- Supplementary Materials -

Synthesis and Characterisation of Molecular Polarised-Covalent Thorium-Rhenium and -Ruthenium Bonds

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Table S1. Final Coordinates and Energy from a Single Point Energy Calculation on Geometry Optimised ThRe

1.C	0.032281	-0.380946	-6.323796
2.C	2.009360	0.944724	-5.553529
3.C	0.843464	0.049305	-5.079402
4.C	-0.853943	2.633908	-4.616031
5.C	1.417250	-1.215079	-4.409415
6.C	-1.892546	-0.072726	-3.639425
7.C	1.453197	2.268323	-2.207499
8.C	2.789770	1.648215	-1.800232
9.C	2.388424	-3.990776	-1.573430
10.C	-0.621390	-3.691025	-1.487666
11.C	-3.585880	2.776906	-0.900957
12.C	-4.106469	-0.796322	-0.694749
13.C	-2.172114	2.792879	-0.633908
14.C	3.269738	-0.445525	-0.537550
15.C	-2.731399	-1.150933	-0.445998
16.C	-4.265199	2.849652	0.364729
17.C	-4.731363	-0.573481	0.580739
18.C	2.515845	-1.393494	0.394202
19.C	0.467028	-5.951961	0.722612
20.C	3.131329	1.707413	0.654617
21.C	-1.986310	2.850344	0.796353
22.C	-2.509824	-1.120039	0.986063
23.C	0.881852	-4.516746	1.119069
24.C	-3.284826	2.869847	1.416703
25.C	1.968090	2.414547	1.348352
26.C	-3.750522	-0.738647	1.619051
27.C	2.249390	-4.590057	1.835870
28.C	-0.157861	-3.950580	2.107468
29.C	-0.748006	0.094151	3.779357
30.C	-0.037732	3.067452	4.077165
31.C	2.676396	-0.495026	4.296435
32.C	3.283600	1.922857	4.566440
33.C	2.126065	0.902185	4.648483
34.C	1.629481	0.867932	6.114161

35.H	0.692042	-0.892489	-7.048098
36.H	-0.417377	0.478644	-6.844731
37.H	2.646645	0.394848	-6.269972
38.H	1.649837	1.850657	-6.065131
39.H	-0.776747	-1.081007	-6.067761
40.H	-1.279958	2.480648	-5.620250
41.H	2.084732	-1.755595	-5.104231
42.H	2.659149	1.264428	-4.725032
43.H	-0.021043	3.345254	-4.722342
44.H	-2.479953	-0.030680	-4.569118
45.H	-1.625344	3.122503	-4.001419
46.H	0.624101	-1.916198	-4.109784
47.H	1.993192	-0.973411	-3.505334
48.H	-1.681812	-1.134964	-3.445236
49.H	1.597170	2.783459	-3.173304
50.H	-2.520836	0.310526	-2.819987
51.H	3.088041	0.931651	-2.575864
52.H	2.405531	-3.428322	-2.520224
53.H	-0.689253	-2.985624	-2.330306
54.H	2.251187	-5.054435	-1.826678
55.H	-4.050479	2.788334	-1.881493
56.H	-0.576923	-4.700366	-1.924768
57.H	3.581113	2.417166	-1.732334
58.H	-4.593902	-0.783644	-1.663973
59.H	3.191966	-0.837089	-1.559286
60.H	1.210022	3.086665	-1.496874
61.H	-1.389139	2.819410	-1.389804
62.H	3.381919	-3.896012	-1.109930
63.H	-2.049106	-1.535834	-1.201430
64.H	-1.551320	-3.627247	-0.906865
65.H	4.344337	-0.396155	-0.269363
66.H	1.180265	-6.408847	0.018672
67.H	-0.530946	-5.982551	0.260388
68.H	-5.341982	2.870254	0.504041
69.H	3.915037	2.421616	0.339344
70.H	3.123187	-2.309083	0.475523
71.H	-5.769910	-0.292266	0.731266
72.H	1.543790	3.172010	0.656343
73.H	3.044577	-4.973107	1.177838
74.H	0.434470	-6.598161	1.618692
75.H	3.581578	1.015241	1.378789
76.H	2.507122	-0.962288	1.408281
77.H	-1.036205	2.935842	1.318878
78.H	-1.632002	-1.499091	1.512222
79.H	-1.167247	-3.909855	1.671183
80.H	2.569210	-3.611608	2.223038
81.H	2.373408	3.008091	2.185273
82.H	-3.486434	2.962760	2.478871
83.H	2.185223	-5.274874	2.701157
84.H	-3.928145	-0.681414	2.687636

85.H	0.113580	-2.933538	2.428670
86.H	-0.217546	-4.580513	3.013217
87.H	-1.628702	0.343893	3.166959
88.H	3.085757	-0.529430	3.276760
89.H	-0.429304	-0.929954	3.531713
90.H	3.770301	1.924231	3.579569
91.H	-0.968061	3.319150	3.547292
92.H	0.676412	3.883201	3.886320
93.H	1.906401	-1.276885	4.373009
94.H	2.951193	2.949901	4.782746
95.H	-1.061886	0.087114	4.833746
96.H	3.493385	-0.771248	4.987230
97.H	-0.262240	3.073523	5.155139
98.H	4.064078	1.671062	5.307646
99.H	0.821225	0.136758	6.264531
100.H	1.265471	1.849392	6.453119
101.H	2.460359	0.578935	6.782956
102.N	0.377407	1.256078	-2.246965
103.N	2.657412	0.912038	-0.514199
104.N	1.124023	-1.679397	-0.076770
105.N	0.952266	1.429567	1.772264
106.Re	-3.108109	0.935259	0.290678
107.Si	-0.329317	0.977069	-3.831969
108.Si	0.950734	-3.390841	-0.469502
109.Si	0.617250	1.373556	3.498442
110.Th	-0.053048	0.375202	-0.091063

Energy: –613.11853305 eV

Table S2. Final Coordinates and Energy from a Single Point Energy Calculation on Geometry Optimised ThRu

1.C	2.583221	3.760416	-4.198654
2.C	-0.545813	0.054100	-3.625527
3.C	3.202208	0.576267	-3.512743
4.C	-0.067627	1.418529	-3.140638
5.C	2.756155	3.537007	-2.678453
6.C	-1.209969	-2.100828	-2.616286
7.C	4.214172	3.904623	-2.312388
8.C	-2.703659	-0.117886	-2.452141
9.C	0.164250	-2.609158	-2.177688
10.C	1.802755	4.485030	-1.925631
11.C	3.025377	-4.589895	-1.893286
12.C	-2.892083	0.619212	-1.119361
13.C	3.930840	-2.616502	-0.631154
14.C	-4.709547	-2.130077	-0.391899
15.C	3.089918	-3.902357	-0.511035
16.C	3.358374	1.318102	-0.555280
17.C	0.284763	-5.059347	0.172445
18.C	3.785814	-4.865336	0.477438
19.C	-0.167359	3.293653	0.980101
20.C	-5.344785	0.954218	1.429687

21.C	-1.334873	2.941368	1.717118
22.C	-2.584225	-2.559037	1.759736
23.C	0.803333	3.782680	1.920717
24.C	1.465553	-2.810465	1.916842
25.C	-4.684406	-0.270855	2.098392
26.C	-5.794712	-1.203384	2.632624
27.C	2.125815	0.828288	2.569910
28.C	-1.089751	3.233255	3.104039
29.C	0.215202	3.785142	3.225322
30.C	-3.829463	0.212902	3.286767
31.C	-0.179086	0.089953	3.444487
32.H	3.250992	3.116279	-4.790259
33.H	2.826843	4.807733	-4.453732
34.H	1.552480	3.579745	-4.539042
35.H	-1.160819	0.131334	-4.544334
36.H	2.670545	0.639671	-4.474722
37.H	0.489722	1.888910	-3.968793
38.H	0.338472	-0.552927	-3.859280
39.H	4.251780	0.852895	-3.704053
40.H	-1.449538	-2.462845	-3.636957
41.H	3.193461	-0.477222	-3.193382
42.H	-2.924965	0.545835	-3.304389
43.H	-0.939435	2.079493	-2.973362
44.H	4.435927	4.936164	-2.640561
45.H	0.929766	-2.271464	-2.900110
46.H	4.946760	3.243404	-2.802464
47.H	2.596813	-3.934377	-2.665399
48.H	2.015460	5.536640	-2.189132
49.H	-3.396318	-0.967713	-2.505342
50.H	4.042867	-4.863571	-2.227325
51.H	0.749300	4.288447	-2.175211
52.H	0.127555	-3.707167	-2.288261
53.H	2.431407	-5.516532	-1.868128
54.H	-1.961507	-2.502682	-1.925351
55.H	4.394173	3.858486	-1.227801
56.H	3.475218	-1.901140	-1.331467
57.H	-4.134490	-2.763918	-1.084948
58.H	1.909176	4.395624	-0.835124
59.H	-5.325449	-1.444802	-0.995603
60.H	4.944630	-2.847686	-1.004699
61.H	-2.323919	1.577528	-1.182962
62.H	-3.941470	0.943052	-1.016435
63.H	0.101774	-5.471140	-0.831704
64.H	4.444200	1.395401	-0.717201
65.H	3.185782	0.290712	-0.195134
66.H	-5.401061	-2.793820	0.150153
67.H	4.794150	-5.122915	0.105790
68.H	-0.041311	3.254597	-0.098852
69.H	3.094206	2.003649	0.260868
70.H	4.049435	-2.109379	0.338495

71.H	3.232379	-5.809922	0.595741
72.H	-5.965376	0.674885	0.563688
73.H	-0.693763	-4.889322	0.646155
74.H	0.798345	-5.841920	0.753048
75.H	-4.596798	1.687478	1.092322
76.H	-1.944536	-3.113799	1.057583
77.H	3.909920	-4.417918	1.475089
78.H	-2.264413	2.558007	1.305954
79.H	-6.494966	-1.511169	1.841058
80.H	1.793425	4.156456	1.675276
81.H	-6.004770	1.471340	2.149364
82.H	2.111972	-1.924769	2.010667
83.H	-3.265130	-3.285925	2.227995
84.H	0.484805	-2.568655	2.353450
85.H	1.906148	-3.584278	2.564457
86.H	-1.947528	-2.151660	2.557610
87.H	-5.383891	-2.115214	3.094182
88.H	-6.384606	-0.683464	3.408950
89.H	-2.983405	0.831313	2.956233
90.H	-1.797414	3.085591	3.914602
91.H	-3.415717	-0.626244	3.863794
92.H	-4.442758	0.818376	3.978599
93.H	0.686779	4.126714	4.141634
94.N	-1.300873	-0.619522	-2.543153
95.N	0.741546	1.272567	-1.909319
96.N	0.513967	-2.204949	-0.794441
97.N	-2.411757	-0.192886	0.010133
98.O	3.206538	0.383990	2.716894
99.O	-0.525495	-0.796385	4.138187
100.Ru	0.416262	1.560299	2.466006
101.Si	2.437931	1.683577	-2.164597
102.Si	1.319296	-3.461305	0.148174
103.Si	-3.565305	-1.229783	0.842122
104.Th	-0.103312	-0.048547	-0.149004

Energy: –581.99703677 eV