Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for

Ethylenediamine complexes of the beryllium halides and pseudo-halides

Magnus R. Buchner* and Matthias Müller

Philipps-Universität Marburg, Germany

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1 X-ray Crystallographic Details

Table S1 Crystal data and details of the structure determination of $BeF_2(en)$, $[Be(en)_3]Cl_2$ and $[Be(en)_3]Br_2$.

	$BeF_2(en)$	$[Be(en)_3]Cl_2$	$[Be(en)_3]Br_2$
Empirical formula	$BeF_2(C_2H_8N_2)$	$[Be(C_2H_8N_2)_2]Cl_2$	$[Be(C_2H_8N_2)_2]Br_2$
Relative molecular mass	107.12	260.22	349.14
Crystal system	monoclinic	triclinic	triclinic
Space group (No.)	$C2/c$ (15)	$P\bar{1}$ (2)	$P\bar{1}$ (2)
Radiation / Å	1.54178	1.54178	1.54178
a / Å	8.7146(4)	7.3971(2)	7.5193(3)
b / Å	6.1071(3)	7.4939(2)	7.6801(4)
c / Å	8.9467(5)	12.4382(3)	12.6503(5)
α / deg	—	101.461(2)	79.817(4)
β / deg	93.483(4)	97.088(2)	83.317(3)
γ / deg	—	90.561(2)	89.851(4)
V / Å^3	475.27(4)	670.16(3)	714.03(6)
T / K	100(2)	100(2)	100(2)
Z	4	2	2
$F(000)$ / e	224	280	352
$d_{calc.}$ / g cm^{-1}	1.50	1.29	1.62
μ / mm^{-1}	1.3	4.2	7.1
ϑ / deg	8.872–78.274	3.656–77.319	3.575–76.561
Range of Miller indices	$-10 \leq h \leq 10$	$-9 \leq h \leq 7$	$-9 \leq h \leq 9$
	$-7 \leq k \leq 5$	$-9 \leq k \leq 8$	$-9 \leq k \leq 6$
	$-10 \leq l \leq 11$	$-15 \leq l \leq 15$	$-15 \leq l \leq 15$
Reflections collected / unique	2315 / 504	11859 / 2791	7894 / 2883
Restraints / parameters	0 / 49	0 / 233	0 / 153
R_{int}	0.0099	0.0351	0.0151
R_1 ($I > 2\sigma(I)$)	0.0330	0.0358	0.0215
R_1 (all data)	0.0357	0.0389	0.0238
wR_2 ($I > 2\sigma(I)$)	0.0846	0.0932	0.0543
wR_2 (all data)	0.0864	0.0960	0.0556
S	1.134	1.071	1.067
$\Delta\rho_{min,\,max}$ / e Å^{-3}	−0.27, 0.23	−0.48, 0.45	−0.53, 0.51

Table S2 Crystal data and details of the structure determination of $[Be(en)_2]I_2 \cdot en$ and $[Be(en)_2](N_3)_2 \cdot en$.

	$[Be(en)_2]I_2 \cdot en$	$[Be(en)_2](N_3)_2 \cdot en$
Empirical formula	$[Be(C_2H_8N_2)_2]I_2 \cdot C_2H_8N_2$	$[Be(C_2H_8N_2)_2](N_3)_2 \cdot C_2H_8N_2$
Relative molecular mass	443.12	273.38
Crystal system	monoclinic	monoclinic
Space group (No.)	$C2/c$ (15)	$C2/c$ (15)
Radiation / Å	1.54178	1.54178
a / Å	11.5044(3)	10.5030(4)
b / Å	8.39210(10)	9.3016(3)
c / Å	15.9669(4)	14.8498(6)
β / deg	100.712(2)	105.734(3)
V / Å^3	1514.68(6)	1396.39(9)
T / K	100(2)	100(2)
Z	4	4
$F(000)$ / e	848	592
$d_{calc.}$ / g cm^{-1}	1.94	1.30
μ / mm^{-1}	32.5	0.8
ϑ / deg	5.640–78.776	6.192–76.083
Range of Miller indices	$-14 \leq h \leq 13$	$-13 \leq h \leq 13$
	$-7 \leq k \leq 10$	$-10 \leq k \leq 5$
	$-20 \leq l \leq 20$	$-18 \leq l \leq 18$
Reflections collected / unique	1626 / 1578	1428 / 1250
Restraints / parameters	0 / 118	0 / 135
R_{int}	0.0463	0.0207
R_1 ($I > 2\sigma(I)$)	0.0392	0.0308
R_1 (all data)	0.0398	0.0355
wR_2 ($I > 2\sigma(I)$)	0.1152	0.0853
wR_2 (all data)	0.1165	0.0883
S	1.042	1.036
$\Delta\rho_{min,\ max}$ / e Å^{-3}	−1.67, 2.33	−0.19, 0.19

Table S3 Crystal data and details of the structure determination of $[Be(en)_2]_4(SCN)_7Cl$ and $[Be_3(OH)_3(en)_3][C_2H_9N_2](SCN)_4$.

	$[Be(en)_2]_4(SCN)_7Cl$	$[Be_3(OH)_3(en)_3][C_2H_9N_2](SCN)_4$
Empirical formula	$[Be(C_2H_8N_2)_2]_4(SCN)_7Cl$	$[Be_3(OH)_3(C_2H_8N_2)_3][C_2H_9N_2](SCN)_4$
Relative molecular mass	958.88	551.80
Crystal system	monoclinic	triclinic
Space group (No.)	$P2_1/c$ (14)	$P\bar{1}$ (2)
Radiation / Å	1.54178	1.54178
a / Å	13.9529(2)	10.5372(3)
b / Å	14.0186(3)	11.0027(3)
c / Å	48.6062(7)	13.3669(3)
α / deg	—	104.350(2)
β / deg	90.185(1)	109.886(2)
γ / deg	—	97.482(2)
V / Å^3	9507.3(3)	1372.15(7)
T / K	100(2)	100(2)
Z	8	2
$F(000)$ / e	4064	584
$d_{calc.}$ / g cm^{-1}	1.34	1.33
μ / mm^{-1}	4.0	3.5
ϑ / deg	2.727–78.499	3.703–79.056
Range of Miller indices	$-17 \leq h \leq 11$	$-12 \leq h \leq 6$
	$-17 \leq k \leq 15$	$-13 \leq k \leq 13$
	$-60 \leq l \leq 61$	$-15 \leq l \leq 16$
Reflections collected / unique	19416 / 15177	5678 / 4827
Restraints / parameters	363 / 1130	0 / 376
R_{int}	0.0317	0.0253
R_1 ($I > 2\sigma(I)$)	0.0554	0.0307
R_1 (all data)	0.0775	0.0403
wR_2 ($I > 2\sigma(I)$)	0.1331	0.0727
wR_2 (all data)	0.1498	0.0775
S	1.031	1.013
$\Delta\rho_{min,\ max}$ / e Å^{-3}	−0.79, 1.02	−0.28, 0.28

2 NMR Spectra

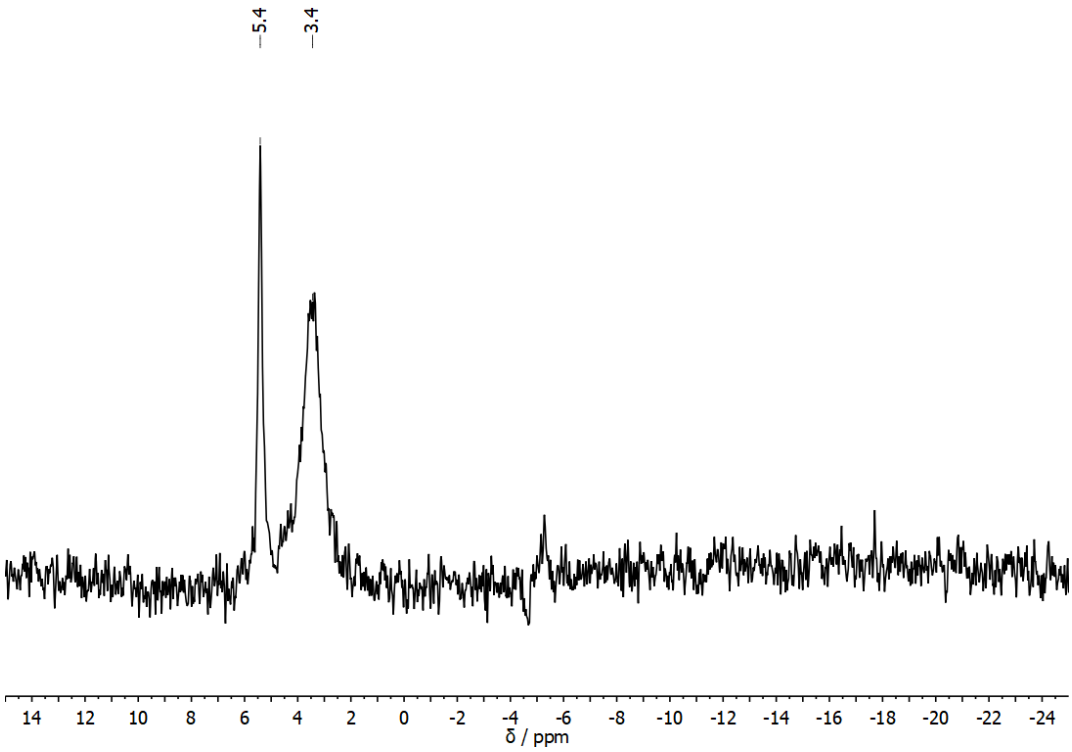

Figure S1 ^{9}Be NMR spectrum of $BeCl_2$ in ethylenediamine.

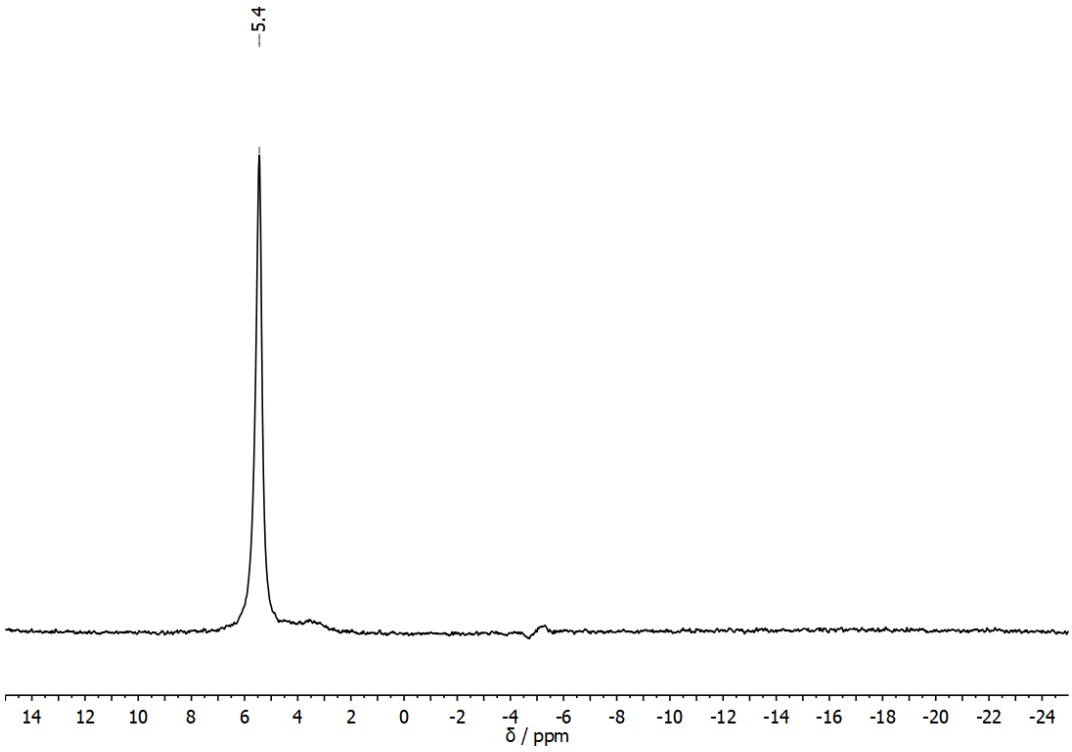

Figure S2 ^{9}Be NMR spectrum of $BeBr_2$ in ethylenediamine.

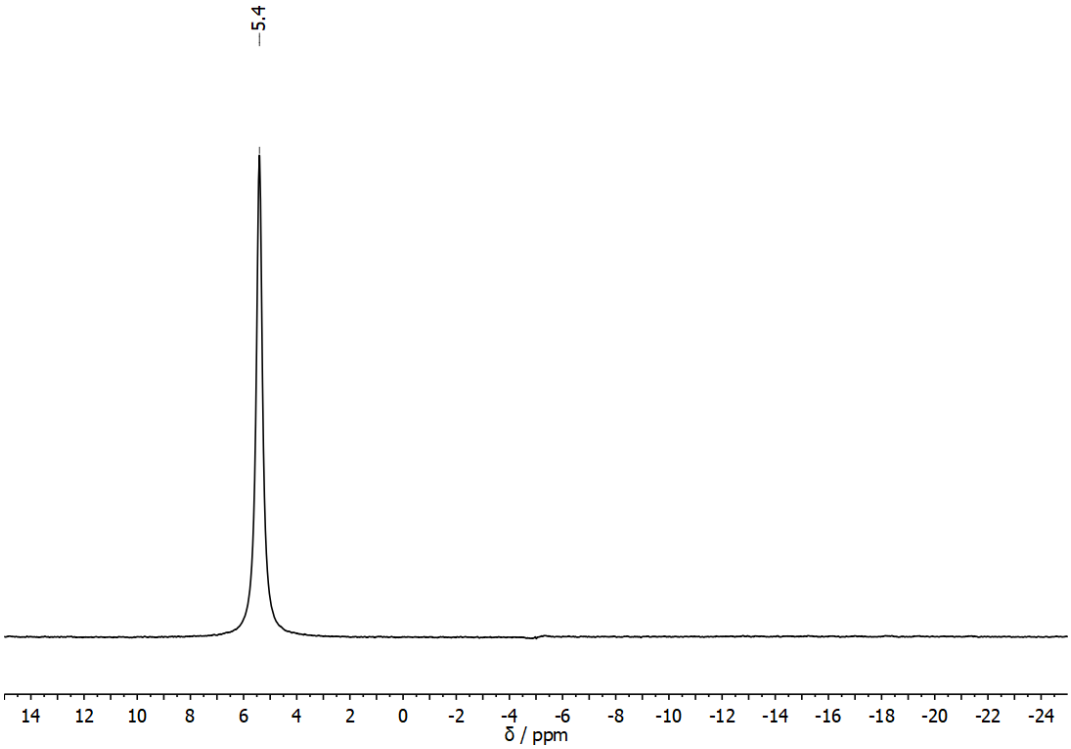

Figure S3 ^{9}Be NMR spectrum of BeI_2 in ethylenediamine.

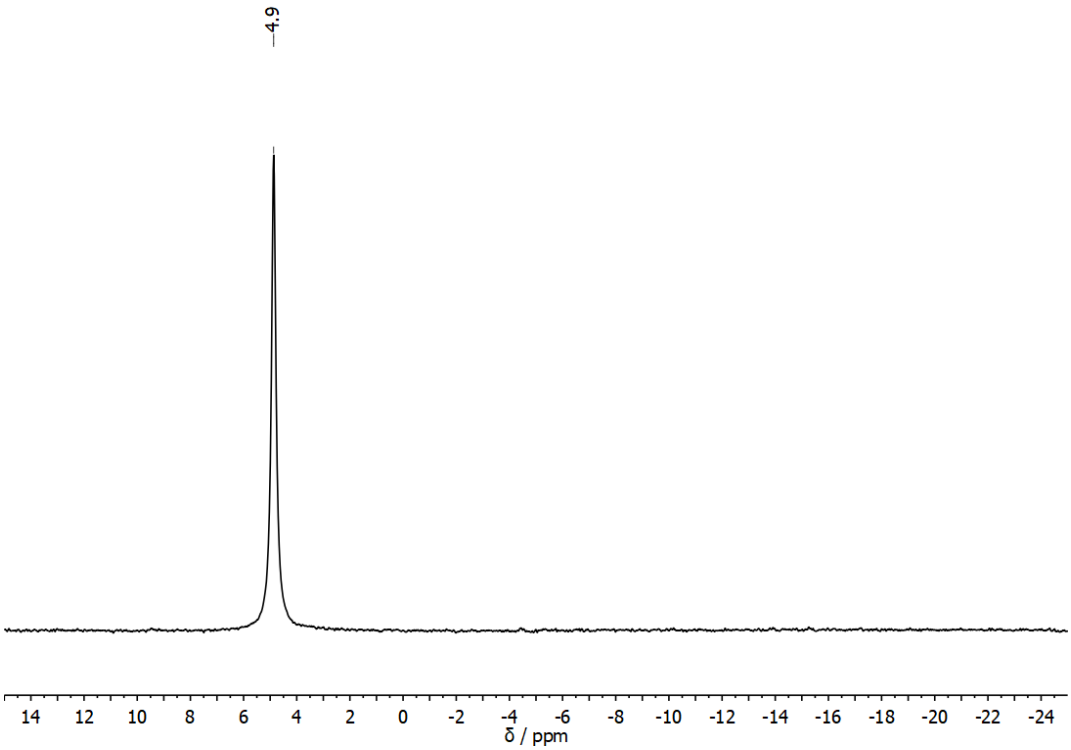

Figure S4 ^{9}Be NMR spectrum of $[Be(NH_3)_4](N_3)_2$ in ethylenediamine.

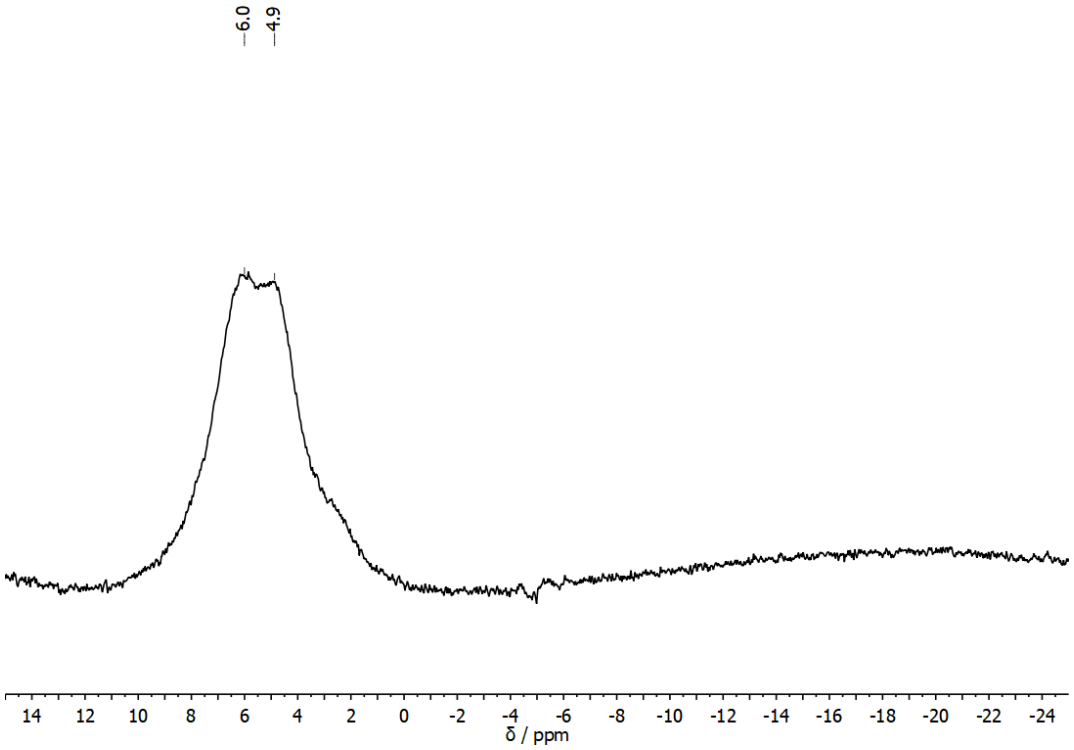

Figure S5 ^{9}Be NMR spectrum of $[Be(NH_3)_4](CN)_2$ in ethylenediamine.

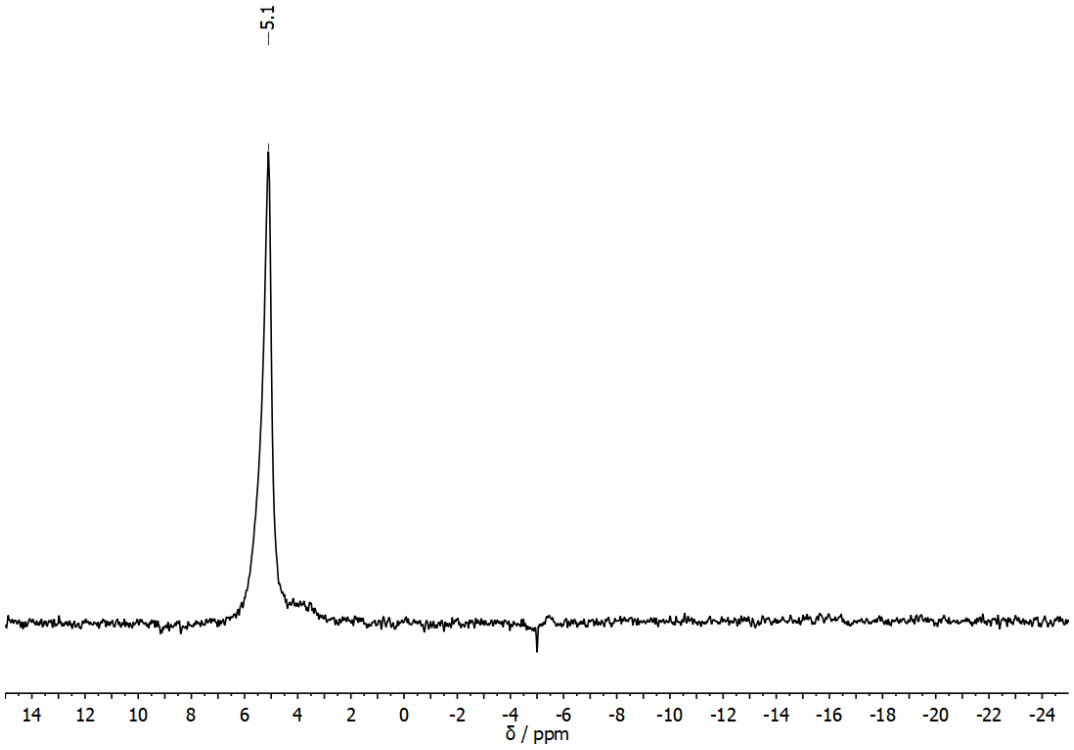

Figure S6 ^{9}Be NMR spectrum of $[Be(NH_3)_4](SCN)_2$ in ethylenediamine.

3 IR Spectra

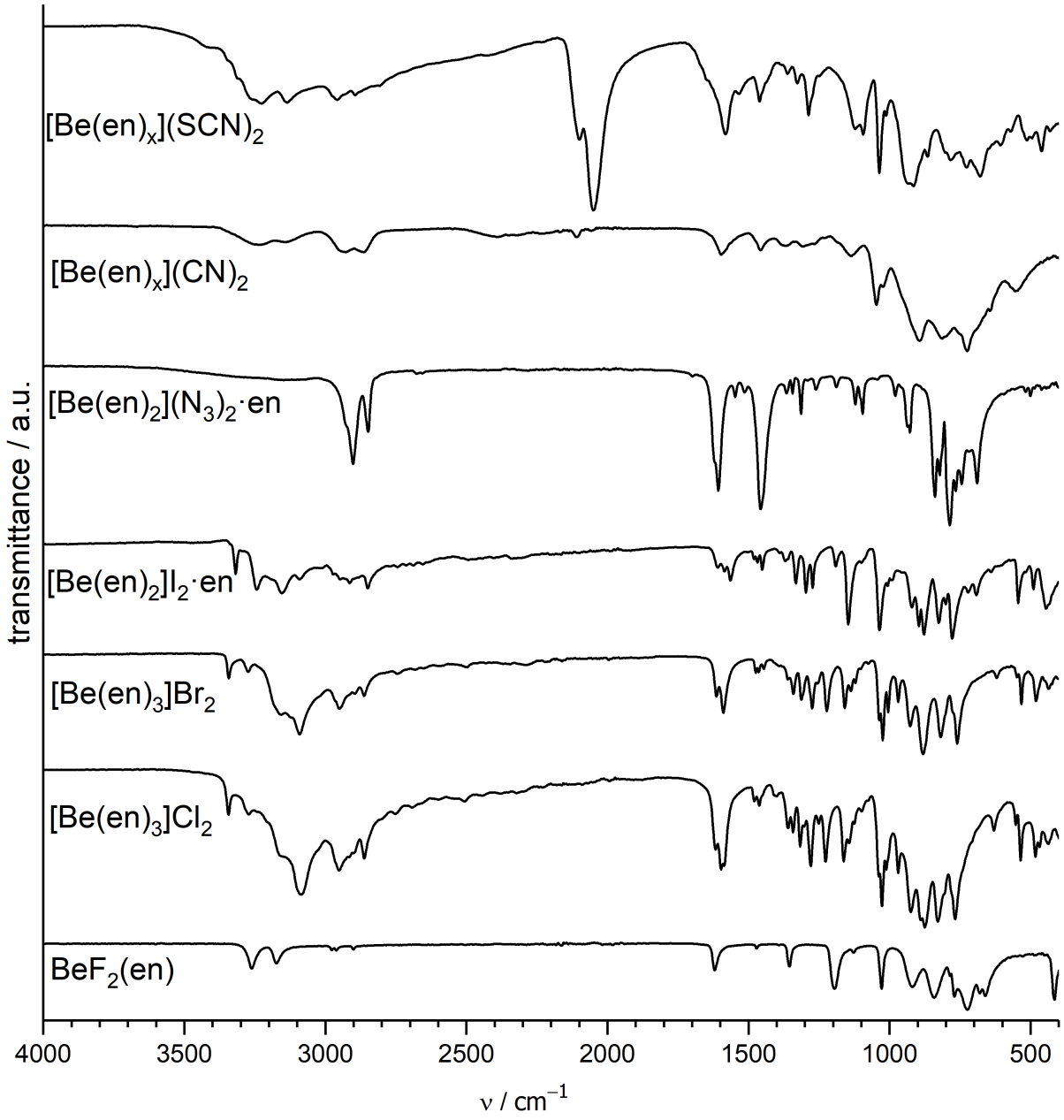

Figure S7 IR spectra of the reaction products of ethylenediamine with $[Be(NH_3)_4](SCN)_2$ and $[Be(NH_3)_4](CN)_2$, respectively, as well as of $[Be(en)_2](N_3)_2 \cdot en$, $[Be(en)_2](I)_2 \cdot en$, $[Be(en)_3]Br_2$, $[Be(en)_3]Cl_2$ and $BeF_2(en)$ (from top to bottom).

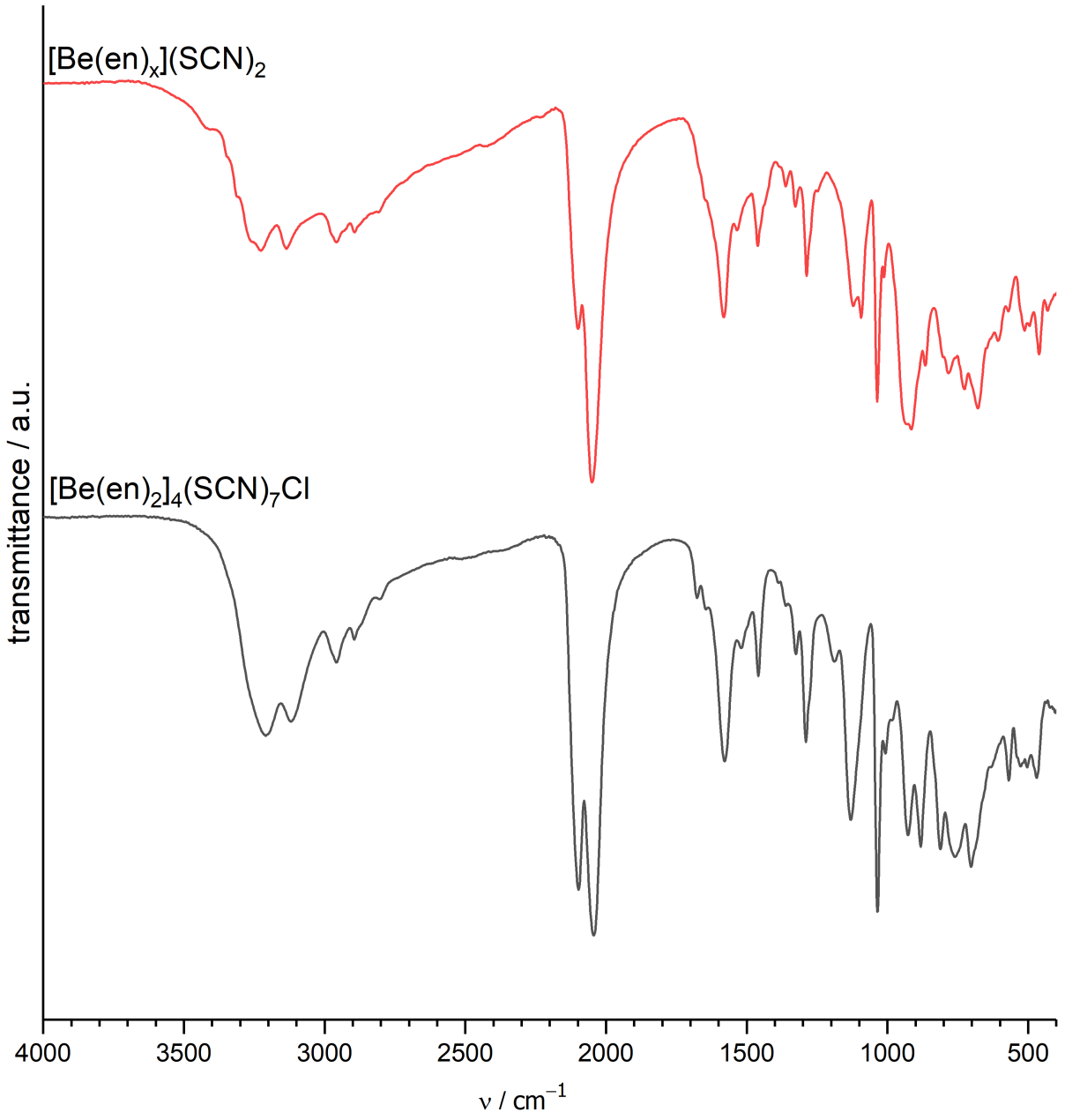

Figure S8 IR spectra of the reaction product of ethylenediamine with $[Be(NH_3)_4](SCN)_2$ (top) and of $[Be(en)_2]_4(SCN)_7Cl$ (bottom).