Supplementary Material for:

Structures of isolated $Co_2(alcohol)_1$ cluster anions

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1) Calculated frequencies of the cobalt/alcohol cluster anions

The frequencies (freq) are given in cm^{-1}, the intensities in km/mol

$[Co_2MeOH_1]^-$		$[Co_2EtOH_1]^-$	
freq (cm^{-1})	**inten.**	**freq (cm^{-1})**	**inten.**
28.9	1.68	21.8	0.91
61.7	0.19	40.0	0.53
76.5	1.41	62.7	1.99
126.4	2.17	75.8	0.06
132.9	0.92	91.7	0.10
341.1	0.03	259.9	0.30
775.8	2.98	341.0	0.00
1002.8	69.09	416.1	3.62
1077.3	4.22	786.9	1.06
1136.2	0.11	865.0	12.47
1374.3	0.88	890.2	9.37
1434.0	3.55	999.0	54.60
1461.6	1.20	1075.9	41.32
1473.1	12.28	1151.0	0.29
2872.9	96.26	1273.9	5.54
2904.3	54.45	1287.9	1.46
2966.4	132.21	1356.2	0.59
3258.1	555.47	1415.9	23.49
		1442.4	4.73
		1467.3	3.13
		1492.8	3.18
		2871.2	40.91
		2890.9	27.04
		2939.8	75.85
		2997.6	55.16
		3006.0	43.08
		3247.1	756.17

[anti-$Co_2PropOH_1$]$^-$		[gauche-$Co_2PropOH_1$]$^-$	
freq (cm^{-1})	**inten.**	**freq (cm^{-1})**	**inten.**
17.5	0.52	15.8	0.44
33.3	0.07	25.2	0.49
48.0	1.72	41.7	0.16
68.9	0.09	60.0	2.08
81.1	0.46	84.7	0.67
127.8	1.06	154.7	1.48
221.2	0.02	192.8	0.57
280.8	1.26	222.6	2.35
341.0	0.00	316.7	0.53
447.2	4.39	431.6	15.81
751.2	0.16	474.0	2.69
855.6	5.84	755.4	0.52
866.8	3.80	830.3	1.76
991.1	34.72	898.1	2.15
1017.3	63.74	945.8	58.60
1033.1	6.83	1024.9	31.86
1075.2	13.22	1085.0	13.62
1154.9	0.02	1131.8	0.86
1237.6	0.08	1224.0	1.20
1256.2	3.55	1239.3	0.60
1313.1	0.39	1293.8	4.48
1351.7	4.00	1333.9	6.17
1367.6	1.88	1360.8	7.09
1417.2	12.86	1411.4	14.31
1459.0	0.64	1439.9	2.85
1463.5	5.84	1456.3	5.34
1473.3	1.72	1477.6	6.17
1490.3	6.42	1485.2	6.57
2861.4	41.90	2859.1	39.88
2885.5	20.58	2889.4	20.44
2938.1	53.18	2924.8	73.91
2940.2	39.08	2938.8	61.55
2965.0	8.15	2955.4	44.23
2992.1	77.54	2986.9	79.99
2996.5	71.90	3030.7	32.33
3243.8	804.73	3214.1	942.60

2) Binding energies, electron affinities and selected bond parameters

The experimentally observed electron affinity (EA) of Co_2 is 63.87 kJ mol^{-1} (D.G. Leopold, W.C. Lineberger, *J. Chem. Phys.*, 1986, **85**, 51). The calculated value at the DFT (BLYP/ 6-311+G(d)) is 76 kJ/mol, i.e. the value is overestimated by about 12 kJ/mol. This "correction term" has also been taken into account for the clusters of Co_2 with methanol, ethanol and propanol leading to an estimate for the electron affinities of the neutral clusters. (The geometries of the clusters are calculated with the 6-311+G(d) basis set for Co and the 6-311G(d,p) basis set for the alcohol; the binding energies are ZPE corrected.)
The calculated EAs and "corrected" EAs of the neutral clusters, the calculated binding energies and the Co-Co distances of neutral and anionic species as well as the Co-O distances of the neutral clusters are given in the following table:

	EA/kJ mol^{-1}	EA/kJ mol^{-1} corr.	ΔE/kJ mol^{-1}	d(Co-Co)/Å	d(Co-O)/Å
Co_2	76	64			
Co_2MeOH_1	50	38	63	2.024	2.125
Co_2EtOH_1	49	37	64	2.020	2.118
anti-$Co_2PropOH_1$	48	36	64	2.020	2.117
gauche-$Co_2PropOH_1$	57	45	62	2.018	2.112
$[Co_2MeOH_1]^-$	-	-	37	2.049	-
$[Co_2EtOH_1]^-$	-	-	37	2.049	-
anti-$[Co_2PropOH_1]^-$	-	-	36	2.049	-
gauche-$[Co_2PropOH_1]^-$	-	-	43	2.132	-

3) Cartesian coordinates of all calculated cluster species (neutral and anions)

Co_2MeOH_1 coordinates

Atomic number	X	Y	Z
27	0.000000	0.000000	0.000000
27	0.000000	0.000000	2.023623
8	1.062695	0.000000	3.864265
1	1.838176	0.575812	3.726885
6	1.494388	-1.211784	4.595904
1	2.055647	-0.883423	5.483652
1	2.159008	-1.801420	3.946484
1	0.599048	-1.784220	4.881883

Co_2EtOH_1 coordinates

Atomic number	X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.528025
8	1.364266	0.000000	2.091199
27	2.637462	1.685042	2.250528
27	3.900743	3.255066	2.109126
1	1.838300	-0.791644	1.774666
1	-0.533127	-0.870671	1.939188
1	-0.457355	0.909424	1.933622
1	-1.035250	0.026404	-0.372916
1	0.533990	0.876329	-0.390926
1	0.475053	-0.907998	-0.402095

anti-$Co_2PropOH_1$ coordinates

Atomic number	X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.528571
8	1.365367	0.000000	2.093259
27	2.757190	1.599450	1.976250
27	4.207912	2.927371	1.502650
1	1.824269	-0.814804	1.813028
1	-0.535713	-0.868697	1.938396
1	-0.458658	0.909398	1.932693
6	-1.366420	0.054451	-0.482111
1	0.546610	0.869685	-0.388453
1	0.462295	-0.914594	-0.401983
1	-1.367393	0.054490	-1.571111
1	-1.914453	-0.813581	-0.118652
1	-1.843643	0.963339	-0.118652

gauche-$Co_2PropOH_1$ coordinates

Atomic number	X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.541992
6	1.393716	0.000000	2.182706
8	2.157507	-1.231122	1.903720
27	3.535280	-1.685536	0.368891
27	4.664005	-2.258809	-1.202774
1	1.662544	-1.999254	2.243316
1	1.331651	0.115768	3.275610
1	2.022919	0.804613	1.782716
1	-0.525222	0.894620	1.918194
1	-0.570639	-0.864363	1.925646
1	-1.028053	-0.012471	-0.388477
1	0.498284	0.897893	-0.394412
1	0.526599	-0.875265	-0.404964

$[Co_2MeOH_1]^-$ coordinates

Atomic number	X	Y	Z
6	0.000000	0.000000	0.000000
1	0.000000	0.000000	1.107177
1	1.047033	0.000000	-0.343214
1	-0.473139	0.942839	-0.336210
8	-0.624542	-1.160695	-0.553443
1	-1.568696	-1.160499	-0.243800
27	-3.496850	-1.458395	1.462809
27	-4.039191	-0.377847	-0.191657

$[Co_2EtOH_1]^-$ coordinates

Atomic number	X	Y	Z
6	0.000000	0.000000	0.000000
1	0.000000	0.000000	1.107731
1	1.060166	0.000000	-0.321117
8	-0.698206	1.136915	-0.518049
1	-0.236570	1.945023	-0.175528
27	1.787231	3.649246	0.047675
27	0.563723	3.649246	1.696668
6	-0.703911	-1.257409	-0.522282
1	-0.694036	-1.270682	-1.622798
1	-0.209771	-2.171808	-0.155644
1	-1.754308	-1.270682	-0.193806

anti-$[Co_2PropOH_1]^-$ coordinates

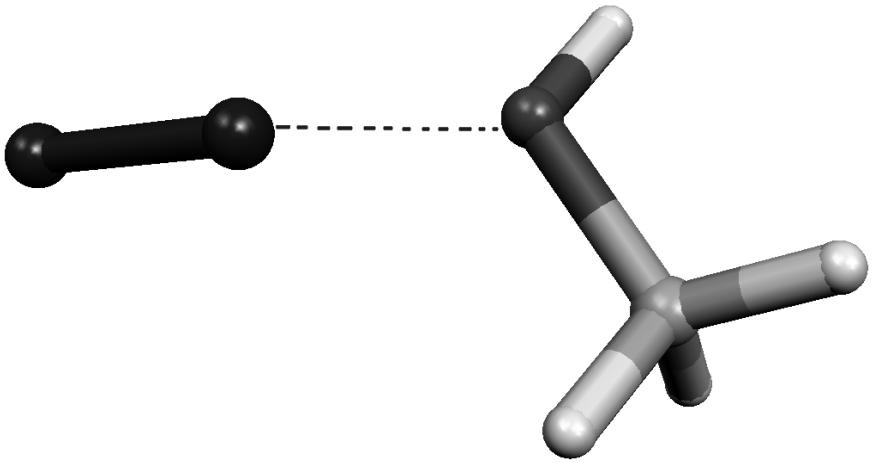
Atomic number	X	Y	Z
6	0.000000	0.000000	0.000000
1	0.000000	0.000000	1.108781
1	1.061324	0.000000	-0.320915
8	-0.699105	1.134772	-0.518975
1	-0.238617	1.944260	-0.177136
27	1.762196	3.665989	0.029480
27	0.538251	3.665989	1.678240
6	-0.699494	-1.264773	-0.519264
1	-0.702285	-1.229206	-1.621199
1	-1.755073	-1.229206	-0.203002
6	-0.041100	-2.571363	-0.030510
1	-0.048869	-2.635284	1.069165
1	-0.565527	-3.458049	-0.419815
1	1.009260	-2.635284	-0.356226

gauche-$[Co_2PropOH_1]^-$ coordinates

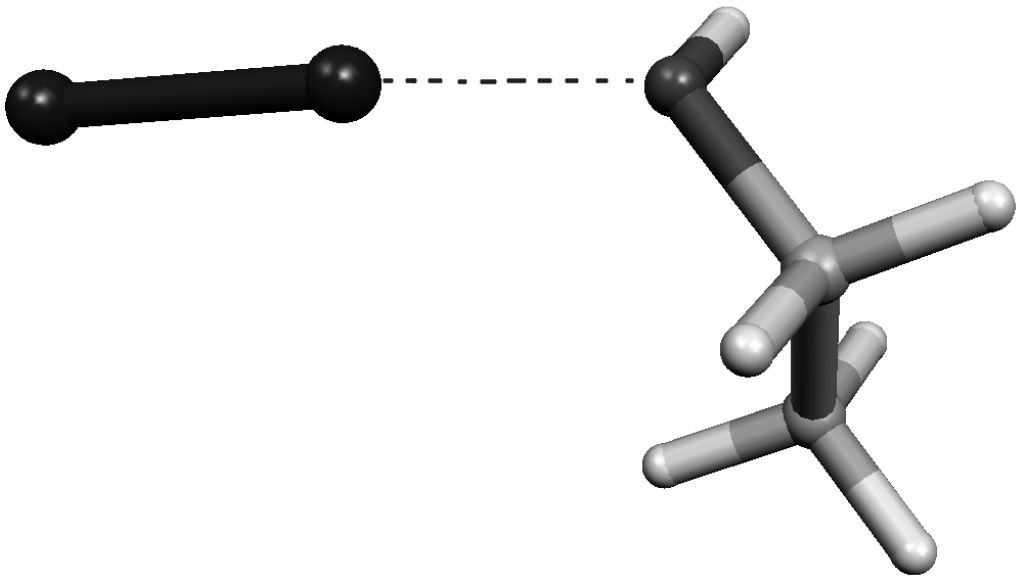
Atomic number	X	Y	Z
6	0.000000	0.000000	0.000000
1	0.000000	0.000000	1.108259
1	1.059345	0.000000	-0.324444
8	-0.695421	1.140111	-0.517119
1	-0.146608	1.940984	-0.311250
6	-0.704852	-1.266438	-0.513090
1	-1.753296	-1.238233	-0.170391
1	-0.236844	-2.147545	-0.038975
6	-0.667769	-1.405873	-2.049449
1	-1.235418	-2.285904	-2.392604
1	-1.093830	-0.507918	-2.515043
1	0.368148	-1.508475	-2.410247
27	1.987542	3.479463	-0.492063
27	0.938047	3.793244	1.245026

4) Geometries of the neutral species (Figures, for coordinates see above)

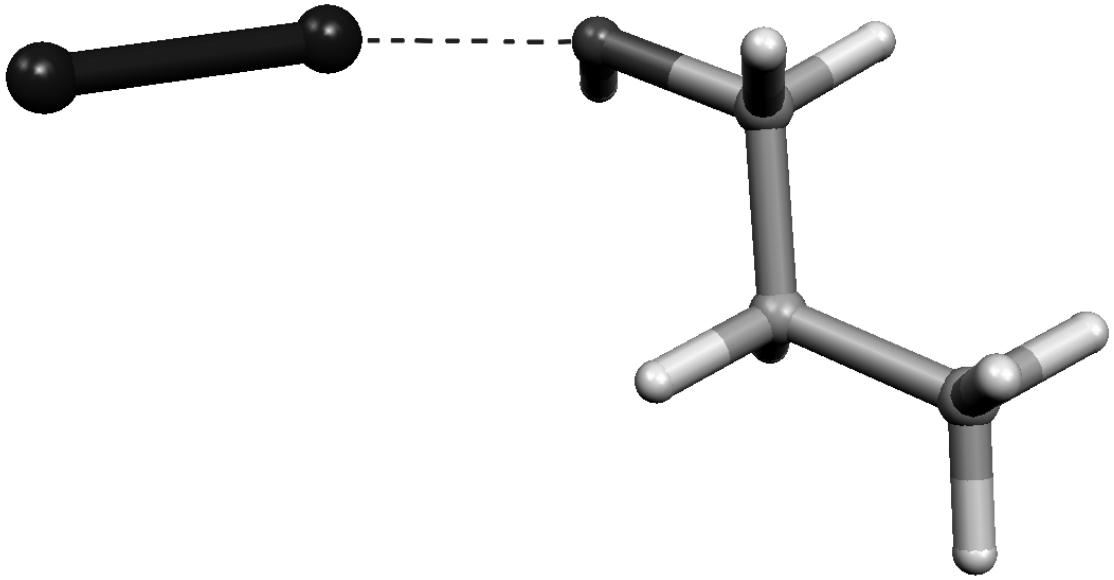
Co_2MeOH_1



Co_2EtOH_1



anti-$Co_2PropOH_1$



gauche-$Co_2PropOH_1$