775100	-1.17021600
H	-4.88680700	2.32672600	0.58027200
H	-4.69329000	3.88851600	-0.22693300
C	-2.11336700	3.59025200	-1.10628700
H	-2.47236300	4.62528400	-1.15760100
H	-1.03020900	3.60675600	-0.95793000
H	-2.31890500	3.11476600	-2.07316600
C	-2.52638600	3.54889100	1.38176200
H	-1.45369200	3.56246300	1.59158800
H	-2.88670400	4.58385700	1.34656600
H	-3.03374600	3.04653300	2.21494200
C	1.39289000	-3.12994100	-0.05702700
H	0.31690100	-3.31946000	-0.05605000
H	1.83948400	-3.70138700	-0.88895600
H	1.81460400	-3.54811800	0.87424100

## VII-Me-TS



B3LYP/6-31G(d) free energy: -2816.284841 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.489541 (a.u.)

Number of imaginary frequencies: 1 (-939.5794)

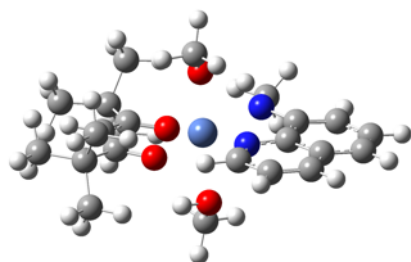
M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2816.282659 (a.u.)

N	1.67523200	-1.72575200	-0.39248100
C	2.96560700	-1.24462900	-0.21713200
C	3.10656100	0.18292400	-0.08439900

C	4.12630000	-2.01137600	-0.15366900
C	4.39575800	0.78573700	0.01211400
C	5.39772100	-1.40806400	-0.03173400
H	4.06172700	-3.09167300	-0.22223300
C	4.44076200	2.19917600	0.10777000
C	5.54921700	-0.04013200	0.03044400
C	2.04078900	2.24104100	0.08562100
H	6.27583500	-2.04837400	-0.00162000
C	3.27180200	2.92651600	0.13373300
H	5.40684300	2.69494000	0.16798600
H	6.53212800	0.41605600	0.10701600
H	1.09335100	2.76726500	0.15000500
H	3.28101800	4.00921400	0.20927200
Ni	0.22333000	-0.17338600	0.08733200
N	1.96155800	0.92350100	-0.01820200
C	0.51262900	0.30698500	-2.94295700
H	0.62074100	-0.22584200	-3.90173400
H	-0.27502100	1.06437300	-3.07840200
H	1.45778000	0.84728100	-2.75760600
O	0.17037500	-0.58191100	-1.91267800
H	1.11154500	-1.28581800	-1.38342800
O	0.36117200	0.12524400	2.26804400
H	-0.34653300	0.79339800	2.23206700
C	0.01786200	-0.89616000	3.21082900
H	0.84393000	-1.60963600	3.20838900
H	-0.08293700	-0.47377100	4.21800800
H	-0.90218000	-1.41407600	2.92262500
C	-2.23688700	1.40622400	0.06766800
C	-3.00150600	0.24345800	-0.09718700
H	-4.04230000	0.36607600	-0.34631400
C	-2.52636300	-1.08055600	0.06937900
C	-3.48201400	-2.28722700	-0.09981000
C	-2.87670300	2.80847100	-0.06907700
O	-1.33032600	-1.38790800	0.36642400
O	-0.98359500	1.42269100	0.35391900
C	-3.00935700	-3.06773600	-1.34888800

H	-1.96542800	-3.37450100	-1.24538800
H	-3.62689400	-3.96347200	-1.48967200
H	-3.08818800	-2.45169900	-2.25166600
C	-3.35057000	-3.18700800	1.14863400
H	-3.70369400	-2.66807400	2.04887200
H	-3.95517500	-4.09359100	1.02648200
H	-2.31034400	-3.48071600	1.30839300
C	-4.96028200	-1.90091200	-0.28131100
H	-5.33845900	-1.31902300	0.56708900
H	-5.12459800	-1.32146500	-1.19637300
H	-5.56906000	-2.80960700	-0.35732000
C	-4.39183700	2.78482800	-0.33392200
H	-4.63446900	2.28246200	-1.27671000
H	-4.93992300	2.28523200	0.47269100
H	-4.76822900	3.81228500	-0.40299400
C	-2.17566600	3.53003000	-1.24337400
H	-2.55990000	4.55237000	-1.34419300
H	-1.09520900	3.57967200	-1.08414400
H	-2.35487000	3.00597200	-2.18959000
C	-2.61170800	3.58411800	1.24133400
H	-1.54144800	3.62901900	1.45966900
H	-2.99231000	4.60915700	1.15939700
H	-3.11634100	3.10664000	2.09063800
C	1.46597300	-3.16227100	-0.25961200
H	0.39476800	-3.35511500	-0.34683100
H	1.98832100	-3.74381200	-1.03535000
H	1.80520300	-3.52612400	0.72005800

### VIII-Me



B3LYP/6-31G(d) free energy: -2816.284056 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.492741 (a.u.)

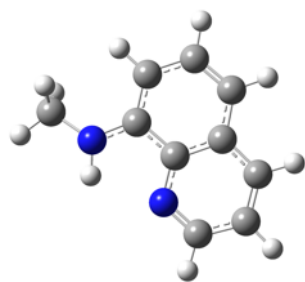
Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -2816.289751 (a.u.)

N	1.75291000	-1.76777900	-0.46695400
C	3.03350800	-1.24561200	-0.21742200
C	3.13333900	0.18236800	-0.11124900
C	4.18506000	-1.99787600	-0.05110000
C	4.40591100	0.80399900	0.05405800
C	5.43979500	-1.37656600	0.15217000
H	4.13547200	-3.08003200	-0.10234100
C	4.43283800	2.22020200	0.10868800
C	5.56415100	-0.00661900	0.18088800
C	2.03836400	2.22720800	-0.06151100
H	6.32055800	-2.00296200	0.26520700
C	3.25707100	2.93141200	0.03655600
H	5.38799400	2.72861000	0.21640800
H	6.53297600	0.46706700	0.31290800
H	1.08366600	2.74418300	-0.06021000
H	3.24822400	4.01584600	0.07766100
Ni	0.21987100	-0.17723900	-0.05563600
N	1.97608500	0.90762700	-0.13049100
C	0.22337500	0.49527600	-2.94540100
H	0.27671300	0.06701600	-3.96280300
H	-0.65067600	1.17467400	-2.93946200
H	1.12040200	1.13877000	-2.82960000
O	0.12365200	-0.50787600	-1.98794900
H	1.34553200	-1.41916700	-1.38606000
O	0.43653800	0.13256100	2.18271000
H	-0.25554200	0.81341600	2.09334200
C	0.03726600	-0.83183100	3.15955900
H	0.84346800	-1.56591000	3.22162100
H	-0.08678700	-0.36254700	4.14385600
H	-0.88594000	-1.34226900	2.86688800
C	-2.24308600	1.38324700	0.10168700
C	-3.00279700	0.21508800	-0.04142800

H	-4.05672900	0.33147900	-0.23111300
C	-2.50972100	-1.10839000	0.07946400
C	-3.46481200	-2.31957300	-0.06024700
C	-2.90784800	2.77940400	0.04202300
O	-1.29973700	-1.41091300	0.31521600
O	-0.97356200	1.41091200	0.30955700
C	-3.03303900	-3.09155100	-1.32914200
H	-1.98403100	-3.39149500	-1.26434900
H	-3.64984400	-3.99049600	-1.45194000
H	-3.14694500	-2.47170500	-2.22542700
C	-3.28220600	-3.22363100	1.17863500
H	-3.60693600	-2.71137500	2.09330100
H	-3.88341700	-4.13475900	1.07422400
H	-2.23443900	-3.50914600	1.29983400
C	-4.95100800	-1.94213600	-0.18646900
H	-5.30398700	-1.37201600	0.68059800
H	-5.15023900	-1.35426100	-1.08912000
H	-5.55589900	-2.85436600	-0.25109900
C	-4.43560800	2.74081700	-0.13387500
H	-4.72675000	2.26168700	-1.07502200
H	-4.92851700	2.21069200	0.68869500
H	-4.82877200	3.76419500	-0.15103100
C	-2.28793400	3.54668900	-1.14843200
H	-2.69317000	4.56488900	-1.19514000
H	-1.20093200	3.61008200	-1.05110700
H	-2.51263300	3.04746100	-2.09804000
C	-2.57669700	3.52040800	1.35766000
H	-1.49597900	3.57755500	1.51276500
H	-2.97720500	4.54077800	1.32980600
H	-3.02190700	3.00955800	2.22071400
C	1.54076200	-3.20252600	-0.29924900
H	0.47931800	-3.39976800	-0.45891800
H	2.12492100	-3.81041500	-1.00624400
H	1.80346600	-3.50782700	0.71967500

***N*-Methyl-8-aminoquinoline (QuinNHMe)**



B3LYP/6-31G(d) free energy: -496.453105 (a.u.)

B3LYP/6-31G(d) thermal correction to the Gibbs free energy: 0.14591 (a.u.)

Number of imaginary frequencies: 0

M06/6-311+G(d,p)/SMD(MeOH) single point energy: -496.3578915 (a.u.)

N	1.99064800	-1.13809700	-0.09464800
C	1.17627000	-0.04148200	-0.04214500
C	-0.24943400	-0.27468600	-0.01996500
C	1.63406900	1.27358000	-0.01950700
C	-1.14937300	0.83411900	0.00096700
C	0.72478100	2.35369800	0.00221800
H	2.69973200	1.47738300	-0.02522500
C	-2.53372500	0.52628900	0.01749400
C	-0.63900800	2.15889200	0.00918500
C	-1.96671900	-1.80674200	0.00650800
H	1.12407200	3.36492300	0.01425400
C	-2.94618700	-0.78709400	0.01832100
H	-3.25680200	1.33883300	0.03080700
H	-1.32827700	2.99856500	0.02468100
H	-2.26892700	-2.85332400	0.01414300
H	-4.00028400	-1.04826400	0.03105700
N	-0.66828300	-1.56801800	-0.01230400
H	1.50376000	-2.01833600	0.01129600
C	3.42176600	-1.08332900	0.07671600
H	3.89863600	-0.50747600	-0.72824000
H	3.71664800	-0.62880000	1.03598300
H	3.82025200	-2.10017200	0.04116000