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Electronic supplementary information for:

Strong chemisorption of CO on $M@B_n^-$(M=Co, Ir, Rh, Ru, Ta, Nb, n=8-10) clusters: An implication for the wheel boron clusters as CO gas detector

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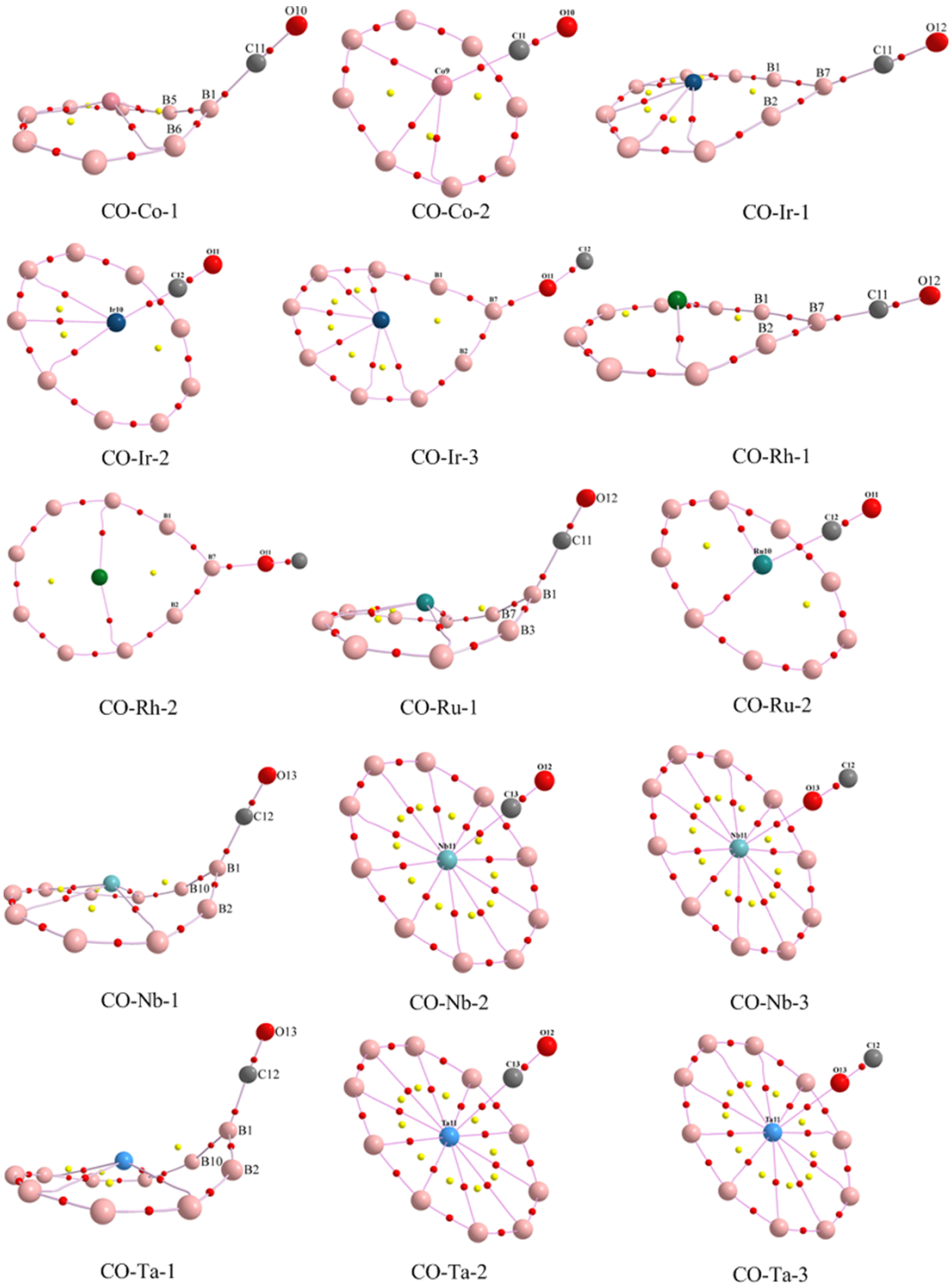

Fig. S1 The molecular graphs of the formed complexes of boron clusters with the CO molecule, where the BCP and RCP are denoted as small red and yellow dots, respectively.

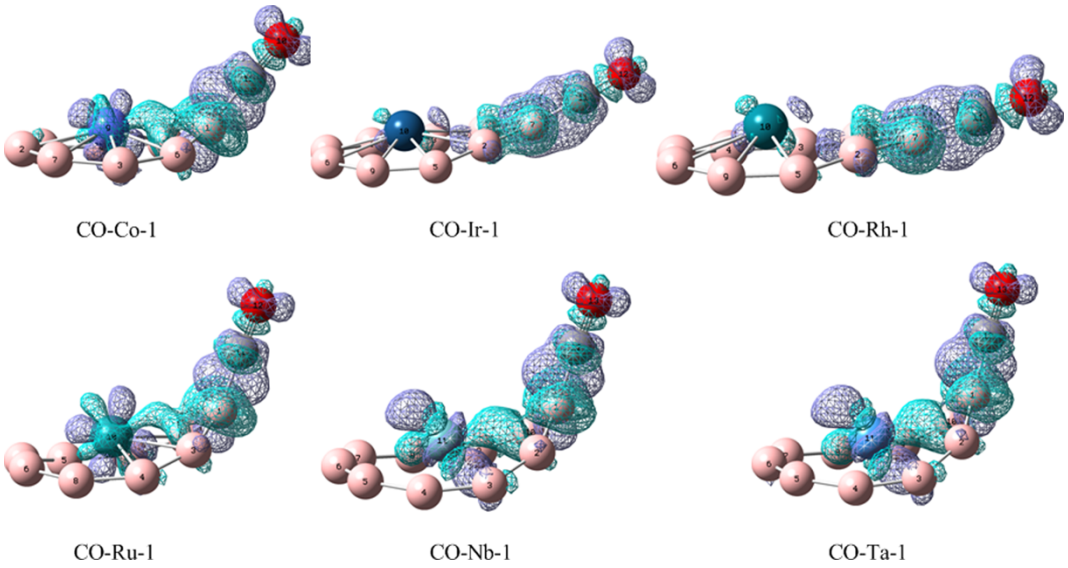

Fig. S2 Electron density difference map for the formation of the CO-M-1 complexes. The blue and purple regions represent the depleted and increased electron density, respectively. The isodensity contours are 0.004 electron/bohr^3.

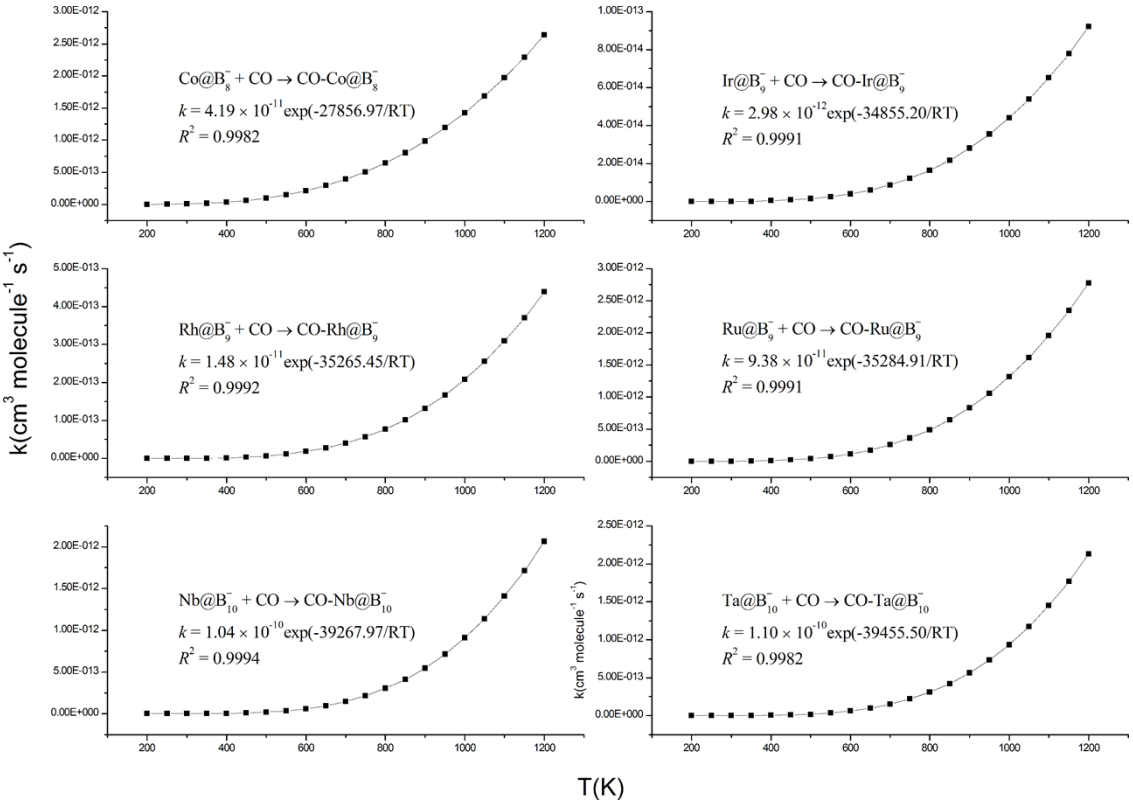

Fig. S3 The dependence of the rate constants versus temperatures ranging from 200.0 to 1200.0 K for the formation of the CO-M-1(M=Co, Ir, Rh, Ru, Ta, Nb) complexes.

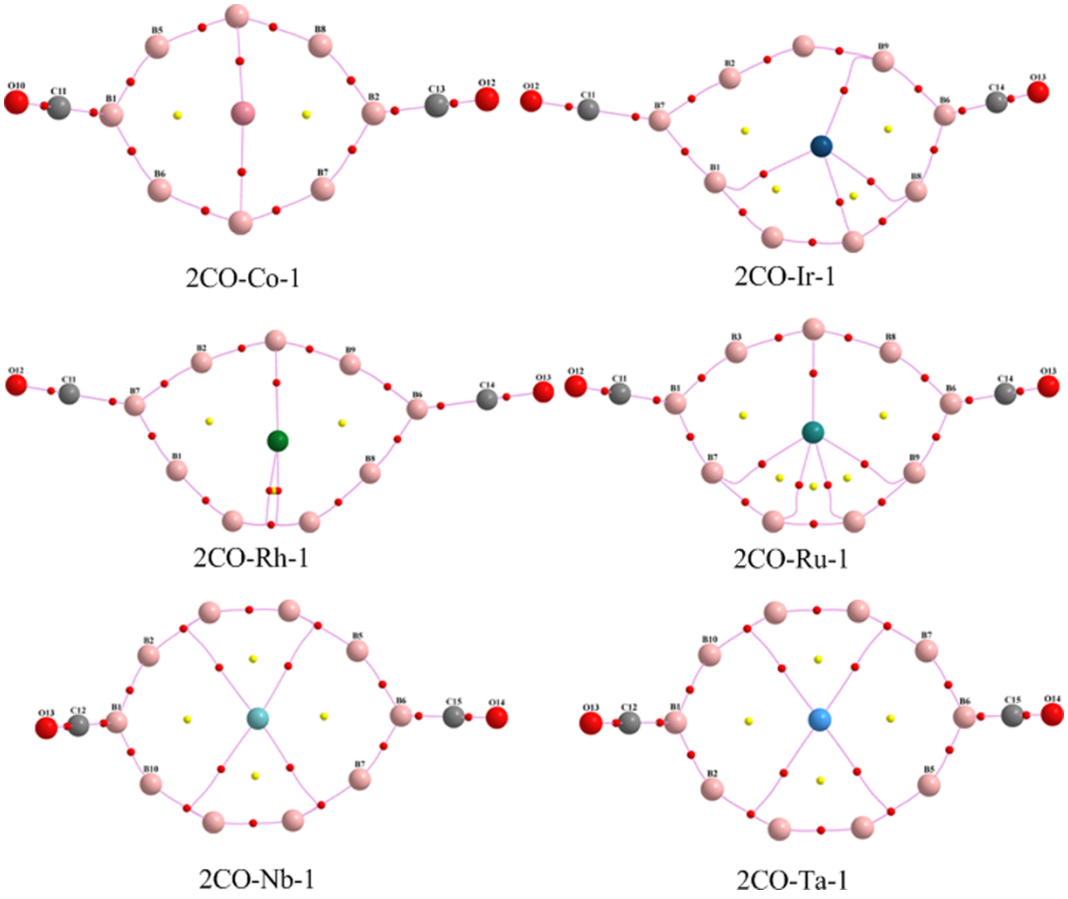

Fig. S4 The molecular graphs of the formed complexes of boron clusters with two CO gas molecules.

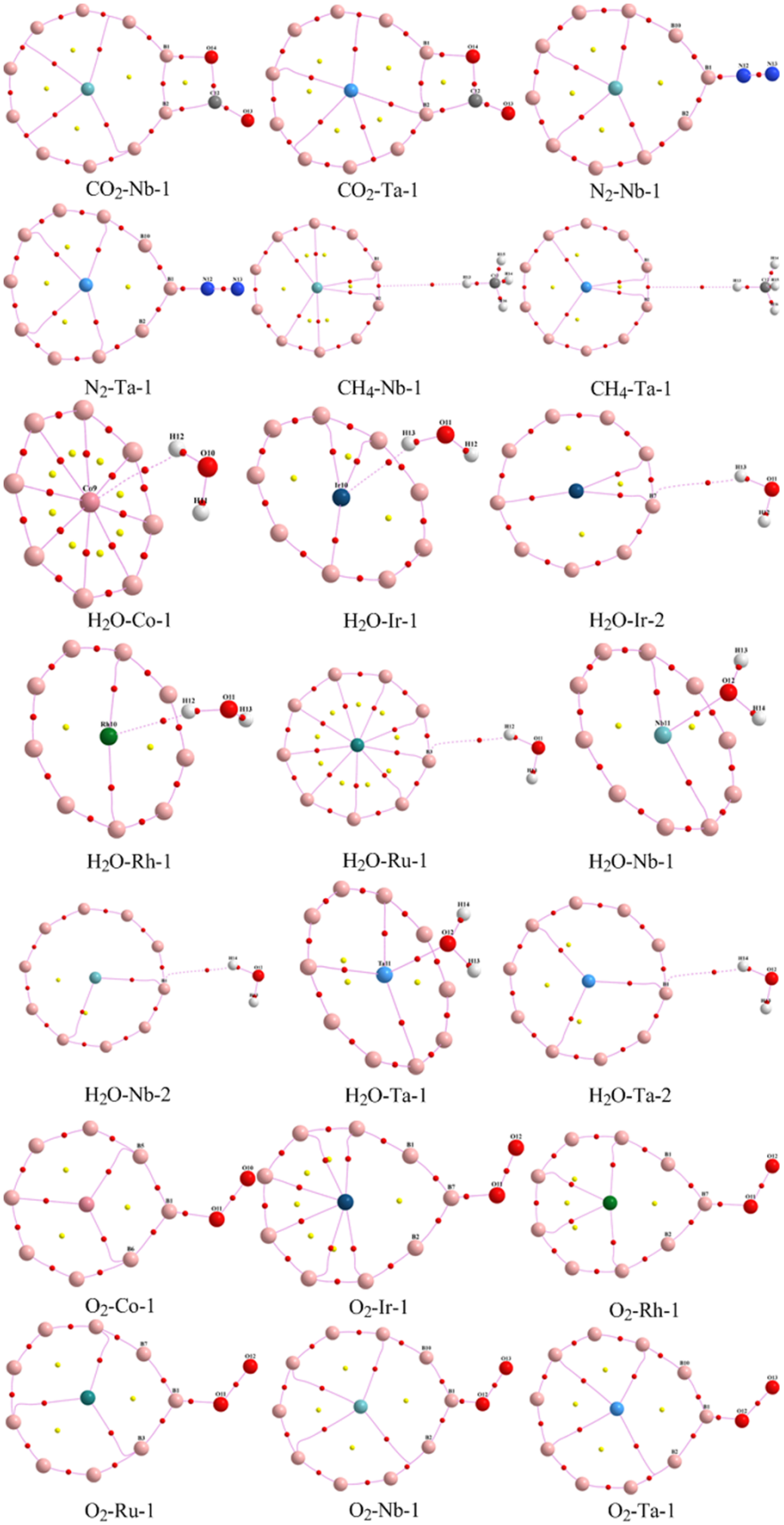

Fig. S5 The molecular graphs of the formed complexes of boron clusters with the CO_2, N_2, CH_4, H_2O, and O_2 gas molecules, where the BCP and RCP are denoted as small red and yellow dots, respectively. Only the formed singlet and doublet complexes involving O_2 have been given due to their similar geometries.

Table S1. The calculated topological parameters at the BCPs for the formed complexes of boron clusters with small gas molecules[a]

Complexes	BCP	ρ_{bcp}	$\nabla^2\rho_{bcp}$	V_{bcp}	G_{bcp}	H_{bcp}
CO-Co-2	Co9···C11	0.1382	0.4897	-0.2502	0.1863	-0.0639
CO-Ir-2	Ir10···C12	0.1894	0.4857	-0.3266	0.2240	-0.1026
CO-Ir-3	B7···O11	0.1376	0.8366	-0.3556	0.2824	-0.0732
CO-Rh-2	B7···O11	0.1322	0.7684	-0.3331	0.2626	-0.0705
CO-Ru-2	Ru10···C12	0.1506	0.5227	-0.2410	0.1858	-0.0552
CO-Nb-2	Nb11···C13	0.0844	0.2843	-0.0971	0.0841	-0.0130
CO-Nb-3	Nb11···O13	0.0342	0.2314	-0.0404	0.0491	0.0087
CO-Ta-2	Ta11···C13	0.0941	0.2607	-0.1045	0.0848	-0.0197
CO-Ta-3	Ta11···O13	0.0422	0.2588	-0.0488	0.0567	0.0080
2CO-Co-1	B2···C13	0.1718	0.4950	-0.4133	0.2685	-0.1448
2CO-Ir-1	B6···C14	0.1707	0.4833	-0.4087	0.2648	-0.1439
2CO-Rh-1	B6···C14	0.1810	0.4695	-0.4368	0.2771	-0.1597
2CO-Ru-1	B6···C14	0.1759	0.4885	-0.4243	0.2732	-0.1511
2CO-Nb-1	B6···C15	0.1749	0.5148	-0.4262	0.2775	-0.1488
2CO-Ta-1	B6···C15	0.1745	0.5138	-0.4249	0.2767	-0.1482
CO_2-Nb-1	B2···C12	0.1655	-0.1444	-0.2875	0.1257	-0.1618
	B1···O14	0.1832	0.6844	-0.4641	0.3176	-0.1465
CO_2-Ta-1	B2···C12	0.1737	-0.0795	-0.3239	0.1520	-0.1719
	B1···O14	0.1923	0.7032	-0.4943	0.3351	-0.1593
N_2-Nb-1	B1···N12	0.1520	0.8794	-0.4115	0.3157	-0.0958
N_2-Ta-1	B1···N12	0.1508	0.8734	-0.4076	0.3130	-0.0946
CH_4-Nb-1	B2···H13	0.0025	0.0055	-0.0008	0.0011	0.0003
CH_4-Ta-1	B2···H13	0.0024	0.0053	-0.0008	0.0010	0.0003
H_2O-Co-1	Co9···H12	0.0099	0.0180	-0.0059	0.0052	-0.0007
H_2O-Ir-1	Ir10···H13	0.0119	0.0268	-0.0053	0.0060	0.0007
H_2O-Ir-2	B7···H13	0.0111	0.0240	-0.0042	0.0051	0.0009
H_2O-Rh-1	Rh10···H12	0.0094	0.0212	-0.0042	0.0047	0.0006
H_2O-Ru-1	B3···H12	0.0114	0.0242	-0.0043	0.0052	0.0009
H_2O-Nb-1	Nb11···O12	0.0483	0.2468	-0.0509	0.0563	0.0054
H_2O-Nb-2	B1···H14	0.0119	0.0251	-0.0045	0.0054	0.0009
H_2O-Ta-1	Ta11···O12	0.0556	0.2540	-0.0568	0.0601	0.0034
H_2O-Ta-2	B1···H14	0.0117	0.0251	-0.0045	0.0054	0.0009
O1-Co-1	B1···O11	0.2036	1.0268	-0.5751	0.4159	-0.1592
		0.1608	*0.6725*	*-0.3954*	*0.2817*	*-0.1136*
O1-Ir-1	B7···O11	0.1693	0.7411	-0.4291	0.3072	-0.1219
		0.1718	*0.7532*	*-0.4377*	*0.3130*	*-0.1247*
O1-Rh-1	B7···O11	0.1721	0.7611	-0.4403	0.3153	-0.1250
		0.1755	*0.7714*	*-0.4517*	*0.3223*	*-0.1294*
O1-Ru-1	B1···O11	0.1936	0.9940	-0.5384	0.3935	-0.1449
		0.1719	*0.7637*	*-0.4401*	*0.3155*	*-0.1246*
O1-Nb-1	B1···O12	0.1914	0.9906	-0.5315	0.3896	-0.1419
O1-Ta-1	B1···O12	0.1903	0.9825	-0.5271	0.3864	-0.1407
		0.1725	*0.7605*	*-0.4416*	*0.3159*	*-0.1257*

[a] The data with italics refer to the results of the triplet and quartet complexes involving O_2. The ρ_{bcp}, $\nabla^2\rho_{bcp}$, V_{bcp}, G_{bcp}, and H_{bcp} is electron density, the Laplacian of the electron density, potential energy density, kinetic energy density, and energy density at the BCP, respectively.

Table S2. The calculated adsorption energies and thermodynamic parameters for the CO, CO_2, N_2, CH_4, H_2O, and O_2 adsorption on the boron clusters[a]

Complexes	ΔE_{ads}	ΔH	ΔG
CO-Co-2	14.16	10.40	18.42
CO-Ir-2	12.78	4.33	15.53
CO-Ir-3	25.43	22.97	35.68
CO-Rh-2	26.09	24.00	35.75
CO-Ru-2	9.66	7.56	15.77
CO-Nb-2	-30.48	-32.81	-23.15
CO-Nb-3	-4.47	-6.26	2.68
CO-Ta-2	-36.84	-39.76	-30.16
CO-Ta-3	-5.93	-8.44	0.81
2CO-Co-1	-25.13	-26.98	-16.80
2CO-Ir-1	-26.58	-28.35	-18.16
2CO-Rh-1	-34.40	-35.95	-27.08
2CO-Ru-1	-30.80	-32.58	-22.63
2CO-Nb-1	-30.81	-32.66	-22.05
2CO-Ta-1	-30.23	-32.11	-21.44
CO_2-Nb-1	-11.86	-14.34	-5.71
CO_2-Ta-1	-11.50	-14.30	-3.97
N_2-Nb-1	4.39	2.28	12.12
N_2-Ta-1	4.60	2.44	12.32
CH_4-Nb-1	0.09	0.68	1.59
CH_4-Ta-1	0.04	0.68	1.46
H_2O-Co-1	-4.00	-5.40	-1.19
H_2O-Ir-1	-4.82	-5.97	1.55
H_2O-Ir-2	-4.66	-5.36	1.75
H_2O-Rh-1	-4.55	-5.33	1.46
H_2O-Ru-1	-5.13	-5.66	-0.31
H_2O-Nb-1	-16.85	-19.34	-10.45
H_2O-Nb-2	-5.20	-5.82	-0.08
H_2O-Ta-1	-20.45	-23.50	-14.74
H_2O-Ta-2	-5.24	-5.80	-0.10
O_2-Co-1	-17.48/-17.64	-19.73/-19.85	-10.66/-11.04
O_2-Ir-1	-42.32/-5.85	-45.20/-8.42	-31.55/4.13
O_2-Rh-1	-41.43/-14.18	-44.03/-16.40	-31.28/-5.27
O_2-Ru-1	-11.08/-22.29	-13.29/-24.45	-3.27/-14.90
O_2-Nb-1	-9.65	-11.85	-1.78
O_2-Ta-1	-9.06/-14.68	-11.33/-16.65	-1.24/-7.70

[a] All the energy units are in kcal/mol. The data behind the slash refer to the results of the triplet and quartet complexes involving O_2.