Supporting Information for the Paper Entitled "Revealing the thermodynamic driving force for ligand-based reductions in quinoids; conceptual rules for designing redox active and non-innocent ligands "

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Contents:

I. Computational protocol

Geometry optimizations were carried out using the TPSSh[1] density-functional coupled with the relativistic core potential containing cc-pVDZ-pp[2] basis set for Ru and the cc-pVDZ basis[3] for light atoms. The energies of the optimized structures were reevaluated using the triple-ζ basis set cc-pVTZ(-pp)[4] (-pp applies for Ru). Analytical vibrational frequency calculations within the harmonic approximation were computed with the cc-pVDZ(-pp) basis to confirm minima on the potential energy surface. All of these calculations were carried out with Gaussian09[5]. Solvent effects were simulated at the TPSSh/cc-pVTZ(-pp) level of theory using the SMD implicit solvation model[6].As is the case for all continuum models, the solvation energies are subject to empirical parametrization of the atomic radii that are used to generate the solute surface. In our calculations the Solvent Accessible Surface (SAS) method was used to create the molecular surface representing the solute-solvent boundary. We employed radii for H (1.400 Å), O (2.000Å), N (2.000Å), C (2.300Å), Cl (2.400Å), and Ru(1.800Å) and a solvent radius of 1.8 Å for acetonitrile.

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II. Energy Decomposition and NOCV Analyses

Energy decomposition analysis was performed at the PBE[7]/TZ2P(small core)/ZORA[8] level as implemented in ADF2013[9]. Within fragment-based approaches, such as the one available in ADF, the potential energy change ΔE can be expressed in terms of the strain energy ΔE_{strain} [10] which is the energy associated with the geometrical deformation of the fragments from their starting (equilibrium) structure, and the interaction energy between the fragments ΔE_{int}, Eq. (1) .

$$\Delta E = \Delta E_{\text{strain}} + \Delta E_{\text{int}} \quad (1)$$

$$\Delta E_{\text{int}} = \Delta E_{\text{Pauli}} + \Delta V_{\text{elstat}} + \Delta E_{\text{oi}} \quad (2)$$

The interaction energy can be further decomposed into three physically meaningful terms, Eq. (2), ΔE_{Pauli}, ΔV_{elstat} and ΔE_{oi}, using the Ziegler-Rauk decomposition scheme[11]. The electrostatic interaction contribution (ΔV_{elstat}) represents the classical Coulomb interaction between the fragments with unperturbed charge distributions. The Pauli repulsion term, ΔE_{Pauli}, embodies the repulsive filled-filled orbital interaction, which is the origin of the steric effect evolving between the reactants[12]. The orbital interaction energy, ΔE_{oi}, calculated in the energy decomposition analysis corresponds to the stabilization caused by the interactions between the occupied molecular orbitals on one fragment and the unoccupied molecular orbitals of the other fragment, as well as by the mixing of occupied and virtual orbitals within the same fragment (intrafragment polarization) upon the formation of the assembled structure from the fragments. The density reorganization which is associated with the latter process and which gives raise to ΔE_{oi} can be expressed in Natural Orbitals for Chemical Valence (NOCV), defined as the eigenvectors that diagonalize the deformation density (5)[13],

$$\Delta\rho(r) = \rho - \rho^0 \quad (3)$$

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being the difference between the total density ρ of the supermolecule and the sum ρ^0 of the densities of the initial fragments. It is a general property of a subtraction of two idempotent density matrices that eigenvalues appear pairwise, so that the deformation density (5) can be expressed as a sum of pairs of complementary eigenfunctions (ψ_k, ψ_{-k}) corresponding to the eigenvalues ν_k and $-\nu_k$:

$$\Delta\rho(r) = \sum_{k=1}^{M/2} \nu_k \left[-\psi_{-k}^2(r) + \psi_k^2(r) \right] = \sum_{k=1}^{M/2} \Delta\rho_k(r) \qquad (4)$$

This implies that the eigenvalue ν_k is the number of electrons that is transferred from orbital ψ_k to $-\psi_k$ upon bond formation. In this study the expression of an NOCV is simply used for the density deformation, $\Delta\rho_i$, represented by a complementary NOCV pair:

$$\Delta\rho_i(r) = \nu_i \left[-\psi_{-i}^2(r) + \psi_i^2(r) \right] \qquad (5)$$

We carried out the Energy Decomposition Analysis and NOCV analysis using L_{NN}^0 and $(en)_2Ru^{+2}$ fragments for $(en)_2RuL_{NN}^{+2}$ and L_{NN}^{-2} and $(en)_2Ru^{+2}$ fragments for $(en)_2RuL_{NN}^0$.

III. Computing redox potentials

We followed an established protocol for computing redox potentials described in details by Roy *et al.*[14] and Baik and Friesner[15]. The standard one-electron reduction potential (E^0) of a half cell, Eq. (1), can be evaluated through the Nernst equation, Eq. (2);

$$A + e^- \rightarrow A^- \tag{6}$$

$$E^0(A \rightarrow A^-) = -\frac{\Delta G^0_{sol}(A \rightarrow A^-)}{nF} \tag{7}$$

where

$$\Delta G^0_{sol} = G^0_{sol}(A^-) - G^0_{sol}(A) \tag{8}$$

and

$$G^0_{sol} = G^0_{gas} + \Delta G^0_{solv} \tag{9}$$

where ΔG^0_{solv} is solvation energy. ΔG^0_{solv} was evaluated in acetonitrile using the method described in section I.

We used the ferrocene-ferrocenium couple, Fc/Fc^+, as reference to derive reduction potentials from computed half-cell potentials. We used the recently published computed value of 4.96 V for the Fc/Fc^+ couple in acetonitrile[16] agreeing well with the experimental value of 4.98 V. Thus, the reduction potentials are evaluated as:

$$E^0 = E^0(A \rightarrow A^-) - E^0(Fc^+ \rightarrow Fc) \tag{10}$$

Figure S1 shows the computed and experimental reduction potentials vs. Fc/Fc^+ for the $(bpy)_2RuL_{NN}^{+3/+2/+1/0}$ redox series, analogous to the series investigated for the octahedral ruthenium-benzoquinonediimine complex $(en)_2RuL_{NN}^{+3/+2/+1/0}$. Conversion from SCE to Fc/Fc^+ couple was required for the experimental value since the redox potentials for the $(bpy)_2RuL_{NN}^{n}$ system were measured against SCE reference electrode in acetonitrile with 0.1 M $TBAPF_6$ supporting electrolyte. We used a formal potential of 0.40V for Fc/Fc^+ vs SCE to convert the measured values to the Fc/Fc^+ couple as proposed by Geiger and Connelly[17] and others[18] for such conditions.

As Figure S1 shows the method used can reproduce experimental redox potentials reasonably well for pure electrode processes.

[14] Roy, L. E.; Jakubikova, E.; Guthrie, M. G.; Batista, E. R. *J. Phys. Chem. A* **2009**, *113*, 6745.
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[16] Namazian, M.; Lin, C. Y.; Coote, M. L. *J. Chem. Theory Comput.* **2010**, *6*, 2721
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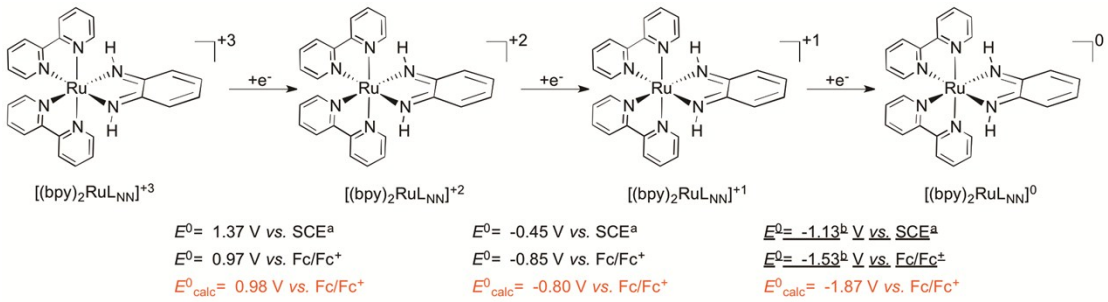

Figure S1. Measured and computed (red) redox potentials for $(bpy)_2RuL_{NN}^{+3/+2}$, $(bpy)_2RuL_{NN}^{+2/+1}$ and $(bpy)_2RuL_{NN}^{+1/0}$ couples. [a] H. Masui, A. B. Lever and E. S. Dodsworth, *Inorg. Chem.*, 1993, **32**, 258. [b] Quasi-reversible transition in experiments corresponding to a coupled electrode-chemical (EC) process, whereas in simulation it is a pure electrode process as indicate in the figure.

IV. Computing Nucleus Independent Chemical Shift values

The Nucleus Independent Chemical Shift (NICS) method has been introduced by Schleyer and co-workers and has been shown to provide a reliable measure for aromaticity based on magnetic criteria[19]. In this study the NICS values were computed at the centre of the benzo-C_6 ring of the quinoid derivatives, as shown for L_{NN} in Figure S2, at the TPSSh/ cc-pVTZ(-pp) level of theory. A NICS value of -8.3 ppm was calculated for benzene at the same level.

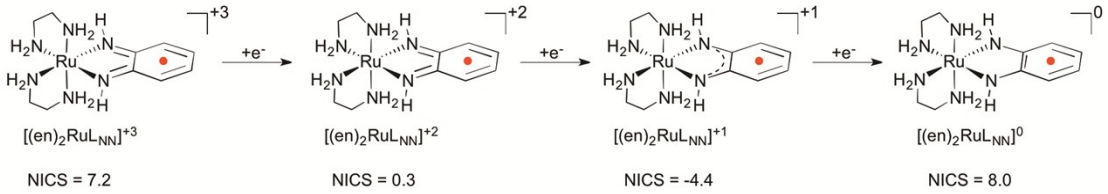

Figure S2. NICS values computed at the middle of the benzo-C_6 ring (red dot) for the $(en)_2RuL_{NN}^{+3/+2/+1/0}$ systems.

[19] Schleyer, P. v. R.; Puhlhofer, F., *Org. Lett.*, **2002**, ***4,*** 2873.

V. Computing theoretical square schemes

The method of theoretical square scheme has been introduced by Baik, Schauer and Ziegler in order to reveal the origins of two-electron potential inversions in various systems[20]. Within this technique the reduction process (diagonal) is partitioned to semi-adiabatic electron attachment and structural relaxation steps, which correspond to moving horizontally and vertically in the square scheme, respectively (Figure S3). To partition the reduction process, a single point calculation is carried out using the optimized geometry of the oxidized form, e.g. $(en)_2RuL_{NN}^{+3}$, but with the total charge of the reduced form, i.e. +2. This energy is corrected with solvation energy, ΔG_{solv}, to get ΔG_{sol}* values to the electron attachment and structural relaxation steps, which does not contain thermal corrections. Thus, ΔG_{sol}* and ΔG_{sol} differ in the thermal corrections, which cannot be evaluated reliably for the non-equilibrium structures.

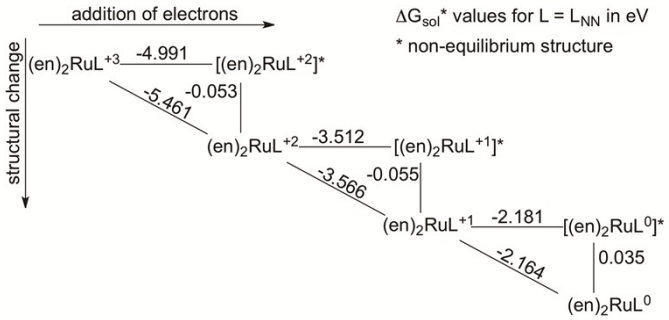

Figure S3. Representative theoretical square scheme for $[(en)_2RuL_{NN}]^{+3/+2/+1/0}$.

Electron density accumulation plots have been computed and given in Figure 3 for the semi-adiabatic electron attachment step (horizontal) where the density change upon structural change does not interfere.

[20] Baik, M.-H.; Schauer, C. K.; Ziegler, T. *J. Am. Chem. Soc.* **2002**, *124*, 11167

V. Cartesian coordinates for optimized structures

$[(en_2]RuL_{NN}]^{+3}$

C	2.134135	0.448403	0.577924
C	2.129213	-0.503699	-0.549321
C	3.359755	-0.967313	-1.097147
C	4.534631	-0.506511	-0.535466
C	4.539338	0.417375	0.571202
C	3.369256	0.894420	1.129533
H	3.368817	-1.668029	-1.934931
H	5.493463	-0.846671	-0.934056
H	5.501585	0.744632	0.972370
H	3.385840	1.594953	1.967360
H	0.890113	1.468954	1.746815
H	0.871098	-1.502901	-1.724059
N	0.895000	-0.839063	-0.936921
N	0.903717	0.803256	0.960752
Ru	-0.652784	0.002856	-0.000326
C	-1.478052	2.842416	-0.637375
H	-1.787946	3.587359	-1.385510
H	-0.767499	3.326603	0.049484
C	-2.672538	2.274979	0.103939
H	-3.187797	3.052511	0.687426
H	-3.404778	1.842547	-0.595535
H	-1.818353	1.596217	1.868562
H	-3.010422	0.643925	1.340365
H	-1.246332	1.465185	-2.181152
H	0.170154	2.029351	-1.622504
C	-2.234406	-2.528668	-0.526203
H	-1.393863	-3.074092	-0.981617
H	-3.165568	-3.027960	-0.832848
C	-2.104026	-2.479380	0.983546
H	-2.969507	-1.979978	1.445648
H	-2.031695	-3.488899	1.415195
H	-0.909556	-1.408696	2.317111
H	-0.046359	-2.287077	1.263684
H	-3.140654	-0.708265	-0.933173
H	-2.076791	-1.151947	-2.068398
N	-2.198036	-1.107116	-1.046242
N	-0.871640	-1.674651	1.322843
N	-0.752208	1.698441	-1.307755
N	-2.186158	1.164063	1.008798

$[(en_2]RuL_{NN}]^{+2}$

C	2.123718	0.471696	0.557056
C	2.123320	-0.501284	-0.538855
C	3.366791	-0.972015	-1.069199
C	4.532214	-0.505363	-0.519841
C	4.532319	0.443225	0.568625
C	3.366619	0.926439	1.102489
H	3.371916	-1.690631	-1.891158
H	5.491153	-0.854166	-0.906469
H	5.491154	0.778044	0.967575
H	3.370989	1.644975	1.924554
H	0.901786	1.510516	1.709703
H	0.898125	-1.513164	-1.714246
N	0.897360	-0.847528	-0.931386
N	0.898337	0.836832	0.933055
Ru	-0.673784	0.004257	-0.005052
C	-1.475770	2.818663	-0.674461
H	-1.800495	3.578629	-1.401210
H	-0.724436	3.277983	-0.014437
C	-2.653643	2.296664	0.129644
H	-3.131334	3.105462	0.702937
H	-3.416414	1.864585	-0.537381
H	-1.737672	1.637859	1.861486
H	-2.984082	0.712122	1.413495
H	-1.343305	1.433427	-2.213674
H	0.105201	1.946223	-1.694050
C	-2.167968	-2.568322	-0.499785
H	-1.291201	-3.080901	-0.923770
H	-3.066075	-3.129367	-0.799431
C	-2.055126	-2.486138	1.012319
H	-2.943036	-1.996223	1.442757
H	-1.978923	-3.489401	1.458202
H	-0.894227	-1.392927	2.343814
H	-0.014573	-2.226888	1.267771
H	-3.145453	-0.810351	-0.965252
H	-2.035369	-1.229359	-2.064896
N	-2.185343	-1.169953	-1.049807
N	-0.859841	-1.647499	1.349468
N	-0.820709	1.655674	-1.356868
N	-2.162957	1.200308	1.033829

$[(en_2]RuL_{NN}]^{+1}$

C	2.084959	0.446769	0.547991
C	2.075703	-0.531659	-0.516132
C	3.309266	-1.001075	-1.034446
C	4.505679	-0.534375	-0.510885
C	4.514228	0.414070	0.542671
C	3.325340	0.897751	1.066866
H	3.304215	-1.735522	-1.844717
H	5.451897	-0.901328	-0.912608
H	5.466442	0.767245	0.942336
H	3.330706	1.632359	1.877082
H	0.874177	1.505792	1.736543
H	0.844686	-1.562388	-1.710853
N	0.830741	-0.911391	-0.920775
N	0.847469	0.847064	0.952143
Ru	-0.736874	0.005492	-0.000466
C	-1.248633	2.864300	-0.651714
H	-1.460204	3.685754	-1.355155
H	-0.496824	3.214925	0.071377
C	-2.515605	2.441053	0.076623
H	-2.957800	3.294514	0.616474
H	-3.265299	2.073228	-0.642742
H	-1.731540	1.698801	1.835227
H	-3.059824	0.909812	1.347743
H	-1.132073	1.537882	-2.242176
H	0.315308	1.846528	-1.552115
C	-2.156155	-2.592258	-0.493711
H	-1.274383	-3.050091	-0.966942
H	-3.039162	-3.197768	-0.755541
C	-1.963308	-2.545835	1.015322
H	-2.846666	-2.100668	1.501718
H	-1.838476	-3.565049	1.416596
H	-0.737446	-1.483857	2.314216
H	0.075945	-2.181610	1.080122
H	-3.228403	-0.871529	-0.876758
H	-2.151922	-1.227576	-2.035179
N	-2.261809	-1.193061	-1.015134
N	-0.792295	-1.678297	1.308851
N	-0.673120	1.671760	-1.333866
N	-2.180953	1.309136	0.997401

$[(en_2]RuL_{NN}]^{0}$

C	2.062977	0.426141	0.546149
C	2.044934	-0.568337	-0.490184
C	3.265234	-1.011615	-1.027799
C	4.495155	-0.551892	-0.526170
C	4.513400	0.363921	0.530488
C	3.304535	0.845471	1.059160
H	3.247093	-1.757716	-1.831316
H	5.430114	-0.920881	-0.956858
H	5.463600	0.717309	0.940893
H	3.317240	1.588083	1.865918
H	0.839508	1.324078	1.868481
H	0.788333	-1.488606	-1.767248
N	0.778366	-1.053397	-0.839102
N	0.817881	0.926421	0.923193
Ru	-0.782219	0.009284	0.000071

C	-1.088509	2.884202	-0.647586
H	-1.221988	3.732099	-1.342913
H	-0.348736	3.165010	0.118425
C	-2.409240	2.538443	0.029541
H	-2.819520	3.430335	0.540174
H	-3.149926	2.204134	-0.715976
H	-1.670867	1.761550	1.787643
H	-3.079627	1.086870	1.331591
H	-0.881044	1.604280	-2.275185
H	0.483651	1.759534	-1.354650
C	-2.181022	-2.590196	-0.481746
H	-1.300816	-3.011308	-0.990844
H	-3.058132	-3.223056	-0.711740
C	-1.919159	-2.565666	1.020487
H	-2.793394	-2.152091	1.553404
H	-1.762065	-3.599194	1.382544
H	-0.585901	-1.567258	2.269434
H	0.095889	-2.088765	0.831641
H	-3.298034	-0.882405	-0.784218
H	-2.282087	-1.218044	-2.006392
N	-2.337908	-1.192810	-0.982141
N	-0.761182	-1.685923	1.266327
N	-0.541551	1.675003	-1.310684
N	-2.173533	1.402806	0.966698

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$[(en_2]RuL_{OO}]^{+3}$

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C	2.087395	0.506545	0.541929
C	2.080777	-0.578999	-0.512562
C	3.297248	-1.096423	-1.030699
C	4.453532	-0.579244	-0.495392
C	4.459629	0.450925	0.550301
C	3.309920	0.994803	1.073556
H	3.294435	-1.862718	-1.807632
H	5.422421	-0.942064	-0.850026
H	5.432744	0.791474	0.915314
H	3.317261	1.760510	1.851000
Ru	-0.681498	0.000914	-0.008376
C	-1.368158	2.872168	-0.605797
H	-1.654862	3.654319	-1.324603
H	-0.614176	3.290318	0.077624
C	-2.573900	2.353449	0.151740
H	-3.017285	3.130950	0.791541
H	-3.357720	1.987061	-0.529009
H	-1.651125	1.558663	1.840247
H	-2.952016	0.700761	1.374066
H	-1.253590	1.520349	-2.189488
H	0.200495	1.994281	-1.653340
C	-2.204285	-2.542611	-0.533140
H	-1.360324	-3.085102	-0.984531
H	-3.137906	-3.025412	-0.857455
C	-2.088590	-2.489879	0.976955
H	-2.956020	-1.990205	1.435320
H	-2.014272	-3.498319	1.411034
H	-0.868224	-1.445956	2.313016
H	-0.032270	-2.291173	1.204135
H	-3.097959	-0.710658	-1.011054
H	-1.940119	-1.153777	-2.060358
N	-2.151113	-1.116785	-1.050241
N	-0.856531	-1.681950	1.309705
N	-0.730268	1.704721	-1.320840
N	-2.120673	1.180931	1.000363
O	0.913147	0.905065	0.857912
O	0.901239	-0.952108	-0.839349

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$[(en_2]RuL_{OO}]^{+2}$

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C	2.046279	0.502230	0.536189
C	2.048636	-0.527642	-0.521430
C	3.277343	-1.034173	-1.028746
C	4.437896	-0.531844	-0.489443
C	4.434960	0.474137	0.550832
C	3.271146	0.994067	1.065867
H	3.272937	-1.791388	-1.813307
H	5.402011	-0.896041	-0.849410
H	5.396896	0.823877	0.930336
H	3.262161	1.752070	1.849615
Ru	-0.679036	0.002231	-0.009510
C	-1.408724	2.824771	-0.667308
H	-1.732373	3.595331	-1.382736
H	-0.615419	3.249125	-0.033926
C	-2.571300	2.337836	0.179298
H	-2.991536	3.154547	0.785008
H	-3.378134	1.936823	-0.454324
H	-1.552869	1.631233	1.837956
H	-2.886630	0.766125	1.488656
H	-1.397052	1.421660	-2.202828
H	0.090329	1.896510	-1.765887
C	-2.067970	-2.590454	-0.517970
H	-1.160464	-3.058921	-0.926598
H	-2.938531	-3.176206	-0.848706
C	-1.998201	-2.514223	0.996251
H	-2.910605	-2.057802	1.410847
H	-1.890973	-3.514710	1.441233
H	-0.901437	-1.373805	2.352699
H	0.025222	-2.189279	1.297469
H	-3.098206	-0.860539	-1.008709
H	-1.914029	-1.230430	-2.061104
N	-2.123438	-1.185858	-1.055283
N	-0.838463	-1.632840	1.360306
N	-0.825255	1.636437	-1.375612
N	-2.073767	1.218271	1.051175
O	0.877894	-0.898700	-0.923041
O	0.872396	0.894122	0.908891

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$[(en_2]RuL_{OO}]^{+1}$

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C	-1.953240	-0.559612	0.485418
C	-1.973896	0.470781	-0.519923
C	-3.211416	0.967804	-0.986598
C	-4.390037	0.457071	-0.459825
C	-4.368142	-0.555928	0.531432
C	-3.166167	-1.065606	1.002643
H	-3.214212	1.744661	-1.753478
H	-5.349398	0.839166	-0.813766
H	-5.310421	-0.938783	0.927577
H	-3.132254	-1.846695	1.764477
Ru	0.734004	0.004740	-0.012941
C	1.381771	-2.814525	-0.669319
H	1.684875	-3.614822	-1.362788
H	0.561598	-3.187272	-0.037993
C	2.552648	-2.377618	0.198717
H	2.937531	-3.226794	0.786188
H	3.376449	-1.995605	-0.425893
H	1.507756	-1.652373	1.826276
H	2.909665	-0.860192	1.553941
H	1.434344	-1.436381	-2.223790
H	-0.077885	-1.822170	-1.756848
C	1.826619	2.720199	-0.478144
H	0.880204	3.032906	-0.943144
H	2.613397	3.438593	-0.758264
C	1.664114	2.654733	1.032926
H	2.599187	2.320538	1.510628
H	1.413982	3.647719	1.439445
H	0.609206	1.426371	2.341121
H	-0.315642	2.062365	1.155009
H	3.126324	1.155753	-0.868950
H	1.974778	1.349129	-2.004461
N	2.123250	1.343544	-0.988417
N	0.608520	1.647509	1.339573
N	0.860544	-1.616789	-1.391890
N	2.092915	-1.257800	1.076701
O	-0.801648	0.898076	-0.983651
O	-0.760323	-1.003543	0.875947

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$[(en_2]RuL_{OO}]^{0}$

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C	1.919520	0.435447	0.516677
C	1.888822	-0.630189	-0.444184
C	3.102681	-1.157410	-0.916125

C	4.334369	-0.662169	-0.460455
C	4.364333	0.375472	0.477381
C	3.163208	0.916974	0.960525
H	3.058689	-1.969061	-1.648928
H	5.265695	-1.089032	-0.842886
H	5.319461	0.767185	0.838245
H	3.167297	1.726558	1.697056
Ru	-0.792696	0.014955	-0.000608
C	-0.880486	2.883998	-0.697502
H	-0.980720	3.731544	-1.398334
H	-0.065790	3.095359	0.010674
C	-2.176701	2.674919	0.078048
H	-2.446050	3.603133	0.615981
H	-3.004316	2.426010	-0.607352
H	-1.325198	1.794959	1.735102
H	-2.875352	1.320769	1.469446
H	-0.984982	1.550810	-2.288180
H	0.494449	1.619679	-1.583694
C	-2.027808	-2.618609	-0.499382
H	-1.076553	-2.967411	-0.928875
H	-2.836224	-3.312501	-0.793071
C	-1.893722	-2.558288	1.017785
H	-2.815702	-2.156856	1.471682
H	-1.729555	-3.574948	1.420220
H	-0.717850	-1.457716	2.338901
H	0.109397	-2.062963	1.040817
H	-3.233773	-0.994213	-0.930398
H	-2.063975	-1.260153	-2.035791
N	-2.240564	-1.237836	-1.025194
N	-0.784057	-1.631732	1.331172
N	-0.513718	1.615815	-1.380156
N	-1.987638	1.518558	0.995946
O	0.751340	0.943633	0.973613
O	0.690686	-1.101593	-0.873968

$[(en_2]RuL_{NO}]^{+3}$

C	-2.124450	-0.545625	0.562526
C	-2.081293	0.475902	-0.522048
C	-3.278514	0.969005	-1.089783
C	-4.467133	0.476233	-0.582595
C	-4.519700	-0.508563	0.484176
C	-3.381005	-1.020787	1.056894
H	-3.247512	1.708857	-1.891059
H	-5.414664	0.837896	-0.991652
H	-5.501054	-0.841038	0.831075
H	-3.424062	-1.758739	1.861156
H	-0.904026	-1.641897	1.676483
N	-0.908037	-0.914248	0.945737
Ru	0.663536	-0.020742	0.040318
C	1.641110	-2.797024	-0.649326
H	1.981778	-3.513849	-1.411507
H	0.988899	-3.335357	0.055087
C	2.813764	-2.149255	0.060669
H	3.398095	-2.886993	0.630558
H	3.494328	-1.662273	-0.654988
H	1.954568	-1.534225	1.850595
H	3.068782	-0.498557	1.298898
H	1.261385	-1.431506	-2.175890
H	-0.091617	-2.094008	-1.573553
C	1.998414	2.610863	-0.581305
H	1.098849	3.052824	-1.034505
H	2.874102	3.177019	-0.931554
C	1.908450	2.599556	0.930982
H	2.822378	2.193843	1.391380
H	1.749758	3.610700	1.334876
H	0.820781	1.481737	2.321017
H	-0.120288	2.231983	1.227879
H	3.061076	0.863687	-0.983672
H	1.885324	1.168741	-2.062894
N	2.080971	1.172415	-1.050158
N	0.756861	1.698650	1.315471
N	0.816606	-1.703112	-1.286535
N	2.275639	-1.075676	0.984917
O	-0.895574	0.859470	-0.866109

$[(en_2]RuL^{OMe}]^{+2}$

C	-1.426482	-0.838306	0.796482
C	-1.686559	0.212143	-0.198233
C	-3.021763	0.541015	-0.552035
C	-4.055574	-0.138530	0.074372
C	-3.796344	-1.165056	1.074484
C	-2.528181	-1.507975	1.430062
H	-4.668014	-1.645680	1.520795
H	-2.340409	-2.280754	2.178131
H	0.029878	-1.795993	1.713220
H	-0.732076	1.470418	-1.390682
N	-0.562790	0.753517	-0.676614
N	-0.135787	-1.066275	1.007560
Ru	1.212278	0.026579	-0.001144
C	2.224401	-2.601729	-1.036323
H	2.535169	-3.256651	-1.864615
H	1.620425	-3.200581	-0.337613
C	3.431812	-2.009477	-0.330949
H	4.068661	-2.800654	0.093204
H	4.046522	-1.429956	-1.038056
H	2.685693	-1.622771	1.556062
H	3.753077	-0.517847	1.060000
H	1.746690	-1.119353	-2.404682
H	0.440017	-1.845216	-1.775021
C	2.307481	2.804675	-0.398533
H	1.333685	3.221303	-0.697709
H	3.091261	3.504955	-0.725118
C	2.355703	2.594730	1.104291
H	3.336238	2.195939	1.408799
H	2.200039	3.543494	1.640175
H	1.476271	1.265394	2.433151
H	0.398255	2.043213	1.500768
H	3.453908	1.237051	-1.098464
H	2.196148	1.581223	-2.056779
N	2.451906	1.467387	-1.068058
N	1.316469	1.581680	1.469688
N	1.363642	-1.475319	-1.519813
N	2.946899	-1.065055	0.732738
H	-3.209770	1.313886	-1.296907
C	-5.786768	1.023505	-1.108341
H	-6.879827	0.972889	-1.094727
H	-5.403409	0.760027	-2.106011
H	-5.446034	2.026194	-0.808146
O	-5.355167	0.043556	-0.138700

$[(en_2]RuL_{NO}]^{+2}$

C	-2.080355	-0.575284	0.524826
C	-2.070950	0.429084	-0.544340
C	-3.301762	0.902044	-1.072478
C	-4.469722	0.395930	-0.545974
C	-4.482205	-0.588428	0.508247
C	-3.317679	-1.074333	1.042906
H	-3.297182	1.645084	-1.870218
H	-5.427845	0.747071	-0.934481
H	-5.444251	-0.945213	0.878623
H	-3.319238	-1.819369	1.841435
H	-0.845546	-1.632281	1.654728
N	-0.845648	-0.923681	0.906508
Ru	0.678425	-0.022896	0.032281
C	1.724666	-2.735013	-0.704141
H	2.130179	-3.434900	-1.450215
H	1.015160	-3.287874	-0.069585
C	2.836138	-2.124673	0.132189
H	3.381419	-2.897688	0.694239
H	3.562592	-1.603040	-0.510937
H	1.840803	-1.601010	1.869301
H	2.991416	-0.543688	1.456762
H	1.473624	-1.319042	-2.201944
H	0.075397	-1.977959	-1.718731
C	1.844085	2.680216	-0.543747
H	0.900542	3.035286	-0.983630
H	2.655209	3.344561	-0.876901

C	1.746975	2.645516	0.969713
H	2.687276	2.287507	1.418028
H	1.539062	3.645739	1.378587
H	0.714489	1.473241	2.343743
H	-0.245494	2.140687	1.211907
H	3.058299	1.051757	-0.949313
H	1.872223	1.266211	-2.041151
N	2.057361	1.273234	-1.029671
N	0.663756	1.675438	1.338268
N	0.967899	-1.617796	-1.357911
N	2.228300	-1.104287	1.056378
O	-0.905703	0.822703	-0.944854

$[(en_2]RuL_{NO}]^{+1}$

C	-2.018598	-0.610081	0.505186
C	-2.018171	0.402307	-0.518629
C	-3.248123	0.864550	-1.029336
C	-4.440585	0.342812	-0.535440
C	-4.442767	-0.648737	0.473724
C	-3.246946	-1.123011	0.991877
H	-3.241252	1.629144	-1.808362
H	-5.390813	0.704580	-0.933244
H	-5.390702	-1.040845	0.845655
H	-3.238172	-1.889175	1.772579
H	-0.784800	-1.695527	1.661822
N	-0.767519	-0.985486	0.921700
Ru	0.734680	-0.008548	0.039990
C	1.634381	-2.749711	-0.702931
H	1.983269	-3.495877	-1.434875
H	0.917475	-3.242305	-0.028523
C	2.805908	-2.188753	0.090913
H	3.337937	-2.994590	0.622335
H	3.524807	-1.700706	-0.586812
H	1.886669	-1.612739	1.848816
H	3.097662	-0.630604	1.410224
H	1.387586	-1.368463	-2.231207
H	-0.023402	-1.919262	-1.632865
C	1.659533	2.757476	-0.539369
H	0.684482	2.983782	-0.995034
H	2.389177	3.518434	-0.859351
C	1.527344	2.734259	0.975587
H	2.489865	2.476349	1.446918
H	1.222189	3.723959	1.352231
H	0.559483	1.505649	2.345102
H	-0.406021	2.017880	1.126753
H	3.057199	1.272713	-0.897335
H	1.879385	1.350229	-2.020214
N	2.042133	1.387585	-1.007077
N	0.542975	1.675739	1.334412
N	0.917184	-1.616119	-1.352773
N	2.292644	-1.142180	1.030380
O	-0.841464	0.857506	-0.940021

$[(en_2]RuL_{NO}]^{0}$

C	1.971173	0.180129	0.595910
C	1.898577	-0.864887	-0.386521
C	3.100999	-1.369886	-0.916451
C	4.348941	-0.898496	-0.478668
C	4.413524	0.094265	0.503759
C	3.227151	0.627038	1.035699
H	3.049816	-2.156268	-1.678953
H	5.265293	-1.310843	-0.910153
H	5.380776	0.465518	0.853455
H	3.256427	1.416889	1.792665
H	0.617564	-1.782836	-1.629259
N	0.611510	-1.312176	-0.717971
Ru	-0.790901	0.037363	-0.024291
C	-0.334492	2.888839	-0.682016
H	-0.246267	3.742680	-1.377043
H	0.462694	2.954081	0.072773
C	-1.688995	2.910818	0.017955
H	-1.819183	3.873318	0.547626
H	-2.506954	2.814131	-0.716256
H	-1.081040	1.876005	1.692924
H	-2.687981	1.719309	1.376793
H	-0.572773	1.601747	-2.295692
H	0.850663	1.404440	-1.496969
C	-2.630692	-2.255018	-0.503843
H	-1.826411	-2.850250	-0.962334
H	-3.601816	-2.715203	-0.763535
C	-2.434860	-2.236077	1.009290
H	-3.239295	-1.652291	1.489189
H	-2.488012	-3.269397	1.400147
H	-1.003585	-1.441015	2.297440
H	-0.355697	-2.147719	0.925778
H	-3.379750	-0.368458	-0.879427
H	-2.411324	-0.929846	-2.058588
N	-2.495292	-0.867711	-1.037903
N	-1.146876	-1.576560	1.291634
N	-0.154650	1.578254	-1.360615
N	-1.763577	1.741016	0.933101
O	0.818842	0.713991	1.057479

$[(en_2]RuL^{OMe}]^{+3}$

C	-1.499795	-0.620173	0.720763
C	-1.616057	0.354039	-0.376110
C	-2.871120	0.741564	-0.833582
C	-4.029930	0.189124	-0.215931
C	-3.916949	-0.764063	0.881171
C	-2.692422	-1.155896	1.335488
H	-4.821956	-1.165116	1.338893
H	-2.605821	-1.871071	2.156848
H	-0.165212	-1.588913	1.809135
H	-0.462154	1.456716	-1.593746
N	-0.403584	0.779566	-0.822622
N	-0.252234	-0.913153	1.037135
Ru	1.218936	0.014989	-0.000771
C	2.161290	-2.757702	-0.768132
H	2.462502	-3.472432	-1.548510
H	1.523141	-3.290864	-0.046996
C	3.368936	-2.143945	-0.087389
H	3.965952	-2.906813	0.434049
H	4.026034	-1.648489	-0.819222
H	2.587625	-1.570955	1.743848
H	3.693231	-0.537417	1.179644
H	1.765683	-1.361927	-2.256407
H	0.418549	-2.010998	-1.625209
C	2.611609	2.640194	-0.536165
H	1.706531	3.151182	-0.897980
H	3.484425	3.208650	-0.890316
C	2.605047	2.528079	0.976446
H	3.532383	2.063981	1.346873
H	2.515756	3.516603	1.451174
H	1.573740	1.356303	2.359976
H	0.590833	2.203021	1.388097
H	3.578533	0.894388	-1.089643
H	2.406115	1.319913	-2.118542
N	2.610592	1.244053	-1.112562
N	1.452949	1.641438	1.378772
N	1.340995	-1.640697	-1.361228
N	2.879599	-1.092229	0.880436
H	-3.009014	1.455992	-1.647311
C	-6.480736	0.155090	-0.208631
H	-6.563315	-0.932204	-0.340210
H	-7.188342	0.685929	-0.851746
H	-6.588968	0.463760	0.839901
O	-5.162112	0.598814	-0.701969

$[(en_2]RuL^{OMe}]^{+1}$

C	-1.389144	-0.850838	0.793026
C	-1.647666	0.202103	-0.163133
C	-2.985642	0.522225	-0.508057
C	-4.034928	-0.168609	0.094326
C	-3.781856	-1.192204	1.051974
C	-2.484928	-1.522896	1.392860
H	-4.637906	-1.699912	1.497021

H	-2.294234	-2.312905	2.124366
H	0.088723	-1.814939	1.735463
H	-0.726294	1.499610	-1.374310
N	-0.528472	0.801319	-0.652989
N	-0.068099	-1.095848	1.022441
Ru	1.260125	0.042257	-0.007278
C	2.061518	-2.646323	-1.003353
H	2.294190	-3.362166	-1.808496
H	1.454351	-3.165944	-0.246618
C	3.340832	-2.116421	-0.371864
H	3.947955	-2.945283	0.028386
H	3.948792	-1.588717	-1.124994
H	2.683856	-1.646146	1.525900
H	3.832247	-0.642174	0.983439
H	1.581289	-1.212304	-2.422168
H	0.280616	-1.786599	-1.619757
C	2.243277	2.849429	-0.391512
H	1.256685	3.209402	-0.720717
H	2.997455	3.598263	-0.684287
C	2.240790	2.648971	1.117295
H	3.227363	2.293243	1.457033
H	2.032576	3.602723	1.629866
H	1.334053	1.318124	2.427887
H	0.290424	1.988606	1.361365
H	3.487492	1.342145	-1.051091
H	2.243846	1.629821	-2.050775
N	2.476727	1.529192	-1.056089
N	1.240698	1.600689	1.446690
N	1.256098	-1.491382	-1.489535
N	2.975676	-1.126230	0.688974
H	-3.168793	1.312923	-1.237306
C	-5.698214	1.054822	-1.104821
H	-6.793740	1.058076	-1.146925
H	-5.289020	0.816407	-2.101946
H	-5.336056	2.046866	-0.783811
O	-5.354250	0.049481	-0.154274

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$[(en_2]RuL^{OMe}]^0$

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C	-1.414565	-0.664334	0.672794
C	-1.543692	0.345899	-0.341981
C	-2.824621	0.710373	-0.787581
C	-3.978726	0.157600	-0.207338
C	-3.868819	-0.774120	0.829471
C	-2.582564	-1.174479	1.251260
H	-4.748488	-1.207044	1.307280
H	-2.495974	-1.931730	2.038887
H	-0.029653	-1.425930	1.917364
H	-0.458773	1.415208	-1.659676
N	-0.349377	0.921446	-0.768933
N	-0.105044	-1.086683	0.950718
Ru	1.345106	0.022548	-0.010261
C	1.920551	-2.790998	-0.746546
H	2.110043	-3.606003	-1.467537
H	1.248220	-3.160956	0.043536
C	3.225248	-2.320701	-0.116652
H	3.753428	-3.174131	0.349501
H	3.889572	-1.885395	-0.881419
H	2.471944	-1.675633	1.687031
H	3.788188	-0.844694	1.208974
H	1.511307	-1.505056	-2.331011
H	0.211375	-1.820391	-1.356205
C	2.417995	2.774481	-0.480487
H	1.468544	3.102482	-0.930313
H	3.201955	3.512093	-0.733667
C	2.240732	2.682072	1.031640
H	3.181385	2.353705	1.506850
H	1.989837	3.681453	1.434301
H	1.104649	1.504143	2.315554
H	0.282153	1.997398	0.948771
H	3.709666	1.223033	-0.903746
H	2.583047	1.459691	-2.049741
N	2.708678	1.418897	-1.032256
N	1.201902	1.671483	1.308733
N	1.223613	-1.632075	-1.355638
N	2.907587	-1.242919	0.863118
H	-2.946926	1.468331	-1.567651
C	-6.361027	0.102701	-0.154666
H	-6.434892	-0.995459	-0.276041
H	-7.195472	0.581819	-0.686667
H	-6.433332	0.340058	0.924503
O	-5.180131	0.619859	-0.730883

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$[(en_2]RuL^{NO2}]^{+2}$

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C	-1.262914	-0.804159	0.776231
C	-1.467599	0.246221	-0.222939
C	-2.793178	0.615693	-0.607172
C	-3.824080	-0.036735	0.007076
C	-3.653183	-1.058034	1.000921
C	-2.394686	-1.438555	1.384207
H	-4.550275	-1.508861	1.425972
H	-2.247077	-2.215461	2.136694
H	0.171742	-1.781882	1.721686
H	-0.477137	1.490113	-1.399411
N	-0.329097	0.765610	-0.685488
N	0.025116	-1.055767	1.008991
Ru	1.397155	0.019425	0.000418
C	2.386112	-2.629760	-1.022485
H	2.693677	-3.285724	-1.850794
H	1.760752	-3.219052	-0.334825
C	3.593163	-2.059044	-0.301196
H	4.207642	-2.858721	0.138927
H	4.231289	-1.492920	-0.998150
H	2.821274	-1.655339	1.572702
H	3.915388	-0.568196	1.091757
H	1.956753	-1.132881	-2.393887
H	0.628435	-1.839417	-1.788124
C	2.572220	2.773606	-0.377427
H	1.608885	3.228452	-0.653924
H	3.373593	3.450156	-0.710589
C	2.641889	2.540638	1.120450
H	3.616561	2.113425	1.404385
H	2.517028	3.483324	1.674276
H	1.753764	1.205622	2.443308
H	0.679306	2.038845	1.560706
H	3.653169	1.177234	-1.118356
H	2.392893	1.575932	-2.050600
N	2.659902	1.439912	-1.067296
N	1.580310	1.548719	1.490829
N	1.553505	-1.484705	-1.516078
N	3.105435	-1.103095	0.753067
H	-2.999282	1.384515	-1.353632
N	-5.218521	0.336303	-0.379719
O	-6.116448	-0.267361	0.190025
O	-5.334326	1.208372	-1.229107

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$[(en_2]RuL^{NO2}]^{+1}$

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C	-1.228216	-0.794485	0.767746
C	-1.435672	0.260026	-0.203139
C	-2.748636	0.617449	-0.573357
C	-3.811310	-0.045528	0.022119
C	-3.635610	-1.063783	0.985695
C	-2.354751	-1.431745	1.354597
H	-4.518801	-1.536335	1.412559
H	-2.199696	-2.220152	2.095340
H	0.205863	-1.786356	1.738568
H	-0.452150	1.533452	-1.393705
N	-0.286137	0.820743	-0.677433
N	0.075107	-1.068291	1.019689
Ru	1.447608	0.030393	-0.003948
C	2.210528	-2.681730	-0.977683
H	2.438436	-3.402729	-1.778939
H	1.581394	-3.187555	-0.229751
C	3.490778	-2.175342	-0.330510
H	4.074048	-3.012671	0.085746
H	4.122225	-1.665169	-1.076195
H	2.819749	-1.682148	1.556971
H	3.990402	-0.699680	1.021599

H	1.785947	-1.239451	-2.406721
H	0.459776	-1.790756	-1.633680
C	2.525008	2.804656	-0.387283
H	1.546519	3.201315	-0.697750
H	3.299550	3.526825	-0.691858
C	2.545154	2.595257	1.119372
H	3.524655	2.202828	1.438203
H	2.379278	3.550044	1.643993
H	1.630485	1.275498	2.436989
H	0.580357	2.011398	1.430294
H	3.705564	1.258887	-1.076340
H	2.454036	1.590690	-2.051135
N	2.701595	1.478829	-1.061024
N	1.513280	1.579342	1.464441
N	1.436353	-1.511017	-1.480491
N	3.129505	-1.171837	0.720497
H	-2.950850	1.398142	-1.307584
N	-5.176924	0.330835	-0.368921
O	-6.106324	-0.265505	0.173852
O	-5.301753	1.217725	-1.214544

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$[(en_2]RuL^{NO2}]^0$

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C	-1.206373	-0.712172	0.835421
C	-1.403833	0.367451	-0.108541
C	-2.699112	0.684104	-0.512553
C	-3.801651	-0.006029	0.036074
C	-3.631199	-1.013809	0.995017
C	-2.340600	-1.355817	1.390011
H	-4.511608	-1.512461	1.397658
H	-2.187997	-2.156591	2.121440
H	0.207117	-1.728234	1.827352
H	-0.390822	1.562578	-1.361131
N	-0.236280	1.022630	-0.504085
N	0.099192	-1.020442	1.095543
Ru	1.500232	0.023943	0.008229
C	1.896310	-2.750586	-0.960749
H	1.985559	-3.515044	-1.752724
H	1.296604	-3.172650	-0.139842
C	3.277269	-2.364685	-0.442529
H	3.811494	-3.261407	-0.077995
H	3.877151	-1.921688	-1.254704
H	2.811341	-1.782671	1.480643
H	4.051168	-0.950611	0.842067
H	1.415067	-1.331348	-2.397409
H	0.171205	-1.697051	-1.387371
C	2.612438	2.754608	-0.457158
H	1.633632	3.129352	-0.792236
H	3.390909	3.473338	-0.770555
C	2.598000	2.605950	1.060027
H	3.575630	2.237103	1.415921
H	2.420548	3.592418	1.526121
H	1.574907	1.396577	2.411842
H	0.621166	1.972274	1.166596
H	3.796607	1.173935	-1.054867
H	2.581697	1.496997	-2.082717
N	2.796068	1.410093	-1.083042
N	1.566318	1.610435	1.409722
N	1.186002	-1.529438	-1.417785
N	3.122048	-1.324273	0.615462
H	-2.891454	1.476371	-1.237609
N	-5.132619	0.336995	-0.398743
O	-6.098125	-0.264104	0.103637
O	-5.259716	1.222759	-1.262658

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$[(en_2]RuL^{NO2}]^{+3}$

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C	-1.275621	-0.774262	0.800636
C	-1.479739	0.231046	-0.257732
C	-2.793810	0.567077	-0.676868
C	-3.830935	-0.061838	-0.021722
C	-3.663039	-1.025077	1.028200
C	-2.398810	-1.392568	1.432104
H	-4.556927	-1.446260	1.494725
H	-2.256001	-2.134105	2.221179
H	0.175761	-1.704614	1.789907
H	-0.454489	1.430963	-1.476596
N	-0.329949	0.728770	-0.733839
N	0.014515	-1.007661	1.048905
Ru	1.378480	0.021261	0.000989
C	2.434907	-2.669395	-0.894126
H	2.743291	-3.337596	-1.712168
H	1.848080	-3.260616	-0.174908
C	3.631699	-2.015197	-0.233614
H	4.279376	-2.760789	0.251265
H	4.243589	-1.469351	-0.968406
H	2.894356	-1.527480	1.643071
H	3.917837	-0.421639	1.062660
H	1.921875	-1.239640	-2.316829
H	0.627819	-1.986913	-1.679786
C	2.610114	2.747973	-0.475830
H	1.673103	3.219308	-0.809239
H	3.445035	3.371066	-0.829631
C	2.639710	2.587005	1.031032
H	3.596972	2.163432	1.371842
H	2.500932	3.551462	1.542263
H	1.707147	1.302366	2.386656
H	0.653527	2.138610	1.482277
H	3.665700	1.075288	-1.099377
H	2.451925	1.463400	-2.096268
N	2.678368	1.367918	-1.095791
N	1.543132	1.624030	1.422053
N	1.535594	-1.575702	-1.422751
N	3.123533	-1.012879	0.780490
H	-2.994937	1.273149	-1.486005
N	-5.220806	0.307604	-0.395419
O	-6.010345	0.319804	0.535438
O	-5.413986	0.576611	-1.567708

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$[(en_2]Rubpy^{Me}]^{+2}$

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C	-2.671534	0.444135	-0.478967
C	-0.764208	1.859163	-0.110913
C	-3.017376	2.813861	-0.325969
C	-3.565912	1.489521	-0.559437
H	-3.038862	-0.580189	-0.642225
H	-3.683074	3.682079	-0.322806
C	2.666193	0.677095	0.167372
C	0.622379	1.918765	-0.037028
C	3.452999	1.793537	0.334848
H	3.143757	-0.311748	0.214196
C	2.771907	3.073545	0.245322
H	3.347301	4.000795	0.321649
N	1.322674	0.659464	-0.084104
C	-1.676464	2.977153	-0.118971
H	-1.270819	3.978847	0.044159
C	1.417110	3.116071	0.074294
H	0.906455	4.081341	0.026422
N	-1.338603	0.544714	-0.211288
H	-2.247863	-2.506068	-0.228120
H	-1.131508	-3.430353	0.507595
C	-2.079721	-2.106451	1.778573
H	-2.653753	-2.943576	2.215193
H	-2.769207	-1.268070	1.596709
C	-0.980596	-1.659681	2.735160
H	-1.429026	-1.351992	3.697177
H	-0.286149	-2.492829	2.939267
N	-0.210777	-0.574617	2.088426
H	-0.759154	0.299124	2.082278
H	0.646668	-0.368083	2.611931
N	-1.481714	-2.463712	0.454584
C	2.198851	-2.490355	-1.416756
H	2.771053	-3.413088	-1.622314
H	2.886569	-1.634286	-1.491062
C	1.075132	-2.320894	-2.432941
H	1.499889	-2.287175	-3.452729
H	0.380539	-3.176671	-2.384259
N	0.316271	-1.102077	-2.082739
H	0.884859	-0.259979	-2.268235
H	-0.529657	-1.013440	-2.657122

H	1.305993	-3.418617	0.196665
H	2.404863	-2.299283	0.620682
N	1.633016	-2.470435	-0.033544
Ru	0.045165	-0.945290	0.018319
C	-5.020768	1.281714	-0.872700
H	-5.327669	1.779794	-1.814096
H	-5.256605	0.208916	-0.980769
H	-5.682790	1.686065	-0.081104
C	4.935592	1.705005	0.563091
H	5.244915	2.172883	1.518723
H	5.274086	0.654786	0.588578
H	5.514362	2.217133	-0.231662

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$[(en_2]Rubpy^{Me}]^{+1}$

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C	2.663591	0.603443	0.301321
C	0.709348	1.919554	0.064998
C	2.883969	2.985283	0.337726
C	3.502081	1.698712	0.422312
H	3.087944	-0.402850	0.369390
H	3.492137	3.888813	0.417133
C	-2.663629	0.602987	-0.302004
C	-0.709666	1.919437	-0.065242
C	-3.502341	1.698126	-0.422666
H	-3.087743	-0.403375	-0.370450
C	-2.884506	2.984799	-0.337656
H	-3.492859	3.888230	-0.416760
N	-1.317042	0.657634	-0.108841
C	1.522526	3.082557	0.168358
H	1.051064	4.064770	0.118654
C	-1.523074	3.082302	-0.168294
H	-1.051804	4.064595	-0.118357
N	1.316965	0.657866	0.108290
H	2.295947	-2.435929	0.478183
H	1.148854	-3.439413	-0.061701
C	2.097038	-2.407236	-1.573312
H	2.637998	-3.327570	-1.847785
H	2.815695	-1.573728	-1.576161
C	0.979027	-2.121370	-2.565555
H	1.391240	-2.015749	-3.582838
H	0.254612	-2.951788	-2.580388
N	0.260541	-0.900320	-2.115853
H	0.832936	-0.071332	-2.326845
H	-0.599259	-0.776640	-2.662025
N	1.520175	-2.488304	-0.192521
C	-2.096710	-2.406839	1.574016
H	-2.637463	-3.327168	1.848902
H	-2.815553	-1.573499	1.576344
C	-0.978888	-2.120158	2.566250
H	-1.391320	-2.013854	3.583374
H	-0.254408	-2.950503	2.581858
N	-0.260452	-0.899323	2.115860
H	-0.832857	-0.070233	2.326392
H	0.599338	-0.775352	2.661976
H	-1.147614	-3.439380	0.063270
H	-2.295499	-2.437259	-0.477465
N	-1.519709	-2.488465	0.193320
Ru	0.000098	-0.919418	-0.000034
C	4.984087	1.546977	0.635245
H	5.303082	2.012912	1.583419
H	5.282210	0.487544	0.664326
H	5.557233	2.036745	-0.170595
C	-4.984280	1.546150	-0.635941
H	-5.302901	2.010463	-1.585044
H	-5.282471	0.486688	-0.663317
H	-5.557652	2.037313	0.168868

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$[(en_2]Rubpy^{Me}]^{0}$

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C	-2.653558	0.634539	-0.263562
C	-0.729596	1.942550	-0.073676
C	-2.884911	3.008435	-0.349388
C	-3.496213	1.742460	-0.391680
H	-3.078934	-0.369006	-0.298674
H	-3.486421	3.914409	-0.444131
C	2.653703	0.634308	0.263345
C	0.729825	1.942480	0.073847
C	3.496463	1.742161	0.391463
H	3.079040	-0.369260	0.298325
C	2.885243	3.008176	0.349475
H	3.486821	3.914096	0.444305
N	1.308834	0.701096	0.102602
C	-1.507178	3.102807	-0.193773
H	-1.031445	4.082684	-0.171806
C	1.507493	3.102661	0.194031
H	1.031828	4.082576	0.172287
N	-1.308692	0.701226	-0.102619
H	-2.283119	-2.420238	-0.487865
H	-1.102861	-3.410741	-0.020714
C	-2.039477	-2.485197	1.564171
H	-2.549163	-3.433961	1.791807
H	-2.782460	-1.676066	1.634274
C	-0.900485	-2.230719	2.537133
H	-1.278026	-2.178581	3.570273
H	-0.159446	-3.044746	2.492951
N	-0.213955	-0.966441	2.132143
H	-0.785192	-0.169239	2.442075
H	0.660467	-0.873577	2.662395
N	-1.491426	-2.475600	0.164727
C	2.039109	-2.485467	-1.564226
H	2.548648	-3.434313	-1.791843
H	2.782177	-1.676437	-1.634558
C	0.900003	-2.230949	-2.537036
H	1.277396	-2.178912	-3.570234
H	0.158879	-3.044887	-2.492687
N	0.213713	-0.966560	-2.132003
H	0.785043	-0.169449	-2.442007
H	-0.660767	-0.873547	-2.662133
H	1.102980	-3.410815	0.021101
H	2.283180	-2.420035	0.487728
N	1.491336	-2.475650	-0.164661
Ru	-0.000052	-0.893230	0.000054
C	-4.981078	1.580680	-0.568797
H	-5.308372	2.034416	-1.517744
H	-5.280731	0.523508	-0.570679
H	-5.525058	2.093146	0.240372
C	4.981349	1.580233	0.568244
H	5.309040	2.034588	1.516753
H	5.280816	0.523010	0.570766
H	5.525168	2.092020	-0.241469

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$[(en_2]Ru^{t}bpy^{CH2=}]^{+2}$

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C	-0.698598	1.859345	-0.103054
C	-2.854915	2.994026	-0.375849
C	-3.517494	1.719432	-0.547603
H	-3.455532	3.907730	-0.358730
C	0.697754	1.859571	0.102951
C	3.516670	1.720603	0.547734
C	2.853676	2.994963	0.375945
H	3.453990	3.908868	0.358905
N	1.329836	0.617698	0.106180
C	-1.489311	3.050320	-0.247277
H	-0.992456	4.020252	-0.188812
C	1.488050	3.050800	0.247292
H	0.990861	4.020561	0.188843
N	-1.330244	0.617264	-0.106374
H	-2.241133	-2.424670	-0.729820
H	-1.244513	-3.461549	0.028608
C	-2.342486	-2.283762	1.319114
H	-2.983237	-3.148499	1.568400
H	-2.986891	-1.404986	1.165089
C	-1.370629	-1.993687	2.456012
H	-1.936486	-1.804769	3.386620
H	-0.713439	-2.862841	2.631599
N	-0.523891	-0.849677	2.056880
H	-1.097626	0.011805	2.002246
H	0.213167	-0.684964	2.748937
N	-1.579237	-2.488264	0.051776
C	2.343617	-2.283244	-1.318524

H	2.984584	-3.147899	-1.567562
H	2.987884	-1.404445	-1.164039
C	1.372350	-1.993163	-2.455902
H	1.938731	-1.804000	-3.386144
H	0.715463	-2.862447	-2.631988
N	0.525123	-0.849436	-2.057142
H	1.098673	0.012129	-2.001418
H	-0.211223	-0.684559	-2.749921
H	1.244907	-3.461252	-0.028868
H	2.241201	-2.424604	0.730310
N	1.579696	-2.487979	-0.051634
Ru	0.000034	-0.955968	-0.000184
C	-2.564087	0.582495	-0.885129
H	-2.357323	0.639633	-1.984923
H	-3.075829	-0.381962	-0.721994
C	2.563604	0.583319	0.885030
H	2.356758	0.640357	1.984803
H	3.075688	-0.380987	0.721977
C	-4.859651	1.529046	-0.502161
H	-5.547646	2.357824	-0.312197
C	4.858903	1.530663	0.502597
H	5.546675	2.359696	0.312885
H	5.301739	0.544168	0.668230
H	-5.302191	0.542415	-0.667805

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$[(en_2)Ru^{t}bpy^{CH2=}]^{+1}$

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C	0.698308	1.889438	0.163853
C	2.840118	3.042179	0.435499
C	3.510850	1.759043	0.521430
H	3.436705	3.956841	0.424160
C	-0.698092	1.889452	-0.164184
C	-3.510609	1.758892	-0.521923
C	-2.839985	3.042073	-0.435727
H	-3.436624	3.956698	-0.424219
N	-1.267827	0.659143	-0.264727
C	1.481232	3.094200	0.324569
H	0.975903	4.057946	0.270583
C	-1.481093	3.094170	-0.324765
H	-0.975853	4.057957	-0.270619
N	1.268057	0.659149	0.264254
H	2.196859	-2.407914	0.837275
H	1.169243	-3.441001	0.131203
C	2.333291	-2.404021	-1.219029
H	2.913478	-3.323114	-1.401567
H	3.043282	-1.570524	-1.108843
C	1.393182	-2.121463	-2.381578
H	1.969594	-1.995987	-3.313110
H	0.696437	-2.962745	-2.530735
N	0.588068	-0.915708	-2.050755
H	1.171811	-0.072802	-2.145853
H	-0.165786	-0.802813	-2.736569
N	1.542002	-2.485153	0.050482
C	-2.333868	-2.402381	1.219635
H	-2.914626	-3.321028	1.402591
H	-3.043309	-1.568507	1.108792
C	-1.393833	-2.119688	2.382203
H	-1.970356	-1.993429	3.313562
H	-0.697521	-2.961222	2.531926
N	-0.588069	-0.914502	2.050892
H	-1.171429	-0.071263	2.145384
H	0.165718	-0.801602	2.736775
H	-1.169964	-3.440792	-0.129627
H	-2.196980	-2.407747	-0.836636
N	-1.542333	-2.484730	-0.049642
Ru	0.000030	-0.924440	0.000080
C	2.593515	0.608937	0.891758
H	2.464111	0.626145	1.997377
H	3.076617	-0.349536	0.649113
C	-2.593102	0.609037	-0.892610
H	-2.463428	0.626848	-1.998187
H	-3.076161	-0.349601	-0.650568
C	4.842416	1.590163	0.363671
H	5.503004	2.440683	0.180244
C	-4.842148	1.589783	-0.364162
H	-5.502868	2.440160	-0.180529
H	-5.308420	0.603503	-0.431244
H	5.308838	0.603933	0.430420

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$[(en_2)Ru^{t}bpy^{CH2=}]^{0}$

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C	-0.706923	1.914573	-0.201483
C	-2.825835	3.082301	-0.477676
C	-3.498498	1.797325	-0.484168
H	-3.418645	3.999500	-0.479399
C	0.706922	1.914639	0.201026
C	3.498580	1.797941	0.483322
C	2.825588	3.082721	0.477573
H	3.418189	4.000055	0.479747
N	1.231990	0.700257	0.319136
C	-1.468237	3.132897	-0.403660
H	-0.948844	4.089309	-0.389719
C	1.467976	3.133045	0.403605
H	0.948370	4.089346	0.390087
N	-1.231755	0.700139	-0.320171
H	-2.175185	-2.367828	-0.898236
H	-1.110267	-3.406531	-0.272522
C	-2.288547	-2.504005	1.160533
H	-2.824084	-3.458015	1.281047
H	-3.039216	-1.700376	1.115037
C	-1.338554	-2.263746	2.321384
H	-1.890857	-2.218101	3.272776
H	-0.604550	-3.081075	2.401036
N	-0.583835	-0.999295	2.059902
H	-1.190726	-0.197427	2.275100
H	0.186039	-0.923808	2.734708
N	-1.507909	-2.468840	-0.123611
C	2.288309	-2.505692	-1.159070
H	2.823673	-3.459937	-1.278460
H	3.039101	-1.702099	-1.114865
C	1.337993	-2.266824	-2.319942
H	1.889953	-2.222685	-3.271604
H	0.603722	-3.084053	-2.398136
N	0.583737	-1.001790	-2.059947
H	1.190863	-0.200419	-2.276318
H	-0.186262	-0.926874	-2.734670
H	1.110360	-3.406169	0.275543
H	2.175548	-2.366718	0.899540
N	1.508025	-2.468704	0.125257
Ru	0.000061	-0.889066	-0.000044
C	-2.608124	0.631655	-0.861251
H	-2.510396	0.611777	-1.966025
H	-3.063913	-0.319753	-0.559026
C	2.608601	0.631653	0.859532
H	2.511383	0.610470	1.964328
H	3.064526	-0.319277	0.556000
C	-4.820107	1.660884	-0.245243
H	-5.456462	2.534797	-0.089548
C	4.820253	1.662075	0.244442
H	5.456344	2.536302	0.089394
H	5.307138	0.684437	0.213744
H	-5.306637	0.683049	-0.215147

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$[(en_2)RuL^{Cl}]^{+3}$

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C	-1.490540	-0.706274	0.779573
C	-1.664035	0.281069	-0.300593
C	-2.953518	0.647648	-0.727712
C	-4.049926	0.057158	-0.088695
C	-3.887245	-0.906524	0.984580
C	-2.641903	-1.282929	1.413209
H	-4.785642	-1.326054	1.442151
H	-2.524241	-2.009731	2.220152
H	-0.085618	-1.651587	1.807929
H	-0.586488	1.436232	-1.528276
N	-0.488438	0.746850	-0.770989
N	-0.218116	-0.964632	1.052117
Ru	1.188852	0.018835	-0.002012
C	2.181745	-2.718641	-0.825594
H	2.477273	-3.416334	-1.623446

H	1.578062	-3.275897	-0.093168
C	3.392278	-2.078622	-0.175754
H	4.020836	-2.828611	0.327065
H	4.018312	-1.564129	-0.921284
H	2.658349	-1.531511	1.684836
H	3.712867	-0.464846	1.085816
H	1.710166	-1.314881	-2.286173
H	0.395902	-2.011499	-1.632994
C	2.485377	2.700782	-0.524026
H	1.560700	3.186680	-0.870630
H	3.335591	3.299433	-0.883491
C	2.502520	2.569863	0.986573
H	3.448899	2.132975	1.341054
H	2.383605	3.548076	1.476074
H	1.533880	1.337491	2.364725
H	0.504974	2.173001	1.431988
H	3.504582	0.993886	-1.110578
H	2.305510	1.391018	-2.120639
N	2.524598	1.309766	-1.117628
N	1.384280	1.639428	1.391816
N	1.313483	-1.617379	-1.385150
N	2.905456	-1.042204	0.812802
H	-3.105835	1.372044	-1.529720
Cl	-5.621677	0.459502	-0.559000

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$[(en_2]RuL^{Cl}]^{+2}$

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C	-1.472797	-0.728199	0.753055
C	-1.656072	0.273118	-0.301038
C	-2.970101	0.637333	-0.714761
C	-4.038161	0.038978	-0.087546
C	-3.866992	-0.939980	0.966273
C	-2.619931	-1.316532	1.379692
H	-4.760331	-1.369994	1.419954
H	-2.491749	-2.056241	2.172406
H	-0.073984	-1.686031	1.763156
H	-0.626707	1.430262	-1.533095
N	-0.502323	0.747696	-0.776079
N	-0.194784	-0.989489	1.016363
Ru	1.213577	0.015371	-0.003671
C	2.210288	-2.684260	-0.860695
H	2.540636	-3.383734	-1.643536
H	1.563841	-3.236910	-0.161793
C	3.399129	-2.080092	-0.134354
H	3.999965	-2.859167	0.358720
H	4.055947	-1.549865	-0.842483
H	2.577662	-1.582028	1.694944
H	3.690539	-0.524475	1.193141
H	1.824479	-1.263146	-2.320548
H	0.476093	-1.928520	-1.712599
C	2.403839	2.740216	-0.504642
H	1.450790	3.171548	-0.846543
H	3.216346	3.398834	-0.846968
C	2.413853	2.601772	1.006977
H	3.376137	2.193253	1.353706
H	2.270856	3.578034	1.494467
H	1.472947	1.355682	2.376415
H	0.435023	2.125621	1.396498
H	3.515722	1.104841	-1.098919
H	2.293457	1.440857	-2.104667
N	2.521134	1.367347	-1.105134
N	1.338175	1.634431	1.397313
N	1.396310	-1.565122	-1.436182
N	2.888105	-1.072414	0.857493
H	-3.122809	1.374385	-1.503845
Cl	-5.648639	0.439954	-0.537710

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$[(en_2]RuL^{Cl}]^{+1}$

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C	-1.431881	-0.742590	0.741554
C	-1.617697	0.262852	-0.280811
C	-2.930438	0.615998	-0.677961
C	-4.011034	0.002665	-0.062181
C	-3.846213	-0.970648	0.952832
C	-2.568350	-1.334824	1.346726
H	-4.724855	-1.423400	1.410948
H	-2.431024	-2.088788	2.126347
H	-0.018398	-1.712011	1.771348
H	-0.609696	1.446674	-1.540194
N	-0.460981	0.784346	-0.774351
N	-0.129088	-1.023836	1.020210
Ru	1.268789	0.027073	-0.005826
C	2.087967	-2.717385	-0.836705
H	2.355233	-3.467144	-1.598768
H	1.439827	-3.203119	-0.091626
C	3.337355	-2.165572	-0.166675
H	3.919271	-2.977001	0.300397
H	3.984214	-1.673872	-0.911528
H	2.588953	-1.605134	1.673085
H	3.772525	-0.635010	1.144984
H	1.693604	-1.344223	-2.338837
H	0.348347	-1.873384	-1.582558
C	2.316689	2.794681	-0.495723
H	1.350538	3.146672	-0.887813
H	3.093580	3.515410	-0.798425
C	2.247452	2.680992	1.020004
H	3.213983	2.336876	1.423176
H	2.027783	3.663602	1.468644
H	1.270384	1.433829	2.363052
H	0.280299	2.060876	1.223600
H	3.566588	1.236674	-1.011651
H	2.374071	1.482441	-2.081750
N	2.559872	1.435062	-1.073213
N	1.219384	1.663447	1.364916
N	1.317826	-1.579501	-1.412992
N	2.927537	-1.125938	0.829453
H	-3.089856	1.366395	-1.454065
Cl	-5.633943	0.440610	-0.545680

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$[(en_2]RuL^{Cl}]^{0}$

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C	-1.404045	-0.736912	0.751638
C	-1.592036	0.287158	-0.242150
C	-2.896600	0.616394	-0.649750
C	-3.997447	-0.002280	-0.041204
C	-3.843350	-0.946835	0.970150
C	-2.538799	-1.303472	1.356858
H	-4.713917	-1.405620	1.439648
H	-2.401850	-2.067136	2.130551
H	0.026424	-1.561461	1.900352
H	-0.577800	1.412655	-1.568024
N	-0.428370	0.908532	-0.689093
N	-0.082828	-1.099767	0.991333
Ru	1.315940	0.035376	-0.013099
C	1.920814	-2.753162	-0.817569
H	2.099319	-3.551684	-1.559312
H	1.285901	-3.153211	-0.011660
C	3.239592	-2.268357	-0.228818
H	3.797831	-3.117587	0.208199
H	3.868720	-1.816239	-1.013362
H	2.563605	-1.652893	1.616723
H	3.831269	-0.788070	1.077925
H	1.439119	-1.445835	-2.361924
H	0.173761	-1.808795	-1.362706
C	2.321969	2.810797	-0.484557
H	1.352445	3.131103	-0.895197
H	3.085520	3.561882	-0.758464
C	2.205132	2.696405	1.031646
H	3.169716	2.380708	1.465502
H	1.951069	3.684962	1.457396
H	1.147442	1.476470	2.343401
H	0.257237	1.977458	1.024986
H	3.618649	1.282578	-0.971844
H	2.451049	1.517933	-2.075874
N	2.611255	1.465802	-1.063766
N	1.197466	1.661874	1.336303
N	1.181036	-1.597347	-1.381626
N	2.943699	-1.204912	0.773910
H	-3.055227	1.381193	-1.414280
Cl	-5.630520	0.451021	-0.573094

[(en_2)RuL^{Me}]$^{+3}$

C	-1.783726	-0.623718	0.714845
C	-1.902015	0.351058	-0.385584
C	-3.175093	0.744894	-0.852386
C	-4.322345	0.212957	-0.256077
C	-4.184300	-0.739570	0.838453
C	-2.967100	-1.153601	1.319351
H	-3.262614	1.461962	-1.671735
H	-5.098261	-1.136332	1.287697
H	-2.896946	-1.870546	2.140452
H	-0.431378	-1.592200	1.793666
H	-0.763844	1.454083	-1.599254
N	-0.705100	0.773985	-0.829173
N	-0.524309	-0.912703	1.025306
C	1.875149	-2.761811	-0.754823
H	2.176997	-3.477624	-1.533976
H	1.237172	-3.294238	-0.033074
C	3.082015	-2.142313	-0.077918
H	3.678902	-2.901412	0.449249
H	3.739551	-1.651046	-0.812148
H	2.305358	-1.556295	1.753433
H	3.407129	-0.525033	1.178454
H	1.477047	-1.371249	-2.249402
H	0.128849	-2.023197	-1.619672
C	2.320811	2.646112	-0.532328
H	1.421651	3.147379	-0.921553
H	3.198346	3.214961	-0.874003
C	2.281666	2.548018	0.980556
H	3.203158	2.094008	1.376721
H	2.172709	3.539559	1.444819
H	1.235925	1.369377	2.347955
H	0.260424	2.214058	1.367267
H	3.313674	0.899433	-1.042795
H	2.164575	1.306774	-2.106164
N	2.344144	1.241965	-1.094143
N	1.125568	1.656514	1.365443
N	1.049745	-1.648660	-1.354386
N	2.593732	-1.083506	0.885009
C	-5.688864	0.588147	-0.702511
H	-6.258067	1.010466	0.147663
H	-5.686874	1.304732	-1.531880
H	-6.247844	-0.319277	-1.001009
Ru	0.934562	0.011078	-0.000604

[(en_2)RuL^{Me}]$^{+2}$

C	-1.768864	-0.651027	0.689770
C	-1.896881	0.341330	-0.381350
C	-3.193216	0.735133	-0.832352
C	-4.316273	0.194762	-0.247558
C	-4.168987	-0.778103	0.826158
C	-2.951503	-1.194262	1.287662
H	-3.280649	1.468313	-1.637525
H	-5.078312	-1.186601	1.272304
H	-2.869010	-1.927142	2.092943
H	-0.426131	-1.633925	1.749729
H	-0.805716	1.452843	-1.598483
N	-0.718895	0.776369	-0.830402
N	-0.506479	-0.944357	0.991203
C	1.894445	-2.730680	-0.792152
H	2.225784	-3.451976	-1.554585
H	1.212501	-3.252985	-0.103842
C	3.080576	-2.151538	-0.040858
H	3.643990	-2.941336	0.478767
H	3.771868	-1.651689	-0.738255
H	2.222258	-1.601624	1.756490
H	3.383151	-0.587401	1.273847
H	1.590943	-1.323006	-2.283721
H	0.207201	-1.937304	-1.701162
C	2.242579	2.688803	-0.507966
H	1.314055	3.143768	-0.884784
H	3.084898	3.317820	-0.833751
C	2.201908	2.573677	1.005479
H	3.140885	2.142847	1.387530
H	2.074272	3.561825	1.473029
H	1.184031	1.377853	2.364149
H	0.198901	2.162073	1.342363
H	3.319919	1.010931	-1.044663
H	2.140222	1.370734	-2.092484
N	2.335071	1.304997	-1.085584
N	1.086751	1.645033	1.377468
N	1.130676	-1.597303	-1.406563
N	2.573840	-1.114565	0.921968
C	-5.702284	0.573699	-0.675885
H	-6.263717	0.993935	0.175709
H	-5.695748	1.308205	-1.491180
H	-6.256974	-0.320103	-1.008146
Ru	0.957401	0.009135	-0.003559

[(en_2)RuL^{Me}]$^{+1}$

C	-1.724516	-0.661445	0.675513
C	-1.853937	0.338451	-0.358110
C	-3.148124	0.723550	-0.791691
C	-4.290584	0.170067	-0.225094
C	-4.145864	-0.802697	0.807176
C	-2.899091	-1.210481	1.249434
H	-3.238842	1.475091	-1.582288
H	-5.042617	-1.236147	1.256160
H	-2.808798	-1.961697	2.039270
H	-0.372306	-1.661644	1.757709
H	-0.778517	1.481737	-1.599309
N	-0.668428	0.822705	-0.823726
N	-0.439432	-0.980712	0.994856
C	1.738430	-2.768220	-0.768300
H	1.988470	-3.547874	-1.506060
H	1.048266	-3.202989	-0.029567
C	2.995809	-2.262141	-0.076937
H	3.526848	-3.090840	0.419833
H	3.683255	-1.816310	-0.814013
H	2.231271	-1.629894	1.732677
H	3.469898	-0.724892	1.213569
H	1.452112	-1.408194	-2.306621
H	0.061649	-1.859660	-1.578934
C	2.149784	2.748848	-0.496068
H	1.199147	3.114945	-0.912467
H	2.947965	3.450520	-0.788581
C	2.042804	2.653806	1.018891
H	2.990251	2.287937	1.447716
H	1.840228	3.647364	1.451660
H	0.996956	1.449617	2.350043
H	0.055428	2.087773	1.175008
H	3.375479	1.156376	-0.962317
H	2.217848	1.419157	-2.066477
N	2.375912	1.378406	-1.053018
N	0.979683	1.668651	1.348447
N	1.039281	-1.608466	-1.388447
N	2.611341	-1.184715	0.888167
C	-5.669290	0.579545	-0.679040
H	-6.252630	1.000954	0.156933
H	-5.624054	1.334087	-1.477595
H	-6.234654	-0.287666	-1.059841
Ru	1.018325	0.018079	-0.004889

[(en_2)RuL^{Me}]^{0}

C	-1.724464	-0.661292	0.675642
C	-1.853843	0.338619	-0.357982
C	-3.148019	0.723663	-0.791654
C	-4.290496	0.170141	-0.225131
C	-4.145820	-0.802592	0.807179
C	-2.899064	-1.210339	1.249512
H	-3.238699	1.475203	-1.582260
H	-5.042585	-1.236053	1.256130
H	-2.808790	-1.961535	2.039372
H	-0.372265	-1.661410	1.757963
H	-0.778414	1.482031	-1.599045
N	-0.668327	0.822956	-0.823496

N	-0.439396	-0.980537	0.995054
C	1.738029	-2.768386	-0.768683
H	1.988049	-3.547725	-1.506774
H	1.047971	-3.203539	-0.030075
C	2.995466	-2.262524	-0.077242
H	3.526468	-3.091360	0.419341
H	3.682904	-1.816545	-0.814232
H	2.230616	-1.630633	1.732356
H	3.469673	-0.725832	1.213873
H	1.451177	-1.408060	-2.306674
H	0.060991	-1.859364	-1.578318
C	2.149797	2.748855	-0.496245
H	1.199061	3.114956	-0.912416
H	2.947897	3.450539	-0.788947
C	2.043168	2.653821	1.018736
H	2.990685	2.287844	1.447312
H	1.840789	3.647396	1.451563
H	0.997402	1.449821	2.350124
H	0.055784	2.087855	1.175061
H	3.375447	1.156492	-0.962996
H	2.217207	1.419035	-2.066593
N	2.375822	1.378419	-1.053221
N	0.980045	1.668763	1.348515
N	1.038784	-1.608434	-1.388332
N	2.611077	-1.185309	0.888099
C	-5.669181	0.579546	-0.679214
H	-5.623893	1.334241	-1.477622
H	-6.234362	-0.287672	-1.060271
H	-6.252695	1.000717	0.156753
Ru	1.018412	0.018080	-0.004761

$[(en_2)Ru^{i}L^{CH2=}]^{+3}$

C	-1.801919	-0.652314	0.631674
C	-1.926850	0.321140	-0.469395
C	-4.452794	0.156241	-0.216524
C	-4.224513	-0.764640	0.844985
C	-2.954660	-1.174909	1.253383
H	-5.093311	-1.169594	1.371275
H	-2.854824	-1.891510	2.072044
H	-0.439929	-1.642283	1.699398
H	-0.841228	1.417498	-1.693036
N	-0.775675	0.749302	-0.913821
N	-0.525834	-0.949856	0.944211
C	2.031610	-2.709654	-0.746139
H	2.428332	-3.397239	-1.507852
H	1.347872	-3.278024	-0.097463
C	3.149720	-2.070756	0.055663
H	3.717710	-2.825762	0.619393
H	3.858821	-1.547216	-0.605229
H	2.191024	-1.545044	1.816033
H	3.305758	-0.471076	1.365623
H	1.722565	-1.295865	-2.240623
H	0.348583	-2.000135	-1.751969
C	2.301952	2.676790	-0.470671
H	1.434219	3.159687	-0.944920
H	3.198679	3.253931	-0.740802
C	2.128381	2.592445	1.032512
H	3.014866	2.151486	1.513732
H	1.968293	3.586590	1.475890
H	0.965746	1.431042	2.308632
H	0.088162	2.235639	1.202336
H	3.364089	0.947124	-0.887825
H	2.276648	1.316827	-2.029398
N	2.393016	1.267062	-1.007601
N	0.953590	1.690579	1.313014
N	1.228619	-1.607562	-1.392274
N	2.542870	-1.047943	0.986026
C	-5.745636	0.509076	-0.518679
H	-5.986152	1.211386	-1.322010
H	-6.585074	0.093228	0.045261
Ru	0.935982	-0.004447	-0.009824
C	-3.277562	0.712574	-1.002415
H	-3.346847	1.812444	-1.061829
H	-3.349707	0.355490	-2.047647

$[(en_2)Ru^{i}L^{CH2=}]^{+2}$

C	-1.782404	-0.748728	0.593534
C	-1.901035	0.210186	-0.507335
C	-4.419038	0.159891	-0.217889
C	-4.203673	-0.804523	0.841124
C	-2.970363	-1.265109	1.213863
H	-5.085061	-1.159670	1.380316
H	-2.871349	-1.986868	2.027580
H	-0.450800	-1.664831	1.717200
H	-0.836970	1.342900	-1.703057
N	-0.748651	0.684365	-0.918079
N	-0.525397	-1.003854	0.934015
C	2.062343	-2.686332	-0.709213
H	2.461002	-3.404504	-1.441978
H	1.390692	-3.232239	-0.029066
C	3.187268	-2.023712	0.067292
H	3.777942	-2.769811	0.620397
H	3.871222	-1.497558	-0.618115
H	2.235411	-1.492015	1.822338
H	3.352361	-0.420622	1.360256
H	1.723054	-1.338448	-2.245321
H	0.362396	-2.020209	-1.684318
C	2.131219	2.745378	-0.457857
H	1.211278	3.147553	-0.909234
H	2.961651	3.416001	-0.726772
C	1.980182	2.644827	1.050052
H	2.906652	2.263158	1.507940
H	1.774657	3.632342	1.490885
H	0.923770	1.416046	2.345705
H	-0.020615	2.142214	1.246213
H	3.328095	1.118580	-0.883809
H	2.226856	1.413226	-2.030603
N	2.337167	1.364052	-1.010142
N	0.885715	1.668794	1.351233
N	1.253392	-1.614632	-1.373827
N	2.588617	-1.001141	0.990938
C	-5.646611	0.691681	-0.421034
H	-5.836190	1.431180	-1.202174
H	-6.495336	0.396222	0.199294
Ru	0.954273	0.011480	-0.013907
C	-3.241609	0.512994	-1.114726
H	-3.290042	1.562125	-1.444507
H	-3.322239	-0.102302	-2.033075

$[(en_2)Ru^{i}L^{CH2=}]^{+1}$

C	-1.734595	-0.764274	0.559136
C	-1.855439	0.199480	-0.476070
C	-4.390720	0.139800	-0.206368
C	-4.176556	-0.882328	0.804411
C	-2.926782	-1.315128	1.151986
H	-5.052314	-1.275692	1.325211
H	-2.811973	-2.071332	1.934637
H	-0.401788	-1.693935	1.730898
H	-0.820866	1.376617	-1.704007
N	-0.701474	0.725636	-0.922423
N	-0.454679	-1.064577	0.925024
C	1.953190	-2.709401	-0.709169
H	2.300497	-3.466787	-1.430792
H	1.269365	-3.200292	-0.000247
C	3.133118	-2.101221	0.035559
H	3.704553	-2.883445	0.562476
H	3.815478	-1.605416	-0.673876
H	2.232021	-1.522076	1.799536
H	3.424422	-0.528144	1.335957
H	1.605707	-1.397679	-2.277532
H	0.236673	-1.945918	-1.573480
C	2.017013	2.811114	-0.436681
H	1.081149	3.132547	-0.918581
H	2.797409	3.553233	-0.673602
C	1.812538	2.710485	1.068665
H	2.749190	2.401865	1.561181
H	1.526269	3.691870	1.481940

H	0.781527	1.431930	2.336012
H	-0.147799	2.040259	1.140587
H	3.347127	1.280253	-0.808293
H	2.267765	1.492544	-1.998420
N	2.347807	1.455076	-0.975632
N	0.790330	1.664462	1.337024
N	1.186471	-1.613648	-1.366093
N	2.620452	-1.053125	0.971869
C	-5.599867	0.718178	-0.391417
H	-5.755847	1.502673	-1.135521
H	-6.465841	0.412491	0.199935
Ru	1.003246	0.025519	-0.010968
C	-3.200434	0.505658	-1.085105
H	-3.253845	1.564113	-1.388187
H	-3.282838	-0.083448	-2.021325

$[(en_2)Ru^{r}L^{CH2=}]^{0}$

C	-1.684647	-0.702672	0.576192
C	-1.793512	0.277693	-0.394160
C	-4.357079	0.192247	-0.195498
C	-4.152648	-0.864179	0.777164
C	-2.886867	-1.277330	1.116039
H	-5.027275	-1.284541	1.281218
H	-2.768953	-2.073307	1.861656
H	-0.318319	-1.156607	1.983209
H	-0.756329	1.383392	-1.720309
N	-0.640911	0.907691	-0.819385
N	-0.372840	-1.137606	0.950273
C	1.637471	-2.785073	-0.734528
H	1.857065	-3.588847	-1.459290
H	0.943431	-3.162584	0.032193
C	2.915586	-2.309943	-0.056780
H	3.428519	-3.163909	0.425292
H	3.607818	-1.866736	-0.791832
H	2.045236	-1.680869	1.696335
H	3.412783	-0.864131	1.328960
H	1.261807	-1.493817	-2.323494
H	-0.059972	-1.819324	-1.383691
C	2.104873	2.803920	-0.431835
H	1.163355	3.133414	-0.897233
H	2.887770	3.553169	-0.653546
C	1.896783	2.687109	1.074981
H	2.827880	2.350324	1.562304
H	1.637278	3.679439	1.489421
H	0.755899	1.484195	2.326165
H	-0.061886	2.011544	0.977831
H	3.416749	1.269127	-0.850052
H	2.313365	1.514775	-2.017442
N	2.418313	1.461381	-0.998307
N	0.854732	1.669673	1.321743
N	0.950468	-1.624612	-1.356196
N	2.552489	-1.242134	0.917188
C	-5.558375	0.786712	-0.415202
H	-5.674293	1.597538	-1.139773
H	-6.455080	0.462931	0.120668
Ru	1.038326	0.032729	-0.009735
C	-3.134318	0.584609	-1.023954
H	-3.187624	1.652015	-1.299805
H	-3.194914	0.023438	-1.982170

$[(en_2)Rubpy^{Me}]^{+3}$

C	-2.662146	0.624819	-0.276084
C	-0.726361	1.947098	-0.083266
C	-2.886168	3.000939	-0.364100
C	-3.505206	1.733646	-0.409131
H	-3.087373	-0.378436	-0.308133
H	-3.488507	3.907184	-0.459556
C	2.662121	0.624989	0.275890
C	0.726247	1.947140	0.083247
C	3.505115	1.733875	0.408979
H	3.087445	-0.378227	0.307871
C	2.885990	3.001121	0.364073
H	3.488255	3.907405	0.459619
N	1.315058	0.705152	0.116411
C	-1.508943	3.103656	-0.202825
H	-1.040699	4.087150	-0.176427
C	1.508746	3.103744	0.202861
H	1.040426	4.087205	0.176579
N	-1.315082	0.705077	-0.116541
H	-2.250430	-2.422356	-0.536681
H	-1.074116	-3.409449	-0.050979
C	-2.070910	-2.517896	1.531593
H	-2.542938	-3.492483	1.724407
H	-2.853898	-1.746725	1.581606
C	-0.967476	-2.227125	2.531485
H	-1.368975	-2.144699	3.552727
H	-0.204123	-3.020302	2.534720
N	-0.297587	-0.944873	2.116402
H	-0.880642	-0.146932	2.406183
H	0.572397	-0.826369	2.654720
N	-1.475931	-2.481253	0.139370
C	2.070975	-2.518180	-1.531372
H	2.542831	-3.492886	-1.724014
H	2.854107	-1.747169	-1.581593
C	0.967546	-2.227454	-2.531284
H	1.369029	-2.145239	-3.552550
H	0.204116	-3.020556	-2.534359
N	0.297793	-0.945067	-2.116402
H	0.880969	-0.147233	-2.406240
H	-0.572143	-0.826509	-2.654791
H	1.074410	-3.409318	0.051613
H	2.250652	-2.421905	0.536845
N	1.476099	-2.481147	-0.139109
Ru	0.000007	-0.886588	-0.000032
C	-4.986843	1.580054	-0.592106
H	-5.301980	2.038719	-1.543545
H	-5.299283	0.527409	-0.591768
H	-5.526515	2.107295	0.211262
C	4.986761	1.580353	0.591941
H	5.301845	2.038804	1.543504
H	5.299286	0.527734	0.591347
H	5.526411	2.107845	-0.211274

$[(en_2)Ru^{r}bpy^{CH2=}]^{+3}$

C	-0.712694	1.910518	-0.195599
C	-2.838509	3.063784	-0.411992
C	-3.510151	1.795326	-0.479385
H	-3.427198	3.982642	-0.349763
C	0.713016	1.910508	0.193889
C	3.510647	1.795799	0.478639
C	2.838781	3.063957	0.411003
H	3.427275	3.982968	0.349144
N	1.244044	0.686900	0.317111
C	-1.466592	3.119492	-0.354862
H	-0.959756	4.080777	-0.303127
C	1.466767	3.119395	0.353152
H	0.959849	4.080621	0.301093
N	-1.243519	0.687038	-0.318893
H	-2.161883	-2.403302	-0.876065
H	-1.074825	-3.406488	-0.234564
C	-2.275951	-2.512455	1.192769
H	-2.791835	-3.477137	1.308447
H	-3.043430	-1.725448	1.141800
C	-1.323724	-2.256556	2.346143
H	-1.866995	-2.186753	3.300521
H	-0.584493	-3.066538	2.442040
N	-0.572943	-0.983040	2.063422
H	-1.166622	-0.178204	2.306319
H	0.219962	-0.914089	2.715354
N	-1.491332	-2.475004	-0.098935
C	2.275081	-2.515228	-1.190769
H	2.791215	-3.479983	-1.304734
H	3.042323	-1.727800	-1.142544
C	1.321605	-2.262432	-2.343832
H	1.863872	-2.195136	-3.298960
H	0.582382	-3.072766	-2.436793
N	0.570962	-0.988231	-2.063723

H	1.164233	-0.184001	-2.309591
H	-0.222760	-0.920975	-2.714829
H	1.075448	-3.406163	0.239734
H	2.163120	-2.401667	0.878003
N	1.491819	-2.474964	0.101678
Ru	0.000305	-0.882652	0.000091
C	-2.627172	0.620537	-0.858482
H	-2.530258	0.608167	-1.963075
H	-3.084176	-0.329819	-0.557984
C	2.627963	0.620223	0.856051
H	2.531528	0.605937	1.960654
H	3.085168	-0.329470	0.553760
C	-4.851981	1.689130	-0.299613
H	-5.468431	2.580407	-0.157439
C	4.852811	1.690370	0.300243
H	5.468906	2.582058	0.159102
H	5.371867	0.728647	0.305578
H	-5.370517	0.727127	-0.304840

$[(bpy_2]RuL_{NN}]^{+3}$

C	-0.754376	2.597401	0.630922
C	-2.082954	0.711013	0.182747
C	-3.142554	2.810238	0.759466
C	-1.872775	3.387620	0.873371
H	0.245675	3.021458	0.717488
H	-4.042716	3.400395	0.941801
H	-1.744080	4.435723	1.147460
C	-0.754376	-2.597401	-0.630922
C	-2.082954	-0.711012	-0.182747
C	-1.872776	-3.387619	-0.873371
H	0.245674	-3.021458	-0.717489
C	-3.142554	-2.810238	-0.759466
H	-1.744082	-4.435723	-1.147460
H	-4.042717	-3.400394	-0.941801
N	-0.836541	-1.284749	-0.290911
C	-3.241946	1.461750	0.411807
H	-4.223460	0.996573	0.325690
C	-3.241946	-1.461749	-0.411807
H	-4.223461	-0.996572	-0.325690
N	-0.836541	1.284749	0.290910
H	2.294649	2.144290	0.858286
H	3.285576	1.057729	0.202663
C	2.385522	2.273992	-1.215252
H	3.357431	2.774846	-1.335522
H	1.611110	3.052512	-1.147162
C	2.101247	1.329043	-2.367401
H	2.010067	1.876747	-3.317442
H	2.901474	0.582789	-2.486926
N	0.825679	0.590270	-2.055182
H	0.021261	1.195109	-2.273990
H	0.725822	-0.200640	-2.707881
N	2.354894	1.478736	0.074483
C	2.385521	-2.273992	1.215253
H	3.357430	-2.774847	1.335522
H	1.611109	-3.052512	1.147162
C	2.101245	-1.329044	2.367401
H	2.010065	-1.876748	3.317443
H	2.901473	-0.582790	2.486927
N	0.825678	-0.590271	2.055182
H	0.021260	-1.195109	2.273989
H	0.725821	0.200640	2.707881
H	3.285576	-1.057729	-0.202662
H	2.294649	-2.144290	-0.858286
N	2.354894	-1.478736	-0.074483
Ru	0.763455	0.000000	0.000000

$[(bpy_2]RuL_{NN}]^{+2}$

C	-0.762638	2.591066	0.617057
C	-2.076905	0.714500	0.172474
C	-3.150330	2.812786	0.727608
C	-1.881176	3.386274	0.844611
H	0.238059	3.012547	0.710535
H	-4.051327	3.402526	0.899938
H	-1.751290	4.435577	1.110942
C	-0.762642	-2.591064	-0.617061
C	-2.076906	-0.714496	-0.172475
C	-1.881181	-3.386270	-0.844614
H	0.238054	-3.012546	-0.710541
C	-3.150334	-2.812780	-0.727609
H	-1.751298	-4.435573	-1.110945
H	-4.051333	-3.402519	-0.899938
N	-0.830024	-1.278973	-0.281719
C	-3.240616	1.463558	0.391105
H	-4.218121	0.990942	0.303126
C	-3.240619	-1.463552	-0.391105
H	-4.218123	-0.990936	-0.303125
N	-0.830022	1.278975	0.281717
H	2.284852	2.180230	0.829863
H	3.279546	1.084045	0.195965
C	2.361089	2.248105	-1.236796
H	3.311033	2.785259	-1.380552
H	1.553292	2.994987	-1.199019
C	2.113051	1.267532	-2.370816
H	2.060405	1.795645	-3.335528
H	2.930687	0.532534	-2.437721
N	0.850389	0.520186	-2.079005
H	0.051792	1.122202	-2.318968
H	0.772629	-0.272167	-2.727762
N	2.345123	1.496355	0.065480
C	2.361081	-2.248110	1.236800
H	3.311023	-2.785266	1.380558
H	1.553283	-2.994990	1.199020
C	2.113042	-1.267536	2.370819
H	2.060392	-1.795650	3.335530
H	2.930680	-0.532540	2.437727
N	0.850383	-0.520188	2.079005
H	0.051784	-1.122201	2.318965
H	0.772623	0.272165	2.727761
H	3.279544	-1.084050	-0.195958
H	2.284851	-2.180234	-0.829859
N	2.345121	-1.496360	-0.065477
Ru	0.763879	-0.000001	0.000000

$[(bpy_2]RuL_{NN}]^{+1}$

C	0.730754	2.587830	-0.683967
C	2.052283	0.691639	-0.169398
C	3.124256	2.805151	-0.746798
C	1.836667	3.385741	-0.912915
H	-0.274132	2.999974	-0.811012
H	4.024828	3.398704	-0.910850
H	1.708363	4.425181	-1.213245
C	0.730755	-2.587830	0.683969
C	2.052283	-0.691639	0.169395
C	1.836669	-3.385741	0.912916
H	-0.274131	-2.999974	0.811016
C	3.124257	-2.805151	0.746797
H	1.708365	-4.425180	1.213248
H	4.024829	-3.398703	0.910849
N	0.786622	-1.284640	0.307025
C	3.219836	1.480280	-0.384961
H	4.200222	1.018534	-0.264692
C	3.219837	-1.480280	0.384958
H	4.200223	-1.018534	0.264687
N	0.786621	1.284639	-0.307026
H	-2.305296	2.181070	-0.847260
H	-3.307041	1.121229	-0.148917
C	-2.309317	2.308437	1.211137
H	-3.244657	2.863397	1.389542
H	-1.494056	3.040467	1.107689
C	-2.009668	1.369814	2.371434
H	-1.908924	1.944628	3.307011
H	-2.831339	0.647907	2.509612
N	-0.778622	0.601754	2.045060
H	0.042990	1.209982	2.164836
H	-0.648713	-0.157681	2.722833
N	-2.361908	1.520507	-0.063316
C	-2.309320	-2.308436	-1.211138

H	-3.244662	-2.863394	-1.389541
H	-1.494061	-3.040467	-1.107691
C	-2.009671	-1.369812	-2.371433
H	-1.908929	-1.944626	-3.307011
H	-2.831341	-0.647904	-2.509611
N	-0.778623	-0.601755	-2.045059
H	0.042987	-1.209984	-2.164837
H	-0.648714	0.157680	-2.722833
H	-3.307041	-1.121229	0.148920
H	-2.305296	-2.181072	0.847260
N	-2.361909	-1.520508	0.063318
Ru	-0.788806	0.000000	0.000000

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$[(bpy_2]RuL_{NN}]^0$

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C	-0.571555	2.623323	0.714723
C	-1.991824	0.771928	0.139036
C	-2.958926	2.954412	0.733437
C	-1.627469	3.469263	0.969240
H	0.454822	2.983152	0.870614
H	-3.830343	3.599932	0.871539
H	-1.451031	4.487496	1.316982
C	-0.803922	-2.533596	-0.794362
C	-2.053242	-0.579505	-0.160990
C	-1.932034	-3.283673	-1.041282
H	0.185945	-2.974108	-0.979180
C	-3.210295	-2.665119	-0.763736
H	-1.848830	-4.304286	-1.415775
H	-4.134903	-3.234387	-0.891053
N	-0.788512	-1.259026	-0.317057
C	-3.119397	1.657018	0.338059
H	-4.122788	1.260233	0.164987
C	-3.254618	-1.366262	-0.343417
H	-4.217918	-0.892224	-0.139708
N	-0.670793	1.343198	0.261449
H	2.393233	2.099386	0.852604
H	3.386649	1.032684	0.133606
C	2.377149	2.245710	-1.198577
H	3.318112	2.788492	-1.400921
H	1.575057	2.986886	-1.062293
C	2.026900	1.332491	-2.368388
H	1.917721	1.935573	-3.288028
H	2.834243	0.600358	-2.540717
N	0.800006	0.583190	-2.022663
H	-0.017160	1.213155	-2.036530
H	0.608896	-0.152215	-2.712342
N	2.446363	1.445923	0.063072
C	2.039454	-2.476843	1.260617
H	2.891658	-3.137168	1.502905
H	1.154881	-3.105196	1.075833
C	1.752360	-1.530021	2.420012
H	1.537434	-2.115234	3.332561
H	2.631822	-0.895845	2.624681
N	0.636175	-0.643311	2.028289
H	-0.248463	-1.173706	2.006573
H	0.503799	0.111532	2.710316
H	3.258489	-1.385944	0.000451
H	2.194178	-2.329894	-0.783263
N	2.273901	-1.686380	0.012703
Ru	0.820660	-0.036331	0.004077