Supporting Information for the Manuscript:

The Catalytic Role of Nickel in the Decarbonylative Addition of Phthalimides to Alkynes

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Computational Details

All the density functional theory (DFT) calculations were performed using the Gaussian09 package.[i] The BP86 GGA functional of Becke and Perdew[ii] was used with the standard split-valence basis set with a polarization function of Ahlrichs and coworkers for H, C, N and P atoms (SVP keyword in Gaussian)[iii] while the quasi relativistic small-core Stuttgart effective core potential (ECP) was used for Nickel (SDD keyword in Gaussian09), for geometry optimizations.[iv] The reported energies have been obtained via single point energy calculations with the M06 functional[v] with the triple-ζ basis set of Ahlrichs for main group atoms (TZVP keyword in Gaussian09).[vi] Solvent effects, toluene, were included with the default Gaussian PCM implementation.[vii] The M06 energy calculations were carried out with the scf=tight, and integral(grid=ultrafinegrid) keywords. Zero point energies and thermal corrections calculated at the BP86 level were added to the M06 in solvent energies to approximate free energies in solvent. As reference system we used the separated reactants, instead of using the pre-reactant complex approach.

In some cases we discuss the change in the local aromaticity of a given ring. As a structure-based measure, we used the harmonic oscillator model of aromaticity (HOMA) index, defined by Kruszewski and Krygowski as:[viii]

$$HOMA = 1 - \frac{\alpha}{n}\sum_{i=1}^{n}\left(R_{opt} - R_i\right)^2, \qquad (1)$$

where n is the number of bonds considered, and α is an empirical constant (for CC bonds α = 257.7 and for CN bonds α= 93.2) fixed to give HOMA = 0 for a model nonaromatic system, and HOMA = 1 for a system with all bonds equal to an optimal value R_{opt}, which is 1.388 Å for CC bonds (1.334 Å for CN bonds), assumed to be achieved for fully aromatic systems.[viiia] R_i stands for a running bond length. HOMA calculations have proved to be useful in similar studies.**¡Error! Marcador no definido.**[d,ix]

To evaluate the strength of bonds, a Mayer Bond Order (MBO) analysis has been envisaged. This index is derivated from the definition of bond order due to Wiberg[x] based on the P matrix.

$$P_{st} = \sum_{i}^{occupied} n_i c_{rs} c_{rt} \qquad (2) \qquad (3)$$

The Wiberg bond order, applicable to NDO-type theories where the atomic orbital basis forms an orthonormal set, uses the square of the off-diagonal elements of P,

$$B_{AB}^{Wiberg} = \sum_{s}^{onA}\sum_{t}^{onB} \mathrm{P}_{\mathrm{st}}^{\ 2} \qquad (3) \qquad (4)$$

Mayer[xi] has suggested a method for calculating bond orders from the P matrix,

$$B_{AB}^{Mayer} = \sum_{s}^{onA}\sum_{t}^{onB} (\mathrm{PS})_{\mathrm{st}} (\mathrm{PS})_{\mathrm{ts}} \qquad (4)$$

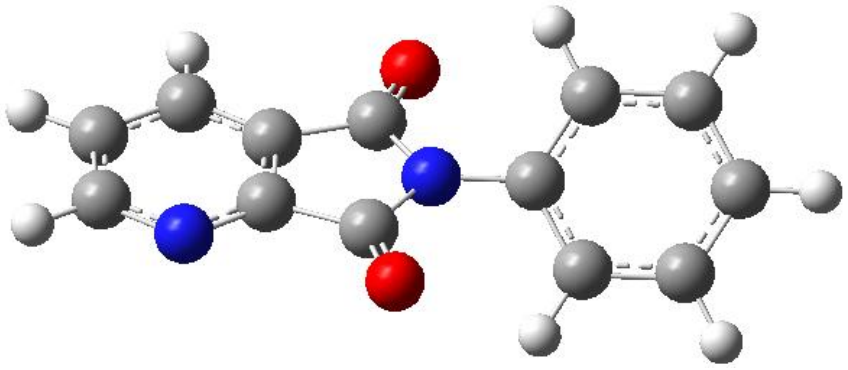
The Mayer definition can be seen as an extension of the Wiberg index. This leads to the classical integer values for homonuclear diatomics when minimal or small basis sets are used. Non-integer values are found for larger basis sets and in more complicated molecules and these reflect the polarized character of the bonds as well as delocalization and multicenter effects. Mayer bond orders are a valuable tool in the analysis of the bonding in main group[xii] and transition metal[ixa,xiii] systems.

It is worth mentioning here that for all the species presented in the manuscript, we have computed the closed-shell singlet and the triplet electronic states. Since the triplet state is always much higher in energy, in the following sections, we confine our discussion only to the singlet ground state.

Figure S1. Potential parallel stationary points the reaction pathway. Free energies in solution (toluene as the solvent) relative to species **3** are given. The imaginary frequency characterizing the transition state structures is given in brackets. Selected distances are given in Å.

Table S1. xyz coordinate data sets and absolute energies in a.u. for DFT optimized complexes.

1



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C	0.484147	1.173217	0.183905
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H	3.136684	2.490818	0.393241
C	4.177032	-0.764603	-0.122596
H	5.095608	-1.370818	-0.219383
C	-2.453521	1.064509	-0.601335
H	-1.906551	1.897631	-1.061649
C	-3.856998	1.056036	-0.593332
H	-4.403114	1.890466	-1.060987
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C	-3.851759	-1.064450	0.590926
H	-4.393668	-1.902521	1.056906
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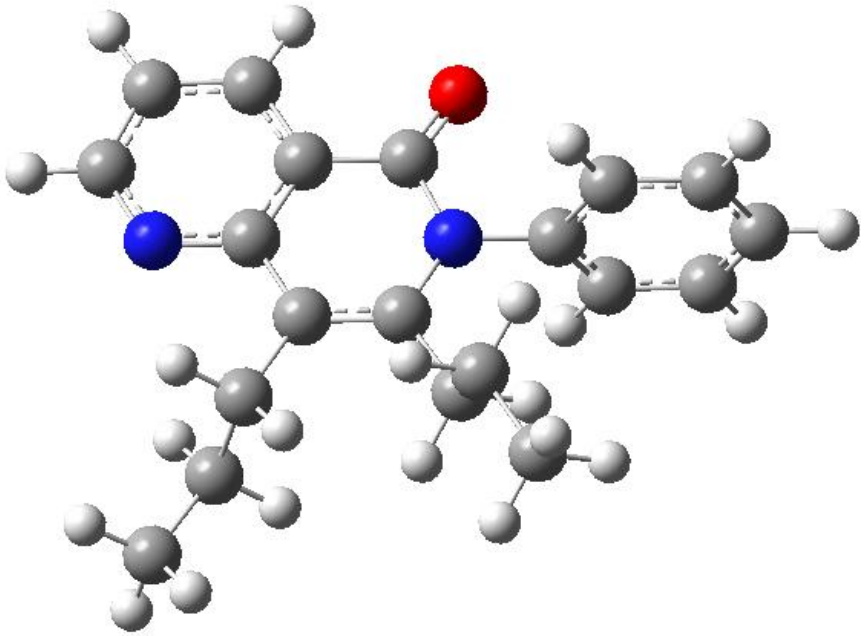
O	0.077990	-2.295722	-0.357872

2



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H	2.037252	-0.413564	2.379838
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H	4.531649	-0.412494	2.696040
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H	-1.998307	2.426788	1.898612
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H	2.200216	4.147581	-2.298724
H	2.858409	3.680874	-0.699859
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H	-3.177778	4.372862	0.723090
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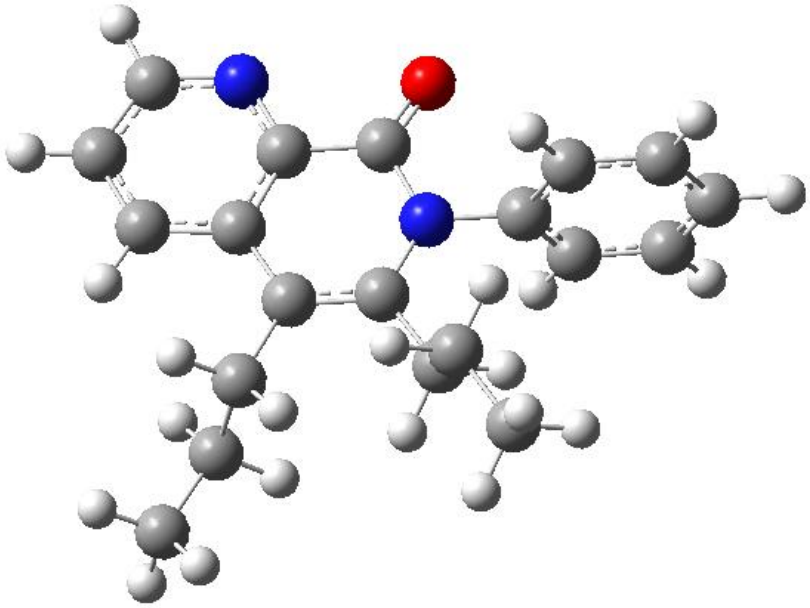

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C	-2.086401	-0.687303	-0.207373
C	0.138268	-1.889323	-0.014446
C	-1.407001	0.596156	-0.146402
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C	2.147371	-0.571547	0.216585
C	-2.224151	1.876661	-0.190280
H	-3.064215	1.751637	-0.908909
H	-1.623610	2.709267	-0.610356
C	0.762096	1.915675	0.028588
H	1.672878	1.782058	0.646315
H	0.156472	2.686537	0.547046
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C	2.987200	-0.690079	-0.905142
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C	4.381710	-0.708525	-0.734771
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H	6.031382	-0.632974	0.684340
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H	4.524992	-0.457390	2.686582
C	1.177222	2.450539	-1.362683
H	1.791923	1.681997	-1.878341
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H	-3.388254	1.476937	1.612293
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H	2.239611	4.134195	-2.288543
H	2.891635	3.648617	-0.692886
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H	-3.091208	4.439446	0.695517
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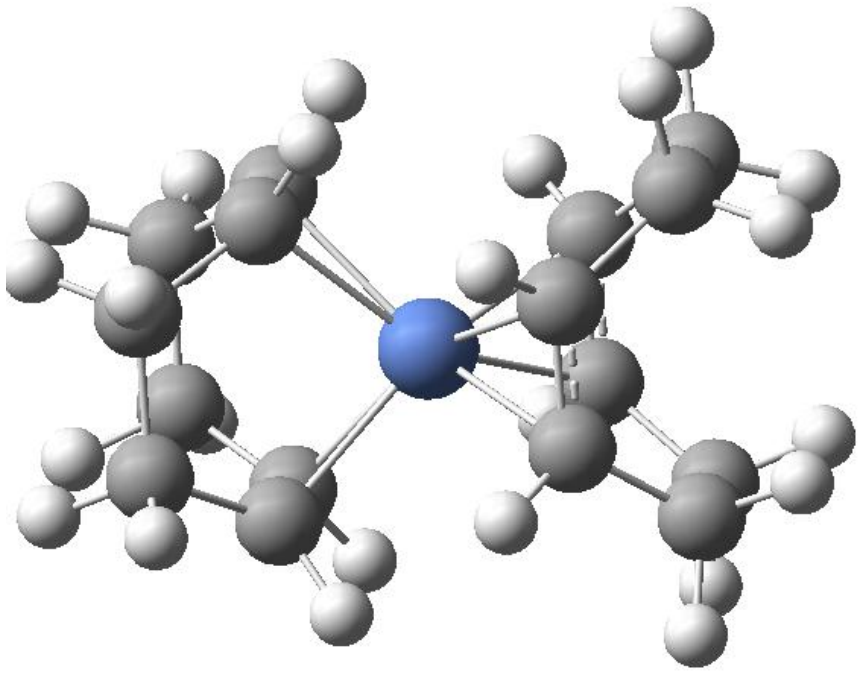
3



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C	-1.491224	0.376213	-1.483848
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C	-2.613403	-0.655554	-1.385433
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C	1.490824	0.376668	1.483757
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C	2.612873	-0.655357	1.386128
C	2.227394	1.874136	-0.510367
C	2.613197	0.655332	-1.385824
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H	0.962287	-0.403759	-2.450819
H	0.732107	-2.332497	-1.071394
H	-0.962107	-0.403871	2.450821
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H	0.732017	2.332653	1.071135
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H	3.145669	-2.406045	0.160046
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H	1.680259	-2.613251	1.134796
H	3.535452	-0.176972	0.996453
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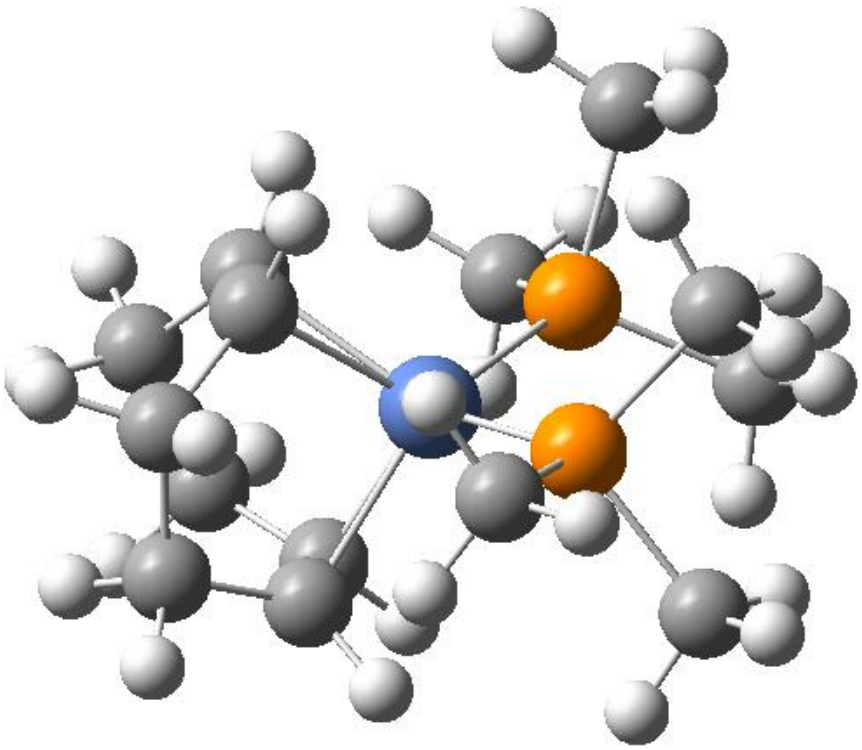
4



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H	3.213876	2.106971	-0.980296
H	3.741830	0.447682	-0.696520
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H	3.571358	1.196756	1.546330
H	2.313230	2.380382	1.163272
C	1.530620	0.418286	1.529694
H	0.983458	0.813900	2.404989
C	1.494942	-0.974715	1.321176
H	0.912169	-1.570859	2.045667
C	2.573139	-1.735525	0.545641
H	2.700072	-2.748414	0.984947
H	3.554206	-1.232804	0.690055
C	2.267517	-1.874374	-0.973970
H	3.224023	-1.959790	-1.546731
H	1.735322	-2.831143	-1.150368
C	1.407636	-0.747322	-1.529151
H	0.785167	-1.014312	-2.402616
P	-1.385200	-1.576395	0.039470
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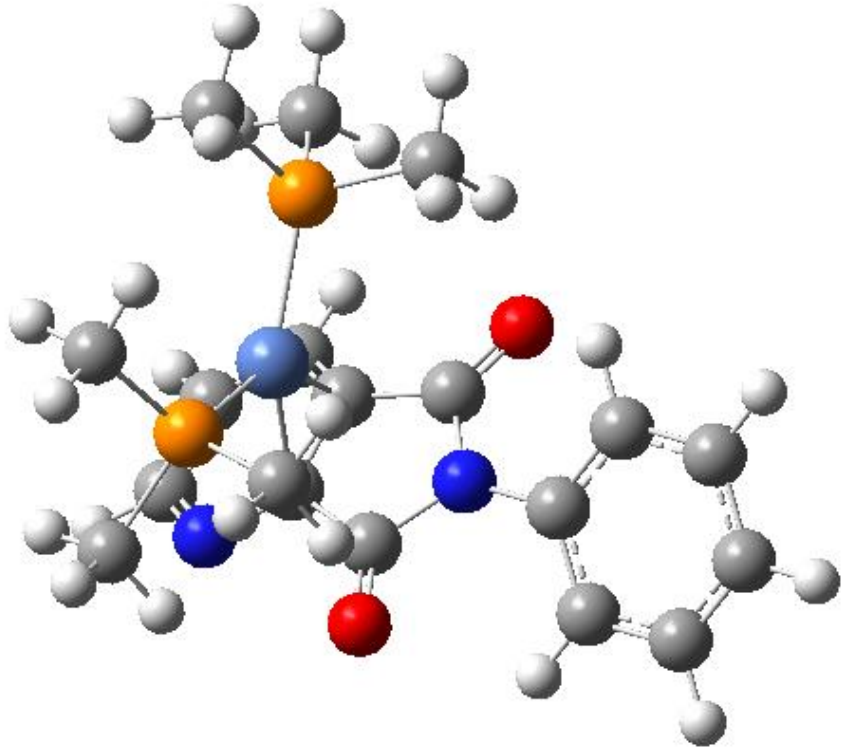
5



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C	-0.988889	-1.373176	0.785805
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Ni	1.119593	-0.029984	-0.042849
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P	1.390062	-1.564089	-1.603720
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H	4.008746	1.632129	-1.616898
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H	3.358049	3.252522	-2.085814
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H	-0.311640	-0.744745	-3.187185
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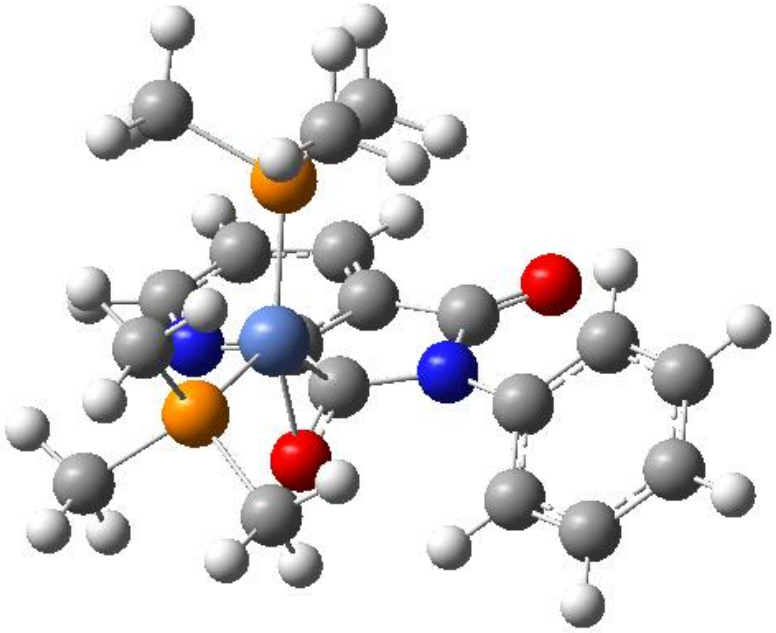
5isomer



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C	-2.142111	-3.541728	-1.483179
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H	-1.895487	4.785857	2.035711
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H	-0.489583	6.022536	0.355641
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H	-0.261228	2.410384	-2.061173
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H	0.322428	4.819846	-1.698563
C	-0.800411	-0.136259	-0.969624
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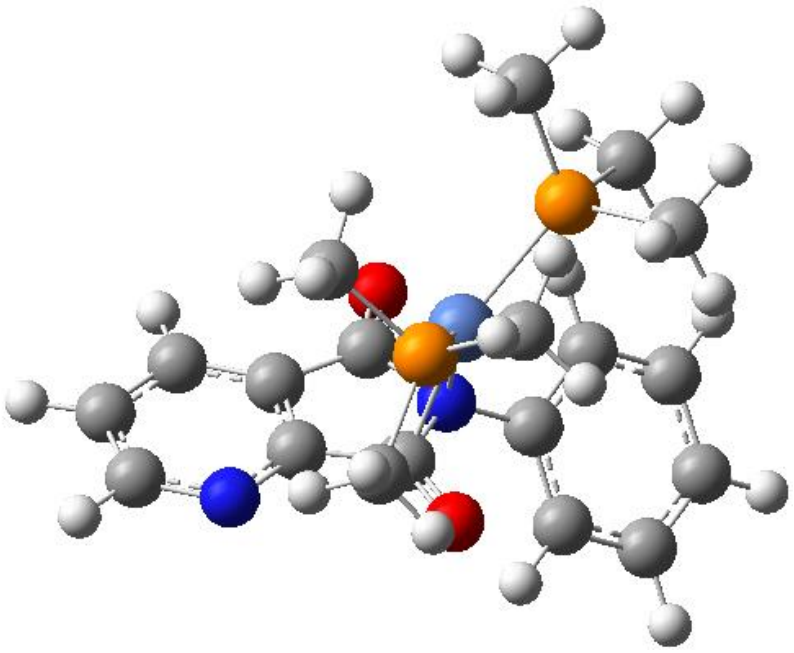
Ni	0.977634	-0.385833	-0.112335
P	3.080832	-0.140007	-0.733538
C	3.431377	-1.210182	-2.207529
H	4.431470	-1.004589	-2.644413
H	3.370232	-2.276449	-1.910407
H	2.643326	-1.024255	-2.964363
C	4.571627	-0.453497	0.332855
H	5.516548	-0.295903	-0.229002
H	4.556884	0.231564	1.204695
H	4.550599	-1.496511	0.708448
C	3.434954	1.558910	-1.386471
H	3.369447	2.294041	-0.559307
H	4.437112	1.623998	-1.860318
H	2.653173	1.812609	-2.129250
P	0.805124	-1.083851	1.907975
C	1.792694	-0.163037	3.186781
H	1.489336	0.903277	3.179342
H	1.633714	-0.579648	4.203913
H	2.870911	-0.217713	2.937271
C	1.335230	-2.841706	2.199196
H	1.206990	-3.139805	3.261378
H	0.731391	-3.511288	1.554555
H	2.399946	-2.961428	1.914964
C	-0.877565	-1.069889	2.690957
H	-1.265294	-0.031553	2.705184
H	-1.571373	-1.683788	2.082691
H	-0.854047	-1.464086	3.728594

5-6



-1852.9689424

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C	0.672758	1.920272	0.642564
C	-0.740236	2.330965	0.359763
N	-2.493862	2.055038	-1.311600
C	2.339761	0.555701	-0.618795
C	-2.774001	3.586009	0.567790
H	-3.418900	4.321370	1.073107
C	-1.493496	3.274084	1.066886
H	-1.073316	3.757481	1.963086
C	-3.217357	2.953863	-0.610092
H	-4.215233	3.194899	-1.020221
C	3.457833	1.393407	-0.372272
H	3.316226	2.340161	0.165241
C	4.736282	0.992184	-0.788747
H	5.596471	1.650439	-0.585091
C	4.931110	-0.230977	-1.456507
H	5.939139	-0.534839	-1.779858
C	2.539312	-0.673085	-1.295112
H	1.662855	-1.307005	-1.502105
C	3.822929	-1.059015	-1.709095
H	3.956380	-2.015461	-2.239925
C	-0.399094	0.719864	-1.470843
O	-0.168133	0.528845	-2.657335
Ni	-0.381322	-0.503028	0.044914
P	-1.787764	-1.846949	-0.922709
C	-3.400091	-1.126450	-1.475218
H	-3.955442	-1.842242	-2.116627
H	-4.013048	-0.883432	-0.583558
H	-3.211960	-0.179030	-2.020817
C	-2.349607	-3.387088	-0.049316
H	-3.026344	-3.984637	-0.695460
H	-1.471799	-4.005883	0.221282
H	-2.889105	-3.112806	0.879482
C	-1.069096	-2.524703	-2.486900
H	-0.215895	-3.188409	-2.240010
H	-1.822671	-3.096517	-3.067305
H	-0.692248	-1.667897	-3.083450
P	0.163151	-1.195524	2.137882
C	-0.780348	-0.286921	3.456748
H	-0.473676	-0.605855	4.475432
H	-0.585517	0.798374	3.343155
H	-1.867545	-0.460915	3.327946
C	-0.011269	-2.960153	2.702106
H	0.349298	-3.083822	3.745208
H	-1.072188	-3.275257	2.649791
H	0.581583	-3.622472	2.038978
C	1.916949	-0.829802	2.613533
H	2.602442	-1.395791	1.951647
H	2.110876	0.252445	2.462506
H	2.114182	-1.099788	3.672096

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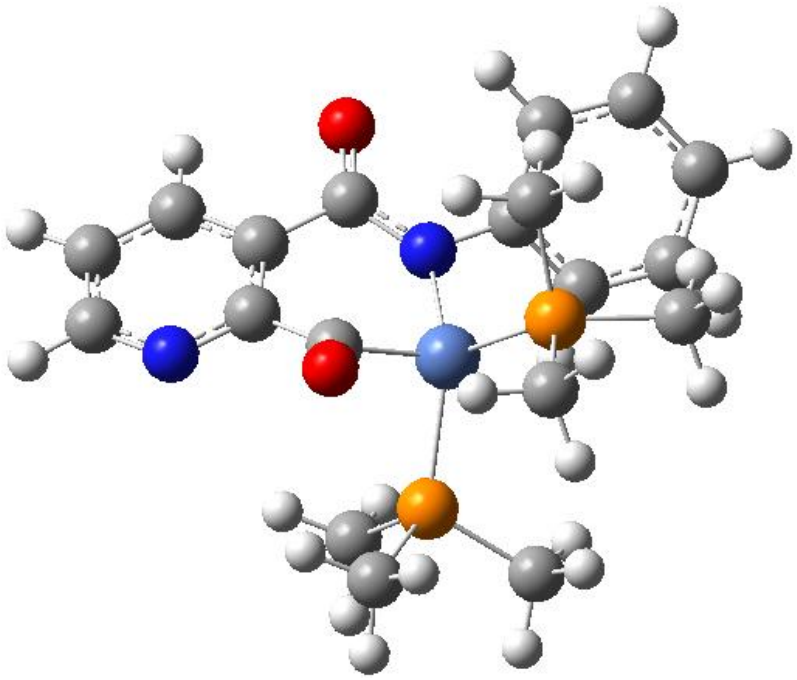

-1852.9618545

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C	-0.757119	2.363590	-0.075103
C	-2.156858	1.856844	0.179140
N	-3.781712	0.117057	0.733568
C	1.501177	1.714040	-0.596410
C	-4.537890	2.346393	0.174793
H	-5.383945	3.037802	0.036134
C	-3.216112	2.774823	0.016729
H	-2.948297	3.810651	-0.245569
C	-4.767244	0.995365	0.511064
H	-5.798695	0.611388	0.618370
C	2.219254	2.771865	0.026847
H	1.692333	3.430367	0.729724
C	3.572493	2.978154	-0.276214
H	4.113847	3.804127	0.213692
C	4.247752	2.151103	-1.198032
H	5.309036	2.330471	-1.432202
C	2.187194	0.902132	-1.541115
H	1.608307	0.133840	-2.082765
C	3.546525	1.110798	-1.831177
H	4.053057	0.470892	-2.571944
C	-1.470811	-0.490451	0.926354
O	-1.599436	-1.317414	1.812428
Ni	0.084513	-0.541152	-0.040741
P	-0.691459	-2.165692	-1.352239
P	1.711729	-1.196247	1.476258
C	-1.824877	-1.607126	-2.712674
H	-1.316981	-0.824747	-3.311605
H	-2.130452	-2.442115	-3.378823
H	-2.727224	-1.152999	-2.256443
C	-1.662021	-3.535164	-0.575064
H	-2.548134	-3.107386	-0.066158
H	-1.990123	-4.277126	-1.332246
H	-1.040117	-4.035970	0.192397
C	0.617637	-3.086517	-2.297288
H	1.298464	-3.588311	-1.580936
H	0.174855	-3.846353	-2.975294
H	1.216175	-2.373977	-2.900312
C	1.408636	-2.797834	2.367701
H	2.116720	-2.947095	3.210633
H	0.368300	-2.792872	2.748611
H	1.514585	-3.642700	1.656930
C	3.501045	-1.365841	1.005960
H	4.132668	-1.630977	1.880464
H	3.607330	-2.152727	0.231785
H	3.855220	-0.410212	0.569674
C	1.808347	-0.000137	2.891044
H	2.539757	-0.322600	3.661953
H	2.100345	0.994927	2.499135
H	0.804512	0.088773	3.352587

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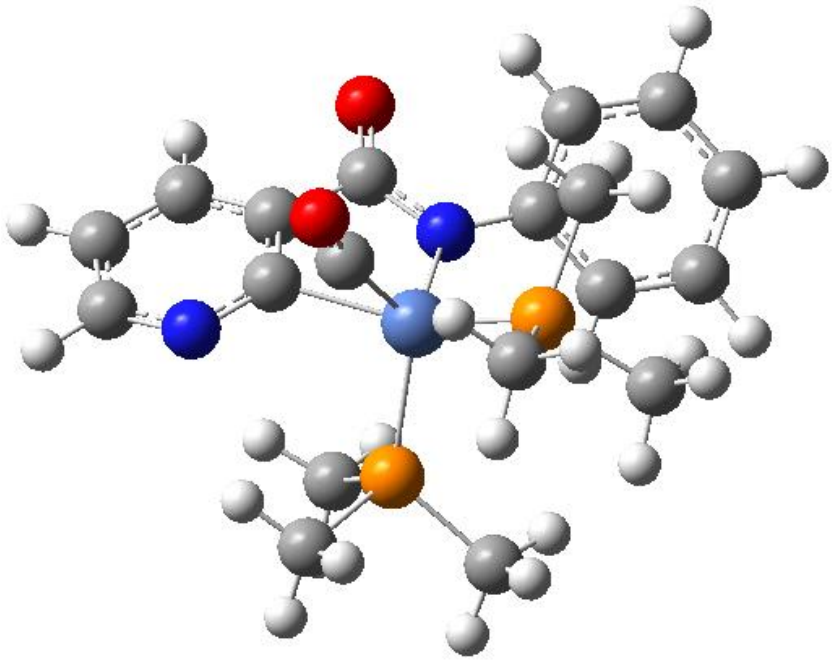

-1852.9539663

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C	0.168717	2.363092	-0.213451
C	1.622582	1.984715	-0.341216
N	3.332385	0.253014	-0.480644
C	-1.978369	1.423424	0.341885
C	3.967559	2.565589	-0.145162
H	4.777981	3.299261	-0.012484
C	2.623395	2.959416	-0.170012
H	2.297572	4.004885	-0.039776
C	4.268337	1.191488	-0.270105
H	5.313318	0.836934	-0.208715
C	-2.601409	0.510025	1.236532
H	-1.965655	-0.250856	1.716351
C	-3.971016	0.585457	1.531995
H	-4.416160	-0.130998	2.242624
C	-4.770757	1.579199	0.937923
H	-5.846106	1.643928	1.167497
C	-2.797852	2.436012	-0.236835
H	-2.333649	3.176621	-0.899633
C	-4.169216	2.497706	0.057251
H	-4.780384	3.287733	-0.409888
C	1.234245	-0.382444	-1.747740
O	1.560907	-0.511020	-2.881302
Ni	0.356838	-0.514697	-0.263627
P	-1.127391	-1.869138	-1.196066
P	1.083310	-1.393273	1.699430
C	-2.121888	-1.021261	-2.502451
H	-2.831923	-1.720368	-2.991455
H	-2.682111	-0.183092	-2.041567
H	-1.432066	-0.604601	-3.262686
C	-2.431477	-2.706216	-0.181077
H	-3.037362	-3.383938	-0.818212
H	-1.964982	-3.295857	0.631943
H	-3.088362	-1.935803	0.266794
C	-0.374227	-3.295858	-2.104537
H	-1.146932	-3.887557	-2.637894
H	0.365705	-2.911130	-2.833401
H	0.154600	-3.952056	-1.384513
C	0.024106	-2.490569	2.763343
H	-0.911343	-1.963659	3.039414
H	-0.244584	-3.408704	2.203100
H	0.556446	-2.786006	3.691866
C	1.620781	-0.106207	2.918795
H	2.033545	-0.557177	3.845095
H	2.392934	0.534431	2.448329
H	0.754269	0.537324	3.171234
C	2.608013	-2.423335	1.491683
H	3.325189	-1.844135	0.873551
H	3.068861	-2.693417	2.465066
H	2.348964	-3.348973	0.938616

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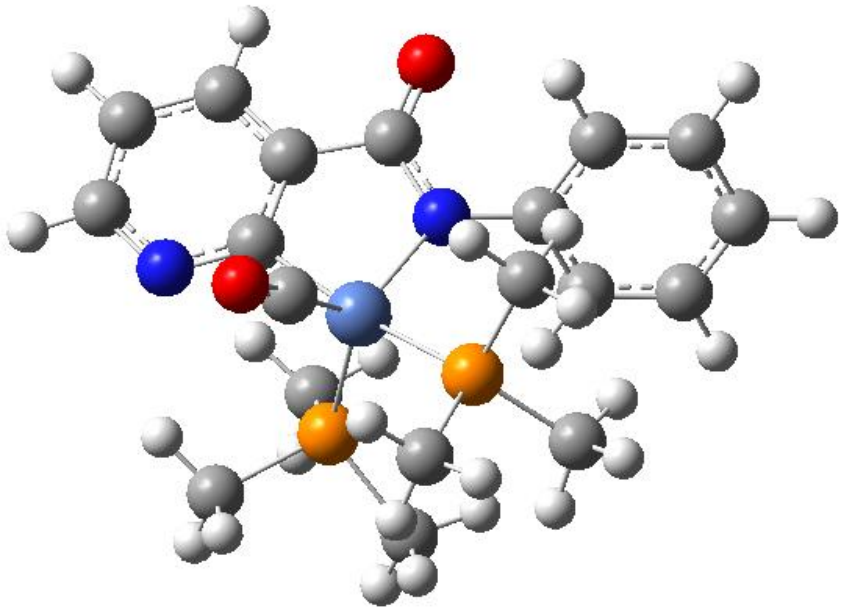

-1852.9709803

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C	1.631336	2.053341	-0.325471
N	3.314124	0.325115	-0.242520
C	-1.937932	1.385218	0.237224
C	3.973377	2.654925	-0.314819
H	4.786978	3.396756	-0.334589
C	2.623509	3.045040	-0.350241
H	2.300431	4.099352	-0.385930
C	4.269965	1.282836	-0.244970
H	5.316407	0.931564	-0.196557
C	-2.806656	2.155734	-0.582561
H	-2.392269	2.661465	-1.465900
C	-4.165228	2.294596	-0.256386
H	-4.817609	2.899035	-0.907950
C	-4.698307	1.682827	0.893975
H	-5.763448	1.802273	1.147786
C	-2.487550	0.788076	1.400021
H	-1.812080	0.221197	2.059893
C	-3.847153	0.932318	1.725038
H	-4.241659	0.464848	2.642525
C	1.301046	-0.967381	-1.873334
O	1.869017	-1.293839	-2.838424
Ni	0.492774	-0.499635	-0.386315
P	-1.275002	-1.810031	-1.029839
P	1.100552	-1.347330	1.644868
C	-2.674003	-2.305316	0.076303
H	-3.423142	-2.883124	-0.504331
H	-2.296754	-2.935095	0.905191
H	-3.149955	-1.401409	0.503168
C	-2.149831	-1.041276	-2.462605
H	-1.419682	-0.838593	-3.270710
H	-2.957118	-1.699664	-2.845230
H	-2.583409	-0.075144	-2.134080
C	-0.752383	-3.462383	-1.690934
H	-1.622071	-4.024626	-2.089455
H	-0.002971	-3.331309	-2.495559
H	-0.283942	-4.053200	-0.877948
C	1.523581	-0.050580	2.896882
H	0.643513	0.603606	3.058354
H	1.835699	-0.502527	3.861027
H	2.345079	0.577068	2.500999
C	-0.001209	-2.460753	2.650193
H	0.490999	-2.742953	3.604794
H	-0.956821	-1.948128	2.880269
H	-0.223780	-3.387575	2.084277
C	2.651407	-2.348774	1.538271
H	3.385163	-1.745644	0.963230
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H	2.444650	-3.280810	0.974297

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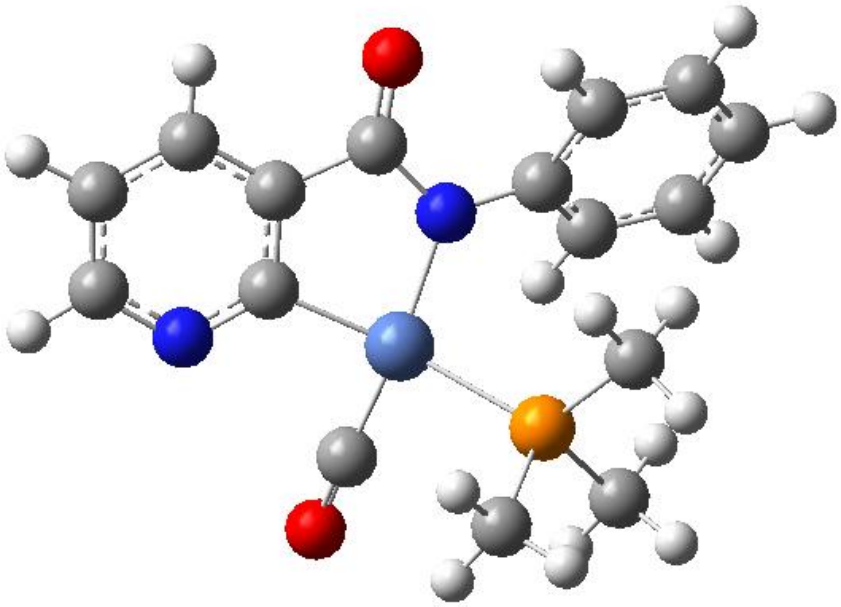

-1391.93073

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C	0.808001	-2.023912	0.356795
C	2.187878	-1.462756	0.215960
N	3.458065	0.464527	-0.483439
C	-1.469119	-1.404857	-0.257682
C	4.594972	-1.553319	0.238496
H	5.548361	-2.074120	0.418624
C	3.360100	-2.183078	0.478277
H	3.277591	-3.217039	0.853378
C	4.592126	-0.233260	-0.244860
H	5.542182	0.292166	-0.450619
C	-2.181633	-2.383965	0.485943
H	-1.657508	-2.939806	1.273208
C	-3.533116	-2.639328	0.204322
H	-4.068330	-3.399108	0.797206
C	-4.211118	-1.940752	-0.812551
H	-5.271594	-2.150532	-1.023260
C	-2.152806	-0.732662	-1.306234
H	-1.581802	-0.026340	-1.932302
C	-3.507421	-0.988420	-1.572616
H	-4.010495	-0.456394	-2.396804
C	1.271914	2.174178	-0.867620
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Ni	0.554684	0.707148	-0.255969
P	-1.240443	1.868474	0.651243
C	-2.347001	2.877082	-0.436506
H	-3.036262	3.504530	0.165879
H	-1.732901	3.531216	-1.087440
H	-2.939715	2.194918	-1.077576
C	-2.417159	0.978710	1.761891
H	-3.026130	1.709892	2.333197
H	-3.081267	0.324052	1.165728
H	-1.846161	0.342344	2.466343
C	-0.519123	3.141121	1.791667
H	0.115734	3.846261	1.218882
H	-1.316356	3.708955	2.314956
H	0.121094	2.635135	2.542299

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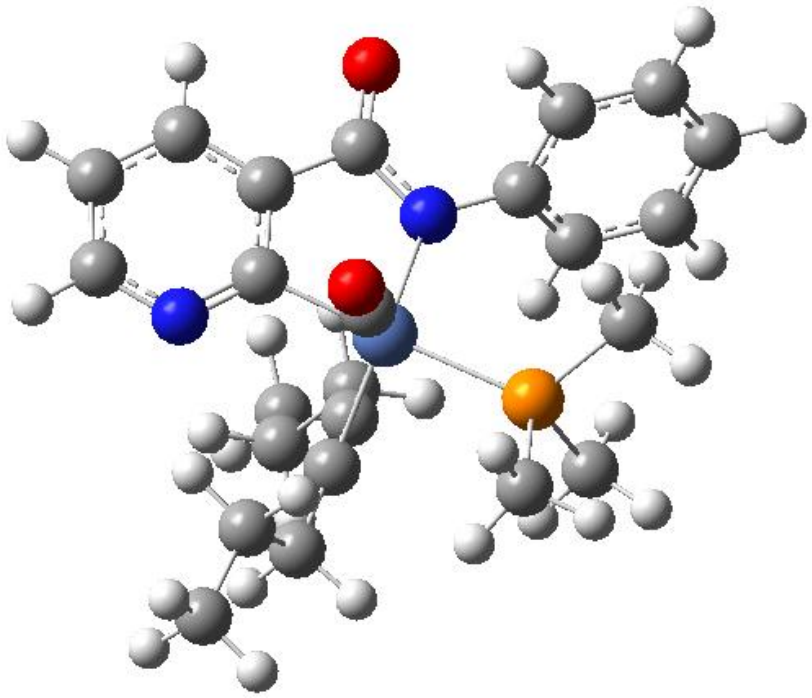

-1704.9993718

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C	-0.27625600	2.66293900	0.45376900
N	-2.40328900	1.73950600	1.11358200
C	2.67739000	0.58026000	-0.24452200
C	-3.17964100	-1.34800500	0.38947100
H	-2.96937200	-2.20532400	1.06802700
H	-3.47215100	-0.49626600	1.04738600
C	-0.71023500	-0.05397300	-2.54490800
H	-0.20125100	0.92888900	-2.43143800
H	0.08626700	-0.75126200	-2.89421400
C	-2.15328800	4.13231900	0.85317300
H	-2.61201700	5.13203500	0.90536500
C	-0.80314600	3.96294700	0.50136700
H	-0.13101100	4.80445900	0.26167900
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H	-3.98163500	3.07817200	1.43324900
C	3.00808300	-0.14470200	-1.41444500
H	2.22078100	-0.31765700	-2.16351900
C	4.31886900	-0.60151000	-1.64157300
H	4.54965400	-1.16080800	-2.56336800
C	5.33675600	-0.32815300	-0.71114200
H	6.36473600	-0.68154300	-0.88909700
C	3.72088200	0.87220200	0.67198800
H	3.48562900	1.46207400	1.57047600
C	5.02940400	0.42179100	0.44101800
H	5.82191100	0.66013100	1.16925200
C	-1.82541100	0.03566500	-3.61183200
H	-2.60739700	0.73793300	-3.25009200
H	-2.32132400	-0.95557900	-3.70438600
C	-4.34150900	-1.70659100	-0.56440700
H	-4.02291300	-2.53084400	-1.24029300
H	-4.54511500	-0.83248000	-1.22021600
C	-1.29652900	0.49161500	-4.97662400
H	-0.53134600	-0.20999900	-5.37254400
H	-2.11298600	0.55206400	-5.72535300
H	-0.82433400	1.49482000	-4.91358200
C	-5.61521000	-2.10710400	0.18925500
H	-5.96892900	-1.28732800	0.84982700
H	-6.43935900	-2.35182200	-0.51209100
H	-5.44659500	-2.99895100	0.83024400
Ni	-0.23156600	-0.14379900	0.62510500
C	-0.39720100	-0.17109100	2.39549900
O	-0.50081700	-0.16392200	3.55255900
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H	0.21216100	-3.07536600	-1.51329500
H	1.45084900	-4.14537300	-0.73903200
H	1.94345300	-2.56314700	-1.46221500
C	2.42944000	-2.38106200	1.60231800
H	2.77405700	-3.43567300	1.63056700
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C	-0.22840100	-3.48465200	1.56422100
H	-0.46830500	-3.13293000	2.58722400
H	0.28774300	-4.46524200	1.62788000
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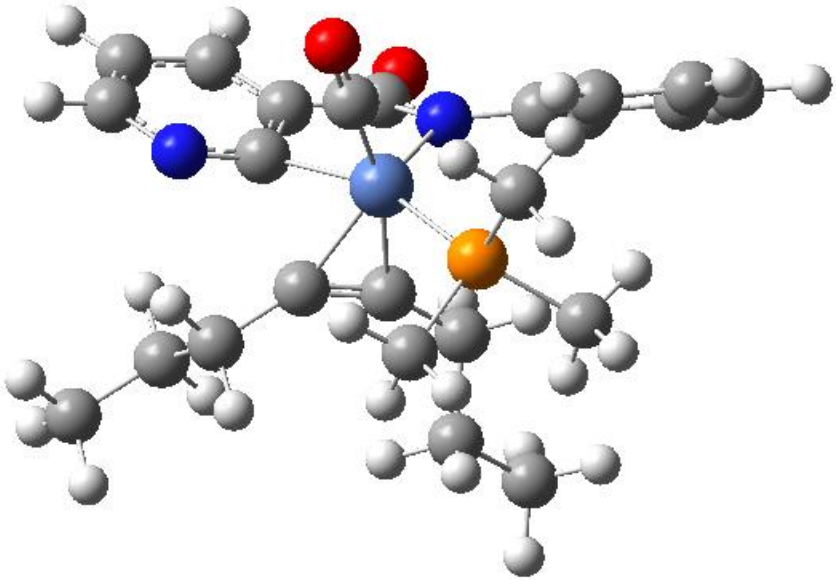

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C	3.58198300	-1.62590600	2.12073400
H	4.54246400	-1.38664500	2.61199700
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C	-4.50960900	0.12021200	0.83724700
H	-5.05937000	0.91200600	1.37299500
C	-5.19773900	-0.75955100	-0.02031400
H	-6.28352200	-0.65609000	-0.17412600
C	-3.09515600	-1.93629700	-0.46629900
H	-2.54860900	-2.76601300	-0.93111500
C	-4.47787200	-1.78485100	-0.66004800
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H	-0.16701400	-2.20271300	-2.42864400
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H	2.93753100	2.11876700	-2.27017900
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H	-0.94262900	-0.73632100	-5.06964400
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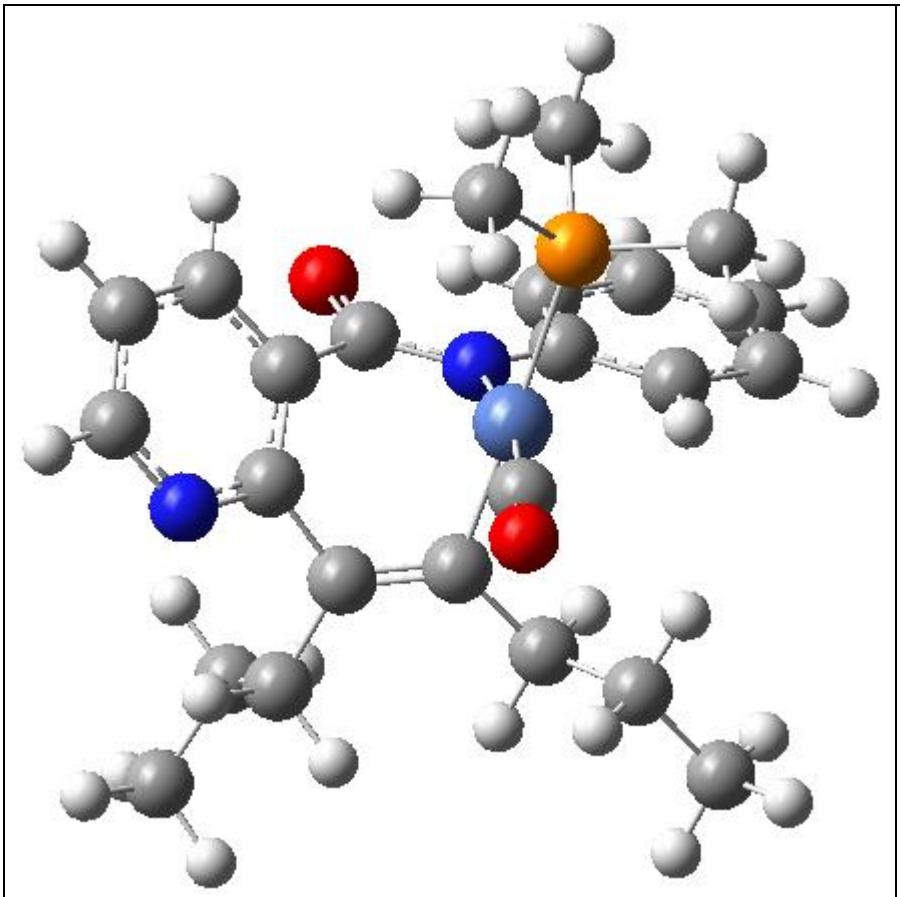

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N	3.358564	-1.571347	0.149441
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H	3.456295	2.169545	1.021119
C	0.674413	2.376983	1.284682
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H	2.805622	-4.431280	-1.612159
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H	0.882813	-3.013197	-2.490631
C	3.509212	-2.818362	-0.314545
H	4.392225	-3.374413	0.052629
C	-2.489399	1.532649	-0.413384
H	-2.241369	1.310250	0.641381
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H	-4.180257	2.793511	0.092613
C	-3.868278	2.676303	-2.062894
H	-4.713723	3.336593	-2.311893
C	-1.977517	1.287811	-2.785029
H	-1.357287	0.852960	-3.577981
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H	-3.277753	2.364991	-4.133587
C	0.129884	2.524283	2.720452
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H	2.923556	2.647862	-1.410522
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H	0.738102	4.611815	3.035398
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H	-3.652790	-2.990524	-0.825479
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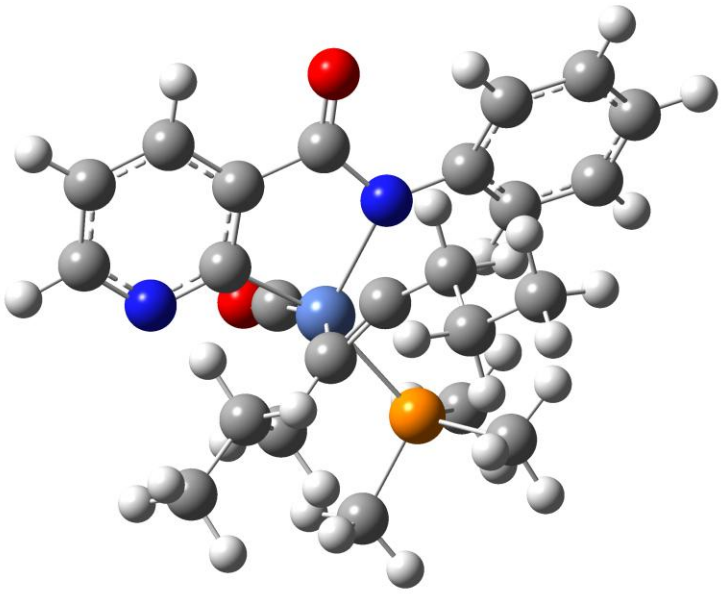

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N	3.06617800	0.11253700	1.40775400
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C	2.30632100	0.05589100	-1.83114600
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H	2.99944100	0.67351000	-1.21819500
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H	4.12227000	-2.65483000	3.09510900
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C	-4.56075900	-1.74574100	0.88520000
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C	-5.18810500	-0.50224500	0.69098700
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C	-2.99651700	0.55777100	0.68818100
H	-2.36187700	1.45533700	0.64740500
C	-4.39250400	0.65413300	0.59697300
H	-4.86482300	1.64143900	0.46384500
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H	-0.55480200	-1.34927800	-3.66767600
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H	2.35873000	-1.85816700	-2.87749300
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C	-1.66797600	-3.22558900	-3.62961600
H	-2.67944500	-2.76715400	-3.64189300
H	-1.41257400	-3.50705300	-4.67196200
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H	-1.62348300	4.78384700	-0.89288800
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C	1.02449400	3.59577700	-1.60507500
H	1.61697900	4.06082800	-0.79203000
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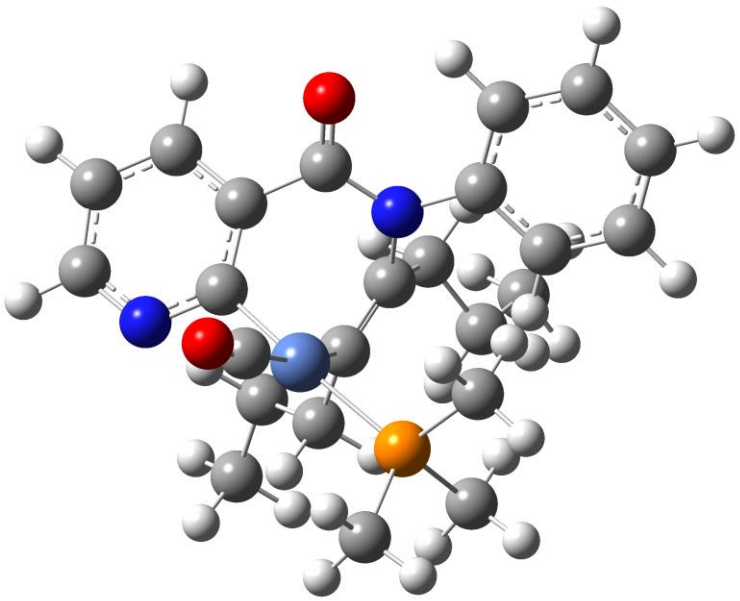
10‘



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C	0.51541000	-0.41149300	-0.84863800
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N	3.27921700	-0.54726000	0.85836400
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H	2.09431100	0.02408700	-2.25262400
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H	-0.53797900	-3.23741000	-0.75609300
H	-2.12374700	-2.57077600	-0.36309000
C	3.23854200	-2.27409800	2.55521700
H	3.79301900	-3.00887500	3.15916400
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C	3.90081000	-1.49331400	1.59408300
H	4.98419600	-1.62091800	1.41433400
C	-3.25739800	-0.50947500	2.19496600
H	-2.80353700	-0.89163300	3.11452000
C	-4.60505500	-0.11445600	2.16990200
H	-5.19934600	-0.21028700	3.09310500
C	-5.20198500	0.38817900	1.00151700
H	-6.26100100	0.69030400	0.99581400
C	-3.07223100	0.10839900	-0.15053100
H	-2.46873100	0.19290800	-1.06562700
C	-4.42183100	0.49226300	-0.16233500
H	-4.86414600	0.87841700	-1.09513400
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C	2.04910200	-2.12506400	-2.07755700
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C	-2.38810500	-3.62491800	-2.83322300
H	-3.32773400	-3.71087300	-2.24692200
H	-2.66252500	-3.61892500	-3.90854200
H	-1.79662700	-4.54665300	-2.64544700
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Ni	1.19178200	1.13246000	0.09601900
C	1.93355700	2.27369900	1.23803200
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P	0.15407800	2.67980000	-1.17946400
C	-0.53501400	2.19075000	-2.82462300
H	0.29193100	1.86026700	-3.48370200
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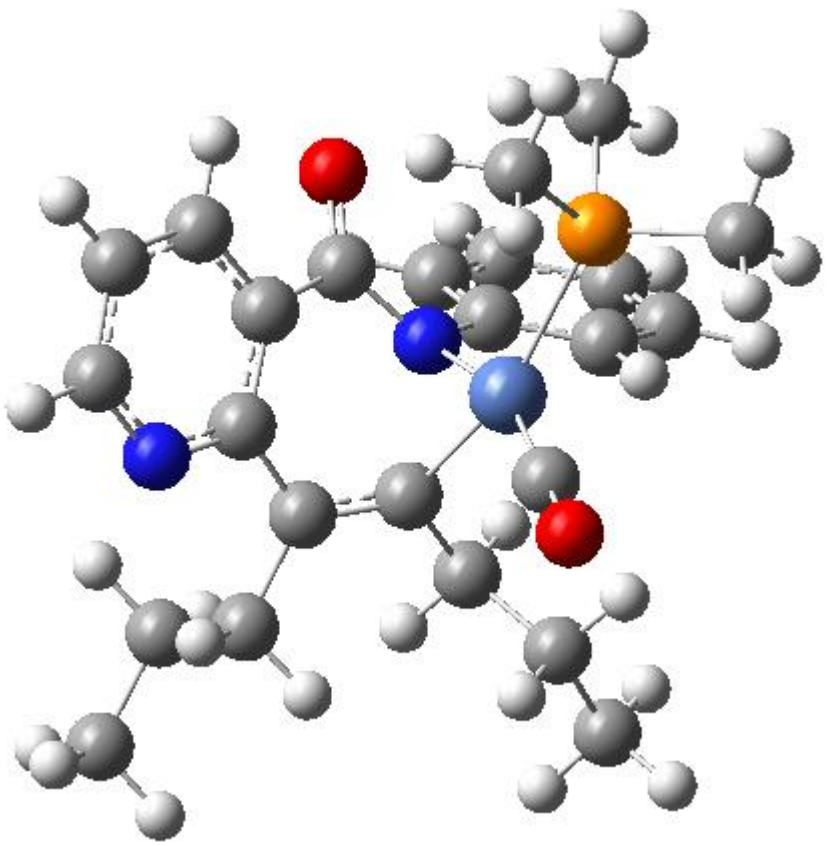

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C	-0.050439	-0.876953	-1.645937
C	2.146145	0.180552	0.212245
C	1.116405	-1.669480	-1.173331
N	3.330622	-1.883474	-0.167806
C	-1.305417	1.216206	-1.376514
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H	3.343597	1.618117	1.332568
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C	1.265701	-2.961162	-1.732176
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H	-3.742951	4.024699	-2.675367
C	-2.247417	1.819194	-0.507574
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C	-3.116902	2.822441	-0.968724
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C	0.553486	2.644580	2.226786
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H	4.323023	0.688284	-1.450498
H	3.526154	2.243920	-1.139814
C	0.528417	4.157473	2.475406
H	1.493920	4.630405	2.195081
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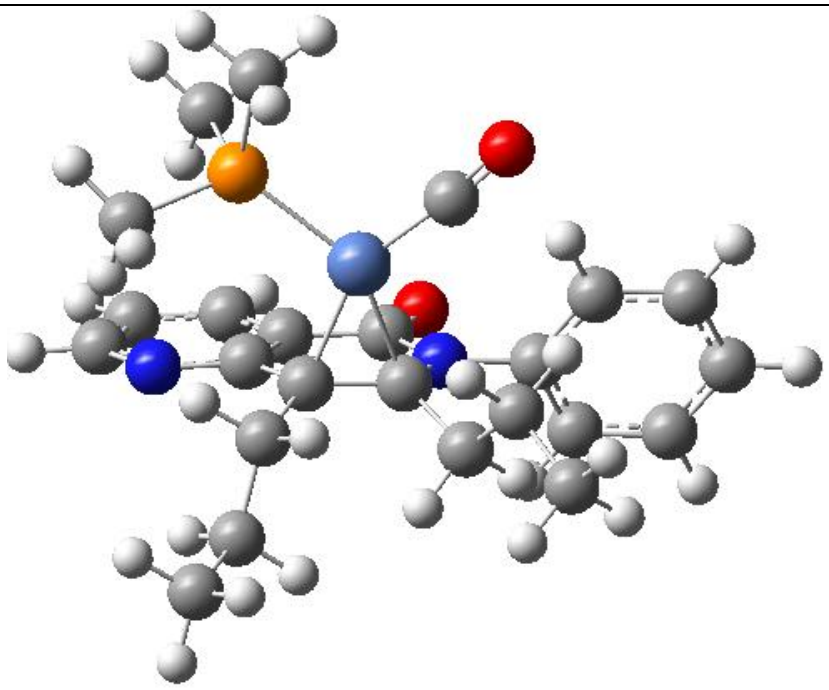

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C	-2.816945	0.793302	-0.405826
C	1.348976	-0.336652	2.250466
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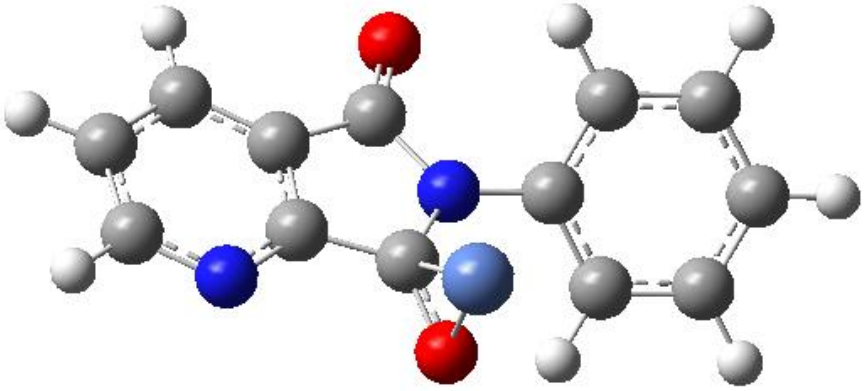
H	0.899741	-1.328931	2.467941
C	-1.602782	-0.662525	1.766759
H	-2.570601	-0.120920	1.805733
H	-1.147059	-0.512159	2.767895
C	2.582021	3.711620	-0.649692
H	3.120428	4.584082	-1.050040
C	1.249226	3.449478	-0.988939
H	0.665368	4.095428	-1.663476
C	3.217754	2.822052	0.241029
H	4.266604	3.002251	0.544071
C	-3.753256	1.704401	0.124246
H	-3.398463	2.540373	0.745581
C	-5.120377	1.544633	-0.147705
H	-5.845927	2.261199	0.268910
C	-5.562647	0.476406	-0.949718
H	-6.636334	0.351443	-1.161686
C	-3.255835	-0.265504	-1.220601
H	-2.520140	-0.956006	-1.654185
C	-4.627806	-0.424936	-1.485383
H	-4.963469	-1.257309	-2.124136
C	-1.899496	-2.162705	1.595118
H	-2.410430	-2.325495	0.622977
H	-0.939520	-2.722212	1.528779
C	1.279884	0.554609	3.511857
H	1.788695	1.515807	3.287080
H	0.219859	0.810318	3.736109
C	-2.757811	-2.725295	2.734905
H	-2.260045	-2.603246	3.721169
H	-2.958313	-3.807470	2.594068
H	-3.740056	-2.209458	2.795295
C	1.924951	-0.100827	4.738865
H	1.420369	-1.054667	5.005485
H	1.876981	0.561185	5.628455
H	2.995631	-0.334446	4.554937
Ni	0.528745	-1.129104	-0.446930
C	-0.389065	-2.330735	-1.324855
O	-0.888764	-3.186661	-1.946807
P	2.592561	-1.336940	-1.291420
C	4.089799	-1.175564	-0.212410
H	4.101728	-2.003923	0.524627
H	5.025555	-1.207369	-0.809219
H	4.019832	-0.212968	0.336087
C	2.936685	-2.924874	-2.187804
H	2.171931	-3.081112	-2.974783
H	3.944901	-2.923549	-2.652386
H	2.868893	-3.770582	-1.473709
C	2.903491	-0.070797	-2.610577
H	2.853183	0.943251	-2.166615
H	3.896754	-0.212954	-3.086136
H	2.112737	-0.147226	-3.383678

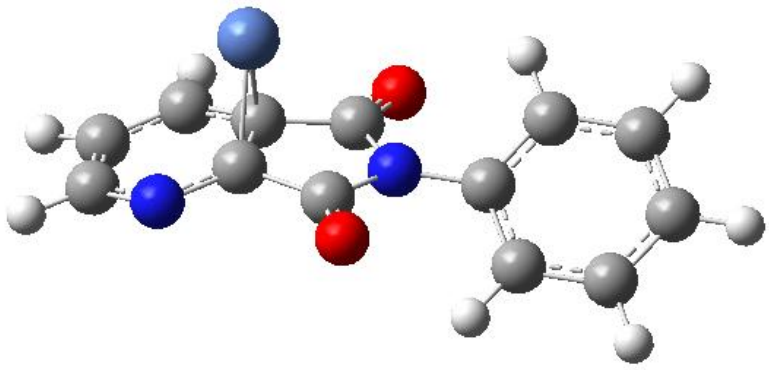
12



-930.8258456

O	-0.045280	2.812410	-0.297854
N	-0.367574	0.520477	0.179788
C	1.876552	-0.110883	0.301570
C	0.399702	1.698279	-0.059695
C	1.822745	1.271742	0.034233
N	3.000423	-0.821119	0.466056
C	-1.793699	0.486531	0.170072
C	4.204526	1.272462	0.083262
H	5.185126	1.766796	0.005638
C	3.012631	1.998475	-0.088639
H	3.002507	3.078804	-0.302887
C	4.142168	-0.114149	0.361016
H	5.078441	-0.683611	0.502831
C	-2.511016	1.243559	-0.783734
H	-1.967727	1.863196	-1.509127
C	-3.914172	1.214183	-0.784174
H	-4.465002	1.810613	-1.528781
C	-4.613992	0.430120	0.149823
H	-5.715174	0.408849	0.142198
C	-2.493716	-0.292894	1.118691
H	-1.933219	-0.876109	1.860883
C	-3.897346	-0.322454	1.096231
H	-4.434494	-0.936460	1.836523
C	0.478084	-0.636329	0.346734
O	0.085751	-1.738651	0.936268
Ni	0.222180	-2.205339	-0.796709

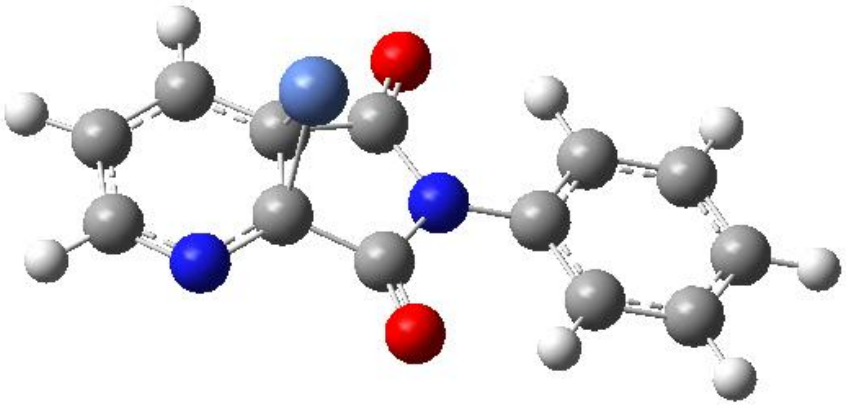
12isomer



-930.8300458

O	-0.338339	-2.160164	-0.948620
N	-0.715489	0.061775	-0.228553
C	1.519136	0.771901	-0.051210
C	0.083081	-1.068390	-0.599562
C	1.508236	-0.619054	-0.476644
N	2.581929	1.627857	-0.215922
C	-2.142007	0.046213	-0.174670
C	3.776003	-0.276483	-1.210215
H	4.717723	-0.613596	-1.669973
C	2.703730	-1.153369	-1.061378
H	2.739990	-2.195216	-1.418373
C	3.661667	1.088643	-0.777401
H	4.527733	1.762767	-0.913711
C	-2.822643	-1.110189	0.268077
H	-2.253686	-2.005008	0.551979
C	-4.225186	-1.115998	0.319393
H	-4.747363	-2.023979	0.660620
C	-4.959741	0.022429	-0.055205
H	-6.060099	0.013251	-0.008832
C	-2.876592	1.189467	-0.560515
H	-2.349130	2.090361	-0.899334
C	-4.278415	1.171784	-0.491575
H	-4.842578	2.069798	-0.789413
C	0.083276	1.211046	0.122630
O	-0.352481	2.288235	0.482478
Ni	1.733772	-0.460656	1.422040

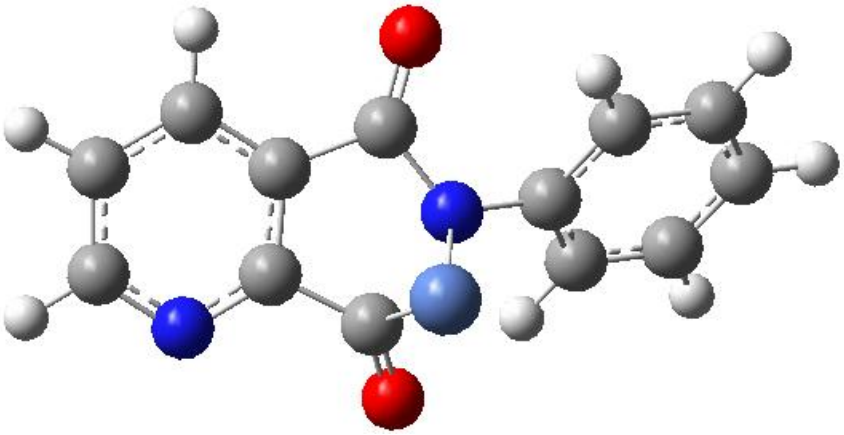
12isomerTS **(rotation phenyl, barrier of 0.1 kcal/mol)**



-930.8249604

O	0.288950	2.349190	-0.279348
N	0.722051	0.001068	-0.236008
C	-1.535021	-0.717172	-0.276029
C	-0.095701	1.188455	-0.262807
C	-1.519066	0.730432	-0.275531
N	-2.601704	-1.486665	-0.675174
C	2.158782	-0.001245	-0.182350
C	-3.789171	0.630602	-1.063951
H	-4.730853	1.090861	-1.400417
C	-2.711046	1.421352	-0.673460
H	-2.739740	2.522093	-0.711406
C	-3.681014	-0.802387	-1.047521
H	-4.552177	-1.403693	-1.367685
C	2.884818	1.217975	-0.174937
H	2.346039	2.170086	-0.217626
C	4.286836	1.203380	-0.115129
H	4.825572	2.164579	-0.110486
C	4.999159	-0.005457	-0.064279
H	6.099577	-0.007199	-0.018964
C	2.879247	-1.222675	-0.134085
H	2.336673	-2.173491	-0.145096
C	4.281358	-1.212045	-0.075028
H	4.815667	-2.174986	-0.038245
C	-0.105017	-1.193036	-0.243339
O	0.284371	-2.346658	-0.226566
Ni	-1.719812	0.027200	1.498792

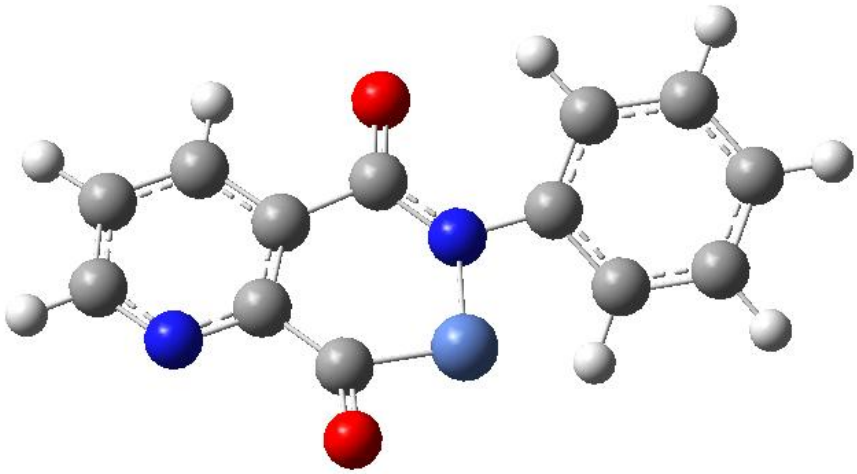
12-13



-930.8032047

O	0.033786	2.469105	-0.048457
N	0.433538	0.137292	0.052900
C	-1.947684	-0.511404	-0.387944
C	-0.376832	1.317487	-0.042320
C	-1.796024	0.887092	-0.229250
N	-3.111233	-1.131532	-0.617072
C	1.849514	0.153285	-0.171796
C	-4.157521	1.073036	-0.573824
H	-5.086373	1.656883	-0.664918
C	-2.922175	1.709323	-0.340217
H	-2.826523	2.802559	-0.249619
C	-4.196412	-0.330520	-0.699029
H	-5.159579	-0.839840	-0.882533
C	2.666842	1.124154	0.453276
H	2.210288	1.875487	1.111886
C	4.048147	1.132306	0.206615
H	4.678347	1.895686	0.690103
C	4.627309	0.176529	-0.647902
H	5.712933	0.185169	-0.833354
C	2.426369	-0.804837	-1.035789
H	1.787335	-1.562289	-1.509464
C	3.811914	-0.789207	-1.263322
H	4.256044	-1.541114	-1.934870
C	-0.656900	-1.264671	-0.213162
O	-0.281688	-2.328768	-0.673745
Ni	-0.182310	-0.781107	1.559556

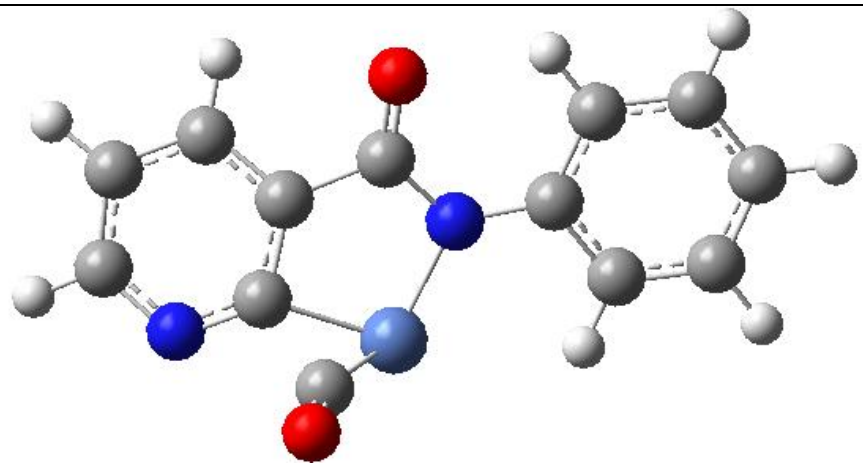
13



-930.8369394

O	0.069840	2.523751	0.082067
N	-0.581896	0.308058	0.204659
C	2.338066	-0.425542	-0.065153
C	0.342994	1.312701	0.113454
C	1.810462	0.892522	0.067295
N	3.655431	-0.722386	-0.117819
C	-1.975359	0.454103	0.134881
C	4.122940	1.640734	0.083138
H	4.878921	2.439849	0.137502
C	2.757098	1.937825	0.132141
H	2.374656	2.966566	0.218691
C	4.523139	0.291998	-0.040874
H	5.595039	0.026314	-0.083161
C	-2.689978	1.603374	-0.289610
H	-2.130488	2.522787	-0.502729
C	-4.085570	1.533729	-0.421428
H	-4.632875	2.431766	-0.751071
C	-4.797333	0.348240	-0.150208
H	-5.891750	0.317942	-0.265365
C	-2.708959	-0.727716	0.450282
H	-2.178881	-1.596007	0.920029
C	-4.100875	-0.791667	0.288482
H	-4.641602	-1.719414	0.532746
C	1.398831	-1.559752	-0.149934
O	1.522440	-2.771709	-0.309373
Ni	-0.329955	-1.484612	0.003183

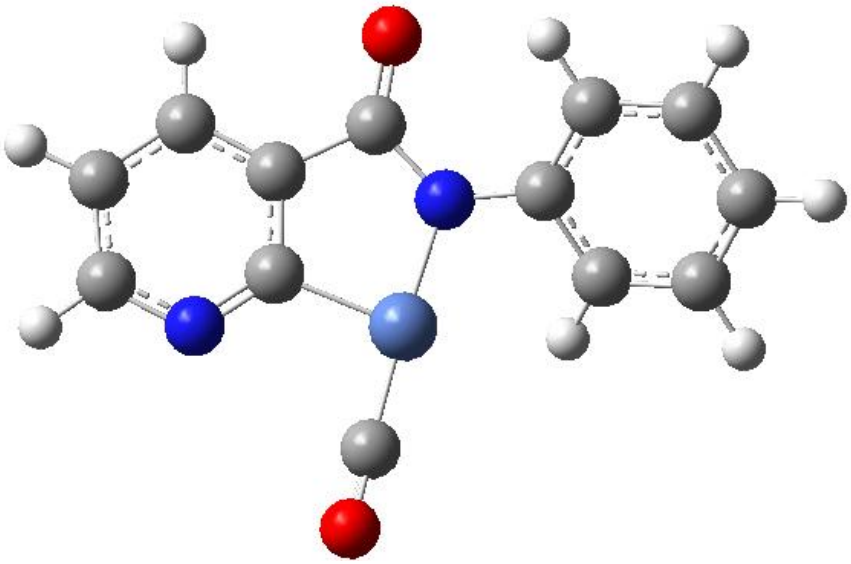
13-14



-930.7983166

O	0.272756	2.383991	0.683861
N	0.721952	0.200807	-0.103908
C	-2.105919	-0.369879	-0.031310
C	-0.083698	1.261157	0.308097
C	-1.563882	0.949283	0.142353
N	-3.351255	-0.616949	-0.475199
C	2.127363	0.223675	-0.067279
C	-3.795048	1.756608	-0.378214
H	-4.522152	2.574212	-0.500677
C	-2.470930	2.016942	0.001317
H	-2.082507	3.037987	0.150460
C	-4.173688	0.424050	-0.658901
H	-5.185312	0.192161	-1.036859
C	2.919371	1.359888	0.257953
H	2.413644	2.295897	0.523355
C	4.320076	1.268876	0.223040
H	4.917344	2.160793	0.472959
C	4.967432	0.069631	-0.121984
H	6.067129	0.012903	-0.138781
C	2.796485	-0.984509	-0.404132
H	2.181833	-1.877803	-0.628732
C	4.192089	-1.063855	-0.436535
H	4.679597	-2.016534	-0.697832
C	-1.513993	-1.703358	0.811047
O	-1.848770	-2.214136	1.827272
Ni	-0.398225	-1.288447	-0.430426

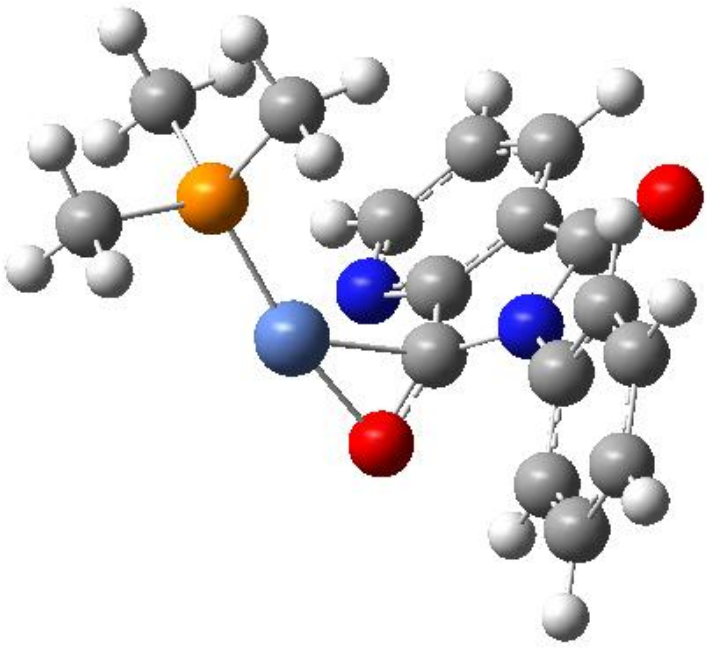
14



-930.8628093

O	-0.155163	-2.905628	-0.194839
N	-0.560178	-0.596404	-0.321224
C	1.853505	0.113050	0.017416
C	0.224919	-1.734441	-0.211611
C	1.653014	-1.284240	-0.099072
N	3.023529	0.679366	0.170121
C	-1.942741	-0.500926	-0.176774
C	4.050654	-1.502505	0.084122
H	4.969814	-2.107408	0.118528
C	2.784224	-2.106968	-0.052608
H	2.653977	-3.200317	-0.117199
C	4.129275	-0.103947	0.194378
H	5.099188	0.408381	0.314654
C	-2.774083	-1.469383	0.448276
H	-2.336673	-2.430814	0.749078
C	-4.128775	-1.180565	0.652832
H	-4.771748	-1.937902	1.129891
C	-4.682926	0.060242	0.268429
H	-5.750221	0.266916	0.443040
C	-2.520974	0.726683	-0.615261
H	-1.900663	1.424561	-1.213828
C	-3.872430	1.016835	-0.364388
H	-4.299235	1.974963	-0.700505
C	0.873360	2.691536	0.157468
O	1.283092	3.754596	0.350759
Ni	0.220948	1.067032	-0.097591

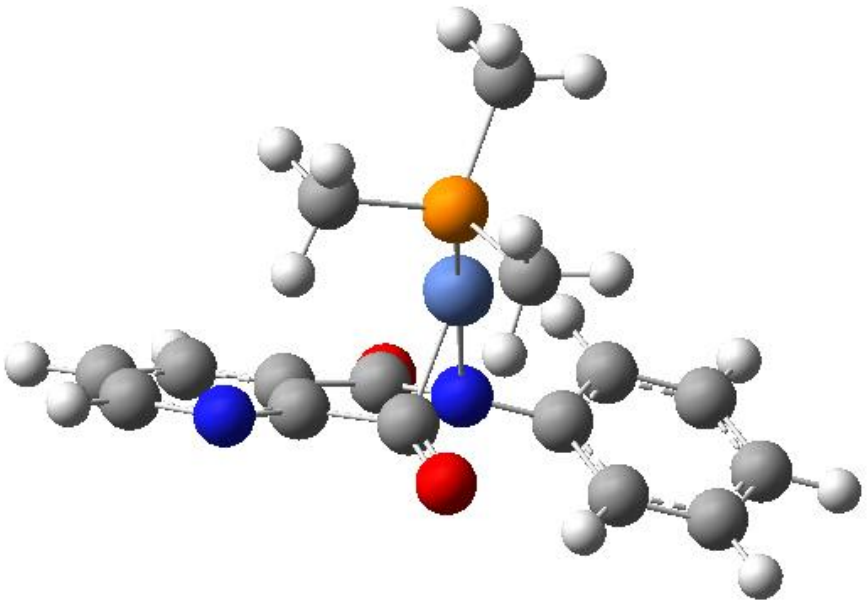
15



-1391.9191025

O	-1.17088200	-2.56669200	1.83059200
N	-1.01863200	-1.13780700	-0.04761600
C	1.19580700	-1.59631200	-0.63249100
C	-0.54170200	-2.09603200	0.89053000
C	0.86186800	-2.38213800	0.49009500
N	2.37404500	-1.63093300	-1.27182300
C	-2.33480100	-0.59100700	-0.02954700
C	3.05398400	-3.30911400	0.37320100
H	3.85492500	-3.97696500	0.72617200
C	1.80953600	-3.26162700	1.02621600
H	1.57784500	-3.88328300	1.90559400
C	3.27599500	-2.48985000	-0.76024000
H	4.24895600	-2.53706400	-1.28253100
C	-2.98025200	-0.33224000	1.20183700
H	-2.46912100	-0.56794300	2.14400700
C	-4.27982800	0.19777400	1.21120600
H	-4.77527300	0.39032800	2.17632000
C	-4.94653200	0.48291900	0.00670800
H	-5.96594100	0.89991400	0.02090300
C	-3.00729200	-0.31642000	-1.24286300
H	-2.50507000	-0.51900400	-2.19748400
C	-4.30240000	0.22491000	-1.21568800
H	-4.81529300	0.43871500	-2.16702600
C	0.02438900	-0.73406300	-0.96946100
O	-0.20146600	-0.13443200	-2.09458600
Ni	0.55686700	1.17964300	-1.01538400
P	1.43098400	2.40709000	0.47638200
C	1.52205000	4.21995000	0.06909500
H	1.98891100	4.79805300	0.89386500
H	2.11679900	4.36299100	-0.85565100
H	0.50017000	4.60912100	-0.11365800
C	3.18909400	2.02421600	0.93591200
H	3.56937500	2.71401600	1.71872500
H	3.24820900	0.98091300	1.30520500
H	3.82728300	2.10208600	0.03320000
C	0.59282600	2.42423000	2.13271400
H	0.58063100	1.39647400	2.54755400
H	1.11252900	3.09903800	2.84530600
H	-0.45752100	2.75525500	2.00922100

15-16



-1391.8994509

O	1.304274	-2.649533	-1.414970
N	1.017571	-0.766450	-0.017052
C	-1.288258	-1.390896	0.733943
C	0.617434	-1.953248	-0.676403
C	-0.793649	-2.251767	-0.272484
N	-2.514466	-1.473600	1.271527
C	2.380494	-0.340742	0.075000
C	-2.894223	-3.397866	-0.181034
H	-3.587154	-4.191085	-0.501425
C	-1.602699	-3.293513	-0.735418
H	-1.225914	-3.992394	-1.498629
C	-3.296562	-2.469373	0.799498
H	-4.309408	-2.536014	1.236449
C	3.239028	-0.414817	-1.048807
H	2.859633	-0.828194	-1.992722
C	4.571016	0.013935	-0.938612
H	5.233027	-0.055499	-1.816775
C	5.061402	0.527697	0.275208
H	6.107134	0.864624	0.353769
C	2.873524	0.169112	1.299251
H	2.201801	0.228816	2.166136
C	4.205402	0.604344	1.387999
H	4.578480	1.001948	2.345618
C	-0.307923	-0.323848	1.142536
O	-0.098901	0.165051	2.241042
Ni	-0.209172	0.673681	-0.468964
P	-1.596699	2.293035	-0.386903
C	-3.360653	1.783185	-0.152065
H	-4.016001	2.660551	0.030234
H	-3.709043	1.245161	-1.056539
H	-3.416969	1.082611	0.706358
C	-1.687924	3.482583	-1.809073
H	-2.429376	4.285600	-1.614995
H	-0.691789	3.940300	-1.974086
H	-1.976110	2.936925	-2.730027
C	-1.279371	3.394460	1.066364
H	-0.296194	3.890446	0.940330
H	-2.071960	4.163494	1.178279
H	-1.229808	2.764861	1.977257

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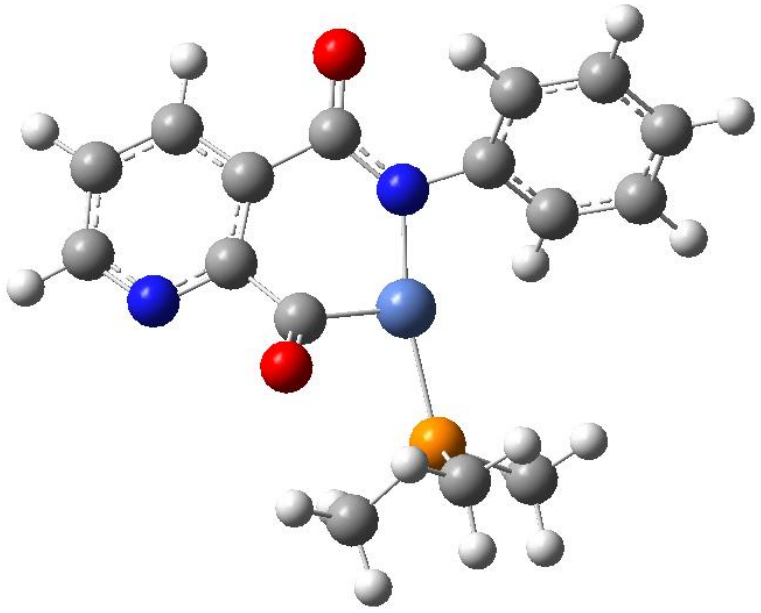
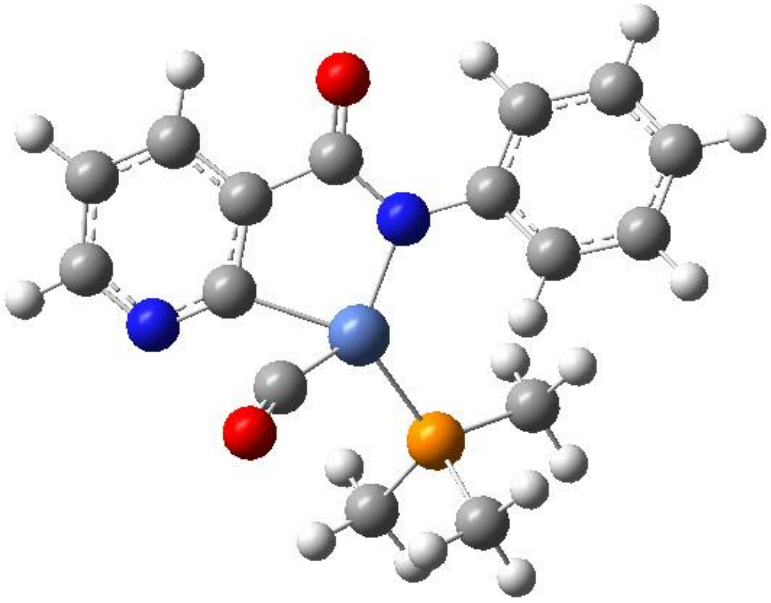


-1391.9210368

O	0.85353100	-3.37481500	-0.04327500
N	-0.19653800	-1.30321900	-0.19682500
C	2.41275900	-0.05560800	0.22440400
C	0.88567900	-2.13651000	-0.09442500
C	2.21679500	-1.41546200	-0.12398400
N	3.60772100	0.56776400	0.17293500
C	-1.52548300	-1.75532500	-0.10356200
C	4.60437700	-1.51875400	-0.54145700
H	5.51397400	-2.06675900	-0.83335800
C	3.36142100	-2.15909000	-0.47329800
H	3.22982200	-3.23106100	-0.68943400
C	4.66959800	-0.14597000	-0.22757800
H	5.63020100	0.39782000	-0.28918900
C	-1.96297900	-2.82227200	0.72463200
H	-1.21796800	-3.41766700	1.26829200
C	-3.33167900	-3.10452800	0.82925300
H	-3.66017800	-3.93531300	1.47480100
C	-4.29240700	-2.34372400	0.13085000
H	-5.36355400	-2.58126700	0.22611400
C	-2.49881400	-1.02111500	-0.83939300
H	-2.14436500	-0.26738900	-1.56859200
C	-3.87026000	-1.29792800	-0.70673600
H	-4.60659800	-0.71766600	-1.28580700
C	1.28099100	0.79911900	0.75843800
O	1.42167300	1.59393500	1.66927600
Ni	-0.30991800	0.55521800	-0.12605000
P	-0.86628500	2.66632800	-0.12961300
C	0.45133500	3.86224300	-0.62700700
H	0.08728600	4.90874000	-0.56826100
H	1.31819100	3.73272900	0.05036400
H	0.77904000	3.64243700	-1.66257700
C	-2.28492800	3.10844200	-1.23828800
H	-2.53731100	4.18605700	-1.15505500
H	-2.02152900	2.87729400	-2.29006200
H	-3.17194300	2.50526200	-0.95864700
C	-1.40452400	3.28161700	1.52741100
H	-1.63374600	4.36718100	1.50255700
H	-2.30143800	2.72068300	1.85749400
H	-0.57909000	3.08230900	2.23860300

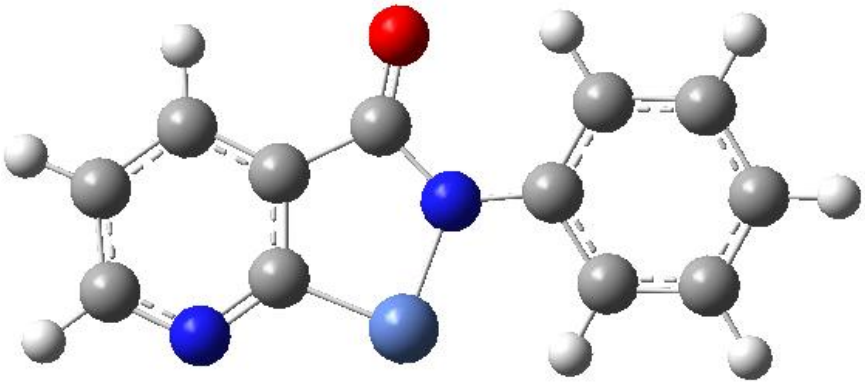
16-8



-1391.8913545

O	0.10155900	-3.34863000	0.14171600
N	-0.49986400	-1.07426200	0.06642600
C	2.25374900	-0.34805100	0.21683400
C	0.37931100	-2.14425700	0.10333500
C	1.82637100	-1.69257100	0.03576200
N	3.48157700	0.08115100	-0.10247700
C	-1.89655200	-1.29862900	0.10193500
C	4.11015700	-2.19022100	-0.62991800
H	4.89513300	-2.89607200	-0.94283700
C	2.80181100	-2.62158200	-0.37321300
H	2.47748300	-3.66760200	-0.50382000
C	4.39124100	-0.81479000	-0.52147600
H	5.38963900	-0.41694700	-0.77702600
C	-2.52783600	-2.36239800	-0.59308800
H	-1.91060200	-3.08601800	-1.14082700
C	-3.92522300	-2.49308300	-0.57048400
H	-4.39543700	-3.32340900	-1.12227600
C	-4.72713600	-1.58520200	0.14499700
H	-5.82249700	-1.69984300	0.16102700
C	-2.71329200	-0.39901800	0.83249400
H	-2.21878400	0.39789600	1.41256400
C	-4.11006400	-0.53724200	0.85215800
H	-4.72024900	0.17045100	1.43705100
C	1.63874400	1.00461900	1.23646100
O	2.14781800	1.42835800	2.21630300
Ni	0.40833300	0.60283300	0.12419500
P	-0.48413200	2.50074500	-0.46742900
C	-1.07762700	3.54792900	0.93538900
H	-0.24123800	3.71717800	1.64248000
H	-1.45888100	4.52448800	0.57154100
H	-1.88790200	3.01869300	1.47506100
C	-1.95099900	2.39787600	-1.58961900
H	-2.73566500	1.78456500	-1.10258300
H	-2.35239200	3.40538500	-1.82701900
H	-1.65448800	1.89015400	-2.52930200
C	0.66890000	3.62945400	-1.37435700
H	1.04063100	3.11898400	-2.28521000
H	0.16749200	4.57689200	-1.66326100
H	1.54008300	3.85166600	-0.72664200

17



-817.5113576

O	0.105496	2.528884	0.186678
N	-0.433779	0.253279	0.167044
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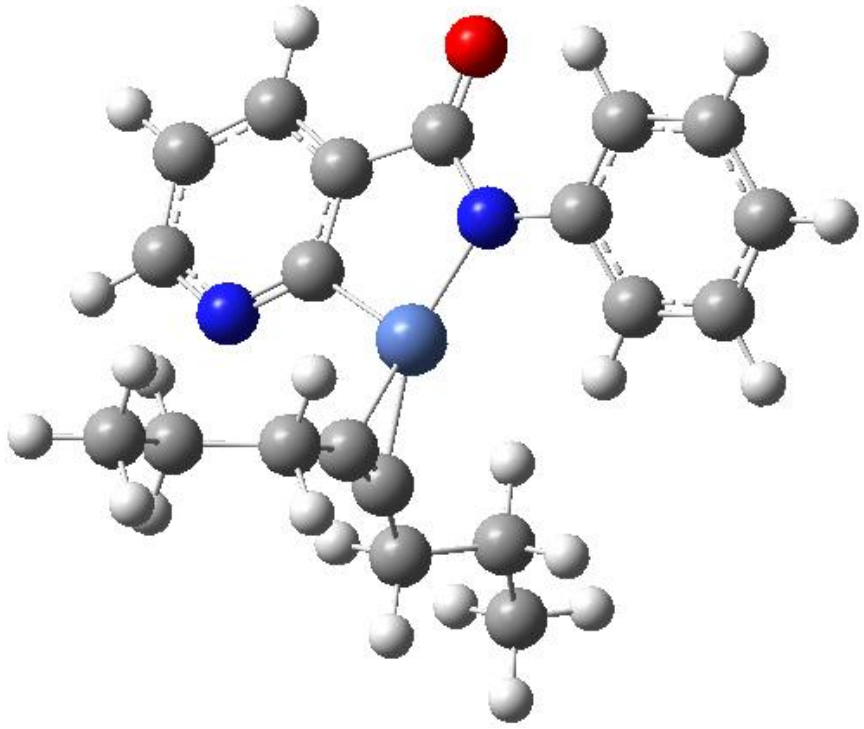
C	0.432999	1.340391	0.148338
C	1.836750	0.817124	0.065966
N	3.039235	-1.276978	-0.158532
C	-1.824693	0.245093	0.095432
C	4.244457	0.815024	-0.046353
H	5.215000	1.334581	-0.051353
C	3.035072	1.538591	0.058963
H	3.014590	2.638794	0.131324
C	4.208453	-0.586846	-0.154133
H	5.136926	-1.176457	-0.243188
C	-2.642262	1.372989	-0.180753
H	-2.164691	2.355482	-0.288704
C	-4.029947	1.203264	-0.295591
H	-4.656938	2.085052	-0.505364
C	-4.633320	-0.061741	-0.153479
H	-5.724254	-0.172640	-0.251005
C	-2.445938	-1.022646	0.273347
H	-1.821450	-1.896672	0.574591
C	-3.830817	-1.181724	0.131364
H	-4.286040	-2.175582	0.265789
Ni	0.304737	-1.407328	-0.020313

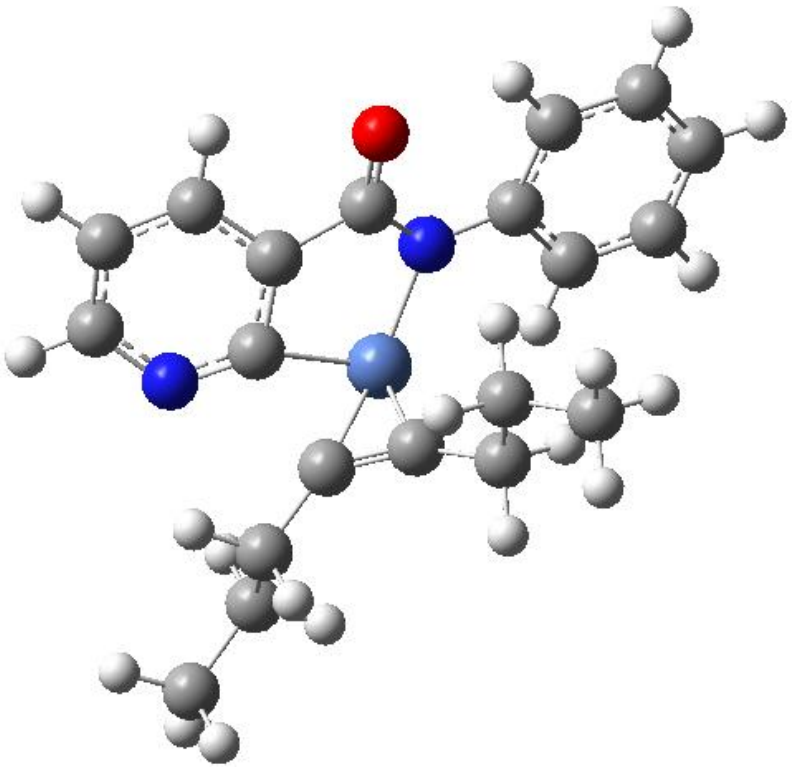
18



-1130.6356344

O	2.015683	3.033161	-0.480871
N	1.357003	0.797808	-0.131848
C	-1.327295	-1.484279	0.996624
C	-1.143368	1.254046	-0.455563
C	1.164008	2.141990	-0.412192
C	-1.336229	-1.799775	-0.238967
C	-0.300447	2.372527	-0.641368
N	-2.447930	1.273532	-0.624723
C	2.598572	0.225478	0.202260
C	-1.754301	-2.445778	-1.502495
H	-2.562387	-1.811285	-1.936286
H	-2.228906	-3.423711	-1.255277
C	-1.705760	-1.453500	2.428849
H	-0.930379	-0.916198	3.017757
H	-1.705411	-2.502719	2.806532
C	-2.286689	3.618873	-1.202068
H	-2.800586	4.545733	-1.500707
C	-0.889554	3.585117	-1.015875
H	-0.246738	4.470399	-1.155918
C	-3.026054	2.441571	-1.000589
H	-4.121096	2.427486	-1.141647
C	3.700116	0.958155	0.722047
H	3.617181	2.048535	0.811024
C	4.877366	0.288335	1.087398
H	5.722866	0.874270	1.483580
C	4.995183	-1.108459	0.957505
H	5.925821	-1.619978	1.249281
C	2.737630	-1.180938	0.050161
H	1.906821	-1.753262	-0.399785
C	3.914111	-1.840290	0.435147
H	3.992051	-2.932130	0.307860
C	-3.088538	-0.805368	2.677240
H	-3.080614	0.222849	2.257870
H	-3.855593	-1.364313	2.098582
C	-0.638111	-2.644914	-2.548620
H	-0.174067	-1.658613	-2.768809
H	0.166594	-3.270698	-2.103790
C	-3.460038	-0.775369	4.163798
H	-3.496658	-1.797726	4.597572
H	-4.456013	-0.311936	4.318078
H	-2.724206	-0.189927	4.755235
C	-1.148964	-3.289173	-3.841766
H	-1.594159	-4.289259	-3.651157
H	-0.328367	-3.423850	-4.575529
H	-1.930320	-2.664615	-4.324972
Ni	-0.174094	-0.277615	0.038726

18-19



-1130.5771123

O	1.613872	2.311792	1.295221
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C	-0.694804	-1.486457	0.402619
C	-1.606539	1.009938	-0.046187
C	0.887242	1.638656	0.552392
C	-1.858346	-0.921098	0.115102
C	-0.625187	1.879090	0.551384
N	-2.820373	1.439674	-0.369106
C	2.609355	0.357406	-0.674860
C	-3.301721	-1.317051	0.080783
H	-3.917877	-0.451568	0.404566
H	-3.455640	-2.138870	0.816435
C	0.115179	-2.415290	1.220767
H	0.994225	-2.768629	0.639219
H	-0.512380	-3.316221	1.427018
C	-2.397105	3.546075	0.714498
H	-2.768940	4.531946	1.033204
C	-1.076843	3.142134	0.974475
H	-0.336747	3.805238	1.452754
C	-3.216498	2.679615	-0.026439
H	-4.229279	2.981374	-0.347391
C	2.822795	-0.670201	-1.633878
H	1.937484	-1.123458	-2.115403
C	4.112482	-1.096771	-1.972100
H	4.242777	-1.896042	-2.719644
C	5.235923	-0.503595	-1.364501
H	6.252879	-0.833444	-1.629369
C	3.750271	0.950585	-0.065979
H	3.598634	1.744715	0.674885
C	5.039193	0.516908	-0.417816
H	5.909653	0.991408	0.064430
C	0.591511	-1.798136	2.560117
H	1.192653	-0.891048	2.338438
H	-0.296197	-1.452033	3.132689
C	-3.776690	-1.764586	-1.319027
H	-3.611034	-0.922900	-2.025309
H	-3.133898	-2.601481	-1.670910
C	1.414978	-2.783478	3.396846
H	0.828930	-3.690638	3.657995
H	1.748183	-2.315466	4.345576
H	2.323684	-3.116305	2.852217
C	-5.250404	-2.186133	-1.335967
H	-5.439738	-3.039505	-0.649821
H	-5.567740	-2.498921	-2.352112
H	-5.913757	-1.352944	-1.020406
Ni	-0.306505	-0.211095	-0.838038

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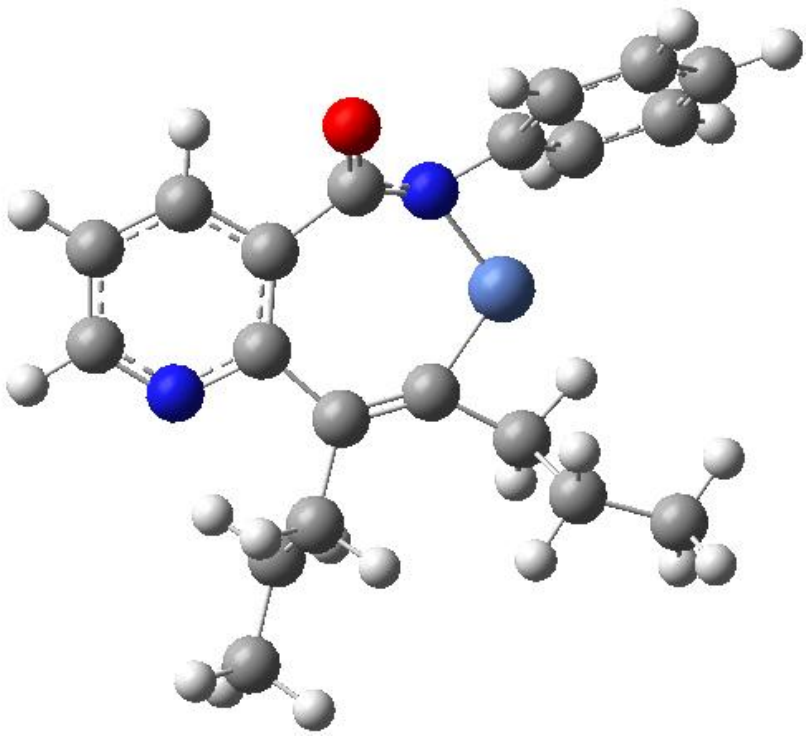

-1130.6388419

O	-0.996565	-2.974117	0.978762
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C	0.639669	1.019132	-0.013291
C	2.053790	-1.055713	0.122490
C	-0.448008	-2.074214	0.326731
C	1.830564	0.416628	0.209431
C	1.066027	-2.105932	0.160242
N	3.377522	-1.366545	0.053596
C	-2.543847	-0.922172	-0.293254
C	3.058371	1.290434	0.474652
H	3.734800	0.749501	1.168128
H	2.737689	2.223338	0.987397
C	0.099063	2.403640	-0.056956
H	-1.008172	2.353354	-0.508805
H	0.580517	3.028238	-0.845007
C	2.910296	-3.724245	0.022552
H	3.278768	-4.760783	-0.019111
C	1.548133	-3.437392	0.131064
H	0.803547	-4.243670	0.209424
C	3.791931	-2.632375	-0.012438
H	4.884889	-2.787806	-0.087368
C	-3.419313	-1.356130	0.748005
H	-3.040617	-2.082712	1.477996
C	-4.722845	-0.859233	0.796703
H	-5.395208	-1.204141	1.599357
C	-5.200929	0.079653	-0.151514
H	-6.233475	0.455681	-0.082463
C	-3.048002	-0.011671	-1.287537
H	-2.452927	0.151283	-2.207691
C	-4.365820	0.496259	-1.191927
H	-4.738797	1.184969	-1.966839
C	-0.055153	3.181081	1.270621
H	-0.502822	2.504905	2.028903
H	0.966885	3.420973	1.635909
C	3.849623	1.662346	-0.797464
H	4.163728	0.720486	-1.293386
H	3.173782	2.185047	-1.511834
C	-0.881528	4.464724	1.136987
H	-0.441973	5.158287	0.388666
H	-0.936133	5.007647	2.102558
H	-1.924358	4.246209	0.820819
C	5.074314	2.536555	-0.502389
H	4.789370	3.490402	-0.006832
H	5.623314	2.795153	-1.431863
H	5.787361	2.015676	0.171769
Ni	-1.028712	0.661295	-0.521354

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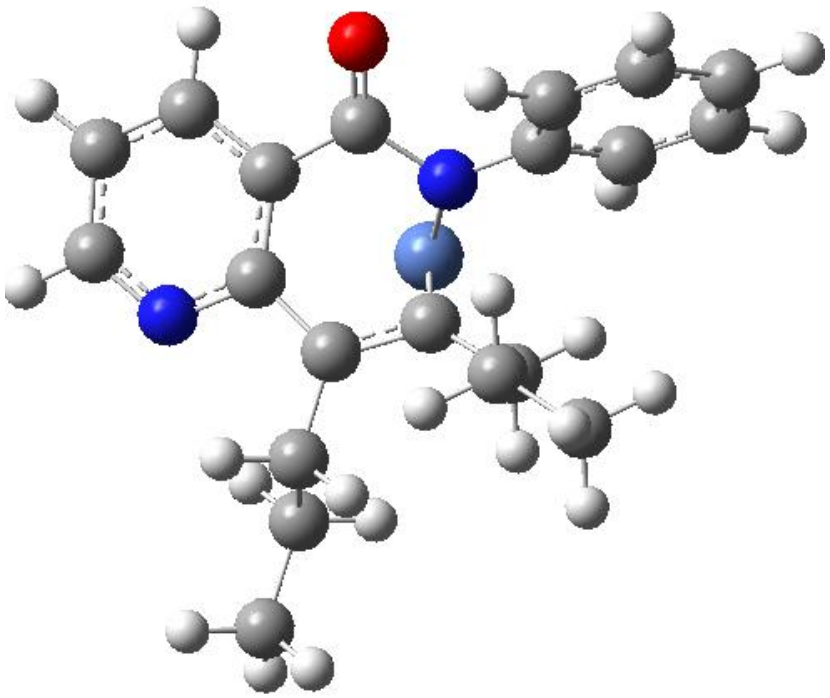

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C	-1.994638	-0.718291	-0.281812
C	0.354106	-1.843500	-0.516352
C	-1.464292	0.654198	-0.211701
C	-1.142361	-1.876015	-0.430508
N	-3.352173	-0.836034	-0.316643
C	2.344057	-0.570842	0.191550
C	-2.412182	1.807116	-0.514618
H	-3.131228	1.474271	-1.292531
H	-1.839403	2.661615	-0.934399
C	0.733983	2.073583	-0.093301
H	1.667728	1.989661	0.501528
H	0.198966	2.959957	0.319542
C	-3.156047	-3.233725	-0.612063
H	-3.662071	-4.203358	-0.735515
C	-1.761391	-3.130964	-0.620906
H	-1.109340	-4.004779	-0.775429
C	-3.901524	-2.046570	-0.456734
H	-5.007320	-2.081253	-0.455667
C	3.155272	-0.780818	-0.950264
H	2.696876	-1.127868	-1.885571
C	4.541016	-0.573914	-0.870025
H	5.162965	-0.749792	-1.762359
C	5.139802	-0.148276	0.330408
H	6.228413	0.010479	0.382141
C	2.952256	-0.152957	1.397275
H	2.305953	-0.011588	2.282362
C	4.337351	0.063678	1.465523
H	4.792154	0.388278	2.414935
C	1.085060	2.322319	-1.578315
H	1.619966	1.431014	-1.970279
H	0.144965	2.398901	-2.167745
C	-3.211206	2.282223	0.718885
H	-3.772460	1.409126	1.114363
H	-2.496424	2.590596	1.515688
C	1.940150	3.577600	-1.783569
H	1.418870	4.490241	-1.422595
H	2.178439	3.731993	-2.856146
H	2.903122	3.505334	-1.234799
C	-4.177202	3.430390	0.404777
H	-3.641363	4.323065	0.015423
H	-4.738443	3.746477	1.308610
H	-4.922317	3.130747	-0.362546
Ni	-0.267776	-0.255124	1.542957

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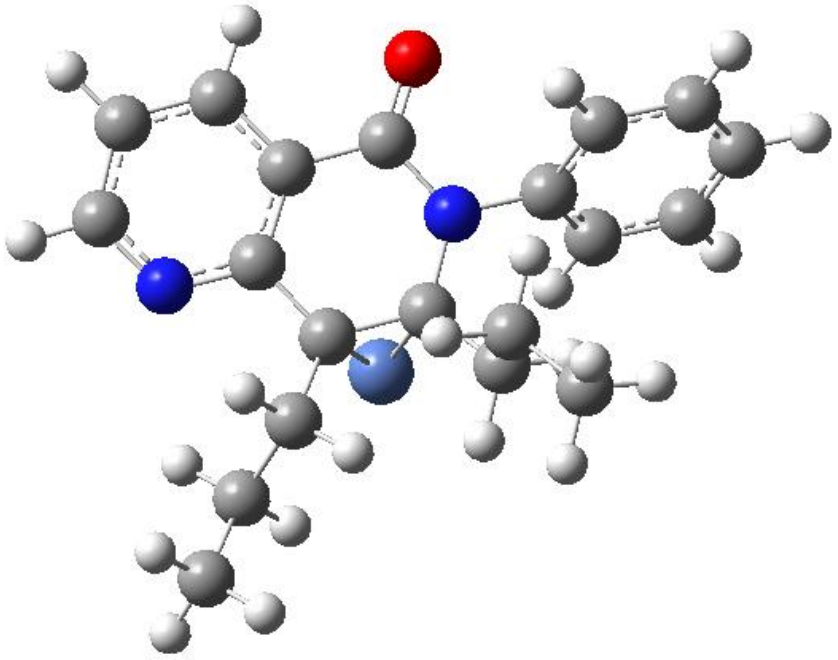

-1130.6594499

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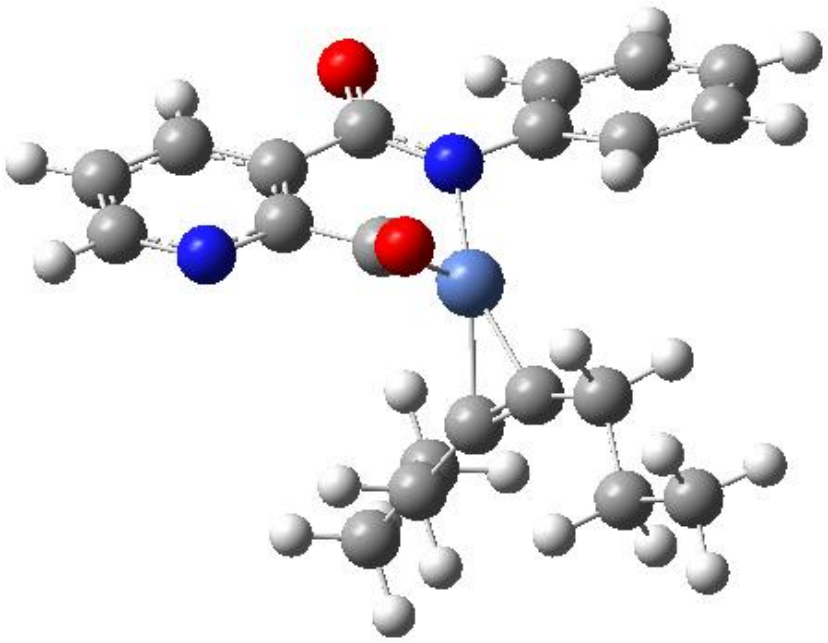
C	0.127248	-0.596103	-0.013868
C	-1.840687	0.965515	0.221656
C	0.537300	1.864021	0.425733
C	-1.330574	-0.412264	0.056384
C	-0.936921	2.045471	0.431590
N	-3.187259	1.152555	0.238926
C	2.400128	0.410530	-0.102409
C	-2.285936	-1.535656	0.478263
H	-2.836476	-1.191497	1.383300
H	-1.706775	-2.430915	0.783787
C	0.762255	-1.919997	0.414702
H	1.740752	-2.051221	-0.091352
H	0.125644	-2.752210	0.050638
C	-2.840879	3.526314	0.617453
H	-3.290073	4.520298	0.765293
C	-1.454609	3.340001	0.628200
H	-0.742622	4.164939	0.787006
C	-3.657249	2.391572	0.421925
H	-4.758513	2.497753	0.421005
C	3.363019	0.725865	0.876048
H	3.036614	1.086240	1.861656
C	4.729308	0.590128	0.580384
H	5.477147	0.840597	1.349350
C	5.144461	0.139198	-0.685318
H	6.217301	0.032680	-0.910645
C	2.816797	-0.021060	-1.377989
H	2.050309	-0.238411	-2.141987
C	4.183586	-0.166702	-1.665121
H	4.498308	-0.509830	-2.663459
C	0.961477	-2.044015	1.942384
H	1.608937	-1.210362	2.290558
H	-0.017709	-1.901544	2.451068
C	-3.324280	-1.954849	-0.583690
H	-3.894528	-1.051395	-0.884420
H	-2.776451	-2.305490	-1.491642
C	1.575218	-3.386746	2.355684
H	0.932269	-4.239787	2.049472
H	1.710011	-3.449671	3.455417
H	2.571349	-3.538421	1.887859
C	-4.279665	-3.047097	-0.090259
H	-3.732109	-3.965711	0.213618
H	-5.006875	-3.337223	-0.876851
H	-4.863214	-2.703572	0.790797
Ni	-0.694719	-0.574379	-1.737979

21



-1243.9547488

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C	1.741207	-1.567289	-1.049332
C	2.253315	0.890628	-0.316816
C	-1.449300	-1.189924	1.123886
C	2.612852	-0.571409	-0.542826
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C	0.401817	2.503274	-0.292636
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H	-0.226478	-2.538353	2.211058
H	-1.863069	-2.300180	2.870600
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H	-2.926740	-1.178873	-1.805068
H	-3.705452	0.157929	-0.935845
C	4.327062	-2.289492	-0.530597
H	5.358067	-2.625916	-0.339034
C	3.947059	-0.959396	-0.308479
H	4.649456	-0.188029	0.043991
C	3.362152	-3.196048	-1.013069
H	3.626062	-4.253551	-1.195571
C	-0.872496	2.750772	-0.870083
H	-1.363192	1.937403	-1.432817
C	-1.485652	4.007988	-0.764325
H	-2.473151	4.171584	-1.225067
C	-0.833876	5.057011	-0.092463
H	-1.307703	6.048074	-0.013633
C	1.057333	3.570971	0.375618
H	2.053753	3.400048	0.799788
C	0.436343	4.826841	0.466541
H	0.961131	5.643607	0.988541
C	-4.483398	-1.820162	-0.392903
H	-4.081211	-2.849570	-0.272906
H	-4.857356	-1.513879	0.608528
C	-0.436377	-0.725974	3.411912
H	0.422674	-0.203838	2.936365
H	-1.207229	0.054864	3.591223
C	-5.630845	-1.816591	-1.409148
H	-6.069010	-0.802399	-1.525616
H	-6.447226	-2.498767	-1.094913
H	-5.285274	-2.146701	-2.411696
C	-0.002788	-1.357245	4.738913
H	-0.851642	-1.862774	5.247193
H	0.394405	-0.591381	5.435864
H	0.793838	-2.116667	4.587775
Ni	-0.423245	-0.106908	-0.119892
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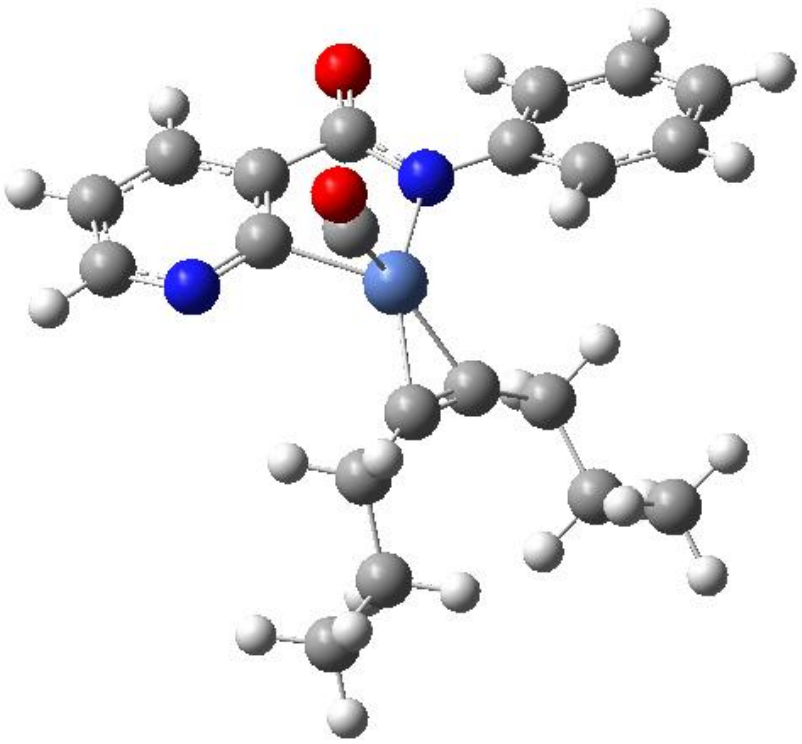
21-22



-1243.9271053

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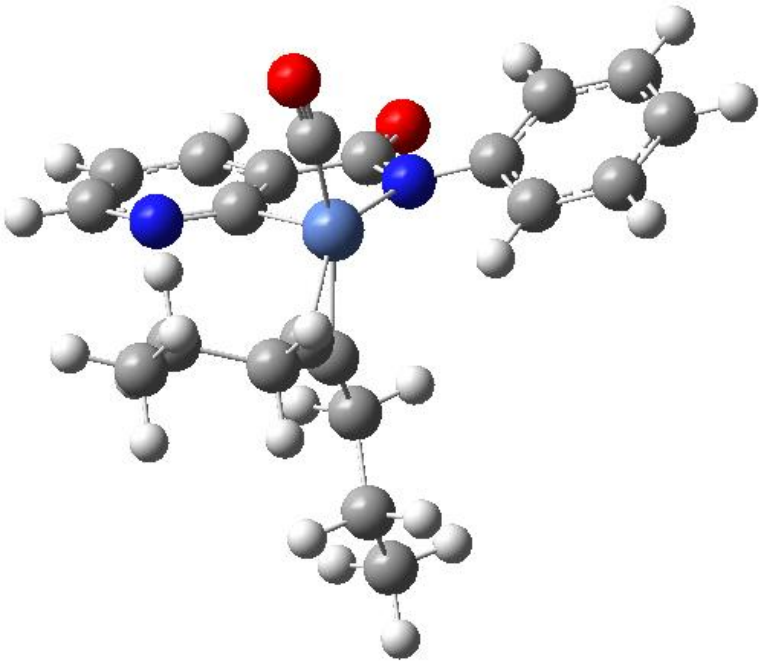
C	1.329644	-1.888657	0.078234
C	-1.118028	-2.265417	-0.575981
C	0.390422	1.686420	-0.244952
C	0.339036	-2.660080	-0.576327
N	2.633616	-2.095046	0.011309
C	-2.557199	-0.458402	0.215358
C	-0.649893	2.512452	-0.897744
H	-1.591348	2.438303	-0.307567
H	-0.900336	2.049899	-1.879616
C	2.981824	1.644504	0.542239
H	3.570963	0.743556	0.256016
H	3.080922	1.708032	1.650387
C	2.183872	-4.024082	-1.367817
H	2.579091	-4.883119	-1.931718
C	0.805080	-3.764710	-1.312801
H	0.055866	-4.375738	-1.843405
C	3.069007	-3.148648	-0.708501
H	4.161574	-3.298973	-0.754238
C	-2.668146	0.553886	1.207516
H	-1.765028	0.825247	1.780291
C	-3.894035	1.176551	1.480580
H	-3.947555	1.950731	2.263277
C	-5.051012	0.805275	0.770668
H	-6.016900	1.289471	0.984664
C	-3.736494	-0.835930	-0.486202
H	-3.673177	-1.635772	-1.233725
C	-4.957237	-0.201939	-0.206686
H	-5.856675	-0.507581	-0.766073
C	3.572735	2.911372	-0.112199
H	3.460076	2.831759	-1.215712
H	2.969166	3.792941	0.195702
C	-0.251218	3.992379	-1.089999
H	-0.009583	4.431395	-0.097048
H	0.687058	4.041850	-1.684828
C	5.046297	3.127741	0.251620
H	5.181568	3.242387	1.348327
H	5.451711	4.040154	-0.231870
H	5.674275	2.270334	-0.071496
C	-1.352520	4.811207	-1.773524
H	-1.590489	4.409694	-2.781520
H	-1.048184	5.870717	-1.898816
H	-2.292848	4.799077	-1.182672
Ni	0.430304	-0.145039	0.429349
C	0.993691	-1.061948	1.779073
O	1.241021	-1.484310	2.840309

22



-1243.9388897

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C	0.791059	1.570984	-0.424143
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C	1.070935	-0.753107	1.145221
C	-0.223584	2.449826	0.005876
N	1.997634	1.922511	-0.761776
C	-2.646204	-0.323556	-0.098874
C	0.820577	-0.335951	2.542749
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H	1.184985	0.711451	2.657353
C	2.666577	-2.288759	-0.403700
H	2.176150	-3.003874	-1.100348
H	3.111815	-2.900763	0.414476
C	1.432335	4.201210	-0.219826
H	1.744112	5.254893	-0.151898
C	0.119032	3.806379	0.102430
H	-0.661751	4.522641	0.410636
C	2.346422	3.229379	-0.662078
H	3.377085	3.495782	-0.952009
C	-2.416231	-1.728920	-0.051774
H	-1.397057	-2.097587	0.158348
C	-3.464490	-2.642414	-0.238400
H	-3.255821	-3.723911	-0.202933
C	-4.775804	-2.180545	-0.444059
H	-5.604142	-2.894378	-0.575305
C	-3.982180	0.132861	-0.295313
H	-4.175190	1.213071	-0.292597
C	-5.020585	-0.792383	-0.461149
H	-6.048072	-0.420848	-0.607615
C	3.790194	-1.540928	-1.158046
H	3.332211	-0.918342	-1.955995
H	4.277851	-0.824948	-0.461990
C	1.489456	-1.243815	3.598179
H	1.121255	-2.284445	3.462844
H	2.584362	-1.276683	3.405877
C	4.829491	-2.495605	-1.755923
H	5.325330	-3.105469	-0.970552
H	5.622545	-1.938013	-2.295088
H	4.366047	-3.200249	-2.479249
C	1.219437	-0.773950	5.032291
H	1.608122	0.252555	5.203454
H	1.703315	-1.442658	5.773447
H	0.131564	-0.757610	5.255534
Ni	0.209638	-0.253788	-0.513622
C	0.155486	-0.492933	-2.334422
O	0.203661	-0.563472	-3.486232

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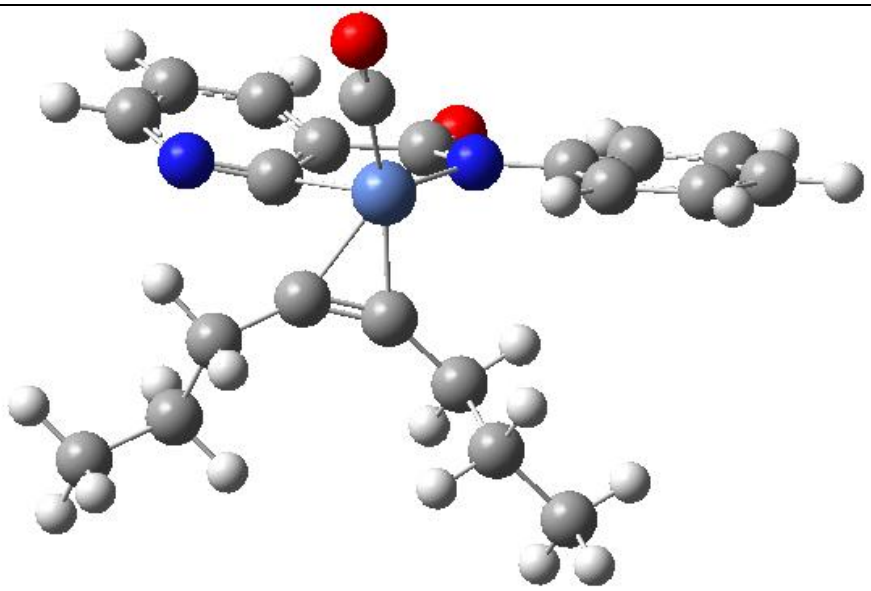

-1243.9143858

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C	1.714956	-0.977406	0.005490
C	-0.530618	-1.602159	-1.194144
C	1.527659	1.027122	0.298091
C	0.963489	-1.730795	-0.948552
N	2.955786	-1.249897	0.339273
C	-2.539443	-0.682140	-0.117941
C	2.866556	1.621498	0.571031
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C	3.012092	-3.013565	-1.289129
C	1.671265	-2.750690	-1.613864
C	3.614644	-2.254416	-0.273581
C	-3.019579	0.075390	0.987645
C	-4.380512	0.371451	1.135800
C	-5.310953	-0.079470	0.180696
C	-3.490924	-1.130713	-1.081407
C	-4.851342	-0.828051	-0.918550
C	-0.993545	3.450036	-0.247826
C	3.531302	2.258821	-0.668316
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C	4.898312	2.875628	-0.349112
Ni	0.210049	-0.179957	1.042479
C	0.334878	-1.093965	2.586422
O	0.381657	-1.589332	3.632263
H	2.740775	2.383643	1.372896
H	3.516748	0.816080	0.980436
H	-0.121616	2.352716	-1.935515
H	-1.528768	1.550703	-1.171602
H	3.577185	-3.809672	-1.797797
H	1.114292	-3.335707	-2.364102
H	4.649909	-2.446087	0.057561
H	-2.285799	0.422536	1.737544
H	-4.717860	0.957495	2.006070
H	-6.382249	0.149988	0.293541
H	-3.129809	-1.719358	-1.933784
H	-5.569831	-1.189637	-1.672584
H	-0.072472	4.022565	-0.001684
H	-1.476579	3.202472	0.721945
H	2.855919	3.034064	-1.093101
H	3.640014	1.481468	-1.455884
H	-2.874245	3.762040	-1.333909
H	-2.206265	5.243653	-0.578233
H	-1.464131	4.586830	-2.070220
H	5.602751	2.114670	0.048494
H	5.361414	3.320980	-1.253536
H	4.813760	3.678907	0.413713

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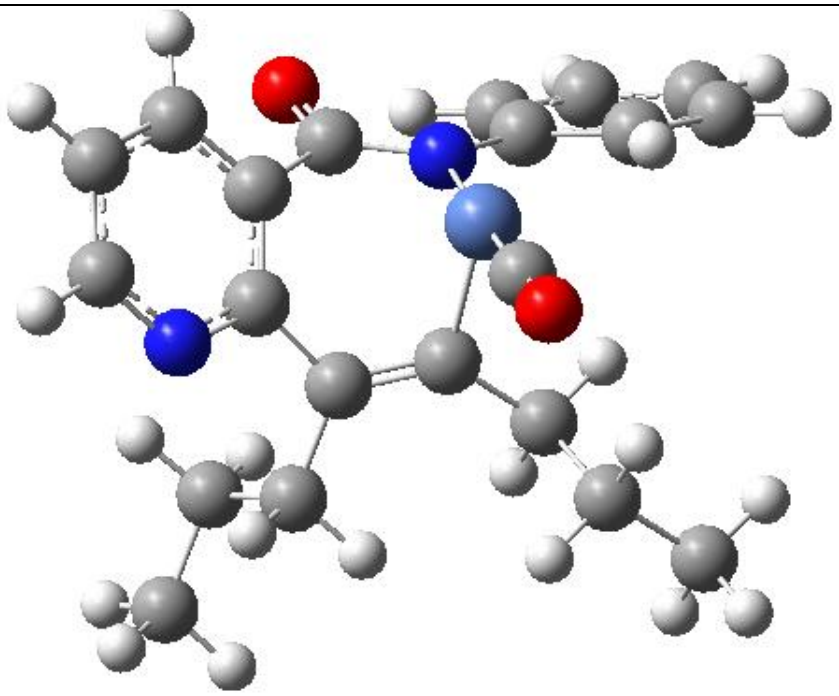

-1243.9818507

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C	2.148307	-1.297557	0.284814
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H	-3.159253	1.909759	1.010970
H	-1.647655	2.752385	1.457855
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H	0.502196	2.574358	1.340387
C	-3.775317	-2.432115	-0.946252
H	-4.443446	-3.235524	-1.292707
C	-2.435154	-2.684401	-0.631169
H	-2.017072	-3.702119	-0.680214
C	-4.255380	-1.121884	-0.769716
H	-5.313635	-0.879270	-0.979697
C	3.239176	-0.963605	-0.558172
H	3.036869	-0.732511	-1.617778
C	4.551304	-0.943985	-0.064333
H	5.383067	-0.683458	-0.738078
C	4.804439	-1.273450	1.279768
H	5.835065	-1.270191	1.667943
C	2.411932	-1.628460	1.639002
H	1.581458	-1.906974	2.300288
C	3.729434	-1.615744	2.120812
H	3.918232	-1.877235	3.174419
C	1.271187	3.202525	-0.603168
H	1.712084	2.729641	-1.508504
H	0.356769	3.733319	-0.948682
C	-2.223405	1.148752	2.827007
H	-2.694503	0.143080	2.763196
H	-1.195794	0.977552	3.218757
C	2.269212	4.204031	-0.010207
H	1.845862	4.724785	0.875218
H	2.551022	4.980728	-0.750505
H	3.202217	3.698306	0.318126
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H	-2.551326	3.033051	3.913136
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H	-4.057393	2.184950	3.449702
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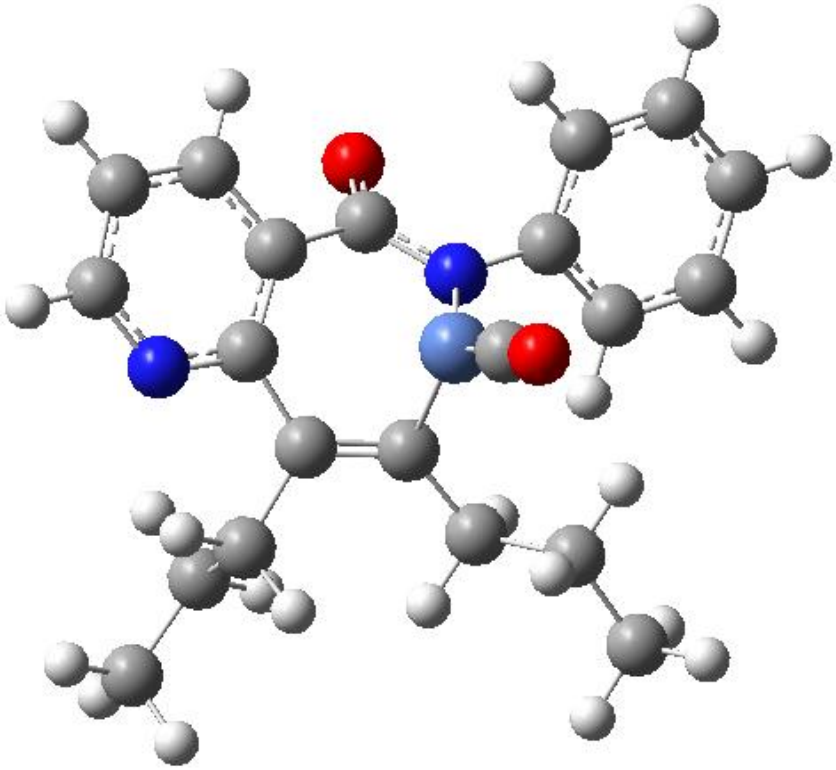
23-24



-1243.9752382

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N	3.515050	-0.248409	0.009428
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C	2.079689	2.044612	-0.842680
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H	1.536411	2.971084	-0.563619
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H	-1.909725	1.414381	-0.581002
H	-0.618523	2.508324	-1.097210
C	3.799260	-2.649284	0.163161
H	4.483874	-3.502744	0.282149
C	2.426902	-2.834720	-0.024076
H	1.978620	-3.837543	-0.100038
C	4.289749	-1.327094	0.162643
H	5.373206	-1.136271	0.276916
C	-2.394571	-1.159313	-1.911626
H	-1.566230	-1.294507	-2.621207
C	-3.721408	-1.133403	-2.364966
H	-3.927064	-1.246003	-3.441304
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H	-5.824625	-0.941450	-1.823411
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H	-2.964446	-0.773230	1.452790
C	-4.513803	-0.821394	-0.087214
H	-5.338496	-0.693369	0.631612
C	-1.325827	2.846320	0.944853
H	-1.742125	2.237959	1.778030
H	-0.393179	3.304615	1.341656
C	2.275791	1.994435	-2.373922
H	2.820138	1.060643	-2.634404
H	1.282966	1.918325	-2.871999
C	-2.323577	3.940270	0.547655
H	-1.919841	4.588178	-0.259755
H	-2.568107	4.595563	1.408902
H	-3.275591	3.504200	0.176666
C	3.039718	3.208848	-2.915993
H	2.506818	4.158276	-2.693218
H	3.168651	3.149036	-4.016666
H	4.051231	3.283689	-2.463270
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C	0.178089	0.409352	3.118206
O	0.497180	0.923299	4.110622

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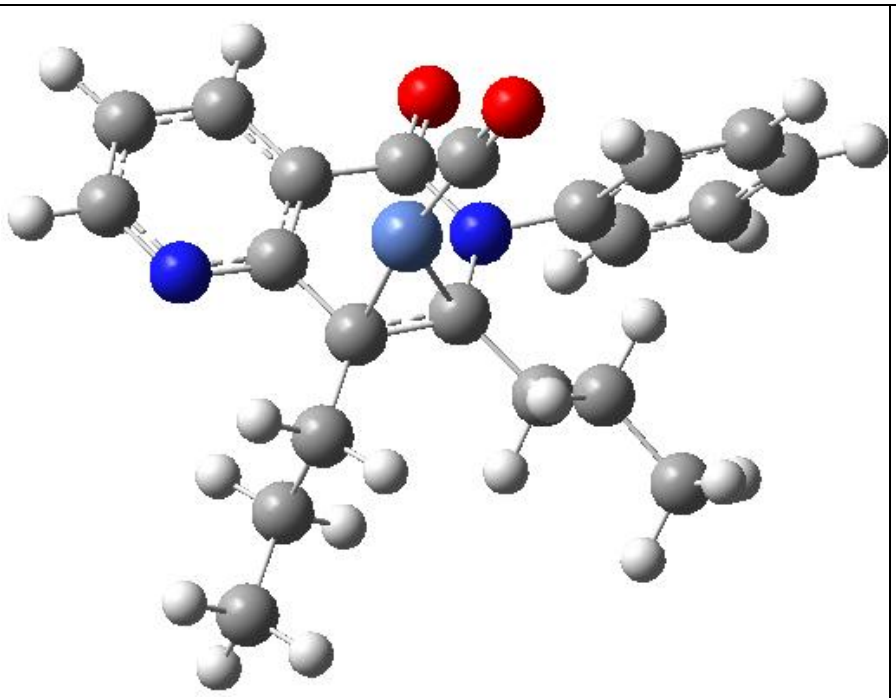

-1244.0273003

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C	2.011381	-0.713376	-0.220152
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C	1.302643	0.568474	-0.308317
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N	3.360459	-0.694508	-0.005132
C	-2.247260	-0.741613	-0.657818
C	2.121781	1.835126	-0.529556
H	3.026973	1.776232	0.109357
H	1.557692	2.732011	-0.201068
C	-0.917559	1.802572	-0.717139
H	-1.806349	1.523379	-1.318883
H	-0.290430	2.434153	-1.381826
C	3.386496	-3.124154	-0.105999
H	3.981651	-4.048054	-0.048626
C	2.008663	-3.155571	-0.340328
H	1.448773	-4.092973	-0.482898
C	4.005345	-1.862878	0.054881
H	5.094234	-1.805330	0.240745
C	-2.896809	-0.975098	-1.884544
H	-2.297628	-1.113409	-2.796820
C	-4.298668	-1.034408	-1.928258
H	-4.806161	-1.217664	-2.888410
C	-5.051830	-0.865934	-0.751976
H	-6.151530	-0.913902	-0.789774
C	-2.994645	-0.591167	0.524663
H	-2.467221	-0.446407	1.479740
C	-4.398336	-0.646700	0.472712
H	-4.981949	-0.528183	1.399200
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H	-2.046269	2.049908	1.127795
H	-0.499156	2.909767	1.112944
C	2.573223	2.009088	-1.998452
H	3.159487	1.112576	-2.294847
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H	-1.447117	4.581751	-0.584399
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H	-3.009573	3.708131	-0.555812
C	3.409922	3.274329	-2.219437
H	2.840491	4.191795	-1.956708
H	3.728253	3.371348	-3.278094
H	4.327678	3.264851	-1.593710
Ni	0.729123	0.353459	1.581497
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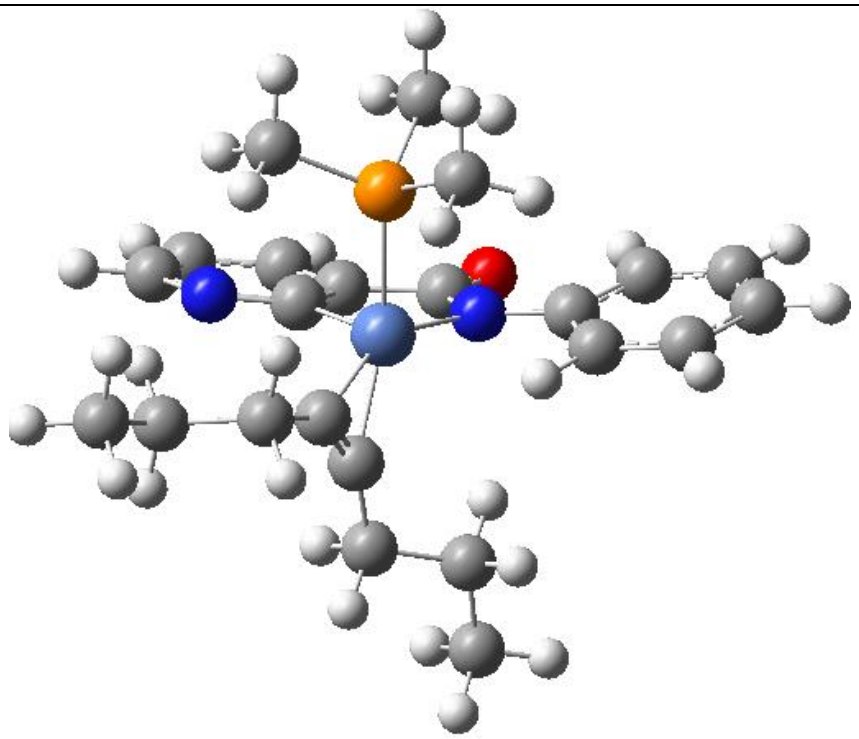

-1591.6826859

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C	-0.862455	1.230334	-1.506621
C	0.004420	1.161942	2.162761
N	-2.292204	0.650069	1.621293
C	2.601578	-0.186603	-0.078609
C	-0.472990	2.626915	-1.825000
H	-0.855658	3.275722	-1.002323
H	-1.013422	2.953002	-2.744916
C	-2.811498	-0.445027	-2.270193
H	-2.776516	-1.551330	-2.161887
H	-2.788676	-0.241666	-3.366826
C	-1.772659	1.829243	3.665517
H	-2.133830	2.306020	4.589896
C	-0.399256	1.769564	3.360363
H	0.381672	2.172480	4.027727
C	-2.688029	1.246989	2.772384
H	-3.772209	1.251040	2.980877
C	3.885317	-0.257562	0.539580
H	4.002399	0.163147	1.546333
C	4.965492	-0.836939	-0.142894
H	5.947696	-0.879903	0.356526
C	4.821677	-1.354903	-1.444286
H	5.681195	-1.802270	-1.967869
C	2.476671	-0.693945	-1.405020
H	1.504049	-0.601009	-1.919911
C	3.565534	-1.274308	-2.072214
H	3.433284	-1.652644	-3.099263
C	-4.139133	0.084884	-1.677660
H	-4.115800	-0.053065	-0.575577
H	-4.186141	1.183566	-1.842126
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H	1.553753	2.509865	-1.067207
H	1.423643	2.232742	-2.813921
C	-5.373410	-0.592067	-2.284066
H	-5.422476	-0.443936	-3.384345
H	-6.310263	-0.184564	-1.850992
H	-5.371186	-1.687950	-2.098920
C	1.382892	4.338182	-2.252063
H	0.897649	4.711989	-3.179720
H	2.476748	4.482372	-2.366699
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Ni	-0.335030	-0.111355	-0.256951
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H	1.096735	-3.368151	-1.020602
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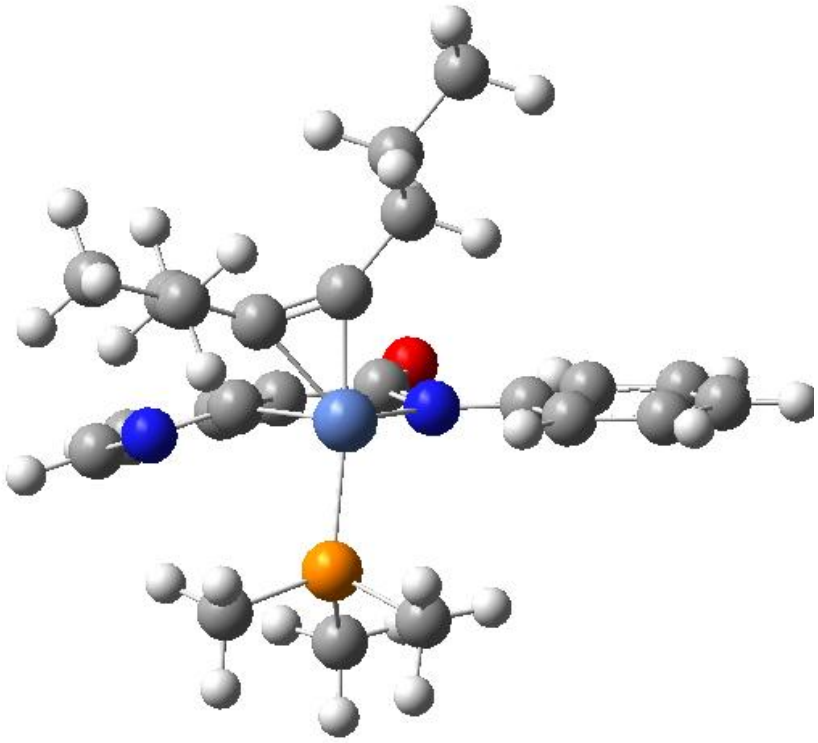

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N	2.749384	-0.259429	1.312483
C	-2.640890	-0.353987	0.010364
C	2.884004	1.806116	-0.732977
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H	2.980033	2.838672	-0.323619
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H	-1.729476	2.194699	-1.286280
H	-0.422351	3.345805	-1.675905
C	2.268172	-0.376835	3.672397
H	2.635822	-0.513591	4.701082
C	0.908082	-0.146877	3.404305
H	0.140135	-0.126473	4.195142
C	3.148462	-0.469515	2.582944
H	4.215751	-0.714502	2.729993
C	-2.778214	-0.548712	-1.394139
H	-1.854446	-0.601035	-1.998930
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C	-5.207127	-0.579337	-1.222355
H	-6.198734	-0.666747	-1.693842
C	-3.834600	-0.267787	0.786713
H	-3.740148	-0.109590	1.868210
C	-5.088172	-0.385074	0.166393
H	-5.996504	-0.319872	0.788302
C	-1.113148	3.453953	0.394426
H	-1.478475	2.756562	1.177747
H	-0.171480	3.898491	0.785150
C	3.240949	1.809667	-2.235364
H	3.107745	0.779161	-2.632512
H	2.513824	2.444291	-2.788820
C	-2.155552	4.550088	0.145947
H	-1.808693	5.281136	-0.616069
H	-2.372653	5.113225	1.076808
H	-3.113765	4.120104	-0.214723
C	4.669713	2.297156	-2.503372
H	4.819287	3.336542	-2.140167
H	4.905672	2.285871	-3.587715
H	5.418952	1.657714	-1.989675
Ni	0.345438	-0.263935	-0.516234
P	0.868721	-2.402866	-0.816917
C	0.384745	-3.516196	0.579256
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H	0.584260	-4.582687	0.346341
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H	0.320480	-2.641289	-3.198978
H	0.322975	-4.254902	-2.385058
H	-1.062797	-3.112600	-2.153702
C	2.652842	-2.813213	-1.087306
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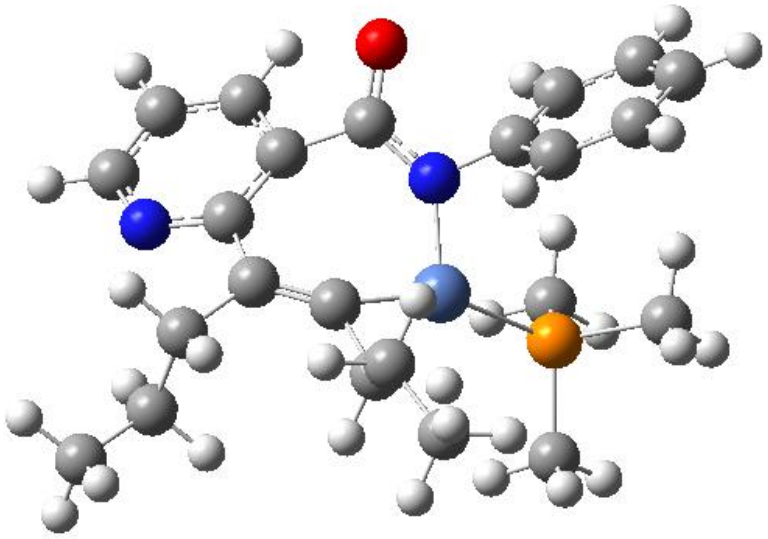

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H	4.423545	-0.185124	-1.291926
H	3.520236	-1.715473	-1.489161
C	0.922411	-2.268160	-0.563174
H	-0.111096	-2.435601	-0.008723
H	1.578585	-2.898629	0.080860
C	3.084467	3.880796	0.788102
H	3.334280	4.889038	1.153407
C	1.781503	3.542594	0.412241
H	0.975247	4.290977	0.423355
C	4.072683	2.894419	0.637894
H	5.131268	3.111983	0.875825
C	-2.623478	0.236168	-1.715321
H	-1.924110	-0.478027	-2.179238
C	-3.976383	0.263884	-2.099335
H	-4.342915	-0.449507	-2.855153
C	-4.852562	1.205640	-1.533907
H	-5.911065	1.234561	-1.837248
C	-3.011484	2.095766	-0.196924
H	-2.624231	2.829885	0.524902
C	-4.359045	2.124353	-0.585915
H	-5.033569	2.878270	-0.148373
C	0.751979	-2.877410	-1.972463
H	0.098016	-2.210452	-2.573061
H	1.746545	-2.854242	-2.468658
C	4.425061	-1.440898	0.473804
H	4.630105	-0.589927	1.155946
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C	0.199782	-4.307066	-1.962260
H	0.854007	-4.992587	-1.382265
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H	-0.814094	-4.348458	-1.508407
C	5.726904	-2.184184	0.151137
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H	6.211854	-2.575955	1.069741
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Ni	-0.438422	-0.727138	0.165295
P	-2.076161	-1.204851	1.678922
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H	-3.880641	-2.410769	0.534420
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C	-2.235293	0.141224	2.939023
H	-2.946841	-0.135884	3.744439
H	-1.239319	0.351645	3.376790
H	-2.591780	1.059443	2.432194
C	-1.666890	-2.679453	2.733783
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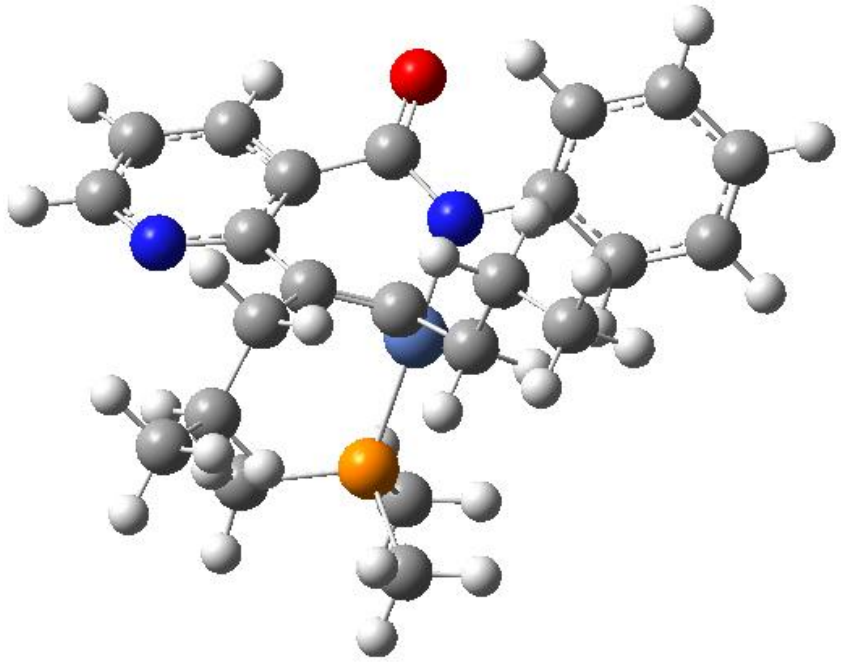
26-27



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N	-2.813299	1.873893	0.933776
C	2.623834	0.562352	-0.310270
C	-1.712289	-0.117137	2.591635
H	-2.104425	0.781936	3.113286
H	-0.991632	-0.604052	3.281694
C	0.890305	-1.413902	1.489210
H	1.563483	-1.912561	0.759140
H	0.184111	-2.210134	1.823778
C	-2.678049	3.727509	-0.620849
H	-3.173719	4.591147	-1.090403
C	-1.348009	3.403207	-0.905981
H	-0.726612	4.019236	-1.574595
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H	-4.398413	3.176750	0.610747
C	3.506151	1.417007	0.395761
H	3.109025	2.306555	0.903267
C	4.880206	1.137700	0.426392
H	5.555198	1.815939	0.972801
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H	6.482010	-0.205836	-0.198420
C	3.155511	-0.564777	-0.978251
H	2.461368	-1.207238	-1.548152
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H	1.788389	-2.846940	3.778058
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P	-1.397660	-1.764230	-2.021435
C	-1.419971	-3.513529	-1.400883
H	-2.171224	-4.126965	-1.941259
H	-0.416595	-3.966652	-1.528044
H	-1.664988	-3.509604	-0.319848
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C	-3.178500	-1.272884	-1.865739
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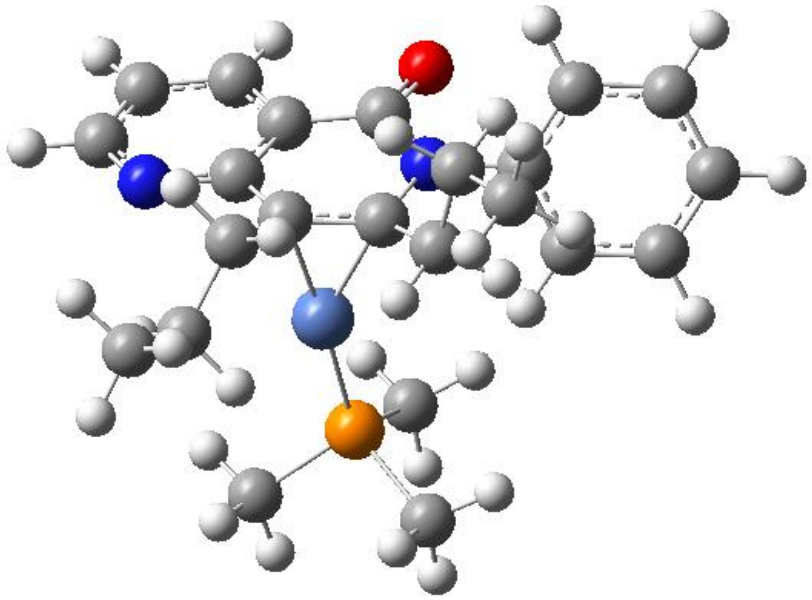

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N	-2.859831	-1.535157	1.213882
C	2.579489	-0.204914	0.489596
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H	6.244992	1.128372	0.097752
C	2.814347	1.071568	-0.059430
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P	-1.059106	2.848893	-0.405949
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H	-2.787837	4.641410	-0.330357
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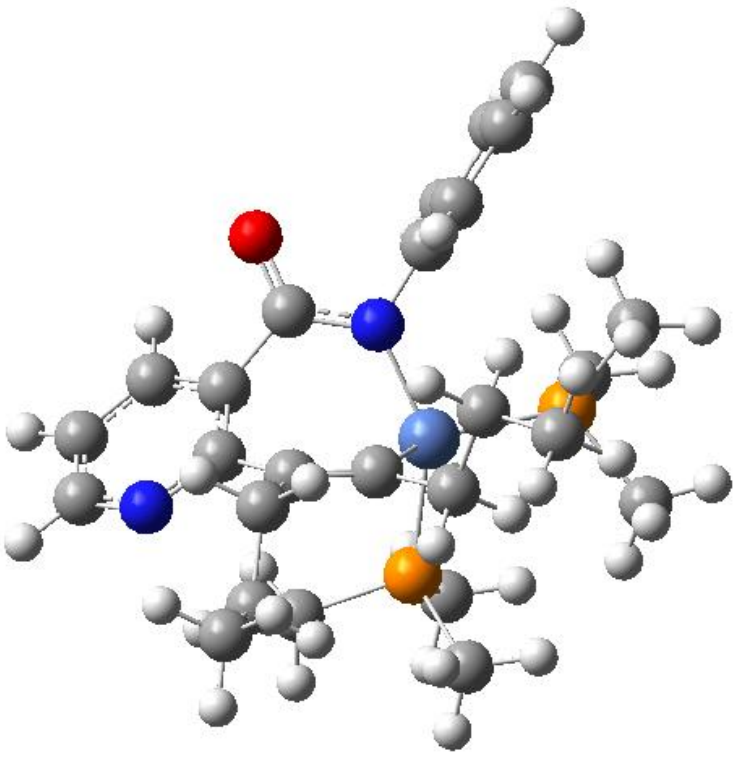

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H	-2.721179	0.135507	2.945894
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H	-0.165028	-2.255016	1.490489
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H	-3.316410	3.795368	-3.143871
C	-1.681123	3.035318	-1.906717
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C	4.824275	2.367869	1.246533
H	5.841025	2.642277	1.569648
C	3.216734	1.931482	-0.534905
H	2.957383	1.892175	-1.604586
C	4.512845	2.282911	-0.123860
H	5.285271	2.503409	-0.878891
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H	1.020021	-0.460006	2.776406
H	-0.495926	0.014576	3.559263
C	-4.328808	-0.629007	1.689108
H	-4.814348	-0.334037	0.735452
H	-3.891812	-1.640957	1.524256
C	0.275687	-1.914344	4.219889
H	-0.685798	-2.303235	4.619264
H	0.849021	-1.501495	5.075897
H	0.844191	-2.785904	3.828014
C	-5.368960	-0.694704	2.814431
H	-4.909409	-0.996386	3.780951
H	-6.174755	-1.423769	2.586219
H	-5.850691	0.293668	2.974465
Ni	0.380279	-0.514496	-0.405610
P	2.437020	-1.603598	-0.681743
P	-0.890925	-1.843614	-1.614205
C	3.648817	-1.376572	0.708023
H	4.047507	-0.344950	0.710683
H	3.131984	-1.549921	1.672905
H	4.487300	-2.097906	0.609652
C	3.537380	-1.385533	-2.166729
H	2.978773	-1.626529	-3.093121
H	3.855858	-0.325908	-2.218059
H	4.438014	-2.032219	-2.104304
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H	3.310659	-3.934332	-0.642738
H	1.809838	-3.757111	0.338286
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H	-2.126351	-3.997125	-1.658756
H	-0.678079	-4.082321	-0.578920
C	-2.458161	-1.089467	-2.245926
H	-2.221639	-0.162240	-2.804311
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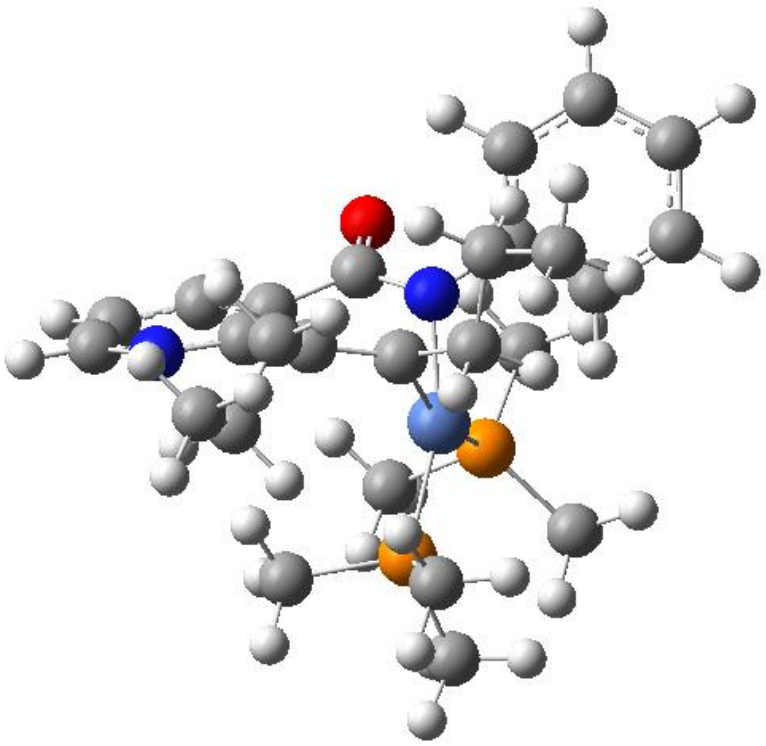
28-29



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C	-2.095379	1.363210	0.579408
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H	3.373445	2.331717	1.121935
H	2.640477	2.832082	-0.417416
C	0.327674	2.062807	-1.348295
H	-0.531867	1.758538	-1.983564
H	1.194468	2.097938	-2.047113
C	2.285811	-1.545516	3.800493
H	2.475553	-2.209495	4.657905
C	0.990593	-1.252053	3.371718
H	0.101911	-1.626759	3.903909
C	3.354888	-0.911931	3.123852
H	4.395810	-1.069563	3.467607
C	-2.577754	2.239315	1.586422
H	-2.051714	2.299363	2.548623
C	-3.727978	3.007138	1.361280
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C	-4.421132	2.934051	0.136346
H	-5.321171	3.545863	-0.032187
C	-2.802363	1.288400	-0.644542
H	-2.432226	0.596701	-1.421437
C	-3.949548	2.069477	-0.865665
H	-4.479433	1.995687	-1.829232
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H	-0.841396	3.479145	-0.173888
H	0.896806	3.808794	-0.160197
C	4.187523	1.325744	-0.602041
H	4.549408	0.457887	-0.012379
H	3.846198	0.927738	-1.584414
C	-0.127215	4.507624	-1.951814
H	0.776837	4.576301	-2.595357
H	-0.332129	5.523728	-1.555331
H	-0.980487	4.229804	-2.607273
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H	4.996775	3.206975	-1.411195
H	6.182113	1.863429	-1.365294
H	5.720042	2.705411	0.146069
Ni	-0.369966	-0.651789	-0.602218
P	1.018131	-1.616342	-1.985726
C	1.784847	-0.561949	-3.307888
H	2.501617	-1.145480	-3.922412
H	0.992162	-0.150469	-3.964427
H	2.321656	0.281709	-2.832997
C	0.504831	-3.082355	-3.012395
H	-0.317997	-2.789180	-3.695019
H	1.354584	-3.463428	-3.616553
H	0.143968	-3.898264	-2.355066
C	2.499399	-2.294276	-1.102856
H	2.968643	-1.487215	-0.505963
H	2.170305	-3.087578	-0.402451
H	3.240971	-2.713939	-1.814077
P	-2.001565	-2.256593	-0.274785
C	-2.903814	-3.118822	-1.659840
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H	-3.468940	-2.367816	-2.248722
H	-2.192604	-3.627544	-2.339129
C	-1.286181	-3.693398	0.665330
H	-0.826900	-3.309763	1.598584
H	-2.061948	-4.444963	0.923145
H	-0.490480	-4.183760	0.068694
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H	-3.035951	-1.297492	1.733446
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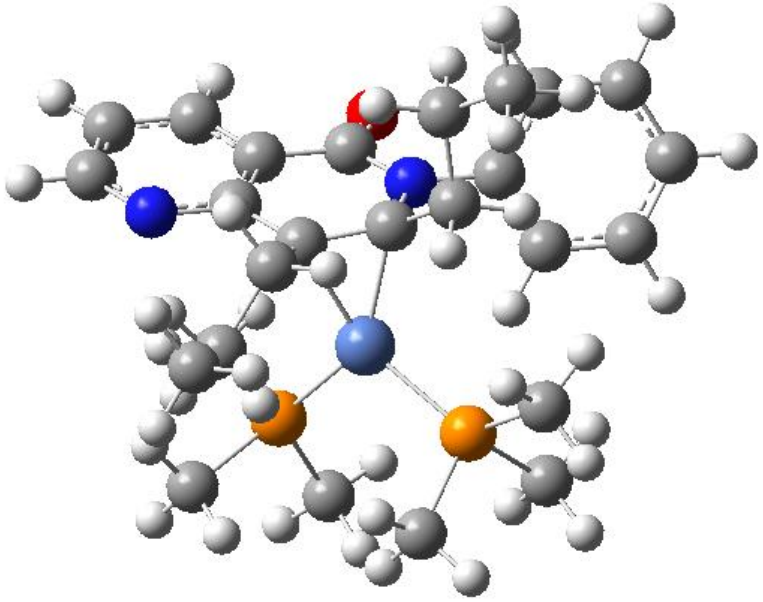

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C	0.779453	-0.825778	1.066099
C	0.635328	-2.687154	-0.612950
N	2.641076	-2.354520	0.711946
C	-2.620650	-0.832202	-0.636074
C	1.453804	-0.425795	2.385266
H	1.704634	-1.359564	2.939453
H	0.734320	0.130336	3.020416
C	-1.570728	-0.176870	1.992908
H	-2.486631	0.300535	1.585045
H	-1.101310	0.588010	2.641077
C	2.517815	-4.181440	-0.889242
H	3.014491	-5.046852	-1.353925
C	1.216434	-3.800970	-1.241791
H	0.621140	-4.338945	-1.996372
C	3.175975	-3.417433	0.097476
H	4.201140	-3.691998	0.412341
C	-3.717775	-1.677783	-0.381301
H	-3.551372	-2.645890	0.113545
C	-5.008668	-1.288732	-0.773852
H	-5.862621	-1.954486	-0.571282
C	-5.212138	-0.060865	-1.429350
H	-6.225845	0.239977	-1.738162
C	-2.820047	0.383402	-1.314445
H	-1.935574	1.002961	-1.532034
C	-4.113396	0.771938	-1.704056
H	-4.262548	1.723217	-2.240238
C	-1.970840	-1.395600	2.852863
H	-2.408775	-2.178104	2.195986
H	-1.053243	-1.848099	3.289253
C	2.740030	0.414470	2.273908
H	3.471976	-0.153396	1.663485
H	2.507649	1.347013	1.710355
C	-2.963028	-1.044385	3.968153
H	-2.543123	-0.284723	4.662512
H	-3.229243	-1.935680	4.573836
H	-3.906576	-0.628112	3.554516
C	3.346220	0.756209	3.640318
H	2.637117	1.334965	4.272369
H	4.272061	1.360824	3.539905
H	3.610756	-0.163907	4.204745
Ni	0.485504	0.844820	-0.118551
P	2.073057	0.992160	-1.664048
P	-0.335353	2.855858	0.169035
C	-1.468248	3.270259	1.594992
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H	-1.007462	2.933131	2.545172
C	1.048950	4.055259	0.533628
H	1.732266	4.112415	-0.336843
H	0.663138	5.072733	0.756725
H	1.631924	3.688456	1.402237
C	-1.225430	3.793225	-1.183186
H	-1.382381	4.857186	-0.904599
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H	0.812482	1.925320	-3.568821
H	1.730799	3.212997	-2.716929
H	2.587184	2.101389	-3.847144
C	3.788356	1.505894	-1.150123
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H	4.176557	0.776083	-0.412614
C	2.457492	-0.555589	-2.620925
H	2.890274	-1.313006	-1.938863
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H	3.176441	-0.350357	-3.441964

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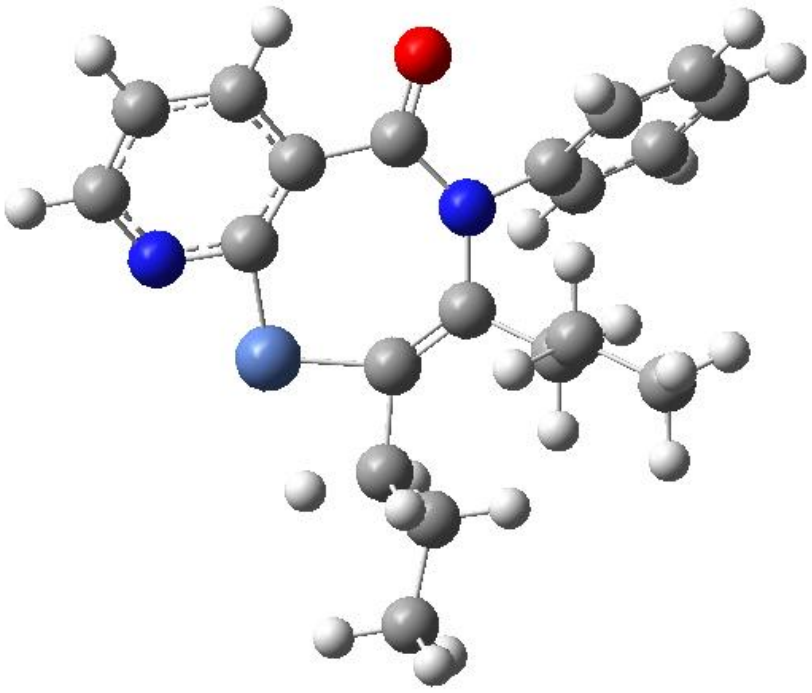

-1130.6059737

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N	3.598832	-1.116335	-0.164844
C	-2.208517	-0.826541	-0.475113
C	1.241156	2.669786	0.077887
H	2.385179	2.660204	-0.088087
H	1.169370	3.059114	1.121069
C	-1.518921	1.508914	0.991225
H	-2.507433	1.442967	0.487959
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H	3.792187	-4.359978	0.778568
C	1.935554	-3.241750	0.521348
H	1.263596	-4.079726	0.764314
C	4.147788	-2.300135	0.164050
H	5.248559	-2.377629	0.143997
C	-3.186808	-1.525292	0.258534
H	-2.915483	-2.002886	1.209841
C	-4.496593	-1.621046	-0.239782
H	-5.256826	-2.171469	0.337159
C	-4.839224	-1.024503	-1.466711
H	-5.868177	-1.103182	-1.852090
C	-2.547234	-0.238100	-1.709627
H	-1.769116	0.295972	-2.276925
C	-3.860202	-0.332739	-2.200881
H	-4.115963	0.130391	-3.167290
C	-1.678054	1.080523	2.467333
H	-1.940192	0.000968	2.506072
H	-0.693100	1.170741	2.977361
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H	0.777443	3.271367	-1.956614
H	-0.409332	3.800437	-0.751499
C	-2.738126	1.897345	3.215906
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H	-2.829101	1.572936	4.273361
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C	1.363779	5.066534	-0.856580
H	1.255144	5.520754	0.151495
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H	2.451814	4.992984	-1.071863
Ni	2.397234	0.734682	-0.427604

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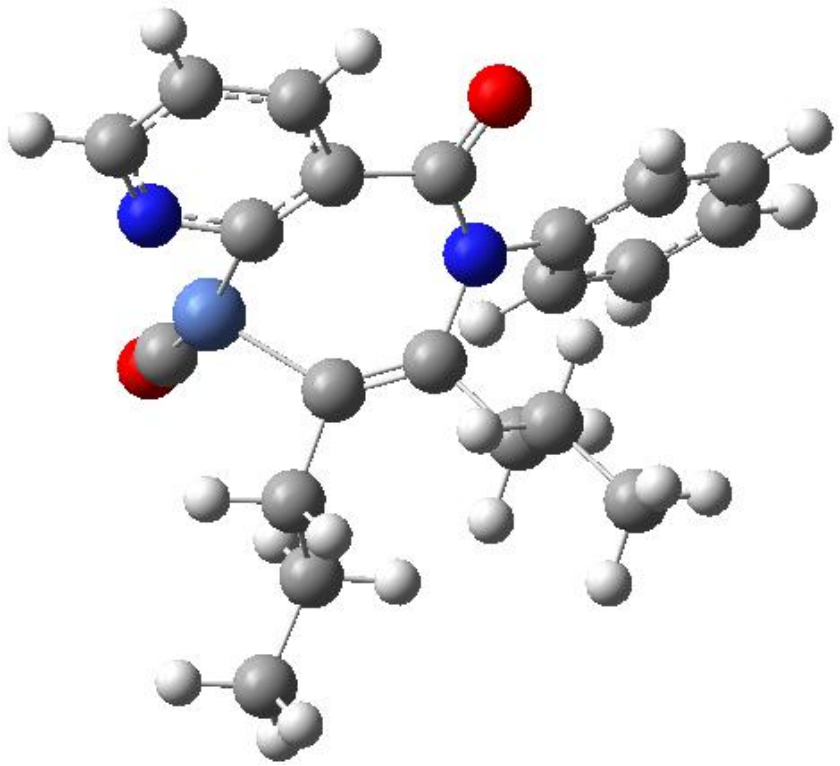

-1243.9501615

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C	-0.825367	-1.957863	0.185132
C	0.775110	0.891410	0.311976
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C	-2.409379	-0.309205	-0.721041
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H	1.188648	1.989116	2.149599
C	-1.385534	1.218336	1.610332
H	-2.360645	1.482137	1.143411
H	-0.925911	2.182232	1.906423
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H	2.744517	-4.919642	0.966544
C	1.045847	-3.561953	0.750782
H	0.274906	-4.303339	1.014900
C	3.345047	-2.963451	0.228454
H	4.415030	-3.202446	0.109857
C	-3.614588	-1.022797	-0.534992
H	-3.641702	-1.871393	0.157688
C	-4.761907	-0.650537	-1.257337
H	-5.695647	-1.215663	-1.105833
C	-4.731955	0.428320	-2.156774
H	-5.637518	0.712699	-2.715603
C	-2.379943	0.777099	-1.626421
H	-1.436442	1.326133	-1.766905
C	-3.533353	1.142713	-2.335340
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C	1.237689	3.424233	0.499953
H	1.514623	3.432607	-0.576587
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H	-2.086759	2.032840	4.244623
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H	1.730998	4.555056	2.320454
H	1.817739	5.519772	0.814372
H	3.109252	4.340324	1.198896
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O	2.700120	2.010161	-2.966171

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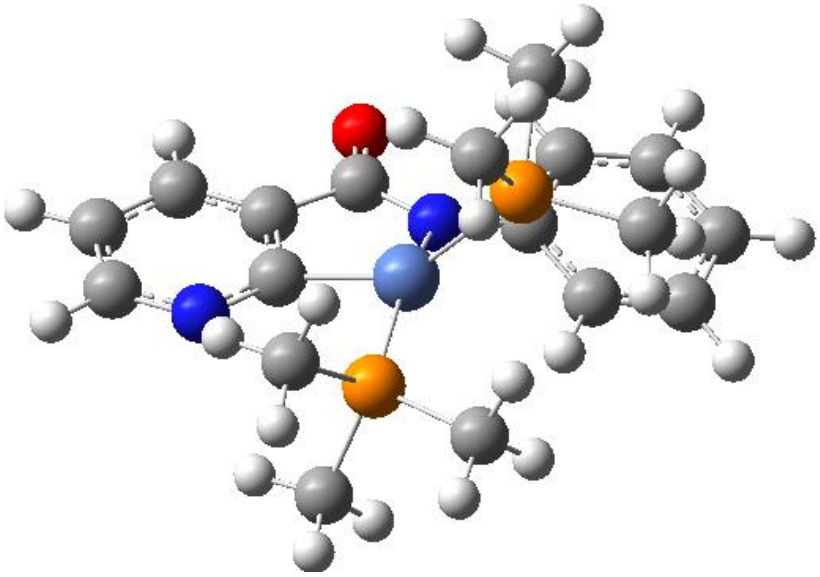

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C	-1.066682	2.415911	0.247736
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H	-3.885307	4.322725	0.634487
C	-1.832806	3.553430	0.530376
H	-1.312385	4.486018	0.806626
C	-3.789369	2.223497	0.063477
H	-4.884949	2.109333	-0.033168
C	3.330489	1.718209	-0.083191
H	3.142974	2.595723	0.547945
C	4.628749	1.391256	-0.506115
H	5.470905	2.020657	-0.173698
C	4.871508	0.282955	-1.338730
H	5.895208	0.039034	-1.663799
C	2.476831	-0.175578	-1.357427
H	1.615164	-0.756563	-1.729619
C	3.780591	-0.496603	-1.765646
H	3.943012	-1.351596	-2.442893
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P	-1.941498	-1.651535	-0.786690
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H	1.490275	-3.697400	0.157086
H	2.810147	-2.477618	0.189725
C	-0.284409	-2.538027	2.488459
H	0.318416	-3.006254	3.294868
H	-1.010129	-1.834510	2.944016
H	-0.852082	-3.334239	1.966245
C	-1.272147	-3.328879	-1.232022
H	-0.933645	-3.868118	-0.325364
H	-2.047977	-3.940051	-1.738901
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C	-3.432743	-2.065477	0.222890
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H	-4.119480	-2.735388	-0.335215
H	-3.129929	-2.553926	1.170009
C	-2.657819	-1.117651	-2.405312
H	-3.350313	-1.886923	-2.805684
H	-3.199540	-0.168727	-2.229573
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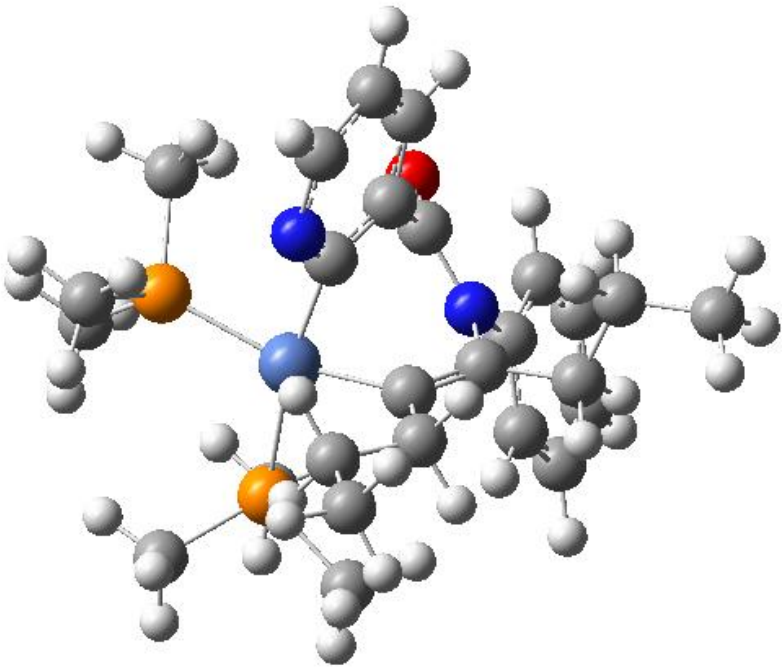

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C	1.116329	0.758230	-1.673891
C	0.149016	0.537242	1.227171
C	0.026838	1.761823	-1.409788
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C	2.887158	-0.668188	-0.704253
C	-0.293673	1.148344	2.553005
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H	0.290833	0.690549	3.388379
C	2.540604	1.403217	1.546525
H	3.509677	0.870421	1.419291
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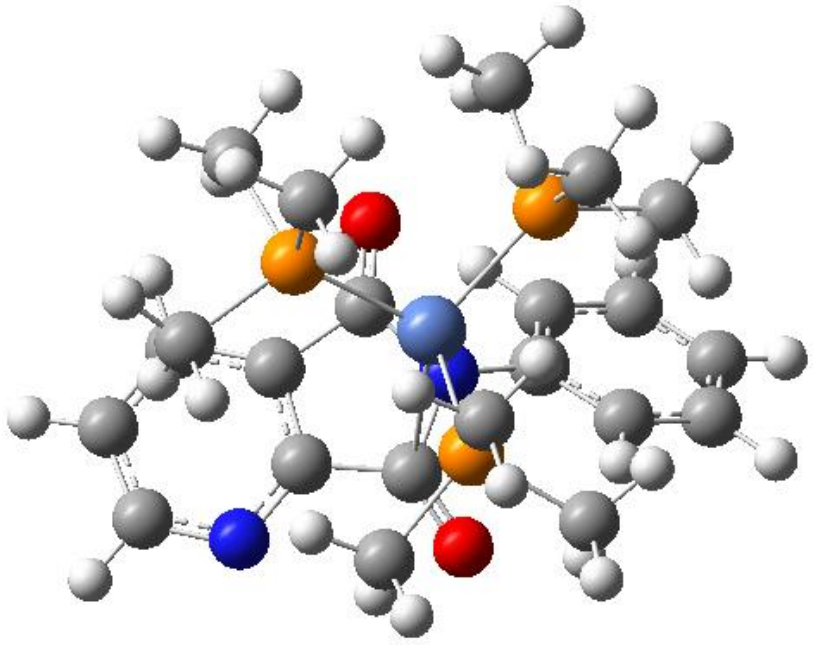

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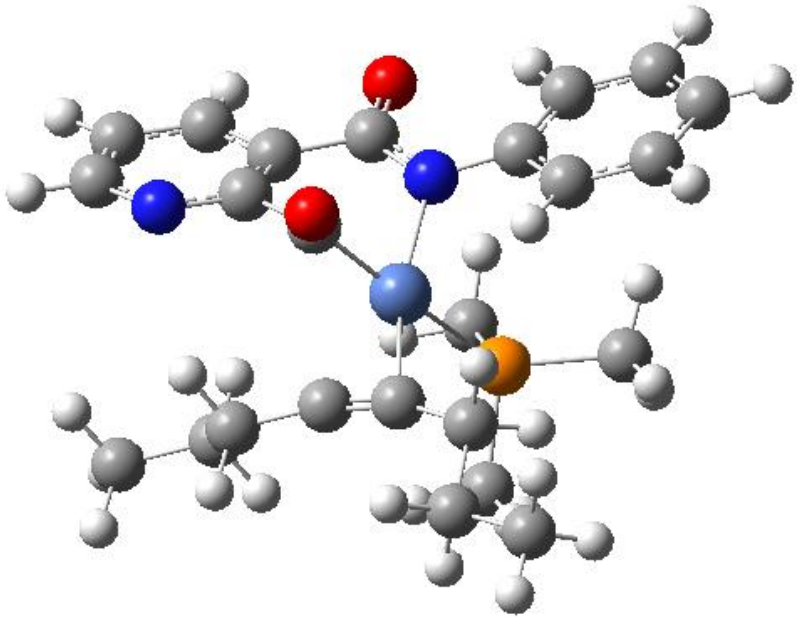

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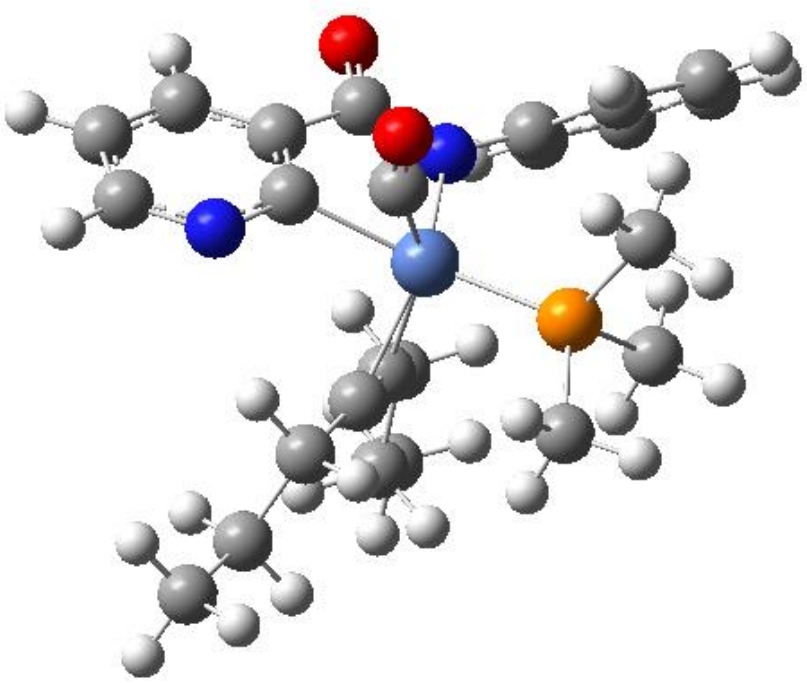
35-9



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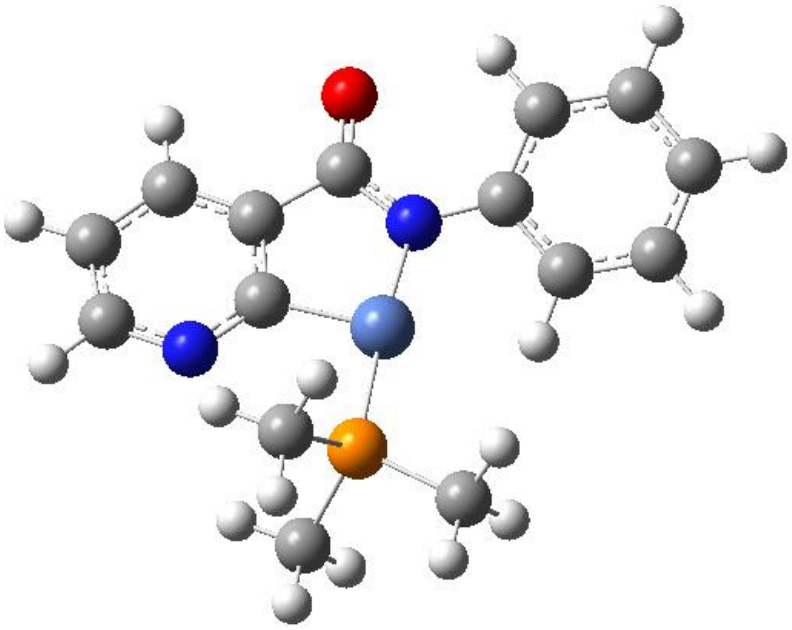

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rmsd

Standard deviations for the distances and for the angles, $s_{n-1} = \sqrt{\frac{\sum_{i=1}^{N}(CV - EV)^2}{N-1}}$, where CV means calculated value, EV experimental value (X-Ray data), and N is the number of distances or angles taken into account.

Table S2. Comparison between the X-Ray data of complex **2** and the corresponding computed geometry (Distances in Å and angles in degrees).

Distances	**OPT**	**X-Ray**
N2-O1	1.232	1.224
N2-C5	1.425	1.388
C5-C7	1.473	1.456
C7-C18	1.411	1.394
C18-C16	1.395	1.363
C16-C20	1.416	1.380
C20-N8	1.333	1.322
N8-C4	1.365	1.359
C4-C6	1.452	1.441
C6-C3	1.388	1.352
C3-N2	1.408	1.413
C7-C4	1.427	1.398
C6-C10	1.516	1.508
C10-C35	1.545	1.516
C35-C42	1.533	1.512
C3-C13	1.516	1.505
C13-C32	1.547	1.523
C32-C38	1.533	1.505
N2-C9	1.450	1.449
C9-C22	1.406	1.380
C22-C24	1.405	1.384
C24-C26	1.406	1.367
C26-C30	1.406	1.376
C30-C28	1.405	1.383
C28-C9	1.407	1.373

Angles	OPT	X-Ray
N2-C5-C7	114.5	115.3
C5-C7-C18	119.3	120.1
C7-C18-C16	118.9	119.3
C18-C16-C20	117.9	117.8
C16-C20-N8	124.3	125.3
C20-N8-C4	118.4	117.1
N8-C4-C6	118.7	118.5
C4-C6-C3	118.8	119.0
C6-C3-N2	120.9	120.6
C3-N2-C5	124.3	123.7
N2-C5-O1	120.8	121.1
C7-C5-O1	124.7	123.6
C3-C6-C10	123.1	122.4
C6-C3-C13	121.9	122.5
C5-N2-C9	114.2	115.7
C3-N2-C9	121.5	120.5
C5-C7-C4	121.6	120.9
N8-C4-C7	121.3	121.4
N2-C9-C22	119.9	119.5
C9-C22-C24	119.8	119.0
C24-C26-C30	119.9	120.2
C30-C28-C9	119.8	119.5
C6-C10-C35	113.8	114.3
C3-C13-C32	114.1	113.4
C10-C35-C42	113.0	112.4

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