

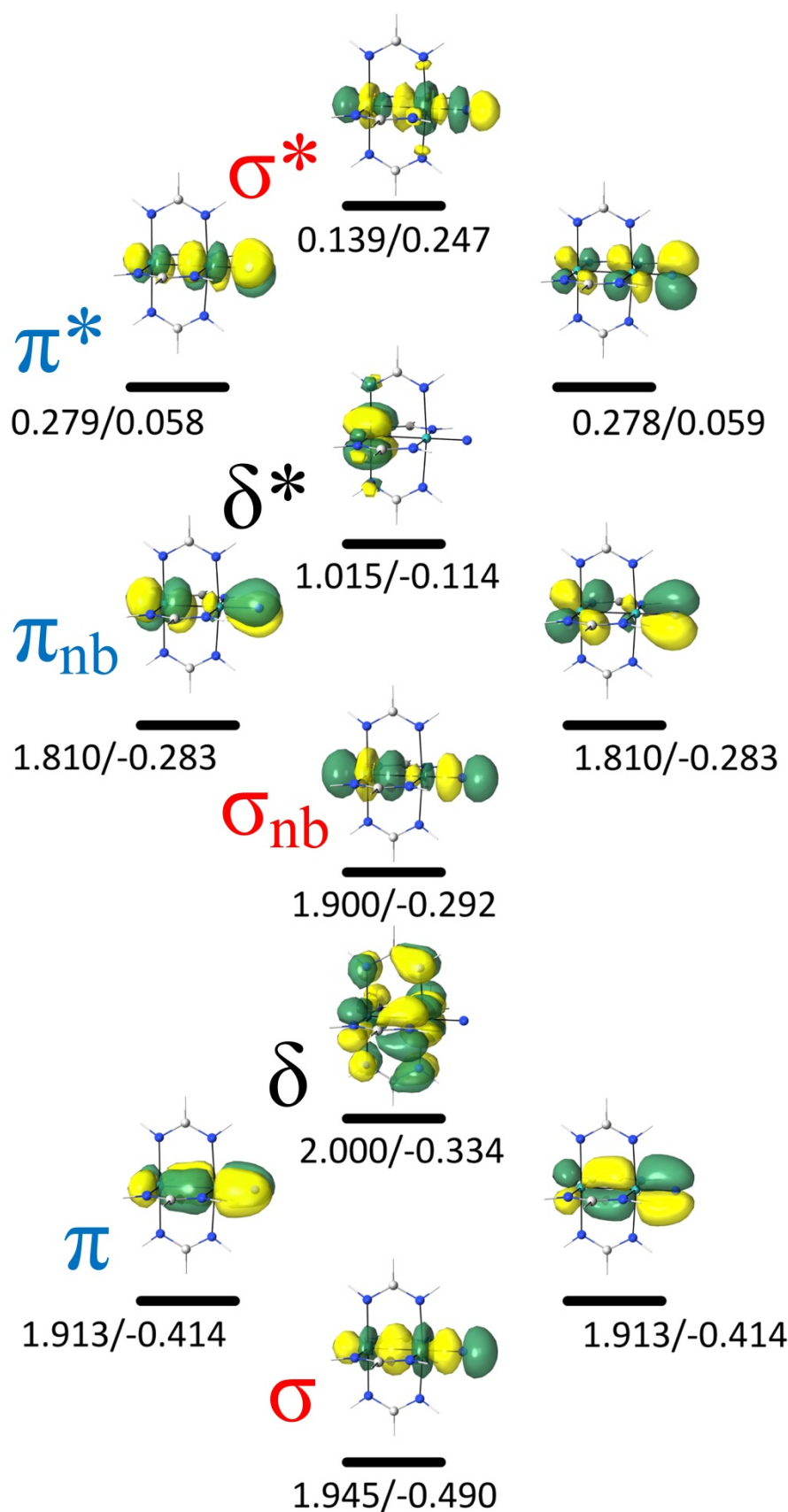


Fig. S1 CASSCF (13,10) active space orbitals with Ru-Ru distance of 2.4 Å. Occupation numbers are on the left and energies in Hartrees are on the right of each orbital. The δ orbital is also included here, even though it was not included in the active space since its occupation number was found to stay very close to 2.0.

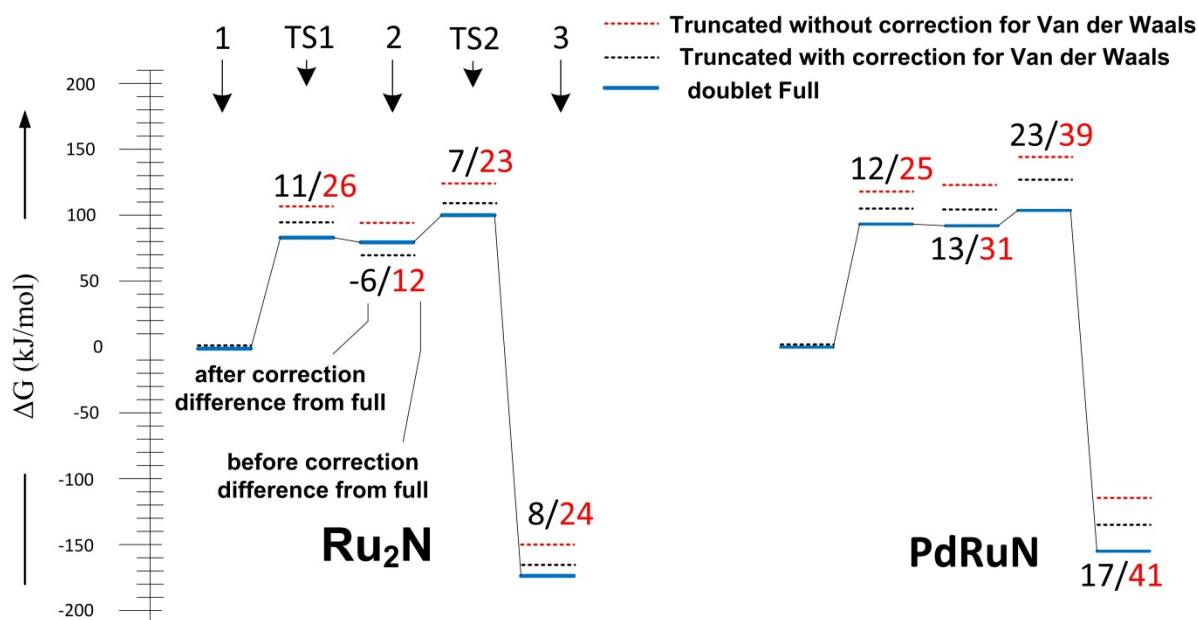


Fig. S2 The reaction coordinates of **1a**-Ru₂N (left) and **1a**-PdRuN (right). For TS1, 2, TS2, and 3 energies of **1b**-Ru₂N (left) and **1b**-PdRuN (right) are presented relative to **1**. The red dotted lines are uncorrected energies. The black dotted lines are energies for **1b** complexes that take into account Van der Waals force differences relative to **1b**, compared to Van der Waals forces differences of the full reaction coordinates.

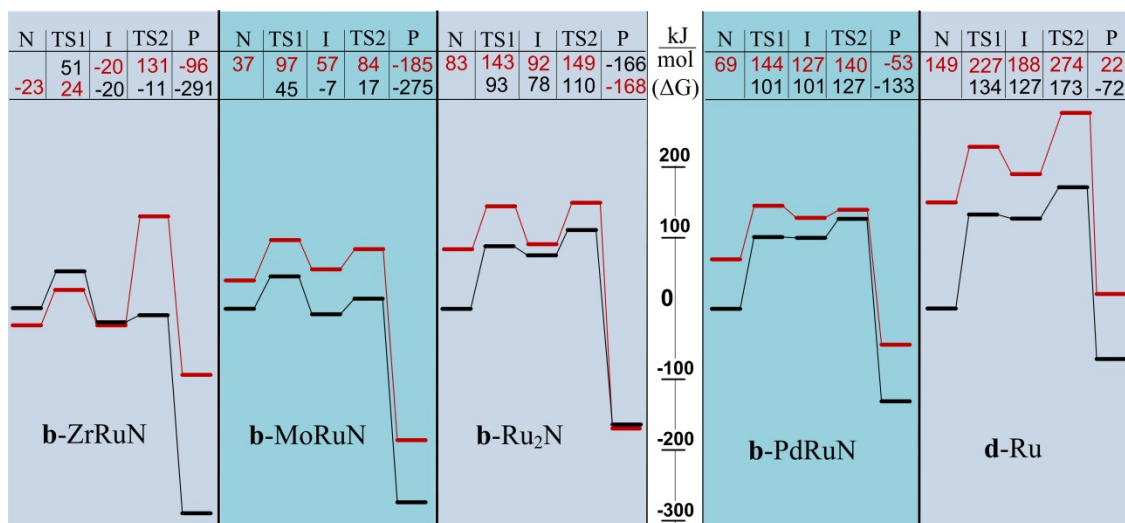


Fig. S3 This figure corresponds to the top half of Figure 5 and shows both doublet (black) and quartet (red) reaction coordinates. The energies in ΔG (kJ/mol) are presented at the top.

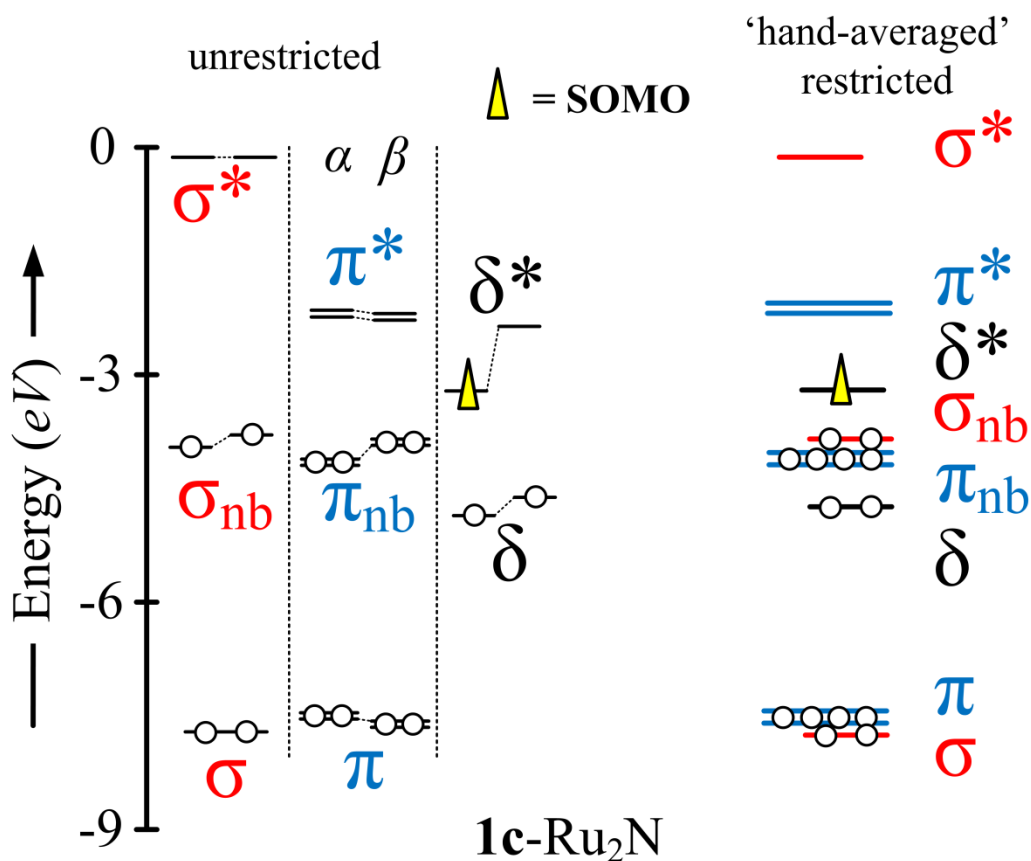


Fig. S4 A representation of how the orbital diagrams were obtained. At the left are unrestricted Kohn-Sham orbitals from the final single point DFT calculations.

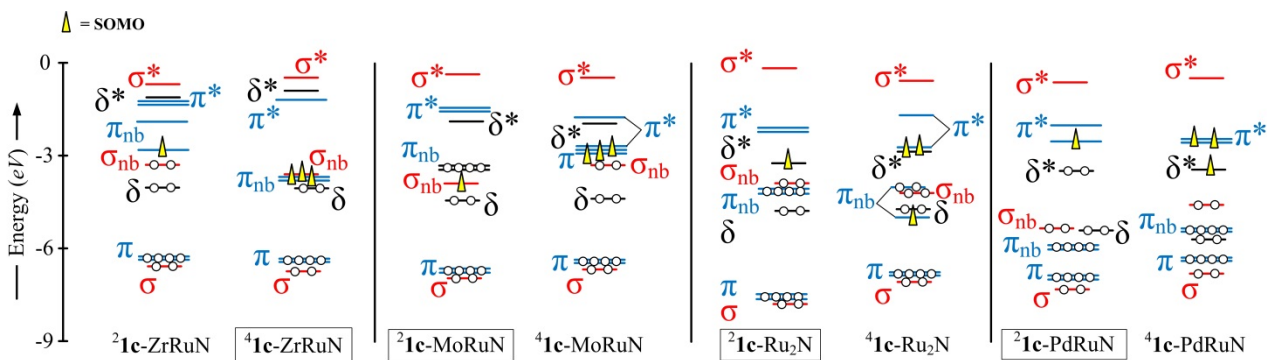


Fig. S5 This figure is an extension of Figure 6 and includes the quartet orbital diagram for the dimetallic complexes. The boxed name designates the ground state, which is clarified in the text and happens only here for $M = \text{Zr}$ (as well as $1b\text{-Mo}_2\text{N}$)

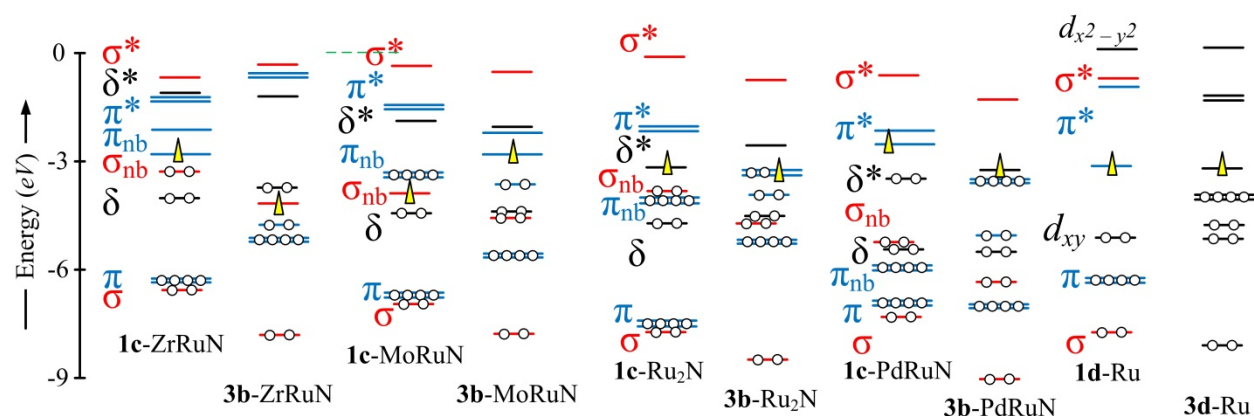


Fig. S6 This figure is an extension of Figure 6 and includes **3b** diagrams for M = Zr, Mo, Ru, Pd and mononuclear complex **3d**.

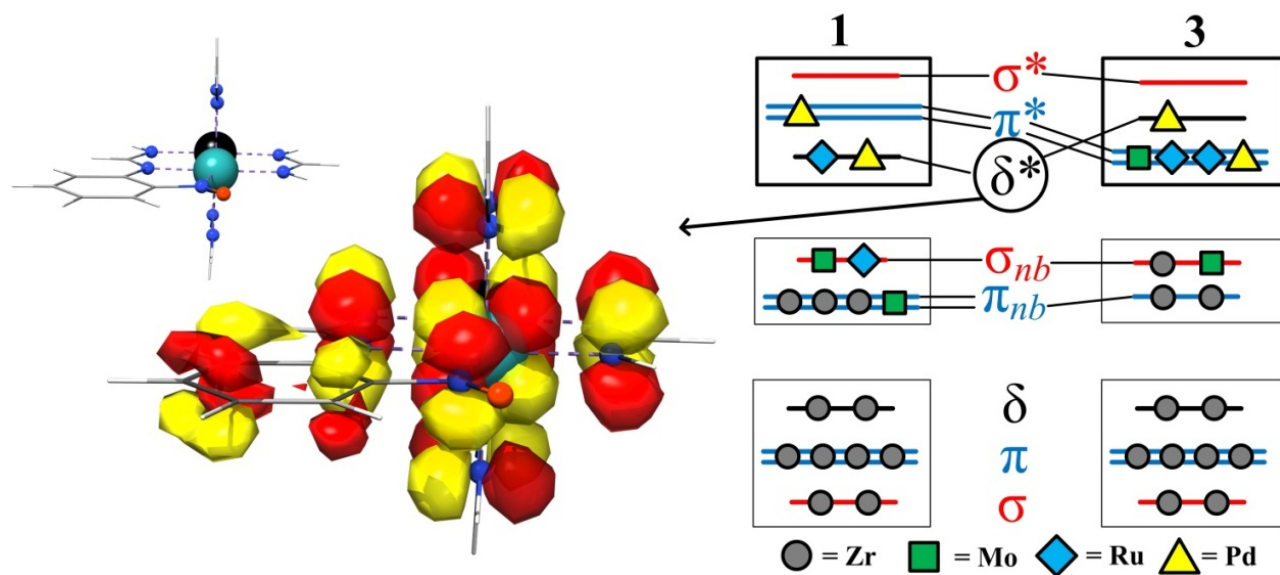


Fig. S7 A representative δ^* orbital (from **3b**-Ru₂N) of product complex **3** that is raised in energy relative to reactant nitrido complex **1** due an antibonding π -type interaction of the amide N after it has inserted into the phenyl ring C—H bond. This orbital ordering change is seen at the right of this figure, which is taken from Figure 9A.

XYZ files of optimized structures from DFT-BP/def2-tzvp on metals and reaction atoms (C,N,H); def2-sv(p) on the rest.

²**1a**-Ru₂N

Ru	0.010572	0.000160	1.103258	C	-2.811431	0.470934	-2.489167
Ru	-0.004809	0.011731	-1.341857	C	-3.806212	1.479190	-2.480021
N	-2.104596	0.035884	1.011525	H	-4.011357	2.028917	-1.546878
N	-2.067932	0.156463	-1.327139	C	-4.492134	1.810774	-3.661647
N	0.021536	-0.005177	2.798955	H	-5.256873	2.606045	-3.639043
N	-0.026460	-2.114303	0.988612	C	-4.189532	1.155629	-4.870758
N	0.044167	2.115357	1.006041	H	-4.720129	1.426974	-5.798818
N	2.124166	-0.039701	0.985556	C	-3.195079	0.156697	-4.884267
N	-0.150567	-2.051266	-1.349324	H	-2.947786	-0.365972	-5.823969
N	0.139312	2.074491	-1.333554	C	-2.514008	-0.187448	-3.706200
N	2.057913	-0.134683	-1.353480	H	-1.737910	-0.966336	-3.715045
C	-2.722443	0.110482	-0.162216	C	-0.103671	-2.718857	-0.192035
H	-3.832767	0.137723	-0.169143	C	0.105101	2.731200	-0.169479
C	-2.890774	-0.214689	2.163637	C	2.727105	-0.105541	-0.196431
C	-3.819286	-1.281412	2.178808	H	3.837007	-0.140793	-0.217478
H	-3.924576	-1.912576	1.281128	H	0.130904	3.841530	-0.178643
C	-4.563331	-1.556628	3.339721	H	-0.132333	-3.828992	-0.211401
H	-5.277824	-2.397438	3.341579	C	2.928845	0.182293	2.131501
C	-4.379787	-0.779542	4.499522	C	-0.190937	2.904148	2.159572
H	-4.954670	-1.002632	5.414054	C	0.225359	-2.913944	2.131016
C	-3.455586	0.284753	4.484347	C	3.872564	1.234608	2.155429
H	-3.313430	0.904966	5.385640	C	-1.259088	3.830558	2.188614
C	-2.714616	0.571751	3.326123	C	1.288661	-3.846721	2.131624
H	-2.005584	1.413204	3.301507	H	3.975748	1.883350	1.269998

H	-1.903967	3.932425	1.300336	C	-0.466790	-2.781120	-2.519543
H	1.914992	-3.945504	1.229859	C	3.769796	-1.458854	-2.543386
C	4.637522	1.470862	3.311599	C	1.442913	3.815161	-2.505105
C	-1.518008	4.576872	3.351844	C	-1.474817	-3.776176	-2.520645
C	1.566723	-4.603540	3.283520	H	3.981907	-2.020788	-1.619114
H	5.365116	2.300289	3.323372	H	2.000827	4.026434	-1.578218
H	-2.360096	5.289717	3.364842	H	-2.023106	-3.992527	-1.589191
H	2.404868	-5.321042	3.273995	C	4.436638	-1.783814	-3.737709
C	4.457488	0.668797	4.454308	C	1.759854	4.498169	-3.692432
C	-0.722810	4.397916	4.500038	C	-1.808116	-4.448066	-3.709832
C	0.796187	-4.428643	4.449059	H	5.193966	-2.586453	-3.734148
H	5.048764	0.858896	5.365672	H	2.551649	5.266736	-3.680268
H	-0.933092	4.974728	5.416388	H	-2.603183	-5.213197	-3.695067
H	1.021679	-5.013386	5.356679	C	4.124068	-1.112569	-4.935409
C	3.514528	-0.378303	4.424743	C	1.094720	4.187880	-4.894134
C	0.343210	3.476029	4.470987	C	-1.154974	-4.130919	-4.916293
C	-0.264886	-3.500587	4.448293	H	4.639483	-1.378709	-5.873477
H	3.370022	-1.020863	5.309197	H	1.354659	4.716250	-5.826717
H	0.977524	3.337564	5.362958	H	-1.427659	-4.650505	-5.850171
H	-0.880244	-3.365527	5.353970	C	3.139290	-0.104074	-4.924576
C	2.758283	-0.620239	3.275285	C	0.100609	3.188516	-4.894365
C	0.613520	2.732678	3.310290	C	-0.156401	-3.136031	-4.919565
C	-0.554785	-2.746692	3.299097	H	2.884513	0.431232	-5.855106
H	2.039670	-1.438981	3.242626	H	-0.429685	2.935009	-5.828104
H	1.456454	2.025434	3.273552	H	0.364619	-2.877333	-5.857073
H	-1.393832	-2.034586	3.285745	C	2.477270	0.233361	-3.733759
C	2.784466	-0.441483	-2.528264	C	-0.229006	2.510339	-3.710517
C	0.439328	2.815547	-2.500841	C	0.189444	-2.468905	-3.734050

H	1.708320	1.019257	-3.723698	C	-2.726667	0.516502	-2.359886
H	-1.003983	1.730281	-3.709064	C	-3.555728	1.663205	-2.335906
H	0.968006	-1.692463	-3.735011	H	-3.632037	2.251179	-1.406447
² TS1a-Ru ₂ N				C	-4.230472	2.074538	-3.498548
Ru	0.142434	-0.079591	1.041448	H	-4.862638	2.978557	-3.468675
Ru	0.088838	-0.050097	-1.394287	C	-4.081980	1.356180	-4.700715
N	-1.947003	0.002690	1.117663	H	-4.601539	1.689149	-5.614872
N	-1.973463	0.132662	-1.224900	C	-3.259276	0.211983	-4.726457
N	0.473050	0.002193	2.793523	H	-3.138186	-0.362239	-5.660753
N	0.081092	-2.175042	0.948638	C	-2.589817	-0.210064	-3.566691
N	0.146295	2.043239	0.919483	H	-1.945613	-1.101267	-3.583941
N	2.219531	-0.095956	0.872554	C	-0.034449	-2.783678	-0.230167
N	-0.084409	-2.110688	-1.383046	C	0.167079	2.664485	-0.253725
N	0.214560	2.012604	-1.420647	C	2.840882	-0.122105	-0.306024
N	2.150150	-0.190746	-1.451706	H	3.950016	-0.113142	-0.331392
C	-2.594744	0.123103	-0.040561	H	0.136236	3.774910	-0.260825
H	-3.701155	0.222468	-0.020246	H	-0.099836	-3.891876	-0.248627
C	-2.704858	-0.215828	2.292473	C	2.859569	0.146667	2.080180
C	-3.757000	-1.163852	2.304580	C	-0.156831	2.819587	2.066108
H	-3.975514	-1.734420	1.386885	C	0.300719	-2.977370	2.094794
C	-4.485333	-1.403939	3.482988	C	3.957144	1.015004	2.243864
H	-5.297713	-2.150890	3.477394	C	-1.331747	3.603684	2.104790
C	-4.164390	-0.714129	4.667463	C	1.273171	-4.006326	2.077928
H	-4.727381	-0.910494	5.595585	H	4.450116	1.437205	1.351856
C	-3.113105	0.225585	4.657657	H	-1.991369	3.619189	1.221516
H	-2.856349	0.775867	5.578959	H	1.857172	-4.178731	1.159008
C	-2.386523	0.478898	3.483621	C	4.357209	1.406595	3.530335
H	-1.569356	1.213102	3.475698	C	-1.675855	4.308188	3.272121

C	1.519222	-4.769391	3.233318		H	4.171944	-1.973363	-1.727383
H	5.197265	2.109861	3.653762		H	1.894069	4.127401	-1.696753
H	-2.603016	4.905995	3.294794		H	-1.961927	-4.061241	-1.602122
H	2.286756	-5.561688	3.207742		C	4.587748	-1.726859	-3.852927
C	3.638447	0.943961	4.674679		C	1.583708	4.561900	-3.808901
C	-0.856770	4.227420	4.414697		C	-1.829923	-4.447041	-3.742685
C	0.810261	-4.507178	4.421237		H	5.390094	-2.484464	-3.852567
H	3.954269	1.271644	5.680125		H	2.296120	5.404787	-3.807673
H	-1.135058	4.766359	5.336067		H	-2.620699	-5.216427	-3.720391
H	1.012169	-5.097683	5.330682		C	4.225841	-1.081486	-5.051120
C	2.563676	0.079559	4.539828		C	0.939686	4.183114	-5.002573
C	0.321206	3.454302	4.372871		C	-1.229869	-4.086367	-4.964750
C	-0.154297	-3.479351	4.440288		H	4.747492	-1.322503	-5.992509
H	2.029079	-0.303921	5.424420		H	1.135394	4.731361	-5.939410
H	0.977344	3.393777	5.257727		H	-1.539907	-4.576390	-5.902916
H	-0.718239	-3.267984	5.364590		C	3.183914	-0.132215	-5.036425
C	2.111525	-0.359842	3.230433		C	0.050920	3.089133	-4.988119
C	0.676532	2.757955	3.206167		C	-0.237477	-3.085420	-4.977379
C	-0.414134	-2.718708	3.288824		H	2.889573	0.382332	-5.966960
H	1.872651	-1.435125	3.178652		H	-0.462645	2.779537	-5.914264
H	1.610195	2.177832	3.164500		H	0.240906	-2.791190	-5.927068
H	-1.168712	-1.919622	3.300790		C	2.514906	0.172780	-3.841061
C	2.874373	-0.473009	-2.634532		C	-0.198506	2.388426	-3.798163
C	0.445977	2.764121	-2.594493		C	0.155312	-2.456893	-3.785633
C	-0.446590	-2.813500	-2.554751		H	1.702888	0.914443	-3.826222
C	3.916645	-1.432472	-2.653208		H	-0.896135	1.538325	-3.785880
C	1.348850	3.856466	-2.615576		H	0.929968	-1.675681	-3.792064
C	-1.451051	-3.812856	-2.546610	² 2a -Ru ₂ N				

Ru	0.071973	0.038432	3.425245	H	3.566761	4.528343	-1.206739
Ru	0.063142	0.070434	0.986338	C	1.793722	4.025309	-2.374161
N	0.305889	2.108881	3.488652	H	2.173018	4.485168	-3.302189
N	0.388383	2.118486	1.146056	C	0.529233	3.403076	-2.354214
N	0.111151	-0.367873	5.224359	H	-0.092253	3.382340	-3.265645
N	-2.018505	0.244470	3.350629	C	0.047208	2.807048	-1.177554
N	2.182524	-0.105265	3.278166	H	-0.937901	2.318569	-1.158739
N	-0.132074	-2.027244	3.280808	C	-2.639545	0.381459	2.180514
N	-1.982026	0.384158	1.017881	C	2.788658	-0.154234	2.096841
N	2.121022	-0.174397	0.938531	C	-0.276725	-2.646560	2.095132
N	-0.239348	-1.946955	0.960085	H	-0.456015	-3.739349	2.061246
C	0.467273	2.740390	2.324698	H	3.899149	-0.167028	2.078065
H	0.679267	3.831015	2.336733	H	-3.741820	0.515750	2.178934
C	0.184651	2.891409	4.661601	C	-0.079867	-2.681325	4.481375
C	-0.623975	4.055264	4.670473	C	2.987087	0.159479	4.413702
H	-1.171914	4.335596	3.755770	C	-2.809704	0.088418	4.513054
C	-0.757595	4.822634	5.841005	C	0.199656	-4.044142	4.714464
H	-1.395451	5.723272	5.830224	C	3.823373	1.297584	4.449338
C	-0.102067	4.431565	7.023794	C	-3.886550	-0.830559	4.535676
H	-0.214766	5.026696	7.945860	H	0.303687	-4.740923	3.865441
C	0.693038	3.266985	7.019300	H	3.855922	1.961588	3.569801
H	1.213324	2.950472	7.939558	H	-4.109146	-1.418691	3.630118
C	0.840014	2.499633	5.853405	C	0.451442	-4.492243	6.016712
H	1.453896	1.589831	5.853992	C	4.557222	1.602960	5.609400
C	0.833953	2.816729	-0.001625	C	-4.635365	-1.019003	5.711428
C	2.098984	3.449776	-0.021477	H	0.699967	-5.552405	6.189624
H	2.723237	3.424816	0.886917	H	5.195666	2.502711	5.629524
C	2.571429	4.051828	-1.200361	H	-5.465806	-1.745596	5.716227

C	0.503395	-3.562847	7.118036
C	4.455208	0.781431	6.748329
C	-4.310941	-0.305353	6.881095
H	0.808644	-3.933758	8.112112
H	5.017832	1.029585	7.664120
H	-4.890289	-0.462246	7.806498
C	0.224115	-2.230017	6.945672
C	3.630863	-0.361695	6.709968
C	-3.234222	0.604431	6.861573
H	0.285033	-1.502405	7.771399
H	3.552932	-1.019923	7.591992
H	-2.971703	1.169258	7.772196
C	-0.271136	-1.722034	5.627011
C	2.905607	-0.677238	5.549901
C	-2.486906	0.805743	5.689878
H	-1.379979	-1.576896	5.745267
H	2.282477	-1.584435	5.509070
H	-1.645336	1.512352	5.672898
C	-0.628283	-2.615235	-0.230731
C	2.840773	-0.423101	-0.250016
C	-2.659743	0.799928	-0.148100
C	-1.811831	-3.388767	-0.271200
C	3.949983	-1.306733	-0.289959
C	-3.615461	1.846858	-0.130058
H	-2.420243	-3.490626	0.642152
H	4.262953	-1.829942	0.628137
H	-3.852367	2.349646	0.821630
C	-2.229729	-3.974289	-1.478778

C	4.622020	-1.552190	-1.500164
C	-4.218127	2.278733	-1.324379
H	-3.162611	-4.562930	-1.502533
H	5.478864	-2.247793	-1.510161
H	-4.952263	3.102112	-1.292617
C	-1.477673	-3.793187	-2.655415
C	4.193085	-0.942484	-2.695092
C	-3.869014	1.691102	-2.555997
H	-1.813517	-4.244902	-3.603840
H	4.716002	-1.146876	-3.644472
H	-4.333521	2.043105	-3.492342
C	-0.297153	-3.024293	-2.613509
C	3.078941	-0.079624	-2.664071
C	-2.911203	0.657212	-2.579387
H	0.301505	-2.877823	-3.528478
H	2.725831	0.404855	-3.590248
H	-2.624840	0.188333	-3.536142
C	0.128741	-2.438651	-1.410752
C	2.411599	0.180955	-1.457823
C	-2.314920	0.211289	-1.390045
H	1.045050	-1.831716	-1.373750
H	1.544072	0.857093	-1.436677
H	-1.566798	-0.595353	-1.407432

²**TS2a**-Ru₂N

Ru	0.132524	0.015600	3.451322
Ru	0.100872	0.047574	0.965107
N	0.317430	2.074408	3.482170
N	0.451537	2.075347	1.141521

N	0.257791	-0.455282	5.310325	H	0.015252	3.368224	-3.268499
N	-1.946391	0.187691	3.396953	C	0.130273	2.781933	-1.181823
N	2.210962	-0.072010	3.266135	H	-0.865578	2.315439	-1.168648
N	-0.078709	-2.040554	3.282533	C	-2.571952	0.353819	2.230030
N	-1.920603	0.385796	1.063795	C	2.811959	-0.164782	2.082267
N	2.137544	-0.233524	0.928651	C	-0.289022	-2.641106	2.101317
N	-0.247671	-1.949234	0.957402	H	-0.504412	-3.726814	2.061501
C	0.496627	2.705402	2.318327	H	3.922247	-0.149322	2.055445
H	0.689810	3.799401	2.329770	H	-3.673180	0.496051	2.233675
C	0.127706	2.862336	4.643792	C	-0.049959	-2.741758	4.479061
C	-0.735585	3.984985	4.617163	C	3.018400	0.322000	4.366224
H	-1.263539	4.234541	3.682025	C	-2.750230	-0.002462	4.545884
C	-0.947619	4.747785	5.779018	C	-0.045408	-4.139340	4.675849
H	-1.628585	5.615517	5.743184	C	3.716748	1.548636	4.326337
C	-0.313363	4.393088	6.984696	C	-3.864783	-0.877752	4.514365
H	-0.487038	4.984615	7.899554	H	-0.133226	-4.826426	3.817815
C	0.539234	3.270283	7.013422	H	3.647958	2.169163	3.417562
H	1.043008	2.983957	7.952450	H	-4.100938	-1.414006	3.580643
C	0.763481	2.507521	5.856908	C	0.130959	-4.665793	5.963418
H	1.419316	1.627641	5.881787	C	4.444515	1.987389	5.446897
C	0.912025	2.771222	-0.003110	C	-4.636601	-1.089633	5.669107
C	2.190215	3.376020	-0.012368	H	0.144925	-5.758602	6.108796
H	2.806618	3.336018	0.901015	H	4.976004	2.953543	5.408958
C	2.683231	3.969419	-1.187355	H	-5.496118	-1.780350	5.627979
H	3.688721	4.423924	-1.187159	C	0.353540	-3.798064	7.076483
C	1.910962	3.963525	-2.364896	C	4.474605	1.207832	6.618287
H	2.305342	4.417383	-3.289570	C	-4.301708	-0.446426	6.877195
C	0.632071	3.371008	-2.353707	H	0.549986	-4.234874	8.070919

H	5.033076	1.556960	7.503147	H	-4.786213	3.305818	-1.126509
H	-4.902231	-0.622058	7.785526	C	-1.587534	-3.762865	-2.637563
C	0.358328	-2.420910	6.925547	C	4.233325	-1.044007	-2.681198
C	3.789257	-0.024081	6.653763	C	-3.814731	1.858827	-2.438879
C	-3.188021	0.414295	6.916314	H	-1.948831	-4.205125	-3.581075
H	0.537740	-1.734555	7.768596	H	4.762735	-1.259888	-3.624445
H	3.819725	-0.647860	7.563316	H	-4.278180	2.255742	-3.357633
H	-2.915206	0.924554	7.855555	C	-0.395533	-3.010699	-2.615977
C	0.039297	-1.832374	5.630127	C	3.127807	-0.169308	-2.667009
C	3.066489	-0.469357	5.535299	C	-2.922284	0.769672	-2.504392
C	-2.413997	0.639119	5.764033	H	0.186244	-2.868019	-3.542379
H	-0.979658	-1.196024	5.762957	H	2.790039	0.313178	-3.599931
H	2.543375	-1.438982	5.556059	H	-2.687941	0.303199	-3.476307
H	-1.550215	1.318147	5.788823	C	0.063004	-2.438412	-1.418964
C	-0.672734	-2.610082	-0.224327	C	2.451195	0.105329	-1.469119
C	2.864818	-0.495293	-0.254904	C	-2.326228	0.266587	-1.337677
C	-2.607481	0.853049	-0.079441	H	0.988961	-1.844666	-1.395173
C	-1.868165	-3.366053	-0.244768	H	1.590952	0.791279	-1.456974
C	3.966608	-1.387320	-0.276185	H	-1.628365	-0.582913	-1.384364
C	-3.501207	1.950496	-0.017444	² 3a -Ru ₂ N			
H	-2.461223	-3.463855	0.679074	Ru	0.005217	-0.117415	1.188344
H	4.267117	-1.901982	0.651005	Ru	-0.150786	-0.013905	-1.283611
H	-3.687932	2.442858	0.950846	N	2.045190	-0.310009	0.998365
C	-2.318198	-3.939321	-1.446848	N	1.878913	-0.316383	-1.342412
C	4.646587	-1.649297	-1.478771	N	-0.286139	-0.075911	3.204330
C	-4.102300	2.442070	-1.189462	N	0.215154	1.955482	1.160553
H	-3.259821	-4.514321	-1.454874	N	-0.167431	-2.175494	1.000345
H	5.497586	-2.352024	-1.476542	N	-2.004443	0.165169	1.288734

N	0.142365	2.016099	-1.180737	C	-0.325715	-2.752637	-0.189770
N	-0.421735	-2.047515	-1.323317	C	-2.719393	0.380192	0.177314
N	-2.153655	0.302882	-1.033340	H	-3.795687	0.634670	0.245658
C	2.597074	-0.390350	-0.214920	H	-0.370807	-3.861080	-0.239563
H	3.697262	-0.523795	-0.292520	H	0.341333	3.729131	0.038534
C	2.907481	-0.159177	2.109546	C	-2.544287	0.270019	2.579519
C	3.974549	0.771117	2.083737	C	0.156382	-3.034402	2.085736
H	4.143726	1.368436	1.172893	C	0.122339	2.726942	2.350349
C	4.771237	0.969780	3.225505	C	-3.898407	0.480433	2.919605
H	5.589501	1.709504	3.194676	C	1.291866	-3.871773	2.014109
C	4.512795	0.250929	4.407786	C	-0.891500	3.700309	2.490888
H	5.130117	0.417353	5.306445	H	-4.668549	0.551623	2.134534
C	3.456043	-0.683041	4.433003	H	1.909603	-3.854338	1.101255
H	3.251565	-1.261894	5.349777	H	-1.599469	3.858706	1.660743
C	2.661340	-0.891929	3.294990	C	-4.274554	0.595672	4.267621
H	1.842609	-1.626154	3.300986	C	1.648764	-4.676992	3.111184
C	2.534311	-0.656572	-2.551326	C	-1.019763	4.423821	3.690467
C	3.344045	-1.814050	-2.643016	H	-5.334314	0.758959	4.526188
H	3.481815	-2.446167	-1.750406	H	2.543719	-5.319266	3.048205
C	3.922118	-2.179878	-3.871570	H	-1.824016	5.172638	3.791299
H	4.538873	-3.093107	-3.930847	C	-3.299048	0.498834	5.291655
C	3.697236	-1.403176	-5.024153	C	0.878599	-4.648543	4.288511
H	4.142114	-1.698574	-5.989266	C	-0.143327	4.176681	4.763325
C	2.892822	-0.248728	-4.934560	H	-3.601794	0.592926	6.348588
H	2.712523	0.371268	-5.829280	H	1.163200	-5.271353	5.153299
C	2.317396	0.125836	-3.710085	H	-0.250364	4.735801	5.708291
H	1.686097	1.023234	-3.636814	C	-1.956867	0.280808	4.970759
C	0.238359	2.623812	0.008642	C	-0.262946	-3.822265	4.354806

C	0.869712	3.206337	4.623195	H	-4.783512	2.064799	-5.341824
H	-1.184384	0.201430	5.754441	H	-1.982402	-4.409392	-5.865035
H	-0.880498	-3.805590	5.269010	H	1.210327	4.678899	-5.699122
H	1.565829	3.009180	5.456319	C	-3.591449	0.452975	-4.474303
C	-1.554931	0.158528	3.617013	C	-0.701471	-2.898135	-4.941853
C	-0.625853	-3.019541	3.261662	C	-0.019123	3.155509	-4.727144
C	1.005693	2.485349	3.426601	H	-3.579784	-0.148035	-5.399388
H	0.397765	-0.120071	3.963420	H	-0.276874	-2.551352	-5.899271
H	-1.516757	-2.375781	3.302500	H	-0.585359	2.908462	-5.641165
H	1.798243	1.732340	3.307717	C	-2.925348	-0.024453	-3.334193
C	-2.925980	0.735822	-2.142114	C	-0.281122	-2.296471	-3.746065
C	-0.811618	-2.721109	-2.503691	C	-0.310520	2.475847	-3.534585
C	0.403887	2.770584	-2.347255	H	-2.389279	-0.984074	-3.356246
C	-3.614019	1.971948	-2.107135	H	0.461441	-1.484497	-3.756690
C	-1.777246	-3.758550	-2.489864	H	-1.091301	1.701316	-3.508984
C	1.417984	3.759881	-2.387136	² 1a -PdRuN			
H	-3.579189	2.581515	-1.189465	Ru	0.014829	0.001885	1.254615
H	-2.236650	-4.061507	-1.534985	Pd	-0.003196	0.014271	-1.436420
H	2.016838	3.961011	-1.484120	N	-2.077837	-0.048149	1.006260
C	-4.281039	2.441411	-3.251701	N	-2.042790	0.142475	-1.348598
C	-2.183791	-4.365065	-3.691318	N	0.028093	-0.001112	2.948274
C	1.694870	4.445401	-3.582858	N	0.054586	-2.098240	1.037008
H	-4.797803	3.415738	-3.217997	N	-0.031529	2.103883	1.053179
H	-2.942622	-5.165800	-3.663100	N	2.103928	0.047396	0.978714
H	2.494373	5.205962	-3.597355	N	-0.131910	-2.033181	-1.327050
C	-4.269683	1.688301	-4.441474	N	0.126412	2.060300	-1.313247
C	-1.651744	-3.939122	-4.923768	N	2.037069	-0.115199	-1.377517
C	0.981598	4.147632	-4.760034	C	-2.673353	0.064111	-0.174574

H	-3.784455	0.086095	-0.192088	H	-0.064559	-3.785076	-0.189004
C	-2.908874	-0.342881	2.124345	C	2.954997	0.307796	2.091132
C	-3.817860	-1.422120	2.074328	C	-0.317692	2.929662	2.171707
H	-3.858631	-2.044069	1.164994	C	0.349079	-2.934655	2.145385
C	-4.625180	-1.719429	3.187284	C	3.883201	1.370109	2.052083
H	-5.323468	-2.572448	3.141186	C	-1.431191	3.798231	2.158887
C	-4.524118	-0.949407	4.359051	C	1.452514	-3.815658	2.108918
H	-5.148590	-1.188862	5.236101	H	3.923986	2.012612	1.157038
C	-3.614231	0.126369	4.407976	H	-2.076954	3.822121	1.265342
H	-3.530576	0.739979	5.320688	H	2.083608	-3.840997	1.205035
C	-2.810258	0.433192	3.300444	C	4.712886	1.622214	3.160033
H	-2.099919	1.274676	3.330322	C	-1.726765	4.589210	3.283650
C	-2.767701	0.538426	-2.492141	C	1.757520	-4.617110	3.223648
C	-3.709560	1.593831	-2.436771	H	5.427918	2.461856	3.125797
H	-3.870795	2.119716	-1.481583	H	-2.601007	5.262110	3.263668
C	-4.393581	1.994133	-3.596585	H	2.623987	-5.299142	3.185159
H	-5.119563	2.823107	-3.539638	C	4.612134	0.823545	4.312009
C	-4.135233	1.365834	-4.828901	C	-0.921955	4.506701	4.434272
H	-4.663940	1.691721	-5.740179	C	0.972695	-4.532953	4.387920
C	-3.190015	0.322743	-4.888396	H	5.254044	1.025092	5.185831
H	-2.981038	-0.182817	-5.846394	H	-1.158238	5.118599	5.321171
C	-2.514236	-0.094406	-3.732317	H	1.216628	-5.152950	5.267054
H	-1.783176	-0.915515	-3.775083	C	3.679244	-0.232652	4.344256
C	-0.049297	-2.673726	-0.153594	C	0.186477	3.636309	4.448662
C	0.055346	2.690241	-0.133307	C	-0.125689	-3.650605	4.425623
C	2.683221	-0.055823	-0.210825	H	3.591346	-0.871573	5.238382
H	3.793704	-0.088062	-0.242923	H	0.825948	3.570567	5.345103
H	0.064951	3.801915	-0.159171	H	-0.750021	-3.583817	5.332601

C	2.858950	-0.488361	3.245371
C	0.491815	2.848828	3.327895
C	-0.440777	-2.852395	3.315142
H	2.136820	-1.305793	3.264230
H	1.362136	2.175109	3.324684
H	-1.303739	-2.170031	3.330892
C	2.742929	-0.506815	-2.534424
C	0.511167	2.795584	-2.453610
C	-0.534533	-2.757421	-2.468563
C	3.671731	-1.574674	-2.502530
C	1.557765	3.748065	-2.397456
C	-1.587412	-3.702536	-2.407336
H	3.839217	-2.111987	-1.554814
H	2.085585	3.909308	-1.443332
H	-2.104958	-3.867290	-1.448169
C	4.333944	-1.972508	-3.675744
C	1.946831	4.444165	-3.553920
C	-1.995483	-4.386584	-3.564451
H	5.049664	-2.811400	-3.637167
H	2.768822	5.177941	-3.494516
H	-2.822258	-5.114620	-3.501035
C	4.066361	-1.328898	-4.898187
C	1.316447	4.189245	-4.785880
C	-1.377772	-4.126633	-4.801756
H	4.577674	-1.652802	-5.820039
H	1.633259	4.727904	-5.694520
H	-1.709428	-4.655660	-5.710759
C	3.134492	-0.272803	-4.934119

C	0.282504	3.234222	-4.847396
C	-0.337394	-3.178967	-4.868132
H	2.918706	0.244766	-5.884165
H	-0.225295	3.026798	-5.804593
H	0.160594	-2.967796	-5.829645
C	2.480639	0.141801	-3.764561
C	-0.123122	2.546232	-3.694402
C	0.087067	-2.503054	-3.714741
H	1.759579	0.972389	-3.789058
H	-0.936953	1.807655	-3.740897
H	0.905680	-1.770135	-3.765333

²**TS1a**-PdRuN

Ru	0.131387	-0.030170	1.161455
Pd	0.061055	-0.022242	-1.483754
N	-1.970915	-0.036242	1.112172
N	-1.984064	0.087764	-1.258114
N	0.448318	0.035004	2.903679
N	0.114895	-2.125891	0.965843
N	0.082074	2.062736	0.923912
N	2.181730	-0.021575	0.911841
N	-0.048334	-2.066625	-1.390220
N	0.147891	2.024534	-1.436539
N	2.132182	-0.124973	-1.441571
C	-2.587322	0.058258	-0.059211
H	-3.698332	0.109918	-0.063074
C	-2.755014	-0.287844	2.263713
C	-3.762426	-1.281037	2.259489
H	-3.927889	-1.871281	1.343047

C	-4.508901	-1.540001	3.422072
H	-5.286481	-2.322855	3.406848
C	-4.249058	-0.823261	4.604064
H	-4.826658	-1.034147	5.519828
C	-3.240247	0.161299	4.610540
H	-3.030461	0.732210	5.530893
C	-2.495298	0.431535	3.453341
H	-1.708805	1.200155	3.451757
C	-2.737366	0.494764	-2.380879
C	-3.580325	1.630075	-2.322781
H	-3.646689	2.197856	-1.380271
C	-4.281761	2.051856	-3.464339
H	-4.927587	2.944628	-3.406422
C	-4.140543	1.360979	-4.682118
H	-4.681374	1.702721	-5.580417
C	-3.298436	0.233153	-4.744036
H	-3.183356	-0.322473	-5.690094
C	-2.605793	-0.203610	-3.605002
H	-1.952586	-1.086988	-3.651333
C	0.008225	-2.711569	-0.219874
C	0.104843	2.659082	-0.259685
C	2.783901	-0.080897	-0.271708
H	3.893852	-0.109336	-0.299124
H	0.072779	3.769865	-0.282979
H	-0.035995	-3.821629	-0.250934
C	2.870550	0.175317	2.112516
C	-0.201009	2.878260	2.055137
C	0.357928	-2.958631	2.089001

C	4.044851	0.926388	2.260720
C	-1.358897	3.683762	2.085393
C	1.379380	-3.935345	2.057779
H	4.557931	1.315676	1.364802
H	-2.037924	3.672286	1.216953
H	1.994497	-4.036312	1.148406
C	4.507614	1.270259	3.546885
C	-1.661114	4.447580	3.227611
C	1.627684	-4.738742	3.185443
H	5.417391	1.883281	3.655208
H	-2.576730	5.062922	3.245242
H	2.431920	-5.493263	3.150063
C	3.766284	0.883979	4.696890
C	-0.815132	4.405028	4.349556
C	0.871567	-4.564133	4.357909
H	4.125520	1.177207	5.698266
H	-1.058987	4.992213	5.250862
H	1.072919	-5.186579	5.245873
C	2.606763	0.127589	4.576359
C	0.344699	3.603991	4.316379
C	-0.137699	-3.580751	4.393735
H	2.046599	-0.204949	5.465446
H	1.021511	3.568838	5.186555
H	-0.737170	-3.435140	5.308075
C	2.109854	-0.270909	3.276292
C	0.655014	2.845575	3.178183
C	-0.396138	-2.778385	3.272249
H	1.809795	-1.338505	3.242461

H	1.569860	2.233039	3.145689
H	-1.179526	-2.007045	3.295362
C	2.850396	-0.447072	-2.610239
C	0.436300	2.758623	-2.604483
C	-0.451078	-2.766850	-2.545015
C	3.865194	-1.437094	-2.606281
C	1.403333	3.794052	-2.606520
C	-1.497058	-3.721305	-2.505400
H	4.087692	-1.976782	-1.671441
H	1.953558	4.017997	-1.678211
H	-2.009031	-3.918828	-1.549632
C	4.545182	-1.761414	-3.791441
C	1.689657	4.495086	-3.789440
C	-1.909807	-4.368999	-3.681346
H	5.326579	-2.540323	-3.771032
H	2.449691	5.294938	-3.774531
H	-2.731302	-5.104257	-3.635380
C	4.216043	-1.123686	-5.002024
C	1.038474	4.162778	-4.991888
C	-1.305881	-4.062237	-4.915037
H	4.744304	-1.389569	-5.932755
H	1.275569	4.706550	-5.921535
H	-1.642675	-4.562457	-5.838324
C	3.197881	-0.149980	-5.012385
C	0.088081	3.122922	-4.996597
C	-0.273377	-3.104565	-4.959134
H	2.928648	0.362453	-5.951519
H	-0.434656	2.852473	-5.929656

H	0.212458	-2.855539	-5.917746
C	2.522958	0.190514	-3.831370
C	-0.217720	2.429547	-3.816557
C	0.157108	-2.465337	-3.787536
H	1.735516	0.958178	-3.840919
H	-0.969143	1.626349	-3.819835
H	0.968810	-1.723169	-3.820312

²**2a**-PdRuN

Ru	0.101276	0.020276	3.531470
Pd	0.079099	0.095694	0.900099
N	0.277350	2.112365	3.503024
N	0.337588	2.123729	1.128232
N	0.166086	-0.328134	5.318183
N	-1.983223	0.201047	3.365273
N	2.190685	-0.075864	3.264092
N	-0.092071	-2.010272	3.310279
N	-1.948791	0.350083	1.011110
N	2.114540	-0.126554	0.905093
N	-0.193291	-1.964756	0.957798
C	0.408802	2.719599	2.330403
H	0.579658	3.818839	2.323035
C	0.126229	2.918804	4.656749
C	-0.753405	4.027530	4.663422
H	-1.336428	4.253468	3.755198
C	-0.911164	4.803013	5.825108
H	-1.604612	5.661469	5.817041
C	-0.207047	4.472509	6.997023
H	-0.337909	5.074417	7.912158

C	0.660224	3.361302	6.994053	H	3.900352	1.970891	3.517237
H	1.218827	3.093535	7.907003	H	-4.034518	-1.518048	3.602727
C	0.829159	2.585464	5.837921	C	0.409924	-4.519082	6.051236
H	1.499429	1.715194	5.831842	C	4.671775	1.583917	5.526711
C	0.815489	2.826812	-0.000676	C	-4.663752	-1.079868	5.649915
C	2.084868	3.450277	0.017378	H	0.625245	-5.587733	6.214436
H	2.691140	3.394297	0.936371	H	5.325196	2.472864	5.529858
C	2.580118	4.082902	-1.134609	H	-5.480823	-1.821211	5.636961
H	3.577363	4.554376	-1.111260	C	0.455734	-3.607758	7.155449
C	1.823461	4.090623	-2.321102	C	4.598449	0.755577	6.660292
H	2.220498	4.574912	-3.228943	C	-4.405861	-0.330638	6.811238
C	0.557395	3.472740	-2.340715	H	0.710570	-3.993158	8.157909
H	-0.049601	3.480438	-3.261852	H	5.199721	0.985741	7.555832
C	0.049714	2.850164	-1.190270	H	-5.024697	-0.473838	7.712874
H	-0.939754	2.370586	-1.201541	C	0.219222	-2.261175	6.985339
C	-2.581281	0.347636	2.190152	C	3.748606	-0.369250	6.645641
C	2.769673	-0.115627	2.072354	C	-3.342777	0.595170	6.818700
C	-0.243715	-2.612168	2.127089	H	0.263515	-1.544470	7.821525
H	-0.430802	-3.705809	2.099797	H	3.689221	-1.033001	7.524682
H	3.880254	-0.126275	2.032857	H	-3.129450	1.186956	7.724665
H	-3.684749	0.478545	2.175685	C	-0.204201	-1.727889	5.663805
C	-0.053975	-2.682506	4.520370	C	2.970933	-0.659148	5.515304
C	3.032533	0.179830	4.380951	C	-2.544915	0.778780	5.679593
C	-2.809489	0.033468	4.506762	H	-1.302644	-1.503204	5.768661
C	0.191044	-4.044285	4.744396	H	2.322050	-1.549813	5.497435
C	3.889678	1.300650	4.392467	H	-1.708310	1.492592	5.681865
C	-3.865224	-0.906679	4.504479	C	-0.607838	-2.635296	-0.210813
H	0.299836	-4.733687	3.889522	C	2.812725	-0.424583	-0.281067

C	-2.611836	0.820575	-0.138144	H	0.982178	-1.776300	-1.420812
C	-1.753952	-3.468688	-0.215884	H	1.610278	0.935360	-1.483024
C	3.866297	-1.373012	-0.306840	H	-1.644133	-0.634542	-1.434428
C	-3.496848	1.925999	-0.086761				
H	-2.333787	-3.590848	0.713480				
H	4.131393	-1.911442	0.617389	² TS2a -PdRuN			
H	-3.673209	2.430484	0.877034	Ru	0.169954	-0.006896	3.512663
C	-2.175199	-4.086328	-1.404512	Pd	0.122810	0.074746	0.896820
C	4.536643	-1.657918	-1.507687	N	0.315684	2.076373	3.487641
C	-4.097920	2.407331	-1.261340	N	0.443570	2.091599	1.118636
H	-3.076239	-4.723196	-1.394487	N	0.296171	-0.396198	5.356755
H	5.351492	-2.402062	-1.508203	N	-1.915713	0.169256	3.399002
H	-4.777581	3.274843	-1.205664	N	2.247578	-0.056645	3.252411
C	-1.474945	-3.873368	-2.606728	N	-0.048442	-2.027625	3.303946
C	4.155867	-1.027447	-2.706841	N	-1.893221	0.388551	1.046696
C	-3.812861	1.813415	-2.505244	N	2.150510	-0.203513	0.898648
H	-1.815883	-4.350631	-3.540541	N	-0.214457	-1.967541	0.956474
H	4.676881	-1.263076	-3.649766	C	0.471950	2.690409	2.320361
H	-4.275515	2.204111	-3.426865	H	0.622737	3.792684	2.318863
C	-0.340794	-3.037307	-2.606145	C	0.085405	2.874223	4.634336
C	3.094370	-0.101589	-2.689679	C	-0.847355	3.937707	4.607793
C	-2.924649	0.721068	-2.560828	H	-1.402652	4.138838	3.676587
H	0.221151	-2.862610	-3.539246	C	-1.091699	4.697046	5.765118
H	2.782025	0.403411	-3.619357	H	-1.827314	5.519039	5.732774
H	-2.692426	0.242950	-3.527461	C	-0.418829	4.395834	6.962967
C	0.094069	-2.425093	-1.421902	H	-0.617273	4.984749	7.874393
C	2.431287	0.203362	-1.492458	C	0.504939	3.331185	6.990951
C	-2.332873	0.222683	-1.391576	H	1.040113	3.088181	7.924603

C	0.759621	2.571425	5.839972
H	1.471598	1.734874	5.857014
C	0.930981	2.799320	-0.001984
C	2.180219	3.460717	0.044393
H	2.768039	3.422255	0.976373
C	2.678861	4.113219	-1.095333
H	3.659849	4.616076	-1.049370
C	1.946638	4.103145	-2.296901
H	2.346379	4.604434	-3.194236
C	0.701782	3.444840	-2.345273
H	0.113690	3.438149	-3.278650
C	0.190833	2.801806	-1.207964
H	-0.783426	2.292232	-1.240191
C	-2.518670	0.353497	2.229554
C	2.818203	-0.131930	2.057740
C	-0.252735	-2.618554	2.123118
H	-0.471413	-3.705549	2.088552
H	3.928393	-0.111108	2.004264
H	-3.621281	0.493565	2.221607
C	-0.052608	-2.721359	4.514427
C	3.079398	0.324109	4.339965
C	-2.741748	-0.047063	4.529781
C	-0.066600	-4.111958	4.725801
C	3.814114	1.528277	4.289919
C	-3.828176	-0.952251	4.476632
H	-0.140690	-4.806266	3.871772
H	3.743604	2.154631	3.385284
H	-4.022655	-1.499843	3.539659

C	0.084791	-4.629524	6.023033
C	4.577029	1.940417	5.396592
C	-4.624832	-1.174509	5.612795
H	0.087569	-5.721126	6.176954
H	5.135436	2.890838	5.351586
H	-5.465798	-1.886576	5.556506
C	0.291363	-3.756781	7.127883
C	4.607379	1.156415	6.563546
C	-4.336250	-0.514736	6.821654
H	0.457664	-4.181893	8.132284
H	5.194874	1.484813	7.437358
H	-4.954309	-0.699477	7.716176
C	0.309896	-2.379591	6.957084
C	3.882114	-0.051332	6.610119
C	-3.245446	0.373368	6.882710
H	0.470188	-1.681572	7.794237
H	3.909296	-0.678868	7.517025
H	-3.008820	0.898369	7.823335
C	0.041911	-1.808285	5.652534
C	3.121604	-0.469127	5.507810
C	-2.448324	0.609628	5.750123
H	-0.945003	-1.115471	5.772772
H	2.564582	-1.418980	5.536614
H	-1.600961	1.309648	5.787775
C	-0.670749	-2.620394	-0.206739
C	2.843657	-0.524193	-0.283269
C	-2.567136	0.884653	-0.085353
C	-1.847321	-3.409472	-0.194073

C	3.900334	-1.469067	-0.291531	H	-1.647470	-0.570422	-1.416380
C	-3.436393	2.000318	-0.003116	² 3a -PdRuN			
H	-2.414688	-3.513030	0.745216	Ru	-0.014406	-0.133522	1.244729
H	4.168413	-1.986160	0.644015	Pd	-0.148560	-0.026399	-1.334419
H	-3.587853	2.493557	0.970737	N	2.055382	-0.289536	1.054021
C	-2.311708	-4.005575	-1.377621	N	1.891994	-0.315069	-1.307979
C	4.569417	-1.774558	-1.488090	N	-0.345911	-0.089152	3.166916
C	-4.055666	2.502128	-1.159533	N	0.147888	1.947516	1.158154
H	-3.235862	-4.607985	-1.354860	N	-0.113240	-2.204820	0.995651
H	5.386983	-2.515599	-1.476326	N	-2.046850	0.103281	1.255779
H	-4.723275	3.377114	-1.080298	N	0.118786	2.000046	-1.200647
C	-1.623841	-3.814215	-2.590602	N	-0.412549	-2.056035	-1.335469
C	4.184919	-1.167428	-2.698130	N	-2.184993	0.264076	-1.083091
C	-3.805072	1.917818	-2.415350	C	2.586291	-0.379386	-0.159942
H	-1.998413	-4.274371	-3.520101	H	3.687056	-0.511573	-0.251052
H	4.705453	-1.419068	-3.637170	C	2.916050	-0.108794	2.157671
H	-4.282755	2.323847	-3.322557	C	3.976693	0.827844	2.120336
C	-0.458529	-3.022395	-2.606803	H	4.137622	1.415708	1.201790
C	3.122242	-0.242582	-2.697145	C	4.774222	1.044359	3.257444
C	-2.932271	0.815193	-2.501858	H	5.588703	1.787778	3.216192
H	0.093907	-2.866382	-3.548855	C	4.521678	0.340012	4.448597
H	2.810202	0.246298	-3.635572	H	5.140498	0.520309	5.343458
H	-2.728189	0.343888	-3.478157	C	3.468770	-0.596838	4.487294
C	0.019224	-2.432087	-1.427903	H	3.268987	-1.167767	5.410019
C	2.460078	0.082361	-1.504717	C	2.672313	-0.824044	3.355125
C	-2.322175	0.296729	-1.350670	H	1.861682	-1.567874	3.371147
H	0.932199	-1.818281	-1.437776	C	2.511692	-0.744189	-2.499887
H	1.641940	0.818456	-1.503520	C	3.282559	-1.930882	-2.539956

H	3.393593	-2.527327	-1.619551
C	3.856901	-2.362474	-3.746952
H	4.448246	-3.293894	-3.764865
C	3.657023	-1.630878	-4.932427
H	4.097895	-1.979744	-5.881188
C	2.884119	-0.453402	-4.896883
H	2.724984	0.134043	-5.817047
C	2.320227	-0.006692	-3.692745
H	1.724393	0.917662	-3.660797
C	0.171620	2.594082	0.001921
C	-0.294027	-2.752994	-0.197846
C	-2.727558	0.344730	0.139271
H	-3.799970	0.625664	0.194577
H	-0.327217	-3.861830	-0.274266
H	0.239322	3.703239	0.018849
C	-2.613222	0.185891	2.539013
C	0.316555	-3.053886	2.046808
C	0.014835	2.727254	2.339463
C	-3.971375	0.345158	2.875109
C	1.487868	-3.831063	1.908780
C	-1.058920	3.629945	2.486421
H	-4.741307	0.380594	2.086891
H	2.047316	-3.781835	0.960126
H	-1.788881	3.726449	1.665834
C	-4.352713	0.452340	4.224130
C	1.953800	-4.609101	2.983137
C	-1.213579	4.359975	3.679016
H	-5.417897	0.577170	4.480685

H	2.877404	-5.201540	2.868048
H	-2.063847	5.054784	3.786497
C	-3.379122	0.395487	5.248170
C	1.258343	-4.614203	4.205409
C	-0.305035	4.185501	4.736930
H	-3.685364	0.485387	6.303850
H	1.629313	-5.215252	5.052543
H	-0.432627	4.748605	5.676719
C	-2.028017	0.221593	4.929551
C	0.081497	-3.849002	4.339743
C	0.766063	3.280484	4.591250
H	-1.252916	0.176097	5.713066
H	-0.479126	-3.859648	5.290006
H	1.489047	3.141026	5.412943
C	-1.630822	0.107872	3.579078
C	-0.391160	-3.073639	3.270150
C	0.928256	2.553675	3.402869
H	0.364312	-0.074173	3.903463
H	-1.309428	-2.475372	3.363466
H	1.763435	1.847587	3.278509
C	-2.895047	0.792788	-2.182202
C	-0.905975	-2.680999	-2.494270
C	0.443903	2.731509	-2.356827
C	-3.487340	2.076567	-2.116130
C	-1.950536	-3.636946	-2.433477
C	1.454868	3.726322	-2.351063
H	-3.404327	2.654792	-1.181418
H	-2.392503	-3.888989	-1.455875

H	2.014119	3.921759	-1.421929	N	2.903058	-0.015337	1.817070
C	-4.115860	2.623997	-3.245843	N	2.940556	0.301082	-0.479312
C	-2.448681	-4.217341	-3.611522	N	0.877169	-0.305215	3.604579
C	1.773161	4.423441	-3.527686	N	0.717345	1.976276	1.945027
H	-4.560398	3.632020	-3.186291	N	0.880674	-2.175643	1.587257
H	-3.266405	-4.955538	-3.547795	N	-1.311635	-0.178188	1.742171
H	2.566310	5.190366	-3.503530	N	0.668555	2.113206	-0.368344
C	-4.151406	1.907319	-4.456867	N	1.124995	-1.948549	-0.705888
C	-1.934968	-3.840530	-4.866691	N	-1.125748	-0.157584	-0.581860
C	1.113637	4.128761	-4.735721	C	3.567429	0.196216	0.690480
H	-4.632641	2.346163	-5.346839	H	4.674721	0.285099	0.733969
H	-2.338817	-4.288602	-5.789873	H	3.468984	-0.067746	2.670001
H	1.375908	4.670034	-5.659989	H	3.562172	0.469611	-1.279102
C	-3.563068	0.629047	-4.524267	C	0.623922	2.690206	0.831056
C	-0.905629	-2.880480	-4.931124	C	1.046620	-2.707461	0.386184
C	0.122954	3.127511	-4.751033	C	-1.855657	-0.232479	0.521441
H	-3.590676	0.054197	-5.465395	H	-2.961757	-0.300859	0.443556
H	-0.489006	-2.577680	-5.906684	H	1.118669	-3.813120	0.295145
H	-0.405968	2.883319	-5.687813	H	0.509590	3.793067	0.909643
C	-2.943445	0.068845	-3.396893	C	-2.160443	-0.236895	2.864794
C	-0.389491	-2.308614	-3.759792	H	0.831596	-2.837011	2.368387
C	-0.215938	2.439475	-3.577155	H	0.675160	2.505943	2.821204
H	-2.486881	-0.930554	-3.444393	C	-3.255956	-1.134410	2.935452
H	0.423388	-1.568341	-3.809486	H	-3.432965	-1.837288	2.104583
H	-0.999974	1.667808	-3.593514	C	-4.091626	-1.150044	4.066896
² 1b -Ru ₂ N				H	-4.936761	-1.859093	4.106596
Ru	0.820681	-0.109874	1.917014	C	-3.842391	-0.285820	5.150022
Ru	0.907079	0.080880	-0.536502	H	-4.493047	-0.303838	6.040374

C	-2.745226	0.597883	5.084424	H	0.585910	3.905917	0.499734
H	-2.534804	1.286420	5.920485	C	-2.201683	-0.174847	2.667325
C	-1.919216	0.620056	3.958868	H	0.618319	-2.539731	2.606080
H	-1.079091	1.310171	3.891455	H	0.363808	2.794133	2.514217
H	-1.688710	-0.178291	-1.441925	C	-3.351748	-0.980961	2.793442
H	1.267226	-2.474351	-1.576399	H	-3.791080	-1.441069	1.891502
H	0.576896	2.771289	-1.151884	C	-3.881551	-1.267751	4.061607
² TS1b -Ru ₂ N				H	-4.763442	-1.923865	4.154143
Ru	0.596785	0.121528	1.872585	C	-3.249464	-0.748074	5.233168
Ru	0.911041	0.055044	-0.563966	H	-3.669533	-0.988813	6.225798
N	2.643505	0.224472	2.091916	C	-2.135956	0.072130	5.138349
N	2.931026	0.123115	-0.213566	H	-1.679103	0.508079	6.043695
N	0.142236	0.000442	3.612440	C	-1.538321	0.396269	3.849679
N	0.482812	2.180050	1.701567	H	-1.289980	1.465175	3.735789
N	0.722489	-1.964112	1.764909	H	-1.610278	-0.061820	-1.675414
N	-1.453935	-0.025704	1.515658	H	1.104973	-2.609172	-1.347829
N	0.834284	2.105990	-0.587983	H	0.948746	2.694605	-1.422379
N	0.993679	-1.990390	-0.536078	² 2b -Ru ₂ N			
N	-1.113024	-0.048217	-0.774139	Ru	0.110198	-0.041780	2.808453
C	3.430446	0.182056	1.022726	Ru	0.097755	0.001751	0.362974
H	4.533295	0.201061	1.164465	N	0.305897	2.000335	2.828808
H	3.128879	0.268165	2.994333	N	0.317498	2.041224	0.505947
H	3.652855	0.082264	-0.944540	N	0.141684	-0.396750	4.631261
C	0.630002	2.795654	0.534105	N	-1.953155	0.138687	2.708583
C	0.870873	-2.627440	0.628177	N	2.182125	-0.218363	2.652193
C	-1.934841	-0.129357	0.267928	N	-0.060275	-2.111368	2.681201
H	-3.030092	-0.227508	0.116401	N	-1.944951	0.229659	0.394026
H	0.896131	-3.739007	0.651073	N	2.141979	-0.191275	0.336689

N	-0.096719	-2.012006	0.367891	Ru	0.147026	-0.011688	2.812057
C	0.392944	2.666547	1.682325	Ru	0.120058	-0.001732	0.316354
H	0.530517	3.769538	1.706820	N	0.267753	2.022411	2.778040
H	0.392018	2.568232	3.679011	N	0.268680	2.029801	0.450946
H	0.411783	2.672041	-0.300454	N	0.220501	-0.379391	4.708568
C	-2.598597	0.257870	1.554680	N	-1.890064	0.101245	2.745036
C	2.811571	-0.261191	1.486524	N	2.196358	-0.118877	2.651419
C	-0.112728	-2.731611	1.485226	N	0.029510	-2.072063	2.694918
H	-0.203418	-3.835531	1.441599	N	-1.912560	0.146463	0.424104
H	3.919787	-0.351223	1.472116	N	2.148095	-0.143903	0.329256
H	-3.702300	0.390426	1.562313	N	-0.040125	-2.011379	0.370991
C	-0.038751	-2.744546	3.896104	C	0.312849	2.675439	1.619764
H	2.780860	-0.258261	3.482369	H	0.391580	3.784211	1.626808
H	-2.532581	0.220456	3.550857	H	0.322811	2.618655	3.612465
C	0.240043	-4.099328	4.159812	H	0.317239	2.660615	-0.360796
H	0.374091	-4.805365	3.321627	C	-2.554057	0.164692	1.594276
C	0.448754	-4.539286	5.477136	C	2.822497	-0.165710	1.481235
H	0.693988	-5.596705	5.671267	C	-0.051080	-2.701963	1.510160
C	0.458734	-3.591802	6.562157	H	-0.140283	-3.806395	1.479039
H	0.731750	-3.944653	7.573072	H	3.933363	-0.210174	1.462615
C	0.174678	-2.261588	6.363934	H	-3.662308	0.249765	1.611350
H	0.201776	-1.531102	7.190930	C	0.041672	-2.730529	3.919286
C	-0.273166	-1.756936	5.021999	H	2.816731	-0.086399	3.468016
H	-1.386401	-1.604830	5.085249	H	-2.473118	0.188925	3.587787
H	-0.181574	-2.592941	-0.478532	C	0.110054	-4.118389	4.156085
H	2.735599	-0.216835	-0.500866	H	0.108060	-4.825051	3.308427
H	-2.546271	0.354280	-0.429311	C	0.238842	-4.616735	5.464627
² TS2b-Ru ₂ N				H	0.302377	-5.704249	5.635554

C	0.344194	-3.710781	6.561573	H	-0.660269	-3.799642	1.489148
H	0.498972	-4.109294	7.580091	H	3.628464	-0.639478	1.639642
C	0.284655	-2.337321	6.374329	H	-3.898656	0.419667	1.453270
H	0.374961	-1.631448	7.217458	C	-0.589757	-2.724792	3.958471
C	0.019594	-1.779171	5.048486	H	2.419438	-0.506691	3.602512
H	-1.027554	-1.205806	5.097412	H	-2.795560	0.230695	3.472862
H	-0.135495	-2.617451	-0.456400	C	-0.813017	-4.102121	4.172504
H	2.756249	-0.158833	-0.500272	H	-0.892197	-4.788838	3.313366
H	-2.542899	0.228280	-0.385073	C	-0.939247	-4.616934	5.477466
² 3b -Ru ₂ N				H	-1.114652	-5.695841	5.626690
Ru	-0.159573	-0.062057	2.807598	C	-0.841582	-3.746685	6.587610
Ru	-0.089710	-0.005084	0.318435	H	-0.940337	-4.145373	7.612359
N	0.123272	1.950440	2.787475	C	-0.620451	-2.375690	6.394856
N	0.183864	1.997041	0.457572	H	-0.543459	-1.687138	7.255619
N	-0.277815	-0.513932	4.811290	C	-0.490555	-1.831619	5.089661
N	-2.175522	0.204143	2.654074	H	-0.218195	0.072564	5.647445
N	1.856397	-0.365403	2.754848	H	-0.434044	-2.628992	-0.432246
N	-0.448330	-2.080305	2.719992	H	2.549329	-0.411554	-0.370057
N	-2.108239	0.253575	0.334952	H	-2.704389	0.321654	-0.500754
N	1.918739	-0.305962	0.436012	² 1b -ZrRuN			
N	-0.371798	-2.017614	0.395407	Ru	0.782796	-0.028867	1.910592
C	0.241798	2.617080	1.640641	Zr	1.005952	0.051272	-0.990516
H	0.392924	3.718746	1.667268	N	1.111102	-0.423084	3.605502
H	0.183913	2.549789	3.620832	C	-1.828999	0.456489	4.057520
H	0.292212	2.644645	-0.335966	H	-0.905974	1.035121	4.059182
C	-2.793617	0.301456	1.480732	N	2.843606	0.180797	1.783503
C	2.533973	-0.446594	1.613466	N	3.131202	0.239857	-0.531874
C	-0.503323	-2.702266	1.531889	N	0.553463	2.019424	1.849851

N	0.880631	-2.080092	1.599045	H	0.746024	2.905049	-1.218445
N	-1.313381	-0.176076	1.759896	² TS1b -ZrRuN			
N	0.746600	2.194652	-0.470914	Ru	0.186883	-0.003634	2.741561
N	1.108882	-2.120962	-0.725991	Zr	0.036728	0.042141	0.261032
N	-1.171724	-0.112694	-0.579831	N	0.293288	-0.253124	4.616909
C	3.617572	0.255675	0.719436	C	-0.649767	-1.997626	4.996738
H	4.716871	0.333139	0.873455	H	-1.539370	-1.407068	4.761242
H	3.356707	0.171547	2.676307	N	0.491764	2.035457	2.757840
H	3.870448	0.290358	-1.246880	N	0.307615	2.252700	0.444057
C	0.540334	2.736488	0.736561	N	-1.868702	0.292428	2.811005
C	1.013055	-2.736932	0.463609	N	2.227286	-0.348983	2.520764
C	-1.875932	-0.159499	0.549056	N	-0.125593	-2.101509	2.659407
H	-2.986242	-0.150540	0.493299	N	-2.180520	0.232827	0.503403
H	1.047773	-3.848643	0.501916	N	2.251771	-0.253716	0.193354
H	0.347857	3.829328	0.818041	N	-0.156533	-2.205185	0.332597
C	-2.157729	-0.261285	2.888620	C	0.493860	2.784531	1.666235
H	0.833749	-2.682578	2.431842	H	0.656531	3.880451	1.772494
H	0.319471	2.554981	2.694096	H	0.640634	2.549757	3.633863
C	-3.330187	-1.060240	2.896042	H	0.348453	2.964620	-0.296359
H	-3.576057	-1.672912	2.013042	C	-2.664907	0.334072	1.753077
C	-4.159280	-1.102713	4.031822	C	2.876112	-0.433399	1.370792
H	-5.063944	-1.735339	4.018299	C	-0.183204	-2.802656	1.526537
C	-3.828649	-0.366015	5.184565	H	-0.286983	-3.908048	1.601417
H	-4.473865	-0.405661	6.078360	H	3.965218	-0.662823	1.389397
C	-2.650704	0.409416	5.185612	H	-3.758998	0.458688	1.914601
H	-2.367166	0.987843	6.081534	C	-0.052922	-2.731381	3.907957
H	-1.790428	-0.054496	-1.405555	H	2.798424	-0.537426	3.352214
H	1.234230	-2.784499	-1.503681	H	-2.348079	0.413398	3.711024

C	0.708697	-3.881934	4.168904	H	0.273629	3.034752	-0.251971
H	1.225774	-4.387712	3.335537	C	-2.631436	0.141451	1.710882
C	0.871585	-4.345167	5.495142	C	2.968253	-0.272622	1.403228
H	1.481486	-5.244078	5.689725	C	-0.120866	-2.804329	1.468430
C	0.278518	-3.640298	6.570627	H	-0.315157	-3.896702	1.535957
H	0.410182	-4.004789	7.604439	H	4.070892	-0.425827	1.433239
C	-0.497347	-2.501016	6.322982	H	-3.733494	0.153563	1.870619
H	-1.003504	-1.976328	7.151253	C	0.051300	-2.712074	3.847356
H	-0.231342	-2.882519	-0.436797	H	2.873275	-0.312534	3.387342
H	2.887819	-0.366050	-0.605323	H	-2.315261	0.171859	3.675411
H	-2.925717	0.251170	-0.203656	C	0.327382	-4.050774	4.144425
² 2b -ZrRuN				H	0.567555	-4.754196	3.328547
Ru	0.237503	0.002367	2.672488	C	0.397961	-4.498976	5.486630
Zr	0.113065	0.079196	0.316402	H	0.631108	-5.556572	5.695328
N	0.256618	-0.382480	4.696861	C	0.235306	-3.579108	6.569886
C	-0.244973	-1.713387	4.955971	H	0.351194	-3.944959	7.605968
H	-1.358252	-1.541921	4.852082	C	-0.046615	-2.247140	6.344386
N	0.408726	2.047180	2.782912	H	-0.158299	-1.526617	7.172547
N	0.269228	2.307885	0.474021	H	-0.267969	-2.842355	-0.485542
N	-1.832024	0.136074	2.769072	H	2.980382	-0.262407	-0.575730
N	2.299584	-0.204658	2.543452	H	-2.869899	0.105299	-0.250425
N	0.031972	-2.106782	2.609888	² TS2b -ZrRuN			
N	-2.132019	0.137763	0.463158	Ru	0.250128	0.009678	2.660163
N	2.336996	-0.164924	0.218736	Zr	0.123391	0.071747	0.313780
N	-0.081038	-2.193637	0.289850	N	0.255583	-0.332384	4.693156
C	0.393936	2.825817	1.711274	C	0.005937	-1.722235	4.977393
H	0.488616	3.927061	1.845403	H	-1.089555	-1.357655	4.954621
H	0.507964	2.540484	3.677907	N	0.362447	2.059422	2.763033

N	0.222791	2.308080	0.453375	H	-0.178209	-2.855516	-0.480018
N	-1.820304	0.090506	2.760878	H	3.006605	-0.204859	-0.566120
N	2.316298	-0.140886	2.550404	H	-2.862679	0.020149	-0.255209
N	0.100467	-2.102894	2.615845	² 3b -ZrRuN			
N	-2.125834	0.078149	0.457887	Ru	0.009509	-0.073674	2.663072
N	2.358096	-0.117919	0.225525	Zr	-0.106996	0.021349	0.346012
N	-0.023636	-2.196444	0.293449	N	-0.045894	-0.558715	4.794462
C	0.327535	2.834233	1.688989	C	-0.500459	-1.824311	5.033266
H	0.387639	3.938298	1.820214	H	-0.388451	0.098113	5.504521
H	0.439337	2.557640	3.657324	N	0.248897	1.970586	2.777699
H	0.207891	3.032365	-0.275001	N	0.110454	2.255985	0.472976
C	-2.623868	0.079988	1.705896	N	-2.052055	0.127129	2.770665
C	2.990235	-0.192575	1.411711	N	2.067281	-0.333621	2.564051
C	-0.049840	-2.803278	1.475286	N	-0.269075	-2.163591	2.672489
H	-0.214010	-3.900119	1.533067	N	-2.350232	0.163996	0.463411
H	4.097914	-0.304151	1.445496	N	2.126674	-0.238065	0.240592
H	-3.725755	0.075505	1.868230	N	-0.322393	-2.248934	0.346920
C	0.088986	-2.706575	3.862336	C	0.273998	2.757142	1.709539
H	2.892525	-0.203899	3.397320	H	0.439740	3.849782	1.850649
H	-2.295458	0.142531	3.671519	H	0.406511	2.459362	3.666804
C	0.142820	-4.085157	4.152342	H	0.154862	2.983999	-0.250011
H	0.209777	-4.818875	3.331848	C	-2.849703	0.147079	1.712390
C	0.184646	-4.552041	5.480054	C	2.747724	-0.369671	1.428106
H	0.234686	-5.636657	5.673716	C	-0.423973	-2.850633	1.529128
C	0.195704	-3.632494	6.566378	H	-0.666675	-3.933528	1.572436
H	0.257296	-4.010858	7.601870	H	3.851900	-0.514737	1.464101
C	0.149787	-2.266177	6.339932	H	-3.952767	0.149092	1.870883
H	0.165767	-1.538870	7.169300	C	-0.483990	-2.752692	3.927606

H	2.630394	-0.462470	3.412353	H	4.700201	0.287280	0.814674
H	-2.537676	0.067671	3.674144	H	3.400177	0.080404	2.704048
C	-0.737859	-4.120996	4.185523	H	3.703119	0.312942	-1.258450
H	-0.686681	-4.860417	3.370077	C	0.581837	2.726785	0.760061
C	-1.084742	-4.563990	5.475960	C	1.002664	-2.720815	0.469718
H	-1.285540	-5.635328	5.647614	C	-1.874894	-0.158008	0.513438
C	-1.199772	-3.637035	6.536416	H	-2.984714	-0.165128	0.462214
H	-1.496247	-3.977387	7.543662	H	1.035835	-3.831696	0.446247
C	-0.930337	-2.281353	6.307361	H	0.425339	3.824568	0.834373
H	-0.996474	-1.543040	7.126541	C	-2.143400	-0.249821	2.854181
H	-0.492463	-2.902883	-0.427954	H	0.865625	-2.721872	2.458779
H	2.782336	-0.295127	-0.547518	H	0.496588	2.547668	2.739106
H	-3.089796	0.171803	-0.249004	C	-3.274143	-1.103998	2.884286
² 1b -MoRuN				H	-3.486659	-1.752232	2.018094
Ru	0.808344	-0.050284	1.895672	C	-4.101547	-1.151490	4.021188
Mo	0.945514	0.057653	-0.626520	H	-4.974417	-1.827184	4.028591
N	1.010094	-0.371184	3.614074	C	-3.808009	-0.362024	5.148834
C	-1.852533	0.524913	3.995171	H	-4.451739	-0.404482	6.043539
H	-0.968375	1.160261	3.971696	C	-2.672575	0.473769	5.124533
N	2.871400	0.107654	1.822612	H	-2.422774	1.097725	5.999555
N	3.022574	0.235613	-0.491095	H	-1.775075	-0.059177	-1.446827
N	0.630027	2.012260	1.874118	H	1.151106	-2.631336	-1.510224
N	0.898915	-2.109286	1.634141	H	0.659017	2.835105	-1.214732
N	-1.303188	-0.164651	1.721206	² TS1b -MoRuN			
N	0.719366	2.154946	-0.446338	Ru	0.168367	0.003037	2.747374
N	1.069227	-2.029177	-0.680322	Mo	0.048226	0.041976	0.424590
N	-1.169544	-0.102519	-0.616772	N	0.247451	-0.252158	4.599771
C	3.594682	0.215131	0.724043	C	-0.612135	-1.975666	5.006972

H	-1.517099	-1.397515	4.801384
N	0.479763	2.034199	2.786721
N	0.321894	2.124421	0.482231
N	-1.892044	0.277360	2.800878
N	2.202950	-0.350045	2.585806
N	-0.145776	-2.094725	2.667303
N	-2.044682	0.254352	0.495465
N	2.125247	-0.264419	0.279882
N	-0.186618	-2.071655	0.357405
C	0.500278	2.735749	1.666234
H	0.667613	3.833957	1.707795
H	0.619589	2.564593	3.654395
H	0.373420	2.765412	-0.320655
C	-2.628835	0.319637	1.704790
C	2.814972	-0.442864	1.419352
C	-0.213400	-2.747613	1.509878
H	-0.324016	-3.853298	1.518380
H	3.900683	-0.679299	1.384001
H	-3.733531	0.410941	1.785971
C	-0.056683	-2.725631	3.907371
H	2.769312	-0.538210	3.421067
H	-2.399984	0.337413	3.691106
C	0.693118	-3.889151	4.148223
H	1.176087	-4.407866	3.302537
C	0.887905	-4.343920	5.471019
H	1.489105	-5.251197	5.653465
C	0.343134	-3.621743	6.561130
H	0.506189	-3.980741	7.592178

C	-0.421963	-2.472733	6.330706
H	-0.891418	-1.932627	7.170384
H	-0.278831	-2.676598	-0.467259
H	2.691146	-0.390602	-0.568640
H	-2.714293	0.272997	-0.283221

²**2b**-MoRuN

Ru	0.214368	0.000593	2.716440
Mo	0.090556	0.055788	0.437247
N	0.208349	-0.425126	4.607954
C	-0.338144	-1.720123	4.959559
H	-1.465666	-1.615768	4.901310
N	0.412844	2.038372	2.811240
N	0.275778	2.154388	0.509700
N	-1.859308	0.148014	2.787941
N	2.266088	-0.233927	2.576659
N	-0.013105	-2.114996	2.627561
N	-2.008396	0.196960	0.489036
N	2.181013	-0.153726	0.274408
N	-0.070953	-2.053533	0.322299
C	0.411994	2.759632	1.701787
H	0.523003	3.864060	1.760653
H	0.518671	2.556442	3.690877
H	0.291730	2.805729	-0.286020
C	-2.600536	0.188327	1.696250
C	2.884981	-0.289773	1.411017
C	-0.100249	-2.755999	1.459383
H	-0.220504	-3.859323	1.442598
H	3.982604	-0.461549	1.373370

H	-3.708758	0.211952	1.776059	N	-0.079926	-2.059148	0.341083
C	-0.002680	-2.725766	3.864350	C	0.324360	2.767118	1.642946
H	2.840493	-0.387500	3.412887	H	0.399277	3.875445	1.687409
H	-2.359903	0.120418	3.683688	H	0.356043	2.608976	3.635408
C	0.337943	-4.050130	4.151074	H	0.312278	2.783247	-0.346976
H	0.596628	-4.744621	3.331868	C	-2.612430	0.161317	1.608032
C	0.446727	-4.485897	5.494320	C	2.887216	-0.233956	1.508786
H	0.731599	-5.529796	5.708719	C	-0.098197	-2.741233	1.493641
C	0.289951	-3.552809	6.572925	H	-0.227194	-3.842813	1.483328
H	0.471014	-3.900109	7.606570	H	3.991626	-0.361984	1.515906
C	-0.044292	-2.235324	6.342369	H	-3.722635	0.191445	1.659532
H	-0.138496	-1.509847	7.169463	C	0.066728	-2.719123	3.895761
H	-0.156650	-2.639133	-0.516970	H	2.792928	-0.202358	3.504153
H	2.747649	-0.249505	-0.577384	H	-2.440002	0.122896	3.599688
H	-2.671200	0.209374	-0.295217	C	0.185746	-4.098322	4.148133
² TS2b -MoRuN				H	0.236608	-4.810955	3.306793
Ru	0.163029	0.021524	2.712096	C	0.300090	-4.585927	5.465286
Mo	0.123334	0.032779	0.401357	H	0.399694	-5.669881	5.642658
N	0.200391	-0.356303	4.676160	C	0.341188	-3.672680	6.557602
C	0.002488	-1.748316	5.016742	H	0.477491	-4.059377	7.583533
H	-1.072745	-1.268617	5.034378	C	0.243228	-2.302870	6.354316
N	0.293056	2.066064	2.766491	H	0.289193	-1.589100	7.194814
N	0.274313	2.141501	0.455348	H	-0.219482	-2.658053	-0.481609
N	-1.902381	0.116924	2.724368	H	2.827716	-0.255727	-0.480776
N	2.227488	-0.140742	2.650674	H	-2.633368	0.193036	-0.381035
N	0.026056	-2.091753	2.655733	² 3b -MoRuN			
N	-1.990318	0.171896	0.419650	Ru	-0.156619	-0.053809	2.704430
N	2.222257	-0.169158	0.344584	Mo	-0.092183	0.003208	0.387527

N	-0.274049	-0.504382	4.788278	C	-0.840613	-3.728490	6.589991
C	-0.487612	-1.820210	5.070641	H	-0.937905	-4.114289	7.620271
H	-0.216497	0.076130	5.627642	C	-0.617511	-2.359097	6.379585
N	0.126728	1.972983	2.785352	H	-0.538274	-1.662621	7.234264
N	0.194303	2.090408	0.480792	H	-0.438996	-2.704302	-0.447888
N	-2.202291	0.205090	2.625259	H	2.630139	-0.443798	-0.381531
N	1.883202	-0.367988	2.723395	H	-2.795059	0.306362	-0.511918
N	-0.450916	-2.113242	2.690226	² 1b -PdRuN			
N	-2.186023	0.264649	0.313823	Ru	0.852096	-0.116966	2.072172
N	1.994980	-0.312546	0.414627	Pd	0.924402	0.088471	-0.670999
N	-0.379530	-2.092833	0.376693	N	0.954529	-0.273383	3.755805
C	0.252175	2.691628	1.679284	C	-1.941842	0.607930	4.029198
H	0.405596	3.791181	1.747176	H	-1.089724	1.285542	3.993979
H	0.183933	2.508829	3.659353	N	2.917670	-0.032969	1.820889
H	0.303940	2.744226	-0.305029	N	2.932096	0.318661	-0.504416
C	-2.857100	0.300910	1.478758	N	0.746032	1.960886	1.893288
C	2.593707	-0.457964	1.610024	N	0.850021	-2.139094	1.557231
C	-0.508237	-2.765369	1.527680	N	-1.280989	-0.165652	1.822173
H	-0.662699	-3.864021	1.507859	N	0.670655	2.086161	-0.441022
H	3.684462	-0.666997	1.662488	N	1.175778	-1.918264	-0.745253
H	-3.964569	0.399434	1.478431	N	-1.087725	-0.179630	-0.536662
C	-0.589659	-2.727105	3.950547	C	3.541452	0.185228	0.672565
H	2.399642	-0.525015	3.596353	H	4.650950	0.264637	0.687622
H	-2.782275	0.202523	3.472044	H	3.535856	-0.110474	2.636520
C	-0.815476	-4.100658	4.181685	H	3.554733	0.487772	-1.300530
H	-0.898214	-4.796783	3.330312	C	0.633432	2.643537	0.762518
C	-0.941547	-4.608738	5.491065	C	1.053955	-2.652180	0.353328
H	-1.118923	-5.686413	5.647451	C	-1.790390	-0.222452	0.587607

H	-2.896959	-0.281992	0.493078	N	-1.934042	0.111192	0.506725
H	1.113883	-3.758573	0.258162	N	2.105176	-0.083097	0.171229
H	0.502846	3.745488	0.828502	N	-0.004371	-2.018531	0.379836
C	-2.165831	-0.230304	2.915782	C	0.383800	2.655089	1.657316
H	0.662701	-2.830404	2.288556	H	0.412968	3.767487	1.643258
H	0.670116	2.529049	2.741303	H	0.630565	2.664095	3.620572
C	-3.267488	-1.122748	2.953619	H	0.057048	2.675035	-0.309071
H	-3.428920	-1.817076	2.112020	C	-2.488929	0.188621	1.712720
C	-4.131561	-1.144593	4.064044	C	2.828383	-0.201019	1.282664
H	-4.983565	-1.846742	4.074805	C	-0.042952	-2.685900	1.527123
C	-3.902286	-0.294391	5.162736	H	-0.101974	-3.794380	1.488392
H	-4.574319	-0.316978	6.037172	H	3.936040	-0.220080	1.183302
C	-2.795421	0.579703	5.133937	H	-3.598343	0.223714	1.779027
H	-2.597975	1.254058	5.984911	C	-0.087798	-2.750953	3.941441
H	-1.669318	-0.197242	-1.381808	H	2.981877	-0.416104	3.243870
H	1.426828	-2.429659	-1.597237	H	-2.331867	0.421294	3.682901
H	0.562344	2.732953	-1.228679	C	0.296283	-4.078169	4.185176
² TS1b -PdRuN				H	0.560599	-4.735992	3.338984
Ru	0.269245	-0.037870	2.946253	C	0.438941	-4.554117	5.507908
Pd	0.084186	0.022493	0.268334	H	0.763580	-5.593361	5.684625
N	0.332172	-0.346682	4.690096	C	0.209585	-3.677849	6.608402
C	-0.383370	-1.828432	5.058690	H	0.342168	-4.054956	7.638135
H	-1.376623	-1.340136	4.943822	C	-0.199946	-2.366670	6.405683
N	0.524760	2.032603	2.819219	H	-0.414157	-1.700354	7.259323
N	0.212628	2.041753	0.481814	H	0.049189	-2.620455	-0.449994
N	-1.783075	0.248538	2.833101	H	2.636521	0.119431	-0.681637
N	2.297591	-0.314038	2.489088	H	-2.589328	-0.054344	-0.264508
N	-0.051388	-2.082085	2.722173	² 2b -PdRuN			

Ru	0.265499	-0.053379	2.925078
Pd	0.110456	0.028152	0.260667
N	0.318410	-0.377848	4.703703
C	-0.227894	-1.751373	5.049017
H	-1.304290	-1.425747	5.060035
N	0.475470	2.019350	2.843707
N	0.227657	2.044669	0.497251
N	-1.789265	0.182447	2.797039
N	2.308800	-0.267759	2.503734
N	-0.001015	-2.087344	2.708995
N	-1.912820	0.104992	0.467018
N	2.134708	-0.059108	0.182196
N	0.032942	-2.016788	0.367380
C	0.353216	2.650411	1.684364
H	0.358235	3.763417	1.679264
H	0.543289	2.647141	3.652964
H	0.076529	2.683315	-0.290192
C	-2.482955	0.129258	1.669572
C	2.849567	-0.130071	1.305095
C	0.006290	-2.692833	1.508927
H	-0.028300	-3.801451	1.463813
H	3.957847	-0.089882	1.218642
H	-3.593623	0.126911	1.724155
C	-0.073148	-2.740934	3.924575
H	2.988028	-0.326560	3.267897
H	-2.352035	0.305384	3.646610
C	0.058674	-4.113196	4.185590
H	0.144568	-4.827597	3.348100

C	0.180715	-4.584489	5.510574
H	0.305846	-5.663768	5.699549
C	0.229269	-3.656016	6.601297
H	0.404476	-4.037617	7.623236
C	0.078015	-2.299154	6.400804
H	0.115965	-1.581472	7.238716
H	0.094787	-2.614678	-0.465375
H	2.664214	0.207001	-0.654762
H	-2.552983	-0.077613	-0.313247

²**TS2b**-PdRuN

Ru	0.214208	-0.042876	2.885802
Pd	0.114747	0.009467	0.249285
N	0.261773	-0.359514	4.753597
C	0.026477	-1.791461	5.062282
H	-0.991283	-1.157999	5.115882
N	0.315638	2.023401	2.814343
N	0.231550	2.024874	0.459705
N	-1.836296	0.119860	2.791870
N	2.271493	-0.128184	2.593973
N	0.059759	-2.067294	2.710993
N	-1.907511	0.107872	0.452103
N	2.139518	-0.093395	0.255688
N	0.025133	-2.025165	0.367909
C	0.287095	2.645811	1.642178
H	0.308644	3.758196	1.623549
H	0.315434	2.659955	3.620477
H	0.212834	2.650574	-0.352190
C	-2.501824	0.140814	1.643780

C	2.833150	-0.110810	1.392870	N	1.839710	-0.301285	2.804158
C	0.028853	-2.686057	1.516379	N	-0.464730	-2.094436	2.727964
H	-0.002519	-3.794669	1.480930	N	-2.110722	0.254815	0.310113
H	3.942938	-0.108673	1.317726	N	1.902483	-0.334227	0.463348
H	-3.612165	0.199667	1.666390	N	-0.402948	-2.051919	0.388474
C	0.015843	-2.735222	3.933607	C	0.253154	2.584858	1.647170
H	2.944469	-0.082787	3.366021	H	0.465410	3.677434	1.627922
H	-2.423028	0.237449	3.627993	H	0.147678	2.623449	3.615915
C	0.004450	-4.123292	4.171597	H	0.417218	2.550986	-0.342968
H	-0.040988	-4.830051	3.324781	C	-2.788382	0.371101	1.453730
C	0.110314	-4.627011	5.482338	C	2.491063	-0.435124	1.656907
H	0.113388	-5.716528	5.653626	C	-0.542547	-2.703240	1.538083
C	0.262733	-3.728820	6.577541	H	-0.733645	-3.795976	1.493595
H	0.398199	-4.132135	7.596781	H	3.587025	-0.627046	1.672690
C	0.263978	-2.352556	6.385047	H	-3.877601	0.587428	1.383835
H	0.382556	-1.647888	7.226056	C	-0.581926	-2.763595	3.958069
H	0.038884	-2.630584	-0.461599	H	2.439519	-0.342379	3.636833
H	2.700027	-0.061086	-0.601921	H	-2.874592	0.400448	3.433051
H	-2.543329	0.071884	-0.351402	C	-0.752287	-4.146179	4.174458
² 3b -PdRuN				H	-0.804846	-4.837754	3.316420
Ru	-0.205530	-0.069484	2.876548	C	-0.854251	-4.662651	5.483330
Pd	-0.100245	-0.038018	0.273353	H	-0.987539	-5.747187	5.635839
N	-0.336506	-0.546545	4.798133	C	-0.781349	-3.785935	6.590379
C	-0.504874	-1.869437	5.086854	H	-0.859126	-4.184964	7.617005
H	-0.280604	0.069510	5.611170	C	-0.607687	-2.407113	6.395369
N	0.075149	1.983044	2.816689	H	-0.547599	-1.714198	7.253974
N	0.186606	1.963937	0.465032	H	-0.522221	-2.639247	-0.444712
N	-2.228497	0.246852	2.649508	H	2.504256	-0.544812	-0.339466

H	-2.658987	0.409781	-0.541832
² 1d -Ru			
Ru	0.032628	0.002167	0.042921
N	0.156727	0.087371	1.757567
C	-2.862512	-2.006747	0.250689
H	-2.092716	-2.027510	1.037590
N	1.641111	-0.005117	-1.059470
N	-0.006093	2.046441	-0.101206
N	0.187846	-2.044638	0.066525
N	-1.804253	-0.013826	-0.717315
C	0.006539	2.786005	-1.158598
C	0.322529	-2.855225	-0.927595
H	0.447913	-3.944987	-0.772458
C	-2.815197	-0.961792	-0.714817
C	-3.870725	-0.902498	-1.673409
H	-3.862302	-0.089364	-2.421171
C	-4.898594	-1.858129	-1.679881
H	-5.698350	-1.784000	-2.438032
C	-4.914808	-2.907164	-0.736760
H	-5.721686	-3.659117	-0.745956
C	-3.888691	-2.964076	0.229492
H	-3.896894	-3.760258	0.994992
H	-0.039516	2.565945	0.795602
H	0.218948	-2.492475	1.000393
H	-2.081477	0.852973	-1.203202
H	2.225063	0.846573	-1.103845
H	2.252511	-0.838825	-1.058091
H	0.051587	2.291988	-2.148961

H	-0.015787	3.892002	-1.093332
H	0.303477	-2.440279	-1.953497
² TS1d -Ru			
Ru	-0.172130	0.013345	-0.133970
N	0.013743	-0.046034	1.678590
C	1.326751	-1.245272	2.045703
H	0.657468	-2.051852	1.721741
N	-1.940934	0.332200	-0.926507
N	-0.522604	-1.989840	-0.319671
N	0.152941	2.020268	-0.207135
N	1.845108	-0.368160	-0.106264
C	0.116338	-2.881114	-1.018220
C	-0.166731	2.903752	-1.101291
H	0.090956	3.973806	-0.975011
C	2.338268	-0.839935	1.051566
C	3.714854	-0.749002	1.438398
H	4.467858	-0.494934	0.670852
C	4.068754	-0.848454	2.781081
H	5.120540	-0.695107	3.080080
C	3.081388	-1.118751	3.785403
H	3.387285	-1.183672	4.843835
C	1.766343	-1.357723	3.419489
H	1.020211	-1.663530	4.173890
H	-1.384949	-2.360047	0.117853
H	0.660476	2.413038	0.606486
H	2.540678	0.085342	-0.714239
H	-2.691668	-0.369109	-1.025201
H	-2.367764	1.273339	-0.894931

H	1.055234	-2.579083	-1.518145
H	-0.256636	-3.920706	-1.104394
H	-0.714260	2.564662	-2.001651
² 2d -Ru			
Ru	0.003724	-0.087330	-0.228581
N	0.144621	-0.251257	1.669919
C	1.344322	-1.103481	2.049654
H	1.054301	-2.151458	1.789080
N	-1.686419	0.105702	-1.185936
N	-0.300155	-2.087465	-0.385779
N	0.166788	1.947980	-0.141023
N	2.050921	-0.247086	-0.019293
C	-0.667014	-2.800364	-1.406953
C	-0.160084	2.867155	-0.993588
H	-0.013707	3.943816	-0.774661
C	2.484139	-0.715721	1.141732
C	3.839972	-0.706560	1.614892
H	4.659618	-0.506945	0.901512
C	4.084623	-0.818867	2.973222
H	5.118374	-0.739622	3.352059
C	2.998741	-0.979385	3.921339
H	3.236669	-1.004610	4.999159
C	1.702557	-1.113192	3.498327
H	0.876778	-1.270540	4.214394
H	-0.273434	-2.634721	0.494543
H	0.575735	2.317026	0.737311
H	2.769045	0.149594	-0.641740
H	-2.360667	-0.666824	-1.329306

H	-2.197494	1.004052	-1.223602
H	-0.758280	-2.303203	-2.391193
H	-0.882888	-3.883163	-1.308147
H	-0.603267	2.553895	-1.959004
² TS2d -Ru			
Ru	-0.194168	0.074093	-0.250649
N	0.049365	-0.211070	1.647701
C	1.364170	-0.806706	2.018994
H	0.494071	-1.613680	1.775806
N	-1.927254	0.271404	-1.109875
N	-0.400047	-1.913322	-0.592791
N	-0.062579	2.107663	-0.111590
N	1.856685	-0.144882	-0.159106
C	0.352545	-2.927326	-0.282254
C	-0.436774	3.040110	-0.932254
H	-0.295738	4.113191	-0.694439
C	2.378186	-0.654582	0.973469
C	3.741921	-0.945984	1.272680
H	4.500261	-0.853770	0.474748
C	4.111649	-1.276978	2.581193
H	5.170754	-1.486142	2.811407
C	3.143355	-1.324783	3.629834
H	3.464808	-1.565483	4.657619
C	1.799470	-1.069011	3.369729
H	1.035384	-1.106330	4.164860
H	-1.287789	-2.204151	-1.043358
H	0.372509	2.475499	0.752996

H	2.533925	0.111767	-0.888299	C	4.165327	0.332449	1.064261
H	-2.600271	-0.478898	-1.347214	H	4.774650	0.205555	0.151711
H	-2.431770	1.174823	-1.121521	C	2.757515	0.150579	0.991558
H	1.345708	-2.746356	0.168716	H	2.531008	-0.437079	-0.947267
H	0.036372	-3.964347	-0.508893	H	-1.557354	2.814238	0.006599
H	-0.907230	2.742679	-1.889178	H	-2.378508	-2.181893	-0.193463
² 3d -Ru				H	-2.065740	-0.472252	-1.580486
Ru	0.002245	0.003821	0.002530	² 1d -Mo			
N	0.645250	0.031672	1.967532	Mo	-0.052223	-0.116642	0.032787
C	1.952652	0.302125	2.188259	N	-0.283155	-0.306532	1.684282
H	0.035108	0.080643	2.782660	C	-3.035588	-1.933841	0.358581
N	-1.506714	0.287835	-1.153943	H	-2.193058	-1.936503	1.070944
N	2.011957	-0.217246	-0.088235	N	1.848246	0.163280	-0.676373
N	0.340069	1.993915	-0.066980	N	-0.192131	2.007046	-0.167544
N	-0.320441	-1.992139	-0.030538	N	0.359306	-2.183923	-0.388096
H	-1.779630	1.188089	-1.586679	N	-1.846161	-0.278302	-0.984479
C	-0.468329	3.008355	-0.030222	C	0.217050	2.763173	-1.140760
C	-1.405663	-2.704275	-0.116250	C	0.975773	-2.695839	-1.405876
H	-1.374264	-3.811782	-0.123818	H	1.095895	-3.791225	-1.523887
H	-0.092688	4.051025	-0.045344	C	-2.956676	-1.068091	-0.774593
H	0.535496	-2.569150	0.060574	C	-4.065095	-1.056791	-1.676915
H	1.343188	2.261001	-0.082739	H	-4.023806	-0.392451	-2.558777
C	2.577912	0.643078	3.412229	C	-5.186440	-1.870206	-1.456185
H	1.955818	0.752997	4.318465	H	-6.025230	-1.839261	-2.173804
C	3.970377	0.824585	3.460176	C	-5.250018	-2.721182	-0.332112
H	4.453169	1.092886	4.415866	H	-6.132163	-3.360898	-0.161909
C	4.762340	0.668388	2.291635	C	-4.163824	-2.738883	0.570102
H	5.854861	0.816772	2.346031	H	-4.197281	-3.395817	1.457201

H	-0.660104	2.524668	0.593751	H	1.060857	-1.618696	4.298649
H	0.003986	-2.883893	0.282326	H	-0.263576	-2.817661	0.231144
H	-1.932191	0.269901	-1.854670	H	0.669790	2.440730	0.507518
H	2.305336	1.079553	-0.535726	H	2.768946	0.083603	-0.565779
H	2.558222	-0.564430	-0.492488	H	-2.513702	-0.536213	-1.107446
H	0.745360	2.285150	-1.988775	H	-2.283242	1.132224	-0.951411
H	0.061245	3.860123	-1.131485	H	-1.060045	-2.010802	-2.496121
H	1.402003	-2.002742	-2.157338	H	-1.019882	-3.760642	-1.712130
² TS1d-Mo				H	-0.608943	2.259592	-2.146312
Mo	-0.048091	-0.137961	0.004898	² 2d-Mo			
N	0.099774	-0.398664	1.754121	Mo	-0.023890	-0.326519	0.047504
C	1.482041	-1.253691	2.163760	N	0.196028	-0.812741	1.779650
H	1.083555	-2.229850	1.826150	C	1.502037	-1.241621	2.328285
N	-1.872633	0.201953	-0.774727	H	1.468798	-2.356279	2.238177
N	-0.427377	-2.124326	-0.521200	N	-1.940773	0.104833	-0.348443
N	0.207302	1.938142	-0.267777	N	-0.415110	-2.049335	-1.008751
N	2.065788	-0.338671	0.056755	N	0.355353	1.648952	-0.499024
C	-0.858600	-2.668364	-1.629697	N	2.113805	-0.473425	0.195432
C	-0.104424	2.713488	-1.272197	C	-1.021530	-2.277563	-2.157210
H	0.122561	3.797504	-1.261065	C	-0.254917	2.497218	-1.316108
C	2.548943	-0.742855	1.247035	H	0.096412	3.541304	-1.423350
C	3.876777	-0.542905	1.723465	C	2.600766	-0.783422	1.393724
H	4.651637	-0.211485	1.008462	C	3.942329	-0.637448	1.868170
C	4.154881	-0.640426	3.088575	H	4.753121	-0.423943	1.148588
H	5.170299	-0.421525	3.460981	C	4.178534	-0.630283	3.236628
C	3.114418	-0.979323	4.019068	H	5.201134	-0.462733	3.615918
H	3.351837	-1.023988	5.096708	C	3.086357	-0.744992	4.186054
C	1.838628	-1.291757	3.586914	H	3.308960	-0.628805	5.261340

C	1.800423	-0.976988	3.775829	H	3.442745	-1.372945	5.191796
H	0.966566	-1.073740	4.492426	C	1.854200	-1.121634	3.746689
H	-0.135582	-2.920138	-0.526339	H	1.029727	-1.293710	4.459113
H	1.157195	2.080818	-0.009826	H	0.136904	-2.747101	-0.148100
H	2.822191	-0.160555	-0.485906	H	0.758026	2.448472	0.136963
H	-2.565471	-0.540725	-0.864589	H	2.821940	0.133701	-0.440851
H	-2.340902	1.056232	-0.372384	H	-2.517771	-0.650644	-0.920389
H	-1.347546	-1.413403	-2.764136	H	-2.324181	1.024892	-0.890773
H	-1.175352	-3.308876	-2.527755	H	-1.360522	-1.807105	-2.510479
H	-1.121414	2.131608	-1.895571	H	-0.894668	-3.597579	-1.991633
² TS2d -Mo				H	-0.998511	2.194861	-2.224399
Mo	0.000825	-0.100460	-0.021462	² 3d -Mo			
N	0.186925	-0.602688	1.823999	Mo	0.210982	-0.142380	-0.033783
C	1.535420	-0.905243	2.363285	N	0.878844	-0.254094	1.961990
H	0.768555	-1.816842	1.974386	C	2.162181	0.141345	2.213265
N	-1.887692	0.120919	-0.644372	H	0.335999	-0.465808	2.800011
N	-0.298338	-2.011384	-0.731980	N	-1.057368	0.107992	-1.541459
N	0.143410	1.916518	-0.502845	N	2.215282	-0.024157	-0.127389
N	2.101049	-0.153115	0.236687	N	0.213488	1.921050	-0.063515
C	-0.886488	-2.508016	-1.799741	N	-0.718545	-1.992441	0.167808
C	-0.341651	2.666448	-1.470778	H	-1.286247	1.001450	-2.009380
H	-0.092480	3.742441	-1.542939	C	-0.733462	2.824038	-0.182400
C	2.597956	-0.570243	1.424934	C	-1.959501	-2.416899	0.042501
C	3.954035	-0.646185	1.855217	H	-2.234486	-3.466800	0.258810
H	4.765257	-0.424659	1.139059	H	-0.516971	3.901963	-0.056637
C	4.237195	-0.944770	3.190948	H	-0.085169	-2.739060	0.502200
H	5.287270	-0.989577	3.527779	H	1.135111	2.330712	0.174301
C	3.188381	-1.166921	4.138224	C	2.779436	0.362930	3.465328

H	2.184175	0.232058	4.386768	H	3.636282	0.051106	2.672023
C	4.129145	0.747326	3.523673	H	3.434626	0.232057	-1.287000
H	4.603170	0.926037	4.504359	C	0.729228	2.714365	0.574254
C	4.886921	0.912801	2.336278	C	0.961250	-2.643030	0.362760
H	5.945883	1.217545	2.396057	C	-1.743917	-0.109544	0.703902
C	4.293452	0.687555	1.081415	H	-2.842793	-0.141330	0.555799
H	4.875519	0.801641	0.149465	H	0.954118	-3.754920	0.351363
C	2.936341	0.295099	1.010034	H	0.630201	3.819768	0.642037
H	2.744351	0.049406	-1.008248	C	-2.165913	-0.243147	3.008622
H	-1.760786	2.481362	-0.404949	H	0.873684	-2.735244	2.316317
H	-2.735940	-1.696503	-0.274984	H	0.698533	2.662839	2.532359
H	-1.722192	-0.619976	-1.857397	C	-3.239113	-1.166637	2.952261
² 1b -Mo ₂ N				H	-3.339698	-1.824634	2.073124
Mo	0.902445	-0.026901	2.185333	C	-4.149092	-1.268328	4.020871
Mo	0.937482	0.092259	-0.996594	H	-4.974278	-1.999321	3.963420
N	0.968461	-0.107138	3.856333	C	-3.999500	-0.458484	5.161801
C	-2.022152	0.555422	4.160085	H	-4.709131	-0.540596	6.002270
H	-1.180633	1.246256	4.202728	C	-2.924016	0.452309	5.221117
N	2.979336	0.064682	1.884266	H	-2.788360	1.094875	6.107782
N	2.854066	0.165499	-0.424182	H	-1.512160	-0.003179	-1.259153
N	0.771704	2.031686	1.724655	H	1.050373	-2.661828	-1.601505
N	0.921579	-2.043079	1.558166	H	0.755916	2.877676	-1.384053
N	-1.243066	-0.105167	1.942981	² TS1b -Mo ₂ N			
N	0.799656	2.163030	-0.643552	Mo	0.250887	0.107191	2.984267
N	1.009352	-2.002514	-0.811375	Mo	0.043056	0.011624	0.270851
N	-0.961772	-0.036236	-0.371323	N	0.171213	-0.394542	4.664200
C	3.574876	0.143355	0.701214	C	-0.627863	-2.031220	5.072170
H	4.680488	0.192380	0.627814	H	-1.594198	-1.549091	4.878231

N	0.518630	2.180245	2.755682	H	-0.903324	-2.057365	7.247945
N	0.270487	2.105890	0.432854	H	-0.225735	-2.721180	-0.395093
N	-1.845929	0.405208	2.818684	H	2.692939	-0.411777	-0.615301
N	2.295962	-0.201274	2.553984	H	-2.745806	0.098857	-0.236440
N	-0.100470	-2.069365	2.735660				
N	-2.044502	0.189581	0.510501	² 2b -Mo ₂ N			
N	2.135947	-0.237111	0.232236	Mo	0.103564	0.102053	2.936163
N	-0.136362	-2.081807	0.407146	Mo	0.106259	-0.017074	0.339435
C	0.470783	2.790295	1.567792	N	-0.045846	-0.532407	4.629827
H	0.600140	3.892924	1.523116	C	-0.382332	-1.891969	5.048102
H	0.674986	2.823329	3.540033	H	-1.502787	-1.880020	5.126460
H	0.255597	2.723131	-0.391327	N	0.341726	2.184062	2.794847
C	-2.595561	0.353601	1.717352	N	0.366030	2.087525	0.464321
C	2.860807	-0.331531	1.352182	N	-1.987260	0.377923	2.679816
C	-0.171438	-2.727786	1.572500	N	2.206290	-0.101548	2.729821
H	-0.299292	-3.831672	1.590677	N	-0.126287	-2.120584	2.693235
H	3.951758	-0.533672	1.285873	N	-1.994229	0.234584	0.363440
H	-3.699951	0.441359	1.810137	N	2.198645	-0.279958	0.415434
C	-0.057764	-2.765340	3.946647	N	-0.177378	-2.100216	0.373016
H	2.957619	-0.338864	3.327056	C	0.441047	2.785233	1.604771
H	-2.397832	0.535189	3.675169	H	0.589466	3.885974	1.566270
C	0.641314	-3.963133	4.163426	H	0.420215	2.824224	3.592791
H	1.118701	-4.470981	3.308002	H	0.456964	2.688297	-0.366210
C	0.818557	-4.461765	5.473805	C	-2.645916	0.386191	1.520578
H	1.395765	-5.388372	5.633610	C	2.858536	-0.263376	1.578983
C	0.290299	-3.750340	6.584790	C	-0.241075	-2.768519	1.522751
H	0.436753	-4.145710	7.605253	H	-0.423775	-3.864081	1.523717
C	-0.441030	-2.578758	6.392324	H	3.962118	-0.399749	1.589911

H	-3.750905	0.511796	1.520958	N	-0.052810	-2.092732	0.387690
C	-0.037873	-2.804379	3.889475	C	0.387081	2.826565	1.562047
H	2.819053	-0.126077	3.553198	H	0.545593	3.927191	1.534809
H	-2.597017	0.506347	3.496607	H	0.526315	2.789412	3.548856
C	0.378382	-4.120487	4.114009	H	0.249903	2.734024	-0.415080
H	0.617851	-4.776481	3.258976	C	-2.650483	0.191161	1.680423
C	0.616234	-4.580105	5.433193	C	2.947858	-0.094935	1.449372
H	0.958263	-5.615803	5.597207	C	-0.036271	-2.803224	1.509074
C	0.540872	-3.672409	6.541684	H	-0.184870	-3.903078	1.487495
H	0.847389	-4.027039	7.542273	H	4.058248	-0.128850	1.385591
C	0.135645	-2.364855	6.377151	H	-3.761842	0.218918	1.732546
H	0.099037	-1.654052	7.220599	C	0.102398	-2.797657	3.894037
H	-0.370519	-2.698627	-0.442115	H	2.986056	-0.029208	3.438699
H	2.808960	-0.484106	-0.386971	H	-2.463818	0.290369	3.662727
H	-2.624206	0.185482	-0.447736	C	0.210210	-4.180764	4.159033
² TS2b -Mo ₂ N				H	0.312432	-4.897020	3.326543
Mo	0.221617	0.079516	2.744223	C	0.265678	-4.650689	5.482695
Mo	0.093606	0.018890	0.492199	H	0.362274	-5.733463	5.670611
N	0.083541	-0.448065	4.675220	C	0.233579	-3.743710	6.579379
C	-0.040237	-1.845662	5.014529	H	0.307125	-4.132063	7.609945
H	-1.141290	-1.467537	4.989306	C	0.126584	-2.375663	6.366881
N	0.373938	2.183084	2.734511	H	0.102616	-1.656996	7.203459
N	0.220793	2.141605	0.423920	H	-0.231402	-2.660442	-0.450902
N	-1.919495	0.227058	2.793406	H	2.764964	-0.200224	-0.525910
N	2.343178	-0.039036	2.638419	H	-2.673508	0.034788	-0.301151
N	0.118662	-2.152765	2.680280	² 3b -Mo ₂ N			
N	-2.031330	0.106806	0.497295	Mo	-0.147247	0.016494	2.691722
N	2.208249	-0.119837	0.333810	Mo	-0.095686	-0.019907	0.488216

N	-0.289645	-0.589261	4.829300
C	-0.500066	-1.905605	5.106414
H	-0.229694	-0.025036	5.680224
N	0.143849	2.121661	2.737289
N	0.197464	2.089911	0.422453
N	-2.264409	0.328766	2.650012
N	1.973976	-0.265090	2.758472
N	-0.459142	-2.138586	2.731216
N	-2.198720	0.248106	0.343860
N	2.004066	-0.337338	0.451226
N	-0.391901	-2.144546	0.416378
C	0.262977	2.766563	1.573763
H	0.417426	3.869087	1.562737
H	0.206141	2.730899	3.561389
H	0.302973	2.681807	-0.410732
C	-2.897354	0.372383	1.481133
C	2.651524	-0.408362	1.622944
C	-0.524472	-2.801667	1.562727
H	-0.690433	-3.899523	1.546220
H	3.748743	-0.595447	1.641808
H	-4.002249	0.503218	1.443996
C	-0.599323	-2.790690	3.971241
H	2.532772	-0.374961	3.612286
H	-2.872641	0.387447	3.474522
C	-0.820118	-4.168273	4.181670
H	-0.899935	-4.857286	3.324561
C	-0.944731	-4.694734	5.485149
H	-1.118039	-5.775379	5.624739

C	-0.846843	-3.832944	6.598043
H	-0.942908	-4.235598	7.621868
C	-0.627387	-2.459405	6.407770
H	-0.549282	-1.774594	7.271890
H	-0.461651	-2.748428	-0.411129
H	2.610692	-0.476868	-0.365529
H	-2.778695	0.284074	-0.502911

²**1b**-RuMoN

Mo	0.896981	-0.087758	2.098247
Ru	0.917390	0.086615	-0.592597
N	0.936864	-0.213856	3.767366
C	-1.999113	0.628558	3.997524
H	-1.179277	1.345543	3.967048
N	2.977844	0.028319	1.784445
N	2.940991	0.228918	-0.535025
N	0.752244	2.013487	1.926921
N	0.929916	-2.147435	1.635012
N	-1.262548	-0.152754	1.805065
N	0.740228	2.104682	-0.400064
N	1.033929	-1.940800	-0.680839
N	-1.110590	-0.075661	-0.536981
C	3.609212	0.167077	0.613127
H	4.718379	0.231464	0.605193
H	3.616749	-0.007895	2.586343
H	3.555386	0.336074	-1.354003
C	0.673285	2.705878	0.784804
C	0.984770	-2.692460	0.415162
C	-1.819432	-0.161509	0.579297

H	-2.927657	-0.206738	0.511259	N	-1.976162	0.223959	0.529643
H	0.991298	-3.799482	0.319756	N	2.069555	-0.221969	0.305639
H	0.552924	3.809398	0.831588	N	-0.143292	-2.002073	0.413840
C	-2.154995	-0.243379	2.901604	C	0.484673	2.766978	1.571828
H	0.881572	-2.842662	2.387776	H	0.630117	3.867015	1.514309
H	0.689810	2.602796	2.764344	H	0.668207	2.793239	3.557562
C	-3.211184	-1.187236	2.931863	H	0.290356	2.642259	-0.390123
H	-3.323614	-1.896331	2.094810	C	-2.597789	0.327046	1.700353
C	-4.088839	-1.241023	4.030887	C	2.819437	-0.385469	1.390261
H	-4.901116	-1.988580	4.041121	C	-0.175122	-2.705176	1.537050
C	-3.923954	-0.361333	5.116861	H	-0.282578	-3.810834	1.507152
H	-4.608113	-0.405864	5.980973	H	3.901261	-0.619848	1.289962
C	-2.867809	0.573428	5.089158	H	-3.706887	0.389968	1.737065
H	-2.723064	1.273632	5.929634	C	-0.065909	-2.756250	3.931987
H	-1.707833	-0.063880	-1.375618	H	2.908638	-0.498760	3.376693
H	1.074557	-2.494354	-1.547725	H	-2.465096	0.387427	3.684769
H	0.662870	2.763429	-1.187421	C	0.630351	-3.955925	4.155100
² TS1b -RuMoN				H	1.081904	-4.486227	3.299284
Mo	0.214944	0.095148	2.899128	C	0.833901	-4.427052	5.470778
Ru	0.049716	0.034261	0.433879	H	1.408333	-5.354570	5.636094
N	0.173850	-0.354238	4.613612	C	0.337242	-3.692068	6.579757
C	-0.608830	-2.000506	5.056559	H	0.507239	-4.067881	7.603759
H	-1.572659	-1.511769	4.871837	C	-0.396740	-2.522118	6.379891
N	0.511091	2.157861	2.767252	H	-0.841464	-1.984180	7.234485
N	0.284762	2.063424	0.461585	H	-0.224791	-2.581894	-0.432078
N	-1.891543	0.342297	2.834493	H	2.581617	-0.358732	-0.576417
N	2.268360	-0.284946	2.604245	H	-2.613699	0.184925	-0.276463
N	-0.127852	-2.077551	2.721215	² 2b -RuMoN			

Mo	0.159143	0.093511	2.861942
Ru	0.105337	0.045602	0.450879
N	0.044704	-0.486004	4.586648
C	-0.363142	-1.814132	5.031981
H	-1.485707	-1.760918	5.095668
N	0.376838	2.165457	2.809383
N	0.304471	2.083435	0.497773
N	-1.952944	0.257313	2.742729
N	2.245637	-0.192459	2.686904
N	-0.081881	-2.101542	2.684930
N	-1.927432	0.212868	0.440054
N	2.133704	-0.177712	0.385606
N	-0.082249	-1.987115	0.383681
C	0.409457	2.787155	1.620064
H	0.523428	3.891541	1.579413
H	0.462737	2.792014	3.617469
H	0.339714	2.663458	-0.352170
C	-2.609304	0.262665	1.580293
C	2.849895	-0.291279	1.499631
C	-0.136761	-2.714506	1.490127
H	-0.253109	-3.817300	1.432936
H	3.942892	-0.485292	1.443519
H	-3.720310	0.293373	1.565228
C	-0.051360	-2.771846	3.889305
H	2.858249	-0.366468	3.491042
H	-2.557737	0.239676	3.571934
C	0.274850	-4.106899	4.139981
H	0.467495	-4.797418	3.300103

C	0.477395	-4.554623	5.470943
H	0.753116	-5.606388	5.656784
C	0.457065	-3.621683	6.559702
H	0.743573	-3.973574	7.567366
C	0.128703	-2.295350	6.368861
H	0.131309	-1.569300	7.200187
H	-0.162110	-2.545274	-0.476787
H	2.677215	-0.312869	-0.477065
H	-2.517740	0.177655	-0.401053

²**TS2b**-RuMoN

Mo	0.171283	0.116957	2.835262
Ru	0.116204	0.019332	0.449697
N	0.173218	-0.471522	4.658538
C	0.033755	-1.863011	5.053571
H	-1.006336	-1.146397	5.029922
N	0.298436	2.199273	2.749258
N	0.252204	2.069728	0.440914
N	-1.937835	0.207105	2.781469
N	2.278086	-0.051525	2.685866
N	0.039232	-2.093904	2.707596
N	-1.932085	0.134296	0.475985
N	2.154649	-0.137684	0.383972
N	-0.029097	-2.006399	0.403256
C	0.316918	2.799257	1.548860
H	0.386564	3.906496	1.486998
H	0.357495	2.843651	3.545894
H	0.271939	2.629109	-0.422584
C	-2.603666	0.182142	1.621771

C	2.879337	-0.164618	1.497891	N	1.947155	-0.331009	2.751359
C	-0.046677	-2.718596	1.520827	N	-0.443594	-2.119767	2.737493
H	-0.138899	-3.823252	1.469944	N	-2.122745	0.256751	0.357200
H	3.982823	-0.287494	1.438437	N	1.938353	-0.296347	0.444845
H	-3.715307	0.194920	1.614541	N	-0.369574	-2.035113	0.431103
C	0.060911	-2.782078	3.915831	C	0.249468	2.717929	1.613531
H	2.918072	-0.109054	3.485989	H	0.396773	3.819930	1.584588
H	-2.542277	0.220586	3.613431	H	0.202628	2.719028	3.600151
C	0.126130	-4.168867	4.147744	H	0.281078	2.614724	-0.363770
H	0.133272	-4.875967	3.300859	C	-2.846891	0.309384	1.471056
C	0.236729	-4.668125	5.464623	C	2.601399	-0.433381	1.589010
H	0.294549	-5.756994	5.631483	C	-0.501982	-2.741770	1.546692
C	0.321860	-3.774489	6.565155	H	-0.660042	-3.839122	1.487696
H	0.453378	-4.175806	7.585316	H	3.692237	-0.647891	1.577430
C	0.265177	-2.393155	6.374387	H	-3.953714	0.395756	1.410923
H	0.340956	-1.686483	7.217870	C	-0.593754	-2.770991	3.968835
H	-0.118330	-2.574450	-0.449322	H	2.523359	-0.519763	3.579473
H	2.703103	-0.258459	-0.477141	H	-2.879345	0.216804	3.463078
H	-2.530631	0.081247	-0.358121	C	-0.825811	-4.145767	4.186817
² 3b -RuMoN				H	-0.906569	-4.835796	3.330397
Mo	-0.140956	0.006242	2.804751	C	-0.959662	-4.652554	5.496900
Ru	-0.089811	0.002343	0.442355	H	-1.142169	-5.730214	5.649299
N	-0.272667	-0.553458	4.799090	C	-0.861624	-3.783328	6.602091
C	-0.495433	-1.885429	5.095749	H	-0.966456	-4.175348	7.628551
H	-0.211770	0.023231	5.642628	C	-0.630723	-2.409839	6.397856
N	0.139343	2.086849	2.792500	H	-0.552778	-1.715363	7.253913
N	0.183900	2.031389	0.477782	H	-0.428322	-2.607579	-0.421540
N	-2.239794	0.240093	2.660705	H	2.516708	-0.419545	-0.395517

H	-2.676183	0.289813	-0.508081
¹ 1b -TcRuN			
Ru	0.823434	-0.050217	1.874650
Tc	0.913460	0.086884	-0.532827
N	0.856236	-0.175619	3.616124
C	-1.940776	0.615430	3.952630
H	-1.131442	1.341401	3.890540
N	2.888145	0.034464	1.825902
N	2.960550	0.217283	-0.478424
N	0.714371	2.022443	1.889373
N	0.877502	-2.111925	1.644629
N	-1.304501	-0.131543	1.726208
N	0.746372	2.136131	-0.421505
N	1.014294	-1.962103	-0.659472
N	-1.142002	-0.052699	-0.596542
C	3.581188	0.155967	0.708588
H	4.690118	0.205451	0.761037
H	3.431546	-0.007795	2.695762
H	3.603127	0.310620	-1.275775
C	0.672231	2.734267	0.776579
C	0.952774	-2.694909	0.462643
C	-1.867114	-0.139693	0.519052
H	-2.975525	-0.187565	0.453593
H	0.964370	-3.804531	0.401904
H	0.578408	3.839744	0.840705
C	-2.143900	-0.245077	2.855669
H	0.831279	-2.738137	2.456214
H	0.662136	2.553685	2.765809

C	-3.184435	-1.202742	2.918876
H	-3.323157	-1.903543	2.078782
C	-4.015160	-1.274438	4.052680
H	-4.821469	-2.027380	4.089827
C	-3.809652	-0.403155	5.139116
H	-4.456198	-0.462435	6.030925
C	-2.764121	0.541512	5.078543
H	-2.590735	1.233125	5.920548
H	-1.719877	-0.030912	-1.447386
H	1.061823	-2.527245	-1.517281
H	0.694765	2.793566	-1.210778
¹ TS1b -TcRuN			
Ru	0.096729	-0.037506	2.785189
Tc	0.045369	0.016329	0.409977
N	0.095333	-0.351226	4.587448
C	-0.562180	-1.903829	5.005589
H	-1.591221	-1.538764	4.847919
N	0.429770	1.990881	2.835117
N	0.383483	2.052791	0.519900
N	-1.954931	0.243676	2.740936
N	2.139032	-0.378889	2.641173
N	-0.189826	-2.112217	2.669956
N	-1.989433	0.337638	0.432369
N	2.079274	-0.322011	0.333703
N	-0.283239	-2.014094	0.363819
C	0.525616	2.670128	1.701374
H	0.736878	3.760835	1.733631
H	0.604671	2.528862	3.691259

H	0.504695	2.683256	-0.284450	N	0.327055	2.069044	0.514661
C	-2.629753	0.366855	1.609841	N	-1.945824	0.173999	2.724703
C	2.757442	-0.483351	1.478217	N	2.187795	-0.278271	2.645391
C	-0.284102	-2.730801	1.498857	N	-0.098463	-2.127948	2.660678
H	-0.395597	-3.835579	1.474376	N	-1.986299	0.277920	0.418796
H	3.846098	-0.704938	1.452836	N	2.133350	-0.228165	0.339983
H	-3.732893	0.495740	1.640201	N	-0.189624	-2.014216	0.356183
C	-0.054642	-2.736863	3.907184	C	0.456014	2.690202	1.691979
H	2.711095	-0.538518	3.476916	H	0.644475	3.785120	1.726524
H	-2.514869	0.262371	3.600637	H	0.584261	2.533614	3.682006
C	0.731979	-3.875685	4.142127	H	0.443938	2.694407	-0.293491
H	1.180156	-4.401175	3.280161	C	-2.625189	0.287600	1.594517
C	0.990399	-4.306100	5.458878	C	2.817251	-0.340221	1.483829
H	1.610331	-5.200053	5.640837	C	-0.192413	-2.747449	1.481389
C	0.464264	-3.556753	6.551802	H	-0.304948	-3.849955	1.441082
H	0.657923	-3.899747	7.584417	H	3.919748	-0.480287	1.462076
C	-0.309175	-2.420509	6.345201	H	-3.731157	0.392675	1.626271
H	-0.742222	-1.875624	7.202290	C	-0.034133	-2.744348	3.890154
H	-0.439376	-2.590665	-0.473476	H	2.765281	-0.377399	3.485798
H	2.658752	-0.416151	-0.509892	H	-2.500851	0.167698	3.587248
H	-2.610691	0.437455	-0.380331	C	0.465789	-4.031603	4.154538
¹ 2b -TcRuN				H	0.763010	-4.676572	3.307940
Ru	0.124355	-0.031155	2.761182	C	0.665113	-4.467091	5.474650
Tc	0.070311	0.001629	0.420599	H	1.077743	-5.469949	5.674321
N	0.091152	-0.431913	4.580285	C	0.422954	-3.555780	6.562150
C	-0.408511	-1.779000	4.991488	H	0.643901	-3.889015	7.593072
H	-1.516034	-1.608560	4.953464	C	-0.050116	-2.279433	6.359259
N	0.381657	2.005455	2.826244	H	-0.222505	-1.592464	7.206459

H	-0.328799	-2.583174	-0.489813
H	2.718662	-0.254133	-0.503689
H	-2.603809	0.374508	-0.395937
¹ TS2b -TcRuN			
Ru	0.110356	0.038377	2.769517
Tc	0.127730	0.002638	0.381981
N	0.180120	-0.391898	4.657639
C	0.008152	-1.787604	5.030649
H	-1.038926	-1.166773	5.037261
N	0.247059	2.077082	2.767031
N	0.314057	2.070715	0.453671
N	-1.938546	0.114319	2.719907
N	2.172910	-0.109115	2.694898
N	-0.004975	-2.078129	2.675536
N	-1.937534	0.200280	0.412394
N	2.177792	-0.212551	0.386350
N	-0.122569	-2.026376	0.359794
C	0.331841	2.734029	1.616341
H	0.432398	3.840841	1.624707
H	0.328770	2.653055	3.612464
H	0.400776	2.684272	-0.368106
C	-2.602105	0.178454	1.573426
C	2.832052	-0.240464	1.554666
C	-0.132659	-2.714792	1.509013
H	-0.259676	-3.816101	1.488501
H	3.938011	-0.354622	1.569285
H	-3.712811	0.228284	1.583732
C	0.061826	-2.731039	3.904556

H	2.748221	-0.129669	3.543752
H	-2.518139	0.114063	3.568916
C	0.214644	-4.110944	4.139537
H	0.264028	-4.812244	3.288772
C	0.356934	-4.607823	5.449870
H	0.483034	-5.690323	5.618093
C	0.396208	-3.700313	6.546194
H	0.554251	-4.089320	7.568038
C	0.271927	-2.328202	6.356089
H	0.319082	-1.620578	7.201211
H	-0.285620	-2.620631	-0.463109
H	2.799679	-0.279392	-0.430260
H	-2.553154	0.298264	-0.406330
¹ 3b -TcRuN			
Ru	-0.155714	-0.051241	2.767389
Tc	-0.087327	0.019791	0.359033
N	-0.273853	-0.497022	4.783827
C	-0.488189	-1.818388	5.070153
H	-0.216010	0.083875	5.625321
N	0.125658	1.963467	2.807375
N	0.188023	2.049036	0.491573
N	-2.191691	0.201086	2.639540
N	1.874712	-0.370821	2.737125
N	-0.447348	-2.089360	2.699243
N	-2.139185	0.256869	0.325710
N	1.950368	-0.307022	0.424269
N	-0.371617	-2.035794	0.382269
C	0.245419	2.659685	1.684114

H	0.395360	3.761110	1.734356	H	-0.912442	1.055496	4.055636
H	0.184236	2.528572	3.663928	N	2.892903	0.158935	1.800357
H	0.295227	2.709595	-0.292145	N	3.015337	0.240607	-0.524504
C	-2.825475	0.285162	1.478259	N	0.575790	1.999408	1.881560
C	2.562391	-0.465442	1.607742	N	0.910906	-2.136198	1.618720
C	-0.502991	-2.721428	1.520562	N	-1.300836	-0.198263	1.762895
H	-0.659639	-3.819910	1.486031	N	0.749711	2.127386	-0.437603
H	3.649615	-0.694989	1.639892	N	1.115617	-2.025834	-0.695765
H	-3.934294	0.362219	1.458120	N	-1.134072	-0.138313	-0.576644
C	-0.588029	-2.717715	3.945328	C	3.590238	0.249861	0.678897
H	2.412844	-0.549012	3.593145	H	4.696088	0.341365	0.753885
H	-2.797136	0.184615	3.468566	H	3.449871	0.152741	2.662380
C	-0.813128	-4.092938	4.172619	H	3.678837	0.321578	-1.303871
H	-0.893897	-4.787254	3.319815	C	0.560845	2.697785	0.750682
C	-0.939451	-4.597260	5.482410	C	1.047927	-2.720812	0.440184
H	-1.116066	-5.675167	5.638882	C	-1.849337	-0.196062	0.538541
C	-0.840873	-3.720995	6.585484	H	-2.957750	-0.198396	0.468604
H	-0.939573	-4.110768	7.613634	H	1.104445	-3.830926	0.404712
C	-0.618147	-2.350871	6.377815	H	0.378990	3.792927	0.810927
H	-0.540045	-1.654130	7.232105	C	-2.152704	-0.257540	2.883544
H	-0.432018	-2.647991	-0.444631	H	0.868463	-2.770934	2.423158
H	2.566104	-0.470164	-0.382430	H	0.311588	2.529093	2.718844
H	-2.738232	0.261490	-0.509487	C	-3.337234	-1.041520	2.889146
³ 1b -TcRuN				H	-3.583199	-1.660780	2.010920
Ru	0.810426	-0.061767	1.953279	C	-4.176292	-1.062766	4.017005
Tc	0.949849	0.045745	-0.638174	H	-5.087976	-1.685122	3.999830
N	1.083058	-0.427875	3.598784	C	-3.848291	-0.320564	5.167542
C	-1.830612	0.469689	4.049799	H	-4.502485	-0.344069	6.055143

C	-2.661892	0.441044	5.171437
H	-2.380158	1.027342	6.062695
H	-1.726409	-0.074998	-1.415150
H	1.239908	-2.606335	-1.533613
H	0.738959	2.796382	-1.216865

³**TS1b**-TcRuN

Ru	0.148137	-0.016388	2.810699
Tc	0.063131	0.037711	0.334555
N	0.366456	-0.232074	4.611368
C	-0.497437	-1.912993	5.056814
H	-1.397970	-1.308676	4.908267
N	0.413281	2.024253	2.794685
N	0.302263	2.090226	0.475629
N	-1.905380	0.233470	2.810333
N	2.196755	-0.307342	2.558734
N	-0.120833	-2.084263	2.701162
N	-2.004329	0.231985	0.492024
N	2.122098	-0.198888	0.241367
N	-0.084301	-2.043319	0.382115
C	0.448334	2.703191	1.657118
H	0.589723	3.805630	1.686924
H	0.493043	2.591442	3.646469
H	0.345986	2.734613	-0.324847
C	-2.605105	0.297984	1.685346
C	2.802790	-0.354785	1.383044
C	-0.120195	-2.726219	1.521578
H	-0.190010	-3.833847	1.508013
H	3.899026	-0.538549	1.347097

H	-3.710284	0.404284	1.740397
C	-0.087469	-2.729841	3.928274
H	2.800770	-0.461379	3.373820
H	-2.454695	0.312180	3.673703
C	0.494127	-3.997985	4.152598
H	0.851896	-4.595754	3.297462
C	0.708273	-4.456265	5.462963
H	1.198398	-5.431706	5.624224
C	0.336043	-3.655023	6.580289
H	0.518893	-4.025202	7.603784
C	-0.281365	-2.424073	6.378787
H	-0.622781	-1.818283	7.235495
H	-0.086541	-2.653204	-0.446262
H	2.698377	-0.305410	-0.602220
H	-2.663965	0.260269	-0.295819

³**2b**-TcRuN

Ru	0.184708	-0.021893	2.762848
Tc	0.102483	0.058836	0.350152
N	0.219704	-0.356886	4.669459
C	-0.237443	-1.698942	4.999764
H	-1.361796	-1.576691	5.014873
N	0.364002	2.003207	2.829888
N	0.271821	2.106240	0.516684
N	-1.872479	0.113763	2.752824
N	2.231411	-0.222389	2.592592
N	-0.006117	-2.085171	2.652924
N	-1.959914	0.180783	0.442025
N	2.157377	-0.134435	0.281635

N	-0.043631	-2.016597	0.339611	N	0.225509	-0.335694	4.710466
C	0.379750	2.711714	1.709160	C	0.018748	-1.731096	5.024071
H	0.481404	3.817472	1.758297	H	-1.061767	-1.294518	5.079585
H	0.448448	2.545638	3.698720	N	0.303524	2.022845	2.794961
H	0.298177	2.764869	-0.273872	N	0.244508	2.092525	0.477040
C	-2.576800	0.166013	1.631851	N	-1.867317	0.101378	2.745736
C	2.850029	-0.258323	1.422347	N	2.233322	-0.145944	2.622292
C	-0.074679	-2.720247	1.468888	N	0.048959	-2.073831	2.665636
H	-0.176770	-3.824530	1.440978	N	-1.952794	0.127893	0.432695
H	3.952335	-0.397198	1.387414	N	2.177526	-0.120108	0.307832
H	-3.686588	0.198188	1.680447	N	-0.012944	-2.029068	0.345520
C	-0.006831	-2.706539	3.880326	C	0.312082	2.715095	1.662652
H	2.833341	-0.339350	3.415279	H	0.373845	3.824518	1.698292
H	-2.422013	0.108316	3.620562	H	0.349148	2.586441	3.653165
C	0.215686	-4.064072	4.153209	H	0.258385	2.742719	-0.320577
H	0.365741	-4.778756	3.325000	C	-2.569918	0.135295	1.620949
C	0.351341	-4.511437	5.484721	C	2.862693	-0.189313	1.456643
H	0.546785	-5.578600	5.683958	C	-0.029161	-2.716616	1.487374
C	0.336986	-3.574929	6.574007	H	-0.113993	-3.822058	1.464662
H	0.544396	-3.942838	7.595069	H	3.970052	-0.284091	1.433023
C	0.107636	-2.234043	6.362298	H	-3.679847	0.172911	1.666989
H	0.122526	-1.502994	7.189472	C	0.048566	-2.707149	3.898670
H	-0.106328	-2.609891	-0.498960	H	2.842211	-0.187065	3.447191
H	2.738793	-0.206018	-0.563233	H	-2.420614	0.153223	3.610658
H	-2.608349	0.203502	-0.355227	C	0.089787	-4.091757	4.154335
³ TS2b -TcRuN				H	0.085404	-4.809508	3.315995
Ru	0.182963	-0.006882	2.760232	C	0.201303	-4.577775	5.470150
Tc	0.116428	0.035805	0.329488	H	0.242957	-5.664959	5.650804

C	0.311636	-3.666434	6.562630	H	-0.654878	-3.835267	1.501213
H	0.452048	-4.060707	7.584824	H	3.656457	-0.642151	1.664888
C	0.271931	-2.296397	6.360844	H	-3.932557	0.418770	1.483958
H	0.364411	-1.583115	7.197905	C	-0.590309	-2.727068	3.953490
H	-0.084042	-2.635629	-0.482708	H	2.403823	-0.486049	3.613613
H	2.770689	-0.188912	-0.529052	H	-2.777022	0.246155	3.490875
H	-2.601098	0.123744	-0.364981	C	-0.816371	-4.103214	4.171268
³ 3b -TcRuN				H	-0.898600	-4.791836	3.313692
Ru	-0.158021	-0.050754	2.746289	C	-0.943470	-4.620648	5.475618
Tc	-0.095239	-0.015317	0.349255	H	-1.121249	-5.699175	5.624793
N	-0.275252	-0.517052	4.804678	C	-0.843303	-3.746921	6.582836
C	-0.488862	-1.827753	5.081193	H	-0.942056	-4.142346	7.609363
H	-0.217053	0.073462	5.635561	C	-0.620270	-2.377079	6.387929
N	0.127024	1.970732	2.771957	H	-0.542138	-1.688605	7.249006
N	0.187667	2.032920	0.456679	H	-0.431276	-2.668868	-0.443381
N	-2.184246	0.213050	2.652707	H	2.590191	-0.412472	-0.363213
N	1.864952	-0.357618	2.748700	H	-2.750737	0.324877	-0.490205
N	-0.449973	-2.095222	2.703815	¹ 1b -RhRuN			
N	-2.150088	0.249872	0.340723	Ru	0.800619	-0.284952	1.971231
N	1.953400	-0.316502	0.438078	Rh	0.889853	0.052276	-0.558182
N	-0.375489	-2.060974	0.384818	N	0.866593	-0.735582	3.562531
C	0.250075	2.655685	1.640291	C	-1.826691	0.661489	3.933040
H	0.406351	3.755903	1.676514	H	-0.912044	1.246290	3.854565
H	0.189081	2.541508	3.623629	N	2.900815	-0.222848	1.783889
H	0.298191	2.667750	-0.344796	N	2.870828	0.491646	-0.432557
C	-2.826996	0.301243	1.495693	N	0.808514	1.805373	2.047081
C	2.561883	-0.451049	1.623818	N	0.780149	-2.327657	1.392194
C	-0.503611	-2.737099	1.531596	N	-1.318990	-0.240337	1.731216

N	0.417683	2.020611	-0.231305	Ru	0.107011	-0.044386	2.900927
N	1.363512	-1.910887	-0.818233	Rh	0.104629	-0.009619	0.315345
N	-1.089796	-0.421666	-0.584158	N	0.388353	-0.332183	4.626975
C	3.502162	0.294742	0.713074	C	-0.346704	-1.856056	5.085127
H	4.579760	0.559101	0.794519	H	-1.334170	-1.366787	5.048362
H	3.464849	-0.196303	2.639636	N	0.288912	2.009385	2.808978
H	3.435106	0.944442	-1.160292	N	0.335366	2.005729	0.466544
C	0.471085	2.538168	0.984534	N	-1.942047	0.189043	2.765911
C	1.244651	-2.731751	0.212528	N	2.186080	-0.238760	2.608657
C	-1.831037	-0.446207	0.503036	N	-0.111458	-2.094618	2.735133
H	-2.926973	-0.593471	0.407577	N	-1.925476	0.229173	0.436929
H	1.520674	-3.803038	0.091531	N	2.128108	-0.200680	0.281363
H	0.241535	3.615572	1.137377	N	-0.064775	-2.011174	0.408371
C	-2.175590	-0.169174	2.844285	C	0.366396	2.637845	1.637223
H	0.799426	-3.040103	2.128254	H	0.446138	3.747857	1.638663
H	0.813761	2.301907	2.942648	H	0.191581	2.632921	3.618365
C	-3.378227	-0.921557	2.941280	H	0.419444	2.636436	-0.340058
H	-3.656547	-1.618875	2.134522	C	-2.563073	0.329728	1.595465
C	-4.198261	-0.816613	4.078061	C	2.789436	-0.288015	1.429164
H	-5.122131	-1.418794	4.131778	C	-0.096600	-2.709085	1.528551
C	-3.839205	0.022495	5.150567	H	-0.163753	-3.815142	1.486059
H	-4.480509	0.096062	6.044754	H	3.896089	-0.404468	1.405870
C	-2.639337	0.757138	5.064350	H	-3.656003	0.536120	1.598972
H	-2.332955	1.422403	5.889759	C	-0.106364	-2.754676	3.939584
H	-1.620692	-0.596234	-1.446436	H	2.806062	-0.335960	3.417860
H	1.826970	-2.313935	-1.640064	H	-2.513872	0.410588	3.588173
H	0.078505	2.668578	-0.951673	C	0.305263	-4.093687	4.154556
¹ TS1b -RhRuN				H	0.491208	-4.757871	3.293905

C	0.581871	-4.547869	5.448513
H	0.947079	-5.578064	5.598151
C	0.442406	-3.671536	6.573568
H	0.688637	-4.043757	7.583311
C	-0.026442	-2.381699	6.405800
H	-0.189398	-1.720931	7.274919
H	-0.090549	-2.612580	-0.428040
H	2.713893	-0.252445	-0.559212
H	-2.528133	0.372993	-0.381998

¹**2b**-RhRuN

Ru	0.118132	-0.082841	2.870521
Rh	0.125014	-0.016596	0.285218
N	0.262799	-0.372382	4.688749
C	-0.171902	-1.748480	5.065910
H	-1.262922	-1.520672	5.210109
N	0.271171	1.964794	2.831380
N	0.288140	1.997711	0.483782
N	-1.923985	0.127184	2.703090
N	2.187968	-0.200317	2.628830
N	-0.051275	-2.098951	2.720941
N	-1.902422	0.162121	0.375284
N	2.149972	-0.138472	0.302023
N	-0.005544	-2.013004	0.391188
C	0.322918	2.611548	1.668571
H	0.390685	3.722253	1.681364
H	0.244017	2.578320	3.655213
H	0.343458	2.648817	-0.309293
C	-2.547732	0.243108	1.532500

C	2.808482	-0.173469	1.455537
C	-0.046392	-2.717328	1.507729
H	-0.096137	-3.823417	1.460542
H	3.920846	-0.179154	1.441170
H	-3.645760	0.419125	1.530406
C	-0.086827	-2.740324	3.924664
H	2.808891	-0.166862	3.442753
H	-2.504894	0.343397	3.520965
C	0.036479	-4.126724	4.180314
H	0.023787	-4.846743	3.343746
C	0.276723	-4.585218	5.479113
H	0.399807	-5.665194	5.665844
C	0.466172	-3.648067	6.560369
H	0.764588	-4.033477	7.551739
C	0.309548	-2.297210	6.374543
H	0.461432	-1.573413	7.194200
H	-0.015115	-2.616862	-0.445207
H	2.750019	-0.098457	-0.529917
H	-2.505001	0.281029	-0.447899

¹**TS2b**-RhRuN

Ru	0.170767	-0.073414	2.845501
Rh	0.118376	-0.009434	0.258828
N	0.227921	-0.366060	4.752796
C	0.033274	-1.779446	5.062924
H	-1.007888	-1.195604	5.147346
N	0.271062	1.966516	2.802099
N	0.240685	1.999791	0.454380
N	-1.857108	0.099343	2.744255

N	2.210269	-0.129456	2.624842	H	-2.531011	0.191948	-0.392880
N	0.044118	-2.076743	2.712785	¹ 3b -RhRuN			
N	-1.896428	0.116262	0.412213	Ru	-0.164466	-0.086878	2.842870
N	2.133814	-0.111594	0.292565	Rh	-0.095294	-0.051456	0.278338
N	0.011922	-2.009941	0.378025	N	-0.283374	-0.551354	4.828381
C	0.286504	2.615902	1.638013	C	-0.495330	-1.859823	5.104088
H	0.335758	3.727269	1.647705	H	-0.219253	0.044775	5.656210
H	0.280373	2.583848	3.624503	N	0.122986	1.934603	2.777531
H	0.265115	2.652100	-0.339851	N	0.178097	1.944108	0.433264
C	-2.515861	0.175947	1.587296	N	-2.160450	0.240565	2.673127
C	2.812337	-0.120739	1.436237	N	1.849861	-0.329598	2.773587
C	-0.001499	-2.698496	1.508929	N	-0.452699	-2.084422	2.739764
H	-0.058598	-3.804922	1.469850	N	-2.096442	0.232005	0.339585
H	3.923653	-0.110242	1.399768	N	1.901109	-0.324099	0.439795
H	-3.619834	0.305662	1.607635	N	-0.375861	-2.037880	0.405965
C	0.021613	-2.735607	3.932550	C	0.238250	2.569059	1.608925
H	2.854658	-0.030762	3.417426	H	0.391601	3.671161	1.611378
H	-2.438041	0.276879	3.574579	H	0.189715	2.563912	3.587475
C	0.032053	-4.126938	4.171370	H	0.284558	2.576886	-0.369800
H	-0.018683	-4.834347	3.325578	C	-2.762313	0.341247	1.487056
C	0.165713	-4.623541	5.477083	C	2.514000	-0.401105	1.618931
H	0.185267	-5.712051	5.652931	C	-0.506312	-2.706766	1.542977
C	0.331393	-3.718554	6.571585	H	-0.662270	-3.803980	1.502849
H	0.497636	-4.122902	7.585899	H	3.619840	-0.519495	1.638826
C	0.312189	-2.346244	6.383604	H	-3.857440	0.533070	1.452576
H	0.443534	-1.640905	7.222105	C	-0.595994	-2.748641	3.965500
H	-0.030290	-2.622364	-0.450204	H	2.454048	-0.335236	3.606044
H	2.730379	-0.095390	-0.544281	H	-2.782089	0.409443	3.475045

C	-0.819942	-4.128657	4.169320
H	-0.900261	-4.810510	3.306156
C	-0.945181	-4.650690	5.469407
H	-1.121130	-5.730097	5.613851
C	-0.845660	-3.783916	6.587635
H	-0.944039	-4.191547	7.609158
C	-0.624711	-2.414303	6.409415
H	-0.546964	-1.732836	7.275763
H	-0.438136	-2.651123	-0.419365
H	2.541426	-0.386193	-0.361987
H	-2.689853	0.340661	-0.492699

¹**1b**-TcMoN

Mo	0.889519	-0.088170	1.960750
Tc	0.924268	0.086641	-0.490885
N	0.884489	-0.217868	3.635442
C	-1.983688	0.632405	3.966310
H	-1.165743	1.349642	3.908310
N	2.997847	0.020513	1.802615
N	2.981185	0.243467	-0.490494
N	0.723144	2.035611	1.927246
N	0.941951	-2.187366	1.618360
N	-1.302828	-0.162361	1.764485
N	0.726514	2.142330	-0.376075
N	1.048592	-1.967069	-0.672550
N	-1.137424	-0.087331	-0.553000
C	3.660760	0.163682	0.654749
H	4.770613	0.214802	0.655137
H	3.596966	-0.033434	2.633570

H	3.580516	0.348379	-1.320549
C	0.635637	2.753408	0.807232
C	1.002841	-2.745529	0.410507
C	-1.872452	-0.171360	0.549694
H	-2.980785	-0.208871	0.476005
H	1.013485	-3.851797	0.306087
H	0.490574	3.853789	0.859607
C	-2.167815	-0.244490	2.877713
H	0.886381	-2.858289	2.392170
H	0.640047	2.585383	2.789371
C	-3.226754	-1.184574	2.938605
H	-3.360774	-1.896601	2.107031
C	-4.078525	-1.230326	4.058176
H	-4.893688	-1.974254	4.091003
C	-3.884183	-0.346986	5.136639
H	-4.547251	-0.385738	6.017408
C	-2.826466	0.584739	5.078789
H	-2.660484	1.288931	5.912172
H	-1.705080	-0.065396	-1.411140
H	1.079982	-2.491961	-1.557219
H	0.646694	2.784357	-1.176355

¹**TS1b**-TcMoN

Mo	0.213079	0.105232	2.833015
Tc	0.075436	0.048027	0.482882
N	0.193708	-0.286510	4.565933
C	-0.632405	-2.064031	5.055020
H	-1.530840	-1.470438	4.872693
N	0.475999	2.179316	2.743702

N	0.319745	2.106382	0.440848	H	-0.308747	-2.574422	-0.426401
N	-1.909165	0.345560	2.812072	H	2.631965	-0.446582	-0.532523
N	2.284902	-0.277650	2.633701	H	-2.625821	0.230358	-0.297168
N	-0.133450	-2.116019	2.719049	¹ 2b -TcMoN			
N	-1.992833	0.247807	0.512634	Mo	0.229480	0.137886	2.779832
N	2.124427	-0.249311	0.340986	Tc	0.135738	0.032974	0.499795
N	-0.151590	-2.016260	0.424270	N	0.206550	-0.447564	4.632460
C	0.463789	2.812654	1.564071	C	-0.064413	-1.774618	5.013399
H	0.571121	3.918188	1.525522	H	-1.198384	-1.769973	5.127138
H	0.578568	2.797041	3.556822	N	0.342577	2.220157	2.748540
H	0.329039	2.686711	-0.409236	N	0.249182	2.113944	0.444475
C	-2.622100	0.353123	1.684286	N	-1.896709	0.221285	2.796229
C	2.861768	-0.420084	1.438045	N	2.344614	-0.010679	2.655160
C	-0.179875	-2.744446	1.535847	N	0.056437	-2.143945	2.679521
H	-0.310155	-3.847111	1.494164	N	-1.951850	0.107976	0.500253
H	3.935006	-0.699266	1.359213	N	2.207205	-0.119600	0.362232
H	-3.730080	0.440112	1.720494	N	-0.010485	-2.021845	0.392952
C	-0.073100	-2.775508	3.925907	C	0.326210	2.839841	1.559633
H	2.893508	-0.494320	3.431137	H	0.374248	3.950080	1.511604
H	-2.467480	0.424674	3.670108	H	0.398007	2.848962	3.557864
C	0.631791	-3.980522	4.151855	H	0.240778	2.681988	-0.413721
H	1.084191	-4.511566	3.297600	C	-2.601120	0.172355	1.662378
C	0.850427	-4.432353	5.464727	C	2.949869	-0.121591	1.470589
H	1.442112	-5.349600	5.629535	C	-0.042830	-2.772145	1.484564
C	0.361179	-3.702568	6.579332	H	-0.161421	-3.873279	1.420242
H	0.557831	-4.065330	7.602443	H	4.054095	-0.240799	1.407555
C	-0.398762	-2.547820	6.371512	H	-3.713338	0.163423	1.686968
H	-0.848047	-2.007694	7.221893	C	0.023845	-2.768953	3.872819

H	2.973931	-0.064011	3.464206
H	-2.462073	0.245142	3.653114
C	0.057823	-4.162872	4.150346
H	0.075904	-4.893559	3.323802
C	0.184382	-4.614352	5.465804
H	0.235561	-5.699281	5.660922
C	0.298279	-3.700011	6.568351
H	0.447856	-4.102707	7.585242
C	0.247323	-2.339936	6.364266
H	0.338127	-1.620481	7.196471
H	-0.107983	-2.567986	-0.474304
H	2.743483	-0.279773	-0.499786
H	-2.565754	-0.010285	-0.314923

¹**TS2b**-TcMoN

Mo	0.222271	0.115861	2.746890
Tc	0.124501	0.030313	0.510668
N	0.233952	-0.439439	4.675994
C	0.057488	-1.813544	5.028269
H	-1.030836	-1.418198	5.061146
N	0.323791	2.206577	2.741818
N	0.225681	2.113944	0.441199
N	-1.905704	0.191777	2.798224
N	2.339891	-0.018955	2.646272
N	0.091973	-2.131398	2.686433
N	-1.962873	0.098305	0.502555
N	2.197969	-0.103628	0.353850
N	0.001576	-2.034105	0.396502
C	0.302944	2.835735	1.558985

H	0.347999	3.945975	1.515293
H	0.382106	2.827952	3.556770
H	0.212286	2.679457	-0.417744
C	-2.612448	0.158546	1.665262
C	2.944286	-0.114414	1.459764
C	-0.008488	-2.767430	1.500815
H	-0.105688	-3.871412	1.446662
H	4.048980	-0.224035	1.392365
H	-3.724404	0.161846	1.689492
C	0.074241	-2.774552	3.893306
H	2.969023	-0.076906	3.455061
H	-2.469754	0.226397	3.655614
C	0.077183	-4.165732	4.151688
H	0.072004	-4.885878	3.316129
C	0.155573	-4.645098	5.468608
H	0.166856	-5.733645	5.648582
C	0.248691	-3.747863	6.571786
H	0.335610	-4.151727	7.595372
C	0.247314	-2.375476	6.369315
H	0.318906	-1.664049	7.209689
H	-0.093685	-2.587446	-0.464873
H	2.730335	-0.237726	-0.514503
H	-2.574407	0.005744	-0.317272

¹**3b**-TcMoN

Mo	-0.143534	0.005240	2.697723
Tc	-0.095599	-0.019259	0.530898
N	-0.277483	-0.566455	4.785395
C	-0.494345	-1.884491	5.083838

H	-0.216986	0.020287	5.619332	C	-0.626494	-2.418151	6.389242
N	0.140597	2.098984	2.769603	H	-0.548106	-1.724558	7.246225
N	0.189517	2.053495	0.465888	H	-0.439729	-2.640353	-0.437997
N	-2.253591	0.267619	2.659818	H	2.545494	-0.442856	-0.376109
N	1.958208	-0.311264	2.759880	H	-2.709500	0.280815	-0.500209
N	-0.451323	-2.145847	2.718758				
N	-2.160439	0.252370	0.366634				
N	1.970404	-0.315835	0.464634				
N	-0.380492	-2.078229	0.419268				
C	0.256300	2.745957	1.603155				
H	0.406328	3.847427	1.583121				
H	0.202349	2.702157	3.597611				
H	0.286658	2.624629	-0.382326				
C	-2.882454	0.334638	1.485413				
C	2.635527	-0.424134	1.615979				
C	-0.513658	-2.784249	1.541316				
H	-0.674234	-3.881227	1.490907				
H	3.730207	-0.619677	1.617533				
H	-3.988041	0.442657	1.435461				
C	-0.595012	-2.781954	3.962654				
H	2.510193	-0.455198	3.612511				
H	-2.861649	0.282107	3.485810				
C	-0.823119	-4.156004	4.184525				
H	-0.904578	-4.847880	3.329390				
C	-0.952732	-4.665942	5.494218				
H	-1.132308	-5.743825	5.647581				
C	-0.852999	-3.790751	6.595245				
H	-0.953346	-4.179353	7.624015				