Supplementary Information

Table 1 Fractional atomic coordinates of $[Co(C_2H_8N_2)_2(NH_3)Br]Br_2$ in the crystal structure of phase III of **2**, determined directly from powder XRD data of the reaction product [$P2_1/n$; *a*= 7.6704(5) Å, *b* = 12.4028(7) Å, *c* = 13.9885(10) Å, β = 98.726(6)°].

Atom	x	y	z
Co1	–0.04164(8)	0.27753(7)	0.42615(5)
Br2	0.1318(19)	0.3690(11)	0.5598(8)
Br3	0.7065(22)	–0.0493(12)	0.3805(11)
Br4	0.0834(21)	–0.1812(12)	0.2315(12)
N5	0.01590(5)	0.394935(26)	0.340631(25)
N6	–0.14014(5)	0.164323(28)	0.503681(33)
N7	–0.25269(5)	0.362414(29)	0.445997(35)
N8	0.16337(6)	0.190840(39)	0.404806(35)
N9	–0.16655(5)	0.202645(38)	0.310893(27)
C10	–0.27663(5)	0.214545(31)	0.554991(29)
C11	–0.37884(4)	0.293820(31)	0.487726(30)
C12	0.10506(6)	0.101765(30)	0.336340(27)
C13	–0.03819(5)	0.147489(34)	0.261117(25)
H14	–0.04621	0.38363	0.27649
H15	–0.01872	0.46282	0.36486
H16	0.14056	0.39538	0.33899
H17	–0.04755	0.1346	0.55007
H18	–0.19288	0.10826	0.46161
H19	–0.30848	0.39045	0.38497
H20	–0.21705	0.42118	0.48918
H21	0.1883	0.1626	0.46877
H22	0.26929	0.22408	0.38757
H23	–0.23063	0.2543	0.26811
H24	–0.24716	0.15088	0.33056
H25	–0.22057	0.25104	0.61197
H26	–0.35456	0.15988	0.57258
H27	–0.45186	0.25629	0.43738
H28	–0.4501	0.33738	0.52254
H29	0.05929	0.0437	0.37015
H30	0.20195	0.07696	0.30587
H31	0.01229	0.19771	0.22072
H32	–0.09497	0.0901	0.22216