Electronic Supplementary Material for PCCP

Supporting Information

Crystal Structure Information for the Methylcobalt Complexes

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Experimental

Structures for *trans*-$[Co(en)_2(CH_3)(NO_2)]ClO_4$, **1**, *trans*-$[Co(en)_2(CH_3)(N_3)]PF_6$, **2**, *trans*-$[Co(cyclam)(CH_3)(CN)]ClO_4$ (cyclam = 1,4,8,11-tetraazacyclotetradecane), **3,** and *trans*-$[Co(tn)_2(CH_3)(N_3)]ClO_4$ (tn = 1,3-propanediamine), **4**, have been determined using low-temperature X-ray diffraction. The compounds were prepared as previously described.[1,2] Dimensions of the crystals used for the measurements were approximately 40 × 25 × 15 mm.

Table S1. X-ray data for Complexes **1** to **4**.

Complex:	**1**	**2**	**3**	**4**
Space Group	$P2_1/n$	$P2_1/c$	*Pbca*	*Cc*
a/Å	7.995(2)	9.268(5)	13.462(1)	13.538(4)
b/Å	15.676(3)	11.151(8)	10.995(5)	8.522(6)
c/Å	10.8310(19)	15.227(6)	23.182(2)	12.721(1)
α/°	90.00	90.00	90.00	90.00
β/°	110.04(2)	117.61(6)	90.00	101.45(1)
γ/°	90.00	90.00	90.00	90.00
Z	4	4	8	4
cell volume/Å^3	1275.3(5)	1394.5(16)	3431.3(16)	1438.4(10)
R factor/%	2.73	4.67	4.29	1.91

Table S2. Selected Bond Distances (Å) and Angles (°) for the Cations of Complexes **1** to **4**.

Complex **1**			
Co1–C14	1.9894(11)	Co1–N9	2.0439(10)
Co1–N10	1.9526(9)	N9–O7	1.2559(11)
Co1–N11	1.9612(9)	N9–O8	1.2416(12)
Co1–N12	1.9678(10)	Co1–N13	1.9517(9)
C14–Co1–N9	179.00(4)	O7–N9–O8	117.89(9)
Complex **2**			
Co1–C16	1.973(3)	Co1–N9	2.096(2)
Co1–N12	1.970(2)	N9–N10	1.184(3)
Co1–N13	1.957(2)	N10–N11	1.172(4)
Co1–N14	1.959(2)	Co1–N15	1.961(2)
Co1–N9–N10	129.7(2)	N9–N10–N11	177.4(3)
Complex **3**			
Co1–C12	1.994(2)	Co1–C13	1.998(2)
Co1–N8	1.988(2)	C13–N7	1.151(3)
Co1–N9	1.985(2)	Co1–N10	1.979(2)
Co1–N11	1.983(2)		
C12–Co1–C13	177.3(1)	Co1–C13–N7	177.9(2)
Complex **4**			
Co1–C14	1.981(3)	Co1–N7	2.112(2)
Co1–N10	2.004(2)	N7–N8	1.213(3)
Co1–N11	1.979(2)	N8–N9	1.158(2)
Co1–N12	1.971(2)	Co1–N13	1.985(2)
Co1–N7–N8	119.6(2)	N7–N8–N9	179.5(2)

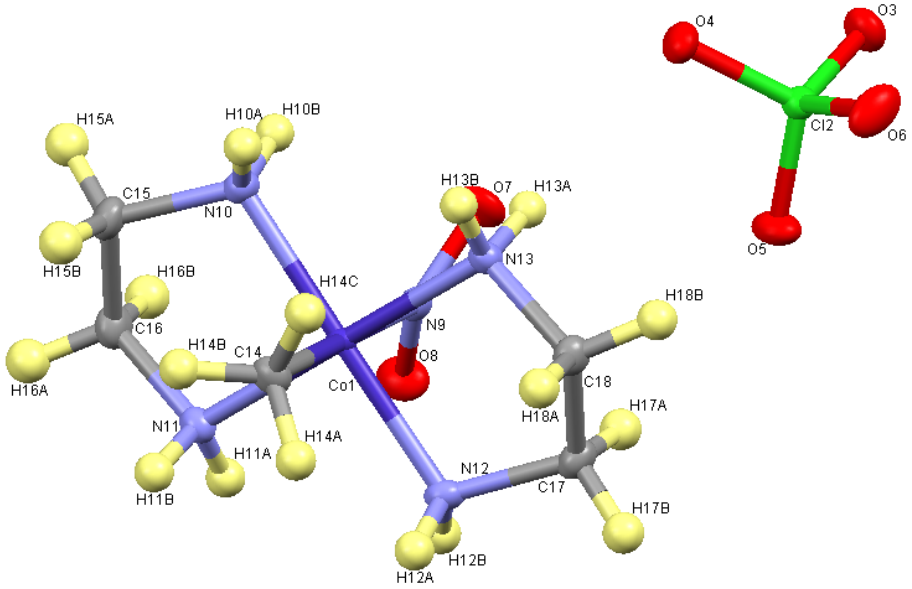

Fig. S1. Structure and labelling, with 50 % probability ellipsoids for non-hydrogen atoms, for Complex **1**.

Table S3. Atomic Positions, in Cartesian Coordinates (Å), for Complex **1**.

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Co1	1.2505	13.52	2.2152	C15	-0.4125	15.5351	3.2854
O7	0.3486	13.7966	-0.5161	H15A	-0.9793	16.3187	3.075
O8	-0.7739	12.3096	0.5355	H15B	-0.0085	15.6697	4.179
N9	0.1168	13.1743	0.5499	C16	-1.2401	14.2725	3.2707
N10	0.6514	15.378	2.2578	H16A	-1.855	14.2589	4.0467
H10A	1.3607	15.9284	2.4573	H16B	-1.7798	14.2275	2.4421
H10B	0.3241	15.618	1.4327	C17	2.8401	11.5125	1.0465
N11	-0.3073	13.1178	3.3367	H17A	2.405	11.4435	0.1598
H11A	-0.7258	12.3574	3.0332	H17B	3.3878	10.7004	1.1915
H11B	-0.0417	12.9766	4.2064	C18	3.7082	12.7454	1.1072
N12	1.8115	11.6366	2.1156	H18A	4.2427	12.7509	1.9404
H12A	2.1621	11.3682	2.9233	H18B	4.3259	12.7712	0.3337
H12B	1.0885	11.1017	1.9211	Cl2	3.8617	13.9213	-2.5818
N13	2.7856	13.9085	1.0745	O3	3.4078	14.1399	-3.9278
H13A	2.5052	14.0629	0.2116	O4	3.4663	15.0436	-1.7573
H13B	3.2187	14.6618	1.3767	O5	3.278	12.7148	-2.0561
C14	2.3794	13.8687	3.8158	O6	5.2991	13.804	-2.5553
H14A	2.736	13.0221	4.1556				
H14B	1.8373	14.2965	4.5107				
H14C	3.1216	14.4595	3.5695				

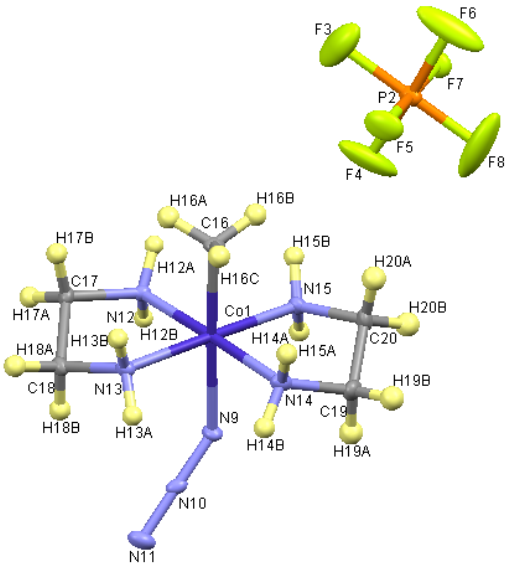

Fig. S2. Structure and labelling, with 50 % probability ellipsoids for non-hydrogen atoms, for Complex **2**.

Table S4. Atomic Positions, in Cartesian Coordinates (Å), for Complex **2**.

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Co1	2.3195	7.7049	1.7306	C17	3.799	7.6317	4.1572
N9	2.3905	5.6346	1.4135	H17A	3.9665	7.111	4.9816
N10	3.3223	4.931	1.2144	H17B	3.9339	8.5918	4.3582
N11	4.2167	4.1939	1.039	C18	4.7511	7.1924	3.0616
N12	2.4083	7.3976	3.6743	H18A	5.6714	7.4935	3.2653
H12A	1.8304	7.9685	4.1059	H18B	4.7514	6.2044	2.9846
H12B	2.155	6.5345	3.8644	C19	0.9023	7.4433	-0.6814
N13	4.2724	7.8102	1.7936	H19A	0.894	6.4542	-0.7259
H13A	4.633	7.3652	1.074	H19B	0.7045	7.8012	-1.5827
H13B	4.5396	8.6889	1.7541	C20	-0.1244	7.9373	0.3211
N14	2.2208	7.9272	-0.2129	H20A	-0.2185	8.9219	0.2618
H14A	2.3257	8.8138	-0.4331	H20B	-1.0062	7.5247	0.143
H14B	2.8932	7.4466	-0.618	P2	-2.4509	10.8493	2.2297
N15	0.3663	7.5459	1.6688	F3	-1.8524	11.3696	3.6215
H15A	0.1187	6.6783	1.8499	F4	-1.794	9.4427	2.5245
H15B	-0.0102	8.0912	2.3073	F5	-1.1682	11.3305	1.4166
C16	2.1982	9.6545	2.001	F6	-3.1201	12.2728	2.0442
H16A	2.6025	9.8909	2.8619	F7	-3.7584	10.3907	3.0536
H16B	1.2568	9.9277	1.997	F8	-3.0742	10.2991	0.9233
H16C	2.674	10.1151	1.2791				

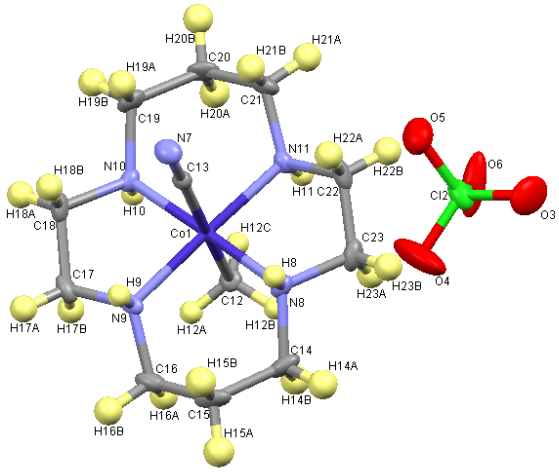

Fig. S3. Structure and labelling, with 50 % probability ellipsoids for non-hydrogen atoms, for Complex **3**.

Table S5. Atomic Positions, in Cartesian Coordinates (Å), for Complex **3**.

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Co1	6.8003	1.7486	14.4255	H17A	8.1014	3.249	11.3151
N7	5.0386	-0.1297	12.6159	H17B	8.2697	3.9868	12.7316
N8	7.7553	0.1353	15.0862	C18	6.3016	3.5085	12.3027
H8	7.4781	-0.5618	14.5374	H18A	6.0916	4.4211	11.9828
N9	8.0523	1.9604	12.9003	H18B	5.8277	2.8565	11.7278
H9	7.7958	1.3194	12.2772	C19	4.4088	3.4161	13.8406
N10	5.8779	3.3506	13.7191	H19A	4.0036	2.7202	13.2647
H10	6.2181	4.0813	14.1827	H19B	4.0951	4.2979	13.5174
N11	5.578	1.4843	15.9647	C20	3.943	3.2149	15.2735
H11	5.8937	2.0264	16.6516	H20A	4.4317	3.8461	15.8588
C12	7.8598	2.9752	15.5857	H20B	2.9805	3.4381	15.3303
H12A	8.4555	3.5195	15.0289	C21	4.1476	1.8131	15.7897
H12B	8.3936	2.4486	16.2158	H21A	3.6845	1.7163	16.6586
H12C	7.252	3.5624	16.0814	H21B	3.7424	1.171	15.1541
C13	5.6612	0.5717	13.2837	C22	5.7577	0.0781	16.4159
C14	9.2363	0.1012	15.0606	H22A	5.304	-0.5432	15.7939
H14A	9.5499	-0.7828	15.3789	H22B	5.374	-0.0451	17.3193
H14B	9.5917	0.7905	15.6757	C23	7.2439	-0.1924	16.4349
C15	9.7694	0.3496	13.6632	H23A	7.6881	0.3705	17.1176
H15A	10.7481	0.1946	13.6658	H23B	7.4189	-1.1435	16.647
H15B	9.3642	-0.3112	13.0468	Cl2	6.5003	1.8418	19.9041
C16	9.5042	1.7339	13.1268	O3	6.4968	0.6454	20.683
H16A	9.8448	2.4057	13.7701	O4	7.6181	1.9846	19.07
H16B	9.9915	1.8538	12.2726	O5	5.3471	1.8834	19.0568
C17	7.7891	3.2644	12.2533	O6	6.447	2.9467	20.8021

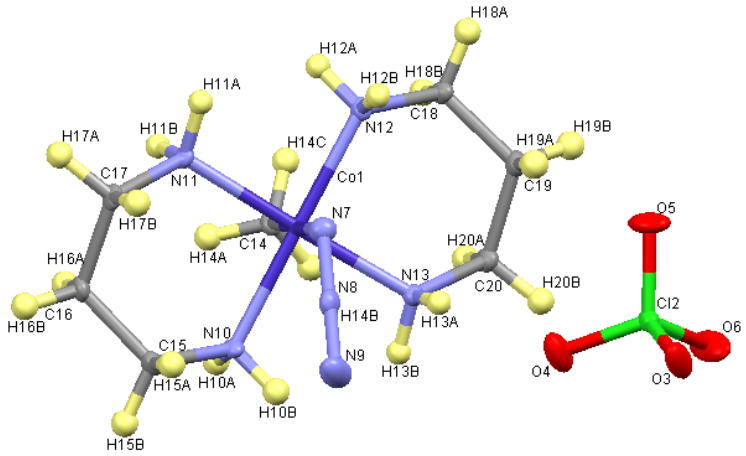

Fig. S4. Structure and labelling, with 50 % probability ellipsoids for non-hydrogen atoms, for Complex **4**.

Table S6. Atomic Positions, in Cartesian Coordinates (Å), for Complex **4**.

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Co1	0.3758	0.0051	7.4406	H15A	3.4536	0.3213	8.5754
N7	1.9546	-0.1287	6.0444	H15B	3.1587	0.2148	10.1451
N8	2.9149	-0.8283	6.29	C16	2.4075	1.9515	9.3051
N9	3.8312	-1.4922	6.5339	H16A	1.6718	2.0896	9.9531
N10	1.585	-0.3809	8.9916	H16B	3.19	2.4671	9.6227
H10A	1.0621	-0.3767	9.7486	C17	1.983	2.4808	7.9611
H10B	1.8934	-1.2417	8.8858	H17A	1.9475	3.4702	7.9969
N11	0.6569	1.9609	7.55	H17B	2.6568	2.2259	7.2825
H11A	0.466	2.3146	6.7227	C18	-2.0212	-0.4653	5.6276
H11B	0.0332	2.2975	8.1378	H18A	-2.4158	-0.1713	4.7689
N12	-0.8312	0.3741	5.927	H18B	-2.6992	-0.3272	6.3349
H12A	-1.1361	1.2357	6.0369	C19	-1.6912	-1.9405	5.5405
H12B	-0.3103	0.375	5.1679	H19A	-0.9989	-2.0726	4.845
N13	0.1224	-1.9532	7.2413	H19B	-2.5008	-2.433	5.2552
H13A	0.7361	-2.2404	6.6192	C20	-1.1903	-2.5344	6.8547
H13B	0.3597	-2.3367	8.043	H20A	-1.8512	-2.3563	7.5692
C14	-1.1153	0.1738	8.735	H20B	-1.0995	-3.5153	6.7588
H14A	-0.8411	0.7568	9.4731	Cl2	1.062	-4.6529	4.2371
H14B	-1.3447	-0.7124	9.0853	O3	2.2297	-5.2521	3.6093
H14C	-1.8947	0.5599	8.2849	O4	1.4849	-3.9517	5.4098
C15	2.7683	0.4747	9.2727	O5	0.4629	-3.7531	3.2956
				O6	0.1202	-5.6774	4.5738

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References

1. Kofod, P.; Harris, P.; Larsen, S. *Inorg. Chem*. **1997**, *36,* 2258-2266.

2. Kofod, P.; Harris, P. *Inorg Chem.* **2004**, *43*, 2680-2688.