Supporting information for: Structural Phase Transition of Ruthenium Cluster Hydrides

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Cartesian coordinates

Cartesian coordinates are given in bohr units for capped icosahedral and hexagonal cluster structures, $Ru_{14}^{ico}H_x^-$ and $Ru_{14}^{hex}H_x^-$, with coverages of $x = 0 - 40$ hydrogen atoms.

1. $Ru_{14}^{hex}H_x^-$ structures with double-layered hexagonal core motif

Ru_{14}^{hex-}
Energy = −1330.766993047 E_h; Spin multiplicity $2S + 1 = 7$

Ru	−0.0000000	0.0000000	−1.1347305
Ru	−0.0000000	0.0000000	1.1347305
Ru	1.4733730	−2.0473342	1.1252724
Ru	1.4733730	−2.0473342	−1.1252724
Ru	−1.4733730	2.0473342	−1.1252724
Ru	−2.4889343	−0.2379830	1.1257432
Ru	−2.4889343	−0.2379830	−1.1257432
Ru	−1.4733730	2.0473342	1.1252724
Ru	−1.0570911	−2.2932392	1.1251145
Ru	−1.0570911	−2.2932392	−1.1251145
Ru	2.4889343	0.2379830	1.1257432
Ru	1.0570911	2.2932392	−1.1251145
Ru	1.0570911	2.2932392	1.1251145
Ru	2.4889343	0.2379830	−1.1257432

$Ru_{14}^{hex}H_2^-$
Energy = −1331.994420533 E_h; Spin multiplicity $2S + 1 = 5$

Ru	0.0145179	0.0221832	−0.9410896
Ru	2.4156842	0.7921310	−0.8898456
Ru	1.8957518	−1.6619377	−0.9467065
Ru	−0.4912174	−2.4484865	−0.9890653
Ru	−2.3888837	−0.7439361	−0.9715276
Ru	−2.4024595	−0.7962349	1.2790513
Ru	−0.0062311	−0.0258036	1.3218295
Ru	−0.5213830	−2.4890706	1.2611243
Ru	1.8541776	−1.6988697	1.3091216
Ru	2.3823272	0.7540927	1.3584697
Ru	0.5136115	2.4391539	1.3717070
Ru	−1.8652690	1.6519933	1.3419284
Ru	−1.8582372	1.7116393	−0.9145816
Ru	0.5283682	2.4928254	−0.8772479
H	2.2174939	2.4706808	−1.6296509
H	−2.1705978	−2.4131030	−1.7344796

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_4^-$
Energy = −1333.221747111 E_h; Spin multiplicity $2S+1=3$

Ru	0.9316704	−1.1448716	2.1668918
Ru	0.9438030	1.1124282	2.1968701
Ru	0.9316704	−1.1448716	−2.1668918
Ru	−0.2914589	1.1420753	0.0000000
Ru	−1.5874020	1.1585489	2.1619702
Ru	−1.5897603	−1.1148329	2.1685022
Ru	−0.3055440	−1.1168377	0.0000000
Ru	−2.8110390	1.1454590	0.0000000
Ru	−2.8467323	−1.1231734	0.0000000
Ru	−1.5897603	−1.1148329	−2.1685022
Ru	2.2217026	−1.1023513	0.0000000
Ru	2.1983958	1.1705538	0.0000000
Ru	0.9438030	1.1124282	−2.1968701
Ru	−1.5874020	1.1585489	−2.1619702
H	−0.2902466	−1.8803051	3.2849958
H	−0.2902466	−1.8803051	−3.2849958
H	2.5483476	1.8585561	−1.6659335
H	2.5483476	1.8585561	1.6659335

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_6^-$
Energy = −1334.446920301 E_h; Spin multiplicity $2S+1=1$

Ru	2.3086670	−0.4299388	−1.1368542
Ru	2.3652518	−0.4441393	1.1434438
Ru	−1.0820247	2.2683607	−1.1234264
Ru	−0.1228783	−0.0553282	1.1442964
Ru	0.7403741	−2.4186003	1.1369223
Ru	0.7498818	−2.4090821	−1.1369284
Ru	−0.1650959	−0.0678899	−1.1107321
Ru	−1.7086244	−2.0258915	1.1649462
Ru	−1.7270465	−2.0450819	−1.1082325
Ru	−2.6505372	0.3036841	−1.0979071
Ru	1.4338811	1.8776572	−1.1465145
Ru	1.4343090	1.9072990	1.1395807
Ru	−1.0830155	2.2679409	1.1315819
Ru	−2.6155694	0.3082593	1.1916945
H	−3.2961021	−1.2661149	−1.7601916
H	2.4045902	−2.2308634	1.7819447
H	2.4672993	−2.0082933	−1.9525430
H	−2.7151033	2.0546891	−1.8237220
H	0.2715951	3.2245555	1.8361413
H	2.9901479	1.1887777	1.7264999

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{8}^{-}$
Energy = −1335.664090961 E_{h}; Spin multiplicity $2S+1=1$

Ru	2.2475695	1.1307967	0.0000000
Ru	2.3107640	−1.1415837	0.0000000
Ru	−1.5156039	1.1178382	2.1893223
Ru	−0.2281303	−1.1526212	0.0000000
Ru	0.9934482	−1.1590233	−2.1967304
Ru	1.0068444	1.1163443	−2.1905464
Ru	−0.2635039	1.0970935	0.0000000
Ru	−1.5274352	−1.1395279	−2.1747442
Ru	−1.5156039	1.1178382	−2.1893223
Ru	−2.7706189	1.0960067	0.0000000
Ru	1.0068444	1.1163443	2.1905464
Ru	0.9934482	−1.1590233	2.1967304
Ru	−1.5274352	−1.1395279	2.1747442
Ru	−2.7740554	−1.1848863	0.0000000
H	−3.1690717	1.7960470	−1.6259511
H	2.6458007	−1.6852991	−1.7622334
H	2.6541078	1.8737561	1.5692168
H	−0.3380869	−1.8473641	−3.3267131
H	2.6541078	1.8737561	−1.5692168
H	−3.1690717	1.7960470	1.6259511
H	−0.3380869	−1.8473641	3.3267131
H	2.6458007	−1.6852991	1.7622334

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{10}^{-}$
Energy = −1336.884035624 E_{h}; Spin multiplicity $2S+1=1$

Ru	1.1379423	2.1092966	1.1421109
Ru	−1.4011495	1.9923676	1.1323435
Ru	−2.5365157	−0.2947388	1.1154524
Ru	−1.3886109	1.9636322	−1.1358482
Ru	−2.5016766	−0.2909512	−1.1529404
Ru	1.1480275	2.1442343	−1.1307846
Ru	0.0341933	−0.1348636	−1.1202461
Ru	−1.1252797	−2.4060827	1.1164500
Ru	−0.0176768	−0.1398596	1.1198125
Ru	−1.1208141	−2.3932703	−1.1484124
Ru	1.4055566	−2.2470968	−1.1173890
Ru	1.3996189	−2.2339385	1.1501235
Ru	2.5570856	0.0163157	−1.1189288
Ru	2.5268862	0.0156346	1.1466890
H	−0.2663594	3.2182043	−1.7229130
H	−0.1276364	3.2229455	1.7319886
H	2.7323300	1.6493881	1.9857814
H	−2.9215032	1.3111749	−1.9701244
H	−3.0417446	1.3716977	1.7037043
H	2.8599225	1.7377371	−1.6854588
H	0.2023893	−3.4341976	−1.9037330
H	−2.7883180	−2.0384013	1.6806822
H	3.0134991	−1.6822222	−1.6863405
H	0.2198336	−3.4570060	1.8679810

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{12}^{-}$
Energy = −1338.089984705 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.0536338	−0.0094136	−1.1128997
Ru	−0.0539521	0.0131851	1.1123741
Ru	−2.3154426	−1.1332643	1.0805374
Ru	−2.2253658	−1.1249160	−1.1887591
Ru	2.3170065	1.1305054	−1.0934878
Ru	0.1168417	2.5413471	1.1232228
Ru	0.1704427	2.5181408	−1.1498324
Ru	2.2307912	1.1299973	1.1762782
Ru	−2.1680848	1.4096382	1.0802344
Ru	−2.0856522	1.3727936	−1.1891114
Ru	−0.1724177	−2.5214390	1.1472757
Ru	2.1671513	−1.4117093	−1.0675370
Ru	2.0801880	−1.3665731	1.2009817
Ru	−0.1159509	−2.5444508	−1.1213472
H	−1.5772782	3.0785373	1.5797666
H	−3.4941719	0.1855417	1.4952466
H	−1.8639096	−2.8429317	1.6956056
H	1.4288217	−2.8484812	2.0420954
H	3.0891651	−0.1430732	2.1767394
H	1.7477618	2.7272313	1.9548432
H	1.5757786	−3.0733252	−1.5895919
H	−1.7626522	−2.7448924	−1.9254290
H	−3.0842016	0.1689436	−2.1798310
H	−1.4176628	2.8275408	−2.0667785
H	1.8644020	2.8503862	−1.6859524
H	3.4947583	−0.1893185	−1.4946437

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{14}^{-}$
Energy = −1339.296566223 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.0000000	−0.0000000	−1.0829038
Ru	0.0000000	−0.0000000	1.1645428
Ru	1.2939578	2.1930253	1.1488518
Ru	1.2725134	2.1815494	−1.1168422
Ru	−1.2725134	−2.1815494	−1.1168422
Ru	1.2939578	−2.1930253	1.1488518
Ru	1.2725134	−2.1815494	−1.1168422
Ru	−1.2939578	−2.1930253	1.1488518
Ru	2.7347355	−0.0000000	1.0594573
Ru	2.5785375	−0.0000000	−1.1726790
Ru	−1.2939578	2.1930253	1.1488518
Ru	−2.5785375	−0.0000000	−1.1726790
Ru	−2.7347355	−0.0000000	1.0594573
Ru	−1.2725134	2.1815494	−1.1168422
H	2.9809622	−1.6541436	1.5832913
H	2.9809622	1.6541436	1.5832913
H	−0.0000000	3.3894590	1.5139638
H	−2.9809622	1.6541436	1.5832913
H	−2.9809622	−1.6541436	1.5832913
H	−0.0000000	−3.3894590	1.5139638
H	−2.9015127	1.6762116	−1.8103460
H	−0.0000000	3.2394649	−1.8712966
H	2.9015127	1.6762116	−1.8103460
H	2.9015127	−1.6762116	−1.8103460
H	−0.0000000	−3.2394649	−1.8712966
H	−2.9015127	−1.6762116	−1.8103460
H	4.2473976	−0.0000000	1.6520061
H	−4.2473976	−0.0000000	1.6520061

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{16}^{-}$
Energy = −1340.496854043 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.0104874	−0.1657041	−1.1358660
Ru	0.0104874	−0.1657041	1.1358660
Ru	−0.0303356	−2.7573160	1.1220898
Ru	−0.0303356	−2.7573160	−1.1220898
Ru	−0.0243058	2.7701702	−1.1263357
Ru	−2.0857812	1.2803626	1.1322171
Ru	−2.0857812	1.2803626	−1.1322171
Ru	−0.0243058	2.7701702	1.1263357
Ru	−2.1908433	−1.3039856	1.1375750
Ru	−2.1908433	−1.3039856	−1.1375750
Ru	2.2392602	−1.2649385	1.1423861
Ru	2.0913803	1.2849552	−1.1333807
Ru	2.0913803	1.2849552	1.1333807
Ru	2.2392602	−1.2649385	−1.1423861
H	−3.2540709	0.0075710	1.7438350
H	−1.6909914	−3.0322273	1.5706716
H	1.6333593	−2.9055439	1.6834705
H	3.3470386	0.0389808	1.5942410
H	1.6219564	2.9568866	1.7281388
H	−1.6898483	3.0027939	1.6485042
H	3.3470386	0.0389808	−1.5942410
H	1.6333593	−2.9055439	−1.6834705
H	−1.6909914	−3.0322273	−1.5706716
H	−3.2540709	0.0075710	−1.7438350
H	−1.6898483	3.0027939	−1.6485042
H	1.6219564	2.9568866	−1.7281388
H	0.0103914	−4.1706707	1.9392351
H	−0.0159976	4.2957342	1.6329221
H	0.0103914	−4.1706707	−1.9392351
H	−0.0159976	4.2957342	−1.6329221

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{18}^{-}$
Energy = −1341.697583223 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.0065517	−1.1175386	0.0669064
Ru	0.0039014	1.1527104	0.0644477
Ru	0.0955148	1.1256200	2.6154755
Ru	−0.0140332	−1.0966962	2.6215745
Ru	−0.0804753	−1.1349270	−2.8893083
Ru	−2.0986297	1.1374902	−1.3746967
Ru	−2.0917417	−1.1220773	−1.3377130
Ru	−0.1029732	1.1220178	−2.9150240
Ru	−2.2354554	1.1459557	1.2070757
Ru	−2.2011216	−1.1472671	1.2457721
Ru	2.2915966	1.2021286	1.0833080
Ru	2.0358392	−1.1094748	−1.4582891
Ru	2.0148678	1.1507876	−1.4647429
Ru	2.3350146	−1.0973408	1.0632093
H	−3.2920122	1.7314158	−0.0234960
H	−1.5698075	1.5519189	2.8441753
H	1.7475740	1.5918101	2.8572544
H	3.3335606	1.6522675	−0.2648356
H	1.5333464	1.7476281	−3.1392018
H	−1.8083468	1.5890871	−3.1267594
H	3.3843202	−1.5700253	−0.2143515
H	1.6552321	−1.6470062	2.6261026
H	−1.6363804	−1.4770578	3.0479329
H	−3.2779136	−1.7324840	−0.0598398
H	−1.7362161	−1.7255736	−3.0371556
H	1.5904318	−1.7167513	−3.1291622
H	0.0120675	1.9444616	4.0272123
H	−0.1270984	1.5703750	−4.4576634
H	0.2125347	−1.8763535	4.0411309
H	−0.1346845	−1.6651010	−4.4058884
H	3.3189693	−2.1692411	1.8099091
H	−3.1308944	2.2691274	1.9909547

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{20}^{-}$
Energy = −1342.878525041 E_{h}; Spin multiplicity $2S + 1 = 3$

Ru	−0.0014878	0.0393928	−1.1403147
Ru	−0.0399132	0.0753200	1.1287975
Ru	0.0175949	−2.4412615	1.1519661
Ru	0.0594326	−2.5246016	−1.0427719
Ru	−0.0838550	3.0465025	−1.2116824
Ru	−2.0554440	1.4674602	1.1074392
Ru	−2.0757700	1.4600394	−1.1731393
Ru	−0.1223736	3.1286446	1.0369155
Ru	−2.3861726	−1.0626143	1.0994881
Ru	−2.2731441	−1.1134239	−1.1823432
Ru	2.3565854	−0.9260155	1.1938889
Ru	1.9890294	1.5675619	−1.1146030
Ru	1.8991714	1.5793052	1.1660774
Ru	2.3395323	−0.9881269	−1.0860219
H	−3.4003742	0.2724848	1.6591438
H	−1.6429326	−2.6523495	1.6383250
H	1.6685338	−2.5534952	1.6985873
H	3.3003676	0.4623973	1.7446160
H	1.4102295	3.2373566	1.8717007
H	−1.6813239	3.1405443	1.8423637
H	3.3136596	0.3227454	−1.6384983
H	1.7198745	−2.6886727	−1.5068398
H	−1.5598460	−2.8023301	−1.5647997
H	−3.2917073	0.1529489	−1.7726403
H	−1.7769770	3.1949171	−1.7104853
H	1.6098771	3.2878198	−1.6636856
H	0.0473314	−3.8163888	2.0371588
H	−0.1674639	4.6035810	1.6734876
H	0.1419070	−4.0064427	−1.7233220
H	−0.1233938	4.5863640	−1.6677585
H	3.3420186	−1.7056482	−2.1582021
H	−3.4461239	−2.2256290	1.4969941
H	3.4471961	−2.0450601	1.6394626
H	−3.1738842	−1.8357252	−2.3389859

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{22}^{-}$
Energy = −1344.080677343 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.0337461	0.0609111	1.1809753
Ru	2.4466628	−0.9237979	1.2095032
Ru	2.4723073	−0.9741828	−1.0409517
Ru	0.5258271	−2.5459200	−1.0505663
Ru	−2.0598087	−1.6259705	−1.0781267
Ru	−2.4142842	0.9119841	−1.1561120
Ru	−0.4330438	2.5451492	−1.1202109
Ru	1.9429610	1.8010625	−1.1027909
Ru	−0.0030937	0.0555948	−1.0963050
Ru	1.9902014	1.7916144	1.1438232
Ru	−0.4468909	2.5385235	1.2054186
Ru	−2.5076064	0.9170447	1.1222640
Ru	−2.0530984	−1.6517965	1.1646788
Ru	0.4395483	−2.4924804	1.2097377
H	3.1952905	2.6411850	1.8260812
H	−2.1985534	2.5538435	1.6606407
H	−0.5647860	3.6131241	2.4375417
H	−3.9647596	1.4201051	1.6020673
H	−3.2464732	−2.5801624	1.7381132
H	3.8792730	−1.2653196	1.8941857
H	3.1886621	2.4600747	−1.9105724
H	3.8754908	−1.1575491	−1.8381296
H	0.5564904	−3.8771608	−1.9924284
H	−3.0588371	−2.5922612	−1.9088420
H	−3.6059010	1.1144961	−2.2527233
H	−3.4235598	−0.5699373	1.4405930
H	−1.2414771	−3.0952485	1.7219408
H	2.2466308	−2.5902937	1.6213057
H	3.1828004	0.6222173	1.7274971
H	1.2110284	3.3085947	1.3912965
H	2.2599258	−2.7014379	−1.3979937
H	−1.0809361	−2.9410046	−1.7161173
H	−3.4361273	−0.6822864	−1.3606330
H	−2.1859064	2.5415562	−1.7385484
H	1.2893030	3.3394369	−1.4405164
H	3.0852103	0.5331083	−1.6738790

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{24}^{-}$
Energy = −1345.268773329 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.0064509	0.0137289	1.1375403
Ru	2.6327122	0.1153411	1.1392136
Ru	0.0194046	0.0078746	−1.1324339
Ru	1.3617503	2.2860822	1.1345237
Ru	−1.3779627	2.2693309	1.1186178
Ru	−2.6339957	0.1030206	1.1210773
Ru	−1.2927965	−2.2876821	1.1340490
Ru	1.2247625	−2.3173796	1.1361312
Ru	2.6430975	0.1151833	−1.1129379
Ru	1.2328844	−2.3196328	−1.1148423
Ru	−1.2826947	−2.2991654	−1.1288064
Ru	−2.6223107	0.0932122	−1.1473762
Ru	−1.3677572	2.2584964	−1.1513873
Ru	1.3746261	2.2846570	−1.1284632
H	4.0615287	−0.1760925	1.8504676
H	−0.0124314	3.2148111	1.7554568
H	1.9405157	3.5678673	1.9395696
H	−1.9259269	3.6176260	1.8339361
H	−4.0696757	−0.0891509	1.8525245
H	−2.1213549	−3.4210148	1.9437582
H	2.1686863	−3.4322229	1.8416010
H	4.0701679	−0.1713917	−1.8307504
H	2.2000101	−3.4042908	−1.8364818
H	−2.1267921	−3.4581368	−1.8820856
H	−4.0507022	−0.1255172	−1.8856699
H	−1.9077916	3.5885681	−1.9086613
H	1.9573657	3.5930348	−1.8848018
H	−3.0796044	1.8093501	1.3365842
H	−2.7762401	−1.5512266	1.7594640
H	−0.0240205	−3.5207166	1.4351300
H	2.6957894	−1.5472989	1.7626741
H	3.0612642	1.7963934	1.4375331
H	−0.0097352	−3.5306251	−1.4206643
H	−2.7610527	−1.5688484	−1.7682005
H	−3.0677348	1.7971108	−1.3832186
H	0.0074656	3.2018896	−1.7757463
H	3.0776492	1.7966483	−1.4101723
H	2.7036152	−1.5444222	−1.7366836

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{26}^{-}$
Energy = −1346.436486903 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.1823795	−0.0396257	−1.7469008
Ru	2.3786908	−1.1189429	−1.1084944
Ru	2.1202615	1.4738819	−1.0926481
Ru	2.0581664	1.4228942	1.1578706
Ru	2.2897259	−1.1226063	1.1353619
Ru	0.1356897	−2.5640859	1.1168973
Ru	−2.1715493	−1.5236186	1.1044219
Ru	−2.1324925	−1.4681978	−1.1819887
Ru	−2.4043809	1.0960758	−1.1254541
Ru	−2.4586931	1.1009977	1.1182008
Ru	−0.2852797	2.5435090	1.1390395
Ru	−0.2942013	2.5187994	−1.1206867
Ru	−0.2547169	0.0271709	1.7411974
Ru	0.1503008	−2.5341257	−1.1797456
H	−3.4107939	−0.3009142	1.5854149
H	−1.5176444	−3.1588236	1.2913678
H	1.8210827	−2.7194197	1.7131405
H	3.2819971	0.2485718	1.6627042
H	1.3401931	2.9576065	1.7064136
H	−1.9982388	2.7489162	1.5713163
H	3.3767527	0.3001221	−1.5194111
H	1.8838238	−2.7109724	−1.6598131
H	−1.5052210	−3.1118667	−1.3661547
H	−3.3040791	−0.2669601	−1.8035768
H	−1.9705038	2.7604749	−1.5933294
H	1.3576733	2.9797953	−1.6197664
H	0.2274286	−4.0954609	1.6315554
H	−0.4026858	3.9625752	1.9179487
H	0.2028426	−3.9179813	−2.0284992
H	−0.3594646	4.0312063	−1.6898009
H	3.6414835	−1.7070297	−1.9427550
H	−3.3049718	−2.3449938	1.9311813
H	3.6735653	−1.7707287	1.6230605
H	−3.3522055	−2.4049374	−1.6613594
H	0.3938270	−0.0705926	−3.3046119
H	−0.4534729	0.0609860	3.3001784
H	3.2419243	2.3231898	−1.9020123
H	−3.7088755	1.6944645	1.9655290
H	3.3057470	2.3150878	1.6467482
H	−3.7818919	1.7875898	−1.5658557

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{28}^{-}$
Energy = −1347.615339532 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	−1.8782455	−0.0156916	−0.2267443
Ru	−1.2181121	1.3872077	2.3531450
Ru	−1.2419056	−1.1637787	2.1964853
Ru	1.0208577	−1.2899450	2.2692515
Ru	1.0448381	1.4087210	2.3336427
Ru	0.9746278	2.7137344	0.0716566
Ru	1.0794667	1.3418061	−2.1573774
Ru	−1.1450103	1.3381961	−2.2348631
Ru	−1.1079435	−1.2632063	−2.2904605
Ru	1.1223256	−1.3172238	−2.1993308
Ru	1.0642840	−2.6104428	0.0728295
Ru	−1.2283431	−2.4376447	0.0188507
Ru	1.8633072	0.2562167	0.3082128
Ru	−1.2977197	2.5117961	0.1181292
H	1.5699217	0.0516485	−3.2742792
H	1.4843030	2.9807312	−1.6238679
H	1.4072954	3.0427163	1.7701267
H	1.4310460	0.0422834	3.3968495
H	1.2963466	−2.9620268	1.8055939
H	1.4882575	−2.9704430	−1.6612637
H	−1.9753142	0.0437563	3.2595227
H	−1.7863678	2.9736546	1.7188231
H	−1.7186091	2.8634395	−1.6083501
H	−1.5855023	0.0794150	−3.3826951
H	−1.7054795	−2.7911081	−1.6723902
H	−1.4859004	−2.8329686	1.7379922
H	1.5229485	4.2277326	0.0250095
H	0.9716977	−4.2169651	0.1208944
H	−2.2135324	3.8415269	0.0083275
H	−2.2125829	−3.7206571	0.0627969
H	−1.5938195	2.1638378	3.7024025
H	1.2996749	2.1240829	−3.5448205
H	2.0195796	2.0257749	3.4729619
H	−1.9448849	2.0720681	−3.4393984
H	−3.4228988	−0.1401697	−0.6340211
H	3.4139928	0.3488713	0.5876450
H	−1.9038462	−2.0412025	3.3715744
H	1.3090730	−2.0452531	−3.6109500
H	1.7086385	−1.9719574	3.5604335
H	−1.8974184	−1.9472507	−3.5241225
H	2.3455372	−1.2221245	−0.3594378
H	2.6943101	0.5647457	−1.0987666

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{30}^{-}$
Energy = −1348.815496898 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	−1.9323003	0.2721791	−0.1590033
Ru	−1.2027059	−0.1481688	2.5578747
Ru	−1.1862404	−2.3162848	1.1457317
Ru	1.0368990	−2.4052804	1.1458855
Ru	1.0790492	−0.1773924	2.6393772
Ru	1.1965213	2.0664292	1.4910580
Ru	1.1952925	2.2908535	−1.0856972
Ru	−1.0271671	2.3396409	−1.1726528
Ru	−0.9898480	0.1680893	−2.6935303
Ru	1.2470856	0.1363088	−2.4921264
Ru	1.0158169	−2.2644630	−1.5014322
Ru	−1.2231051	−2.0932234	−1.4166419
Ru	1.9409294	−0.3286716	0.1473615
Ru	−1.0875419	2.1394897	1.5018538
H	1.7202278	1.8220359	−2.7212959
H	1.7327953	3.2774618	0.2790050
H	1.3359651	1.4854486	3.1724755
H	1.4941877	−1.9418259	2.7554033
H	1.4335530	−3.4356952	−0.2371411
H	1.6233144	−1.5557390	−2.9988702
H	−1.7388669	−1.8495695	2.7585318
H	−1.3467227	1.5300375	3.1386486
H	−1.4990863	3.3191883	0.1808757
H	−1.3950049	1.8881841	−2.8448020
H	−1.5904330	−1.4489808	−3.0636086
H	−1.6974075	−3.3172193	−0.2356775
H	1.3459107	3.4416273	2.3080717
H	1.7797267	−3.5072278	−2.1976745
H	−1.9594979	3.3202015	2.1781185
H	−1.5386394	−3.4314858	−2.2463599
H	−1.3718514	−0.3556959	4.1422410
H	1.5417486	3.6698069	−1.8126666
H	1.9370703	−0.3885649	3.9929749
H	−1.8163152	3.6030926	−1.8071712
H	−3.4207604	0.7311676	−0.3971639
H	3.4334041	−0.7844212	0.3634489
H	−1.5312048	−3.7389947	1.7841511
H	1.5739950	0.3085058	−4.0550735
H	1.8262072	−3.6777316	1.7623506
H	−1.7459247	0.3814286	−4.1058267
H	2.8351151	−0.1185299	−1.2735597
H	−2.8190011	−0.9810782	−0.8724566
H	−2.7765089	0.2420330	1.2965859
H	2.7749434	0.8437958	1.0210571

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{32}^{-}$
Energy = −1349.991602140 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.2318631	−2.0996010	−0.2018084
Ru	−0.2579665	1.9512643	−0.0470612
Ru	−0.0514522	1.0412260	2.5704800
Ru	0.0290773	−1.2118936	2.5165034
Ru	−0.0833290	−1.2045877	−2.6487426
Ru	−2.4085297	0.9446763	−1.4355566
Ru	−2.2975451	−1.2945694	−1.3716174
Ru	−0.1988261	1.0441922	−2.6633634
Ru	−2.3071455	0.9182687	1.2738026
Ru	−2.1978488	−1.3141977	1.2832647
Ru	2.1913005	1.1767963	1.2321729
Ru	2.3273886	−1.0385675	−1.3227617
Ru	2.1402293	1.1884405	−1.2818552
Ru	2.3600684	−1.0840940	1.2673064
H	−3.3844375	1.4451202	−0.0303810
H	−1.8259451	1.0834897	2.9355878
H	1.5630198	1.7021153	2.8349790
H	3.3775587	1.4978908	−0.0835910
H	1.4414036	1.6883755	−2.8401480
H	−1.8975155	1.1601940	−3.1443217
H	3.5582369	−1.1938541	−0.0993243
H	1.7362156	−1.6763781	2.8176436
H	−1.6640141	−1.4892087	2.9600849
H	−3.2942020	−1.8617493	−0.0252692
H	−1.7632988	−1.5690379	−3.0517274
H	1.6419922	−1.6255428	−2.8438119
H	−0.1988887	1.8046064	3.9806025
H	0.0761409	1.3919048	−4.2077924
H	−0.0186794	−1.3914801	4.1063486
H	0.0723865	−2.0141974	−4.0399737
H	3.6243272	−1.8342442	1.9276843
H	−3.5735720	1.5310107	2.0519101
H	3.5628026	1.3633600	2.0486177
H	−3.5517558	−1.6346704	2.0792798
H	−3.7070809	−1.6774536	−2.0410828
H	3.3402312	1.7586875	−2.1798481
H	−3.7576056	1.5766444	−2.0675193
H	3.5576924	−1.5970059	−2.2016040
H	−1.0449245	−2.8545180	−0.9598474
H	−0.8917401	2.5648786	−1.4833598
H	−0.3541813	3.5187270	−0.0880858
H	0.3607976	−3.6541089	−0.4136804
H	1.6486458	−2.7478761	0.3165803
H	−0.9986397	2.5826574	1.2857702
H	1.2197204	2.6927760	0.2641891
H	−0.3919013	−2.7367596	1.2202997

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{34}^{-}$
Energy = −1351.194784589 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	−0.4996063	−1.4159454	1.0921614
Ru	−1.1569164	0.4156053	2.7855742
Ru	−2.7733834	−0.3249289	0.8117780
Ru	−1.9591501	−1.7606391	−1.2504914
Ru	0.6074620	−1.8440031	−1.7753993
Ru	0.9372708	0.0762206	−2.7426974
Ru	0.1470503	1.9565754	−0.8950913
Ru	−1.6322559	0.7009890	−2.3491778
Ru	−2.4473271	1.6263394	−0.1709085
Ru	−0.7783257	2.3141052	1.7047891
Ru	1.7607390	1.5759707	1.5259782
Ru	2.4955669	0.7637849	−0.7370940
Ru	2.1351693	−1.7321697	0.3320844
Ru	1.3678532	−0.3743328	2.5040027
H	−3.1956218	1.1674138	−1.8181183
H	−2.3212415	2.9312471	1.1501604
H	0.8226327	2.8913577	2.2691803
H	3.3146458	1.3148064	0.7256956
H	2.6244993	0.4509081	−2.5415331
H	−0.4591559	0.4302823	−3.7197409
H	2.7536819	−1.3349533	1.9566975
H	0.2558700	0.0306190	3.8168803
H	−2.8679497	0.0248816	2.5586449
H	−3.4829206	−1.2949944	−0.5035272
H	−0.8364644	−2.6154261	−2.3770101
H	2.1337980	−2.5425785	−1.2467310
H	−1.2195691	3.2701697	2.9120049
H	1.4618188	0.1036694	−4.2671732
H	−1.7665843	0.3850496	4.2851768
H	1.0472405	−2.8245465	−2.9402335
H	2.0829497	−0.7886866	3.8932026
H	2.7440348	2.2269611	2.5992874
H	−4.2524855	−0.6964502	1.3350225
H	−2.3663208	−3.2799938	−0.9629685
H	3.9356116	1.3394932	−1.0609613
H	−2.5053822	−0.7855509	−2.6728845
H	3.5902044	−2.3767376	0.3541736
H	−3.1081859	−2.5398926	−2.0197362
H	3.4389443	−0.6489944	−0.2200125
H	−2.4920906	1.0959982	−3.6225925
H	2.4213626	−3.2306731	0.7988897
H	−0.9458983	−2.5201239	2.1189426
H	0.4224816	3.2956392	−1.6533723
H	1.8190660	2.4278986	−1.0568484
H	−1.4560958	−2.6701560	0.1412931
H	0.8262581	−2.6825930	0.9463966
H	−1.0646595	2.4362577	−2.0552038
H	−0.2264306	3.2993181	0.0180003

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{36}^{-}$
Energy = −1352.379521125 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	−0.1781708	−1.9764148	−0.2629924
Ru	0.3391370	−1.4916503	2.4110225
Ru	−2.1028309	−1.1614403	1.5639910
Ru	−2.5542528	−0.8811111	−1.0253842
Ru	−0.4624566	−0.6859587	−2.7209731
Ru	−0.2624738	1.4485143	−2.2946826
Ru	0.3961268	2.0726493	0.9310257
Ru	−1.9276902	1.7587619	−0.4546060
Ru	−1.8135747	0.9732891	2.0334926
Ru	0.6191394	0.5944009	3.0783673
Ru	2.6277772	0.8368459	1.3059752
Ru	1.9598324	1.4625781	−1.1790958
Ru	1.9968093	−1.2618596	−1.8674589
Ru	2.3167349	−1.2764917	0.6641269
H	−2.9690325	1.8066747	1.0377949
H	−0.9981097	1.0349583	3.6607364
H	2.3571893	0.8973178	3.0870517
H	3.4603208	1.4575881	−0.0710867
H	1.3438299	2.0657683	−2.7060923
H	−1.7830007	2.3313260	−2.1170555
H	3.2233457	−1.8519517	−0.7631340
H	1.9115506	−2.2032036	2.1359636
H	−1.3268066	−1.9101648	2.9771099
H	−3.4919012	−1.0915326	0.4433934
H	−2.2329738	−0.8019626	−2.7694527
H	1.1366119	−0.9681855	−3.4189818
H	0.9678333	0.9032264	4.6303610
H	−0.5293271	2.0259598	−3.7577361
H	0.6837617	−2.1580081	3.8247047
H	−0.8199476	−1.0119828	−4.2525860
H	3.5296962	−2.0374964	1.3539727
H	4.0181842	1.3351894	1.9695827
H	−3.3268955	−1.9341296	2.2779408
H	−3.5462175	−2.0662247	−1.3889633
H	2.9059308	2.5428767	−1.8246994
H	−3.2704140	0.6919287	−1.1154220
H	3.3514826	−1.1461861	−2.7059861
H	−4.0182334	−0.6870601	−1.6157881
H	2.8491051	0.2005081	−2.2262707
H	−2.9556014	2.9319939	−0.6750854
H	2.5591579	−2.4643493	−2.7393330
H	−0.1955101	−3.5391912	−0.3509628
H	0.8013802	3.4507977	1.5620227
H	1.4491653	2.8790219	−0.3560723
H	−1.6620796	−2.4436387	−1.0608066
H	0.7858433	−2.5648731	−1.6296874
H	−0.8533529	3.0666152	0.0919754
H	−0.6041161	2.5976002	2.1460681

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{38}^{-}$
Energy = −1353.562188210 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	−0.0234627	−1.6925270	−0.4869097
Ru	0.3087524	−1.9056376	1.9675043
Ru	−2.0795520	−1.4228617	1.1334434
Ru	−2.4443934	−0.6944951	−1.4066789
Ru	−0.2487573	−0.6803949	−3.1045400
Ru	−0.1538993	1.3624067	−1.9633272
Ru	0.3316287	1.9183595	1.1847944
Ru	−1.9581963	1.6807810	−0.1795329
Ru	−1.8252439	0.7713410	2.2267255
Ru	0.4932069	0.1624865	3.1837533
Ru	2.6141533	0.8081209	1.6557601
Ru	2.0401248	1.5576830	−0.8675947
Ru	2.1741225	−0.9616500	−2.0274391
Ru	2.4078584	−1.1292124	0.5644987
H	−3.0448955	1.5969682	1.2136667
H	−1.1716543	−0.0247721	3.6910257
H	2.2379962	0.5525618	3.3754943
H	3.4300095	1.6361598	0.3482794
H	1.2926801	2.3133767	−2.2437209
H	−1.4292746	2.4783783	−1.6955023
H	3.2169636	−1.7623218	−0.9354607
H	2.0101885	−2.4181469	1.6532672
H	−1.3502827	−2.2856891	2.4725150
H	−3.4241338	−1.0013451	−0.0068431
H	−1.9448987	−1.1884745	−3.0497628
H	1.4398972	−0.4367459	−3.6092711
H	0.5484595	0.0149824	4.7747267
H	−0.2714615	2.3829410	−3.1564121
H	0.3261297	−3.3149149	2.7106777
H	−0.2734776	−1.0509638	−4.6639691
H	3.6999421	−1.9329527	1.0178535
H	3.9738246	1.2418312	2.4298087
H	−3.1982671	−2.4363886	1.6253043
H	−3.7291447	−1.5474749	−1.7625596
H	2.9917033	2.6883971	−1.4215353
H	−3.3309934	0.6890567	−1.0637014
H	3.6567416	−0.9273973	−2.6007615
H	−3.4919050	−0.1865651	−2.4869436
H	3.0507584	0.4935724	−2.0690618
H	−2.9683078	2.8840757	−0.3381819
H	2.7787229	−1.9852466	−3.0962263
H	−0.0188324	−3.2664055	−0.4510593
H	0.5880314	3.3084591	1.8724368
H	1.4794073	2.8654373	0.0680888
H	−1.6606119	−2.2591681	−0.7018417
H	0.7299648	−2.1561105	−2.0686604
H	−1.0390504	2.9744554	0.4320718
H	−0.4410165	1.9786382	2.7410516

$\mathbf{Ru}_{14}^{\mathrm{hex}}\mathbf{H}_{40}^{-}$
Energy = −1354.731966882 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	−0.0724614	−1.9930387	−0.0070634
Ru	2.1941090	−1.2395059	1.2800692
Ru	2.3689640	−1.2352620	−1.2899315
Ru	2.2485443	1.3461029	−1.1524628
Ru	2.2962899	1.2061718	1.3760222
Ru	0.0191382	1.1450674	2.6879917
Ru	−2.2049462	1.3840894	1.4385937
Ru	−2.2098305	1.4173257	−1.1111956
Ru	0.0528582	2.1325830	0.1120416
Ru	−0.0077669	1.2115475	−2.4670374
Ru	−0.0926439	−1.1456336	−2.6035275
Ru	−2.4736494	−1.2168943	−1.3818805
Ru	−2.3021023	−1.1155490	1.1988878
Ru	−0.1189591	−1.2925237	2.5086796
H	−3.4343963	1.5842292	0.1611470
H	−1.7028311	1.1600174	3.1140456
H	1.6440013	1.7801432	2.9185038
H	3.5214182	1.1669626	0.0158799
H	1.5247371	2.0871996	−2.5863909
H	−1.5448933	2.0382653	−2.6234239
H	3.4951565	−1.1456499	0.0398622
H	1.5996008	−1.8557364	2.7680345
H	−1.8584558	−1.4548698	2.8489833
H	−3.5971374	−1.0253788	−0.0711770
H	−1.6895237	−1.6995410	−2.9611981
H	1.5455127	−1.5653367	−2.9039663
H	−0.0264951	1.6202281	4.1997818
H	0.0349726	2.0419100	−3.8148768
H	−0.2675777	−2.3370464	3.7028017
H	0.1181503	−1.8565063	−4.0022984
H	3.4271067	−2.0150945	1.9076924
H	3.5230451	1.9435291	2.0716676
H	−3.5316774	−1.8755328	1.8491641
H	−3.3031578	−2.5386933	−1.7302058
H	3.4526173	2.1680879	−1.7758019
H	−3.1166843	0.1804511	−2.1325924
H	3.8712762	−1.5691331	−1.6415970
H	−3.8402077	−1.2960222	−2.1817067
H	3.0926591	0.0534119	−2.1754532
H	−3.3492998	2.3543230	−1.6760557
H	2.7977313	−2.5442230	−2.0978898
H	−0.1252519	−3.5345216	0.2786155
H	0.1833657	3.6956383	0.1051035
H	1.7702173	2.6519931	0.0788115
H	−1.7670080	−2.4756534	−0.1082089
H	−0.0426119	−2.7106379	−1.5676782
H	−1.4085169	2.8885194	−0.5553940
H	−0.7383520	2.6526328	1.6223072

$\mathbf{Ru_{14}^{ico}H_x^-}$ structures with icosahedral-plus-one core motif

$\mathbf{Ru_{14}^{ico-}}$
Energy = −1330.595358873 E_h; Spin multiplicity $2S + 1 = 9$

Ru	0.0217956	−0.3116959	0.0125682
Ru	−1.0688877	1.7477101	1.0284542
Ru	1.4649178	1.6681734	0.5431111
Ru	−0.0866311	1.7097106	−1.5213917
Ru	−2.2468587	0.3083687	−0.8565475
Ru	−1.9460830	−0.6692830	1.5941990
Ru	0.3779385	0.2130624	2.4724591
Ru	2.3201992	−0.8583220	0.8966304
Ru	1.9233179	0.1544583	−1.6037517
Ru	−0.3966156	−0.7453687	−2.4644830
Ru	−1.5236478	−2.1860240	−0.5450081
Ru	0.1180770	−2.2504916	1.5676285
Ru	1.1039665	−2.2902452	−1.0298398
Ru	0.0202422	3.6312993	−0.0614537

$\mathbf{Ru_{14}^{ico}H_2^-}$
Energy = −1331.827419263 E_h; Spin multiplicity $2S + 1 = 1$

Ru	−0.1461193	0.2324254	−0.0845692
Ru	2.3288010	0.5350785	0.2630559
Ru	1.3117576	0.3623166	−2.1411286
Ru	−0.8327007	−1.0861961	−2.1302226
Ru	−1.0635060	1.5803995	−1.9608303
Ru	0.9891795	2.4763207	−0.5623261
Ru	−1.4993325	2.2363516	0.5015679
Ru	−2.6532583	0.0247712	−0.5432475
Ru	−1.3624107	−1.9440941	0.2885973
Ru	1.2242781	−1.8086147	−0.5375867
Ru	0.6991693	−1.0053495	1.9034278
Ru	−0.3336281	0.5368608	3.6634296
Ru	0.7073364	1.6679539	1.8486104
Ru	−1.7846860	−0.0105243	1.8648741
H	1.5994341	−2.3731440	1.1610637
H	0.5610582	−0.8397176	−3.2883604

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{4}^{-}$
Energy = −1333.057390563 E_{h}; Spin multiplicity $2S+1=11$

Ru	0.5702839	−2.2980976	0.6691394
Ru	2.1703206	−0.4264685	1.6342785
Ru	2.1619866	1.7015155	−0.0916932
Ru	0.5466596	1.0117000	−2.1619568
Ru	−1.9188922	0.7620093	−1.0812251
Ru	−1.9443677	−1.2131870	0.5437751
Ru	−0.3410521	−0.5666727	2.5386454
Ru	0.7845673	1.7652065	2.1172342
Ru	−0.3103185	2.5742441	−0.1627966
Ru	−1.8336165	1.2005578	1.4186146
Ru	−3.8523216	0.2609814	0.3267216
Ru	0.2103432	0.1650612	0.2201853
Ru	−0.4896389	−1.3793699	−1.6534542
Ru	2.0718671	−0.8382464	−1.0003245
H	1.9478315	−2.2451316	1.8198276
H	1.2661446	2.6144114	−1.5284394
H	−0.8470813	−2.7672469	−0.4430913
H	−0.2322126	−0.3114587	−3.1014249

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{6}^{-}$
Energy = −1334.288044244 E_{h}; Spin multiplicity $2S+1=9$

Ru	0.7789216	−1.5202095	2.0133054
Ru	2.2814801	0.6446885	1.3983898
Ru	2.2245919	0.9660830	−1.2120801
Ru	0.6595862	−0.9327291	−2.2824849
Ru	−1.7917809	−0.5920602	−1.3116715
Ru	−1.7402051	−0.9388872	1.2263498
Ru	−0.1880577	0.9402241	2.3318277
Ru	0.6774636	2.4491730	0.2960218
Ru	−0.2985341	1.4767328	−1.9129173
Ru	−1.7920120	1.4529683	0.2973358
Ru	−3.7096220	−0.0070255	0.0451093
Ru	0.2938938	−0.0209305	0.0387215
Ru	−0.1834619	−2.4699059	−0.2933607
Ru	2.2869533	−1.4667380	−0.2368491
H	−0.7603834	2.5605723	1.6112346
H	0.1125221	3.1473410	−1.2683542
H	0.5037571	−0.3520893	3.3795069
H	0.1593886	0.4506167	−3.3439489
H	0.3402906	−3.1373573	1.3100058
H	0.1325845	−2.6531671	−2.0716318

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{8}^{-}$
Energy = −1335.516713958 E_{h}; Spin multiplicity $2S+1=7$

Ru	0.2896535	1.3130275	−2.1649687
Ru	2.3818964	−0.2033842	−1.2905878
Ru	2.3818964	−0.2033842	1.2905878
Ru	0.2896535	1.3130275	2.1649687
Ru	−1.9350989	0.1660370	1.3422320
Ru	−1.9350989	0.1660370	−1.3422320
Ru	0.1104985	−1.3817512	−2.0861609
Ru	1.3009744	−2.3004241	0.0000000
Ru	0.1104985	−1.3817512	2.0861609
Ru	−1.4305344	−1.9402204	0.0000000
Ru	−3.6607382	−0.9282517	0.0000000
Ru	0.2448563	0.0022464	0.0000000
Ru	−0.8191154	2.2740897	0.0000000
Ru	1.7780981	1.9661222	0.0000000
H	1.0148749	−2.8825343	−1.7247283
H	1.0148749	−2.8825343	1.7247283
H	1.2449564	−0.0821440	−2.9657891
H	1.2449564	−0.0821440	2.9657891
H	−1.2227583	0.7359362	−2.9403968
H	−1.2227583	0.7359362	2.9403968
H	−0.5907928	2.7980320	−1.7397144
H	−0.5907928	2.7980320	1.7397144

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{10}^{-}$
Energy = −1336.744157200 E_{h}; Spin multiplicity $2S+1=5$

Ru	0.4999768	1.5104402	−1.8518975
Ru	1.9834737	−0.6607046	−1.5051158
Ru	2.0712155	−1.3379340	0.9858343
Ru	0.4710026	0.4888867	2.3866897
Ru	−1.9630633	0.3055431	1.4471277
Ru	−2.0295882	0.8659003	−1.0266987
Ru	−0.4873313	−0.8856033	−2.3643625
Ru	0.4058403	−2.6034808	−0.6097035
Ru	−0.3676114	−1.9537311	1.7393798
Ru	−2.0346366	−1.6173325	−0.2807317
Ru	−3.9562976	−0.1463161	0.0412681
Ru	0.0869593	−0.1763303	0.0040455
Ru	−0.3484179	2.2108050	0.5531600
Ru	2.1597560	1.2163780	0.3337092
H	−0.2864961	−2.6631367	−2.3239714
H	−1.0988932	−3.1545638	0.4782912
H	−0.3430367	0.7668491	−3.2114964
H	−1.0897750	0.6212565	3.1269480
H	−0.9976086	2.4941767	−1.2768141
H	0.3126163	2.2940443	2.2255794
H	1.3427943	2.6345481	−0.5661265
H	3.2045315	0.1290134	1.2536273
H	2.0034211	0.8711951	−2.5525047
H	0.5502814	−1.1956927	3.0993576

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{12}^{-}$
Energy = −1337.980624517 E_{h}; Spin multiplicity $2S + 1 = 7$

Ru	0.4293007	1.7273692	−1.8241666
Ru	1.9035887	−0.4732003	−1.4880529
Ru	1.9187167	−1.0623312	1.1402866
Ru	0.3333789	0.7467292	2.4011780
Ru	−2.1115867	0.4903058	1.4597110
Ru	−2.1654338	1.0813704	−1.0368962
Ru	−0.6729225	−0.6700575	−2.3053356
Ru	0.3360318	−2.4106726	−0.5693392
Ru	−0.6461357	−1.6039422	1.7659909
Ru	−2.2292075	−1.3522598	−0.2914394
Ru	−4.1143786	0.1632146	0.0283665
Ru	0.0059193	0.0399619	−0.0045153
Ru	−0.5437286	2.4158151	0.5761277
Ru	1.9902144	1.4747370	0.3464284
H	−0.6360654	−2.4807412	−2.0829008
H	−1.1632117	−2.8911205	0.4305188
H	−0.6934950	1.0032884	−3.0449736
H	−1.2219662	0.4479530	3.1495883
H	−0.9706428	2.7816451	−1.2422517
H	−0.1513365	2.4799631	2.3348049
H	1.5867826	2.7577779	−0.8802953
H	2.8187983	0.4504387	1.5848079
H	1.8482855	−2.3048794	−1.5212039
H	1.3844364	−2.7822089	0.8672144
H	1.8688674	0.9749922	−2.5982778
H	0.8957907	−1.0041480	2.8046248

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{14}^{-}$
Energy = −1339.207842067 E_{h}; Spin multiplicity $2S + 1 = 5$

Ru	0.6701125	0.7348844	−2.3980701
Ru	2.3051173	−1.0888987	−1.1448835
Ru	2.3345960	−0.3690427	1.4824583
Ru	0.7665898	1.7344466	1.7935551
Ru	−1.7796636	1.0112706	1.0587059
Ru	−1.7923031	0.4179071	−1.3860245
Ru	−0.1860182	−1.6938705	−1.7566558
Ru	0.7927955	−2.4162304	0.6218932
Ru	−0.2150325	−0.6825422	2.3370597
Ru	−1.7855597	−1.4174052	0.3654156
Ru	−3.7491828	−0.0362214	0.0143447
Ru	0.4071632	−0.0128302	−0.0087916
Ru	−0.2692169	2.3278593	−0.5689211
Ru	2.3542556	1.4881791	−0.4095834
H	−0.1423882	−3.1938196	−0.7059534
H	−0.6863566	−2.4504675	1.7162201
H	−0.3777090	−0.5209982	−3.1558470
H	−0.3651865	1.0387469	3.0030693
H	−0.7694744	1.8335726	−2.3934761
H	−0.6199074	2.8117526	1.2081511
H	1.4718784	2.3532845	−1.7660762
H	1.9235735	2.7578300	0.8099780
H	2.3590356	−2.6527237	−0.2353413
H	1.6419801	−1.9039596	2.2126709
H	1.4979189	−2.0065495	−2.4555642
H	2.0985898	0.9251412	2.7241643
H	3.0882623	0.4695136	−1.7174544
H	3.5541292	0.7887745	0.7050892

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{16}^{-}$
Energy = −1340.414256565 E_{h}; Spin multiplicity $2S + 1 = 3$

Ru	−0.6564388	2.5084868	0.0333766
Ru	−2.1223258	0.8156959	1.5273538
Ru	−0.5631671	−1.2176687	2.1872504
Ru	0.4637769	1.3177127	2.0139918
Ru	1.8374490	−0.9482152	1.0790271
Ru	−0.3115248	−0.0200712	0.0158718
Ru	0.0660444	−2.4871474	−0.0134455
Ru	−1.0495450	−1.2443535	−2.0656847
Ru	0.0323597	1.2642747	−2.1393747
Ru	−2.4061464	−1.4083621	0.2035757
Ru	−2.3708443	0.8458101	−1.0885647
Ru	3.7256090	−0.0029703	0.0665395
Ru	1.7878163	1.4264382	−0.2340695
Ru	1.5558268	−0.8211332	−1.5883771
H	−0.2371175	2.9402953	1.7472677
H	−2.3572822	−0.1638124	−2.6191930
H	0.4215004	−2.4465271	−1.8475681
H	1.6918193	−2.7289681	0.6436542
H	−2.2786521	−2.3599361	−1.3535170
H	−3.1587107	−0.6538999	1.6682875
H	−1.4073207	2.4335382	−1.7628051
H	−3.3195551	1.4215471	0.3359124
H	−0.5540495	−2.9452729	1.5960643
H	1.1300304	−1.2761044	2.7578842
H	−0.9638475	0.4802168	3.0133346
H	1.9381908	2.1180731	1.4452162
H	1.8641139	1.0545472	−2.1168995
H	3.3772405	−0.9800123	−1.3830387
H	4.7224595	0.6787250	1.1941180
H	0.2451911	−0.4298084	−3.0650841

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{18}^{-}$
Energy = −1341.634012122 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.8851838	1.0165104	−2.1860114
Ru	2.4341243	−0.9974486	−1.2488829
Ru	2.4341243	−0.9974486	1.2488829
Ru	0.8851838	1.0165104	2.1860114
Ru	−1.5931085	0.6272365	1.3664753
Ru	−1.5931085	0.6272365	−1.3664753
Ru	−0.0577222	−1.4158837	−2.1492919
Ru	0.8112838	−2.6569623	0.0000000
Ru	−0.0577222	−1.4158837	2.1492919
Ru	−1.6908153	−1.5769081	0.0000000
Ru	−3.6542336	−0.1617632	0.0000000
Ru	0.4380067	−0.1390525	0.0000000
Ru	−0.0315892	2.3231552	0.0000000
Ru	2.4655506	1.3198790	0.0000000
H	0.8923163	−0.4028923	−3.3139148
H	0.8923163	−0.4028923	3.3139148
H	−1.6344272	−0.7544542	−2.6078665
H	−1.6344272	−0.7544542	2.6078665
H	−0.7161579	1.4448212	−2.7933270
H	−0.7161579	1.4448212	2.7933270
H	−0.8369566	−2.7940837	−1.1854169
H	−0.8369566	−2.7940837	1.1854169
H	1.5047316	−2.5357377	−1.7913670
H	1.5047316	−2.5357377	1.7913670
H	−1.4108009	2.4563207	−1.0639727
H	−1.4108009	2.4563207	1.0639727
H	1.4313915	2.5315685	−1.2173784
H	1.4313915	2.5315685	1.2173784
H	3.4955535	0.4970921	−1.1996616
H	3.4955535	0.4970921	1.1996616
H	−3.5183803	0.7448526	−1.4065657
H	−3.5183803	0.7448526	1.4065657

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{20}^{-}$
Energy = −1342.844950985 E_{h}; Spin multiplicity $2S + 1 = 3$

Ru	0.7051008	1.0576551	−2.2098224
Ru	2.2253950	−0.9435784	−1.3512909
Ru	2.2613355	−0.9660394	1.3364711
Ru	0.7758722	1.0581595	2.2025103
Ru	−1.7559882	0.7195227	1.3810326
Ru	−1.8075384	0.7176534	−1.3337139
Ru	−0.3297319	−1.3736862	−2.0840369
Ru	0.6107869	−2.6044897	−0.0046321
Ru	−0.2917238	−1.3550483	2.1561910
Ru	−1.8261716	−1.4964040	0.0164755
Ru	−3.8481239	−0.0453067	0.0689474
Ru	0.3129073	−0.1162628	0.0169490
Ru	−0.1601391	2.3699882	0.0170649
Ru	2.3304623	1.3341802	−0.0190427
H	−3.6718031	0.9323388	−1.2966385
H	−3.6567721	0.9212119	1.4200729
H	−1.5526238	2.5478451	−0.9823253
H	−1.5549119	2.5582471	1.0162491
H	1.3683024	2.5209903	−1.2065891
H	1.3924866	2.5326567	1.2204793
H	2.1367595	0.0856096	−2.8028121
H	2.2467333	0.0710931	2.7584420
H	0.0397267	−3.0830214	−1.6327070
H	−0.9462889	−2.8259210	1.0439770
H	3.4246771	0.4491230	−1.0813785
H	3.4383563	0.3808882	1.0182302
H	0.1550265	−0.1205847	−3.3797135
H	0.2406165	−0.2031278	3.4052152
H	−0.8837549	1.5730885	−2.7240297
H	−0.8090453	1.6046072	2.7300950
H	−1.9146299	−0.7203380	2.5202323
H	−2.0286249	−0.7186434	−2.3826066
H	1.2854091	−2.3927155	1.9709384
H	2.6064996	−2.2333948	−0.0804899

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{22}^{-}$
Energy = −1344.058566737 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	−0.1202841	0.2820103	0.0383996
Ru	−1.7488170	−1.7658278	−0.3097201
Ru	0.7551695	−1.8539179	−1.1809431
Ru	0.3090690	−1.9347503	1.3280478
Ru	−1.6653609	−0.2930416	1.9164392
Ru	−2.5061317	0.8794356	−0.3467171
Ru	−0.9798050	−0.1590990	−2.2629937
Ru	1.5281128	0.5918939	−1.8480341
Ru	2.3080954	−0.5036225	0.3738185
Ru	0.8817873	0.4396084	2.3493325
Ru	−0.9171349	2.2029031	1.3601893
Ru	−0.4649785	2.3476497	−1.2815917
Ru	1.6635749	2.1421596	0.3515491
Ru	−0.0114973	−3.9419851	0.0884526
H	−2.1157648	−1.9728956	1.4968133
H	−3.2374045	−0.0940127	0.9904919
H	−2.7517180	0.0917789	−1.9508041
H	−1.6371440	−1.8034366	−2.1470864
H	0.8176287	−0.7755382	−2.8348674
H	3.0258251	−0.2028740	−1.2526574
H	2.4609239	−2.0640947	−0.3610552
H	1.9034415	−1.0946219	2.1544120
H	−0.2898309	−0.8019355	3.0334449
H	−1.3698958	1.3256686	2.8336684
H	−2.6764662	2.1733937	0.9046436
H	−0.9377882	3.4649719	0.0353601
H	−2.2599471	2.2506016	−1.4950694
H	0.0312321	1.4590219	−2.8164354
H	1.0491782	3.2804793	−0.9143602
H	2.6836025	1.9289558	−0.9904735
H	2.5591594	1.1494646	1.5395760
H	0.7463056	2.6655147	1.9308386
H	2.9670223	3.0554690	0.6445538
H	1.2583365	−4.9652938	0.2162040
H	−1.7439157	−3.5537425	−0.3183425
H	0.6818093	−3.7221075	−1.4102974

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{24}^{-}$
Energy = −1345.267771832 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	−0.0559253	0.4012297	0.0159232
Ru	2.3892850	−0.3598063	0.3834998
Ru	1.7425915	2.2796285	0.3414049
Ru	−0.3655050	2.4745013	−1.3108167
Ru	−0.8469802	2.3495782	1.3082995
Ru	0.9371471	0.5942831	2.3228256
Ru	−1.6169434	−0.1197001	1.9011672
Ru	−2.4282802	1.0213828	−0.3952684
Ru	−0.8845699	−0.0106662	−2.2950499
Ru	1.6270598	0.7192199	−1.8519708
Ru	0.8377484	−1.7242632	−1.1776433
Ru	0.3870130	−1.7680306	1.3501501
Ru	0.0512694	−3.8715817	−0.0440690
Ru	−1.6980425	−1.6431200	−0.3319409
H	−2.1223711	−1.8081496	1.4154580
H	−3.1776113	0.1803873	1.0448816
H	−2.6274359	0.3399913	−2.0710542
H	−1.6425264	−1.6416862	−2.1317313
H	0.9467244	−0.6609452	−2.8293175
H	3.1160364	−0.0643738	−1.2568543
H	2.5498809	−1.8991483	−0.3941533
H	1.9590140	−0.9585622	2.1587025
H	−0.2522343	−0.6199583	3.0342432
H	−1.4118088	1.4835773	2.7748000
H	−2.5887694	2.3728809	0.7949282
H	−0.8098345	3.6140127	−0.0021995
H	−2.1657419	2.4094982	−1.5190514
H	0.1307045	1.5768834	−2.8486558
H	1.1547366	3.4031266	−0.9504975
H	2.7659215	2.0440372	−0.9932100
H	2.6448794	1.2817892	1.5211056
H	0.8081362	2.7347812	1.9625957
H	3.0368573	3.2069501	0.5790978
H	1.2357860	−4.9401290	0.1229689
H	−1.7367168	−3.3580634	−0.3967629
H	1.1006998	−3.6511869	−1.2831243
H	0.7438517	−3.6888600	1.4285755
H	−3.1753945	−2.2408727	−0.5666707

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{26}^{-}$
Energy = −1346.453083030 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.8430060	1.5373701	−1.9845867
Ru	2.3490242	1.8547683	0.2440625
Ru	−0.2845547	2.6195579	0.1047230
Ru	0.4379529	0.0138174	0.0094722
Ru	1.1136750	−2.4133886	−0.0865714
Ru	−1.5583862	−1.5820289	−0.1829941
Ru	−3.7914540	0.1180792	−0.0126497
Ru	−1.6293552	0.8067325	−1.3082435
Ru	0.1402659	−1.0286040	−2.2207475
Ru	2.5241482	−0.3381814	−1.2751019
Ru	2.3963776	−0.5550503	1.3873345
Ru	−0.1134429	−1.2476907	2.0779331
Ru	−1.6735799	0.7303559	1.2823561
Ru	0.6890347	1.2711431	2.2216276
H	−3.5405594	1.1063188	−1.2942705
H	−3.6615677	1.0172394	1.3288311
H	−3.2583074	−1.7125840	0.0308800
H	−2.0913525	−3.0700160	−0.4956038
H	0.3759906	−2.7427159	−1.6913543
H	−1.2622821	−2.4732463	1.3201556
H	−1.7262846	−1.1122370	−1.9733693
H	−1.6230195	−0.6049937	2.6486810
H	−1.7844708	2.6461299	0.8528783
H	1.9251028	−3.8841096	−0.3231906
H	1.0775677	−4.0989346	0.0898237
H	−0.0285201	0.4795828	−3.2016529
H	0.7323980	−0.2167331	3.2843848
H	−0.7660039	2.5227393	−1.6999685
H	−0.9214477	1.5992169	2.7877043
H	1.6968240	2.9074631	−1.0681186
H	1.2016845	2.9071273	1.3147213
H	2.8991586	−1.7937778	−0.1058743
H	1.5357054	−2.2741767	1.7020752
H	1.8443441	−1.2765662	−2.7037227
H	2.4564908	0.8927042	−2.5493111
H	2.9173360	1.1474667	1.8246634
H	3.6518342	0.9518125	−0.5504195
H	3.4165268	3.0460036	0.3772996
H	−4.9026923	1.2685223	−0.0608506
H	−0.8805103	4.1024531	0.1846820

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{28}^{-}$
Energy = −1347.644241880 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.8555743	1.3419623	−2.0672811
Ru	2.2758990	1.7615642	0.1502140
Ru	−0.2894928	2.5696083	0.0817080
Ru	0.4354119	−0.1005286	−0.0129708
Ru	1.0853804	−2.5522561	−0.0296594
Ru	−1.5489259	−1.6924770	−0.1132573
Ru	−3.7939501	0.0652810	−0.1582452
Ru	−1.6178428	0.6841870	−1.3635244
Ru	0.0731731	−1.1637223	−2.2337493
Ru	2.5262209	−0.5555123	−1.2856542
Ru	2.4080368	−0.6149219	1.4086496
Ru	−0.0906341	−1.2585925	2.1605961
Ru	−1.7180671	0.5544960	1.2705633
Ru	0.6564984	1.2454365	2.1674911
H	−3.6011463	1.0296879	−1.4472179
H	−3.6496226	0.8538039	1.2669573
H	−3.2619531	−1.7403914	−0.2158219
H	−2.3740700	−3.0836375	−0.1300429
H	−0.3257689	−2.7588397	−1.2682910
H	−0.4648333	−2.7700384	1.0421314
H	−1.6253282	−0.7638629	−2.5355701
H	−1.7716171	−0.8621918	2.4876168
H	−1.7163776	2.5276292	−0.8617967
H	−1.4668792	3.1312843	1.0215899
H	1.6069487	−4.1018746	−0.5103561
H	1.1578631	−4.2210375	0.3113226
H	0.4358792	0.0780104	−3.3955060
H	0.2079893	−0.0344508	3.4030760
H	−0.7559007	1.7510744	−2.6248265
H	−0.9752745	1.5935037	2.6588042
H	1.2662820	2.8553833	−1.0650715
H	1.1368074	2.8886443	1.2467230
H	2.6006640	−2.3368128	−0.9577757
H	2.4150968	−2.4465657	1.1210919
H	1.8302177	−1.3877988	−2.7205399
H	1.6833997	−1.3780044	2.8055560
H	2.7141583	0.9391901	−2.1652722
H	2.6123105	1.0814072	2.0129223
H	3.5307256	0.1999345	0.0676124
H	3.5013254	2.8053083	0.1952041
H	−4.8802063	1.2440286	−0.1412778
H	−0.6231491	4.1238494	−0.0251949

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{30}^{-}$
Energy = −1348.846983826 E_{h}; Spin multiplicity $2S + 1 = 3$

Ru	0.5751250	1.2292497	−2.1571703
Ru	2.4166457	1.5666579	−0.2039196
Ru	−0.2699631	2.6219466	−0.0034216
Ru	0.4372381	−0.0353644	0.0003914
Ru	0.8147407	−2.6204457	−0.0100675
Ru	−1.9356892	−1.6850354	0.1625020
Ru	−3.8848272	0.4625583	0.2115492
Ru	−1.7995032	0.7279783	−1.1730971
Ru	−0.3481906	−1.1937045	−2.0629350
Ru	2.2263624	−0.8125509	−1.5091669
Ru	2.3950841	−0.7936103	1.3111543
Ru	−0.0464579	−1.2054246	2.1500315
Ru	−1.6100151	0.7124346	1.3766914
Ru	0.9094534	1.2674581	2.0741236
H	−3.6287598	1.3128028	−1.1789074
H	−3.4757438	1.3112108	1.5473630
H	−2.7618077	−2.6307474	−0.8328277
H	−3.6040378	−1.3988274	0.2453305
H	−0.8017793	−2.7569498	−0.8538491
H	−2.4978361	−3.0205279	0.8415296
H	−1.9782217	−0.6588367	−2.4032320
H	−1.9114149	−1.1057958	1.9466660
H	−0.4238811	3.6535180	−1.2283625
H	−1.7528075	3.2111707	−0.0147004
H	0.5292174	−4.2602534	−0.3383047
H	−0.0145155	−2.9420004	1.5291509
H	−0.0025108	0.0151113	−3.3433256
H	−0.0554808	0.2692320	3.2361619
H	−1.0549610	1.7318741	−2.5365998
H	−0.5424599	2.3959914	1.8033177
H	1.4412523	2.9391941	−0.6620402
H	2.0585514	−2.5902551	−1.3106288
H	2.3853633	−2.5420481	0.8616685
H	1.4078436	−1.4419519	−2.8681593
H	1.7031571	−1.5350460	2.7333900
H	2.5657206	0.9638344	−2.0002426
H	2.5691086	0.4864731	2.4816897
H	3.4919126	2.8428373	−0.5813842
H	2.1752502	2.3939619	1.3406082
H	4.0251392	2.1688800	−0.2117253
H	3.4310436	−0.1106388	−0.0997882
H	1.3754327	−4.2248854	0.0852516
H	−4.8311592	1.7637821	0.3061058
H	−0.2521484	4.1594213	0.4421041

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{32}^{-}$
Energy = −1350.034422722 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	0.6513492	1.2173696	−2.3112920
Ru	2.4654662	1.4989861	−0.3152027
Ru	−0.2178922	2.6100624	−0.2138804
Ru	0.4363688	−0.0416867	−0.1433833
Ru	0.8173064	−2.6566312	−0.1789110
Ru	−1.9302209	−1.7637472	−0.1533197
Ru	−3.8265275	0.3820988	0.1013738
Ru	−1.7664617	0.6620193	−1.3710529
Ru	−0.2482850	−1.1999419	−2.2652351
Ru	2.2800773	−0.8430342	−1.6169643
Ru	2.3767377	−0.8532299	1.1876516
Ru	−0.1290319	−1.2061862	1.9953859
Ru	−1.5931578	0.7401541	1.1994661
Ru	0.9410663	1.2872321	1.9478124
H	−3.6126575	1.1425003	−1.3538884
H	−3.4944572	1.3510995	1.3667650
H	−2.8095613	−2.4932099	−1.2679387
H	−3.5462787	−1.4513736	0.2795716
H	−0.7409880	−2.8047692	−1.1170806
H	−1.7073364	−2.2721519	1.4322054
H	−1.8889281	−0.6924943	−2.6236684
H	−1.6348378	−0.5261059	2.5535030
H	−0.6610832	3.6714326	−1.3265941
H	−1.7125072	3.1105351	0.1076771
H	0.5688402	−4.2712191	−0.5762735
H	0.1785048	−3.0001794	1.3906184
H	0.1042954	0.0344869	−3.5239755
H	0.4231236	0.0646174	3.1509505
H	−0.9498765	1.6955141	−2.7217383
H	−0.6716890	1.7413392	2.4607901
H	1.4549453	2.8368916	−0.9732958
H	0.4334779	2.9479600	1.3859786
H	2.0429778	−2.6406659	−1.4710170
H	2.4069555	−2.5656952	0.6704192
H	1.5194967	−1.4546276	−3.0191577
H	1.7334723	−1.6492107	2.5441691
H	2.6398787	0.9137189	−2.1099846
H	2.5213669	0.3955801	2.4064324
H	3.5698425	2.7268379	−0.7439645
H	2.3421618	2.2538301	1.2948351
H	4.0530760	2.1248716	−0.2001685
H	3.4587517	−0.0971787	−0.1559721
H	−2.5626948	−3.1802793	0.2106788
H	1.3434997	−4.2497118	0.0075370
H	−4.8307459	1.6426163	0.0533334
H	−0.0433594	4.1662168	0.1172858

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{34}^{-}$
Energy = −1351.232501020 E_{h}; Spin multiplicity $2S + 1 = 3$

Ru	1.2491259	1.4592128	−2.2296915
Ru	2.4101168	−0.8325096	−1.4208247
Ru	2.4184533	−0.9116287	1.2976089
Ru	1.1086706	1.4225729	2.1410361
Ru	−1.5788480	1.5128937	1.3507698
Ru	−1.4241746	1.3777215	−1.4536310
Ru	−0.0646883	−0.8196457	−2.2701140
Ru	0.6155330	−2.3755278	−0.0798373
Ru	−0.2072239	−0.9349196	2.2466762
Ru	−1.6501161	−1.0951005	−0.1811975
Ru	−3.6589397	−0.0087628	−0.1861498
Ru	0.3707082	0.2470710	0.1153061
Ru	0.4805456	2.7477307	−0.0081358
Ru	2.6362793	1.3476044	−0.0055802
H	−3.1527016	1.2469661	−1.4427966
H	−3.2738321	1.2389238	1.0759507
H	−4.4151571	−0.4340914	−1.5436226
H	−4.4808721	−0.4647658	1.1243272
H	−0.8581660	−2.3569888	−1.2663969
H	−1.1762405	−1.6098290	3.4968529
H	−1.4852992	0.2128197	−2.7872325
H	−1.6501260	0.1363150	2.4875120
H	−2.3477901	2.8826891	1.6494639
H	−0.8622726	−2.3241828	1.0864962
H	1.0957900	1.1595173	−3.7920826
H	0.4478993	0.1494228	3.4248462
H	−0.2947212	2.3684324	−2.4251991
H	−0.4310329	2.3472985	2.4057320
H	1.6684315	2.9928390	1.4025730
H	2.2646613	−2.4703852	−0.8916017
H	3.2778741	−2.2555793	1.4281132
H	1.4801486	−1.5209856	−2.8253524
H	1.3588469	−1.7424206	2.5079193
H	2.8140762	0.5910669	−2.4910085
H	2.7840846	0.7401728	2.0936613
H	1.7382059	2.5142780	−3.3146875
H	3.6263227	−0.4381663	−0.0060961
H	−4.7055621	−1.2084906	−0.2192765
H	0.8603322	−4.0105382	0.3967401
H	1.9888905	2.8065025	−1.1038300
H	−1.4967544	2.6993027	−0.1379384
H	−2.3973326	1.8443334	2.6898499
H	−2.2088571	2.2987440	−2.4994082
H	−0.3740437	−2.0831171	3.5145411
H	−0.0824180	−0.6489010	−3.8638297
H	3.5183514	−1.2240276	2.4258279
H	3.6760278	−1.5425935	−2.0796246
H	0.9686577	−3.9832108	−0.5451311

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{36}^{-}$
Energy = −1352.430294104 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	1.0766494	1.4178787	−2.1261572
Ru	2.3116821	−0.8941846	−1.1450581
Ru	2.1468151	−0.8760184	1.6448020
Ru	0.9420088	1.4043637	2.2461208
Ru	−1.6608539	1.4443113	1.4379589
Ru	−1.6085305	1.4316567	−1.2816469
Ru	−0.3364367	−0.8757301	−2.1362968
Ru	0.3122166	−2.4107330	0.0996299
Ru	−0.5482819	−0.9206846	2.3039745
Ru	−1.8294755	−0.9714876	−0.0602606
Ru	−3.8456210	0.1291788	−0.0006359
Ru	0.3924112	0.1983045	0.1285258
Ru	0.3457639	2.7337087	0.0908300
Ru	2.5493869	1.3855091	0.1727885
H	−3.3303140	1.4309927	−1.1993023
H	−3.3829125	1.3087121	1.3409177
H	−4.6675557	−0.2284798	−1.3400750
H	−4.6187630	−0.3903846	1.3160187
H	−1.3189816	−2.7837054	−0.3157757
H	−1.7054661	−1.8868958	2.8391497
H	−1.7829226	0.2180032	−2.5310420
H	−1.8881996	0.1870130	2.7098828
H	−2.4892935	2.5214094	2.2587799
H	0.8214193	−2.2280790	−1.6842945
H	−0.3827150	−2.5743005	1.8072064
H	1.0665055	1.5002418	−3.7271054
H	−0.5423754	2.0138136	−2.5781099
H	−0.7241461	2.0468695	2.7587809
H	0.8828772	3.0747834	−1.7696068
H	0.6383800	3.1595755	1.7703903
H	3.5194798	−1.9982663	−1.5441343
H	3.1472731	−1.9110678	2.5327552
H	0.1429782	−1.5681360	−3.6204024
H	1.0215663	−1.5994119	2.8381937
H	2.3575905	0.2624597	−2.5287523
H	2.1856520	0.1375752	3.0216421
H	2.2198870	2.2511346	−2.8682926
H	2.6795029	1.8914752	1.8688080
H	3.6678688	−0.0273560	−0.5924890
H	−4.9100328	−1.0579405	0.0020089
H	0.5488929	−4.0432622	0.6068127
H	2.2590524	−2.1505164	0.2760822
H	2.0649238	3.1602687	0.0827897
H	−1.6139004	2.7777239	0.1103212
H	−2.3929652	2.1941299	−2.4408044
H	−0.7184711	−1.2416017	3.8704416
H	−0.2989342	−0.7508765	−3.8399547
H	3.7244290	−1.2355404	2.1127639

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{38}^{-}$
Energy = −1353.622507841 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	1.1323832	1.3655906	−2.2190471
Ru	2.3780888	−0.9284546	−1.2389043
Ru	2.2113445	−0.9179397	1.5164595
Ru	0.9382086	1.3527705	2.1922498
Ru	−1.7270793	1.5644379	1.3853497
Ru	−1.5505359	1.3675732	−1.3994023
Ru	−0.3002971	−0.9032483	−2.2488924
Ru	0.3652535	−2.4718126	−0.0382421
Ru	−0.4620438	−1.0281088	2.2138101
Ru	−1.7887293	−1.0456053	−0.1592966
Ru	−3.7796379	0.0726912	−0.0937920
Ru	0.4013187	0.1546060	0.0524639
Ru	0.3822530	2.6780814	−0.0259803
Ru	2.5586284	1.3345896	0.0876299
H	−3.2754028	1.3176298	−1.3528160
H	−3.4237002	1.3765564	1.1553329
H	−4.5247111	−0.3709402	−1.4509283
H	−4.5775794	−0.4079227	1.2268246
H	−1.2624975	−2.8100609	−0.5264397
H	−1.6595006	−1.8386970	3.0548594
H	−1.7542970	0.1094974	−2.6489720
H	−1.8830651	0.0522606	2.3275029
H	−2.3215511	3.0025840	1.6915747
H	0.9513036	−2.1984453	−1.8156283
H	−0.3618395	−2.6709184	1.6214610
H	1.0912664	1.3842769	−3.8213398
H	0.0757579	0.2226074	3.3670221
H	−0.4936541	1.9361976	−2.6986259
H	−0.6593762	2.1448513	2.6341117
H	0.9127040	3.0360193	−1.8165785
H	0.7355749	3.0707979	1.6985046
H	3.5657732	−2.0370640	−1.6590479
H	3.2350139	−1.8826965	2.4478358
H	0.1467835	−1.6421147	−3.7081829
H	1.1420917	−1.7180999	2.6844124
H	2.4245964	0.2240358	−2.6225602
H	2.3031590	0.1891071	2.8440943
H	2.2538365	2.2212904	−2.9681056
H	2.6216754	1.9155593	1.7916750
H	3.7358046	−0.0959764	−0.6950222
H	−4.8497581	−1.1092091	−0.0853128
H	0.6212178	−4.0867681	0.4439076
H	2.3209867	−2.1962899	0.1572644
H	2.0963740	3.0944804	−0.0409826
H	−1.5900838	2.7061067	−0.1352832
H	−2.5605925	1.7331420	2.7346377
H	−2.2983921	2.2732006	−2.4771442
H	−0.8684705	−1.8123880	3.6448212

$\mathbf{Ru}_{14}^{\mathrm{ico}}\mathbf{H}_{40}^{-}$
Energy = −1354.821765762 E_{h}; Spin multiplicity $2S + 1 = 1$

Ru	1.1595404	1.2993826	−2.1884642
Ru	2.4041993	−0.9876526	−1.2773426
Ru	2.2679580	−1.0052904	1.5731144
Ru	0.9539564	1.2297012	2.2273214
Ru	−1.6410869	1.4829831	1.4704707
Ru	−1.6087322	1.3730663	−1.4739512
Ru	−0.2342604	−1.0013998	−2.2424668
Ru	0.4249167	−2.5595758	−0.0839451
Ru	−0.5094632	−1.1433282	2.1585797
Ru	−1.7635769	−1.1526975	−0.2730322
Ru	−3.7036756	0.0274237	−0.0006230
Ru	0.4211431	0.0698518	0.0606074
Ru	0.4257334	2.5877922	0.0220309
Ru	2.6036228	1.2298669	0.1343631
H	−3.3069937	1.3027793	−1.3022334
H	−3.3408993	1.3137377	1.2679557
H	−4.5534373	−0.3985068	−1.3033530
H	−4.3825523	−0.5197862	1.3570117
H	−1.1511127	−2.9182549	−0.6395886
H	−1.6956691	−1.9833406	2.9661500
H	−1.8274555	−0.2600584	−2.3547612
H	−1.9138805	−0.1477846	2.3204670
H	−2.0437580	2.8776557	−1.8002201
H	−2.1645287	2.9553713	1.7338543
H	1.0593689	−2.2963010	−1.8339415
H	−0.4012785	−2.7686899	1.5337062
H	1.0812663	1.4540575	−3.7807634
H	0.0567666	0.0334162	3.3528744
H	−0.4600695	1.6728374	−2.7826983
H	−0.5973231	1.9874465	2.7759425
H	0.8870698	2.9644190	−1.7851280
H	0.7332326	2.9780820	1.7241173
H	3.6329320	−2.0416937	−1.6779493
H	3.0605728	−2.0461393	2.6794320
H	0.0607015	−1.7801039	−3.7493319
H	1.0903282	−1.8394343	2.6216571
H	2.2152054	−0.0102161	−2.7647132
H	2.2885281	0.0364463	2.9481466
H	2.3348919	2.0674931	−2.9490517
H	2.5829312	1.8885556	1.8224767
H	3.7199443	0.0367010	−1.0471138
H	3.5999369	0.0280867	1.1640746
H	−4.7899773	−1.1362660	0.0901175
H	0.6629589	−4.2111646	0.3386907
H	2.3665414	−2.2309839	0.1860866
H	2.1682852	2.9608760	−0.0587559
H	−1.6390210	2.4804324	−0.0013032
H	−2.4916637	1.7260024	2.7944573

Further details on genetic algorithm and free energy computations

For hexagonal structures with loadings of up to 16 hydrogen atoms, the minimum energy structures obtained by successively adding hydrogens in preferred binding positions were checked and confirmed using the hybrid ab initio genetic algorithm (HAGA) as implemented in the Turbomole program package. Structures obtained from the genetic algorithm (GA) only showed μ binding in E2 positions and for higher loadings also η binding in A2 positions. For a coverage of 16 hydrogen atoms, the genetic algorithm predicted a bi-icosahedral structure to be lower in energy than clusters with (more or less) distorted hexagonal core motif. It has to be noted that the performed GA computations did not restrict the metal core to the hexagonal or bi-icosahedral motif, but allowed all sorts of mutations and children generated by the standard procedure of cutting and mixing parental structures. Due to this freedom, convergence of the GA was comparatively slow for larger hydrogen loadings so that all bi-icosahedral cluster structures were generated by the described procedure of adding hydrogens successively in preferred binding positions. Analogously to the manually generated candidate structures, the GA computations were performed using the BP86 functional and a def2-SVP basis set. While the GA for the naked Ru_{14}^{-} cluster was started assuming an open-shell configuration with 10 excess majority spins (and applying Fermi smearing during the optimization process), start structures with stepwise smaller spin multiplicities were taken for increasingly larger hydrogen coverages. As summarized in the paper, it furthermore has to be kept in mind that candidate structures resulting from the GA were subsequently a) ensured to represent local minima (including, if necessary, one or more distortion and reoptimization cycles) and b) optimized with respect to the electronic structure, modifying the number of unpaired electrons and keeping it fixed during a further geometry optimization step.

Subsequent to the geometry optimization procedure, free energies were calculated for all

minimum energy structures using the freeh module of Turbomole based on analytical vibrational frequencies obtained with the aoforce module of Turbomole. Frequencies were scaled with the standard scaling factor of 0.9914 for BP86/def2-SVP computations. The different spin multiplicities were taken into account by adding the contribution due to the electronic partition sum. Based on the so obtained free energies for coverages of 2 to 40 hydrogen atoms, free energies for all possible hydrogen loadings were extrapolated using cubic fits. With the fits as input functions, all possible choices for parameters c, b, a and x defining the different equilibria R1, R2 and R3 were calculated using a small stand-alone Fortran program assuming the constraint $x = (1-c)b+ca$ to ensure equilibrium stoichiometry. Such an extrapolation was performed for each temperature and pressure reported in the paper, thus for a temperature range of 100 to 400 K (or 100 to 600 K for Ru_{19}^- clusters) and pressures of 1 Pa, 37 Pa, 10 Pa and 100 Pa.

Trend in spin multiplicities for increasing hydrogen coverages

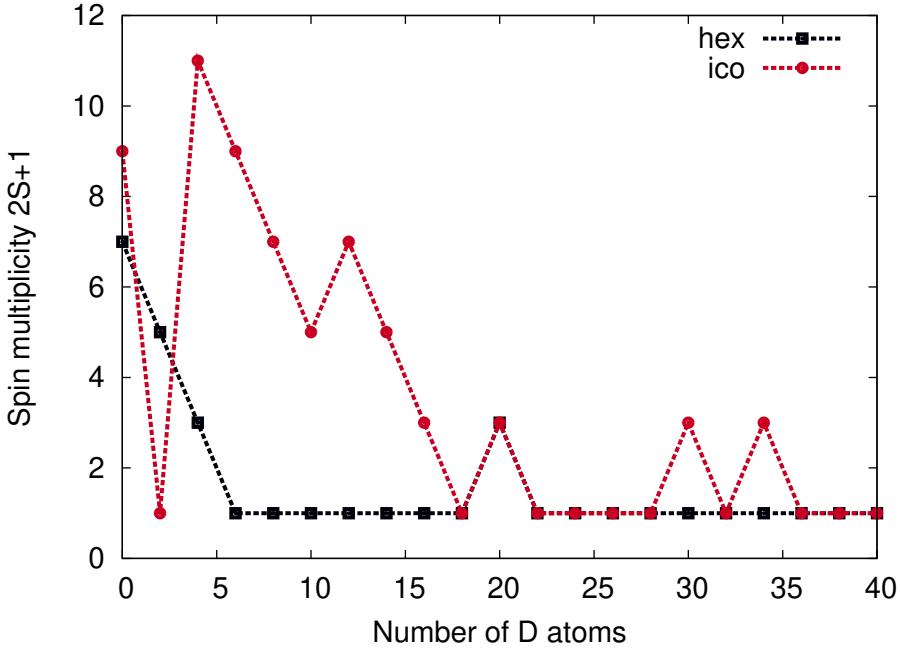

Figure S1: $Ru_{14}D_x^-$: Spin multiplicity as function of the hydrogen coverage for both hexagonal and icosahedral-plus-one Ru clusters.

Dependence of the adsorption energy on the position of the d-band center of $Ru_{14}D_x^-$

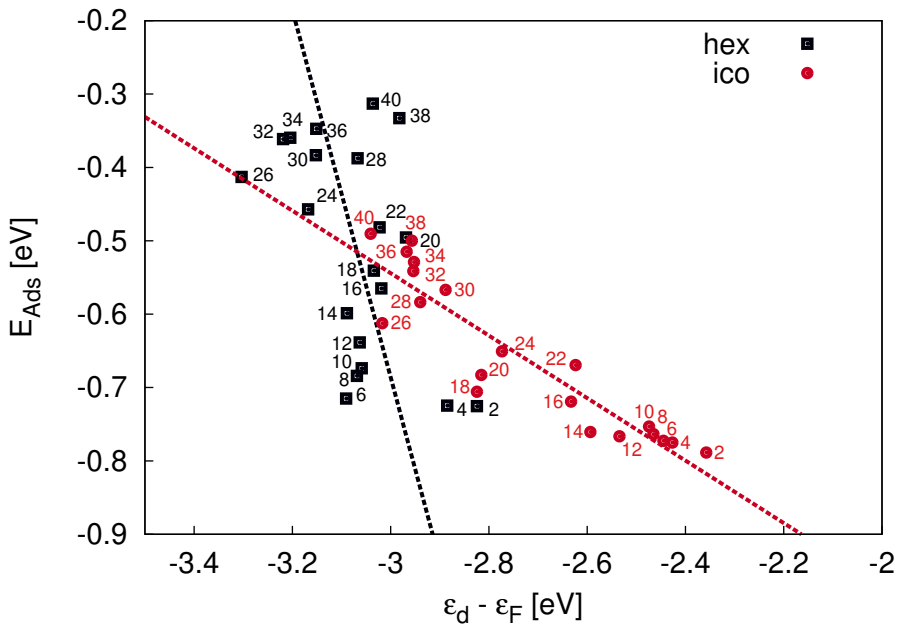

Figure S2: $Ru_{14}D_x^-$: Dependence of the adsorption energy on the position of the d-band center for hydrogen loads of 0 - 40 atoms.

Free energy differences as function of the number of the hydrogen loading $Ru_{14}D_x^-$

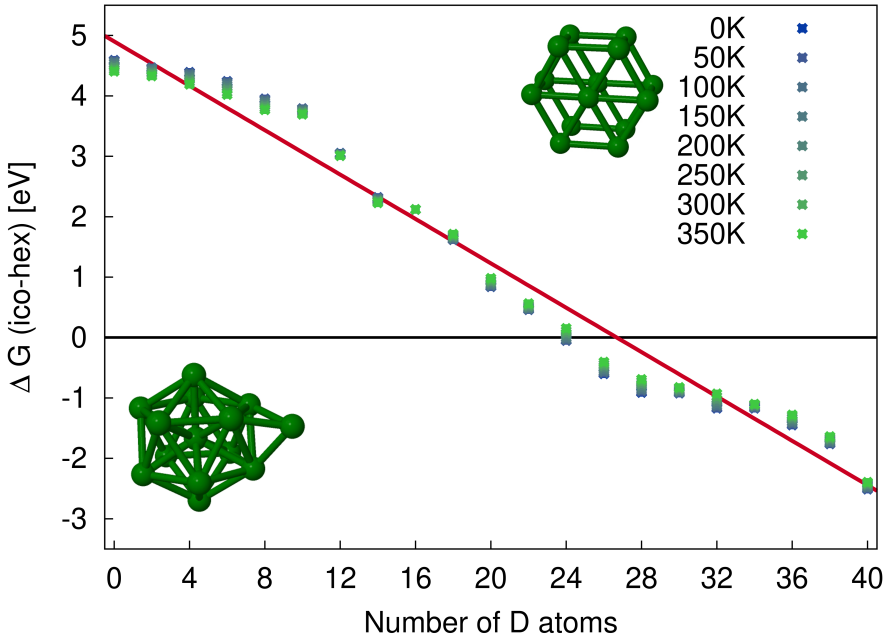

Figure S3: $Ru_{14}D_x^-$: Free energy differences for isomers with icosahedral-plus-one (bottom left) and double-layered hexagonal (top right) Ru core structures as a function of the hydrogen loading for a temperature range of 0 - 350 K.

Minimum free energy differences for $Ru_{14}D_x^-$ for experimentally measured temperatures

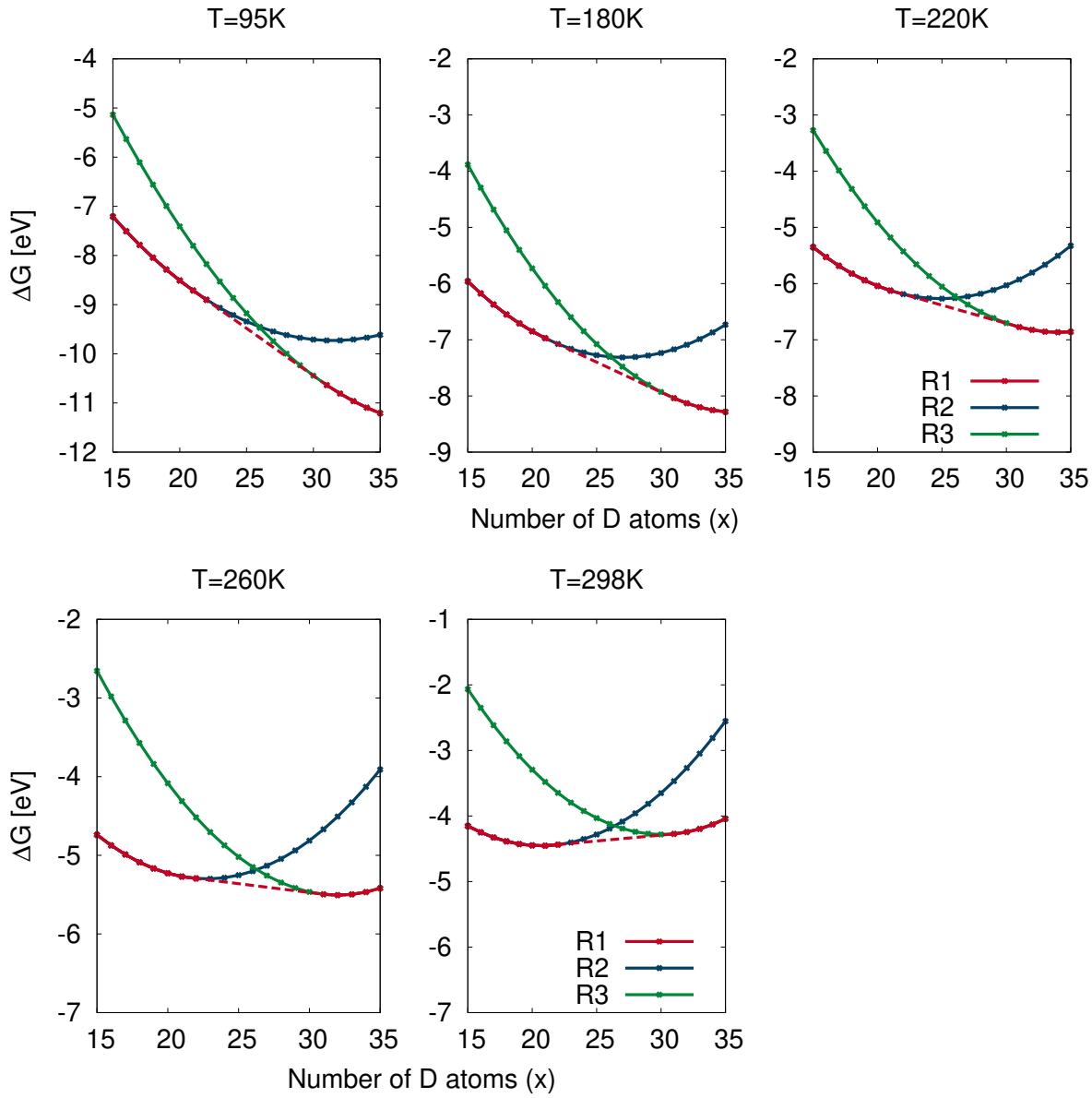

Figure S4: $Ru_{14}D_x^-$: Minimum free energy differences ΔG for the experimentally measured temperatures of 95, 180, 220, 260 and 298 K and a pressure of 37 Pa for R1, R2 and R3, depending on the total number of adsorbed deuterium atoms x.

Phase diagram for $Ru_{14}D_x^-$ at 10 and 100 Pa

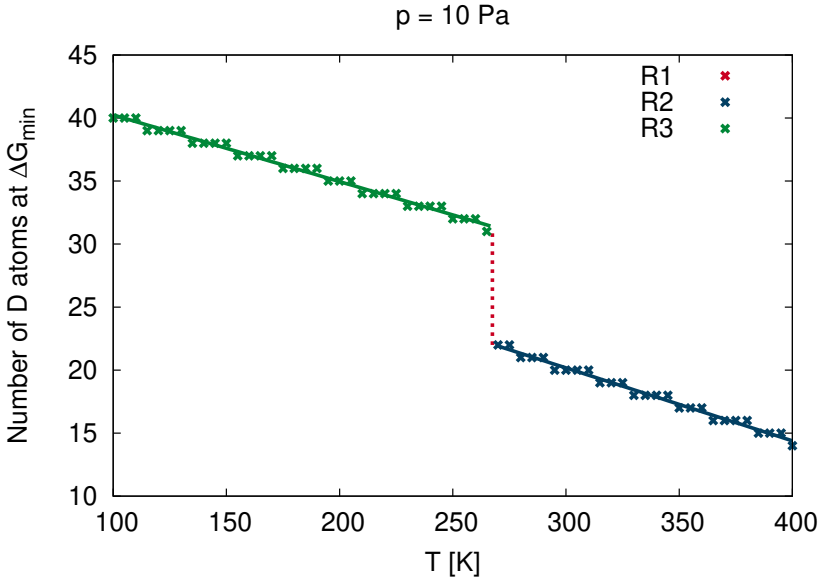

Figure S5: $Ru_{14}D_x^-$: Number of D atoms x at ΔG_{min} for a temperature range of 100 - 400 K at a pressure of 10 Pa. Data points are given in steps of $\Delta T = 5$ K with 265-270 K being the turnover point for the transition from icosahedral to hexagonal core structure.

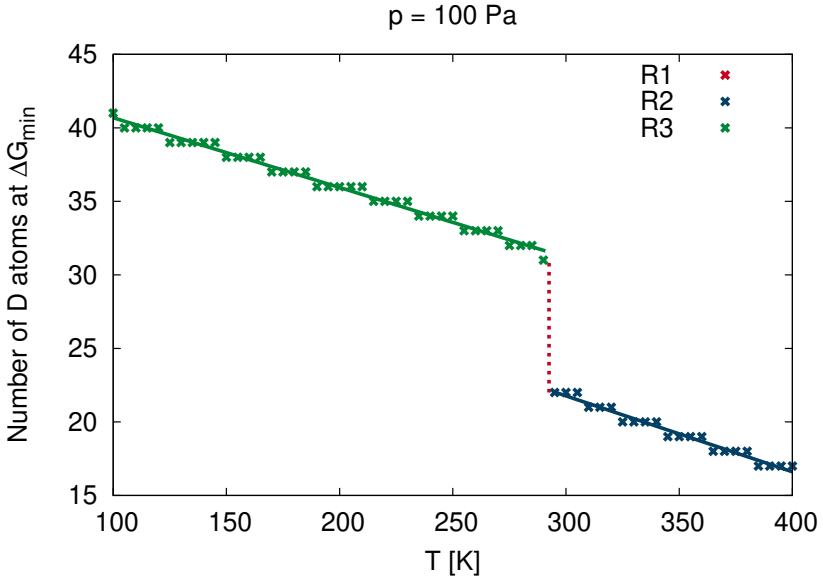

Figure S6: $Ru_{14}D_x^-$: Number of D atoms x at ΔG_{min} for a temperature range of 100 - 400 K at a pressure of 100 Pa. Data points are given in steps of $\Delta T = 5$ K with 290-295 K being the turnover point for the transition from icosahedral to hexagonal core structure.

$Ru_{19}D_x^-$: Free energy computations.

To analyze if a phase equilibrium analogously to the one for $Ru_{14}D_x^-$ can be found for $Ru_{19}D_x^-$ clusters, we extrapolated our earlier published computations on $Ru_{19}D_x^-$ isomers, investigating the following equilibrium reactions R4, R5 and R6 over the significant range of possible hydrogen loads and temperatures:

$$Ru_{19}^{oct-} + \frac{x}{2}D_2 \leftrightarrows cRu_{19}^{biico}D_a^- + (1-c)Ru_{19}^{oct}D_b^- \qquad \text{(R4)},$$

$$Ru_{19}^{oct-} + \frac{x}{2}D_2 \leftrightarrows Ru_{19}^{oct}D_x^- \qquad \text{(R5)},$$

and

$$Ru_{19}^{oct-} + \frac{x}{2}D_2 \leftrightarrows Ru_{19}^{biico}D_x^- \qquad \text{(R6)}.$$

With decreasing temperature, increasing hydrogen loads are found at thermodynamical equilibrium and $Ru_{19}D_x^-$ clusters undergo a structural transition from octahedral (oct) to bi-icosahedral (biico) cluster core. In Figure S7, free energy differences ΔG are depicted for the three equilibria R4, R5 and R6 at temperatures of 300 K, 430 K and 550 K. At 300 K (left picture), a hydrogen load of 22 atoms and a bi-icosahedral cluster core is most stable. At a temperature of 430 K (middle picture), our extrapolations predict a phase equilibrium with an instability region for intermediate hydrogen loads of 15 to 20 atoms. Within this range, the two concurrent cluster motifs of octahedral and bi-icosahedral core are in equilibrium as described by R4 and hydrogen coverages of $Ru_{19}^{oct}D_{15}^-$ and $Ru_{19}^{biico}D_{19}^-$ are found at minimum free energy $\Delta G_{\min}$. Going to higher temperatures, the octahedral cluster motif becomes more and more stable, with R5 being energetically lowest for a temperature of 550 K and coverages of 13 H atoms (right picture).

Within the instability region, R4 is energetically favored over R5 and R6 as depicted in Fig-

ure S8, unraveling that the splitting of the total number of adsorbed hydrogen atoms x with $x = 18$ into two different hydrogen loads of $a = 16$ and $b = 20$ results in a lowering of ΔG by 0.09 eV and 0.03 eV when comparing R4 to R5 and R6, respectively. Furthermore, the temperature dependence of the hydrogen coverages found at ΔG_{min} is plotted in Figure S9, visualizing that the number of D atoms steadily decreases with increasing temperature and that the turnover point between bi-icosahedral and octahedral structure motif is predicted theoretically at a temperature of 431 K when assuming a pressure of 1 Pa. Note that these predictions for $Ru_{19}D_x^-$ clusters are solely based on our computations as the instability gap is – in contrast to the one for $Ru_{14}D_x^-$ clusters – too narrow to allow for experimental evidence.

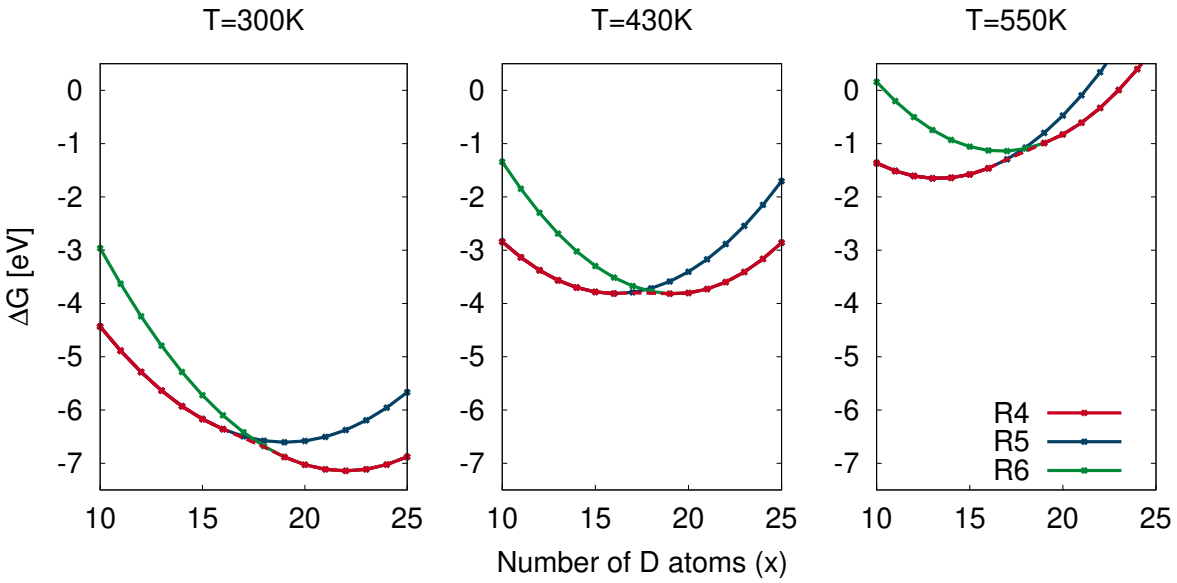

Figure S7: $Ru_{19}D_x^-$: Minimum free energy differences ΔG for temperatures of 300, 430 and 550 K and a pressure of 1 Pa for R4, R5, and R6, depending on the total number of adsorbed deuterium atoms x.

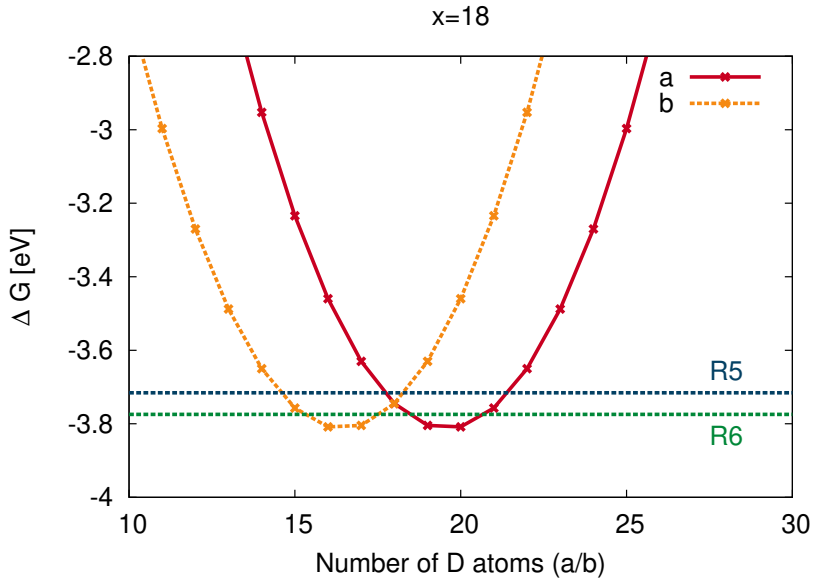

Figure S8: $Ru_{19}D_x^-$: Free energy differences ΔG at $T = 430$ K, $p = 1$ Pa and $x = 18$ for $c = 0.5$ as function of the number of adsorbed deuterium atoms for each isomer a, b of R4. For comparison, free energy differences for R5 and R6 are indicated as blue (R5) and green (R6) horizontal lines.

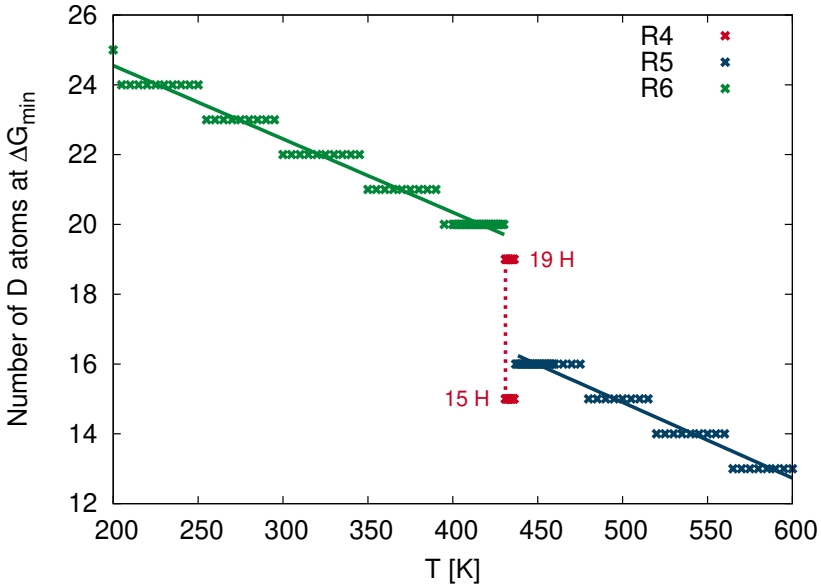

Figure S9: $Ru_{19}D_x^-$: Number of D atoms x at ΔG_{min} for a temperature range of 200 - 600 K at a pressure of 1 Pa. Data points are given in steps of $\Delta T = 5$ K in the range of 200 - 400 K as well as 460 - 600 K and in steps of $\Delta T = 1$ K in the range of 401 - 459 K, with 431 K being the turnover point for the transition from bi-icosahedral to octahedral core structure.