

Supporting information

Unveiling role of amino nitrogen-ruthenium cooperation effect in Methanol steam reforming reaction via. hydride transfer mechanism and Marcus theory

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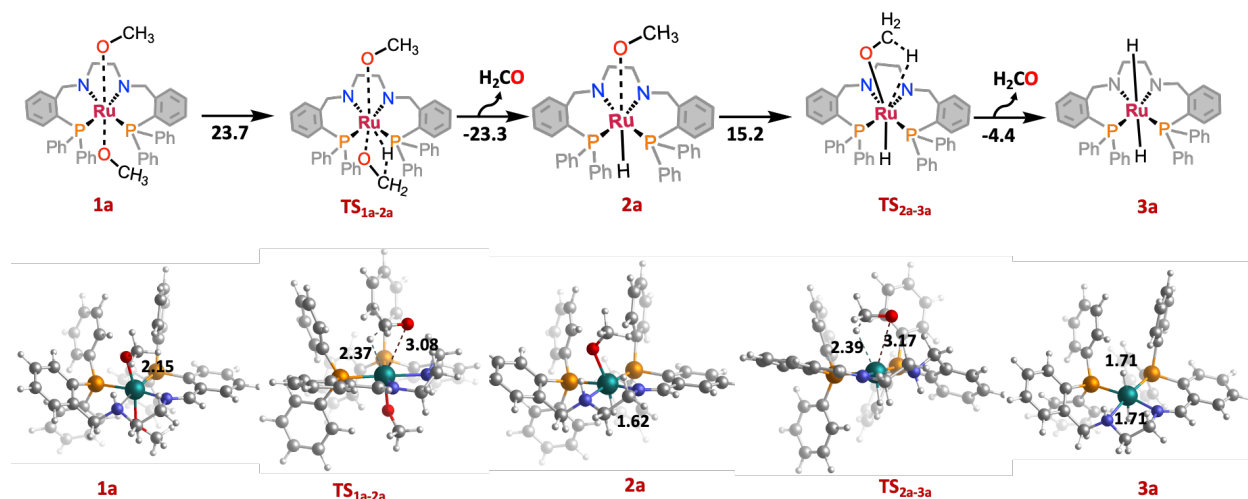


Figure S1. A possible reaction path for the formation of two Ru-H bonds and formaldehyde by catalyst a.

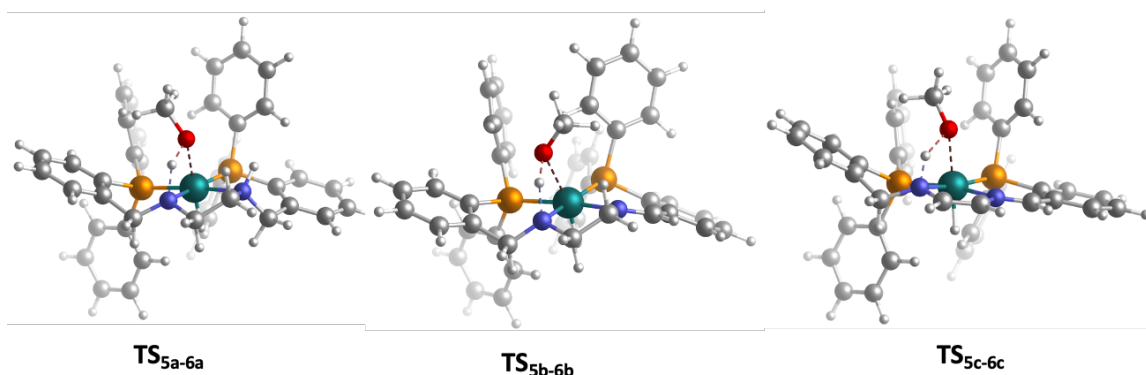


Figure S2. Transition states structures for intramolecular proton transfer reaction from Ru methanol O to ligand N center.

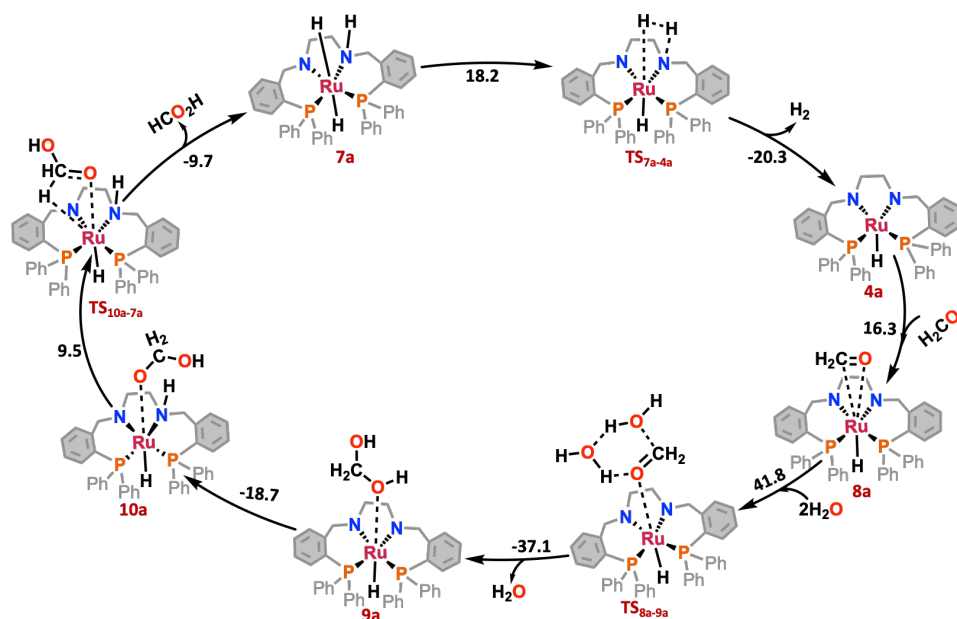


Figure S3. A plausible mechanism of Formic acid formation with reaction of aldehyde and water molecules by catalyst a.

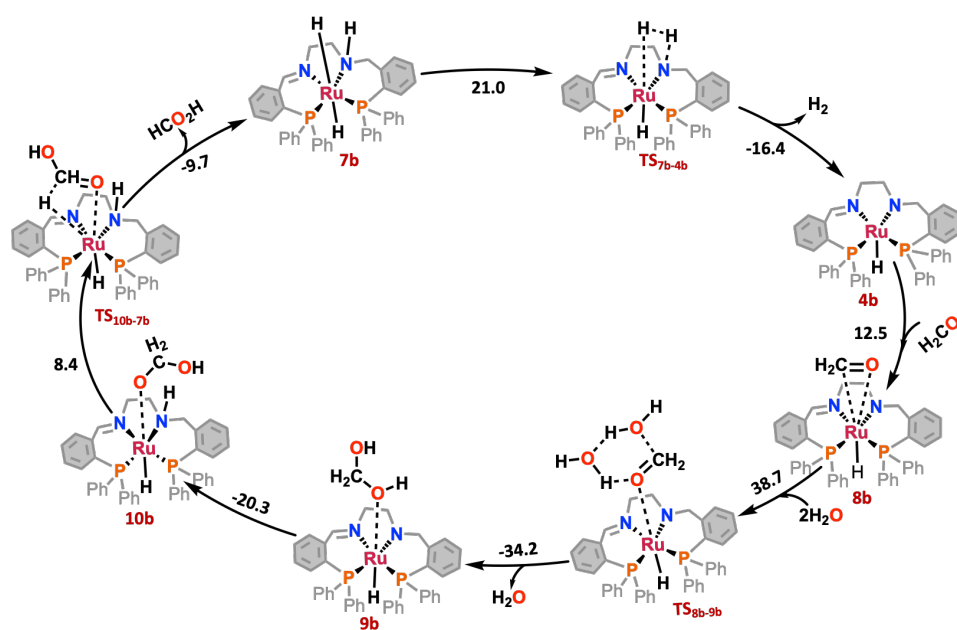


Figure S4. A plausible mechanism of Formic acid formation with reaction of aldehyde and water molecules by catalyst b.

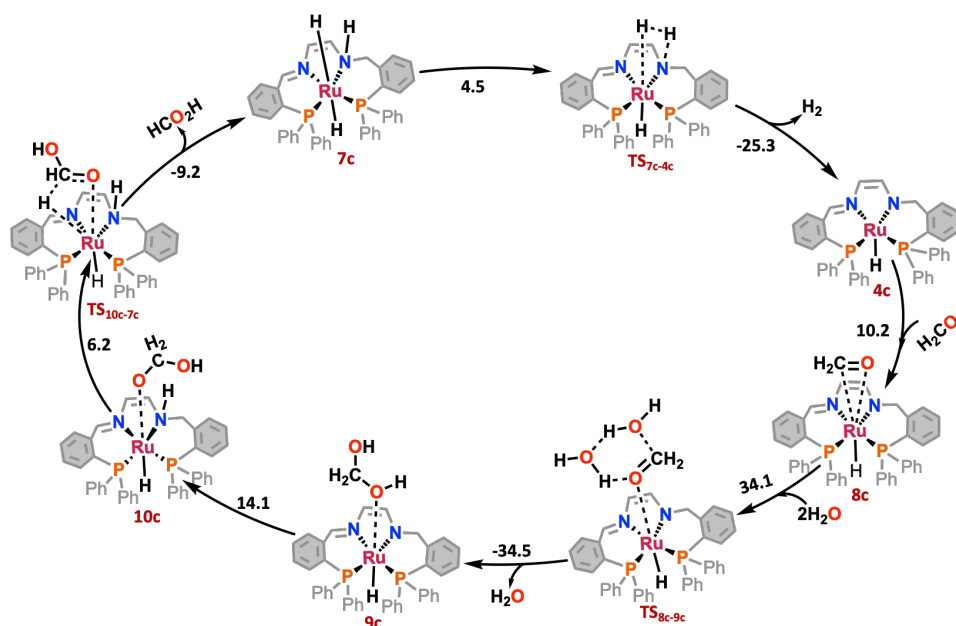


Figure S5. A plausible mechanism of Formic acid formation with reaction of aldehyde and water molecules by catalyst c.

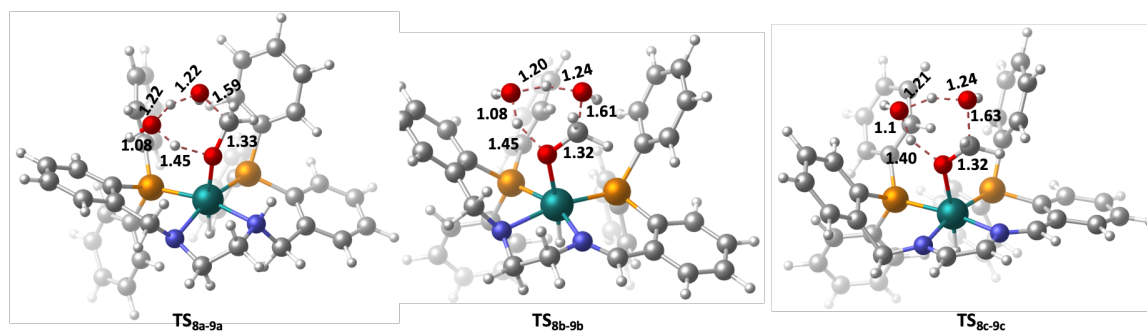


Figure S6. Transition state structures associate with water and metal aldehyde complex addition reaction (all values are in Å).

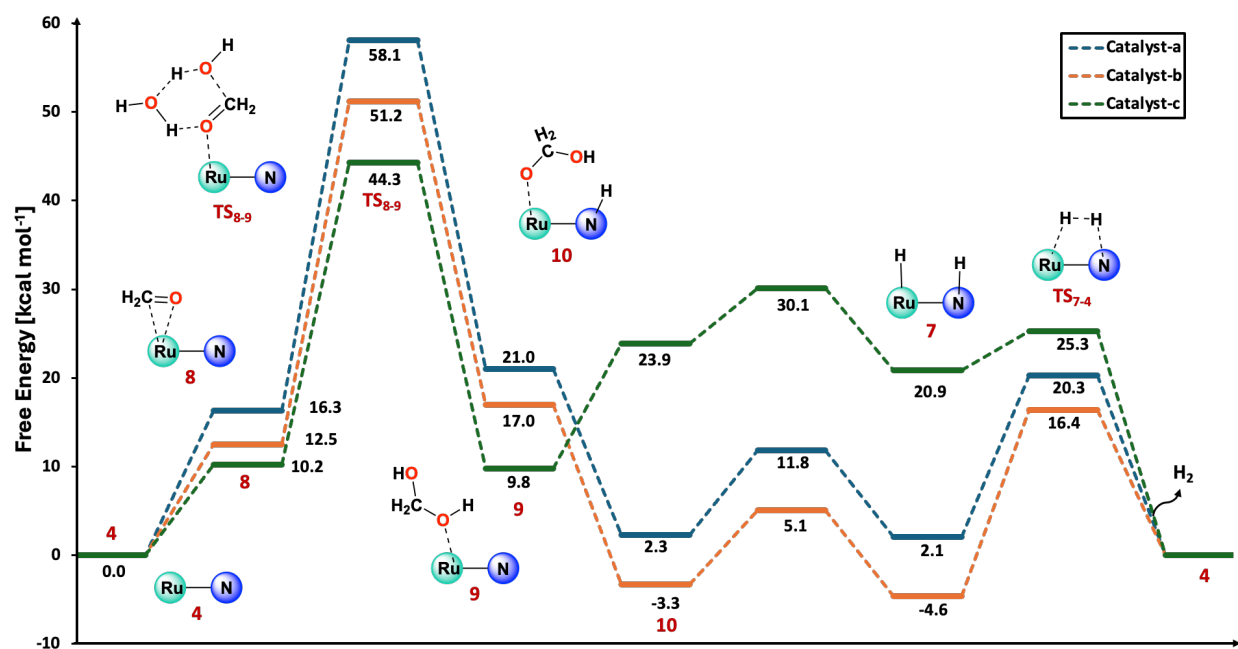


Figure S7. Energy profile diagram of formic acid formation via formaldehyde and water addition reaction, blue, orange, and green lines represent the reaction in the presence of catalyst a, catalyst b, and catalyst c, respectively.

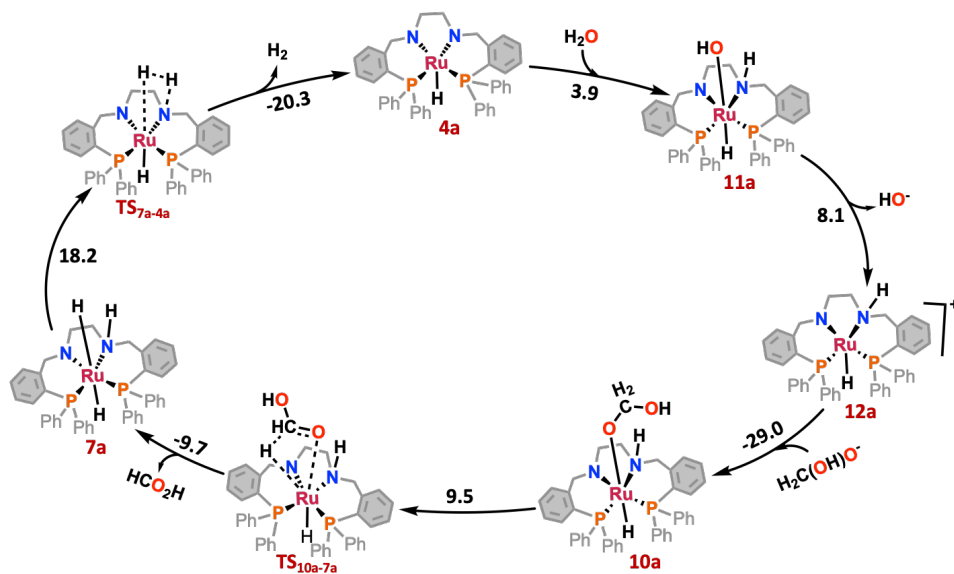


Figure S8. A plausible mechanism of Formic acid formation with reaction via hydroxy methanolate intermediate by catalyst a (all values are in kcal mol⁻¹).

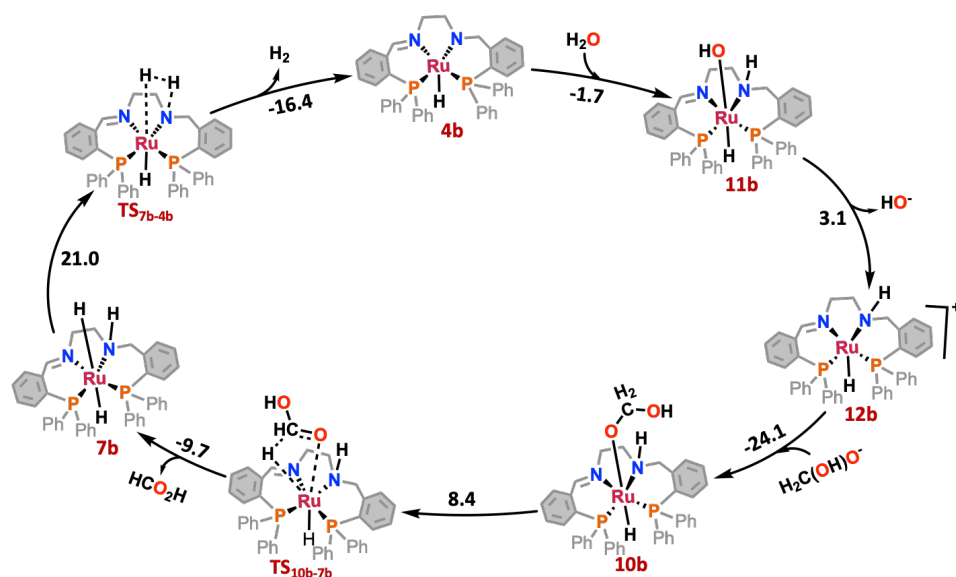


Figure S9. A plausible mechanism of Formic acid formation with reaction via hydroxy methanolate intermediate by catalyst b (all values are in kcal mol⁻¹).

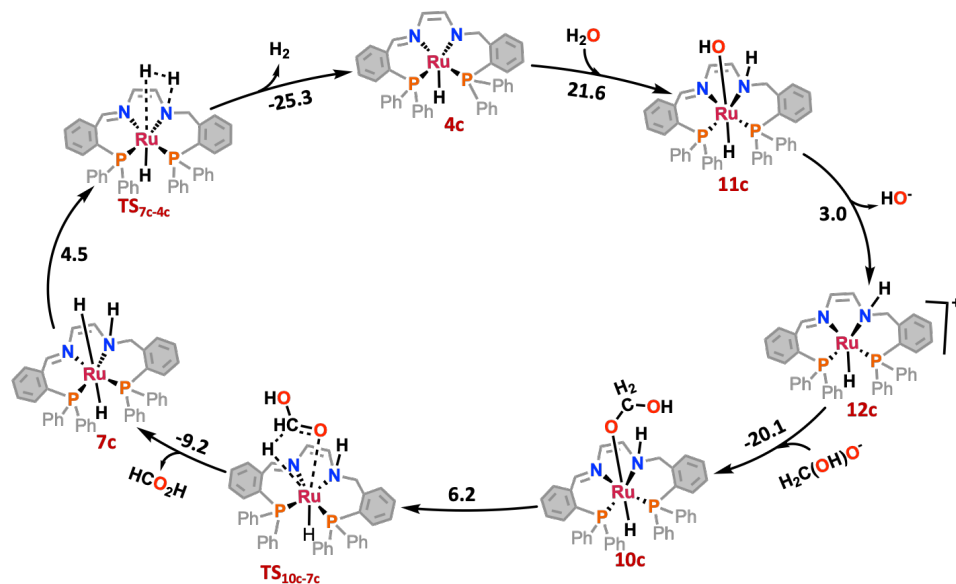


Figure S10. A plausible mechanism of Formic acid formation with reaction via hydroxy methanolate intermediate by catalyst c (all values are in kcal mol⁻¹).

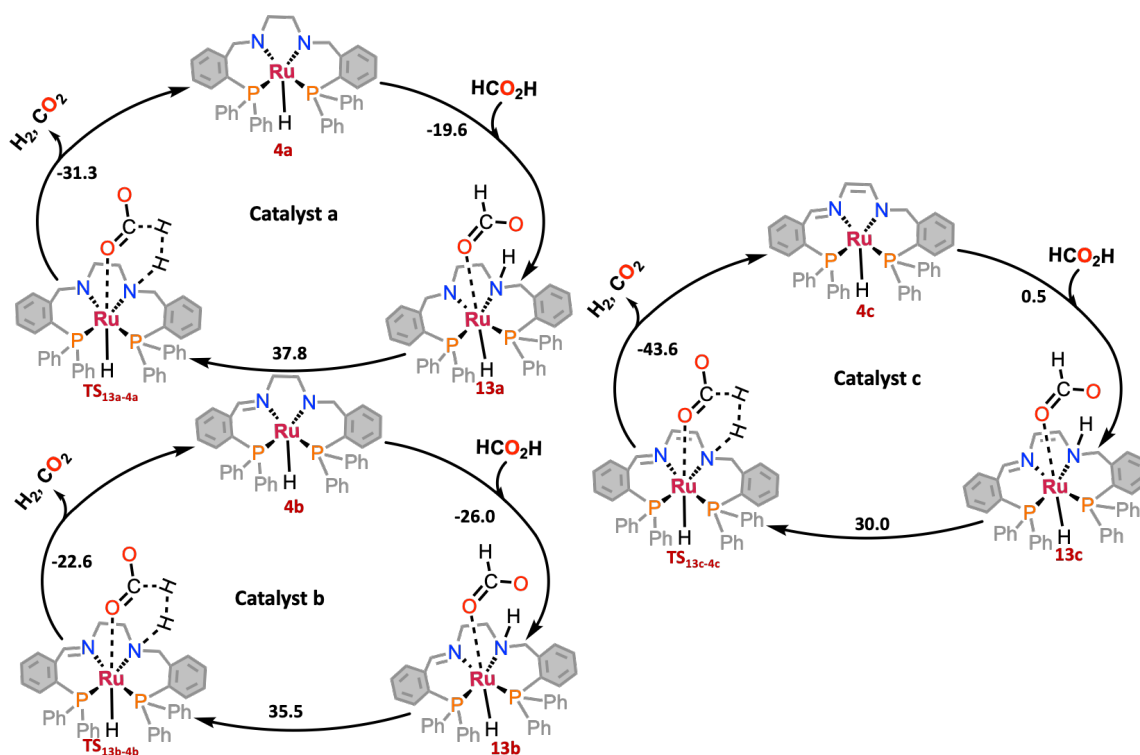


Figure S11. A plausible reaction mechanism of formic acid dehydrogenation to CO_2 via direct dissociation of N-H and C-H through TS_{13b-4b} .

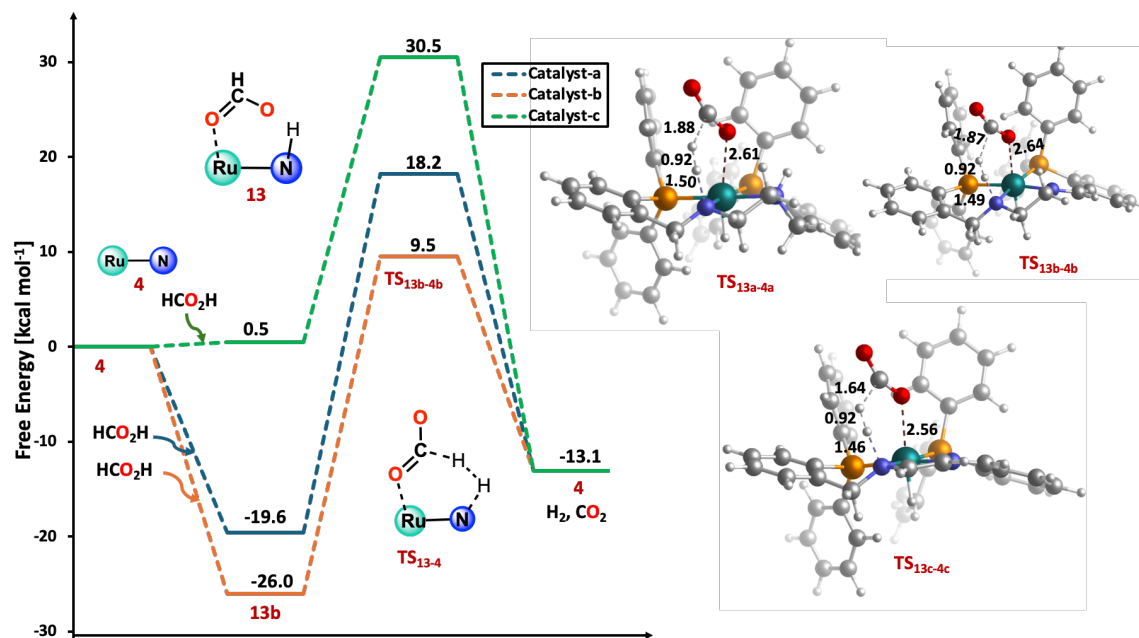


Figure S12. Energy profile diagram of formic acid to CO_2 formation reaction, blue, orange, and green lines represent the reaction in the presence of catalyst a, catalyst b, and catalyst c, respectively.

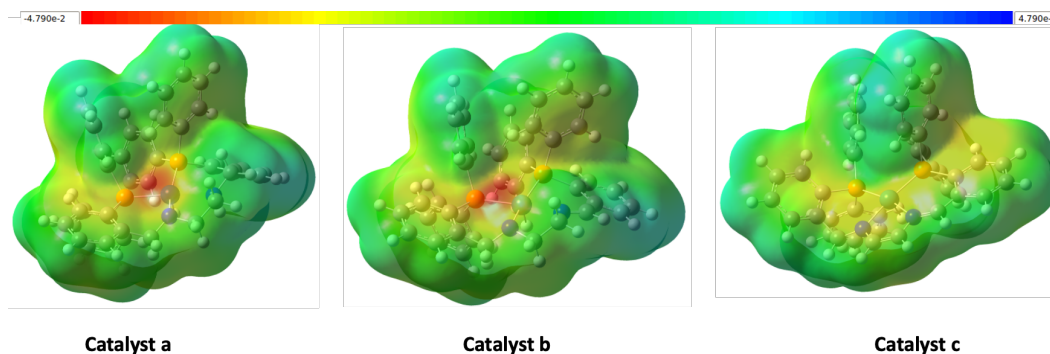


Figure S12. Total charge distribution of catalyst a, catalyst b, and catalyst c. The red region indicates the electron-reached region, and the blue color indicates the electron-deficient region.

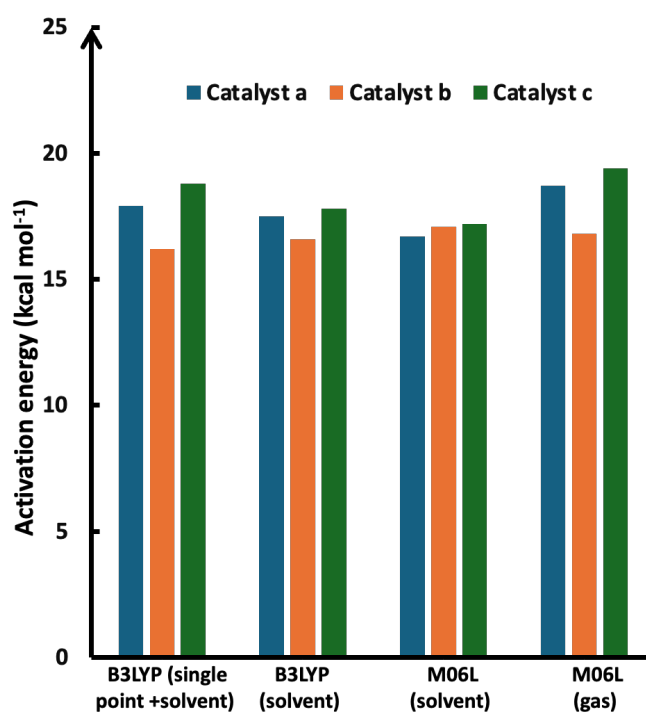


Figure S13. Activation energy associated with TS of the C-H activation process in the formaldehyde formation step with different functionals, blue line, orange, and green line represent activation barrier by catalyst a, catalyst b, and catalyst c, respectively.

Table S1. Quantum Theory of Atoms in Molecules (QTAIM) analysis of catalyst a, catalyst b, and catalyst c. (Topological parameters (in a.u.) at the bond critical points of all the hydrogen-bonded complexes at B3LYP/6-311++G (d, p) level of theory

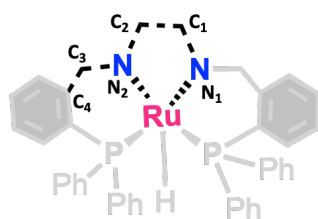
Catalyst	Bond Type	BCP	Electron density (ρ)	Laplacian of electron density ($\nabla^2\rho$)	Kinetic energy density $G(r)$	Potential energy density $V(r)$	Total energy density $H(r)$	Ellipticity (ϵ)
Catalyst a	Ru-N4	181	0.0685	0.3293	0.0879	-0.0934	-0.0056	0.0859
	Ru-N6	182	0.1084	0.4503	0.1352	-0.1578	-0.0226	0.1178
	Ru-P2	161	0.0899	0.21134	0.0829	-0.1129	-0.0300	0.2568
	Ru-P3	164	0.0975	0.2279	0.0905	-0.1241	-0.0336	0.1143
Catalyst b	Ru-N4	185	0.0856	0.4573	0.1225	-0.1307	-0.0082	0.1001
	Ru-N5	182	0.1081	0.4535	0.1356	-0.1579	-0.0223	0.1081
	Ru-P2	161	0.0938	0.2202	0.0864	-0.1177	-0.0313	0.0656
	Ru-P3	167	0.0936	0.2057	0.0842	-0.1170	-0.0328	0.2423
Catalyst c	Ru-N4	174	0.0920	0.4350	0.1214	-0.1340	-0.0126	0.4350
	Ru-N5	178	0.0795	0.3967	0.1063	-0.1134	-0.0071	0.2144
	Ru-P2	160	0.0963	0.2269	0.0901	-0.1235	-0.0334	0.1457
	Ru-P3	159	0.0924	0.2060	0.0827	-0.1139	-0.0312	0.2251

Quantum theory of atoms in molecule (QTAIM) analysis

To gain a deeper understanding of the bonding nature within the Ru coordination sphere in catalysts a, b, and c, a topological analysis was carried out based on the Quantum Theory of Atoms in Molecules (QTAIM). The topological parameters include the electron density (ρ), Laplacian of electron density ($\nabla^2\rho$), kinetic energy density ($G(r)$), potential energy density ($V(r)$), total energy density ($H(r)$), and ellipticity (ϵ) at the bond critical point. The Ru–N and Ru–P bonds in all three catalysts display moderate electron density values ($\rho \approx 0.0685\text{--}0.1084$ a.u.) accompanied by positive Laplacian values ($\nabla^2\rho > 0$), characteristics typically associated with closed-shell interactions. However, the consistently negative $H(r)$ values across these BCPs point toward a partial covalent contribution. According to Bader's criteria, the coexistence of a positive Laplacian and negative total energy density indicates an interaction that is partially covalent in nature.

Ellipticity analysis provides further insights into bond stability. Previous literature suggests that $\varepsilon < 1$ corresponds to stable interactions, whereas $\varepsilon > 1$ denotes unstable or anisotropic bonding pathways. In the present study, all Ru–N and Ru–P bonds exhibit ε values below unity, confirming their structural stability. The kinetic-to-potential energy ratio ($-G(r)/V(r)$) further clarifies the interaction type: values greater than 1 are characteristic of closed-shell or noncovalent interactions, while ratios below 1 indicate partial covalency. For the studied systems, $-G(r)/V(r)$ values predominantly exceed unity, reinforcing the dominance of closed-shell character; however, ratios approaching unity, combined with negative $H(r)$, indicate the presence of partial covalent bonding.

Table S2. Quantitative measure of bond order of 4a, 4b, and 4c with Wiberg bond order (WBO) analysis using Multiwfn.



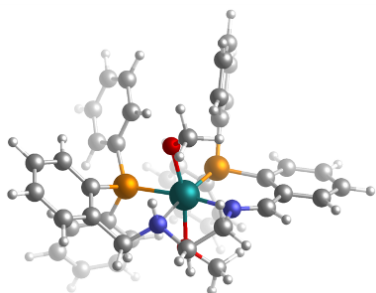
Bond	WBO (Catalyst a)	WBO (Catalyst b)	WBO (Catalyst c)
Ru-N ₁	0.57	0.69	0.64
Ru-N ₂	0.96	0.96	0.72
N ₁ -C ₁	1.22	1.22	1.60
N ₂ -C ₂	1.16	1.14	1.39
N ₂ -C ₃	1.22	1.90	1.71
C ₁ -C ₂	1.13	1.12	1.50
C ₃ -C ₄	1.06	1.13	1.19

Table S3. Activation energy barrier of hydride transfer in the formaldehyde formation step.

SL no.	Methode	Activation energy in Kcal mol ⁻¹ (Catalyst a)	Activation energy in Kcal mol ⁻¹ (Catalyst b)	Activation energy in Kcal mol ⁻¹ (Catalyst c)
1	B3lyp (total)	17.9	16.2	18.8
2	B3LYP (solvent)	17.5	16.6	17.8
3	Mo6-l (solvent)	16.7	17.1	17.2
4	Mo6l (gas phase)	18.7	16.8	19.4

Coordinates and structures of optimized intermediates and transition states involved in our DFT studies.

1a

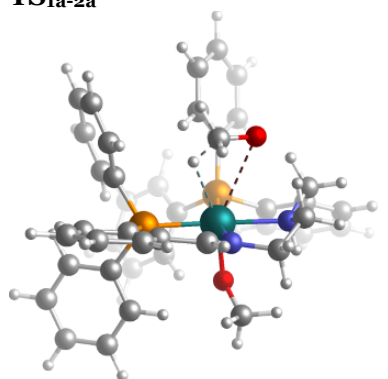


Ru	0.038000	-1.289000	0.071000
P	-1.776000	0.265000	0.079000
P	1.752000	0.223000	-0.030000
N	-1.451000	-2.911000	0.123000
H	-1.602000	-3.048000	1.124000
N	1.351000	-2.907000	0.028000
C	-1.594000	1.824000	1.044000
C	-0.897000	1.743000	2.262000
H	-0.546000	0.770000	2.602000
C	-0.648000	2.900000	3.002000
H	-0.081000	2.830000	3.926000
C	-1.095000	4.143000	2.542000
H	-0.887000	5.044000	3.113000
C	-1.806000	4.224000	1.339000
H	-2.157000	5.187000	0.976000
C	-2.056000	3.069000	0.592000
H	-2.586000	3.147000	-0.352000
C	-2.511000	0.821000	-1.522000
C	-3.876000	1.143000	-1.633000
H	-4.536000	1.028000	-0.778000
C	-4.398000	1.615000	-2.839000
H	-5.455000	1.860000	-2.910000
C	-3.562000	1.770000	-3.950000
H	-3.967000	2.137000	-4.891000
C	-2.207000	1.444000	-3.848000
H	-1.550000	1.552000	-4.707000
C	-1.682000	0.967000	-2.644000
H	-0.647000	0.662000	-2.582000
C	-3.250000	-0.538000	0.864000
C	-4.026000	0.114000	1.830000
H	-3.741000	1.105000	2.168000
C	-5.168000	-0.490000	2.364000
H	-5.757000	0.036000	3.112000
C	-5.548000	-1.761000	1.932000
H	-6.437000	-2.239000	2.337000
C	-4.769000	-2.425000	0.980000

H	-5.054000	-3.424000	0.654000
C	-3.622000	-1.833000	0.440000
C	-2.763000	-2.630000	-0.518000
H	-3.273000	-3.574000	-0.760000
H	-2.549000	-2.110000	-1.459000
C	-0.763000	-4.077000	-0.452000
H	-0.690000	-3.908000	-1.528000
H	-1.326000	-5.008000	-0.276000
C	0.623000	-4.187000	0.173000
H	0.532000	-4.400000	1.244000
H	1.179000	-5.011000	-0.291000
C	2.618000	-3.009000	-0.200000
H	3.035000	-4.019000	-0.264000
C	3.608000	-1.960000	-0.435000
C	4.911000	-2.443000	-0.701000
H	5.084000	-3.517000	-0.683000
C	5.968000	-1.591000	-0.992000
H	6.956000	-1.996000	-1.195000
C	5.744000	-0.211000	-1.022000
H	6.554000	0.476000	-1.251000
C	4.469000	0.283000	-0.750000
H	4.311000	1.356000	-0.770000
C	3.386000	-0.560000	-0.455000
C	1.589000	1.522000	-1.338000
C	1.989000	1.273000	-2.660000
H	2.512000	0.355000	-2.906000
C	1.710000	2.191000	-3.674000
H	2.023000	1.976000	-4.693000
C	1.023000	3.374000	-3.385000
H	0.796000	4.084000	-4.176000
C	0.623000	3.633000	-2.071000
H	0.080000	4.543000	-1.831000
C	0.903000	2.715000	-1.058000
H	0.577000	2.931000	-0.047000
C	2.311000	1.183000	1.462000
C	2.905000	2.454000	1.407000
H	3.007000	2.975000	0.460000
C	3.361000	3.078000	2.571000
H	3.809000	4.067000	2.510000
C	3.241000	2.435000	3.807000
H	3.595000	2.922000	4.713000
C	2.661000	1.165000	3.870000
H	2.555000	0.657000	4.825000
C	2.198000	0.544000	2.707000
H	1.692000	-0.411000	2.758000
O	-0.168000	-1.453000	-2.037000
C	0.789000	-2.031000	-2.852000

H	0.865000	-3.139000	-2.752000
H	0.546000	-1.832000	-3.913000
H	1.817000	-1.654000	-2.682000
O	-0.241000	-1.258000	2.205000
C	0.145000	-2.322000	2.999000
H	1.200000	-2.640000	2.840000
H	0.046000	-2.059000	4.069000
H	-0.471000	-3.244000	2.866000

TS_{1a-2a}

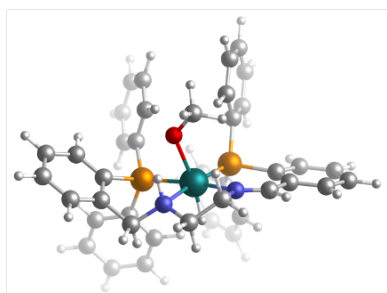


Ru	0.016000	-1.219000	-0.366000
P	1.756000	0.364000	-0.063000
P	-1.805000	0.185000	-0.014000
N	1.569000	-2.749000	-0.684000
H	1.730000	-2.723000	-1.692000
N	-1.219000	-2.924000	-0.523000
C	1.501000	2.077000	-0.690000
C	0.764000	2.229000	-1.876000
H	0.418000	1.343000	-2.401000
C	0.459000	3.506000	-2.353000
H	-0.139000	3.610000	-3.254000
C	0.894000	4.640000	-1.659000
H	0.645000	5.633000	-2.025000
C	1.648000	4.492000	-0.489000
H	1.991000	5.369000	0.054000
C	1.951000	3.216000	-0.005000
H	2.510000	3.113000	0.919000
C	2.423000	0.584000	1.638000
C	3.768000	0.926000	1.862000
H	4.447000	1.050000	1.024000
C	4.245000	1.099000	3.163000
H	5.288000	1.361000	3.324000
C	3.384000	0.928000	4.253000
H	3.757000	1.055000	5.267000
C	2.050000	0.580000	4.035000
H	1.376000	0.424000	4.873000
C	1.572000	0.402000	2.735000
H	0.542000	0.116000	2.584000
C	3.263000	-0.197000	-0.971000
C	4.004000	0.670000	-1.783000

H	3.671000	1.693000	-1.923000
C	5.176000	0.238000	-2.413000
H	5.740000	0.928000	-3.036000
C	5.617000	-1.073000	-2.232000
H	6.528000	-1.419000	-2.712000
C	4.871000	-1.948000	-1.436000
H	5.206000	-2.975000	-1.306000
C	3.694000	-1.532000	-0.801000
C	2.884000	-2.533000	-0.009000
H	3.431000	-3.486000	0.034000
H	2.654000	-2.236000	1.020000
C	0.960000	-4.045000	-0.304000
H	0.918000	-4.033000	0.794000
H	1.570000	-4.887000	-0.669000
C	-0.439000	-4.121000	-0.901000
H	-0.392000	-4.143000	-1.996000
H	-0.940000	-5.039000	-0.567000
C	-2.424000	-3.136000	-0.119000
H	-2.759000	-4.176000	-0.070000
C	-3.465000	-2.178000	0.265000
C	-4.707000	-2.782000	0.575000
H	-4.785000	-3.866000	0.533000
C	-5.824000	-2.036000	0.929000
H	-6.761000	-2.534000	1.163000
C	-5.725000	-0.642000	0.977000
H	-6.585000	-0.036000	1.250000
C	-4.509000	-0.030000	0.677000
H	-4.444000	1.051000	0.729000
C	-3.366000	-0.766000	0.328000
C	-1.688000	1.246000	1.499000
C	-2.095000	0.760000	2.753000
H	-2.587000	-0.203000	2.834000
C	-1.850000	1.497000	3.913000
H	-2.162000	1.098000	4.875000
C	-1.194000	2.730000	3.841000
H	-0.992000	3.296000	4.746000
C	-0.791000	3.223000	2.598000
H	-0.272000	4.176000	2.525000
C	-1.035000	2.487000	1.437000
H	-0.708000	2.884000	0.484000
C	-2.425000	1.342000	-1.324000
C	-3.020000	2.585000	-1.057000
H	-3.107000	2.947000	-0.038000
C	-3.499000	3.384000	-2.099000
H	-3.949000	4.347000	-1.872000
C	-3.398000	2.949000	-3.423000
H	-3.767000	3.573000	-4.234000
C	-2.819000	1.706000	-3.698000
H	-2.733000	1.356000	-4.724000
C	-2.336000	0.910000	-2.656000
H	-1.856000	-0.032000	-2.875000
O	0.904000	-2.617000	2.234000
C	-0.373000	-2.293000	2.513000
H	-1.133000	-3.109000	2.356000

H	-0.558000	-1.918000	3.555000
H	-0.794000	-1.453000	1.858000
O	0.252000	-0.790000	-2.368000
C	-0.137000	-1.726000	-3.320000
H	-1.176000	-2.088000	-3.187000
H	-0.073000	-1.257000	-4.317000
H	0.509000	-2.627000	-3.361000

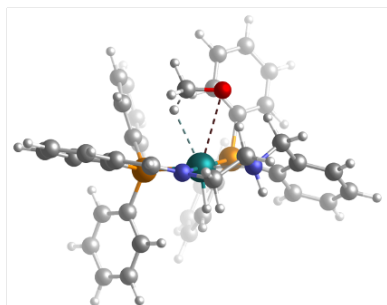
2a



Ru	0.039000	-1.291000	-0.352000
P	-1.729000	0.203000	-0.005000
P	1.756000	0.168000	-0.109000
N	-1.460000	-2.846000	-0.723000
H	-1.524000	-3.057000	0.290000
N	1.331000	-2.871000	-0.769000
C	-1.538000	1.406000	1.377000
C	-1.003000	0.887000	2.569000
H	-0.766000	-0.177000	2.615000
C	-0.775000	1.731000	3.656000
H	-0.343000	1.326000	4.567000
C	-1.070000	3.096000	3.565000
H	-0.877000	3.753000	4.410000
C	-1.607000	3.614000	2.383000
H	-1.837000	4.674000	2.305000
C	-1.846000	2.771000	1.292000
H	-2.250000	3.186000	0.374000
C	-2.383000	1.216000	-1.413000
C	-3.677000	1.768000	-1.384000
H	-4.327000	1.587000	-0.533000
C	-4.141000	2.547000	-2.445000
H	-5.145000	2.965000	-2.408000
C	-3.320000	2.784000	-3.554000
H	-3.682000	3.390000	-4.381000
C	-2.037000	2.233000	-3.593000
H	-1.389000	2.411000	-4.447000
C	-1.574000	1.450000	-2.532000
H	-0.584000	1.011000	-2.572000
C	-3.279000	-0.700000	0.488000
C	-4.102000	-0.227000	1.520000
H	-3.815000	0.663000	2.071000
C	-5.289000	-0.881000	1.860000
H	-5.909000	-0.491000	2.663000
C	-5.671000	-2.029000	1.166000

H	-6.591000	-2.549000	1.421000
C	-4.849000	-2.519000	0.148000
H	-5.134000	-3.426000	-0.381000
C	-3.657000	-1.872000	-0.203000
C	-2.786000	-2.491000	-1.276000
H	-3.287000	-3.392000	-1.660000
H	-2.629000	-1.814000	-2.124000
C	-0.781000	-3.924000	-1.449000
H	-0.671000	-3.617000	-2.495000
H	-1.360000	-4.862000	-1.420000
C	0.587000	-4.145000	-0.815000
H	0.458000	-4.488000	0.218000
H	1.144000	-4.913000	-1.366000
C	2.596000	-2.944000	-1.019000
H	3.005000	-3.927000	-1.271000
C	3.592000	-1.873000	-1.033000
C	4.888000	-2.290000	-1.419000
H	5.049000	-3.339000	-1.660000
C	5.954000	-1.404000	-1.503000
H	6.936000	-1.757000	-1.805000
C	5.745000	-0.056000	-1.192000
H	6.563000	0.658000	-1.251000
C	4.478000	0.369000	-0.800000
H	4.333000	1.417000	-0.559000
C	3.385000	-0.508000	-0.712000
C	1.626000	1.729000	-1.097000
C	2.004000	1.745000	-2.450000
H	2.473000	0.869000	-2.891000
C	1.769000	2.870000	-3.243000
H	2.070000	2.863000	-4.288000
C	1.142000	3.996000	-2.700000
H	0.950000	4.868000	-3.320000
C	0.756000	3.988000	-1.358000
H	0.257000	4.851000	-0.925000
C	0.998000	2.864000	-0.563000
H	0.683000	2.873000	0.474000
C	2.304000	0.763000	1.567000
C	2.949000	1.983000	1.826000
H	3.118000	2.698000	1.027000
C	3.370000	2.303000	3.120000
H	3.856000	3.257000	3.306000
C	3.167000	1.402000	4.170000
H	3.496000	1.653000	5.176000
C	2.532000	0.182000	3.919000
H	2.359000	-0.525000	4.727000
C	2.098000	-0.128000	2.629000
H	1.565000	-1.051000	2.440000
O	-0.494000	-2.179000	1.683000
C	0.267000	-3.050000	2.447000
H	1.284000	-3.243000	2.039000
H	0.421000	-2.683000	3.486000
H	-0.215000	-4.047000	2.557000
H	0.121000	-0.863000	-1.920000

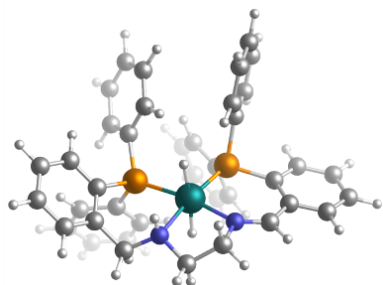
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P	1.735000	0.298000	-0.146000
P	-1.784000	0.166000	-0.075000
N	1.504000	-2.673000	-1.224000
H	1.689000	-2.488000	-2.211000
N	-1.290000	-2.786000	-1.063000
C	1.520000	2.084000	-0.568000
C	0.795000	2.395000	-1.729000
H	0.416000	1.591000	-2.352000
C	0.517000	3.721000	-2.064000
H	-0.074000	3.937000	-2.950000
C	0.970000	4.759000	-1.242000
H	0.742000	5.792000	-1.492000
C	1.709000	4.460000	-0.094000
H	2.064000	5.261000	0.551000
C	1.984000	3.131000	0.242000
H	2.532000	2.913000	1.153000
C	2.411000	0.311000	1.573000
C	3.741000	0.679000	1.846000
H	4.408000	0.960000	1.037000
C	4.218000	0.676000	3.158000
H	5.249000	0.961000	3.357000
C	3.376000	0.297000	4.210000
H	3.751000	0.285000	5.231000
C	2.060000	-0.083000	3.942000
H	1.403000	-0.401000	4.746000
C	1.581000	-0.081000	2.630000
H	0.567000	-0.397000	2.434000
C	3.261000	-0.166000	-1.090000
C	4.049000	0.790000	-1.745000
H	3.743000	1.832000	-1.744000
C	5.235000	0.427000	-2.391000
H	5.834000	1.186000	-2.889000
C	5.645000	-0.906000	-2.386000
H	6.568000	-1.201000	-2.879000
C	4.854000	-1.868000	-1.750000
H	5.166000	-2.910000	-1.759000
C	3.662000	-1.523000	-1.101000
C	2.808000	-2.615000	-0.496000
H	3.327000	-3.578000	-0.601000

H	2.561000	-2.489000	0.565000
C	0.840000	-3.992000	-1.101000
H	0.773000	-4.187000	-0.019000
H	1.422000	-4.775000	-1.613000
C	-0.545000	-3.874000	-1.723000
H	-0.468000	-3.611000	-2.788000
H	-1.082000	-4.829000	-1.645000
C	-2.492000	-3.055000	-0.682000
H	-2.859000	-4.071000	-0.857000
C	-3.487000	-2.174000	-0.064000
C	-4.723000	-2.804000	0.212000
H	-4.831000	-3.863000	-0.012000
C	-5.796000	-2.113000	0.760000
H	-6.730000	-2.629000	0.965000
C	-5.660000	-0.749000	1.038000
H	-6.487000	-0.187000	1.464000
C	-4.450000	-0.112000	0.770000
H	-4.354000	0.944000	1.000000
C	-3.347000	-0.796000	0.233000
C	-1.634000	1.129000	1.498000
C	-1.939000	0.519000	2.728000
H	-2.379000	-0.473000	2.751000
C	-1.659000	1.167000	3.932000
H	-1.894000	0.673000	4.871000
C	-1.065000	2.433000	3.930000
H	-0.835000	2.930000	4.868000
C	-0.759000	3.047000	2.713000
H	-0.289000	4.027000	2.695000
C	-1.041000	2.401000	1.507000
H	-0.786000	2.893000	0.576000
C	-2.425000	1.395000	-1.315000
C	-3.083000	2.584000	-0.968000
H	-3.210000	2.858000	0.075000
C	-3.569000	3.446000	-1.956000
H	-4.064000	4.369000	-1.667000
C	-3.417000	3.124000	-3.308000
H	-3.793000	3.795000	-4.076000
C	-2.779000	1.931000	-3.664000
H	-2.658000	1.667000	-4.712000
C	-2.286000	1.076000	-2.675000
H	-1.773000	0.161000	-2.956000
O	0.830000	-3.173000	1.708000
C	-0.405000	-2.772000	2.058000
H	-1.247000	-3.455000	1.750000
H	-0.560000	-2.596000	3.157000
H	-0.726000	-1.779000	1.584000
H	0.020000	-0.621000	-2.094000

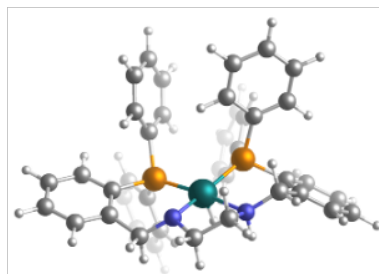
3a



Ru	-0.029000	1.425000	0.098000
P	1.721000	-0.095000	0.100000
P	-1.751000	-0.026000	-0.041000
N	1.481000	3.059000	0.193000
H	1.612000	3.188000	1.197000
N	-1.324000	3.056000	0.042000
C	1.535000	-1.689000	1.026000
C	0.818000	-1.646000	2.232000
H	0.443000	-0.692000	2.585000
C	0.551000	-2.817000	2.944000
H	-0.036000	-2.765000	3.857000
C	1.003000	-4.049000	2.462000
H	0.782000	-4.964000	3.006000
C	1.734000	-4.099000	1.270000
H	2.088000	-5.054000	0.886000
C	1.999000	-2.927000	0.556000
H	2.543000	-2.988000	-0.381000
C	2.470000	-0.654000	-1.509000
C	3.817000	-1.045000	-1.616000
H	4.469000	-0.999000	-0.748000
C	4.334000	-1.493000	-2.835000
H	5.379000	-1.784000	-2.902000
C	3.509000	-1.564000	-3.962000
H	3.910000	-1.915000	-4.910000
C	2.170000	-1.176000	-3.864000
H	1.519000	-1.225000	-4.733000
C	1.658000	-0.715000	-2.649000
H	0.630000	-0.379000	-2.583000
C	3.234000	0.646000	0.891000
C	4.003000	-0.058000	1.829000
H	3.699000	-1.056000	2.128000
C	5.160000	0.498000	2.384000
H	5.738000	-0.071000	3.107000
C	5.568000	1.776000	2.002000
H	6.467000	2.218000	2.423000
C	4.801000	2.493000	1.079000
H	5.109000	3.496000	0.790000
C	3.639000	1.949000	0.518000
C	2.810000	2.804000	-0.417000
H	3.335000	3.755000	-0.595000
H	2.635000	2.325000	-1.386000
C	0.788000	4.235000	-0.353000
H	0.688000	4.090000	-1.434000
H	1.350000	5.165000	-0.164000

C	-0.588000	4.309000	0.296000
H	-0.478000	4.419000	1.383000
H	-1.139000	5.181000	-0.083000
C	-2.585000	3.198000	-0.220000
H	-2.986000	4.216000	-0.241000
C	-3.569000	2.169000	-0.533000
C	-4.855000	2.664000	-0.862000
H	-5.020000	3.740000	-0.842000
C	-5.901000	1.823000	-1.213000
H	-6.874000	2.237000	-1.463000
C	-5.686000	0.440000	-1.240000
H	-6.489000	-0.239000	-1.513000
C	-4.431000	-0.065000	-0.908000
H	-4.282000	-1.139000	-0.930000
C	-3.355000	0.767000	-0.553000
C	-1.591000	-1.385000	-1.292000
C	-1.891000	-1.130000	-2.641000
H	-2.320000	-0.174000	-2.926000
C	-1.623000	-2.084000	-3.624000
H	-1.864000	-1.868000	-4.663000
C	-1.033000	-3.305000	-3.279000
H	-0.811000	-4.042000	-4.046000
C	-0.723000	-3.564000	-1.942000
H	-0.253000	-4.503000	-1.659000
C	-1.004000	-2.614000	-0.956000
H	-0.751000	-2.834000	0.075000
C	-2.383000	-0.916000	1.480000
C	-3.058000	-2.147000	1.455000
H	-3.198000	-2.679000	0.519000
C	-3.544000	-2.720000	2.633000
H	-4.051000	-3.682000	2.594000
C	-3.379000	-2.063000	3.856000
H	-3.756000	-2.509000	4.773000
C	-2.724000	-0.828000	3.889000
H	-2.590000	-0.305000	4.834000
C	-2.230000	-0.262000	2.711000
H	-1.687000	0.680000	2.737000
H	0.051000	1.494000	-1.606000
H	0.068000	1.413000	1.820000

4a

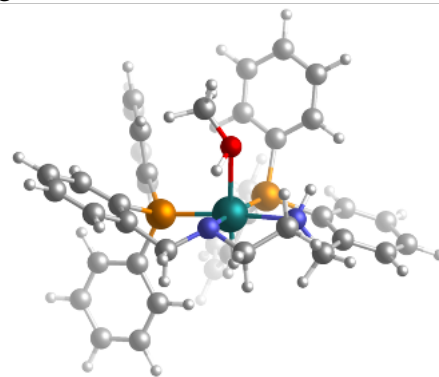


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P	1.798000	0.213000	-0.076000

N	1.577000	-2.872000	-0.552000
N	-1.258000	-2.947000	-0.392000
C	-2.065000	0.546000	-2.908000
H	-1.323000	-0.242000	-2.993000
C	-2.633000	1.106000	-4.058000
H	-2.329000	0.745000	-5.037000
C	-3.585000	2.122000	-3.948000
H	-4.023000	2.562000	-4.841000
C	-3.976000	2.567000	-2.680000
H	-4.721000	3.352000	-2.582000
C	-3.413000	2.000000	-1.535000
H	-3.734000	2.352000	-0.559000
C	-2.438000	0.993000	-1.634000
C	-1.212000	2.883000	0.631000
H	-1.091000	3.084000	-0.428000
C	-0.984000	3.915000	1.546000
H	-0.686000	4.893000	1.179000
C	-1.128000	3.689000	2.918000
H	-0.955000	4.494000	3.627000
C	-1.488000	2.415000	3.368000
H	-1.595000	2.219000	4.432000
C	-1.698000	1.381000	2.454000
H	-1.961000	0.397000	2.823000
C	-1.582000	1.601000	1.070000
C	-3.281000	-0.686000	0.473000
C	-4.238000	-0.024000	1.262000
H	-4.082000	1.011000	1.546000
C	-5.398000	-0.665000	1.699000
H	-6.117000	-0.126000	2.312000
C	-5.622000	-1.995000	1.344000
H	-6.514000	-2.516000	1.684000
C	-4.693000	-2.653000	0.536000
H	-4.876000	-3.686000	0.246000
C	-3.526000	-2.023000	0.078000
C	-2.624000	-2.798000	-0.867000
H	-3.082000	-3.794000	-1.006000
C	-0.564000	-3.967000	-1.167000
H	-0.489000	-3.703000	-2.241000
H	-1.096000	-4.938000	-1.121000
C	0.829000	-4.165000	-0.584000
H	0.735000	-4.500000	0.453000
H	1.397000	-4.923000	-1.143000
C	2.421000	-2.653000	-1.748000
H	1.755000	-2.378000	-2.570000
C	3.510000	-1.605000	-1.576000
C	4.752000	-1.921000	-2.160000
H	4.868000	-2.881000	-2.658000
C	5.834000	-1.045000	-2.120000
H	6.776000	-1.322000	-2.585000
C	5.696000	0.183000	-1.467000
H	6.528000	0.880000	-1.416000
C	4.477000	0.506000	-0.877000
H	4.380000	1.459000	-0.367000
C	3.369000	-0.361000	-0.921000

C	1.686000	1.939000	-0.743000
C	0.996000	2.091000	-1.956000
H	0.568000	1.216000	-2.434000
C	0.825000	3.351000	-2.531000
H	0.272000	3.445000	-3.462000
C	1.341000	4.486000	-1.896000
H	1.198000	5.471000	-2.333000
C	2.040000	4.345000	-0.693000
H	2.445000	5.221000	-0.191000
C	2.216000	3.080000	-0.123000
H	2.751000	2.994000	0.818000
C	2.404000	0.411000	1.664000
C	3.396000	-0.434000	2.188000
H	3.945000	-1.102000	1.530000
C	3.697000	-0.424000	3.552000
H	4.468000	-1.087000	3.937000
C	3.012000	0.433000	4.419000
H	3.246000	0.441000	5.480000
C	2.023000	1.280000	3.907000
H	1.479000	1.952000	4.566000
C	1.719000	1.264000	2.545000
H	0.941000	1.918000	2.170000
H	0.073000	-0.957000	-1.851000
H	-2.657000	-2.316000	-1.866000
O	-0.071000	-2.463000	1.903000
C	-0.638000	-2.045000	3.136000
H	-0.065000	-1.186000	3.500000
H	-1.690000	-1.750000	3.012000
H	-0.586000	-2.851000	3.883000
H	-0.759000	-2.891000	1.294000
H	2.175000	-2.877000	0.275000
H	2.911000	-3.598000	-2.026000

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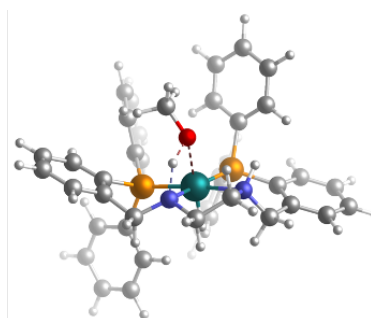


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P	-1.720000	0.177000	-0.114000
P	1.797000	0.199000	-0.064000
N	1.563000	-2.870000	-0.477000
N	-1.265000	-2.956000	-0.317000
C	-2.066000	0.462000	-2.916000
H	-1.317000	-0.322000	-2.977000

C	-2.641000	0.983000	-4.080000
H	-2.339000	0.594000	-5.050000
C	-3.596000	2.000000	-3.998000
H	-4.040000	2.409000	-4.902000
C	-3.982000	2.483000	-2.743000
H	-4.729000	3.270000	-2.667000
C	-3.413000	1.955000	-1.583000
H	-3.728000	2.338000	-0.618000
C	-2.435000	0.948000	-1.655000
C	-1.203000	2.906000	0.544000
H	-1.082000	3.073000	-0.521000
C	-0.980000	3.969000	1.424000
H	-0.688000	4.936000	1.025000
C	-1.126000	3.788000	2.802000
H	-0.959000	4.617000	3.485000
C	-1.481000	2.528000	3.294000
H	-1.588000	2.367000	4.364000
C	-1.684000	1.463000	2.416000
H	-1.940000	0.490000	2.818000
C	-1.566000	1.638000	1.025000
C	-3.271000	-0.660000	0.507000
C	-4.222000	0.037000	1.271000
H	-4.059000	1.082000	1.513000
C	-5.382000	-0.579000	1.742000
H	-6.093000	-0.010000	2.336000
C	-5.615000	-1.922000	1.447000
H	-6.506000	-2.424000	1.815000
C	-4.694000	-2.617000	0.663000
H	-4.883000	-3.660000	0.417000
C	-3.528000	-2.010000	0.171000
C	-2.649000	-2.831000	-0.756000
H	-3.105000	-3.833000	-0.840000
C	-0.569000	-4.017000	-1.039000
H	-0.516000	-3.791000	-2.118000
H	-1.096000	-4.985000	-0.940000
C	0.830000	-4.172000	-0.457000
H	0.747000	-4.469000	0.591000
H	1.400000	-4.943000	-0.995000
C	2.429000	-2.701000	-1.663000
H	1.777000	-2.453000	-2.507000
C	3.517000	-1.651000	-1.512000
C	4.761000	-1.980000	-2.084000
H	4.878000	-2.950000	-2.562000
C	5.844000	-1.104000	-2.056000
H	6.788000	-1.391000	-2.512000
C	5.704000	0.136000	-1.428000
H	6.537000	0.833000	-1.385000
C	4.483000	0.472000	-0.850000
H	4.386000	1.434000	-0.358000
C	3.374000	-0.394000	-0.883000
C	1.688000	1.905000	-0.784000
C	1.006000	2.023000	-2.006000
H	0.577000	1.136000	-2.458000
C	0.845000	3.266000	-2.620000

H	0.298000	3.334000	-3.557000
C	1.365000	4.417000	-2.018000
H	1.230000	5.389000	-2.486000
C	2.057000	4.309000	-0.808000
H	2.465000	5.198000	-0.331000
C	2.222000	3.062000	-0.197000
H	2.752000	3.002000	0.748000
C	2.394000	0.451000	1.671000
C	3.381000	-0.382000	2.225000
H	3.924000	-1.079000	1.591000
C	3.684000	-0.324000	3.588000
H	4.450000	-0.979000	3.996000
C	3.008000	0.570000	4.422000
H	3.243000	0.615000	5.483000
C	2.024000	1.404000	3.881000
H	1.484000	2.103000	4.516000
C	1.717000	1.340000	2.521000
H	0.944000	1.985000	2.123000
H	0.120000	-0.986000	-1.844000
H	-2.686000	-2.396000	-1.771000
O	-0.158000	-2.413000	1.761000
C	-0.700000	-1.975000	2.983000
H	-0.143000	-1.102000	3.350000
H	-1.762000	-1.693000	2.883000
H	-0.635000	-2.768000	3.748000
H	-0.919000	-2.880000	0.964000
H	2.138000	-2.834000	0.366000
H	2.921000	-3.657000	-1.896000

TS_{5a-6a}

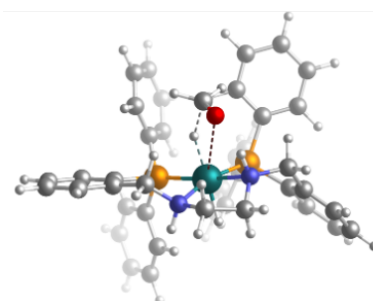


Ru	0.059000	-1.257000	-0.260000
P	-1.720000	0.177000	-0.114000
P	1.797000	0.199000	-0.064000
N	1.563000	-2.870000	-0.477000
N	-1.265000	-2.956000	-0.317000
C	-2.066000	0.462000	-2.916000
H	-1.317000	-0.322000	-2.977000
C	-2.641000	0.983000	-4.080000
H	-2.339000	0.594000	-5.050000
C	-3.596000	2.000000	-3.998000
H	-4.040000	2.409000	-4.902000

C	-3.982000	2.483000	-2.743000
H	-4.729000	3.270000	-2.667000
C	-3.413000	1.955000	-1.583000
H	-3.728000	2.338000	-0.618000
C	-2.435000	0.948000	-1.655000
C	-1.203000	2.906000	0.544000
H	-1.082000	3.073000	-0.521000
C	-0.980000	3.969000	1.424000
H	-0.688000	4.936000	1.025000
C	-1.126000	3.788000	2.802000
H	-0.959000	4.617000	3.485000
C	-1.481000	2.528000	3.294000
H	-1.588000	2.367000	4.364000
C	-1.684000	1.463000	2.416000
H	-1.940000	0.490000	2.818000
C	-1.566000	1.638000	1.025000
C	-3.271000	-0.660000	0.507000
C	-4.222000	0.037000	1.271000
H	-4.059000	1.082000	1.513000
C	-5.382000	-0.579000	1.742000
H	-6.093000	-0.010000	2.336000
C	-5.615000	-1.922000	1.447000
H	-6.506000	-2.424000	1.815000
C	-4.694000	-2.617000	0.663000
H	-4.883000	-3.660000	0.417000
C	-3.528000	-2.010000	0.171000
C	-2.649000	-2.831000	-0.756000
H	-3.105000	-3.833000	-0.840000
C	-0.569000	-4.017000	-1.039000
H	-0.516000	-3.791000	-2.118000
H	-1.096000	-4.985000	-0.940000
C	0.830000	-4.172000	-0.457000
H	0.747000	-4.469000	0.591000
H	1.400000	-4.943000	-0.995000
C	2.429000	-2.701000	-1.663000
H	1.777000	-2.453000	-2.507000
C	3.517000	-1.651000	-1.512000
C	4.761000	-1.980000	-2.084000
H	4.878000	-2.950000	-2.562000
C	5.844000	-1.104000	-2.056000
H	6.788000	-1.391000	-2.512000
C	5.704000	0.136000	-1.428000
H	6.537000	0.833000	-1.385000
C	4.483000	0.472000	-0.850000
H	4.386000	1.434000	-0.358000
C	3.374000	-0.394000	-0.883000
C	1.688000	1.905000	-0.784000
C	1.006000	2.023000	-2.006000
H	0.577000	1.136000	-2.458000
C	0.845000	3.266000	-2.620000
H	0.298000	3.334000	-3.557000
C	1.365000	4.417000	-2.018000
H	1.230000	5.389000	-2.486000
C	2.057000	4.309000	-0.808000

H	2.465000	5.198000	-0.331000
C	2.222000	3.062000	-0.197000
H	2.752000	3.002000	0.748000
C	2.394000	0.451000	1.671000
C	3.381000	-0.382000	2.225000
H	3.924000	-1.079000	1.591000
C	3.684000	-0.324000	3.588000
H	4.450000	-0.979000	3.996000
C	3.008000	0.570000	4.422000
H	3.243000	0.615000	5.483000
C	2.024000	1.404000	3.881000
H	1.484000	2.103000	4.516000
C	1.717000	1.340000	2.521000
H	0.944000	1.985000	2.123000
H	0.120000	-0.986000	-1.844000
H	-2.686000	-2.396000	-1.771000
O	-0.158000	-2.413000	1.761000
C	-0.700000	-1.975000	2.983000
H	-0.143000	-1.102000	3.350000
H	-1.762000	-1.693000	2.883000
H	-0.635000	-2.768000	3.748000
H	-0.919000	-2.880000	0.964000
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H	2.921000	-3.657000	-1.896000

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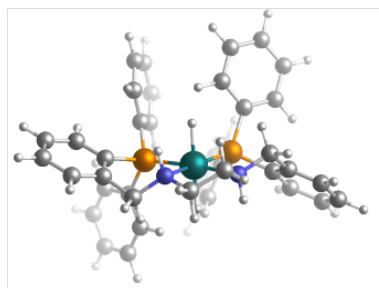


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N	1.533000	-2.771000	-0.516000
N	-1.224000	-2.824000	-1.075000
C	1.481000	2.146000	-0.440000
C	0.754000	2.480000	-1.594000
H	0.415000	1.687000	-2.250000
C	0.443000	3.810000	-1.881000
H	-0.146000	4.043000	-2.764000
C	0.861000	4.828000	-1.016000
H	0.607000	5.863000	-1.227000
C	1.604000	4.506000	0.124000
H	1.937000	5.292000	0.799000
C	1.916000	3.173000	0.410000
H	2.477000	2.936000	1.309000
C	2.583000	0.404000	1.558000

C	3.976000	0.486000	1.704000
H	4.613000	0.513000	0.823000
C	4.554000	0.533000	2.977000
H	5.636000	0.586000	3.077000
C	3.744000	0.517000	4.117000
H	4.193000	0.558000	5.106000
C	2.353000	0.445000	3.978000
H	1.714000	0.435000	4.858000
C	1.777000	0.377000	2.708000
H	0.700000	0.294000	2.602000
C	3.112000	-0.095000	-1.252000
C	3.712000	0.862000	-2.081000
H	3.426000	1.905000	-1.994000
C	4.674000	0.502000	-3.031000
H	5.121000	1.266000	-3.662000
C	5.053000	-0.833000	-3.163000
H	5.794000	-1.128000	-3.902000
C	4.475000	-1.794000	-2.328000
H	4.779000	-2.835000	-2.415000
C	3.514000	-1.446000	-1.373000
C	2.989000	-2.518000	-0.442000
H	3.538000	-3.455000	-0.619000
H	3.186000	-2.225000	0.596000
C	1.090000	-3.603000	-1.652000
C	-0.356000	-4.006000	-1.368000
C	-2.317000	-3.209000	-0.158000
H	-2.741000	-4.172000	-0.480000
C	-3.467000	-2.227000	-0.016000
C	-4.742000	-2.820000	0.075000
H	-4.827000	-3.898000	-0.047000
C	-5.892000	-2.077000	0.329000
H	-6.857000	-2.573000	0.395000
C	-5.787000	-0.695000	0.494000
H	-6.668000	-0.091000	0.700000
C	-4.538000	-0.091000	0.382000
H	-4.472000	0.985000	0.505000
C	-3.364000	-0.824000	0.125000
C	-1.744000	1.099000	1.541000
C	-2.106000	0.450000	2.733000
H	-2.535000	-0.547000	2.696000
C	-1.905000	1.065000	3.971000
H	-2.191000	0.546000	4.882000
C	-1.330000	2.340000	4.038000
H	-1.165000	2.815000	5.002000
C	-0.966000	2.992000	2.858000
H	-0.507000	3.977000	2.894000
C	-1.171000	2.378000	1.620000
H	-0.864000	2.896000	0.718000
C	-2.353000	1.401000	-1.311000
C	-3.020000	2.598000	-1.010000
H	-3.204000	2.881000	0.022000
C	-3.442000	3.458000	-2.029000
H	-3.945000	4.387000	-1.773000
C	-3.216000	3.128000	-3.368000

H	-3.543000	3.797000	-4.160000
C	-2.560000	1.932000	-3.680000
H	-2.371000	1.667000	-4.717000
C	-2.129000	1.082000	-2.659000
H	-1.571000	0.180000	-2.898000
O	0.573000	-4.000000	1.880000
C	0.285000	-2.939000	2.468000
H	-0.712000	-2.790000	2.919000
H	1.065000	-2.247000	2.821000
H	-0.194000	-1.604000	1.257000
H	0.222000	-0.789000	-2.032000
H	-0.772000	-4.595000	-2.197000
H	1.187000	-3.024000	-2.573000
H	-0.364000	-4.634000	-0.471000
H	1.700000	-4.518000	-1.740000
H	1.307000	-3.297000	0.342000
H	-1.621000	-2.485000	-1.950000
H	-1.846000	-3.375000	0.816000

7a

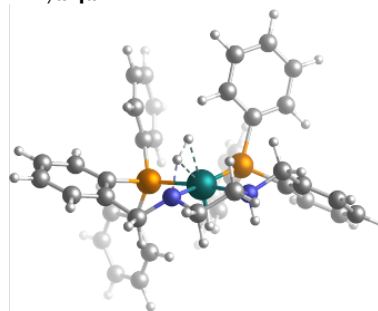


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N	1.439000	-3.076000	-0.003000
H	1.521000	-3.245000	-1.006000
N	-1.399000	-3.076000	0.369000
C	1.543000	1.620000	-1.122000
C	0.848000	1.502000	-2.336000
H	0.503000	0.521000	-2.646000
C	0.566000	2.627000	-3.111000
H	-0.002000	2.517000	-4.032000
C	0.982000	3.893000	-2.684000
H	0.750000	4.774000	-3.278000
C	1.688000	4.020000	-1.485000
H	2.012000	5.000000	-1.143000
C	1.968000	2.891000	-0.707000
H	2.492000	3.012000	0.234000
C	2.554000	0.728000	1.428000
C	3.900000	1.131000	1.452000
H	4.513000	1.040000	0.559000
C	4.468000	1.653000	2.617000
H	5.513000	1.953000	2.621000

C	3.693000	1.788000	3.775000
H	4.133000	2.197000	4.681000
C	2.354000	1.389000	3.759000
H	1.741000	1.489000	4.652000
C	1.792000	0.854000	2.596000
H	0.766000	0.507000	2.592000
C	3.211000	-0.739000	-0.904000
C	3.963000	-0.104000	-1.903000
H	3.670000	0.883000	-2.246000
C	5.089000	-0.713000	-2.465000
H	5.655000	-0.195000	-3.235000
C	5.485000	-1.977000	-2.029000
H	6.361000	-2.460000	-2.454000
C	4.736000	-2.627000	-1.043000
H	5.034000	-3.619000	-0.710000
C	3.604000	-2.029000	-0.474000
C	2.798000	-2.820000	0.536000
H	3.313000	-3.771000	0.740000
H	2.673000	-2.289000	1.487000
C	0.753000	-4.223000	0.617000
H	0.720000	-4.042000	1.698000
H	1.296000	-5.166000	0.439000
C	-0.660000	-4.313000	0.050000
H	-0.620000	-4.395000	-1.043000
H	-1.178000	-5.204000	0.440000
C	-2.703000	-2.985000	-0.324000
H	-3.178000	-3.978000	-0.367000
C	-3.651000	-2.033000	0.378000
C	-4.903000	-2.540000	0.761000
H	-5.133000	-3.584000	0.558000
C	-5.859000	-1.740000	1.389000
H	-6.820000	-2.161000	1.674000
C	-5.564000	-0.400000	1.643000
H	-6.294000	0.245000	2.125000
C	-4.322000	0.115000	1.270000
H	-4.113000	1.161000	1.470000
C	-3.344000	-0.678000	0.647000
C	-1.528000	1.530000	1.228000
C	-1.691000	1.353000	2.613000
H	-2.038000	0.397000	2.995000
C	-1.390000	2.382000	3.505000
H	-1.528000	2.226000	4.573000
C	-0.893000	3.601000	3.031000
H	-0.642000	4.398000	3.726000
C	-0.708000	3.780000	1.658000
H	-0.306000	4.715000	1.275000
C	-1.029000	2.755000	0.763000
H	-0.871000	2.913000	-0.299000
C	-2.403000	0.863000	-1.472000
C	-3.214000	2.010000	-1.463000
H	-3.420000	2.527000	-0.530000
C	-3.758000	2.510000	-2.648000
H	-4.372000	3.407000	-2.622000
C	-3.517000	1.858000	-3.862000

H	-3.942000	2.247000	-4.785000
C	-2.731000	0.703000	-3.878000
H	-2.539000	0.185000	-4.816000
C	-2.177000	0.212000	-2.692000
H	-1.540000	-0.670000	-2.699000
H	-0.093000	-1.638000	-1.655000
H	-2.491000	-2.669000	-1.352000
H	0.099000	-1.396000	1.767000
H	-1.559000	-3.039000	1.376000

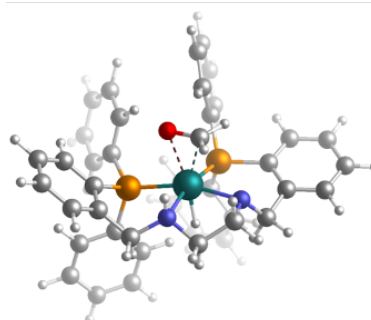
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P	-1.737000	-0.119000	-0.088000
P	1.771000	-0.066000	0.007000
N	-1.463000	3.042000	-0.240000
H	-1.525000	3.153000	-1.253000
N	1.335000	3.104000	0.204000
C	-1.546000	-1.755000	-0.930000
C	-0.838000	-1.768000	-2.143000
H	-0.476000	-0.831000	-2.552000
C	-0.562000	-2.969000	-2.797000
H	0.014000	-2.957000	-3.718000
C	-0.999000	-4.180000	-2.248000
H	-0.773000	-5.119000	-2.747000
C	-1.719000	-4.177000	-1.050000
H	-2.059000	-5.113000	-0.615000
C	-1.991000	-2.972000	-0.393000
H	-2.526000	-2.990000	0.551000
C	-2.523000	-0.579000	1.533000
C	-3.874000	-0.951000	1.646000
H	-4.511000	-0.963000	0.766000
C	-4.412000	-1.304000	2.887000
H	-5.460000	-1.585000	2.960000
C	-3.605000	-1.295000	4.030000
H	-4.024000	-1.571000	4.995000
C	-2.262000	-0.923000	3.926000
H	-1.626000	-0.911000	4.807000
C	-1.728000	-0.560000	2.686000
H	-0.692000	-0.250000	2.612000
C	-3.220000	0.599000	-0.956000
C	-3.964000	-0.140000	-1.887000
H	-3.669000	-1.158000	-2.122000
C	-5.086000	0.406000	-2.518000

H	-5.646000	-0.191000	-3.234000
C	-5.483000	1.709000	-2.223000
H	-6.354000	2.145000	-2.705000
C	-4.744000	2.459000	-1.303000
H	-5.046000	3.480000	-1.078000
C	-3.617000	1.925000	-0.664000
C	-2.834000	2.812000	0.281000
H	-3.361000	3.772000	0.391000
H	-2.736000	2.372000	1.280000
C	-0.809000	4.247000	0.316000
H	-0.817000	4.154000	1.407000
H	-1.363000	5.158000	0.040000
C	0.625000	4.299000	-0.201000
H	0.599000	4.394000	-1.308000
H	1.115000	5.213000	0.183000
C	2.682000	3.054000	-0.326000
H	3.137000	4.057000	-0.264000
C	3.619000	2.097000	0.392000
C	4.845000	2.615000	0.842000
H	5.040000	3.678000	0.714000
C	5.816000	1.812000	1.440000
H	6.752000	2.250000	1.777000
C	5.572000	0.447000	1.598000
H	6.316000	-0.201000	2.054000
C	4.357000	-0.083000	1.168000
H	4.176000	-1.144000	1.306000
C	3.365000	0.719000	0.576000
C	1.567000	-1.446000	1.225000
C	1.737000	-1.177000	2.596000
H	2.090000	-0.200000	2.913000
C	1.447000	-2.147000	3.556000
H	1.589000	-1.919000	4.609000
C	0.963000	-3.401000	3.165000
H	0.726000	-4.153000	3.913000
C	0.778000	-3.673000	1.809000
H	0.390000	-4.637000	1.489000
C	1.080000	-2.705000	0.845000
H	0.921000	-2.937000	-0.202000
C	2.401000	-0.901000	-1.531000
C	3.191000	-2.062000	-1.498000
H	3.412000	-2.546000	-0.552000
C	3.690000	-2.619000	-2.677000
H	4.288000	-3.526000	-2.632000
C	3.425000	-2.012000	-3.909000
H	3.815000	-2.445000	-4.827000
C	2.661000	-0.842000	-3.950000
H	2.454000	-0.358000	-4.902000
C	2.152000	-0.293000	-2.770000
H	1.540000	0.603000	-2.802000
H	-0.049000	1.339000	-1.702000
H	2.660000	2.797000	-1.406000
H	0.260000	1.793000	1.835000
H	0.845000	2.443000	1.340000

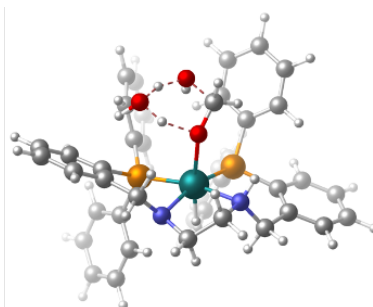
8a



Ru	0.029000	-1.273000	0.475000
P	-1.746000	0.241000	0.005000
P	1.834000	0.110000	0.043000
N	-1.489000	-2.902000	0.602000
H	-1.590000	-3.097000	1.602000
N	1.367000	-2.991000	0.439000
C	-1.636000	2.039000	0.397000
C	-1.052000	2.386000	1.627000
H	-0.736000	1.600000	2.305000
C	-0.864000	3.727000	1.965000
H	-0.389000	3.978000	2.909000
C	-1.250000	4.736000	1.078000
H	-1.088000	5.780000	1.335000
C	-1.839000	4.398000	-0.145000
H	-2.141000	5.177000	-0.840000
C	-2.034000	3.056000	-0.484000
H	-2.476000	2.806000	-1.443000
C	-2.418000	0.226000	-1.721000
C	-3.778000	0.479000	-1.973000
H	-4.458000	0.666000	-1.146000
C	-4.270000	0.489000	-3.281000
H	-5.325000	0.681000	-3.458000
C	-3.407000	0.250000	-4.356000
H	-3.789000	0.257000	-5.374000
C	-2.053000	0.000000	-4.114000
H	-1.372000	-0.184000	-4.940000
C	-1.562000	-0.017000	-2.806000
H	-0.514000	-0.225000	-2.630000
C	-3.234000	-0.304000	0.967000
C	-3.969000	0.573000	1.773000
H	-3.686000	1.619000	1.831000
C	-5.072000	0.125000	2.508000
H	-5.627000	0.825000	3.127000
C	-5.454000	-1.214000	2.440000
H	-6.309000	-1.574000	3.007000
C	-4.725000	-2.097000	1.637000
H	-5.022000	-3.142000	1.582000
C	-3.618000	-1.663000	0.900000
C	-2.854000	-2.668000	0.067000

H	-3.411000	-3.617000	0.046000
H	-2.741000	-2.335000	-0.970000
C	-0.835000	-4.076000	-0.036000
H	-0.792000	-3.877000	-1.111000
H	-1.434000	-4.988000	0.133000
C	0.572000	-4.198000	0.555000
H	0.448000	-4.464000	1.623000
H	1.076000	-5.063000	0.092000
C	2.301000	-3.014000	-0.671000
H	2.669000	-4.043000	-0.818000
C	3.524000	-2.155000	-0.390000
C	4.787000	-2.760000	-0.484000
H	4.840000	-3.813000	-0.752000
C	5.968000	-2.061000	-0.230000
H	6.928000	-2.567000	-0.307000
C	5.901000	-0.717000	0.138000
H	6.806000	-0.154000	0.351000
C	4.657000	-0.094000	0.234000
H	4.624000	0.949000	0.525000
C	3.462000	-0.786000	-0.033000
C	1.743000	0.879000	-1.642000
C	2.277000	0.219000	-2.760000
H	2.853000	-0.692000	-2.630000
C	2.072000	0.722000	-4.049000
H	2.492000	0.195000	-4.902000
C	1.336000	1.895000	-4.240000
H	1.175000	2.284000	-5.243000
C	0.809000	2.564000	-3.132000
H	0.230000	3.475000	-3.264000
C	1.009000	2.059000	-1.846000
H	0.586000	2.588000	-1.000000
C	2.237000	1.567000	1.125000
C	2.857000	2.734000	0.646000
H	3.094000	2.832000	-0.409000
C	3.180000	3.782000	1.512000
H	3.653000	4.678000	1.118000
C	2.904000	3.675000	2.879000
H	3.159000	4.488000	3.554000
C	2.294000	2.517000	3.367000
H	2.065000	2.423000	4.426000
C	1.957000	1.477000	2.497000
H	1.433000	0.614000	2.886000
O	-0.387000	-0.751000	2.688000
C	0.482000	-1.678000	2.658000
H	0.073000	-1.578000	-1.088000
H	1.554000	-1.467000	2.771000
H	0.192000	-2.717000	2.866000
H	1.861000	-2.714000	-1.647000

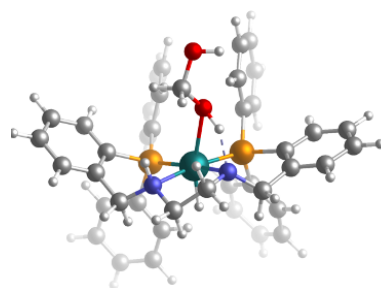
TS_{8a-9a}



Ru	-0.021000	-1.129000	-0.458000
P	1.859000	0.122000	-0.118000
P	-1.722000	0.350000	-0.210000
N	-1.611000	-2.311000	-1.328000
N	1.232000	-2.894000	-1.004000
C	3.616000	-0.372000	2.118000
H	4.175000	-1.044000	1.474000
C	3.975000	-0.267000	3.466000
H	4.805000	-0.859000	3.846000
C	3.276000	0.588000	4.321000
H	3.556000	0.667000	5.369000
C	2.210000	1.340000	3.816000
H	1.650000	2.009000	4.464000
C	1.846000	1.227000	2.473000
H	1.019000	1.820000	2.099000
C	2.546000	0.375000	1.596000
C	1.160000	2.091000	-1.994000
H	0.642000	1.268000	-2.473000
C	1.082000	3.370000	-2.548000
H	0.515000	3.521000	-3.463000
C	1.703000	4.450000	-1.913000
H	1.632000	5.450000	-2.334000
C	2.417000	4.233000	-0.730000
H	2.907000	5.064000	-0.228000
C	2.499000	2.950000	-0.182000
H	3.048000	2.811000	0.744000
C	1.862000	1.862000	-0.798000
C	3.370000	-0.556000	-0.999000
C	4.560000	0.190000	-0.897000
H	4.552000	1.118000	-0.335000
C	5.752000	-0.223000	-1.487000
H	6.649000	0.383000	-1.385000
C	5.777000	-1.421000	-2.203000
H	6.696000	-1.772000	-2.666000
C	4.607000	-2.167000	-2.323000
H	4.631000	-3.096000	-2.889000
C	3.388000	-1.757000	-1.747000
C	2.191000	-2.630000	-2.094000
H	1.629000	-2.158000	-2.907000
C	0.245000	-3.964000	-1.349000
H	-0.103000	-4.381000	-0.400000
H	0.736000	-4.765000	-1.928000
C	-0.942000	-3.341000	-2.103000
H	-0.572000	-2.901000	-3.043000

H	-1.636000	-4.154000	-2.391000
C	-2.608000	-2.857000	-0.448000
H	-3.244000	-3.567000	-1.011000
C	-3.570000	-1.838000	0.155000
C	-4.807000	-2.347000	0.601000
H	-4.991000	-3.415000	0.496000
C	-5.792000	-1.536000	1.155000
H	-6.733000	-1.968000	1.484000
C	-5.564000	-0.159000	1.267000
H	-6.326000	0.498000	1.678000
C	-4.346000	0.363000	0.843000
H	-4.178000	1.432000	0.933000
C	-3.325000	-0.453000	0.310000
C	-1.531000	1.713000	1.045000
C	-1.821000	1.486000	2.403000
H	-2.317000	0.569000	2.705000
C	-1.515000	2.435000	3.382000
H	-1.753000	2.228000	4.422000
C	-0.910000	3.643000	3.022000
H	-0.671000	4.385000	3.780000
C	-0.616000	3.885000	1.677000
H	-0.135000	4.813000	1.378000
C	-0.917000	2.930000	0.702000
H	-0.657000	3.138000	-0.329000
C	-2.331000	1.237000	-1.728000
C	-2.961000	2.490000	-1.701000
H	-3.092000	3.021000	-0.763000
C	-3.424000	3.082000	-2.880000
H	-3.898000	4.060000	-2.841000
C	-3.279000	2.418000	-4.102000
H	-3.637000	2.878000	-5.020000
C	-2.684000	1.152000	-4.132000
H	-2.587000	0.618000	-5.074000
C	-2.215000	0.563000	-2.955000
H	-1.782000	-0.432000	-2.964000
O	-0.127000	-2.595000	1.595000
C	0.588000	-2.322000	2.680000
H	0.119000	-0.571000	-1.942000
H	0.582000	-3.102000	3.456000
H	1.596000	-1.936000	2.504000
H	-2.203000	-3.465000	0.394000
O	-0.097000	-1.148000	3.506000
H	-1.264000	-1.477000	3.331000
O	-2.154000	-2.189000	2.900000
H	-1.459000	-2.564000	2.158000
H	-2.848000	-1.713000	2.406000
H	0.081000	-0.322000	3.012000
H	1.741000	-3.184000	-0.170000
H	2.576000	-3.586000	-2.482000

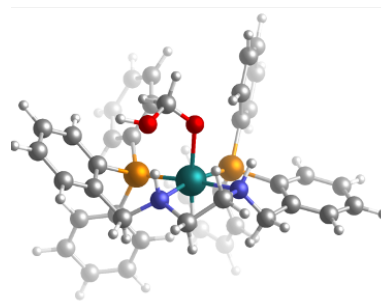
9a



Ru	0.033000	-1.070000	-0.601000
P	-1.765000	0.220000	0.051000
P	1.728000	0.407000	-0.166000
N	-1.384000	-2.650000	-1.292000
H	-1.444000	-3.338000	-0.537000
N	1.436000	-2.579000	-1.277000
C	-1.676000	1.363000	1.503000
C	-1.112000	0.847000	2.682000
H	-0.766000	-0.182000	2.704000
C	-0.977000	1.647000	3.816000
H	-0.530000	1.232000	4.714000
C	-1.376000	2.987000	3.781000
H	-1.251000	3.616000	4.659000
C	-1.919000	3.516000	2.608000
H	-2.224000	4.560000	2.569000
C	-2.076000	2.707000	1.477000
H	-2.507000	3.132000	0.576000
C	-2.634000	1.261000	-1.227000
C	-3.986000	1.622000	-1.084000
H	-4.549000	1.285000	-0.218000
C	-4.621000	2.411000	-2.047000
H	-5.667000	2.678000	-1.921000
C	-3.911000	2.853000	-3.169000
H	-4.404000	3.467000	-3.919000
C	-2.569000	2.498000	-3.322000
H	-2.006000	2.836000	-4.189000
C	-1.937000	1.703000	-2.360000
H	-0.900000	1.417000	-2.490000
C	-3.189000	-0.893000	0.527000
C	-3.922000	-0.721000	1.710000
H	-3.671000	0.090000	2.385000
C	-4.983000	-1.571000	2.039000
H	-5.534000	-1.411000	2.962000
C	-5.333000	-2.611000	1.179000
H	-6.157000	-3.278000	1.423000
C	-4.609000	-2.794000	-0.003000
H	-4.877000	-3.607000	-0.676000
C	-3.543000	-1.953000	-0.342000
C	-2.772000	-2.236000	-1.614000
H	-3.282000	-3.032000	-2.178000
H	-2.708000	-1.357000	-2.264000
C	-0.672000	-3.287000	-2.425000
H	-0.597000	-2.546000	-3.226000
H	-1.232000	-4.163000	-2.798000

C	0.710000	-3.689000	-1.911000
H	0.559000	-4.501000	-1.177000
H	1.285000	-4.137000	-2.735000
C	2.545000	-2.108000	-2.104000
H	3.025000	-2.965000	-2.604000
C	3.642000	-1.388000	-1.339000
C	4.959000	-1.843000	-1.521000
H	5.128000	-2.714000	-2.151000
C	6.051000	-1.214000	-0.923000
H	7.056000	-1.595000	-1.087000
C	5.839000	-0.096000	-0.113000
H	6.674000	0.412000	0.361000
C	4.538000	0.360000	0.093000
H	4.383000	1.222000	0.734000
C	3.430000	-0.268000	-0.505000
C	1.716000	1.955000	-1.180000
C	2.562000	2.111000	-2.288000
H	3.311000	1.357000	-2.509000
C	2.452000	3.235000	-3.114000
H	3.114000	3.337000	-3.971000
C	1.503000	4.223000	-2.838000
H	1.421000	5.098000	-3.479000
C	0.658000	4.077000	-1.734000
H	-0.092000	4.833000	-1.513000
C	0.759000	2.949000	-0.919000
H	0.083000	2.843000	-0.076000
C	1.991000	1.011000	1.573000
C	2.204000	2.348000	1.936000
H	2.184000	3.132000	1.187000
C	2.459000	2.691000	3.269000
H	2.613000	3.734000	3.532000
C	2.525000	1.701000	4.251000
H	2.731000	1.969000	5.285000
C	2.318000	0.363000	3.896000
H	2.359000	-0.418000	4.652000
C	2.045000	0.021000	2.571000
H	1.858000	-1.015000	2.308000
O	1.023000	-4.022000	3.069000
C	0.367000	-3.742000	1.844000
H	-0.103000	-0.408000	-2.035000
H	2.190000	-1.446000	-2.916000
H	1.975000	-4.078000	2.885000
H	-0.675000	-3.550000	2.121000
H	0.420000	-4.617000	1.175000
O	0.906000	-2.617000	1.211000
H	1.391000	-2.809000	0.302000

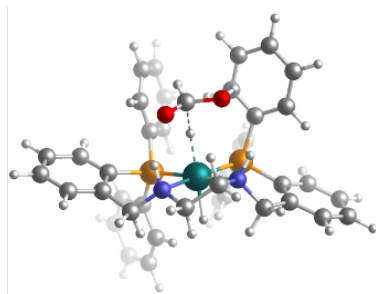
10a



Ru	0.041000	1.182000	-0.342000
P	1.649000	-0.417000	-0.072000
P	-1.832000	-0.091000	-0.029000
N	1.607000	2.624000	-0.898000
H	1.840000	3.035000	0.023000
N	-1.223000	2.949000	-0.692000
C	1.445000	-1.663000	1.278000
C	0.752000	-1.232000	2.420000
H	0.397000	-0.208000	2.471000
C	0.472000	-2.121000	3.460000
H	-0.095000	-1.775000	4.320000
C	0.883000	-3.454000	3.370000
H	0.650000	-4.153000	4.170000
C	1.584000	-3.890000	2.240000
H	1.904000	-4.927000	2.162000
C	1.866000	-3.000000	1.199000
H	2.389000	-3.357000	0.318000
C	2.201000	-1.447000	-1.517000
C	3.513000	-1.940000	-1.623000
H	4.248000	-1.700000	-0.860000
C	3.891000	-2.734000	-2.709000
H	4.912000	-3.102000	-2.778000
C	2.959000	-3.051000	-3.703000
H	3.252000	-3.670000	-4.548000
C	1.653000	-2.562000	-3.607000
H	0.919000	-2.801000	-4.372000
C	1.279000	-1.761000	-2.526000
H	0.273000	-1.365000	-2.468000
C	3.266000	0.392000	0.370000
C	4.043000	-0.041000	1.453000
H	3.706000	-0.881000	2.052000
C	5.246000	0.591000	1.781000
H	5.829000	0.238000	2.628000
C	5.692000	1.671000	1.018000
H	6.627000	2.170000	1.260000
C	4.920000	2.116000	-0.059000
H	5.254000	2.973000	-0.641000
C	3.709000	1.498000	-0.393000
C	2.857000	2.101000	-1.493000
H	3.420000	2.914000	-1.976000
H	2.593000	1.372000	-2.267000
C	0.931000	3.654000	-1.703000
H	0.663000	3.224000	-2.674000

H	1.589000	4.521000	-1.876000
C	-0.304000	4.095000	-0.924000
H	0.010000	4.450000	0.062000
H	-0.821000	4.915000	-1.444000
C	-2.227000	2.780000	-1.761000
H	-2.593000	3.767000	-2.081000
C	-3.434000	1.945000	-1.373000
C	-4.680000	2.447000	-1.797000
H	-4.711000	3.402000	-2.316000
C	-5.870000	1.758000	-1.575000
H	-6.813000	2.175000	-1.918000
C	-5.834000	0.535000	-0.901000
H	-6.748000	-0.022000	-0.713000
C	-4.611000	0.036000	-0.460000
H	-4.599000	-0.911000	0.067000
C	-3.397000	0.714000	-0.681000
C	-1.884000	-1.714000	-0.919000
C	-2.380000	-1.792000	-2.231000
H	-2.849000	-0.924000	-2.686000
C	-2.268000	-2.975000	-2.967000
H	-2.658000	-3.015000	-3.981000
C	-1.655000	-4.099000	-2.405000
H	-1.561000	-5.017000	-2.980000
C	-1.160000	-4.031000	-1.100000
H	-0.673000	-4.894000	-0.652000
C	-1.273000	-2.850000	-0.364000
H	-0.874000	-2.816000	0.643000
C	-2.413000	-0.520000	1.688000
C	-3.070000	-1.709000	2.044000
H	-3.255000	-2.479000	1.301000
C	-3.485000	-1.928000	3.360000
H	-3.985000	-2.858000	3.619000
C	-3.258000	-0.956000	4.340000
H	-3.580000	-1.127000	5.364000
C	-2.607000	0.232000	3.993000
H	-2.414000	0.990000	4.749000
C	-2.183000	0.450000	2.679000
H	-1.613000	1.344000	2.431000
C	1.150000	2.458000	2.437000
H	-0.067000	0.754000	-1.910000
H	-1.714000	2.327000	-2.616000
H	1.763000	1.556000	2.651000
O	0.085000	2.238000	1.666000
H	-1.682000	3.100000	0.208000
H	0.878000	2.942000	3.394000
O	2.105000	3.417000	1.776000
H	3.013000	3.161000	2.010000

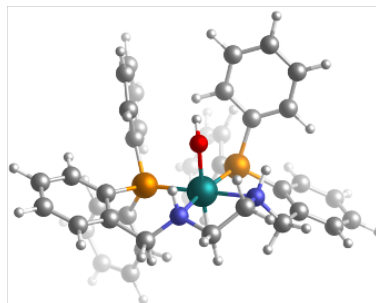
TS_{10a-7a}



Ru	0.065000	-0.998000	-0.639000
P	-1.784000	0.198000	-0.095000
P	1.706000	0.472000	-0.147000
N	1.713000	-2.409000	-1.123000
N	-1.147000	-2.754000	-1.135000
C	-2.104000	1.566000	-2.526000
H	-1.395000	0.820000	-2.880000
C	-2.628000	2.525000	-3.398000
H	-2.337000	2.515000	-4.446000
C	-3.513000	3.498000	-2.924000
H	-3.915000	4.249000	-3.600000
C	-3.883000	3.495000	-1.575000
H	-4.574000	4.244000	-1.197000
C	-3.367000	2.530000	-0.708000
H	-3.669000	2.542000	0.335000
C	-2.460000	1.562000	-1.170000
C	-1.359000	2.291000	1.805000
H	-1.211000	2.957000	0.962000
C	-1.154000	2.778000	3.102000
H	-0.857000	3.814000	3.239000
C	-1.318000	1.939000	4.206000
H	-1.161000	2.320000	5.212000
C	-1.678000	0.600000	4.006000
H	-1.802000	-0.066000	4.857000
C	-1.867000	0.111000	2.714000
H	-2.124000	-0.935000	2.568000
C	-1.723000	0.953000	1.596000
C	-3.337000	-0.840000	0.009000
C	-4.395000	-0.438000	0.843000
H	-4.290000	0.457000	1.447000
C	-5.583000	-1.165000	0.927000
H	-6.379000	-0.826000	1.586000
C	-5.736000	-2.324000	0.165000
H	-6.650000	-2.909000	0.225000
C	-4.699000	-2.729000	-0.675000
H	-4.817000	-3.633000	-1.269000
C	-3.501000	-2.003000	-0.775000
C	-2.464000	-2.507000	-1.759000
H	-2.842000	-3.437000	-2.210000
C	-0.288000	-3.598000	-1.991000
H	-0.215000	-3.114000	-2.970000
H	-0.732000	-4.598000	-2.131000
C	1.080000	-3.741000	-1.339000
H	0.964000	-4.209000	-0.360000

H	1.727000	-4.384000	-1.955000
C	2.537000	-1.991000	-2.276000
H	1.841000	-1.777000	-3.094000
C	3.442000	-0.783000	-2.082000
C	4.621000	-0.802000	-2.851000
H	4.832000	-1.675000	-3.465000
C	5.521000	0.261000	-2.856000
H	6.418000	0.211000	-3.468000
C	5.261000	1.382000	-2.065000
H	5.949000	2.223000	-2.050000
C	4.107000	1.411000	-1.285000
H	3.916000	2.282000	-0.665000
C	3.182000	0.350000	-1.278000
C	1.421000	2.297000	-0.097000
C	0.704000	2.840000	-1.175000
H	0.393000	2.188000	-1.983000
C	0.358000	4.191000	-1.193000
H	-0.222000	4.585000	-2.024000
C	0.734000	5.024000	-0.133000
H	0.456000	6.074000	-0.137000
C	1.468000	4.496000	0.935000
H	1.767000	5.137000	1.761000
C	1.811000	3.140000	0.953000
H	2.365000	2.743000	1.797000
C	2.514000	0.115000	1.493000
C	3.796000	-0.443000	1.615000
H	4.427000	-0.561000	0.740000
C	4.277000	-0.865000	2.863000
H	5.267000	-1.310000	2.934000
C	3.491000	-0.717000	4.009000
H	3.864000	-1.047000	4.975000
C	2.216000	-0.146000	3.899000
H	1.590000	-0.023000	4.780000
C	1.730000	0.253000	2.654000
H	0.729000	0.656000	2.579000
H	0.046000	-0.541000	-2.277000
H	-2.303000	-1.788000	-2.569000
H	0.082000	-1.589000	0.975000
C	0.217000	-3.048000	1.992000
H	-0.080000	-2.363000	2.799000
O	1.586000	-3.216000	1.900000
H	2.022000	-2.442000	2.300000
O	-0.526000	-3.908000	1.524000
H	-1.275000	-3.240000	-0.237000
H	2.301000	-2.500000	-0.293000
H	3.175000	-2.833000	-2.587000

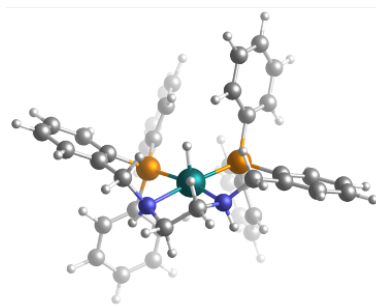
11a



Ru	-0.063000	-1.287000	0.077000
P	1.751000	0.074000	0.037000
P	-1.753000	0.214000	0.121000
N	-1.656000	-2.805000	-0.025000
N	1.215000	-3.048000	-0.043000
C	2.049000	0.471000	2.803000
H	1.370000	-0.375000	2.862000
C	2.551000	1.064000	3.965000
H	2.274000	0.662000	4.937000
C	3.397000	2.173000	3.880000
H	3.782000	2.640000	4.783000
C	3.751000	2.675000	2.623000
H	4.413000	3.534000	2.544000
C	3.257000	2.074000	1.462000
H	3.548000	2.475000	0.496000
C	2.387000	0.975000	1.538000
C	1.274000	2.691000	-1.003000
H	1.110000	3.014000	0.020000
C	1.058000	3.598000	-2.046000
H	0.740000	4.611000	-1.813000
C	1.234000	3.201000	-3.374000
H	1.066000	3.908000	-4.183000
C	1.615000	1.884000	-3.657000
H	1.738000	1.559000	-4.687000
C	1.822000	0.975000	-2.618000
H	2.082000	-0.055000	-2.846000
C	1.670000	1.372000	-1.276000
C	3.340000	-0.817000	-0.398000
C	4.386000	-0.116000	-1.021000
H	4.246000	0.928000	-1.284000
C	5.605000	-0.722000	-1.322000
H	6.391000	-0.148000	-1.806000
C	5.803000	-2.065000	-0.999000
H	6.744000	-2.558000	-1.231000
C	4.776000	-2.775000	-0.377000
H	4.928000	-3.823000	-0.128000
C	3.546000	-2.175000	-0.062000
C	2.518000	-3.034000	0.648000
H	2.916000	-4.058000	0.722000
C	0.370000	-4.195000	0.339000
H	0.247000	-4.173000	1.428000
H	0.849000	-5.152000	0.071000
C	-0.973000	-4.079000	-0.375000

H	-0.801000	-4.043000	-1.454000
H	-1.607000	-4.946000	-0.138000
C	-2.507000	-2.906000	1.172000
H	-1.835000	-3.034000	2.027000
C	-3.432000	-1.730000	1.457000
C	-4.597000	-2.063000	2.173000
H	-4.780000	-3.108000	2.419000
C	-5.519000	-1.102000	2.582000
H	-6.404000	-1.399000	3.138000
C	-5.295000	0.239000	2.262000
H	-6.002000	1.007000	2.565000
C	-4.156000	0.585000	1.539000
H	-3.995000	1.628000	1.285000
C	-3.208000	-0.373000	1.130000
C	-1.507000	1.928000	0.768000
C	-0.803000	2.044000	1.977000
H	-0.481000	1.144000	2.488000
C	-0.485000	3.297000	2.501000
H	0.087000	3.364000	3.423000
C	-0.877000	4.458000	1.823000
H	-0.620000	5.436000	2.221000
C	-1.599000	4.352000	0.631000
H	-1.911000	5.249000	0.100000
C	-1.914000	3.095000	0.106000
H	-2.459000	3.029000	-0.831000
C	-2.561000	0.481000	-1.528000
C	-3.843000	0.008000	-1.848000
H	-4.463000	-0.451000	-1.084000
C	-4.342000	0.126000	-3.151000
H	-5.337000	-0.249000	-3.380000
C	-3.571000	0.724000	-4.150000
H	-3.960000	0.815000	-5.161000
C	-2.292000	1.201000	-3.840000
H	-1.677000	1.666000	-4.606000
C	-1.791000	1.071000	-2.546000
H	-0.794000	1.431000	-2.324000
H	-0.094000	-1.301000	1.731000
H	2.338000	-2.677000	1.668000
H	1.333000	-3.030000	-1.065000
H	-2.201000	-2.528000	-0.843000
H	-3.132000	-3.811000	1.104000
O	-0.044000	-1.812000	-2.061000
H	-0.219000	-1.068000	-2.655000

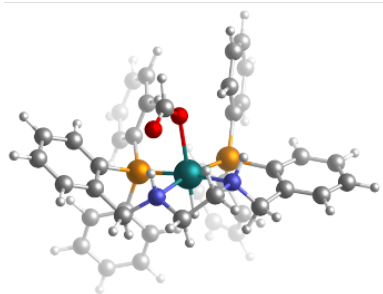
12a



Ru	-0.063000	-1.285000	0.015000
P	1.802000	0.055000	0.049000
P	-1.753000	0.251000	0.086000
N	-1.719000	-2.775000	-0.048000
N	1.175000	-3.118000	-0.085000
C	1.857000	0.598000	2.798000
H	1.211000	-0.271000	2.872000
C	2.248000	1.276000	3.955000
H	1.915000	0.919000	4.927000
C	3.058000	2.411000	3.863000
H	3.358000	2.943000	4.762000
C	3.486000	2.856000	2.608000
H	4.120000	3.735000	2.528000
C	3.104000	2.173000	1.452000
H	3.449000	2.532000	0.487000
C	2.273000	1.044000	1.534000
C	1.289000	2.548000	-1.216000
H	1.041000	2.935000	-0.234000
C	1.104000	3.364000	-2.336000
H	0.724000	4.373000	-2.201000
C	1.395000	2.885000	-3.616000
H	1.252000	3.523000	-4.484000
C	1.873000	1.579000	-3.774000
H	2.105000	1.198000	-4.765000
C	2.057000	0.762000	-2.657000
H	2.432000	-0.249000	-2.794000
C	1.774000	1.239000	-1.364000
C	3.382000	-0.890000	-0.236000
C	4.494000	-0.216000	-0.769000
H	4.407000	0.833000	-1.035000
C	5.713000	-0.862000	-0.975000
H	6.554000	-0.312000	-1.388000
C	5.840000	-2.212000	-0.648000
H	6.781000	-2.732000	-0.806000
C	4.747000	-2.894000	-0.113000
H	4.852000	-3.945000	0.148000
C	3.517000	-2.255000	0.108000
C	2.414000	-3.078000	0.743000
H	2.785000	-4.101000	0.899000
C	0.267000	-4.219000	0.328000
H	0.140000	-4.150000	1.413000
H	0.708000	-5.202000	0.106000
C	-1.075000	-4.078000	-0.382000

H	-0.922000	-4.098000	-1.467000
H	-1.729000	-4.922000	-0.123000
C	-2.473000	-2.819000	1.233000
H	-1.737000	-2.893000	2.040000
C	-3.399000	-1.641000	1.503000
C	-4.555000	-1.955000	2.238000
H	-4.741000	-2.990000	2.515000
C	-5.468000	-0.977000	2.632000
H	-6.348000	-1.256000	3.204000
C	-5.244000	0.354000	2.277000
H	-5.946000	1.130000	2.569000
C	-4.112000	0.682000	1.533000
H	-3.949000	1.718000	1.254000
C	-3.175000	-0.292000	1.141000
C	-1.540000	2.020000	0.521000
C	-0.892000	2.308000	1.733000
H	-0.578000	1.500000	2.384000
C	-0.626000	3.628000	2.096000
H	-0.107000	3.834000	3.029000
C	-1.011000	4.676000	1.252000
H	-0.798000	5.705000	1.529000
C	-1.674000	4.396000	0.054000
H	-1.984000	5.207000	-0.600000
C	-1.939000	3.073000	-0.313000
H	-2.442000	2.869000	-1.253000
C	-2.477000	0.243000	-1.615000
C	-3.775000	-0.216000	-1.893000
H	-4.446000	-0.488000	-1.083000
C	-4.225000	-0.307000	-3.216000
H	-5.234000	-0.656000	-3.417000
C	-3.387000	0.062000	-4.272000
H	-3.741000	-0.004000	-5.297000
C	-2.093000	0.523000	-4.003000
H	-1.436000	0.819000	-4.815000
C	-1.638000	0.604000	-2.686000
H	-0.634000	0.965000	-2.493000
H	-0.024000	-1.356000	1.581000
H	2.126000	-2.680000	1.721000
H	1.466000	-3.293000	-1.051000
H	-2.388000	-2.560000	-0.791000
H	-3.078000	-3.737000	1.259000

13a

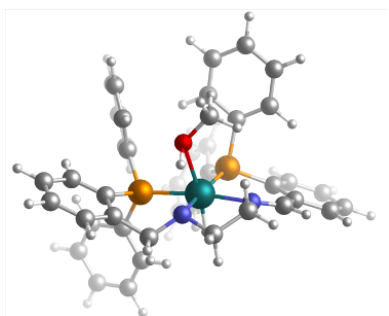


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P	1.817000	0.119000	-0.024000
P	-1.680000	0.393000	-0.043000
N	-1.604000	-2.704000	-0.749000
N	1.248000	-3.008000	-0.589000
C	2.164000	-0.148000	2.728000
H	1.638000	-1.085000	2.572000
C	2.568000	0.210000	4.016000
H	2.397000	-0.478000	4.840000
C	3.171000	1.450000	4.249000
H	3.477000	1.732000	5.253000
C	3.371000	2.329000	3.180000
H	3.834000	3.298000	3.348000
C	2.976000	1.968000	1.889000
H	3.146000	2.665000	1.075000
C	2.365000	0.727000	1.647000
C	1.211000	2.815000	-0.645000
H	0.789000	2.869000	0.352000
C	1.090000	3.915000	-1.496000
H	0.577000	4.807000	-1.145000
C	1.609000	3.863000	-2.792000
H	1.508000	4.717000	-3.457000
C	2.253000	2.702000	-3.230000
H	2.661000	2.649000	-4.236000
C	2.376000	1.601000	-2.377000
H	2.874000	0.704000	-2.734000
C	1.856000	1.643000	-1.074000
C	3.397000	-0.728000	-0.588000
C	4.612000	-0.068000	-0.330000
H	4.598000	0.886000	0.185000
C	5.842000	-0.595000	-0.717000
H	6.758000	-0.050000	-0.501000
C	5.884000	-1.826000	-1.372000
H	6.832000	-2.264000	-1.674000
C	4.691000	-2.498000	-1.632000
H	4.726000	-3.460000	-2.139000
C	3.439000	-1.971000	-1.263000
C	2.231000	-2.792000	-1.676000
H	2.596000	-3.765000	-2.038000
C	0.335000	-4.159000	-0.842000
H	0.039000	-4.559000	0.131000
H	0.852000	-4.949000	-1.405000
C	-0.924000	-3.712000	-1.581000
H	-0.685000	-3.267000	-2.554000
H	-1.573000	-4.587000	-1.752000
C	-2.884000	-2.222000	-1.309000
H	-2.663000	-1.528000	-2.129000
C	-3.711000	-1.571000	-0.217000
C	-4.917000	-2.170000	0.162000
H	-5.248000	-3.067000	-0.357000
C	-5.692000	-1.652000	1.203000
H	-6.622000	-2.139000	1.482000
C	-5.251000	-0.520000	1.888000

H	-5.836000	-0.110000	2.708000	C	-1.124000	2.136000	1.948000
C	-4.048000	0.089000	1.521000	H	-0.846000	2.844000	1.175000
H	-3.715000	0.971000	2.060000	C	-0.900000	2.467000	3.287000
C	-3.271000	-0.416000	0.470000	H	-0.460000	3.431000	3.529000
C	-1.470000	1.717000	1.227000	C	-1.220000	1.562000	4.303000
C	-0.853000	1.335000	2.430000	H	-1.038000	1.820000	5.344000
H	-0.569000	0.297000	2.581000	C	-1.770000	0.319000	3.972000
C	-0.583000	2.287000	3.416000	H	-2.017000	-0.400000	4.749000
H	-0.080000	1.981000	4.329000	C	-1.998000	-0.011000	2.635000
C	-0.926000	3.627000	3.212000	H	-2.430000	-0.978000	2.394000
H	-0.700000	4.370000	3.973000	C	-1.680000	0.893000	1.605000
C	-1.552000	4.011000	2.021000	C	-3.393000	-0.574000	-0.209000
H	-1.822000	5.051000	1.856000	C	-4.463000	-0.098000	0.568000
C	-1.826000	3.060000	1.033000	H	-4.313000	0.755000	1.223000
H	-2.295000	3.372000	0.106000	C	-5.719000	-0.703000	0.531000
C	-2.251000	1.319000	-1.547000	H	-6.526000	-0.317000	1.147000
C	-3.568000	1.801000	-1.658000	C	-5.921000	-1.806000	-0.300000
H	-4.284000	1.613000	-0.862000	H	-6.889000	-2.300000	-0.336000
C	-3.972000	2.516000	-2.788000	C	-4.868000	-2.280000	-1.082000
H	-4.995000	2.878000	-2.859000	H	-5.027000	-3.144000	-1.723000
C	-3.064000	2.762000	-3.824000	C	-3.598000	-1.680000	-1.062000
H	-3.378000	3.318000	-4.704000	C	-2.538000	-2.244000	-1.995000
C	-1.755000	2.283000	-3.723000	H	-2.964000	-3.149000	-2.459000
H	-1.040000	2.469000	-4.520000	C	-0.502000	-3.501000	-2.152000
C	-1.353000	1.562000	-2.596000	H	-0.329000	-3.099000	-3.169000
H	-0.342000	1.180000	-2.533000	H	-1.033000	-4.462000	-2.282000
H	0.054000	-0.848000	-1.818000	C	0.827000	-3.780000	-1.460000
H	-3.454000	-3.064000	-1.731000	H	0.631000	-4.215000	-0.477000
O	-0.233000	-1.952000	2.044000	H	1.439000	-4.487000	-2.040000
C	-0.911000	-2.933000	2.488000	C	2.383000	-2.090000	-2.388000
O	-1.575000	-3.771000	1.834000	H	1.683000	-1.785000	-3.173000
H	-0.895000	-3.046000	3.594000	C	3.383000	-0.967000	-2.144000
H	-1.777000	-3.134000	0.181000	C	4.535000	-1.022000	-2.950000
H	1.700000	-2.311000	-2.502000	H	4.658000	-1.859000	-3.635000
H	1.755000	-3.191000	0.278000	C	5.519000	-0.037000	-2.906000
TS_{13a-4a}				H	6.392000	-0.111000	-3.549000
Ru	0.024000	-1.021000	-0.680000	C	5.374000	1.036000	-2.024000
P	-1.754000	0.301000	-0.146000	H	6.131000	1.814000	-1.967000
P	1.799000	0.292000	-0.072000	C	4.247000	1.098000	-1.207000
N	1.572000	-2.508000	-1.225000	H	4.145000	1.931000	-0.518000
N	-1.280000	-2.577000	-1.334000	C	3.237000	0.118000	-1.249000
C	-1.834000	1.844000	-2.492000	C	1.672000	2.127000	0.088000
H	-1.250000	1.026000	-2.904000	C	1.033000	2.805000	-0.961000
C	-2.197000	2.923000	-3.301000	H	0.691000	2.247000	-1.826000
H	-1.904000	2.933000	-4.349000	C	0.798000	4.178000	-0.885000
C	-2.926000	3.989000	-2.765000	H	0.274000	4.677000	-1.696000
H	-3.203000	4.834000	-3.391000	C	1.209000	4.895000	0.244000
C	-3.304000	3.957000	-1.419000	H	1.015000	5.963000	0.313000
H	-3.877000	4.777000	-0.993000	C	1.866000	4.232000	1.284000
C	-2.950000	2.871000	-0.615000	H	2.193000	4.783000	2.163000
H	-3.258000	2.863000	0.426000	C	2.098000	2.854000	1.208000
C	-2.195000	1.809000	-1.137000	H	2.591000	2.349000	2.032000
				C	2.567000	-0.238000	1.529000
				C	3.848000	-0.801000	1.635000

H	4.495000	-0.859000	0.764000
C	4.312000	-1.288000	2.863000
H	5.307000	-1.723000	2.927000
C	3.506000	-1.210000	4.001000
H	3.868000	-1.588000	4.955000
C	2.227000	-0.651000	3.905000
H	1.583000	-0.595000	4.779000
C	1.758000	-0.183000	2.678000
H	0.753000	0.217000	2.611000
H	0.063000	-0.353000	-2.115000
H	-2.359000	-1.533000	-2.823000
C	-0.625000	-3.044000	2.115000
H	-1.620000	-3.305000	-0.067000
O	-1.188000	-3.448000	3.071000
O	0.211000	-2.489000	1.472000
H	-1.743000	-3.704000	0.751000
H	2.942000	-2.958000	-2.771000
H	2.196000	-2.655000	-0.429000

5b

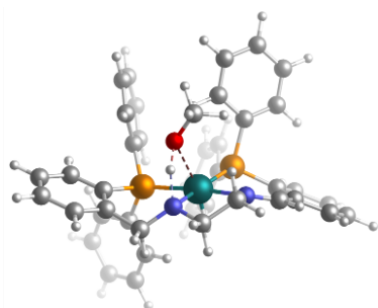


Ru	0.089000	-1.239000	-0.423000
P	-1.768000	0.114000	-0.093000
P	1.764000	0.287000	-0.132000
N	1.544000	-2.696000	-0.879000
N	-1.192000	-2.956000	-0.559000
C	-2.111000	0.815000	-2.800000
H	-1.401000	0.013000	-2.977000
C	-2.661000	1.520000	-3.875000
H	-2.379000	1.255000	-4.891000
C	-3.564000	2.561000	-3.644000
H	-3.987000	3.115000	-4.479000
C	-3.928000	2.881000	-2.331000
H	-4.637000	3.683000	-2.141000
C	-3.386000	2.169000	-1.260000
H	-3.687000	2.424000	-0.248000
C	-2.457000	1.139000	-1.480000
C	-1.311000	2.653000	1.155000
H	-1.220000	3.074000	0.159000
C	-1.108000	3.481000	2.264000
H	-0.867000	4.529000	2.108000
C	-1.206000	2.964000	3.558000
H	-1.054000	3.610000	4.419000

C	-1.486000	1.604000	3.737000
H	-1.545000	1.185000	4.739000
C	-1.673000	0.773000	2.632000
H	-1.852000	-0.287000	2.778000
C	-1.611000	1.293000	1.325000
C	-3.305000	-0.828000	0.365000
C	-4.295000	-0.234000	1.167000
H	-4.149000	0.771000	1.549000
C	-5.469000	-0.910000	1.498000
H	-6.216000	-0.426000	2.122000
C	-5.668000	-2.208000	1.024000
H	-6.572000	-2.756000	1.280000
C	-4.697000	-2.800000	0.218000
H	-4.855000	-3.810000	-0.154000
C	-3.513000	-2.131000	-0.135000
C	-2.550000	-2.836000	-1.072000
H	-2.964000	-3.842000	-1.259000
C	-0.481000	-3.974000	-1.310000
H	-0.460000	-3.762000	-2.399000
H	-0.948000	-4.971000	-1.189000
C	0.951000	-4.045000	-0.801000
H	0.943000	-4.346000	0.254000
H	1.549000	-4.774000	-1.364000
C	2.741000	-2.619000	-1.353000
H	3.223000	-3.552000	-1.665000
C	3.565000	-1.428000	-1.574000
C	4.766000	-1.667000	-2.278000
H	4.993000	-2.681000	-2.599000
C	5.658000	-0.642000	-2.579000
H	6.569000	-0.857000	-3.131000
C	5.367000	0.659000	-2.161000
H	6.050000	1.475000	-2.384000
C	4.193000	0.910000	-1.449000
H	3.987000	1.924000	-1.123000
C	3.275000	-0.106000	-1.146000
C	1.513000	2.074000	-0.550000
C	0.775000	2.336000	-1.715000
H	0.411000	1.504000	-2.308000
C	0.478000	3.645000	-2.097000
H	-0.116000	3.821000	-2.990000
C	0.921000	4.718000	-1.315000
H	0.679000	5.739000	-1.599000
C	1.674000	4.469000	-0.163000
H	2.026000	5.296000	0.448000
C	1.972000	3.156000	0.215000
H	2.551000	2.981000	1.117000
C	2.497000	0.315000	1.572000
C	3.642000	-0.430000	1.898000
H	4.209000	-0.930000	1.118000
C	4.067000	-0.545000	3.225000
H	4.954000	-1.129000	3.457000
C	3.357000	0.089000	4.250000
H	3.687000	-0.001000	5.282000
C	2.218000	0.838000	3.935000

H	1.652000	1.336000	4.718000
C	1.791000	0.943000	2.611000
H	0.899000	1.516000	2.388000
H	0.116000	-0.883000	-1.982000
H	-2.565000	-2.324000	-2.057000
O	-0.362000	-2.081000	1.783000
C	0.652000	-2.628000	2.618000
H	1.441000	-3.123000	2.033000
H	1.106000	-1.799000	3.165000
H	0.227000	-3.345000	3.335000
H	-0.811000	-2.765000	1.192000

TS_{5b-6b}

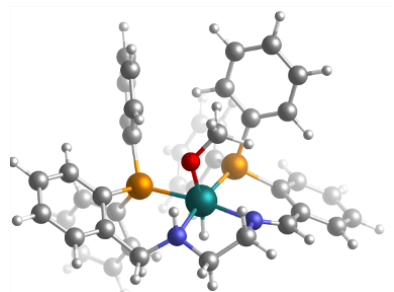


Ru	0.014000	-1.256000	-0.409000
P	-1.756000	0.216000	-0.109000
P	1.779000	0.160000	-0.120000
N	1.391000	-2.808000	-0.761000
N	-1.380000	-2.905000	-0.537000
C	-1.968000	1.026000	-2.788000
H	-1.363000	0.143000	-2.974000
C	-2.399000	1.822000	-3.852000
H	-2.138000	1.545000	-4.871000
C	-3.154000	2.973000	-3.608000
H	-3.482000	3.599000	-4.434000
C	-3.489000	3.312000	-2.293000
H	-4.081000	4.202000	-2.092000
C	-3.068000	2.508000	-1.231000
H	-3.343000	2.784000	-0.218000
C	-2.288000	1.365000	-1.464000
C	-1.079000	2.599000	1.312000
H	-0.893000	3.064000	0.350000
C	-0.812000	3.324000	2.479000
H	-0.429000	4.338000	2.398000
C	-1.023000	2.746000	3.732000
H	-0.815000	3.311000	4.637000
C	-1.495000	1.431000	3.814000
H	-1.652000	0.966000	4.785000
C	-1.754000	0.702000	2.653000
H	-2.078000	-0.332000	2.721000
C	-1.560000	1.285000	1.386000
C	-3.385000	-0.620000	0.228000
C	-4.377000	0.068000	0.947000

H	-4.172000	1.064000	1.326000
C	-5.624000	-0.501000	1.205000
H	-6.369000	0.057000	1.767000
C	-5.897000	-1.788000	0.740000
H	-6.859000	-2.255000	0.938000
C	-4.923000	-2.476000	0.018000
H	-5.138000	-3.480000	-0.343000
C	-3.665000	-1.915000	-0.260000
C	-2.710000	-2.730000	-1.113000
H	-3.177000	-3.717000	-1.269000
C	-0.686000	-4.026000	-1.156000
H	-0.628000	-3.898000	-2.251000
H	-1.207000	-4.982000	-0.965000
C	0.727000	-4.114000	-0.591000
H	0.682000	-4.328000	0.483000
H	1.297000	-4.916000	-1.078000
C	2.604000	-2.823000	-1.198000
H	3.057000	-3.797000	-1.413000
C	3.463000	-1.681000	-1.523000
C	4.625000	-2.005000	-2.256000
H	4.823000	-3.049000	-2.492000
C	5.508000	-1.026000	-2.702000
H	6.388000	-1.306000	-3.275000
C	5.245000	0.314000	-2.410000
H	5.916000	1.096000	-2.755000
C	4.114000	0.649000	-1.660000
H	3.931000	1.693000	-1.428000
C	3.214000	-0.322000	-1.198000
C	1.626000	1.962000	-0.506000
C	0.980000	2.306000	-1.704000
H	0.634000	1.518000	-2.364000
C	0.746000	3.642000	-2.031000
H	0.217000	3.885000	-2.949000
C	1.166000	4.657000	-1.164000
H	0.976000	5.699000	-1.410000
C	1.826000	4.325000	0.023000
H	2.154000	5.108000	0.703000
C	2.054000	2.985000	0.352000
H	2.543000	2.741000	1.290000
C	2.576000	0.179000	1.557000
C	3.953000	0.344000	1.779000
H	4.635000	0.446000	0.940000
C	4.463000	0.378000	3.080000
H	5.532000	0.501000	3.237000
C	3.602000	0.254000	4.176000
H	3.999000	0.284000	5.188000
C	2.231000	0.086000	3.963000
H	1.551000	-0.015000	4.805000
C	1.724000	0.038000	2.662000
H	0.664000	-0.120000	2.500000
H	0.126000	-0.892000	-1.968000
H	-2.629000	-2.272000	-2.115000
O	-0.726000	-2.161000	1.679000
C	0.018000	-2.883000	2.631000

H	1.079000	-2.980000	2.347000
H	-0.010000	-2.366000	3.602000
H	-0.395000	-3.895000	2.783000
H	-1.201000	-2.769000	0.780000

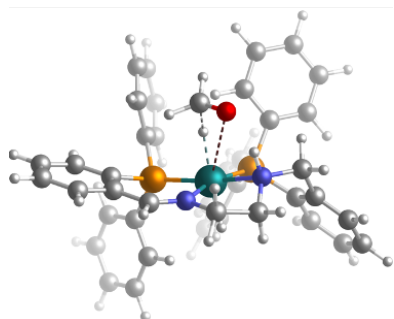
6b



Ru	0.083000	-1.276000	-0.280000
P	-1.743000	0.127000	-0.029000
P	1.770000	0.241000	-0.192000
N	1.486000	-2.794000	-0.549000
N	-1.296000	-2.979000	-0.332000
C	-2.212000	0.598000	-2.767000
H	-1.487000	-0.200000	-2.906000
C	-2.826000	1.195000	-3.871000
H	-2.585000	0.849000	-4.873000
C	-3.740000	2.237000	-3.688000
H	-4.213000	2.708000	-4.546000
C	-4.049000	2.664000	-2.392000
H	-4.766000	3.467000	-2.238000
C	-3.443000	2.058000	-1.290000
H	-3.706000	2.391000	-0.291000
C	-2.502000	1.030000	-1.465000
C	-1.307000	2.750000	1.028000
H	-1.292000	3.117000	0.006000
C	-1.065000	3.643000	2.078000
H	-0.878000	4.690000	1.855000
C	-1.056000	3.190000	3.400000
H	-0.876000	3.887000	4.215000
C	-1.254000	1.829000	3.667000
H	-1.211000	1.461000	4.689000
C	-1.476000	0.931000	2.623000
H	-1.561000	-0.135000	2.815000
C	-1.539000	1.393000	1.294000
C	-3.286000	-0.779000	0.505000
C	-4.224000	-0.155000	1.343000
H	-4.019000	0.836000	1.733000
C	-5.420000	-0.781000	1.699000
H	-6.123000	-0.270000	2.353000
C	-5.701000	-2.058000	1.215000
H	-6.624000	-2.563000	1.486000
C	-4.778000	-2.690000	0.380000
H	-4.992000	-3.689000	0.007000
C	-3.575000	-2.071000	0.009000
C	-2.645000	-2.840000	-0.911000

H	-3.082000	-3.833000	-1.092000
C	-0.537000	-4.128000	-0.845000
H	-0.474000	-4.048000	-1.936000
H	-1.030000	-5.081000	-0.593000
C	0.861000	-4.086000	-0.230000
H	0.776000	-4.146000	0.861000
H	1.466000	-4.929000	-0.591000
C	2.689000	-2.819000	-1.019000
H	3.161000	-3.796000	-1.166000
C	3.511000	-1.683000	-1.434000
C	4.694000	-2.029000	-2.127000
H	4.916000	-3.081000	-2.290000
C	5.570000	-1.063000	-2.611000
H	6.466000	-1.361000	-3.149000
C	5.283000	0.287000	-2.398000
H	5.953000	1.059000	-2.769000
C	4.131000	0.646000	-1.696000
H	3.931000	1.699000	-1.525000
C	3.229000	-0.310000	-1.206000
C	1.493000	1.961000	-0.832000
C	0.695000	2.083000	-1.979000
H	0.310000	1.184000	-2.445000
C	0.373000	3.335000	-2.503000
H	-0.272000	3.401000	-3.376000
C	0.858000	4.495000	-1.889000
H	0.599000	5.474000	-2.285000
C	1.680000	4.386000	-0.764000
H	2.071000	5.281000	-0.284000
C	2.000000	3.129000	-0.241000
H	2.634000	3.068000	0.637000
C	2.584000	0.516000	1.450000
C	3.739000	-0.185000	1.827000
H	4.248000	-0.826000	1.114000
C	4.249000	-0.075000	3.125000
H	5.142000	-0.632000	3.399000
C	3.615000	0.743000	4.064000
H	4.011000	0.827000	5.073000
C	2.464000	1.447000	3.697000
H	1.952000	2.081000	4.416000
C	1.950000	1.327000	2.406000
H	1.049000	1.866000	2.145000
H	0.111000	-1.035000	-1.903000
H	-2.544000	-2.347000	-1.885000
H	-1.326000	-3.022000	0.703000
O	-0.307000	-1.928000	1.824000
C	0.693000	-2.057000	2.779000
H	1.627000	-2.510000	2.380000
H	0.994000	-1.091000	3.224000
H	0.356000	-2.703000	3.614000

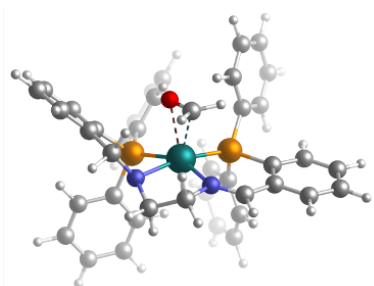
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Ru	0.014000	-1.206000	-0.250000
P	1.750000	0.311000	-0.113000
P	-1.758000	0.168000	-0.015000
N	1.488000	-2.839000	-0.224000
N	-1.198000	-2.837000	-0.680000
C	1.501000	2.059000	-0.652000
C	0.752000	2.277000	-1.819000
H	0.399000	1.424000	-2.386000
C	0.433000	3.571000	-2.231000
H	-0.174000	3.716000	-3.121000
C	0.867000	4.671000	-1.481000
H	0.608000	5.680000	-1.791000
C	1.631000	4.464000	-0.329000
H	1.974000	5.313000	0.259000
C	1.948000	3.166000	0.085000
H	2.522000	3.020000	0.994000
C	2.640000	0.519000	1.495000
C	4.032000	0.681000	1.581000
H	4.638000	0.663000	0.679000
C	4.647000	0.862000	2.824000
H	5.727000	0.976000	2.880000
C	3.876000	0.898000	3.990000
H	4.354000	1.041000	4.956000
C	2.488000	0.746000	3.909000
H	1.879000	0.774000	4.810000
C	1.874000	0.547000	2.670000
H	0.801000	0.405000	2.611000
C	3.100000	-0.284000	-1.244000
C	3.697000	0.561000	-2.189000
H	3.417000	1.608000	-2.228000
C	4.650000	0.079000	-3.093000
H	5.097000	0.755000	-3.817000
C	5.020000	-1.265000	-3.060000
H	5.754000	-1.654000	-3.761000
C	4.439000	-2.113000	-2.111000
H	4.734000	-3.160000	-2.074000
C	3.487000	-1.644000	-1.200000
C	2.946000	-2.593000	-0.153000
H	3.484000	-3.550000	-0.217000
H	3.131000	-2.187000	0.848000
C	1.052000	-3.716000	-1.325000
C	-0.422000	-4.040000	-1.094000
C	-2.474000	-3.033000	-0.579000

H	-2.858000	-4.017000	-0.867000
C	-3.496000	-2.129000	-0.056000
C	-4.771000	-2.722000	0.114000
H	-4.905000	-3.762000	-0.175000
C	-5.844000	-2.023000	0.652000
H	-6.806000	-2.513000	0.776000
C	-5.670000	-0.687000	1.031000
H	-6.495000	-0.121000	1.456000
C	-4.429000	-0.080000	0.850000
H	-4.311000	0.961000	1.136000
C	-3.329000	-0.768000	0.313000
C	-1.646000	1.296000	1.447000
C	-1.883000	0.775000	2.732000
H	-2.255000	-0.240000	2.840000
C	-1.627000	1.539000	3.870000
H	-1.819000	1.119000	4.855000
C	-1.116000	2.837000	3.746000
H	-0.906000	3.429000	4.633000
C	-0.870000	3.360000	2.475000
H	-0.459000	4.360000	2.363000
C	-1.136000	2.597000	1.333000
H	-0.925000	3.019000	0.357000
C	-2.394000	1.253000	-1.390000
C	-3.148000	2.420000	-1.193000
H	-3.353000	2.778000	-0.189000
C	-3.630000	3.148000	-2.284000
H	-4.200000	4.058000	-2.113000
C	-3.380000	2.710000	-3.589000
H	-3.755000	3.278000	-4.437000
C	-2.647000	1.537000	-3.794000
H	-2.449000	1.186000	-4.804000
C	-2.157000	0.816000	-2.702000
H	-1.559000	-0.079000	-2.856000
O	0.348000	-3.887000	2.159000
C	-0.347000	-2.919000	2.519000
H	-1.417000	-2.855000	2.259000
H	-0.017000	-2.254000	3.336000
H	-0.080000	-1.403000	1.466000
H	0.238000	-0.925000	-1.896000
H	-0.860000	-4.479000	-1.998000
H	1.210000	-3.190000	-2.268000
H	-0.500000	-4.765000	-0.275000
H	1.624000	-4.659000	-1.340000
H	1.233000	-3.301000	0.661000

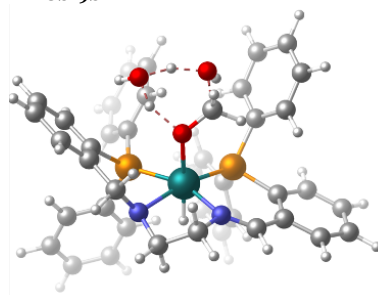
8b



Ru	-0.039000	-1.240000	0.304000
P	1.860000	0.054000	0.119000
P	-1.834000	0.206000	-0.065000
N	-1.760000	-2.460000	0.016000
N	1.000000	-3.050000	-0.030000
C	1.976000	1.142000	2.699000
H	1.325000	0.313000	2.951000
C	2.333000	2.057000	3.694000
H	1.998000	1.895000	4.715000
C	3.096000	3.183000	3.373000
H	3.366000	3.900000	4.144000
C	3.495000	3.389000	2.049000
H	4.076000	4.270000	1.784000
C	3.144000	2.470000	1.058000
H	3.448000	2.662000	0.033000
C	2.385000	1.328000	1.369000
C	1.304000	2.283000	-1.545000
H	0.938000	2.772000	-0.649000
C	1.159000	2.927000	-2.776000
H	0.686000	3.905000	-2.811000
C	1.599000	2.311000	-3.951000
H	1.480000	2.810000	-4.910000
C	2.189000	1.044000	-3.885000
H	2.532000	0.553000	-4.793000
C	2.335000	0.400000	-2.654000
H	2.781000	-0.590000	-2.622000
C	1.896000	1.012000	-1.468000
C	3.412000	-0.981000	-0.061000
C	4.659000	-0.335000	-0.048000
H	4.697000	0.737000	0.100000
C	5.862000	-1.019000	-0.222000
H	6.802000	-0.474000	-0.204000
C	5.845000	-2.400000	-0.426000
H	6.769000	-2.954000	-0.569000
C	4.623000	-3.063000	-0.448000
H	4.609000	-4.139000	-0.607000
C	3.393000	-2.389000	-0.260000
C	2.231000	-3.291000	-0.304000
H	2.487000	-4.317000	-0.592000
C	0.030000	-4.164000	-0.118000
H	-0.142000	-4.529000	0.903000
H	0.445000	-4.989000	-0.716000
C	-1.295000	-3.624000	-0.697000
H	-1.116000	-3.358000	-1.750000
H	-2.036000	-4.443000	-0.685000

C	-2.652000	-2.716000	1.112000
H	-3.371000	-3.504000	0.820000
C	-3.475000	-1.505000	1.520000
C	-4.536000	-1.720000	2.414000
H	-4.703000	-2.730000	2.786000
C	-5.375000	-0.687000	2.826000
H	-6.191000	-0.890000	3.515000
C	-5.161000	0.607000	2.342000
H	-5.807000	1.427000	2.647000
C	-4.104000	0.843000	1.465000
H	-3.935000	1.854000	1.106000
C	-3.250000	-0.196000	1.046000
C	-1.585000	2.014000	0.233000
C	-0.919000	2.365000	1.419000
H	-0.643000	1.586000	2.122000
C	-0.585000	3.694000	1.680000
H	-0.041000	3.942000	2.588000
C	-0.921000	4.694000	0.759000
H	-0.649000	5.729000	0.954000
C	-1.604000	4.356000	-0.413000
H	-1.872000	5.129000	-1.130000
C	-1.936000	3.022000	-0.676000
H	-2.447000	2.769000	-1.600000
C	-2.503000	0.155000	-1.777000
C	-3.863000	-0.057000	-2.035000
H	-4.551000	-0.223000	-1.212000
C	-4.341000	-0.068000	-3.350000
H	-5.398000	-0.244000	-3.536000
C	-3.465000	0.141000	-4.419000
H	-3.837000	0.132000	-5.440000
C	-2.105000	0.356000	-4.166000
H	-1.412000	0.519000	-4.988000
C	-1.626000	0.358000	-2.855000
H	-0.568000	0.515000	-2.674000
O	-0.488000	-0.946000	2.551000
C	0.281000	-1.947000	2.475000
H	0.062000	-1.255000	-1.291000
H	-0.130000	-2.965000	2.514000
H	1.357000	-1.854000	2.698000
H	-2.172000	-3.102000	2.040000

TS_{8b-9b}

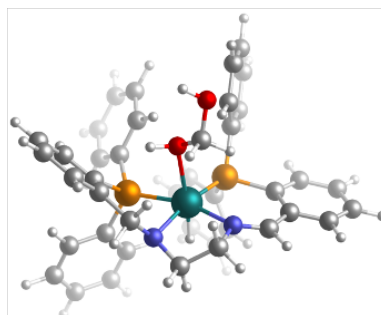


Ru	0.090000	-0.571000	-1.046000
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P	1.852000	0.280000	0.119000
P	-1.808000	0.292000	-0.076000
N	-1.477000	-1.004000	-2.457000
N	1.342000	-1.291000	-2.564000
C	3.537000	-1.530000	1.514000
H	3.929000	-1.758000	0.527000
C	4.013000	-2.259000	2.605000
H	4.752000	-3.040000	2.445000
C	3.544000	-1.990000	3.895000
H	3.912000	-2.557000	4.745000
C	2.592000	-0.984000	4.071000
H	2.215000	-0.754000	5.065000
C	2.113000	-0.258000	2.974000
H	1.374000	0.507000	3.158000
C	2.576000	-0.508000	1.669000
C	0.982000	2.622000	1.580000
H	0.586000	1.970000	2.345000
C	0.718000	3.990000	1.697000
H	0.163000	4.348000	2.560000
C	1.134000	4.878000	0.705000
H	0.920000	5.941000	0.792000
C	1.814000	4.380000	-0.411000
H	2.130000	5.053000	-1.204000
C	2.081000	3.015000	-0.522000
H	2.588000	2.654000	-1.411000
C	1.685000	2.107000	0.479000
C	3.436000	0.304000	-0.866000
C	4.546000	0.959000	-0.303000
H	4.429000	1.450000	0.659000
C	5.785000	1.002000	-0.936000
H	6.617000	1.525000	-0.471000
C	5.945000	0.368000	-2.174000
H	6.903000	0.387000	-2.686000
C	4.863000	-0.287000	-2.748000
H	4.987000	-0.778000	-3.710000
C	3.594000	-0.338000	-2.119000
C	2.571000	-1.061000	-2.881000
H	2.922000	-1.432000	-3.849000
C	0.502000	-1.977000	-3.560000
H	0.245000	-2.963000	-3.155000
H	1.042000	-2.107000	-4.511000
C	-0.789000	-1.139000	-3.720000
H	-0.503000	-0.146000	-4.095000
H	-1.422000	-1.617000	-4.491000
C	-2.330000	-2.135000	-2.200000
H	-2.985000	-2.301000	-3.078000
C	-3.258000	-1.987000	-1.009000
C	-4.258000	-2.967000	-0.871000
H	-4.304000	-3.763000	-1.612000
C	-5.173000	-2.952000	0.177000
H	-5.929000	-3.729000	0.254000
C	-5.109000	-1.927000	1.127000
H	-5.820000	-1.887000	1.949000
C	-4.124000	-0.947000	1.010000

H	-4.088000	-0.156000	1.752000
C	-3.181000	-0.961000	-0.042000
C	-1.849000	0.852000	1.698000
C	-1.255000	0.005000	2.646000
H	-0.766000	-0.901000	2.304000
C	-1.243000	0.331000	4.003000
H	-0.775000	-0.342000	4.718000
C	-1.810000	1.536000	4.434000
H	-1.792000	1.803000	5.488000
C	-2.394000	2.395000	3.498000
H	-2.832000	3.336000	3.823000
C	-2.422000	2.052000	2.142000
H	-2.882000	2.728000	1.429000
C	-2.533000	1.754000	-0.931000
C	-3.870000	1.799000	-1.347000
H	-4.515000	0.938000	-1.198000
C	-4.380000	2.945000	-1.967000
H	-5.417000	2.963000	-2.295000
C	-3.561000	4.060000	-2.166000
H	-3.958000	4.951000	-2.647000
C	-2.225000	4.020000	-1.749000
H	-1.577000	4.880000	-1.901000
C	-1.713000	2.873000	-1.143000
H	-0.672000	2.847000	-0.839000
O	-0.139000	-2.836000	-0.308000
C	0.833000	-3.452000	0.340000
H	0.188000	0.847000	-1.775000
H	0.798000	-4.551000	0.312000
H	1.842000	-3.067000	0.162000
H	-1.789000	-3.096000	-2.057000
O	0.659000	-3.258000	1.929000
H	-0.585000	-3.255000	1.978000
O	-1.686000	-3.365000	1.506000
H	-1.289000	-3.125000	0.532000
H	-2.325000	-2.668000	1.743000
H	1.025000	-2.381000	2.155000

9b

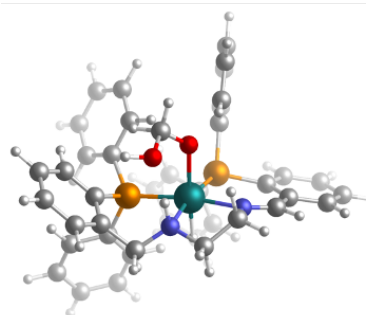


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N	-1.149000	-2.308000	1.834000
C	-2.102000	-0.859000	-2.525000
H	-1.568000	-1.692000	-2.086000
C	-2.490000	-0.924000	-3.865000
H	-2.278000	-1.822000	-4.439000
C	-3.134000	0.165000	-4.461000
H	-3.431000	0.123000	-5.506000
C	-3.393000	1.311000	-3.702000
H	-3.890000	2.165000	-4.155000
C	-3.011000	1.368000	-2.358000
H	-3.215000	2.272000	-1.793000
C	-2.356000	0.284000	-1.752000
C	-1.158000	2.981000	-0.285000
H	-0.830000	2.728000	-1.287000
C	-0.948000	4.279000	0.188000
H	-0.465000	5.008000	-0.457000
C	-1.338000	4.630000	1.483000
H	-1.168000	5.638000	1.853000
C	-1.940000	3.670000	2.303000
H	-2.243000	3.928000	3.315000
C	-2.148000	2.372000	1.831000
H	-2.599000	1.633000	2.486000
C	-1.764000	2.009000	0.528000
C	-3.397000	-0.338000	0.822000
C	-4.569000	0.383000	0.542000
H	-4.508000	1.254000	-0.102000
C	-5.810000	0.028000	1.066000
H	-6.691000	0.617000	0.826000
C	-5.907000	-1.090000	1.902000
H	-6.865000	-1.388000	2.320000
C	-4.760000	-1.815000	2.199000
H	-4.836000	-2.679000	2.856000
C	-3.490000	-1.467000	1.680000
C	-2.403000	-2.336000	2.142000
H	-2.727000	-3.098000	2.859000
C	-0.262000	-3.271000	2.516000
H	0.007000	-4.054000	1.794000
H	-0.776000	-3.747000	3.366000
C	1.018000	-2.518000	2.944000
H	0.732000	-1.763000	3.690000
H	1.696000	-3.236000	3.442000
C	2.551000	-2.736000	1.132000
H	3.317000	-3.105000	1.845000
C	3.330000	-2.119000	-0.026000
C	4.306000	-2.948000	-0.613000
H	4.426000	-3.958000	-0.224000
C	5.125000	-2.510000	-1.650000
H	5.874000	-3.176000	-2.073000
C	4.980000	-1.205000	-2.132000
H	5.614000	-0.837000	-2.935000
C	4.008000	-0.376000	-1.578000
H	3.892000	0.629000	-1.972000
C	3.165000	-0.808000	-0.531000
C	1.613000	1.441000	-1.403000

C	0.894000	0.930000	-2.496000
H	0.523000	-0.090000	-2.463000
C	0.611000	1.731000	-3.602000
H	0.025000	1.325000	-4.422000
C	1.048000	3.061000	-3.630000
H	0.815000	3.694000	-4.483000
C	1.779000	3.573000	-2.555000
H	2.122000	4.605000	-2.571000
C	2.063000	2.768000	-1.446000
H	2.613000	3.182000	-0.607000
C	2.589000	1.413000	1.308000
C	3.970000	1.435000	1.542000
H	4.625000	0.761000	0.997000
C	4.513000	2.315000	2.484000
H	5.586000	2.316000	2.664000
C	3.682000	3.188000	3.191000
H	4.104000	3.873000	3.922000
C	2.302000	3.171000	2.958000
H	1.644000	3.844000	3.504000
C	1.757000	2.285000	2.029000
H	0.685000	2.267000	1.865000
O	0.410000	-2.483000	-1.173000
C	-0.147000	-3.790000	-1.183000
H	-0.102000	0.008000	2.016000
H	0.527000	-4.484000	-0.662000
H	-1.098000	-3.717000	-0.657000
H	2.093000	-3.680000	0.732000
O	-0.449000	-4.240000	-2.481000
H	0.374000	-4.429000	-2.960000
H	1.377000	-2.519000	-1.280000

10b

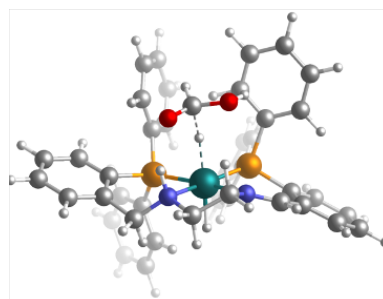


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N	1.169000	-2.809000	-1.060000
C	2.263000	-0.704000	2.558000
H	1.644000	-1.550000	2.263000
C	2.763000	-0.618000	3.860000
H	2.569000	-1.428000	4.560000
C	3.495000	0.502000	4.268000

H	3.877000	0.569000	5.284000
C	3.731000	1.540000	3.360000
H	4.296000	2.417000	3.666000
C	3.239000	1.455000	2.054000
H	3.430000	2.274000	1.367000
C	2.495000	0.338000	1.643000
C	1.290000	2.867000	-0.084000
H	0.992000	2.738000	0.950000
C	1.124000	4.116000	-0.688000
H	0.694000	4.932000	-0.113000
C	1.497000	4.310000	-2.020000
H	1.364000	5.281000	-2.490000
C	2.036000	3.243000	-2.746000
H	2.327000	3.381000	-3.785000
C	2.192000	1.992000	-2.146000
H	2.590000	1.167000	-2.729000
C	1.826000	1.788000	-0.804000
C	3.390000	-0.624000	-0.840000
C	4.542000	0.178000	-0.873000
H	4.486000	1.196000	-0.504000
C	5.759000	-0.287000	-1.370000
H	6.625000	0.369000	-1.383000
C	5.854000	-1.600000	-1.842000
H	6.795000	-1.983000	-2.227000
C	4.730000	-2.415000	-1.807000
H	4.803000	-3.439000	-2.167000
C	3.485000	-1.955000	-1.317000
C	2.413000	-2.950000	-1.360000
H	2.740000	-3.935000	-1.710000
C	0.318000	-4.004000	-1.178000
H	0.108000	-4.343000	-0.156000
H	0.826000	-4.807000	-1.730000
C	-0.990000	-3.618000	-1.862000
H	-0.797000	-3.207000	-2.859000
H	-1.638000	-4.503000	-1.962000
C	-2.881000	-2.034000	-1.586000
H	-2.628000	-1.270000	-2.330000
C	-3.723000	-1.484000	-0.451000
C	-4.941000	-2.106000	-0.148000
H	-5.286000	-2.925000	-0.775000
C	-5.705000	-1.712000	0.954000
H	-6.645000	-2.214000	1.171000
C	-5.244000	-0.683000	1.777000
H	-5.821000	-0.372000	2.645000
C	-4.034000	-0.048000	1.482000
H	-3.684000	0.752000	2.127000
C	-3.267000	-0.429000	0.372000
C	-1.403000	1.545000	1.388000
C	-0.664000	1.036000	2.469000
H	-0.309000	0.012000	2.435000
C	-0.337000	1.854000	3.552000
H	0.266000	1.451000	4.361000
C	-0.748000	3.191000	3.569000
H	-0.479000	3.834000	4.404000

C	-1.496000	3.701000	2.503000
H	-1.816000	4.741000	2.509000
C	-1.823000	2.884000	1.417000
H	-2.379000	3.301000	0.583000
C	-2.232000	1.526000	-1.398000
C	-3.540000	2.041000	-1.430000
H	-4.257000	1.759000	-0.665000
C	-3.936000	2.914000	-2.448000
H	-4.953000	3.299000	-2.460000
C	-3.029000	3.286000	-3.446000
H	-3.337000	3.965000	-4.237000
C	-1.729000	2.774000	-3.422000
H	-1.014000	3.055000	-4.192000
C	-1.336000	1.895000	-2.410000
H	-0.336000	1.483000	-2.409000
H	0.062000	-0.623000	-1.989000
H	-3.449000	-2.825000	-2.099000
O	-0.128000	-2.284000	1.528000
C	-1.193000	-2.524000	2.288000
H	-1.816000	-1.634000	2.524000
H	-0.921000	-3.029000	3.235000
O	-2.143000	-3.474000	1.602000
H	-3.052000	-3.236000	1.851000
H	-1.844000	-3.010000	-0.113000

TS_{10b-7b}

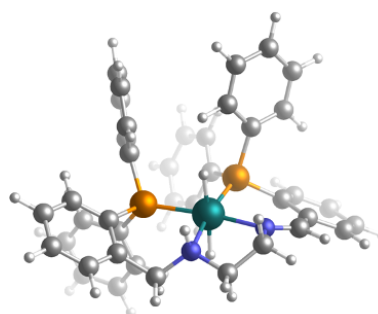


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N	1.603000	-2.300000	-1.388000
N	-1.168000	-2.719000	-1.209000
C	-2.098000	1.701000	-2.468000
H	-1.431000	0.946000	-2.880000
C	-2.602000	2.722000	-3.278000
H	-2.342000	2.749000	-4.334000
C	-3.429000	3.709000	-2.733000
H	-3.815000	4.509000	-3.360000
C	-3.759000	3.658000	-1.375000
H	-4.404000	4.417000	-0.940000
C	-3.263000	2.629000	-0.570000
H	-3.535000	2.607000	0.481000
C	-2.415000	1.646000	-1.103000
C	-1.275000	2.147000	1.919000

H	-1.085000	2.857000	1.120000
C	-1.064000	2.542000	3.244000
H	-0.719000	3.552000	3.449000
C	-1.281000	1.644000	4.291000
H	-1.115000	1.952000	5.321000
C	-1.706000	0.341000	4.006000
H	-1.874000	-0.370000	4.812000
C	-1.909000	-0.057000	2.684000
H	-2.225000	-1.075000	2.473000
C	-1.705000	0.845000	1.622000
C	-3.349000	-0.803000	-0.077000
C	-4.417000	-0.387000	0.736000
H	-4.302000	0.491000	1.362000
C	-5.627000	-1.079000	0.773000
H	-6.431000	-0.730000	1.417000
C	-5.792000	-2.217000	-0.017000
H	-6.724000	-2.777000	0.005000
C	-4.744000	-2.638000	-0.835000
H	-4.870000	-3.528000	-1.447000
C	-3.523000	-1.946000	-0.888000
C	-2.475000	-2.466000	-1.851000
H	-2.854000	-3.397000	-2.298000
C	-0.334000	-3.630000	-2.019000
H	-0.302000	-3.240000	-3.042000
H	-0.765000	-4.643000	-2.038000
C	1.069000	-3.672000	-1.430000
H	1.034000	-4.048000	-0.402000
H	1.713000	-4.333000	-2.027000
C	2.814000	-2.134000	-1.802000
H	3.354000	-3.013000	-2.170000
C	3.558000	-0.878000	-1.908000
C	4.730000	-0.935000	-2.692000
H	5.016000	-1.883000	-3.141000
C	5.516000	0.192000	-2.915000
H	6.407000	0.121000	-3.533000
C	5.147000	1.410000	-2.337000
H	5.748000	2.301000	-2.499000
C	4.006000	1.477000	-1.535000
H	3.743000	2.424000	-1.073000
C	3.197000	0.355000	-1.306000
C	1.468000	2.273000	-0.031000
C	0.732000	2.868000	-1.067000
H	0.400000	2.254000	-1.897000
C	0.396000	4.221000	-1.018000
H	-0.201000	4.655000	-1.815000
C	0.800000	5.001000	0.072000
H	0.527000	6.052000	0.122000
C	1.553000	4.422000	1.098000
H	1.874000	5.023000	1.946000
C	1.888000	3.065000	1.048000
H	2.457000	2.624000	1.860000
C	2.546000	0.029000	1.464000
C	3.867000	-0.429000	1.580000
H	4.514000	-0.457000	0.709000

C	4.364000	-0.870000	2.814000
H	5.385000	-1.238000	2.880000
C	3.556000	-0.838000	3.953000
H	3.941000	-1.183000	4.909000
C	2.240000	-0.366000	3.850000
H	1.596000	-0.335000	4.725000
C	1.739000	0.049000	2.617000
H	0.710000	0.374000	2.544000
H	-0.011000	-0.398000	-2.315000
H	-2.300000	-1.756000	-2.668000
H	0.116000	-1.634000	0.865000
C	0.054000	-2.976000	1.900000
H	-0.148000	-2.238000	2.691000
O	1.380000	-3.361000	1.851000
H	1.934000	-2.605000	2.117000
O	-0.807000	-3.753000	1.474000
H	-1.314000	-3.165000	-0.290000

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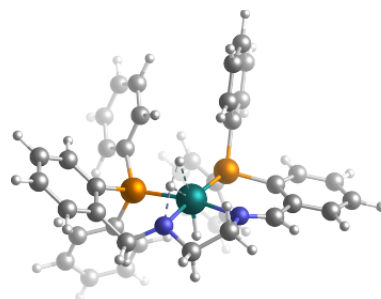


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P	1.770000	0.009000	-0.057000
N	1.372000	-2.975000	0.390000
N	-1.436000	-3.032000	0.560000
C	-2.068000	0.035000	-2.732000
H	-1.403000	-0.823000	-2.661000
C	-2.592000	0.433000	-3.965000
H	-2.344000	-0.132000	-4.862000
C	-3.421000	1.555000	-4.048000
H	-3.822000	1.871000	-5.008000
C	-3.734000	2.267000	-2.886000
H	-4.383000	3.139000	-2.937000
C	-3.220000	1.860000	-1.653000
H	-3.482000	2.421000	-0.761000
C	-2.366000	0.748000	-1.563000
C	-1.092000	2.838000	0.545000
H	-0.950000	2.933000	-0.527000
C	-0.799000	3.930000	1.369000
H	-0.438000	4.852000	0.921000
C	-0.956000	3.832000	2.752000
H	-0.728000	4.681000	3.392000
C	-1.396000	2.626000	3.312000

H	-1.510000	2.533000	4.390000
C	-1.671000	1.532000	2.492000
H	-1.970000	0.588000	2.938000
C	-1.537000	1.628000	1.096000
C	-3.354000	-0.608000	0.657000
C	-4.326000	0.221000	1.239000
H	-4.107000	1.272000	1.399000
C	-5.577000	-0.267000	1.621000
H	-6.305000	0.404000	2.070000
C	-5.883000	-1.613000	1.420000
H	-6.851000	-2.012000	1.713000
C	-4.930000	-2.449000	0.837000
H	-5.167000	-3.500000	0.679000
C	-3.670000	-1.971000	0.446000
C	-2.711000	-2.962000	-0.187000
H	-3.194000	-3.951000	-0.205000
C	-0.682000	-4.276000	0.324000
H	-0.567000	-4.393000	-0.758000
H	-1.215000	-5.154000	0.724000
C	0.691000	-4.140000	0.977000
H	0.579000	-3.963000	2.054000
H	1.270000	-5.064000	0.832000
C	2.598000	-3.151000	0.016000
H	3.050000	-4.134000	0.183000
C	3.442000	-2.213000	-0.719000
C	4.596000	-2.779000	-1.305000
H	4.814000	-3.830000	-1.124000
C	5.441000	-2.039000	-2.125000
H	6.315000	-2.506000	-2.571000
C	5.145000	-0.696000	-2.376000
H	5.786000	-0.101000	-3.022000
C	4.026000	-0.111000	-1.779000
H	3.822000	0.938000	-1.964000
C	3.167000	-0.837000	-0.939000
C	1.574000	1.554000	-1.062000
C	0.901000	1.438000	-2.288000
H	0.568000	0.458000	-2.612000
C	0.633000	2.565000	-3.065000
H	0.083000	2.457000	-3.997000
C	1.045000	3.830000	-2.629000
H	0.828000	4.712000	-3.227000
C	1.733000	3.953000	-1.418000
H	2.055000	4.932000	-1.071000
C	1.994000	2.823000	-0.637000
H	2.506000	2.939000	0.313000
C	2.651000	0.666000	1.448000
C	4.033000	0.914000	1.492000
H	4.661000	0.676000	0.639000
C	4.621000	1.468000	2.633000
H	5.694000	1.645000	2.654000
C	3.833000	1.796000	3.741000
H	4.290000	2.232000	4.627000
C	2.457000	1.553000	3.704000
H	1.832000	1.802000	4.559000

C	1.874000	0.981000	2.571000
H	0.813000	0.759000	2.557000
H	-0.042000	-1.709000	-1.480000
H	-2.461000	-2.692000	-1.219000
H	-0.068000	-1.159000	1.907000
H	-1.638000	-2.952000	1.557000

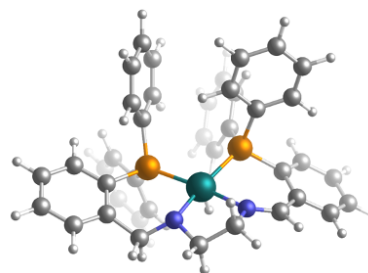
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P	-1.766000	-0.093000	-0.023000
P	1.758000	-0.032000	-0.006000
N	1.309000	3.066000	0.191000
N	-1.468000	3.053000	-0.077000
C	-1.631000	-0.908000	2.660000
H	-0.570000	-0.718000	2.551000
C	-2.130000	-1.396000	3.869000
H	-1.444000	-1.598000	4.688000
C	-3.502000	-1.615000	4.026000
H	-3.893000	-1.986000	4.971000
C	-4.371000	-1.350000	2.964000
H	-5.441000	-1.511000	3.078000
C	-3.870000	-0.876000	1.747000
H	-4.555000	-0.679000	0.928000
C	-2.493000	-0.650000	1.585000
C	-1.974000	-2.929000	-0.452000
H	-2.500000	-2.993000	0.495000
C	-1.702000	-4.097000	-1.170000
H	-2.031000	-5.057000	-0.779000
C	-0.999000	-4.036000	-2.377000
H	-0.774000	-4.947000	-2.925000
C	-0.583000	-2.795000	-2.875000
H	-0.024000	-2.734000	-3.805000
C	-0.858000	-1.630000	-2.159000
H	-0.520000	-0.671000	-2.536000
C	-1.544000	-1.685000	-0.935000
C	-3.243000	0.631000	-0.877000
C	-3.996000	-0.114000	-1.798000
H	-3.719000	-1.139000	-2.018000
C	-5.107000	0.440000	-2.441000
H	-5.676000	-0.157000	-3.149000
C	-5.475000	1.758000	-2.168000
H	-6.334000	2.204000	-2.662000
C	-4.726000	2.507000	-1.256000

H	-5.008000	3.537000	-1.050000
C	-3.612000	1.967000	-0.600000
C	-2.834000	2.837000	0.369000
H	-3.356000	3.806000	0.441000
C	-0.838000	4.198000	0.535000
H	-0.784000	4.090000	1.637000
H	-1.390000	5.133000	0.321000
C	0.573000	4.330000	-0.022000
H	0.520000	4.494000	-1.106000
H	1.104000	5.176000	0.435000
C	2.558000	3.178000	0.486000
H	2.961000	4.191000	0.595000
C	3.554000	2.126000	0.704000
C	4.829000	2.605000	1.087000
H	4.974000	3.677000	1.195000
C	5.895000	1.747000	1.329000
H	6.861000	2.147000	1.626000
C	5.707000	0.369000	1.184000
H	6.525000	-0.323000	1.367000
C	4.459000	-0.117000	0.798000
H	4.329000	-1.189000	0.694000
C	3.365000	0.730000	0.557000
C	1.657000	-1.490000	1.132000
C	1.957000	-1.317000	2.495000
H	2.346000	-0.365000	2.846000
C	1.742000	-2.347000	3.411000
H	1.981000	-2.191000	4.461000
C	1.212000	-3.569000	2.984000
H	1.034000	-4.369000	3.698000
C	0.905000	-3.750000	1.634000
H	0.480000	-4.688000	1.287000
C	1.128000	-2.720000	0.714000
H	0.874000	-2.881000	-0.327000
C	2.346000	-0.754000	-1.623000
C	3.058000	-1.957000	-1.752000
H	3.274000	-2.563000	-0.878000
C	3.480000	-2.405000	-3.006000
H	4.019000	-3.346000	-3.087000
C	3.210000	-1.650000	-4.151000
H	3.538000	-2.001000	-5.127000
C	2.514000	-0.443000	-4.033000
H	2.296000	0.152000	-4.916000
C	2.083000	-0.003000	-2.779000
H	1.514000	0.920000	-2.692000
H	0.084000	1.257000	1.630000
H	-2.856000	2.397000	1.385000
H	-0.393000	1.938000	-1.857000
H	-0.958000	2.539000	-1.290000

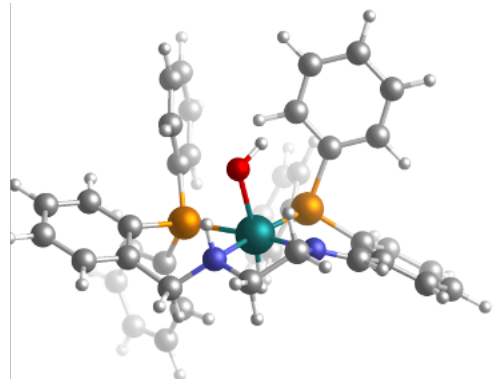
4b



Ru	-0.011000	1.408000	0.115000
P	-1.804000	-0.036000	0.051000
P	1.751000	-0.076000	0.049000
N	1.451000	2.932000	0.076000
N	-1.263000	3.002000	-0.172000
C	-2.037000	-0.442000	2.806000
H	-1.503000	0.503000	2.858000
C	-2.430000	-1.090000	3.980000
H	-2.212000	-0.636000	4.944000
C	-3.092000	-2.320000	3.915000
H	-3.390000	-2.830000	4.828000
C	-3.371000	-2.888000	2.669000
H	-3.888000	-3.842000	2.607000
C	-2.988000	-2.232000	1.496000
H	-3.215000	-2.690000	0.538000
C	-2.304000	-1.008000	1.550000
C	-1.077000	-2.555000	-1.098000
H	-0.829000	-2.886000	-0.096000
C	-0.808000	-3.401000	-2.179000
H	-0.358000	-4.372000	-1.993000
C	-1.103000	-2.997000	-3.483000
H	-0.889000	-3.655000	-4.322000
C	-1.669000	-1.736000	-3.702000
H	-1.901000	-1.408000	-4.712000
C	-1.932000	-0.888000	-2.624000
H	-2.360000	0.093000	-2.809000
C	-1.644000	-1.289000	-1.306000
C	-3.431000	0.746000	-0.377000
C	-4.485000	-0.079000	-0.813000
H	-4.320000	-1.147000	-0.917000
C	-5.738000	0.439000	-1.130000
H	-6.532000	-0.222000	-1.467000
C	-5.954000	1.815000	-1.015000
H	-6.921000	2.245000	-1.266000
C	-4.917000	2.639000	-0.581000
H	-5.090000	3.710000	-0.496000
C	-3.646000	2.132000	-0.249000
C	-2.633000	3.127000	0.292000
H	-3.014000	4.128000	0.029000
C	-0.573000	4.267000	0.021000
H	-0.531000	4.570000	1.088000
H	-1.079000	5.087000	-0.520000
C	0.849000	4.142000	-0.508000
H	0.818000	3.997000	-1.595000

H	1.450000	5.035000	-0.284000
C	2.657000	3.015000	0.521000
H	3.161000	3.987000	0.465000
C	3.449000	1.952000	1.146000
C	4.579000	2.388000	1.867000
H	4.799000	3.453000	1.906000
C	5.406000	1.494000	2.543000
H	6.262000	1.859000	3.103000
C	5.118000	0.128000	2.490000
H	5.750000	-0.588000	3.009000
C	4.020000	-0.323000	1.752000
H	3.824000	-1.389000	1.705000
C	3.170000	0.562000	1.072000
C	1.595000	-1.803000	0.692000
C	0.907000	-1.975000	1.903000
H	0.538000	-1.103000	2.433000
C	0.658000	-3.251000	2.409000
H	0.097000	-3.361000	3.333000
C	1.104000	-4.379000	1.710000
H	0.900000	-5.375000	2.093000
C	1.808000	-4.217000	0.513000
H	2.159000	-5.089000	-0.035000
C	2.054000	-2.937000	0.006000
H	2.582000	-2.826000	-0.936000
C	2.578000	-0.347000	-1.591000
C	3.968000	-0.387000	-1.781000
H	4.638000	-0.251000	-0.937000
C	4.505000	-0.600000	-3.055000
H	5.585000	-0.621000	-3.187000
C	3.660000	-0.787000	-4.153000
H	4.080000	-0.956000	-5.142000
C	2.274000	-0.752000	-3.972000
H	1.605000	-0.898000	-4.817000
C	1.738000	-0.522000	-2.704000
H	0.662000	-0.482000	-2.574000
H	0.158000	1.203000	1.680000
H	-2.678000	3.084000	1.401000

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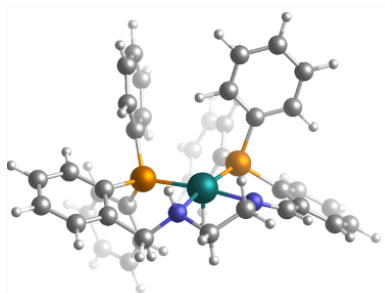


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P	-1.753000	0.097000	-0.023000

P	1.781000	0.135000	-0.132000
N	1.481000	-2.871000	-0.111000
N	-1.310000	-3.035000	0.094000
C	-2.053000	0.430000	-2.797000
H	-1.400000	-0.437000	-2.845000
C	-2.547000	1.010000	-3.970000
H	-2.291000	0.576000	-4.933000
C	-3.358000	2.146000	-3.904000
H	-3.736000	2.604000	-4.815000
C	-3.684000	2.690000	-2.656000
H	-4.318000	3.571000	-2.593000
C	-3.199000	2.102000	-1.486000
H	-3.468000	2.534000	-0.527000
C	-2.363000	0.975000	-1.543000
C	-1.180000	2.709000	0.956000
H	-1.012000	3.004000	-0.075000
C	-0.932000	3.633000	1.976000
H	-0.585000	4.630000	1.718000
C	-1.118000	3.273000	3.313000
H	-0.926000	3.993000	4.105000
C	-1.536000	1.975000	3.627000
H	-1.662000	1.677000	4.665000
C	-1.772000	1.044000	2.613000
H	-2.028000	0.020000	2.862000
C	-1.615000	1.411000	1.262000
C	-3.358000	-0.746000	0.432000
C	-4.376000	-0.006000	1.057000
H	-4.197000	1.032000	1.320000
C	-5.615000	-0.569000	1.361000
H	-6.379000	0.033000	1.847000
C	-5.861000	-1.904000	1.040000
H	-6.818000	-2.363000	1.274000
C	-4.861000	-2.651000	0.418000
H	-5.051000	-3.694000	0.172000
C	-3.612000	-2.096000	0.099000
C	-2.611000	-2.996000	-0.600000
H	-3.039000	-4.008000	-0.654000
C	-0.525000	-4.246000	-0.194000
H	-0.437000	-4.350000	-1.281000
H	-1.018000	-5.148000	0.204000
C	0.858000	-4.083000	0.434000
H	0.743000	-3.919000	1.514000
H	1.474000	-4.975000	0.255000
C	2.692000	-2.963000	-0.551000
H	3.178000	-3.944000	-0.520000
C	3.493000	-1.904000	-1.166000
C	4.649000	-2.339000	-1.849000
H	4.887000	-3.401000	-1.854000
C	5.476000	-1.450000	-2.528000
H	6.353000	-1.816000	-3.056000
C	5.164000	-0.087000	-2.526000
H	5.796000	0.623000	-3.053000
C	4.041000	0.364000	-1.829000
H	3.825000	1.428000	-1.814000

C	3.193000	-0.516000	-1.141000
C	1.553000	1.833000	-0.827000
C	0.848000	1.937000	-2.037000
H	0.508000	1.033000	-2.529000
C	0.554000	3.186000	-2.586000
H	-0.019000	3.245000	-3.507000
C	0.973000	4.352000	-1.933000
H	0.734000	5.327000	-2.351000
C	1.694000	4.256000	-0.739000
H	2.024000	5.157000	-0.227000
C	1.984000	3.004000	-0.188000
H	2.526000	2.945000	0.750000
C	2.622000	0.476000	1.486000
C	3.999000	0.317000	1.707000
H	4.650000	-0.002000	0.899000
C	4.549000	0.568000	2.969000
H	5.617000	0.436000	3.125000
C	3.733000	0.989000	4.023000
H	4.162000	1.185000	5.002000
C	2.359000	1.152000	3.810000
H	1.710000	1.476000	4.619000
C	1.809000	0.889000	2.555000
H	0.742000	1.000000	2.405000
H	0.095000	-1.301000	-1.722000
H	-2.424000	-2.665000	-1.628000
H	-1.425000	-2.948000	1.114000
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H	0.470000	-1.399000	2.643000

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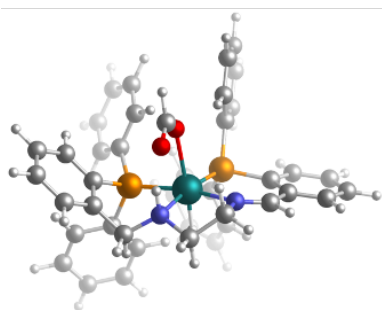


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P	1.796000	0.066000	0.010000
P	-1.772000	0.168000	0.107000
N	-1.531000	-2.870000	0.045000
N	1.277000	-3.111000	-0.189000
C	1.955000	0.478000	2.777000
H	1.357000	-0.427000	2.838000
C	2.371000	1.114000	3.949000
H	2.106000	0.692000	4.915000
C	3.120000	2.292000	3.879000
H	3.439000	2.792000	4.789000
C	3.463000	2.821000	2.630000
H	4.050000	3.734000	2.567000

C	3.056000	2.179000	1.459000
H	3.338000	2.602000	0.500000
C	2.285000	1.008000	1.520000
C	1.159000	2.580000	-1.146000
H	0.911000	2.914000	-0.145000
C	0.922000	3.432000	-2.228000
H	0.500000	4.416000	-2.046000
C	1.217000	3.020000	-3.530000
H	1.032000	3.686000	-4.369000
C	1.752000	1.746000	-3.749000
H	1.988000	1.418000	-4.758000
C	1.987000	0.891000	-2.671000
H	2.404000	-0.095000	-2.856000
C	1.700000	1.301000	-1.355000
C	3.399000	-0.816000	-0.339000
C	4.475000	-0.089000	-0.876000
H	4.346000	0.961000	-1.116000
C	5.713000	-0.685000	-1.115000
H	6.526000	-0.096000	-1.530000
C	5.898000	-2.035000	-0.816000
H	6.855000	-2.516000	-0.999000
C	4.841000	-2.768000	-0.275000
H	4.990000	-3.818000	-0.035000
C	3.591000	-2.180000	-0.021000
C	2.530000	-3.053000	0.616000
H	2.937000	-4.067000	0.734000
C	0.443000	-4.288000	0.162000
H	0.358000	-4.320000	1.253000
H	0.911000	-5.223000	-0.177000
C	-0.943000	-4.125000	-0.454000
H	-0.866000	-4.059000	-1.548000
H	-1.571000	-4.993000	-0.215000
C	-2.716000	-2.930000	0.554000
H	-3.215000	-3.904000	0.570000
C	-3.486000	-1.851000	1.175000
C	-4.632000	-2.272000	1.880000
H	-4.881000	-3.331000	1.902000
C	-5.443000	-1.367000	2.561000
H	-6.314000	-1.719000	3.106000
C	-5.124000	-0.009000	2.530000
H	-5.745000	0.713000	3.054000
C	-4.007000	0.430000	1.812000
H	-3.786000	1.492000	1.781000
C	-3.174000	-0.466000	1.131000
C	-1.565000	1.895000	0.693000
C	-0.883000	2.093000	1.903000
H	-0.538000	1.238000	2.474000
C	-0.623000	3.383000	2.367000
H	-0.075000	3.519000	3.295000
C	-1.051000	4.490000	1.625000
H	-0.842000	5.496000	1.979000
C	-1.750000	4.299000	0.429000
H	-2.091000	5.156000	-0.145000
C	-2.008000	3.007000	-0.038000

H	-2.535000	2.870000	-0.977000
C	-2.541000	0.333000	-1.563000
C	-3.911000	0.146000	-1.803000
H	-4.587000	-0.080000	-0.984000
C	-4.421000	0.257000	-3.101000
H	-5.485000	0.111000	-3.273000
C	-3.572000	0.558000	-4.169000
H	-3.973000	0.645000	-5.176000
C	-2.206000	0.749000	-3.937000
H	-1.538000	0.991000	-4.759000
C	-1.692000	0.631000	-2.645000
H	-0.633000	0.793000	-2.479000
H	-0.005000	-1.388000	1.568000
H	2.251000	-2.693000	1.611000
H	1.556000	-3.205000	-1.170000

13b



Ru	-0.023000	-1.190000	-0.398000
P	1.828000	0.093000	-0.077000
P	-1.683000	0.396000	-0.006000
N	-1.656000	-2.648000	-0.929000
N	1.148000	-2.865000	-0.988000
C	2.215000	-0.446000	2.631000
H	1.631000	-1.333000	2.406000
C	2.683000	-0.235000	3.930000
H	2.492000	-0.985000	4.695000
C	3.377000	0.936000	4.250000
H	3.734000	1.103000	5.264000
C	3.605000	1.894000	3.258000
H	4.141000	2.811000	3.495000
C	3.145000	1.682000	1.956000
H	3.331000	2.442000	1.204000
C	2.439000	0.513000	1.630000
C	1.263000	2.856000	-0.359000
H	0.941000	2.823000	0.676000
C	1.097000	4.038000	-1.085000
H	0.648000	4.901000	-0.602000
C	1.492000	4.104000	-2.423000
H	1.358000	5.022000	-2.990000
C	2.054000	2.977000	-3.032000
H	2.362000	3.015000	-4.074000
C	2.214000	1.793000	-2.308000
H	2.633000	0.920000	-2.800000

C	1.824000	1.719000	-0.960000
C	3.390000	-0.681000	-0.741000
C	4.555000	0.103000	-0.753000
H	4.500000	1.134000	-0.421000
C	5.784000	-0.393000	-1.184000
H	6.660000	0.250000	-1.180000
C	5.878000	-1.721000	-1.612000
H	6.827000	-2.130000	-1.946000
C	4.739000	-2.516000	-1.606000
H	4.810000	-3.549000	-1.940000
C	3.482000	-2.025000	-1.181000
C	2.397000	-3.006000	-1.270000
H	2.722000	-3.982000	-1.647000
C	0.292000	-4.054000	-1.200000
H	0.087000	-4.492000	-0.216000
H	0.798000	-4.798000	-1.828000
C	-1.032000	-3.627000	-1.831000
H	-0.863000	-3.159000	-2.808000
H	-1.675000	-4.511000	-1.967000
C	-2.955000	-2.123000	-1.400000
H	-2.766000	-1.374000	-2.179000
C	-3.728000	-1.547000	-0.228000
C	-4.920000	-2.167000	0.163000
H	-5.280000	-3.023000	-0.403000
C	-5.641000	-1.723000	1.274000
H	-6.561000	-2.226000	1.561000
C	-5.161000	-0.646000	2.019000
H	-5.704000	-0.294000	2.892000
C	-3.972000	-0.016000	1.640000
H	-3.608000	0.823000	2.225000
C	-3.249000	-0.448000	0.521000
C	-1.414000	1.648000	1.322000
C	-0.745000	1.208000	2.477000
H	-0.474000	0.161000	2.571000
C	-0.411000	2.115000	3.484000
H	0.134000	1.766000	4.357000
C	-0.747000	3.467000	3.353000
H	-0.472000	4.175000	4.131000
C	-1.431000	3.906000	2.215000
H	-1.697000	4.955000	2.107000
C	-1.765000	3.000000	1.202000
H	-2.274000	3.357000	0.312000
C	-2.305000	1.405000	-1.430000
C	-3.637000	1.851000	-1.491000
H	-4.338000	1.580000	-0.707000
C	-4.073000	2.640000	-2.559000
H	-5.108000	2.972000	-2.595000
C	-3.184000	2.997000	-3.578000
H	-3.523000	3.611000	-4.408000
C	-1.858000	2.557000	-3.523000
H	-1.156000	2.828000	-4.308000
C	-1.424000	1.761000	-2.460000
H	-0.400000	1.409000	-2.435000
H	0.055000	-0.704000	-1.929000

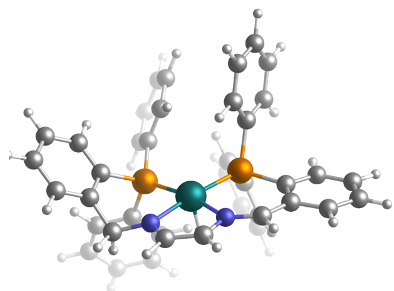
H	-3.549000	-2.931000	-1.853000
O	-0.330000	-2.005000	1.909000
C	-0.962000	-3.044000	2.281000
O	-1.562000	-3.880000	1.566000
H	-0.970000	-3.215000	3.381000
H	-1.791000	-3.122000	-0.013000

TS_{13b-4b}

Ru	0.016000	-1.065000	-0.708000
P	-1.745000	0.316000	-0.131000
P	1.824000	0.220000	-0.115000
N	1.387000	-2.529000	-1.378000
N	-1.383000	-2.584000	-1.284000
C	-1.859000	1.805000	-2.506000
H	-1.329000	0.953000	-2.923000
C	-2.212000	2.879000	-3.327000
H	-1.967000	2.850000	-4.386000
C	-2.870000	3.988000	-2.787000
H	-3.139000	4.829000	-3.422000
C	-3.187000	4.006000	-1.425000
H	-3.705000	4.861000	-0.996000
C	-2.843000	2.926000	-0.609000
H	-3.105000	2.956000	0.444000
C	-2.159000	1.820000	-1.136000
C	-0.992000	2.139000	1.924000
H	-0.691000	2.819000	1.136000
C	-0.727000	2.478000	3.254000
H	-0.230000	3.420000	3.473000
C	-1.079000	1.608000	4.289000
H	-0.864000	1.871000	5.322000
C	-1.704000	0.393000	3.987000
H	-1.977000	-0.298000	4.780000
C	-1.972000	0.055000	2.660000
H	-2.461000	-0.890000	2.443000
C	-1.620000	0.923000	1.610000
C	-3.411000	-0.504000	-0.159000
C	-4.454000	0.026000	0.621000
H	-4.262000	0.883000	1.261000
C	-5.733000	-0.526000	0.605000
H	-6.518000	-0.098000	1.223000
C	-5.989000	-1.631000	-0.209000
H	-6.977000	-2.085000	-0.230000
C	-4.964000	-2.158000	-0.994000
H	-5.166000	-3.023000	-1.622000
C	-3.670000	-1.611000	-0.994000
C	-2.645000	-2.230000	-1.931000
H	-3.106000	-3.134000	-2.361000
C	-0.682000	-3.603000	-2.056000
H	-0.558000	-3.301000	-3.112000
H	-1.237000	-4.559000	-2.050000
C	0.694000	-3.827000	-1.434000

H	0.575000	-4.178000	-0.403000
H	1.276000	-4.568000	-1.998000
C	2.590000	-2.467000	-1.831000
H	3.032000	-3.384000	-2.236000
C	3.456000	-1.286000	-1.927000
C	4.598000	-1.453000	-2.737000
H	4.772000	-2.418000	-3.208000
C	5.496000	-0.412000	-2.961000
H	6.361000	-0.567000	-3.600000
C	5.269000	0.825000	-2.355000
H	5.957000	1.652000	-2.516000
C	4.158000	0.998000	-1.527000
H	4.007000	1.960000	-1.046000
C	3.238000	-0.034000	-1.295000
C	1.724000	2.063000	-0.045000
C	1.072000	2.707000	-1.108000
H	0.699000	2.117000	-1.938000
C	0.864000	4.087000	-1.088000
H	0.328000	4.560000	-1.906000
C	1.318000	4.845000	-0.003000
H	1.146000	5.918000	0.024000
C	1.990000	4.215000	1.050000
H	2.349000	4.798000	1.894000
C	2.194000	2.831000	1.029000
H	2.699000	2.351000	1.862000
C	2.615000	-0.202000	1.506000
C	3.975000	-0.513000	1.659000
H	4.641000	-0.498000	0.801000
C	4.490000	-0.844000	2.917000
H	5.545000	-1.087000	3.019000
C	3.655000	-0.860000	4.037000
H	4.056000	-1.118000	5.015000
C	2.298000	-0.551000	3.893000
H	1.634000	-0.567000	4.753000
C	1.782000	-0.235000	2.636000
H	0.726000	-0.019000	2.534000
H	0.059000	-0.381000	-2.134000
H	-2.460000	-1.549000	-2.781000
C	-0.765000	-3.035000	2.163000
H	-1.741000	-3.260000	-0.008000
O	-1.319000	-3.461000	3.118000
O	0.064000	-2.459000	1.532000
H	-1.885000	-3.663000	0.807000

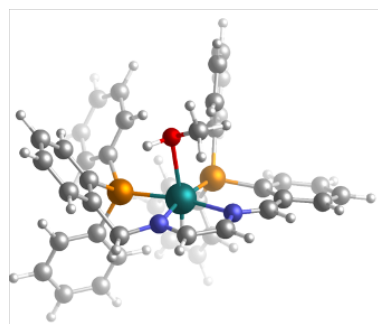
4c



Ru	0.007000	1.414000	0.126000
P	1.787000	-0.021000	0.048000
P	-1.756000	-0.072000	-0.053000
N	-1.404000	2.965000	0.232000
N	1.298000	3.121000	0.355000
C	2.022000	0.073000	-2.726000
H	1.523000	1.032000	-2.598000
C	2.386000	-0.349000	-4.006000
H	2.176000	0.285000	-4.864000
C	3.012000	-1.588000	-4.182000
H	3.288000	-1.925000	-5.178000
C	3.284000	-2.387000	-3.068000
H	3.774000	-3.350000	-3.194000
C	2.929000	-1.955000	-1.787000
H	3.152000	-2.591000	-0.935000
C	2.282000	-0.725000	-1.600000
C	1.104000	-2.687000	0.798000
H	0.818000	-2.850000	-0.235000
C	0.862000	-3.695000	1.736000
H	0.398000	-4.623000	1.411000
C	1.200000	-3.506000	3.078000
H	1.007000	-4.289000	3.807000
C	1.782000	-2.298000	3.478000
H	2.048000	-2.138000	4.520000
C	2.022000	-1.290000	2.542000
H	2.463000	-0.352000	2.867000
C	1.688000	-1.472000	1.188000
C	3.410000	0.735000	0.514000
C	4.508000	-0.116000	0.706000
H	4.356000	-1.190000	0.655000
C	5.791000	0.365000	0.964000
H	6.616000	-0.326000	1.114000
C	5.993000	1.750000	1.018000
H	6.984000	2.155000	1.209000
C	4.921000	2.610000	0.830000
H	5.089000	3.684000	0.881000
C	3.600000	2.143000	0.586000
C	2.606000	3.195000	0.465000
H	3.023000	4.204000	0.539000
C	0.554000	4.280000	0.374000
C	-0.827000	4.159000	0.343000
C	-2.840000	2.844000	0.419000
H	-3.306000	3.839000	0.480000
C	-3.519000	2.054000	-0.688000
C	-4.553000	2.653000	-1.416000

H	-4.830000	3.681000	-1.189000
C	-5.230000	1.965000	-2.427000
H	-6.026000	2.457000	-2.981000
C	-4.875000	0.648000	-2.718000
H	-5.393000	0.096000	-3.497000
C	-3.844000	0.034000	-1.999000
H	-3.581000	-0.992000	-2.232000
C	-3.156000	0.719000	-0.986000
C	-1.571000	-1.689000	-0.929000
C	-0.865000	-1.687000	-2.142000
H	-0.491000	-0.751000	-2.544000
C	-0.610000	-2.877000	-2.824000
H	-0.038000	-2.854000	-3.747000
C	-1.064000	-4.092000	-2.298000
H	-0.856000	-5.024000	-2.818000
C	-1.786000	-4.102000	-1.101000
H	-2.146000	-5.042000	-0.689000
C	-2.040000	-2.907000	-0.419000
H	-2.585000	-2.932000	0.519000
C	-2.562000	-0.578000	1.533000
C	-3.955000	-0.627000	1.693000
H	-4.606000	-0.333000	0.875000
C	-4.514000	-1.051000	2.903000
H	-5.595000	-1.076000	3.017000
C	-3.687000	-1.444000	3.959000
H	-4.122000	-1.776000	4.898000
C	-2.297000	-1.406000	3.802000
H	-1.644000	-1.711000	4.616000
C	-1.737000	-0.968000	2.601000
H	-0.660000	-0.930000	2.492000
H	-1.446000	5.057000	0.426000
H	1.053000	5.243000	0.461000
H	0.038000	1.153000	1.671000
H	-3.033000	2.346000	1.383000

5c

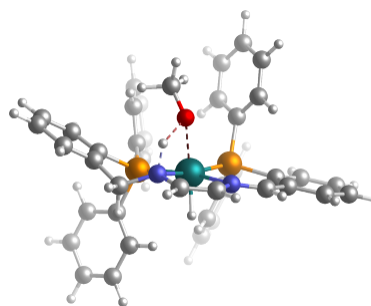


Ru	-0.016000	-1.204000	-0.497000
P	1.793000	0.148000	-0.124000
P	-1.744000	0.239000	0.002000
N	-1.480000	-2.642000	-1.077000
N	1.231000	-2.847000	-1.170000
C	2.109000	-0.372000	2.600000
H	1.569000	-1.278000	2.349000

C	2.526000	-0.156000	3.915000
H	2.334000	-0.913000	4.672000
C	3.174000	1.035000	4.258000
H	3.493000	1.211000	5.282000
C	3.407000	1.999000	3.272000
H	3.909000	2.929000	3.527000
C	2.999000	1.774000	1.955000
H	3.191000	2.537000	1.208000
C	2.337000	0.587000	1.603000
C	1.090000	2.890000	-0.389000
H	0.795000	2.851000	0.653000
C	0.843000	4.053000	-1.123000
H	0.362000	4.898000	-0.636000
C	1.198000	4.124000	-2.472000
H	1.001000	5.027000	-3.044000
C	1.803000	3.020000	-3.084000
H	2.082000	3.063000	-4.134000
C	2.047000	1.856000	-2.352000
H	2.503000	1.000000	-2.841000
C	1.696000	1.777000	-0.994000
C	3.397000	-0.547000	-0.740000
C	4.517000	0.300000	-0.745000
H	4.387000	1.342000	-0.470000
C	5.791000	-0.145000	-1.092000
H	6.632000	0.544000	-1.088000
C	5.965000	-1.491000	-1.433000
H	6.949000	-1.871000	-1.696000
C	4.871000	-2.345000	-1.442000
H	5.016000	-3.385000	-1.724000
C	3.556000	-1.910000	-1.116000
C	2.538000	-2.934000	-1.269000
H	2.930000	-3.898000	-1.609000
C	0.451000	-3.920000	-1.545000
C	-0.929000	-3.763000	-1.529000
C	-2.903000	-2.408000	-1.251000
H	-3.409000	-3.318000	-1.606000
C	-3.559000	-1.950000	0.042000
C	-4.580000	-2.725000	0.604000
H	-4.885000	-3.640000	0.099000
C	-5.211000	-2.352000	1.795000
H	-5.999000	-2.974000	2.211000
C	-4.817000	-1.181000	2.442000
H	-5.297000	-0.874000	3.368000
C	-3.798000	-0.395000	1.895000
H	-3.503000	0.515000	2.407000
C	-3.158000	-0.759000	0.700000
C	-1.537000	1.561000	1.273000
C	-0.818000	1.219000	2.429000
H	-0.468000	0.200000	2.559000
C	-0.524000	2.182000	3.395000
H	0.062000	1.905000	4.267000
C	-0.951000	3.503000	3.216000
H	-0.708000	4.260000	3.958000
C	-1.685000	3.847000	2.076000

H	-2.020000	4.872000	1.932000
C	-1.978000	2.881000	1.108000
H	-2.528000	3.165000	0.217000
C	-2.552000	1.143000	-1.392000
C	-3.939000	1.351000	-1.448000
H	-4.582000	0.942000	-0.674000
C	-4.504000	2.080000	-2.499000
H	-5.581000	2.227000	-2.535000
C	-3.686000	2.620000	-3.497000
H	-4.126000	3.189000	-4.313000
C	-2.303000	2.422000	-3.443000
H	-1.658000	2.838000	-4.212000
C	-1.739000	1.681000	-2.401000
H	-0.668000	1.518000	-2.374000
H	-1.564000	-4.572000	-1.904000
H	0.925000	-4.831000	-1.905000
H	0.034000	-0.618000	-1.968000
H	-3.051000	-1.638000	-2.026000
O	-0.424000	-2.333000	1.794000
C	0.113000	-3.656000	1.937000
H	1.201000	-3.552000	1.953000
H	-0.222000	-4.111000	2.879000
H	-0.163000	-4.287000	1.087000
H	-1.382000	-2.405000	1.645000

TS_{5c-6c}

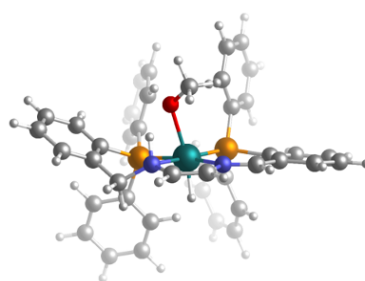


Ru	0.114000	-1.284000	-0.404000
P	-1.695000	0.137000	-0.095000
P	1.806000	0.180000	-0.136000
N	1.436000	-2.840000	-0.971000
N	-1.261000	-3.003000	-0.397000
C	-2.210000	0.390000	-2.886000
H	-1.404000	-0.330000	-2.997000
C	-2.893000	0.868000	-4.010000
H	-2.615000	0.510000	-4.999000
C	-3.923000	1.799000	-3.864000
H	-4.451000	2.174000	-4.738000
C	-4.274000	2.245000	-2.584000
H	-5.078000	2.966000	-2.458000
C	-3.597000	1.762000	-1.465000
H	-3.885000	2.114000	-0.479000
C	-2.546000	0.837000	-1.602000
C	-1.233000	2.898000	0.401000

H	-1.187000	3.010000	-0.677000
C	-1.006000	4.017000	1.206000
H	-0.780000	4.972000	0.738000
C	-1.070000	3.910000	2.598000
H	-0.905000	4.783000	3.224000
C	-1.335000	2.666000	3.178000
H	-1.369000	2.560000	4.260000
C	-1.532000	1.542000	2.374000
H	-1.704000	0.582000	2.844000
C	-1.511000	1.645000	0.972000
C	-3.180000	-0.731000	0.651000
C	-4.064000	-0.055000	1.509000
H	-3.889000	0.987000	1.752000
C	-5.174000	-0.685000	2.073000
H	-5.831000	-0.129000	2.737000
C	-5.429000	-2.024000	1.780000
H	-6.280000	-2.537000	2.220000
C	-4.580000	-2.700000	0.903000
H	-4.786000	-3.740000	0.659000
C	-3.467000	-2.077000	0.318000
C	-2.689000	-2.881000	-0.707000
H	-3.144000	-3.881000	-0.776000
C	-0.595000	-4.088000	-0.985000
H	-1.163000	-4.990000	-1.218000
C	0.735000	-4.039000	-1.191000
H	1.292000	-4.910000	-1.532000
C	2.708000	-2.856000	-1.234000
C	3.673000	-1.766000	-1.188000
C	4.977000	-2.134000	-1.607000
H	5.158000	-3.165000	-1.902000
C	6.022000	-1.222000	-1.653000
H	7.009000	-1.539000	-1.979000
C	5.787000	0.105000	-1.278000
H	6.589000	0.838000	-1.306000
C	4.512000	0.484000	-0.860000
H	4.353000	1.515000	-0.567000
C	3.440000	-0.420000	-0.802000
C	1.708000	1.876000	-0.886000
C	0.990000	1.991000	-2.087000
H	0.522000	1.107000	-2.506000
C	0.850000	3.225000	-2.724000
H	0.278000	3.290000	-3.646000
C	1.425000	4.371000	-2.167000
H	1.307000	5.336000	-2.654000
C	2.154000	4.268000	-0.978000
H	2.607000	5.152000	-0.537000
C	2.299000	3.030000	-0.346000
H	2.864000	2.976000	0.579000
C	2.264000	0.437000	1.638000
C	3.016000	-0.561000	2.282000
H	3.399000	-1.404000	1.714000
C	3.256000	-0.499000	3.654000
H	3.833000	-1.286000	4.134000
C	2.747000	0.562000	4.411000

H	2.934000	0.610000	5.481000
C	1.987000	1.550000	3.783000
H	1.568000	2.372000	4.359000
C	1.740000	1.484000	2.409000
H	1.125000	2.248000	1.949000
H	0.093000	-0.916000	-1.977000
H	-2.790000	-2.418000	-1.698000
O	0.007000	-2.348000	1.602000
C	-0.373000	-1.828000	2.840000
H	0.207000	-0.928000	3.099000
H	-1.448000	-1.555000	2.876000
H	-0.205000	-2.569000	3.644000
H	-0.962000	-2.929000	0.696000
H	3.131000	-3.805000	-1.579000

6c

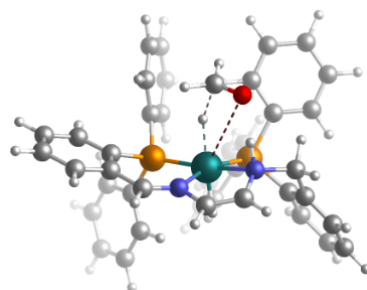


Ru	0.050000	-1.278000	-0.416000
P	1.758000	0.167000	-0.098000
P	-1.740000	0.173000	-0.037000
N	-1.421000	-2.895000	-0.682000
N	1.329000	-2.834000	-1.008000
C	1.903000	-0.205000	2.653000
H	1.301000	-1.076000	2.418000
C	2.287000	0.058000	3.970000
H	2.026000	-0.650000	4.754000
C	2.978000	1.231000	4.281000
H	3.269000	1.442000	5.308000
C	3.285000	2.142000	3.265000
H	3.811000	3.065000	3.498000
C	2.917000	1.872000	1.944000
H	3.162000	2.595000	1.173000
C	2.224000	0.693000	1.624000
C	1.063000	2.889000	-0.484000
H	0.729000	2.875000	0.547000
C	0.849000	4.034000	-1.255000
H	0.353000	4.893000	-0.810000
C	1.259000	4.070000	-2.590000
H	1.089000	4.960000	-3.191000
C	1.883000	2.950000	-3.150000
H	2.203000	2.966000	-4.189000
C	2.089000	1.803000	-2.381000
H	2.555000	0.932000	-2.834000
C	1.686000	1.760000	-1.036000
C	3.408000	-0.508000	-0.647000

C	4.512000	0.359000	-0.641000
H	4.362000	1.400000	-0.378000
C	5.800000	-0.068000	-0.961000
H	6.626000	0.638000	-0.939000
C	6.017000	-1.407000	-1.302000
H	7.014000	-1.762000	-1.547000
C	4.938000	-2.280000	-1.332000
H	5.103000	-3.318000	-1.612000
C	3.621000	-1.862000	-1.018000
C	2.616000	-2.904000	-1.179000
H	3.019000	-3.855000	-1.539000
C	0.594000	-3.984000	-1.370000
C	-0.743000	-3.995000	-1.269000
C	-2.781000	-2.620000	-1.193000
H	-3.262000	-3.557000	-1.507000
C	-3.632000	-1.967000	-0.124000
C	-4.804000	-2.621000	0.278000
H	-5.074000	-3.561000	-0.198000
C	-5.625000	-2.098000	1.280000
H	-6.529000	-2.626000	1.574000
C	-5.264000	-0.905000	1.904000
H	-5.883000	-0.484000	2.692000
C	-4.095000	-0.245000	1.515000
H	-3.828000	0.682000	2.011000
C	-3.269000	-0.752000	0.500000
C	-1.580000	1.420000	1.309000
C	-1.071000	0.947000	2.530000
H	-0.832000	-0.111000	2.627000
C	-0.865000	1.830000	3.591000
H	-0.450000	1.458000	4.524000
C	-1.162000	3.189000	3.443000
H	-0.987000	3.878000	4.267000
C	-1.677000	3.662000	2.232000
H	-1.909000	4.717000	2.112000
C	-1.890000	2.780000	1.168000
H	-2.280000	3.157000	0.227000
C	-2.412000	1.155000	-1.458000
C	-3.753000	1.577000	-1.498000
H	-4.438000	1.294000	-0.705000
C	-4.220000	2.361000	-2.557000
H	-5.261000	2.675000	-2.575000
C	-3.352000	2.739000	-3.587000
H	-3.716000	3.350000	-4.410000
C	-2.019000	2.321000	-3.555000
H	-1.334000	2.609000	-4.348000
C	-1.554000	1.530000	-2.502000
H	-0.525000	1.193000	-2.492000
H	-1.328000	-4.853000	-1.598000
H	1.142000	-4.853000	-1.731000
H	0.071000	-0.796000	-1.964000
H	-2.685000	-1.986000	-2.083000
H	-1.375000	-2.936000	0.374000
O	-0.371000	-2.237000	1.631000
C	0.375000	-3.325000	2.090000

H	1.465000	-3.121000	2.141000
H	0.056000	-3.616000	3.110000
H	0.269000	-4.232000	1.459000

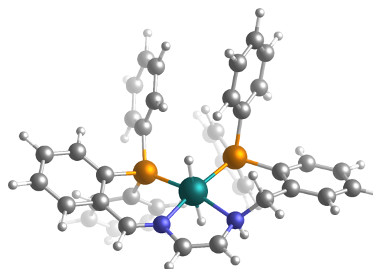
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Ru	0.030000	-1.211000	-0.244000
P	1.730000	0.333000	-0.170000
P	-1.776000	0.091000	0.022000
N	1.546000	-2.834000	-0.223000
N	-1.131000	-2.891000	-0.719000
C	1.419000	2.080000	-0.679000
C	0.626000	2.291000	-1.818000
H	0.282000	1.434000	-2.387000
C	0.254000	3.580000	-2.199000
H	-0.385000	3.718000	-3.067000
C	0.678000	4.681000	-1.446000
H	0.377000	5.686000	-1.731000
C	1.486000	4.482000	-0.323000
H	1.823000	5.333000	0.265000
C	1.857000	3.188000	0.059000
H	2.468000	3.047000	0.946000
C	2.672000	0.546000	1.406000
C	4.071000	0.635000	1.460000
H	4.655000	0.565000	0.546000
C	4.721000	0.813000	2.685000
H	5.807000	0.869000	2.717000
C	3.978000	0.920000	3.865000
H	4.484000	1.059000	4.817000
C	2.582000	0.843000	3.815000
H	1.995000	0.927000	4.727000
C	1.933000	0.647000	2.595000
H	0.852000	0.565000	2.560000
C	3.036000	-0.235000	-1.368000
C	3.569000	0.636000	-2.327000
H	3.279000	1.682000	-2.324000
C	4.469000	0.186000	-3.300000
H	4.865000	0.885000	-4.032000
C	4.848000	-1.155000	-3.324000
H	5.540000	-1.521000	-4.079000
C	4.336000	-2.029000	-2.360000
H	4.645000	-3.072000	-2.365000
C	3.439000	-1.593000	-1.380000
C	3.004000	-2.572000	-0.309000
H	3.543000	-3.520000	-0.441000

H	3.282000	-2.183000	0.676000
C	1.014000	-3.864000	-1.063000
C	-0.312000	-3.920000	-1.248000
C	-2.408000	-3.124000	-0.654000
H	-2.768000	-4.086000	-1.030000
C	-3.440000	-2.274000	-0.071000
C	-4.695000	-2.910000	0.092000
H	-4.805000	-3.940000	-0.240000
C	-5.778000	-2.266000	0.675000
H	-6.723000	-2.788000	0.796000
C	-5.636000	-0.942000	1.104000
H	-6.470000	-0.418000	1.565000
C	-4.418000	-0.289000	0.925000
H	-4.329000	0.744000	1.245000
C	-3.305000	-0.922000	0.349000
C	-1.683000	1.206000	1.493000
C	-1.875000	0.667000	2.778000
H	-2.209000	-0.361000	2.885000
C	-1.617000	1.430000	3.917000
H	-1.773000	0.997000	4.902000
C	-1.148000	2.744000	3.793000
H	-0.936000	3.335000	4.680000
C	-0.946000	3.284000	2.521000
H	-0.566000	4.297000	2.408000
C	-1.214000	2.523000	1.379000
H	-1.034000	2.958000	0.402000
C	-2.481000	1.163000	-1.328000
C	-3.278000	2.295000	-1.103000
H	-3.478000	2.633000	-0.091000
C	-3.812000	3.015000	-2.176000
H	-4.416000	3.898000	-1.984000
C	-3.569000	2.602000	-3.490000
H	-3.984000	3.162000	-4.324000
C	-2.791000	1.463000	-3.723000
H	-2.598000	1.132000	-4.741000
C	-2.250000	0.751000	-2.649000
H	-1.619000	-0.117000	-2.825000
O	1.121000	-3.484000	2.448000
C	0.257000	-2.659000	2.801000
H	-0.818000	-2.905000	2.757000
H	0.522000	-1.790000	3.424000
H	-0.070000	-1.391000	1.473000
H	0.199000	-0.962000	-1.898000
H	1.688000	-4.619000	-1.463000
H	1.382000	-3.144000	0.754000
H	-0.789000	-4.749000	-1.766000

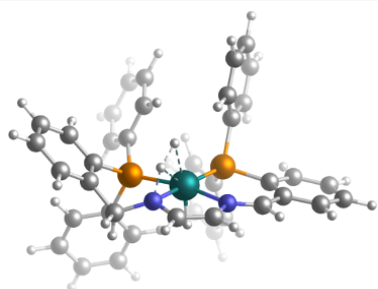
7c



Ru	0.018000	1.420000	-0.216000
P	-1.725000	-0.075000	-0.062000
P	1.778000	0.023000	0.057000
N	1.323000	3.056000	-0.284000
N	-1.421000	3.016000	-0.734000
C	-2.077000	0.013000	2.734000
H	-1.466000	0.909000	2.651000
C	-2.574000	-0.398000	3.975000
H	-2.364000	0.197000	4.861000
C	-3.326000	-1.571000	4.078000
H	-3.706000	-1.897000	5.043000
C	-3.590000	-2.322000	2.928000
H	-4.178000	-3.235000	2.994000
C	-3.103000	-1.903000	1.688000
H	-3.326000	-2.498000	0.808000
C	-2.325000	-0.739000	1.578000
C	-1.033000	-2.777000	-0.595000
H	-0.818000	-2.865000	0.465000
C	-0.742000	-3.854000	-1.439000
H	-0.307000	-4.756000	-1.017000
C	-0.996000	-3.765000	-2.808000
H	-0.767000	-4.602000	-3.464000
C	-1.533000	-2.584000	-3.335000
H	-1.725000	-2.498000	-4.401000
C	-1.807000	-1.504000	-2.495000
H	-2.187000	-0.579000	-2.920000
C	-1.573000	-1.590000	-1.112000
C	-3.373000	0.643000	-0.602000
C	-4.383000	-0.217000	-1.067000
H	-4.175000	-1.276000	-1.169000
C	-5.655000	0.249000	-1.401000
H	-6.409000	-0.448000	-1.757000
C	-5.948000	1.607000	-1.271000
H	-6.932000	1.989000	-1.528000
C	-4.958000	2.475000	-0.810000
H	-5.184000	3.535000	-0.711000
C	-3.675000	2.020000	-0.466000
C	-2.688000	3.057000	0.037000
H	-3.151000	4.051000	-0.050000
C	-0.694000	4.253000	-0.771000
H	-1.245000	5.174000	-0.954000
C	0.634000	4.244000	-0.613000
H	1.210000	5.166000	-0.686000
C	2.577000	3.219000	0.047000
H	2.993000	4.226000	-0.042000

C	3.465000	2.255000	0.672000
C	4.659000	2.808000	1.198000
H	4.865000	3.863000	1.028000
C	5.552000	2.052000	1.947000
H	6.453000	2.510000	2.345000
C	5.267000	0.706000	2.195000
H	5.943000	0.099000	2.792000
C	4.112000	0.134000	1.658000
H	3.917000	-0.919000	1.837000
C	3.206000	0.872000	0.880000
C	1.598000	-1.500000	1.099000
C	0.916000	-1.364000	2.318000
H	0.566000	-0.381000	2.615000
C	0.654000	-2.476000	3.118000
H	0.095000	-2.353000	4.042000
C	1.083000	-3.746000	2.713000
H	0.869000	-4.616000	3.328000
C	1.781000	-3.889000	1.511000
H	2.118000	-4.872000	1.189000
C	2.038000	-2.773000	0.706000
H	2.559000	-2.904000	-0.236000
C	2.608000	-0.679000	-1.457000
C	3.996000	-0.852000	-1.577000
H	4.662000	-0.527000	-0.784000
C	4.546000	-1.443000	-2.721000
H	5.624000	-1.558000	-2.800000
C	3.714000	-1.884000	-3.753000
H	4.140000	-2.348000	-4.639000
C	2.330000	-1.716000	-3.640000
H	1.669000	-2.052000	-4.436000
C	1.785000	-1.108000	-2.509000
H	0.716000	-0.946000	-2.444000
H	-0.112000	1.731000	1.463000
H	-2.421000	2.899000	1.087000
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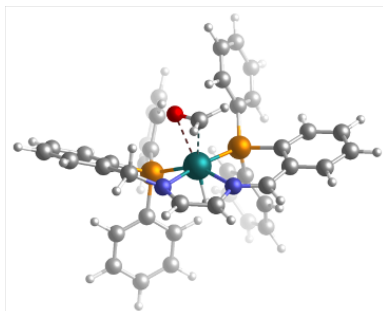


Ru	0.032000	1.422000	0.118000
P	-1.756000	-0.060000	-0.007000
P	1.765000	-0.023000	0.022000
N	1.315000	3.090000	0.404000
N	-1.424000	3.088000	0.035000
C	-1.677000	-0.977000	2.640000

H	-0.609000	-0.824000	2.543000
C	-2.202000	-1.491000	3.828000
H	-1.529000	-1.751000	4.641000
C	-3.583000	-1.661000	3.972000
H	-3.993000	-2.051000	4.900000
C	-4.435000	-1.321000	2.917000
H	-5.511000	-1.445000	3.021000
C	-3.909000	-0.823000	1.720000
H	-4.581000	-0.573000	0.905000
C	-2.524000	-0.645000	1.572000
C	-1.999000	-2.881000	-0.497000
H	-2.523000	-2.960000	0.450000
C	-1.741000	-4.037000	-1.241000
H	-2.077000	-5.002000	-0.868000
C	-1.042000	-3.956000	-2.449000
H	-0.828000	-4.858000	-3.017000
C	-0.616000	-2.710000	-2.923000
H	-0.059000	-2.634000	-3.853000
C	-0.877000	-1.557000	-2.182000
H	-0.530000	-0.593000	-2.538000
C	-1.559000	-1.632000	-0.957000
C	-3.215000	0.716000	-0.874000
C	-3.966000	-0.019000	-1.804000
H	-3.703000	-1.050000	-2.012000
C	-5.054000	0.546000	-2.475000
H	-5.617000	-0.052000	-3.188000
C	-5.408000	1.870000	-2.225000
H	-6.249000	2.326000	-2.742000
C	-4.666000	2.614000	-1.305000
H	-4.937000	3.650000	-1.113000
C	-3.577000	2.061000	-0.620000
C	-2.836000	2.936000	0.375000
H	-3.319000	3.924000	0.404000
C	-0.773000	4.253000	0.343000
H	-1.357000	5.167000	0.461000
C	0.581000	4.283000	0.450000
H	1.120000	5.219000	0.588000
C	2.603000	3.177000	0.591000
H	3.011000	4.181000	0.743000
C	3.592000	2.117000	0.691000
C	4.902000	2.568000	0.998000
H	5.071000	3.638000	1.100000
C	5.963000	1.694000	1.181000
H	6.951000	2.081000	1.418000
C	5.747000	0.317000	1.062000
H	6.562000	-0.388000	1.206000
C	4.471000	-0.147000	0.749000
H	4.317000	-1.217000	0.656000
C	3.382000	0.719000	0.553000
C	1.659000	-1.511000	1.119000
C	1.971000	-1.370000	2.483000
H	2.376000	-0.431000	2.849000
C	1.750000	-2.418000	3.377000
H	2.000000	-2.290000	4.428000

C	1.200000	-3.624000	2.926000
H	1.018000	-4.437000	3.624000
C	0.880000	-3.770000	1.575000
H	0.441000	-4.695000	1.211000
C	1.110000	-2.723000	0.677000
H	0.846000	-2.857000	-0.365000
C	2.301000	-0.700000	-1.631000
C	2.997000	-1.907000	-1.804000
H	3.219000	-2.540000	-0.951000
C	3.399000	-2.323000	-3.076000
H	3.925000	-3.268000	-3.190000
C	3.126000	-1.530000	-4.195000
H	3.439000	-1.855000	-5.184000
C	2.449000	-0.318000	-4.031000
H	2.233000	0.309000	-4.893000
C	2.039000	0.091000	-2.760000
H	1.486000	1.020000	-2.638000
H	0.106000	1.171000	1.732000
H	-2.911000	2.510000	1.387000
H	-0.335000	1.922000	-1.691000
H	-0.997000	2.592000	-1.038000

8c

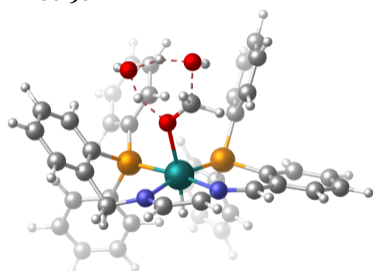


Ru	0.018000	-1.320000	-0.311000
P	-1.848000	0.055000	-0.107000
P	1.795000	0.173000	0.027000
N	1.572000	-2.764000	-0.354000
N	-1.087000	-3.064000	0.257000
C	-1.887000	1.085000	-2.718000
H	-1.285000	0.216000	-2.954000
C	-2.208000	1.990000	-3.734000
H	-1.894000	1.780000	-4.753000
C	-2.908000	3.162000	-3.439000
H	-3.152000	3.869000	-4.229000
C	-3.286000	3.424000	-2.119000
H	-3.825000	4.336000	-1.875000
C	-2.974000	2.516000	-1.105000
H	-3.274000	2.743000	-0.088000
C	-2.270000	1.332000	-1.389000
C	-1.260000	2.288000	1.552000
H	-0.879000	2.771000	0.659000
C	-1.127000	2.936000	2.783000
H	-0.648000	3.912000	2.821000
C	-1.587000	2.328000	3.953000

H	-1.478000	2.830000	4.911000
C	-2.185000	1.065000	3.883000
H	-2.546000	0.580000	4.787000
C	-2.322000	0.418000	2.653000
H	-2.779000	-0.567000	2.616000
C	-1.861000	1.022000	1.472000
C	-3.433000	-0.904000	0.034000
C	-4.649000	-0.214000	-0.100000
H	-4.635000	0.839000	-0.356000
C	-5.887000	-0.825000	0.086000
H	-6.802000	-0.251000	-0.031000
C	-5.928000	-2.180000	0.432000
H	-6.879000	-2.683000	0.590000
C	-4.742000	-2.886000	0.567000
H	-4.783000	-3.941000	0.829000
C	-3.466000	-2.292000	0.363000
C	-2.359000	-3.216000	0.533000
H	-2.652000	-4.200000	0.910000
C	-0.209000	-4.111000	0.443000
H	-0.584000	-5.055000	0.833000
C	1.111000	-3.943000	0.060000
H	1.775000	-4.814000	0.055000
C	2.701000	-2.789000	-1.259000
H	3.347000	-3.645000	-1.004000
C	3.590000	-1.560000	-1.379000
C	4.802000	-1.784000	-2.058000
H	5.036000	-2.797000	-2.383000
C	5.699000	-0.758000	-2.339000
H	6.625000	-0.974000	-2.867000
C	5.397000	0.546000	-1.937000
H	6.080000	1.365000	-2.148000
C	4.208000	0.788000	-1.257000
H	3.982000	1.802000	-0.941000
C	3.294000	-0.246000	-0.965000
C	1.569000	1.968000	-0.321000
C	0.960000	2.299000	-1.541000
H	0.695000	1.508000	-2.235000
C	0.670000	3.628000	-1.849000
H	0.168000	3.864000	-2.783000
C	0.995000	4.644000	-0.942000
H	0.757000	5.679000	-1.175000
C	1.623000	4.323000	0.265000
H	1.883000	5.108000	0.971000
C	1.911000	2.990000	0.577000
H	2.379000	2.748000	1.526000
C	2.437000	0.156000	1.763000
C	3.795000	-0.034000	2.058000
H	4.511000	-0.202000	1.261000
C	4.243000	-0.016000	3.384000
H	5.298000	-0.175000	3.595000
C	3.343000	0.204000	4.429000
H	3.692000	0.220000	5.458000
C	1.987000	0.397000	4.141000
H	1.272000	0.566000	4.942000

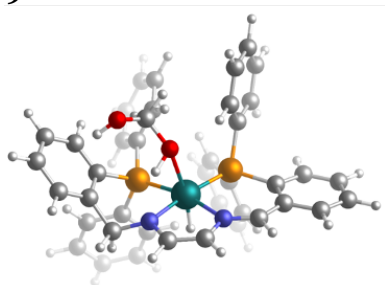
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O	0.358000	-1.148000	-2.573000
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H	0.020000	-1.302000	1.281000
H	-0.123000	-3.142000	-2.366000
H	-1.544000	-1.950000	-2.566000
H	2.334000	-2.979000	-2.283000

TS_{8c-9c}



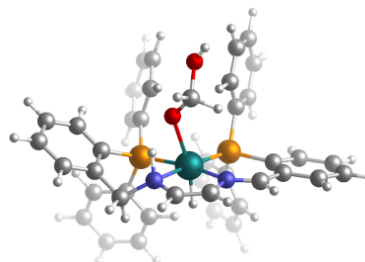
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P	-1.742000	0.324000	-0.061000
N	-1.318000	-1.647000	-2.376000
N	1.380000	-1.838000	-2.330000
C	2.831000	-1.291000	1.785000
H	2.834000	-1.966000	0.933000
C	3.303000	-1.739000	3.020000
H	3.640000	-2.768000	3.129000
C	3.368000	-0.856000	4.107000
H	3.731000	-1.199000	5.072000
C	2.991000	0.474000	3.924000
H	3.060000	1.178000	4.750000
C	2.527000	0.922000	2.680000
H	2.265000	1.967000	2.569000
C	2.415000	0.042000	1.596000
C	0.815000	2.950000	0.791000
H	0.379000	2.404000	1.619000
C	0.530000	4.311000	0.664000
H	-0.097000	4.797000	1.408000
C	1.023000	5.035000	-0.424000
H	0.795000	6.092000	-0.530000
C	1.801000	4.381000	-1.385000
H	2.182000	4.928000	-2.244000
C	2.093000	3.021000	-1.252000
H	2.688000	2.527000	-2.014000
C	1.612000	2.285000	-0.156000
C	3.430000	0.167000	-0.952000
C	4.510000	0.968000	-0.545000
H	4.325000	1.777000	0.158000
C	5.809000	0.761000	-1.002000
H	6.617000	1.409000	-0.674000
C	6.049000	-0.306000	-1.880000
H	7.054000	-0.501000	-2.246000
C	5.001000	-1.119000	-2.283000

H	5.202000	-1.942000	-2.965000
C	3.659000	-0.914000	-1.849000
C	2.697000	-1.841000	-2.407000
H	3.137000	-2.595000	-3.068000
C	0.655000	-2.721000	-3.086000
H	1.168000	-3.429000	-3.734000
C	-0.732000	-2.569000	-3.114000
H	-1.328000	-3.201000	-3.780000
C	-2.741000	-1.406000	-2.480000
H	-2.897000	-0.365000	-2.803000
C	-3.472000	-1.630000	-1.164000
C	-4.493000	-2.585000	-1.103000
H	-4.725000	-3.166000	-1.994000
C	-5.215000	-2.811000	0.072000
H	-6.000000	-3.564000	0.093000
C	-4.921000	-2.064000	1.212000
H	-5.478000	-2.219000	2.133000
C	-3.899000	-1.111000	1.168000
H	-3.686000	-0.531000	2.062000
C	-3.159000	-0.885000	-0.003000
C	-1.617000	0.775000	1.734000
C	-0.803000	-0.046000	2.531000
H	-0.251000	-0.851000	2.056000
C	-0.661000	0.196000	3.899000
H	-0.008000	-0.438000	4.493000
C	-1.320000	1.281000	4.487000
H	-1.201000	1.483000	5.548000
C	-2.120000	2.114000	3.698000
H	-2.627000	2.966000	4.147000
C	-2.274000	1.860000	2.331000
H	-2.895000	2.517000	1.730000
C	-2.547000	1.807000	-0.820000
C	-3.927000	2.048000	-0.706000
H	-4.561000	1.340000	-0.179000
C	-4.498000	3.189000	-1.276000
H	-5.568000	3.359000	-1.186000
C	-3.695000	4.105000	-1.965000
H	-4.139000	4.992000	-2.411000
C	-2.323000	3.869000	-2.086000
H	-1.690000	4.571000	-2.623000
C	-1.752000	2.724000	-1.524000
H	-0.692000	2.535000	-1.642000
O	-0.329000	-2.662000	0.134000
C	0.547000	-3.604000	0.409000
H	0.142000	0.548000	-2.142000
H	0.221000	-4.639000	0.234000
H	1.567000	-3.428000	0.051000
H	-3.191000	-2.050000	-3.251000
O	0.721000	-3.707000	2.030000
H	-0.467000	-3.508000	2.315000
O	-1.635000	-3.282000	2.070000
H	-1.342000	-2.910000	1.077000
H	-2.000000	-2.529000	2.565000
H	1.234000	-2.920000	2.304000

9c

Ru	0.031000	-1.002000	-0.813000
P	1.891000	0.080000	-0.054000
P	-1.628000	0.436000	-0.099000
N	-1.502000	-2.221000	-1.669000
N	1.206000	-2.498000	-1.812000
C	1.968000	-1.260000	2.381000
H	1.447000	-2.027000	1.814000
C	2.269000	-1.472000	3.728000
H	1.992000	-2.412000	4.199000
C	2.918000	-0.478000	4.468000
H	3.145000	-0.638000	5.519000
C	3.278000	0.721000	3.846000
H	3.788000	1.497000	4.411000
C	2.987000	0.929000	2.494000
H	3.277000	1.866000	2.030000
C	2.317000	-0.053000	1.751000
C	1.428000	2.860000	0.390000
H	1.053000	2.589000	1.370000
C	1.332000	4.191000	-0.027000
H	0.888000	4.926000	0.639000
C	1.788000	4.568000	-1.292000
H	1.708000	5.602000	-1.618000
C	2.343000	3.603000	-2.140000
H	2.699000	3.883000	-3.128000
C	2.437000	2.274000	-1.725000
H	2.857000	1.532000	-2.398000
C	1.983000	1.884000	-0.452000
C	3.488000	-0.554000	-0.747000
C	4.659000	0.167000	-0.466000
H	4.581000	1.102000	0.081000
C	5.919000	-0.273000	-0.864000
H	6.803000	0.315000	-0.631000
C	6.025000	-1.484000	-1.558000
H	6.996000	-1.857000	-1.873000
C	4.879000	-2.211000	-1.849000
H	4.970000	-3.147000	-2.395000
C	3.582000	-1.775000	-1.467000
C	2.503000	-2.642000	-1.914000
H	2.849000	-3.516000	-2.475000
C	0.386000	-3.413000	-2.452000
C	-0.976000	-3.207000	-2.413000
C	-2.884000	-1.826000	-1.901000
H	-2.909000	-0.928000	-2.540000
C	-3.611000	-1.537000	-0.599000

C	-4.741000	-2.296000	-0.266000
H	-5.070000	-3.077000	-0.949000
C	-5.444000	-2.080000	0.924000
H	-6.312000	-2.689000	1.161000
C	-5.016000	-1.083000	1.802000
H	-5.547000	-0.902000	2.732000
C	-3.892000	-0.315000	1.482000
H	-3.569000	0.457000	2.174000
C	-3.176000	-0.527000	0.294000
C	-1.437000	1.491000	1.409000
C	-0.769000	0.935000	2.511000
H	-0.400000	-0.082000	2.458000
C	-0.527000	1.690000	3.659000
H	0.014000	1.243000	4.489000
C	-0.949000	3.022000	3.718000
H	-0.748000	3.620000	4.604000
C	-1.623000	3.584000	2.629000
H	-1.953000	4.620000	2.668000
C	-1.869000	2.823000	1.482000
H	-2.379000	3.278000	0.639000
C	-2.246000	1.657000	-1.344000
C	-3.611000	1.926000	-1.526000
H	-4.355000	1.385000	-0.948000
C	-4.027000	2.889000	-2.451000
H	-5.089000	3.081000	-2.588000
C	-3.082000	3.604000	-3.192000
H	-3.405000	4.354000	-3.910000
C	-1.719000	3.346000	-3.009000
H	-0.974000	3.896000	-3.579000
C	-1.304000	2.374000	-2.098000
H	-0.247000	2.170000	-1.974000
H	0.164000	-0.101000	-2.099000
H	-3.427000	-2.615000	-2.443000
O	-0.569000	-2.971000	0.906000
C	-1.336000	-2.873000	2.096000
H	-0.671000	-3.174000	2.908000
H	0.831000	-4.245000	-2.992000
H	-1.635000	-3.864000	-2.987000
O	-2.439000	-3.744000	2.113000
H	-3.190000	-3.311000	1.673000
H	-1.672000	-1.840000	2.247000
H	-1.171000	-2.983000	0.126000

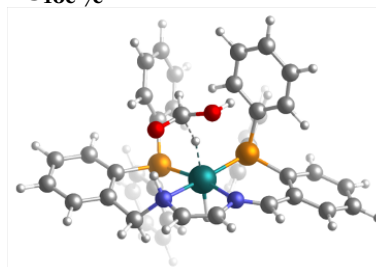
10c

Ru	0.041000	-1.063000	-0.777000
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N	-1.430000	-2.548000	-1.471000
N	1.328000	-2.442000	-1.703000
C	2.017000	-0.693000	2.435000
H	1.507000	-1.557000	2.028000
C	2.414000	-0.713000	3.773000
H	2.222000	-1.607000	4.361000
C	3.014000	0.412000	4.343000
H	3.313000	0.406000	5.389000
C	3.219000	1.555000	3.563000
H	3.677000	2.440000	3.999000
C	2.834000	1.570000	2.220000
H	3.004000	2.468000	1.635000
C	2.225000	0.443000	1.643000
C	0.974000	3.009000	0.034000
H	0.614000	2.765000	1.027000
C	0.751000	4.291000	-0.476000
H	0.223000	5.023000	0.129000
C	1.189000	4.623000	-1.760000
H	1.011000	5.618000	-2.159000
C	1.850000	3.662000	-2.533000
H	2.191000	3.907000	-3.536000
C	2.070000	2.380000	-2.023000
H	2.569000	1.639000	-2.641000
C	1.641000	2.040000	-0.730000
C	3.394000	-0.239000	-0.829000
C	4.493000	0.607000	-0.618000
H	4.336000	1.557000	-0.117000
C	5.783000	0.272000	-1.025000
H	6.606000	0.957000	-0.839000
C	6.007000	-0.952000	-1.665000
H	7.006000	-1.236000	-1.983000
C	4.934000	-1.802000	-1.895000
H	5.105000	-2.748000	-2.403000
C	3.614000	-1.473000	-1.496000
C	2.615000	-2.460000	-1.886000
H	3.026000	-3.303000	-2.450000
C	0.599000	-3.483000	-2.318000
C	-0.742000	-3.493000	-2.273000
C	-2.772000	-2.128000	-1.929000
H	-2.646000	-1.281000	-2.614000
C	-3.647000	-1.774000	-0.743000
C	-4.836000	-2.492000	-0.562000
H	-5.106000	-3.256000	-1.288000
C	-5.672000	-2.258000	0.531000
H	-6.588000	-2.830000	0.649000
C	-5.308000	-1.298000	1.475000
H	-5.937000	-1.109000	2.341000
C	-4.124000	-0.577000	1.309000
H	-3.851000	0.162000	2.055000
C	-3.284000	-0.788000	0.204000
C	-1.562000	1.012000	1.639000
C	-1.074000	0.178000	2.660000

H	-0.851000	-0.865000	2.441000
C	-0.867000	0.693000	3.941000
H	-0.474000	0.043000	4.717000
C	-1.131000	2.040000	4.213000
H	-0.952000	2.440000	5.208000
C	-1.617000	2.872000	3.199000
H	-1.822000	3.920000	3.403000
C	-1.838000	2.359000	1.917000
H	-2.209000	3.014000	1.135000
C	-2.404000	1.593000	-1.099000
C	-3.701000	2.107000	-0.917000
H	-4.347000	1.694000	-0.149000
C	-4.174000	3.146000	-1.722000
H	-5.180000	3.529000	-1.569000
C	-3.358000	3.686000	-2.722000
H	-3.727000	4.494000	-3.350000
C	-2.072000	3.177000	-2.913000
H	-1.427000	3.589000	-3.685000
C	-1.599000	2.136000	-2.110000
H	-0.604000	1.737000	-2.270000
H	0.080000	-0.229000	-2.155000
H	-3.250000	-2.941000	-2.494000
O	-0.474000	-2.563000	0.937000
C	0.241000	-3.627000	1.355000
H	-0.320000	-4.582000	1.247000
H	1.154000	-4.255000	-2.849000
H	-1.320000	-4.248000	-2.806000
O	0.543000	-3.474000	2.783000
H	0.936000	-4.304000	3.102000
H	1.213000	-3.736000	0.824000
H	-1.419000	-2.869000	-0.464000

TS_{10c-7c}

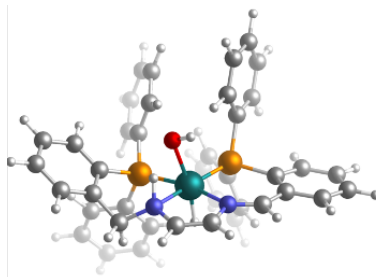


Ru	0.104000	-0.994000	-0.784000
P	-1.775000	0.190000	-0.129000
P	1.762000	0.435000	-0.176000
N	1.559000	-2.297000	-1.599000
N	-1.147000	-2.764000	-1.133000
C	-2.141000	1.676000	-2.503000
H	-1.460000	0.944000	-2.927000
C	-2.686000	2.678000	-3.313000
H	-2.432000	2.710000	-4.370000
C	-3.541000	3.638000	-2.765000
H	-3.959000	4.424000	-3.391000
C	-3.858000	3.580000	-1.403000

H	-4.525000	4.318000	-0.964000
C	-3.322000	2.571000	-0.598000
H	-3.591000	2.544000	0.453000
C	-2.445000	1.612000	-1.135000
C	-1.298000	2.180000	1.858000
H	-1.103000	2.868000	1.043000
C	-1.117000	2.619000	3.175000
H	-0.793000	3.641000	3.356000
C	-1.338000	1.750000	4.247000
H	-1.195000	2.092000	5.269000
C	-1.737000	0.431000	3.993000
H	-1.903000	-0.259000	4.817000
C	-1.915000	-0.008000	2.680000
H	-2.217000	-1.036000	2.500000
C	-1.710000	0.864000	1.595000
C	-3.337000	-0.845000	-0.081000
C	-4.412000	-0.410000	0.717000
H	-4.302000	0.482000	1.324000
C	-5.625000	-1.096000	0.761000
H	-6.431000	-0.730000	1.392000
C	-5.790000	-2.250000	-0.008000
H	-6.725000	-2.804000	0.016000
C	-4.736000	-2.694000	-0.806000
H	-4.861000	-3.597000	-1.399000
C	-3.509000	-2.009000	-0.866000
C	-2.461000	-2.576000	-1.802000
H	-2.822000	-3.540000	-2.183000
C	-0.324000	-3.756000	-1.773000
H	-0.795000	-4.689000	-2.079000
C	0.985000	-3.543000	-1.940000
H	1.631000	-4.303000	-2.377000
C	2.795000	-2.128000	-1.969000
H	3.295000	-2.971000	-2.452000
C	3.594000	-0.910000	-1.918000
C	4.810000	-0.982000	-2.637000
H	5.071000	-1.915000	-3.132000
C	5.666000	0.110000	-2.741000
H	6.589000	0.026000	-3.309000
C	5.324000	1.310000	-2.112000
H	5.978000	2.176000	-2.182000
C	4.138000	1.394000	-1.377000
H	3.900000	2.327000	-0.877000
C	3.260000	0.307000	-1.262000
C	1.508000	2.262000	-0.062000
C	0.784000	2.863000	-1.103000
H	0.426000	2.252000	-1.925000
C	0.499000	4.230000	-1.077000
H	-0.075000	4.675000	-1.885000
C	0.934000	5.015000	-0.002000
H	0.700000	6.076000	0.029000
C	1.667000	4.426000	1.033000
H	2.011000	5.029000	1.871000
C	1.958000	3.058000	1.002000
H	2.524000	2.618000	1.817000

C	2.505000	-0.009000	1.473000
C	3.763000	-0.621000	1.601000
H	4.400000	-0.758000	0.734000
C	4.212000	-1.080000	2.847000
H	5.183000	-1.564000	2.920000
C	3.420000	-0.919000	3.987000
H	3.768000	-1.277000	4.953000
C	2.170000	-0.295000	3.873000
H	1.540000	-0.163000	4.749000
C	1.717000	0.145000	2.629000
H	0.737000	0.598000	2.553000
H	-0.059000	-0.406000	-2.370000
H	-2.294000	-1.920000	-2.662000
H	0.216000	-1.671000	0.793000
C	0.098000	-2.925000	1.962000
H	-0.057000	-2.105000	2.677000
O	1.395000	-3.378000	1.928000
H	1.990000	-2.638000	2.148000
O	-0.812000	-3.691000	1.619000
H	-1.308000	-3.104000	-0.170000

11c

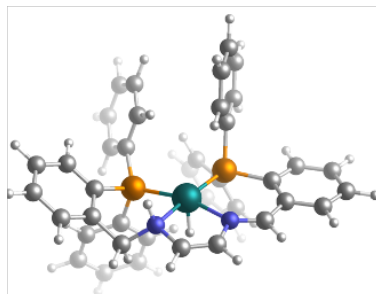


Ru	0.035000	1.376000	0.228000
P	1.764000	-0.068000	0.072000
P	-1.745000	-0.117000	0.022000
N	-1.446000	3.009000	0.262000
N	1.303000	3.016000	0.584000
C	1.969000	0.091000	-2.705000
H	1.341000	0.966000	-2.561000
C	2.386000	-0.276000	-3.987000
H	2.123000	0.352000	-4.835000
C	3.117000	-1.451000	-4.182000
H	3.434000	-1.742000	-5.181000
C	3.428000	-2.260000	-3.084000
H	3.987000	-3.182000	-3.225000
C	3.023000	-1.887000	-1.800000
H	3.272000	-2.533000	-0.964000
C	2.287000	-0.709000	-1.596000
C	1.117000	-2.771000	0.642000
H	0.825000	-2.850000	-0.399000
C	0.898000	-3.856000	1.496000
H	0.438000	-4.759000	1.103000
C	1.256000	-3.776000	2.843000
H	1.083000	-4.618000	3.507000
C	1.833000	-2.599000	3.334000

H	2.113000	-2.524000	4.382000
C	2.042000	-1.512000	2.484000
H	2.468000	-0.595000	2.882000
C	1.691000	-1.586000	1.125000
C	3.393000	0.672000	0.596000
C	4.496000	-0.184000	0.748000
H	4.352000	-1.253000	0.629000
C	5.773000	0.286000	1.047000
H	6.598000	-0.413000	1.154000
C	5.981000	1.661000	1.200000
H	6.971000	2.050000	1.426000
C	4.905000	2.527000	1.068000
H	5.064000	3.595000	1.201000
C	3.597000	2.065000	0.775000
C	2.590000	3.117000	0.751000
H	2.987000	4.115000	0.961000
C	0.560000	4.205000	0.756000
C	-0.782000	4.181000	0.680000
C	-2.821000	2.809000	0.757000
H	-3.309000	3.781000	0.918000
C	-3.641000	2.008000	-0.234000
C	-4.804000	2.591000	-0.754000
H	-5.086000	3.589000	-0.423000
C	-5.599000	1.928000	-1.690000
H	-6.496000	2.404000	-2.078000
C	-5.222000	0.659000	-2.129000
H	-5.821000	0.128000	-2.864000
C	-4.062000	0.068000	-1.622000
H	-3.781000	-0.919000	-1.975000
C	-3.262000	0.717000	-0.670000
C	-1.547000	-1.535000	-1.137000
C	-0.970000	-1.236000	-2.383000
H	-0.721000	-0.204000	-2.617000
C	-0.712000	-2.259000	-3.297000
H	-0.241000	-2.021000	-4.247000
C	-1.030000	-3.584000	-2.979000
H	-0.815000	-4.381000	-3.687000
C	-1.621000	-3.882000	-1.747000
H	-1.873000	-4.910000	-1.496000
C	-1.882000	-2.860000	-0.828000
H	-2.323000	-3.102000	0.134000
C	-2.437000	-0.907000	1.548000
C	-3.790000	-1.270000	1.655000
H	-4.481000	-1.048000	0.847000
C	-4.263000	-1.917000	2.800000
H	-5.315000	-2.185000	2.871000
C	-3.388000	-2.217000	3.850000
H	-3.756000	-2.722000	4.740000
C	-2.041000	-1.859000	3.749000
H	-1.350000	-2.088000	4.557000
C	-1.570000	-1.202000	2.610000
H	-0.530000	-0.908000	2.546000
H	-1.372000	5.072000	0.892000
H	1.101000	5.124000	0.975000

H	0.071000	1.083000	1.824000
H	-2.764000	2.307000	1.731000
H	-1.329000	2.885000	-0.809000
O	-0.416000	2.108000	-1.906000
H	0.241000	2.773000	-2.165000

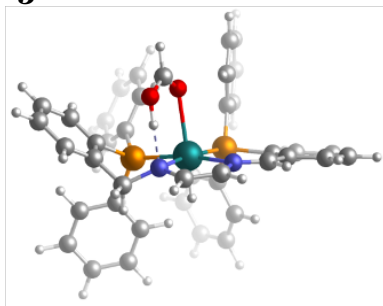
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Ru	0.054000	1.413000	-0.105000
P	1.792000	-0.057000	0.020000
P	-1.743000	-0.101000	-0.062000
N	-1.408000	3.074000	-0.344000
N	1.333000	3.080000	0.170000
C	1.985000	-0.047000	-2.753000
H	1.553000	0.948000	-2.654000
C	2.302000	-0.529000	-4.024000
H	2.112000	0.085000	-4.900000
C	2.864000	-1.803000	-4.166000
H	3.108000	-2.184000	-5.154000
C	3.117000	-2.579000	-3.031000
H	3.558000	-3.567000	-3.134000
C	2.805000	-2.092000	-1.759000
H	3.008000	-2.712000	-0.892000
C	2.224000	-0.825000	-1.607000
C	1.076000	-2.638000	0.938000
H	0.722000	-2.834000	-0.067000
C	0.870000	-3.600000	1.930000
H	0.365000	-4.527000	1.676000
C	1.300000	-3.366000	3.239000
H	1.136000	-4.114000	4.009000
C	1.942000	-2.164000	3.552000
H	2.282000	-1.974000	4.566000
C	2.149000	-1.200000	2.563000
H	2.641000	-0.267000	2.824000
C	1.720000	-1.429000	1.243000
C	3.423000	0.739000	0.416000
C	4.535000	-0.101000	0.561000
H	4.401000	-1.176000	0.485000
C	5.815000	0.399000	0.805000
H	6.652000	-0.286000	0.912000
C	6.011000	1.778000	0.912000
H	7.000000	2.184000	1.101000
C	4.922000	2.630000	0.776000
H	5.074000	3.703000	0.864000
C	3.617000	2.141000	0.524000
C	2.604000	3.182000	0.437000

H	2.985000	4.185000	0.647000
C	0.590000	4.280000	0.250000
C	-0.732000	4.287000	0.053000
C	-2.757000	2.877000	0.287000
H	-3.256000	3.847000	0.404000
C	-3.597000	1.983000	-0.599000
C	-4.748000	2.519000	-1.190000
H	-5.031000	3.546000	-0.968000
C	-5.541000	1.759000	-2.055000
H	-6.432000	2.195000	-2.498000
C	-5.175000	0.445000	-2.345000
H	-5.779000	-0.158000	-3.017000
C	-4.029000	-0.104000	-1.761000
H	-3.764000	-1.132000	-1.986000
C	-3.231000	0.645000	-0.885000
C	-1.609000	-1.749000	-0.867000
C	-0.955000	-1.821000	-2.106000
H	-0.572000	-0.918000	-2.571000
C	-0.766000	-3.050000	-2.741000
H	-0.242000	-3.089000	-3.691000
C	-1.233000	-4.223000	-2.139000
H	-1.078000	-5.183000	-2.625000
C	-1.899000	-4.158000	-0.911000
H	-2.269000	-5.067000	-0.443000
C	-2.090000	-2.928000	-0.276000
H	-2.594000	-2.892000	0.684000
C	-2.403000	-0.482000	1.620000
C	-3.782000	-0.597000	1.862000
H	-4.497000	-0.427000	1.063000
C	-4.251000	-0.931000	3.136000
H	-5.320000	-1.012000	3.311000
C	-3.348000	-1.164000	4.178000
H	-3.714000	-1.426000	5.168000
C	-1.974000	-1.057000	3.942000
H	-1.263000	-1.238000	4.743000
C	-1.504000	-0.712000	2.673000
H	-0.438000	-0.628000	2.507000
H	-1.321000	5.197000	0.146000
H	1.123000	5.197000	0.496000
H	-0.045000	1.398000	1.454000
H	-2.593000	2.460000	1.284000
H	-1.577000	3.137000	-1.354000

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Ru	-0.024000	-1.200000	-0.424000
P	1.845000	0.078000	-0.102000
P	-1.676000	0.362000	-0.001000
N	-1.603000	-2.610000	-0.963000
N	1.128000	-2.873000	-1.150000
C	2.283000	-0.386000	2.615000
H	1.812000	-1.336000	2.394000
C	2.719000	-0.118000	3.914000
H	2.603000	-0.876000	4.685000
C	3.294000	1.119000	4.225000
H	3.627000	1.331000	5.238000
C	3.440000	2.078000	3.220000
H	3.890000	3.042000	3.446000
C	3.011000	1.807000	1.917000
H	3.144000	2.567000	1.154000
C	2.415000	0.577000	1.601000
C	1.233000	2.809000	-0.551000
H	0.848000	2.816000	0.462000
C	1.078000	3.948000	-1.345000
H	0.580000	4.822000	-0.932000
C	1.541000	3.956000	-2.663000
H	1.414000	4.840000	-3.283000
C	2.161000	2.815000	-3.182000
H	2.521000	2.807000	-4.208000
C	2.318000	1.676000	-2.387000
H	2.790000	0.792000	-2.808000
C	1.860000	1.660000	-1.060000
C	3.422000	-0.735000	-0.655000
C	4.599000	0.029000	-0.601000
H	4.535000	1.071000	-0.300000
C	5.849000	-0.500000	-0.912000
H	6.736000	0.125000	-0.856000
C	5.943000	-1.846000	-1.285000
H	6.908000	-2.287000	-1.523000
C	4.791000	-2.617000	-1.358000
H	4.869000	-3.658000	-1.664000
C	3.506000	-2.094000	-1.058000
C	2.416000	-3.034000	-1.286000
H	2.745000	-3.990000	-1.708000
C	0.289000	-3.875000	-1.639000
C	-1.062000	-3.667000	-1.628000
C	-2.948000	-2.173000	-1.355000
H	-2.871000	-1.415000	-2.149000
C	-3.699000	-1.614000	-0.158000
C	-4.869000	-2.250000	0.270000
H	-5.231000	-3.115000	-0.281000
C	-5.569000	-1.812000	1.398000
H	-6.472000	-2.328000	1.712000
C	-5.090000	-0.720000	2.122000
H	-5.618000	-0.369000	3.005000
C	-3.924000	-0.069000	1.704000
H	-3.565000	0.785000	2.270000
C	-3.222000	-0.497000	0.568000
C	-1.422000	1.651000	1.298000

C	-0.725000	1.259000	2.452000
H	-0.402000	0.229000	2.558000
C	-0.416000	2.189000	3.446000
H	0.150000	1.872000	4.317000
C	-0.802000	3.525000	3.298000
H	-0.547000	4.255000	4.063000
C	-1.508000	3.922000	2.158000
H	-1.810000	4.959000	2.036000
C	-1.819000	2.990000	1.163000
H	-2.351000	3.314000	0.273000
C	-2.329000	1.336000	-1.437000
C	-3.674000	1.742000	-1.498000
H	-4.364000	1.459000	-0.708000
C	-4.138000	2.503000	-2.574000
H	-5.183000	2.803000	-2.609000
C	-3.264000	2.874000	-3.600000
H	-3.625000	3.466000	-4.438000
C	-1.925000	2.474000	-3.546000
H	-1.235000	2.755000	-4.337000
C	-1.462000	1.706000	-2.475000
H	-0.428000	1.387000	-2.451000
H	0.013000	-0.692000	-1.925000
H	-3.520000	-3.016000	-1.772000
O	-0.233000	-2.089000	1.950000
C	-0.987000	-3.006000	2.270000
O	-1.799000	-3.646000	1.473000
H	-1.035000	-3.371000	3.307000
H	-1.732000	-3.243000	0.511000
H	0.734000	-4.768000	-2.074000
H	-1.723000	-4.384000	-2.123000

TS_{13c-4c}

Ru	0.041000	-1.125000	-0.663000
P	-1.739000	0.247000	-0.125000
P	1.830000	0.219000	-0.174000
N	1.389000	-2.625000	-1.410000
N	-1.363000	-2.725000	-1.123000
C	-1.955000	1.521000	-2.625000
H	-1.389000	0.666000	-2.980000
C	-2.375000	2.503000	-3.526000
H	-2.143000	2.397000	-4.583000
C	-3.081000	3.620000	-3.070000
H	-3.401000	4.389000	-3.769000
C	-3.379000	3.737000	-1.709000
H	-3.934000	4.598000	-1.343000
C	-2.969000	2.749000	-0.812000
H	-3.217000	2.856000	0.239000
C	-2.236000	1.637000	-1.255000
C	-1.045000	2.292000	1.725000
H	-0.775000	2.897000	0.866000
C	-0.786000	2.780000	3.008000
H	-0.327000	3.759000	3.122000

C	-1.094000	2.010000	4.133000
H	-0.885000	2.388000	5.130000
C	-1.665000	0.743000	3.966000
H	-1.898000	0.126000	4.830000
C	-1.925000	0.254000	2.685000
H	-2.362000	-0.734000	2.576000
C	-1.623000	1.025000	1.547000
C	-3.390000	-0.624000	-0.052000
C	-4.420000	-0.065000	0.724000
H	-4.229000	0.837000	1.297000
C	-5.688000	-0.640000	0.789000
H	-6.459000	-0.184000	1.404000
C	-5.951000	-1.803000	0.064000
H	-6.929000	-2.274000	0.108000
C	-4.942000	-2.362000	-0.720000
H	-5.147000	-3.270000	-1.283000
C	-3.662000	-1.791000	-0.802000
C	-2.667000	-2.452000	-1.741000
H	-3.113000	-3.389000	-2.107000
C	-0.669000	-3.793000	-1.657000
H	-1.229000	-4.658000	-2.017000
C	0.689000	-3.804000	-1.698000
H	1.247000	-4.672000	-2.044000
C	2.651000	-2.578000	-1.730000
H	3.093000	-3.494000	-2.134000
C	3.546000	-1.426000	-1.761000
C	4.771000	-1.656000	-2.430000
H	4.983000	-2.656000	-2.803000
C	5.697000	-0.641000	-2.645000
H	6.623000	-0.854000	-3.171000
C	5.419000	0.650000	-2.188000
H	6.124000	1.460000	-2.354000
C	4.230000	0.891000	-1.495000
H	4.038000	1.890000	-1.117000
C	3.289000	-0.120000	-1.259000
C	1.678000	2.057000	-0.269000
C	0.997000	2.585000	-1.377000
H	0.629000	1.912000	-2.143000
C	0.754000	3.955000	-1.478000
H	0.196000	4.340000	-2.328000
C	1.200000	4.819000	-0.472000
H	1.000000	5.886000	-0.540000
C	1.899000	4.305000	0.625000
H	2.251000	4.971000	1.409000
C	2.138000	2.931000	0.727000
H	2.662000	2.540000	1.593000
C	2.579000	-0.049000	1.501000
C	3.925000	-0.390000	1.707000
H	4.600000	-0.497000	0.865000
C	4.415000	-0.599000	3.001000
H	5.459000	-0.868000	3.141000
C	3.570000	-0.462000	4.105000
H	3.952000	-0.625000	5.110000
C	2.227000	-0.124000	3.908000

H	1.552000	-0.026000	4.754000	O	0.220000	-2.275000	1.609000
C	1.736000	0.070000	2.618000	H	-1.757000	-3.246000	1.142000
H	0.689000	0.305000	2.480000				
H	0.009000	-0.522000	-2.130000				
H	-2.508000	-1.813000	-2.622000				
C	-0.628000	-2.870000	2.224000				
H	-1.662000	-3.091000	0.230000				
O	-1.053000	-3.314000	3.246000				