Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

Hypo-electronic Triple-Decker Sandwich Complexes: Synthesis and Structural Characterization of $[(Cp^*Mo)_2\{\mu\text{-}\eta^6\text{:}\eta^6\text{-}B_4H_4E\text{-}Ru(CO)_3\}]$ (E = S, Se, Te or $Ru(CO)_3$ and $Cp^* = \eta^5\text{-}C_5Me_5$)

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Supplementary Tables

Table S1. DFT calculated and experimental ^{11}B NMR chemical shift δ (ppm) values of compound **3**, **6** and **7**.

	3		**6**		**7**	
	Exp.	*Cal.*	*Exp.*	*Cal.*	*Exp.*	*Cal.*
B1	72.4	67.6	54.5	44.3	104.5	114.8
B2	99.4	105.7	103.4	106.5	101.8	106.7
B3	102.6	112.6	107.5	117.7	101.8	105.1
B4	99.4	102.9	103.4	109.4	63.5	55.2

Table S2. Selected experimental and calculated bond distances (Å) and their computed Wiberg bond index (WBI) values of compound **3**, **6** and **7**. The chalcogen atoms are indicated by E.

	3			**6**			**7**		
	Exp.	*Cal.*	*WBI*	*Exp.*	*Cal.*	*WBI*	*Exp.*	*Cal.*	*WBI*
Mo-Mo	2.77	2.78	0.70	2.76	2.77	0.73	2.77	2.77	0.72
B-E	2.26	2.28	0.66	1.89	1.91	0.78	2.05	2.07	0.72
B-Ru	2.24	2.23	0.46	2.25	2.24	0.44	2.28	2.23	0.45
Ru-E	2.67	2.74	0.59	2.45	2.49	0.52	2.54	2.59	0.55

Table S3: Calculated natural charges (q_{Mo}, q_{Ru}, q_B and q_E), natural valence population (Pop), HOMO – LUMO gaps and vertical ionization potential (IP_v) of **3**, **6** and **7**. The chalcogen atoms are indicated by E.

	q_{Mo}	q_{Ru}	q_E	Pop (Mo_{val})	Pop (Ru_{val})	Pop (E_{val})	ΔE_{H-L} (eV)	IP_v (eV)
2	-0.92, -1.04	-1.49	0.92	6.90, 7.01	9.53	5.06	1.99	7.16
5	-0.82, -0.89	-1.37	0.51	6.80, 6.86	9.40	5.44	1.97	7.20
6	–0.96, -0.86	-1.42	0.68	6.93, 6.85	9.45	5.28	2.01	7.19

IP_v: The vertical ionization potential computed for the compounds **2**, **5** and **6**, corresponds to the removal of one electron from the fixed geometry of the neutral molecule.

Table S4. Molecular orbital energies for **3**, **6** and **7** obtained from Fenske-Hall MO analysis.

3			**6**			**7**		
fragment	*mol orbital*	*energy (eV)*	*fragment*	*mol orbital*	*energy (eV)*	*fragment*	*mol orbital*	*energy (eV)*
CpMo	16	-4.82	CpMo	16	-4.82	CpMo	16	-4.82
	15	-5.82		15	-5.83		15	-5.82
	14	-5.91		14	-5.89		14	-5.90
$[(CpMo)_2B_4H_4$-$TeRu(CO)_3]$	69	-3.62	**$[(CpMo)_2B_4H_4$-$SRu(CO)_3]$**	64	-3.18	**$[(CpMo)_2B_4H_4$-$SeRu(CO)_3\}]$**	69	-3.39
	68	-4.58		63	-4.93		68	-4.79
	67(LUMO)	-5.82		62(LUMO)	-5.78		67(LUMO)	-5.81
	66(HOMO)	-10.14		61(HOMO)	-10.13		66(HOMO)	-10.18
	65	-10.46		60	-10.63		65	-10.57
	64	-10.82		59	-11.10		64	-10.98
	63	-11.74		58	-11.86		63	-11.84
	62	-12.10		57	-12.30		62	-12.32

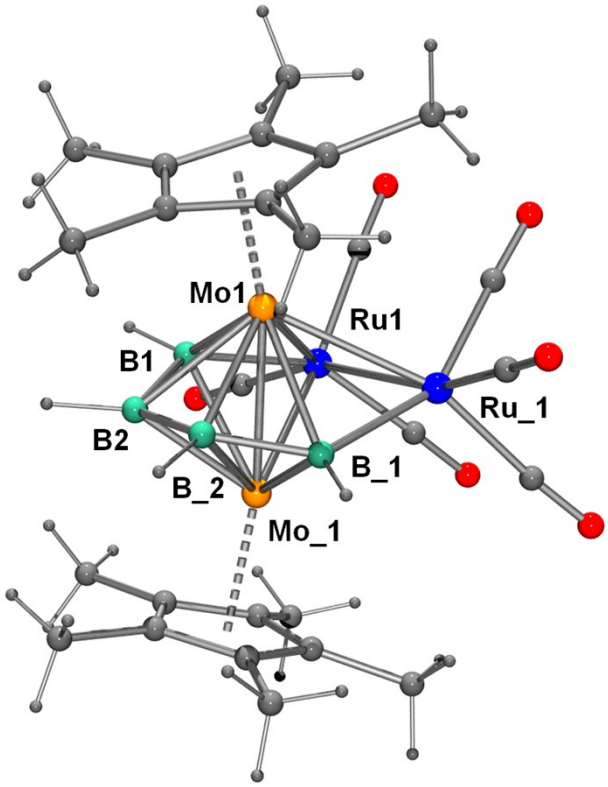

Fig. S1 Molecular structure of **1**. Selected bond lengths (Å) and angles (deg): Mo1-Mo_1 2.7510(5), Mo1-Ru1 2.6625(4), Mo_1-Ru1 2.9529(4), Mo1-B1 2.261(4), Mo1-B2 2.276(4), Mo1-B1 2.261(4), Mo1-B2 2.133(5), Mo_1-B2 2.133(5), Ru1-Ru_1 2.8822(5), B1-B2 1.622(5), B2-B_2 1.679(7), B1-Ru1 2.180(4), B1-B2-B_1 118.5(2), B2-B_1-Ru1 136.9(3), B1-Ru1-Ru_1 93.73(10), B2-B1-Mo1 75.5(2), Mo1-B1-Ru1 88.41(15), B2-B1-Mo1 64.2(2), Mo1-B1-Mo_1 79.08(13), Ru1-B1-Mo1 73.66(12), B1-B2-Mo1 60.9(2), Mo1-B2-Mo1 77.15(15), B1-Mo1-B2 85.32(16), B1-Mo1-B1 100.48(13), B1-Mo1-Ru1 103.59(11), B2-Mo1-Ru1 94.58(11), B1-Mo1-Mo_1 53.79(11), B2-Mo1-Mo_1 53.75(12).

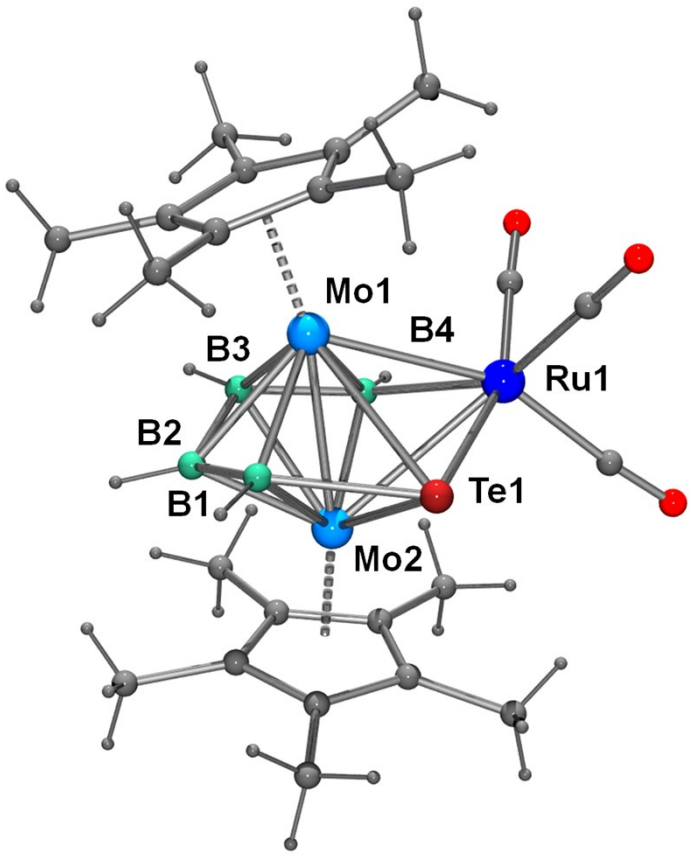

Fig. S2 Molecular structure of **3**. Selected bond lengths (Å) and angles (deg): B(1)-B(2) 1.697(10), B(1)-Mo(1) 2.187(6), B(1)-Te(1) 2.263(7), B(1)-Mo(2) 2.415(6), B(1)-H(1) 1.11(5), B(2)-B(3) 1.725(10), B(2)-Mo(2) 2.107(7), B(2)-Mo(1) 2.317(6), B(2)-H(2) 1.01(5), B(3)-B(4) 1.733(9), B(3)-Mo(1) 2.082(6), B(3)-Mo(2) 2.296(6), B(3)-H(3) 1.02(6), B(4)-Mo(2) 2.142(6), B(4)-Ru(1) 2.243(6), B(4)-Mo(1) 2.422(6), B(4)-H(4) 1.1000, Mo(1)-Ru(1) 2.7492(6), Mo(1)-Mo(2) 2.7787(6), Mo(1)-Te(1) 2.8746(6), Mo(2)-Te(1) 2.6708(5), Mo(2)-Ru(1) 2.9570(6), Ru(1)-Te(1) 2.6794(6), B(2)-B(1)-Mo(1) 72.0(3), B(2)-B(1)-Te(1) 125.9(4), Mo(1)-B(1)-Te(1) 80.5(2), B(2)-B(1)-Mo(2) 58.6(3), Mo(1)-B(1)-Mo(2) 74.10(19), Te(1)-B(1)-Mo(2) 69.54(18), B(1)-B(2)-B(3) 120.5(5), B(1)-B(2)-Mo(2) 78.0(3), B(3)-B(2)-Mo(2) 72.8(3), B(1)-B(2)-Mo(1) 63.8(3), B(3)-B(2)-Mo(1) 59.9(3), Mo(2)-B(2)-Mo(1) 77.7(2), B(2)-B(3)-B(4) 120.8(5), B(2)-B(3)-Mo(1) 74.3(3), B(4)-B(3)-Mo(1) 78.2(3), B(2)-B(3)-Mo(2) 61.3(3), B(4)-B(3)-Mo(2) 62.4(3), Mo(1)-B(3)-Mo(2) 78.6(2), B(3)-B(4)-Mo(2) 71.8(3), B(3)-B(4)-Ru(1) 128.0(4), Mo(2)-B(4)-Ru(1) 84.8(2), B(3)-B(4)-Mo(1) 57.3(3), Mo(2)-B(4)-Mo(1) 74.74(19), Ru(1)-B(4)-Mo(1) 72.12(18), B(3)-Mo(1)-B(1) 88.2(3), B(3)-Mo(1)-B(2) 45.8(3), B(1)-Mo(1)-B(2) 44.1(2), B(3)-Mo(1)-C(2) 122.2(2), B(3)-Mo(1)-B(4) 44.5(2) B(1)-Mo(1)-B(4) 104.5(2), B(2)-Mo(1)-B(4) 78.7(2), B(3)-Mo(1)-Ru(1) 94.64(18), B(1)-Mo(1)-Ru(1) 103.16(18), B(2)-Mo(1)-Ru(1) 112.40(16), B(4)-Mo(1)-Ru(1) 50.92(16), B(3)-Mo(1)-Mo(2) 54.09(16), B(1)-Mo(1)-Mo(2) 56.71(17), B(2)-Mo(1)-Mo(2) 47.80(16), B(4)-Mo(1)-Mo(2) 48.04(14), Ru(1)-Mo(1)-Mo(2) 64.675(15), B(3)-

Mo(1)-Te(1) 110.40(16), B(1)-Mo(1)-Te(1) 50.93(18), B(2)-Mo(1)-Te(1) 85.12(17), B(4)-Mo(1)-Te(1) 89.05(16), Ru(1)-Mo(1)-Te(1) 56.852(15), Mo(2)-Mo(1)-Te(1) 56.352(14), B(2)-Mo(2)-B(4) 90.0(3), B(2)-Mo(2)-B(3) 45.9(3), B(4)-Mo(2)-B(3) 45.8(2), B(2)-Mo(2)-B(1) 43.4(2), B(4)-Mo(2)-B(1) 106.1(2), B(3)-Mo(2)-B(1) 78.1(2), B(2)-Mo(2)-Te(1) 94.72(18), B(4)-Mo(2)-Te(1) 100.97(17), B(3)-Mo(2)-Te(1) 110.86(15), B(1)-Mo(2)-Te(1) 52.55(17), B(2)-Mo(2)-Mo(1) 54.55(17), B(4)-Mo(2)-Mo(1) 57.22(17), B(3)-Mo(2)-Mo(1) 47.26(15), B(1)-Mo(2)-Mo(1) 49.19(16), Te(1)-Mo(2)-Mo(1) 63.638(15), B(2)-Mo(2)-Ru(1) 111.65(17), B(4)-Mo(2)-Ru(1) 49.05(17), B(3)-Mo(2)-Ru(1) 84.94(15), B(4)-Ru(1)-Mo(2) 46.17(15), Te(1)-Ru(1)-Mo(2) 56.309(14), Mo(1)-Ru(1)-Mo(2) 58.146(14), B(1)-Te(1)-Mo(2) 57.92(17), B(1)-Te(1)-Ru(1) 103.24(16), Mo(2)-Te(1)-Ru(1) 67.105(15), B(1)-Te(1)-Mo(1) 48.61(17), Mo(2)-Te(1)-Mo(1) 60.010(13), Ru(1)-Te(1)-Mo(1) 59.215(14).

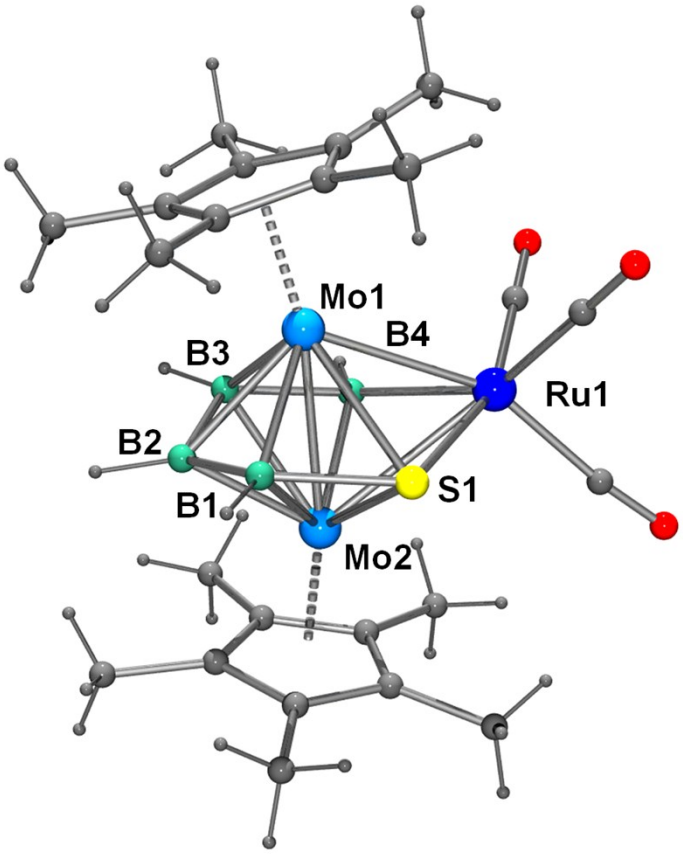

Fig. S3 Molecular structure of **6**. Selected bond lengths (Å) and angles (deg): B1-B2 1.707(6), B1-S1 1.891(4), B1-Mo1 2.218(4), B1-Mo2 2.361(4), B1-H1 1.131(18), B2-B3 1.740(5), B2-Mo2 2.127(4), B2-Mo1 2.280(4), B2-H2 1.115(17), B3-B4 1.741(5), B3-Mo1 2.096(4), B3-Mo2 2.289(4), B3-H3 1.136(17), B4-Mo2 2.154(4), B4-Ru1 2.260(4), B4-Mo1 2.393(4), B4-H4 1.054(17), S1-Mo2 2.4028(8), S1-Ru1 2.4537(9), S1-Mo1 2.5638(8), Mo1-Ru1 2.7137(4), Mo1-Mo2 2.7693(3), Mo2-Ru1 2.8849(3), B2-B1-S1 123.8(2), B2-B1-Mo1 69.63(18), S1-B1-Mo1 76.76(14), B2-B1-Mo2 60.54(17), S1-B1-Mo2 67.79(12), Mo1-B1-Mo2 74.36(11), B2-B1-H1 121.3(18), S1-B1-H1 111.9(17), Mo1-B1-H1 146.3(17), Mo2-B1-H1 139.4(17), B1-B2-B3 121.6(3), B1-B2-Mo2 75.13(19), B3-B2 Mo2 71.80(18), B1-B2-Mo1 65.79(18), B3-B2-Mo1 61.13(16), Mo2-B2-Mo1 77.79(12), B1-B2-H2 119.8(17), B3-B2-H2 116.1(16), Mo2-B2-H2 141.6(16), Mo1-B2-H2 140.2(16), B2-B3-B4 120.5(3), B2-B3-Mo1 72.23(18), B4-B3-Mo1 76.56(18), B2-B3-Mo2 61.96(17), B4-B3-Mo2 62.89(17), Mo1-B3-Mo2 78.18(12), B2-B3-H3 115.4(16), B4 B3 H3 120.7(16), Mo1 B3 H3 141.0(16), Mo2 B3 H3 140.4(16), B3 B4 Mo2 71.11(18), B3-B4-Ru1 127.1(2), Mo2-B4-Ru1 81.61(14), B3-B4-Mo1 58.42(16), Mo2-B4-Mo1 74.84(12), Ru1-B4-Mo1 71.29(11), B3-B4-H4 97.2(16), Mo2-B4-H4 141.4(16), Ru1-B4-H4 129.9(16), Mo1-B4-H4 131.1(16), B1-S1-Mo2 65.45(12), B1-S1-Ru1 118.01(12), Mo2-S1-Ru1 72.88(2), B1-S1-Mo1 57.35(12), Mo2-S1-Mo1 67.69(2), Ru1-S1-Mo1 65.44(2), B3-Mo1-B1 88.43(14), B3-Mo1-B2 46.64(14), B1-Mo1-B2 44.58(14), B3-Mo1-S1 107.25(10), B1-Mo1-S1 45.88(11), B2-Mo1-S1 81.66(10), B4-Mo1-S1 88.02(10), B3-Mo1-Ru1 95.67(10), B1-Mo1-Ru1

97.99(11), B2-Mo1-Ru1 112.13(9), B4-Mo1-Ru1 52.06(9), S1-Mo1-Ru1 55.32(2), B3-Mo1-Mo2 54.01(10), B1-Mo1-Mo2 55.18(10), B2-Mo1-Mo2 48.65(9), B4-Mo1-Mo2 48.64(9), S1-Mo1-Mo2 53.39(2), Ru1-Mo1-Mo2 63.483(9), B2-Mo2-B4 89.84(15), B2-Mo2-B3 46.24(14), B4-Mo2-B3 46.00(14), B2-Mo2-B1 44.32(15), B4-Mo2-B1 106.89(14), B3-Mo2-B1 80.65(14), B2-Mo2-S1 88.75(11), B4-Mo2-S1 98.14(10), B3-Mo2-S1 106.59(9), B1-Mo2-S1 46.76(11), B2-Mo2-Mo1 53.57(10), B4-Mo2-Mo1 56.52(10), B3-Mo2-Mo1 47.81(9), B1-Mo2-Mo1 50.46(10), S1-Mo2-Mo1 58.92(2), B2-Mo2-Ru1 110.88(10), B4-Mo2-Ru1 50.79(10), B3-Mo2-Ru1 87.05(9), B1-Mo2-Ru1 90.24(10), S1-Mo2-Ru1 54.37(2), Mo1-Mo2-Ru1 57.320(8), B4-Ru1-S1 93.88(10), B4-Ru1-Mo1 56.65(9), S1-Ru1-Mo1 59.24(2), B4-Ru1-Mo2 47.60(9), S1-Ru1-Mo2 52.75(2), Mo1-Ru1-Mo2 59.197(9).

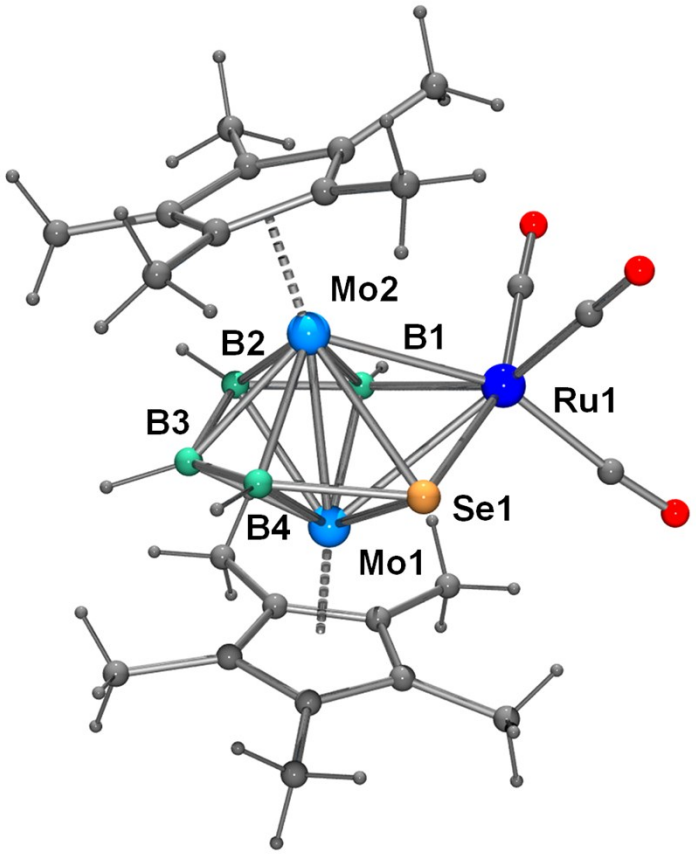

Fig. S4 Molecular structure of **7**. Selected bond lengths (Å) and angles (deg): B1-B2 1.725(10), B1-Mo1 2.155(7), B1-Ru1 2.282(8), B1-Mo2 2.413(7), B1-H1 1.1000, B2-B3 1.724(10), B2-Mo2 2.095(7), B2-Mo1 2.293(7), B2-H2 1.1000, B3-B4 1.703(10), B3-Mo1 2.119(7), B3-Mo2 2.294(7), B3-H3 1.1000, B4-Se1 2.056(8), B4-Mo2 2.215(8), B4-Mo1 2.392(7), B4-H4 1.1000, Mo1-Se1 2.5083(8), Mo1-Mo2 2.7733(7), Mo1-Ru1 2.9173(7), Mo2-Se1 2.6982(8), Mo2-Ru1 2.7226(7), Ru1-Se1 2.5478(8), B2-B1-Mo1 71.5(3), B2-B1-Ru1 126.7(4), Mo1-B1-Ru1 82.2(3), B2-B1-Mo2 58.0(3), Mo1-B1-Mo2 74.5(2), Ru1-B1-Mo2 70.8(2), B2-B1-H1 120.8, Mo1-B1-H1 134.8, Ru1-B1-H1 110.8, Mo2-B1-H1 150.5, B3-B2-B1 121.2(6), B3-B2-Mo2 73.1(3), B1-B2-

Mo2 77.7(4), B3-B2-Mo1 61.8(3), B1-B2-Mo1 63.0(3), Mo2-B2-Mo1 78.2(2), B3-B2-H2 119.9, B1-B2-H2 117.4, Mo2-B2-H2 133.2, Mo1-B2-H2 148.6, B4-B3-B2 122.0(5), B4-B3-Mo1 76.6(4), B2-B3-Mo1 72.5(3), B4-B3-Mo2 65.4(3), B2-B3-Mo2 60.9(3), Mo1-B3-Mo2 77.8(2), B4-B3-H3 116.6, B2-B3-H3 120.2, Mo1-B3-H3 134.3, Mo2-B3-H3 147.9, B3-B4-Se1 124.2(5), B3-B4-Mo2 70.3(3), Se1-B4-Mo2 78.3(3), B3-B4-Mo1 59.5(3), Se1-B4-Mo1 68.2(2), Mo2-B4-Mo1 73.9(2), B3-B4-H4 120.8, Se1-B4-H4 113.9, Mo2-B4-H4 136.6, Mo1-B4-H4 149.4, B3-Mo1-B1 89.3(3), B3-Mo1-B2 45.8(3), B1-Mo1-B2 45.5(3), B3-Mo1-B4 43.8(3), B1-Mo1-B4 106.9(3), B2-Mo1-B4 79.5(3), B3-Mo1-Se1 91.5(2), B1-Mo1-Se1 100.3(2), B2-Mo1-Se1 108.79(17), B4-Mo1-Se1 49.55(19), B3-Mo1-Mo2 53.93(18), B1-Mo1-Mo2 56.99(18), B2-Mo1-Mo2 47.70(17), B4-Mo1-Mo2 50.12(18), Se1-Mo1-Mo2 61.20(2), B3-Mo1-Ru1 111.02(18), B1-Mo1-Ru1 50.8(2), B2-Mo1-Ru1 86.21(17), B4-Mo1-Ru1 91.24(19), Se1-Mo1-Ru1 55.40(2), Mo2-Mo1-Ru1 57.099(16), B2-Mo2-B4 88.1(3), B2-Mo2-B3 46.0(3), B4-Mo2-B3 44.3(3), B2-Mo2-B1 44.3(3), B4-Mo2-B1 104.2(3), B3-Mo2-B1 79.3(2), B2-Mo2-Se1 108.5(2), B4-Mo2-Se1 48.3(2), B3-Mo2-Se1 83.15(18), B1-Mo2-Se1 88.96(19), B2-Mo2-Ru1 95.5(2), B4-Mo2-Ru1 100.6(2), B3-Mo2-Ru1 112.41(18), B1-Mo2-Ru1 52.33(19), Se1-Mo2-Ru1 56.07(2), B2-Mo2-Mo1 54.1(2), B4-Mo2-Mo1 55.96(19), B3-Mo2-Mo1 48.31(18), B1-Mo2-Mo1 48.50(17), Se1-Mo2-Mo1 54.551(19), Ru1-Mo2-Mo1 64.114(18), B1-Ru1-Se1 95.78(17), B1-Ru1-Mo2 56.85(17), Se1-Ru1-Mo2 61.48(2), B1-Ru1-Mo1 47.04(18), Se1-Ru1-Mo1 54.13(2), Mo2-Ru1-Mo1 58.787(16), B4-Se1-Mo1 62.3(2), B4-Se1-Ru1 111.4(2), Mo1-Se1-Ru1 70.47(2), B4-Se1-Mo2 53.5(2), Mo1-Se1-Mo2 64.25(2), Ru1-Se1-Mo2 62.45(2).

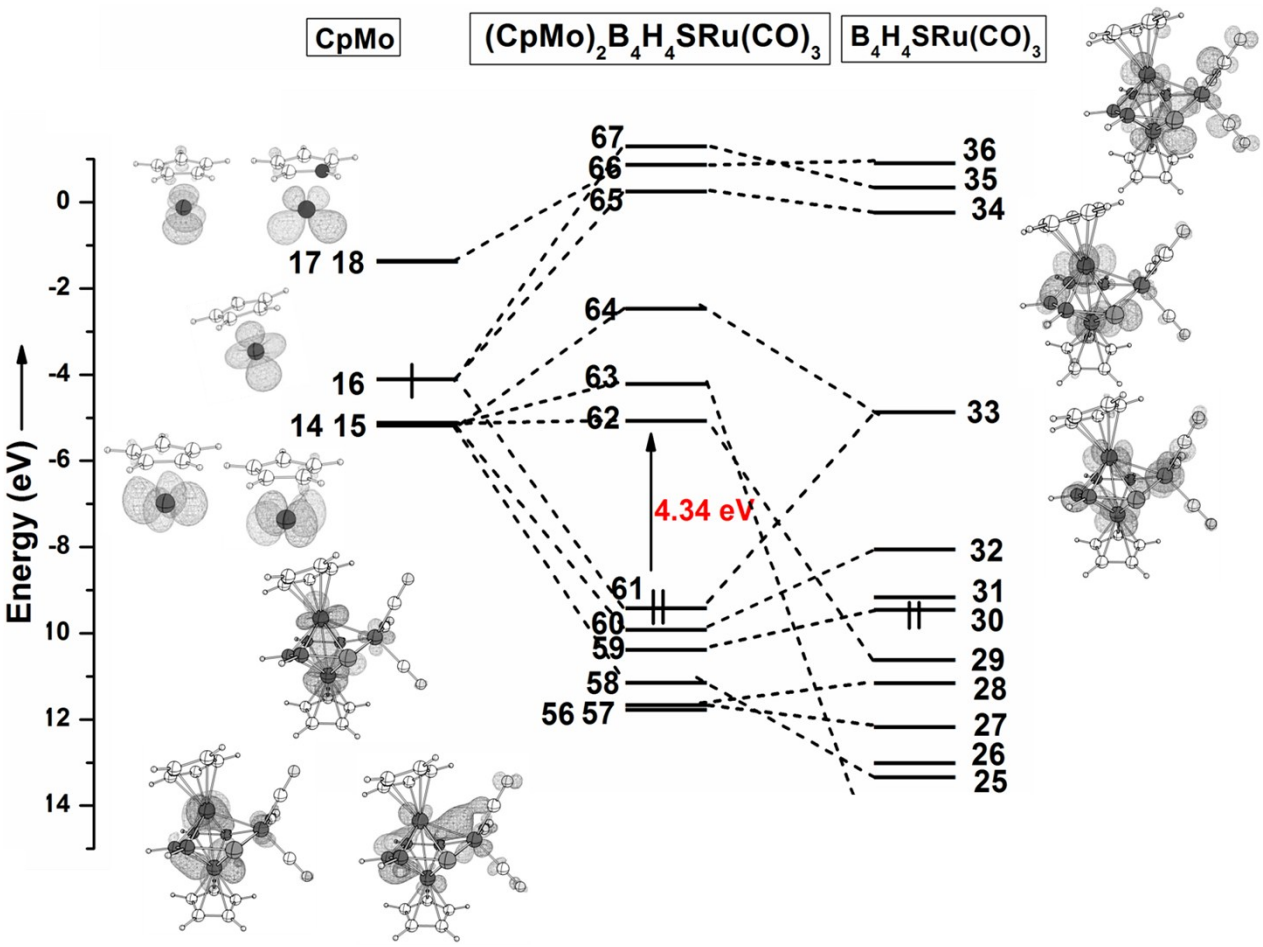

Fig. S5 Molecular orbital scheme resulting from Fenske-Hall calculation on **6**.

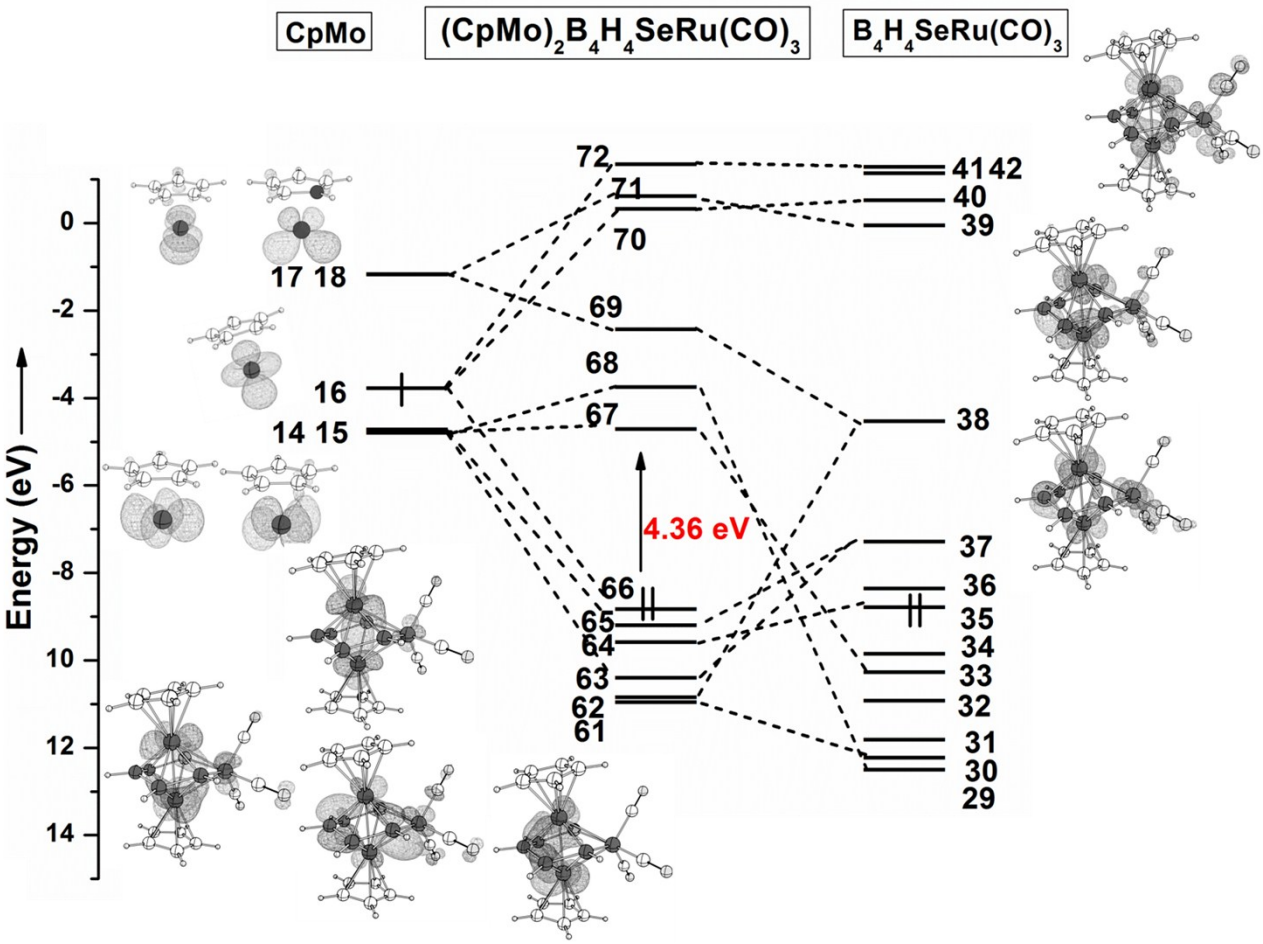

Fig. S6 Molecular orbital scheme resulting from Fenske-Hall calculation on **7**.

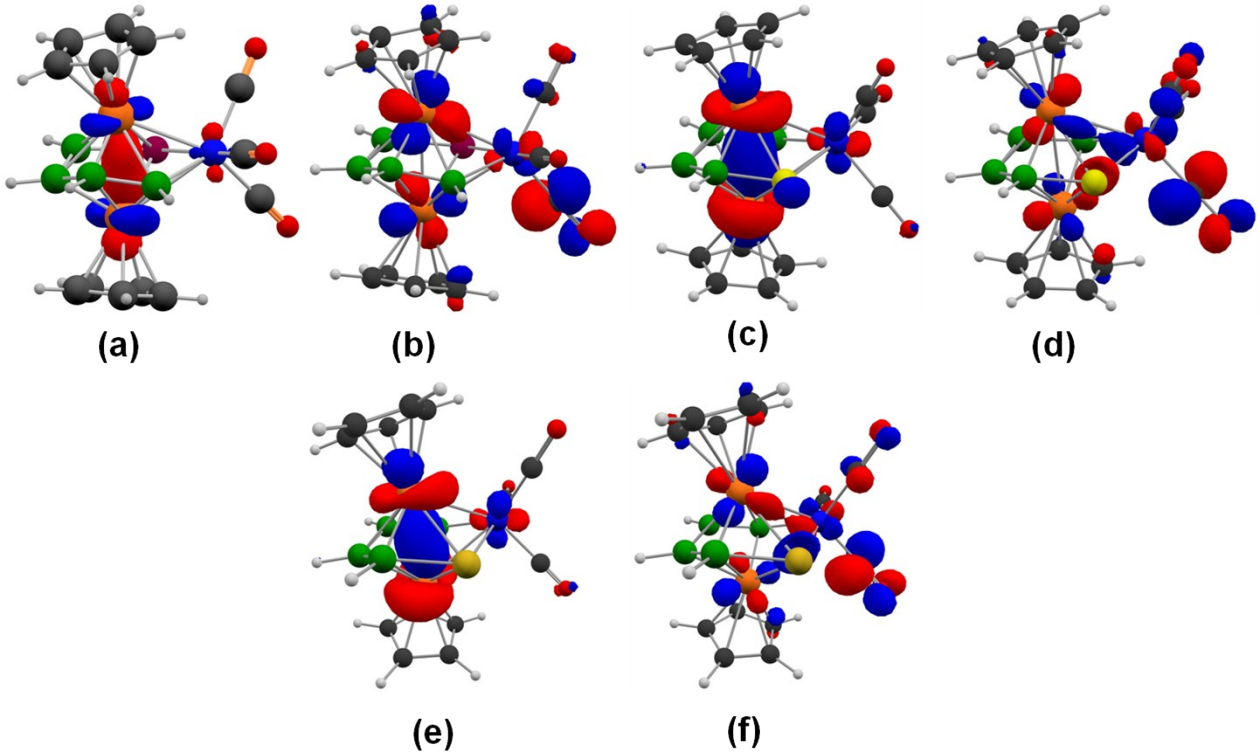

Fig. S7 Mo-Mo bonding and anti-bonding interaction of **3** (a and b), **6** (c and d) and **7** (e and f) obtained from DFT calculations.

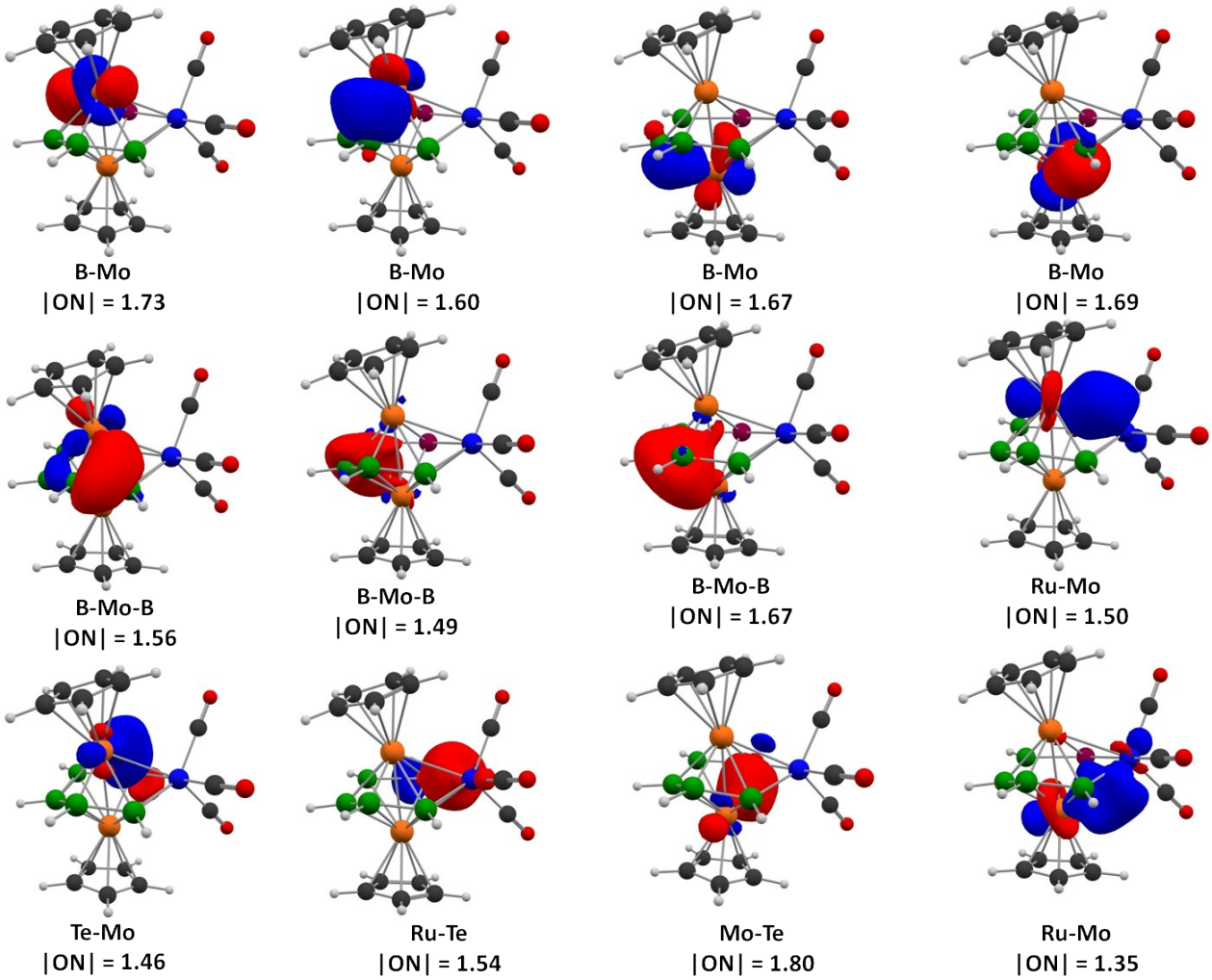

Fig. S8 Chemical bonding analyses of $[Mo_2B_4TeRu]$ core in **3**. ON stands for occupation number.

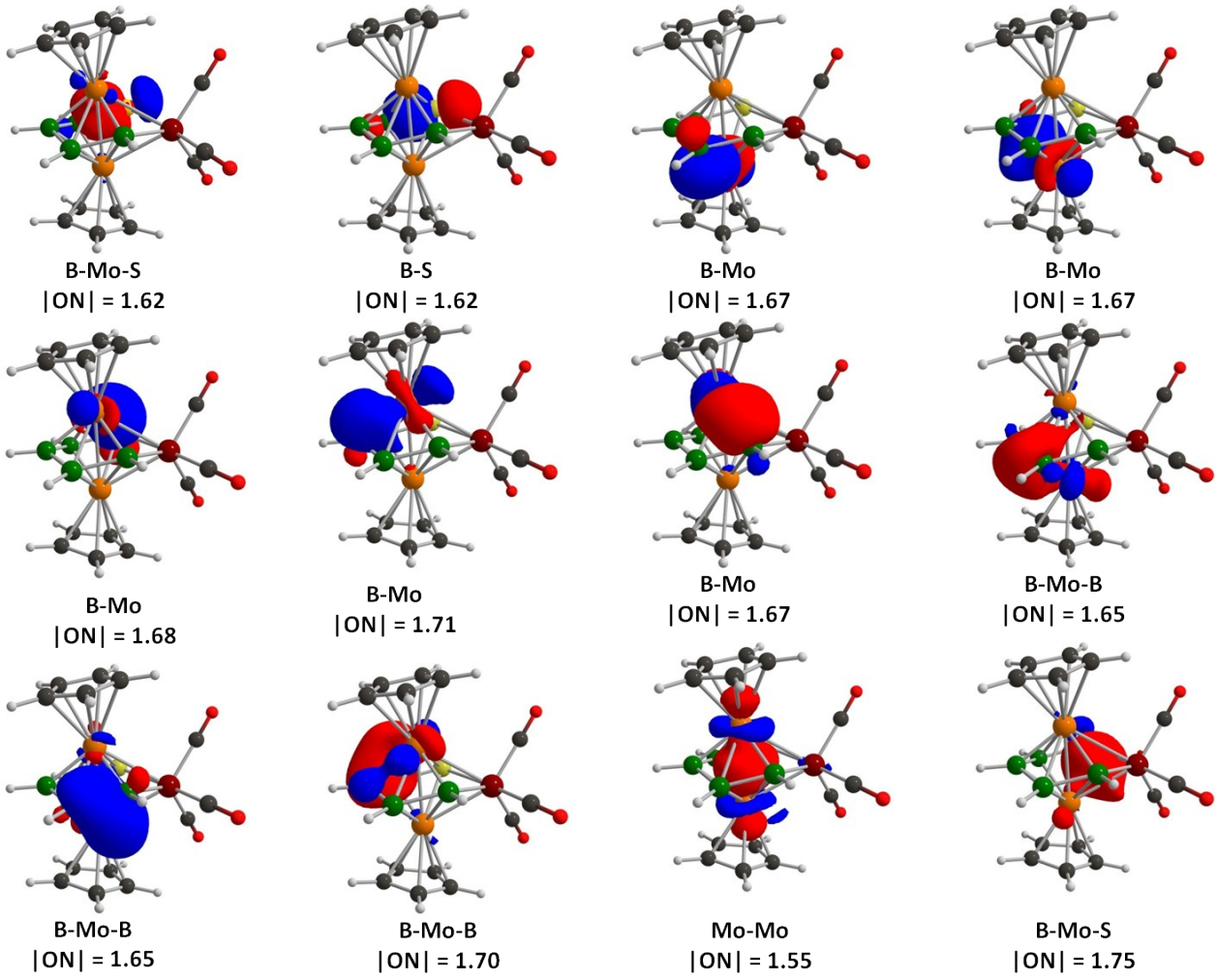

Fig. S9 Chemical bonding analyses of [Mo_2B_4SRu] core in **6**. ON stands for occupation number.

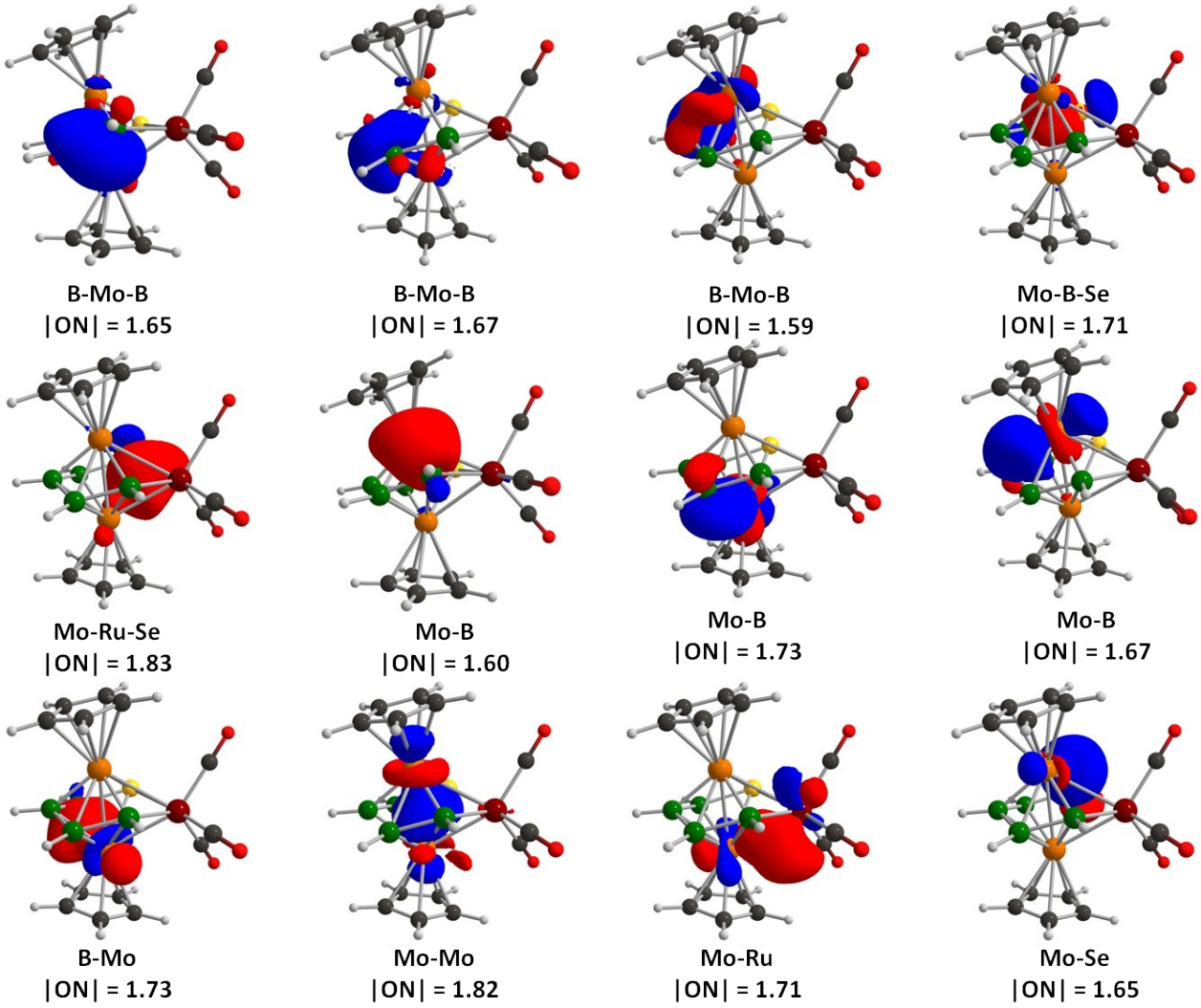

Fig. S10 Chemical bonding analyses of [Mo_2B_4SeRu] core in **7**. ON stands for occupation number.

Cartesian coordinates (xyz) for the optimized geometries of 3, 6 and 7.

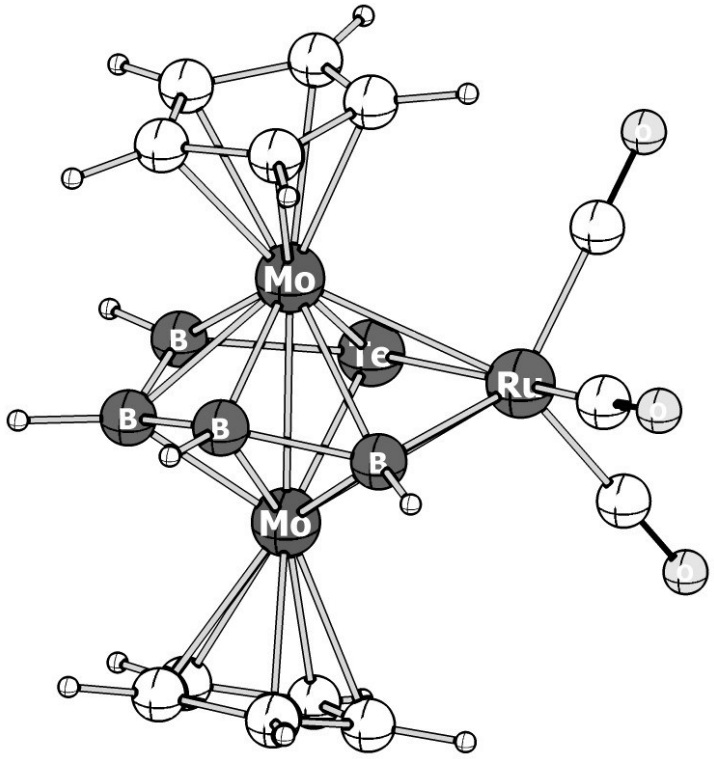

Fig. S11. Optimized geometry of **3.**

6	-3.491615000	-0.534110000	0.676719000
6	-3.057757000	-1.563239000	1.566320000
6	-2.757271000	-2.721361000	0.784956000
6	-2.997282000	-2.408364000	-0.587359000
6	-3.444256000	-1.053459000	-0.652147000
6	3.700908000	-1.471314000	-0.313215000
6	3.751416000	-0.045155000	-0.342509000
6	3.486390000	0.434164000	0.975128000
6	3.267963000	-0.693161000	1.822138000
6	3.400962000	-1.875698000	1.023245000
42	-1.220844000	-1.057796000	0.185507000
42	1.538140000	-0.705877000	0.244334000
44	-0.365426000	1.585012000	0.287878000
52	0.263093000	0.176458000	-1.979937000
5	0.123099000	-1.992039000	-1.282342000
5	0.550311000	-2.577769000	0.277837000
5	0.047245000	-1.722919000	1.716500000
5	0.199840000	0.022437000	1.779980000
6	-0.832461000	2.323030000	1.948406000
8	-1.152337000	2.816620000	2.946512000
6	0.958803000	2.930615000	-0.080005000
8	1.759427000	3.739674000	-0.296449000

1	0.706129000	-3.767953000	0.341845000
1	0.084581000	-2.335619000	2.748140000
1	0.205488000	-2.686369000	-2.257683000
1	0.238607000	0.306763000	2.950006000
6	-1.963316000	2.241860000	-0.528526000
8	-2.950878000	2.636379000	-0.990244000
1	3.311338000	-2.898159000	1.375925000
1	3.846096000	-2.135279000	-1.161144000
1	3.053147000	-0.660008000	2.885679000
1	3.443075000	1.476057000	1.279373000
1	3.955005000	0.570002000	-1.215305000
1	-2.396237000	-3.669694000	1.171403000
1	-2.867664000	-3.081656000	-1.429322000
1	-2.977915000	-1.486901000	2.646458000
1	-3.704316000	-0.509124000	-1.556725000
1	-3.812920000	0.463064000	0.960764000

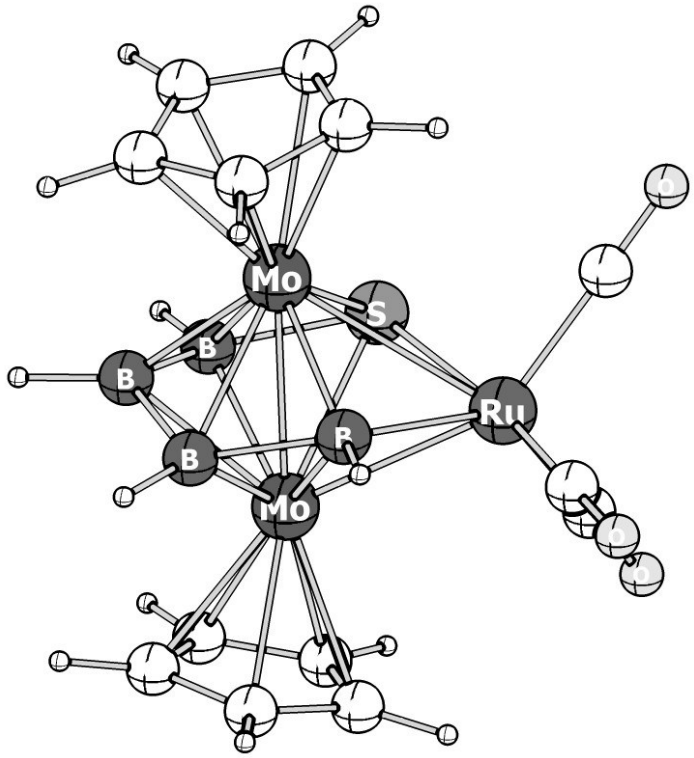

Figure S12. Optimized geometry of **6.**

Mo	1.22887400	-0.98259800	-0.00390300
Mo	-1.52990700	-0.71044700	-0.02050900
Ru	0.27028500	1.58493400	-0.01292700
S	-0.20702000	0.01776400	-1.89101300
O	2.89265000	2.67341000	-1.18823900
C	-3.35130700	-0.68949600	1.46686900
C	2.79404600	-2.60952800	0.63656200

C	3.47829700	-0.92265800	-0.78201900
C	3.04202600	-1.44529000	1.42605700
C	3.06336000	-2.28782700	-0.72851800
C	-3.72625200	-0.13688600	-0.74698400
O	0.74678100	3.08869100	2.57098600
C	-3.64557700	-1.55833400	-0.65663800
C	3.47331100	-0.40433500	0.54834600
C	-3.54877000	0.39837300	0.56422000
C	-3.41069500	-1.90328800	0.70927900
C	1.89933200	2.25859600	-0.76087900
O	-1.87589600	3.59604800	-0.95076500
C	0.54810000	2.50228100	1.59203700
B	-0.46193200	-2.54807000	-0.01393400
B	-0.08395800	-1.70040400	1.47236000
B	-0.09545200	-1.86061400	-1.55193700
C	-1.06770100	2.84891500	-0.59324600
B	-0.23828100	0.04694600	1.54264200
H	-0.57761000	-3.74342900	0.01015300
H	-0.13236800	-2.31641000	2.50146800
H	-0.27953600	0.36571100	2.70250800
H	-0.13516800	-2.51402600	-2.55604900
H	2.44932400	-3.56814800	1.01229200
H	2.97026000	-2.96300300	-1.57409200
H	2.93064300	-1.37161700	2.50362200
H	3.76086100	0.60021000	0.84308500
H	3.75075000	-0.37212000	-1.67916800
H	-3.88818900	0.43804900	-1.65548000
H	-3.72527800	-2.25882100	-1.48376100
H	-3.31222200	-2.90881500	1.10593000
H	-3.19900200	-0.61059500	2.53880200
H	-3.54846400	1.45196500	0.82896600

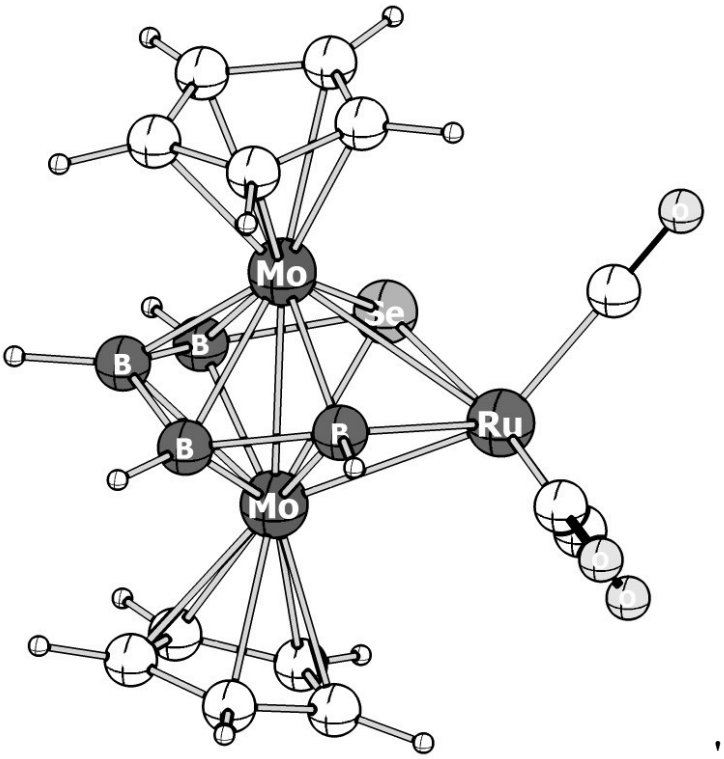

Fig. S13 Optimized geometry of **7.**

B	-0.22476000	0.05264300	1.65725300
H	-0.26738500	0.36743100	2.81865600
B	-0.06689600	-1.69357400	1.60404400
H	-0.11215500	-2.29977400	2.63912700
B	-0.50207700	-2.55533500	0.14518700
H	-0.63459000	-3.74863800	0.19408400
B	-0.09994700	-1.93170500	-1.40769300
H	-0.15623600	-2.61038600	-2.39432900
C	-3.73585100	-0.09135200	-0.55981300
C	-3.66957600	-1.51495400	-0.49220400
C	-3.40653600	-1.88213700	0.86278300
C	-3.31446300	-0.67941200	1.63576600
C	-3.52032200	0.42353600	0.75373400
C	3.46383600	-0.99520900	-0.70879700
C	3.03279400	-2.35342100	-0.61710900
C	2.77807400	-2.63779100	0.75912100
C	3.05242900	-1.45769800	1.51636800
C	3.48576600	-0.44431100	0.60802700
C	-1.02779700	2.88445500	-0.37832600
C	1.92574400	2.24634800	-0.66884700
C	0.67191400	2.44919400	1.74196500
Mo	-1.53279400	-0.70380900	0.10980000
Mo	1.22741500	-1.00921100	0.10054100
O	-1.83695400	3.65523800	-0.68108700

O	2.91572200	2.64527000	-1.11963800
O	0.92243200	3.00714300	2.72572200
Ru	0.31066100	1.58973300	0.11878200
Se	-0.22984300	0.07116800	-1.91730100
H	2.42575300	-3.58204300	1.16312400
H	2.92172100	-3.04777200	-1.44463400
H	2.95588100	-1.35628000	2.59312800
H	3.79205900	0.56280600	0.87331700
H	3.72861200	-0.46937500	-1.62292900
H	-3.31361400	-2.89431400	1.24337200
H	-3.13508100	-0.61742400	2.70458400
H	-3.77717500	-2.20227300	-1.32717000
H	-3.91361800	0.49889700	-1.45539800
H	-3.49993200	1.47320400	1.03267600