Supporting Information for

Probing the electronic boundaries between trigonal and tetrahedral coordination at beryllium

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1 Experimental Procedures

Caution! Beryllium and its compounds are regarded as toxic and carcinogenic. As the biochemical mechanisms that cause beryllium associated diseases are still unknown, special (safety) precautions are strongly advised.[1]

1.1 General Experimental Techniques

All manipulations were performed either under solvent vapor pressure or dry argon using glovebox and *Schlenk* techniques. Dichloromethane, chloroform and NEt_3 were dried over CaH_2 and subsequently distilled under argon. $CDCl_3$ and CD_2Cl_2 were dried over CaH_2 and C_6D_6 over NaK alloy. NMR solvents were transferred directly into the *J. Young* NMR tube via vacuum distillation. $BeCl_2$, $BeBr_2$ and BeI_2 were prepared from the elements according to the literature.[2] Due to the expected extreme toxicity of the obtained compounds no elemental analysis or mass spectrometry could be performed. The purity was therefore determined by NMR and IR spectroscopy.

1.2 NMR Spectroscopy

^{1}H, ^{9}Be and ^{13}C NMR spectra were recorded on *Bruker* Avance III HD 300 and Avance III 500 NMR spectrometers. The latter was equipped with a *Prodigy* cryo-probe. ^{1}H NMR (300 / 500 MHz) and ^{13}C NMR (76 / 126 MHz) chemical shifts are given relative to the solvent signal for C_6D_6 (7.16 and 128.1 ppm) / CD_2Cl_2 (5.32 and 53.8 ppm) / $CDCl_3$ (7.26 and 77.2 ppm) and ^{9}Be (42 MHz) used 0.43 [M] $BeSO_4$ in D_2O as an external standard. NMR spectra were processed with the MestReNova software package.[3]

1.3 IR Spectroscopy

IR spectra were recorded on a *Bruker* alpha FTIR spectrometer equipped with a diamond ATR unit in an argon filled glovebox. Processing of the spectra was performed with the OPUS software package[4] and OriginPro 2017.[5] Single crystals of the compounds were used for the IR spectroscopic measurements.

1.4 Raman spectroscopy

The Raman spectra were recorded on a *S&I* Confocal Raman Microscope MonoVista CRS+ at ambient temperature. The Raman spectrometer was equipped with four laser diodes with excitation lines of 488, 532, 633 and 785 nm. However, all samples showed severe fluorescence at all available wavelengths, which prevented the acquisition of significant spectra.

1.5 Single Crystal X-Ray Diffraction

Single crystals were selected under predried argon in perfluorinated polyether (Fomblin YR 1800, *Solvay Solexis*) and mounted using the *MiTeGen* MicroLoop system at ambient temperature. X-ray diffraction data were collected using the monochromated Cu-K_α (1.54178 Å) radiation of a *Stoe* StadiVari diffractometer equipped with a Xenocs microfocus source and a *Dectris* Pilatus 300K detector. Evaluation, integration and reduction of the diffraction data was carried out using the X-Area software suite.[6] Multi-scan absorption correction was applied with the LANA module of the X-Area software suite. The structures were solved with dual-space methods (SHELXT-2018/2) and refined against F^2 (SHELXL-2018/3) using the ShelXle software package.[7–9] All atoms were located by Difference Fourier synthesis and non-hydrogen atoms refined anisotropically.

2 Synthesis and Characterization

2.1 General Synthetic Procedure for NEt_3 Adducts to Beryllium Halides

BeX_2 (X = Cl, Br, I; 0.125 mmol; 1.0 eq.) was weighed into a *J. Young* NMR tube in a glovebox and the tube was then filled with approx. 600 μL solvent *via* vacuum distillation. Subsequently one (17.3 μL; 0.12 mmol) or two (34.6 μL; 0.24 mmol) eq. NEt_3 was added with a microliter pipette inside a glovebox and NMR spectra were recorded immediately. The reaction mixtures in C_6D_6 were left to stand for several days to yield single crystals of compounds **1a**, **1b** or **2c** respectively. Single crystals were isolated for single crystal diffraction as well as IR and Raman spectroscopy.

2.1.1 $[(NEt_3)BeCl_2]_2$ (1a)

^{1}H NMR (300 MHz, C_6D_6) δ = 0.85 (t, $^3J_{HH}$ = 7.3 Hz, 3H, CH_3), 2.53 (q, $^3J_{HH}$ = 7.3 Hz, 2H, CH_2); ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.10 (bt, $\omega_{1/2}$ = 9.9 Hz,$^3J_{HH}$ = 6.5 Hz, 3H, CH_3), 2.74 (bs, $\omega_{1/2}$ = 37.6 Hz, 2H, CH_2); ^{1}H NMR (300 MHz, CD_2Cl_2) δ = 1.04 (t, $\omega_{1/2}$ = 7.2 Hz,$^3J_{HH}$ = 6.9 Hz, 3H, CH_3), 2.55 – 2.79 (bm, $\omega_{1/2}$ = 21.8 Hz, 2H, CH_2); ^{9}Be NMR (42 MHz, C_6D_6) δ = 8.0 ($\omega_{1/2}$ = 16.8 Hz); ^{9}Be NMR (42 MHz, $CDCl_3$) δ = 8.7 ($\omega_{1/2}$ = 23.3 Hz); ^{9}Be NMR (42 MHz, CD_2Cl_2) δ = 10.0 ($\omega_{1/2}$ = 30.1 Hz); ^{13}C NMR (76 MHz, C_6D_6) δ = 10.3 ($\omega_{1/2}$ = 40.4 Hz, CH_3), 47.4 ($\omega_{1/2}$ = 4.6 Hz, CH_2); ^{13}C NMR (76 MHz, $CDCl_3$) δ = 10.6 ($\omega_{1/2}$ = 45.1 Hz, CH_3), 46.9 ($\omega_{1/2}$ = 8.4 Hz, CH_2); ^{13}C NMR (76 MHz, CD_2Cl_2) δ = 11.3 ($\omega_{1/2}$ = 47.6 Hz, CH_3), 47.1 ($\omega_{1/2}$ = 3.9 Hz, CH_2); FT-IR (cm^{-1}): 3052 (w), 2979 (m), 2943 (w), 2881 (w), 2627 (w), 2601 (w), 2494 (w), 1612 (w), 1471 (m), 1459 (m), 1388 (m), 1362 (m), 1286 (m), 1186 (m), 1165 (m), 1091 (m), 1036 (s), 1013 (s), 886 (m), 851 (m), 834 (m), 803 (m), 784 (m), 741 (m), 682 (m), 592 (vs), 542 (vs), 513 (vs), 468 (s), 428 (m).

2.1.2 $[(NEt_3)BeBr_2]_2$ (1b) & $(NEt_3)BeBr_2$ (2b)

^{1}H NMR (300 MHz, C_6D_6) δ = 0.58 (t, $^3J_{HH}$ = 7.3 Hz, 3H, CH_3), 2.45 (q, $^3J_{HH}$ = 7.3 Hz, 2H, CH_2); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 1.21 (t, $^3J_{HH}$ = 7.3 Hz, 3H, CH_3), 3.08 (bs, $\omega_{1/2}$ = 25.4 Hz, 2H, CH_2); ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 1.18 (t, $^3J_{HH}$ = 7.3 Hz, 3H, CH_3), 3.05 (bq, $\omega_{1/2}$ = 10.0 Hz, $^3J_{HH}$ = 7.3 Hz Hz, 2H, CH_2); ^{9}Be NMR (42 MHz, C_6D_6) δ = 13.5 ($\omega_{1/2}$ = 25.0 Hz); ^{9}Be NMR (42 MHz, $CDCl_3$) δ = 13.5 ($\omega_{1/2}$ = 27.9 Hz); ^{9}Be NMR (42 MHz, CD_2Cl_2) δ = 13.7 ($\omega_{1/2}$ = 21.5 Hz); ^{13}C NMR (126 MHz, C_6D_6) δ = 8.8 ($\omega_{1/2}$ = 8.4 Hz, CH_3), 46.8 ($\omega_{1/2}$ = 3.7 Hz, CH_2); ^{13}C NMR (126 MHz, $CDCl_3$) δ = 9.3 ($\omega_{1/2}$ = 15.9 Hz, CH_3), 47.0 ($\omega_{1/2}$ = 3.3 Hz, CH_2); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 9.6 ($\omega_{1/2}$ = 10.4 Hz, CH_3), 47.3 ($\omega_{1/2}$ = 3.2 Hz, CH_2); FT-IR (cm^{-1}): 3000 (w), 2979 (m), 2942 (w), 2882 (w), 1633 (w), 1472 (m), 1450 (m), 1393 (m), 1367 (w), 1335 (w), 1303 (w), 1182 (w), 1163 (m), 1085 (m), 1067 (w), 1035 (m), 1006 (m), 968 (w), 888 (m), 843 (w), 805 (m), 787 (m), 746 (s), 641 (s), 555 (vs), 492 (vs), 472 (m), 447 (vs), 413 (m).

2.1.3 $(NEt_3)BeI_2$ (2c)

^{1}H NMR (300 MHz, C_6D_6) δ = 0.72 (bs, $\omega_{1/2}$ = 40.0 Hz, 3H, CH_3), 2.45 (q, $^3J_{HH}$ = 7.2 Hz, 2H, CH_2); ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.14 (bs, $\omega_{1/2}$ = 26.5 Hz, 3H, CH_3), 2.45 – 3.36 (bm, $\omega_{1/2}$ = 115.5 Hz, 2H, CH_2); ^{9}Be NMR (42 MHz, C_6D_6) δ = 12.7 ($\omega_{1/2}$ = 27.9 Hz); ^{9}Be NMR (42 MHz, $CDCl_3$) δ = 12.3 ($\omega_{1/2}$ = 28.9 Hz); ^{13}C NMR (76 MHz, C_6D_6) δ = 10.3 ($\omega_{1/2}$ = 137.7 Hz, CH_3), 47.3 ($\omega_{1/2}$ = 3.9 Hz, CH_2); ^{13}C NMR (76 MHz, $CDCl_3$) δ = 10.3

($\omega_{1/2}$ = 167.1 Hz, CH_3), 47.2 ($\omega_{1/2}$ = 52.0 Hz, CH_2); FT-IR (cm^{-1}): 2988 (w), 2970 (m), 2917 (w), 2870 (w), 1634 (w), 1473 (s), 1443 (s), 1390 (s), 1358 (m), 1345 (m), 1322 (m), 1181 (m), 1149 (s), 1108 (w), 1081 (m), 1064 (w), 1040 (m), 1007 (s), 895 (m), 846 (m), 807 (m), 757 (vs), 683 (s), 614 (vs), 506 (s), 472 (m), 436 (m), 410 (m).

2.2 $[Et_3N(CD_2Cl)]_2[Be_2Cl_6]$ (3a) & $[Et_3N(CD_2Cl)]_2[BeCl_4]$ (3b)

32.9 mg BeI_2 (0.125 mmol; 1.0 eq.) was weighed into a *J. Young* NMR tube in a glovebox and the tube was then filled with approx. 600 μL CD_2Cl_2 *via* vacuum distillation. Subsequently one (17.3 μL; 0.12 mmol) or two (34.6 μL; 0.24 mmol) eq. NEt_3 was added with a microliter pipette inside a glovebox and NMR spectra were recorded immediately and then after defined time intervals. After several days single crystals began to form on the wall of the reaction vessels. After NMR spectorscopic reaction monitoring revealed no further changes single crystals of compound **3a** were isolated when one eq. NEt_3 was used. Single crystals which contained co-crystallized compounds **3a** and **3b** were received in case of two eq. NEt_3. These single crystals were used for X-ray diffraction as well as IR and Raman spectroscopy. ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 1.40 (t, $^3J_{HH}$ = 7.2 Hz, 3H, CH_3), 3.50 (q, Hz, 3H, $CH_3$7.2 Hz, 2H, CH_2); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 8.3 (s, CH_3), 53.4 (s, CH_2), 63.4 (p, $^1J_{CD}$ = 26.2 Hz, CD_2Cl); FT-IR (cm^{-1}): 3027 (w), 2998 (w), 2980 (m), 2942 (w), 2884 (w), 1455 (s), 1396 (m), 1356 (m), 1306 (w), 1262 (w), 1185 (m), 1170 (m), 1102 (w), 1088 (w), 1019 (m), 1010 (m), 985 (w), 942 (w), 897 (m), 857 (w), 806 (s), 742 (m), 675 (w), 579 (s), 551 (s), 504 (vs), 471 (s), 431 (w).

2.3 $[Et_3NH][(NEt_3)BeCl_3]$ (4)

8.0 mg $BeCl_2$ (0.10 mmol; 1.0 eq.) was weighed into a *J. Young* NMR tube in a glovebox and the tube was then filled with approx. 600 μL C_6D_6 *via* vacuum distillation. Subsequently 13.8 μL (0.10 mmol; 1 eq.) NEt_3 was added with a microliter pipette inside a glovebox. After several hours of storage of the closed but apparently not sufficiently sealed NMR tube in air, a fluffy, white precipitate had formed and NMR spectroscopy revealed the formation of $[Et_3NH]^+$. ^{1}H NMR (300 MHz, C_6D_6) δ = 0.67 (t, $^3J_{HH}$ = 7.3 Hz, 3H, CH_3), 2.41 (bq, $\omega_{1/2}$ = 6.5 Hz, **J** = 7.3 Hz, 2H, CH_2); ^{9}Be NMR (42 MHz, C_6D_6) δ = 4.9 ($\omega_{1/2}$ = 13.2 Hz); ^{13}C NMR (126 MHz, C_6D_6) δ = 8.9 ($\omega_{1/2}$ = 1.7 Hz, CH_3), 47.7 ($\omega_{1/2}$ = 15.2 Hz, CH_2).

3 X-ray Crystallographic Data

Table S1 Crystal data and details of the structure determination of **1a**,**b** and **2c**.

	1a	**1b**	**2c**
Empirical formula	$C_{12}H_{30}Be_2Cl_4N_2$	$C_{12}H_{30}Be_2Br_4N_2$	$C_6H_{15}BeI_2N$
Relative molecular mass	362.20	540.00	364.00
Radiation / Å	(Cu-Kα), 1.54186	(Cu-Kα), 1.54178	(Cu-Kα), 1.54178
Crystal System	monoclinic	monoclinic	monoclinic
Space group (No.)	$P2_1$/c (14)	$P2_1$/n (14)	$P2_1$/n (14)
a / Å	7.0921(14)	7.8122(3)	7.5575(1)
b / Å	14.229(3)	9.8904(3)	11.6638(2)
c / Å	9.4303(19)	13.0159(5)	13.2585(2)
α / °	90	90	90
β / °	94.57(3)	93.991(3)	98.333(1)
γ / °	90	90	90
V / Å^3	948.6(3)	1003.24(6)	1156.39(3)
T / K	100(2)	100(2)	100(2)
Z	2	2	4
F(000)	384	528	672
$d_{calc.}$ / g·cm^{-1}	1.268	1.788	2.091
μ / mm^{-1}	5.574	9.704	42.248
Θ / °	5.641–74.966	5.623–78.892	5.074–79.606
Range of Miller indices	$-8 \leq h \leq 8$	$-9 \leq h \leq 9$	$-9 \leq h \leq 9$
	$-17 \leq k \leq 10$	$-10 \leq k \leq 12$	$-14 \leq k \leq 9$
	$-11 \leq l \leq 11$	$-16 \leq l \leq 14$	$-16 \leq l \leq 16$
reflections collected / unique	16595 / 1514	9510 / 2107	32549 / 2406
restraints / parameters	0 / 143	0 / 153	0 / 94
R_{Int}	0.0677	0.0145	0.0564
R_1 $I \geq 2\sigma$(I)	0.0456	0.0187	0.0359
R_1 (all data)	0.0634	0.0191	0.0369
wR_2 $I \geq 2\sigma$(I)	0.1189	0.0527	0.0977
S	1.042	1.144	1.055
$\Delta\rho_{min,\ max}$ /e·Å^{-3}	−0.502, 0.453	−0.399, 0.514	−1.767, 1.018

Table S2 Crystal data and details of the structure determination of **3a**, **3a**/**3b** and **4**.

	3a	**3a**/**3b**	**4**
Empirical formula	$C_7H_{17}BeCl_4N$	$C_{28}H_{68}Be_3Cl_{14}N_4$	$C_{12}H_{31}BeCl_3N_2$
Relative molecular mass	266.02	984.19	318.75
Radiation / Å	(Cu-Kα), 1.54178	(Cu-Kα), 1.54178	(Cu-Kα), 1.54178
Crystal System	monoclinic	tetragonal	monoclinic
Space group (No.)	$P2_1$/n (14)	$P\bar{4}$ (81)	$P2_1$/c (14)
a / Å	11.0572(3)	14.0352(2)	12.2229(3)
b / Å	8.7404(2)	14.0352(2)	10.8012(3)
c / Å	13.0930(3)	12.0689(2)	13.2687(3)
α / °	90	90	90
β / °	91.947(2)	90	92.653(2)
γ / °	90	90	90
V / Å^3	1264.63(5)	2377.42(8)	1749.88(8)
T / K	100(2)	100(2)	100(2)
Z	4	4	4
F(000)	552	1028	688
$d_{calc.}$ / g·cm^{-1}	1.397	1.375	1.210
μ / mm^{-1}	8.157	7.627	4.613
Θ / °	5.326–75.694	3.620–78.622	3.149–78.613
Range of Miller indices	$-5 \leq h \leq 13$	$-15 \leq h \leq 13$	$-16 \leq h \leq 17$
	$-10 \leq k \leq 10$	$-12 \leq k \leq 13$	$-17 \leq k \leq 16$
	$-16 \leq l \leq 16$	$-15 \leq l \leq 16$	$-7 \leq l \leq 15$
reflections collected / unique	15955 / 2423	29421 / 5025	19102 / 2973
restraints / parameters	0 / 121	0 / 174	0 / 233
R_{Int}	0.0133	0.0290	0.0148
R_1 $I \geq 2\sigma$(I)	0.0405	0.0318	0.0280
R_1 (all data)	0.0432	0.0429	0.0284
wR_2 $I \geq 2\sigma$(I)	0.1258	0.0824	0.0831
S	1.081	1.039	1.040
$\Delta\rho_{min,\ max}$ /e·Å^{-3}	−1.011, 0.665	−0.347, 0.288	−0.421, 0.695

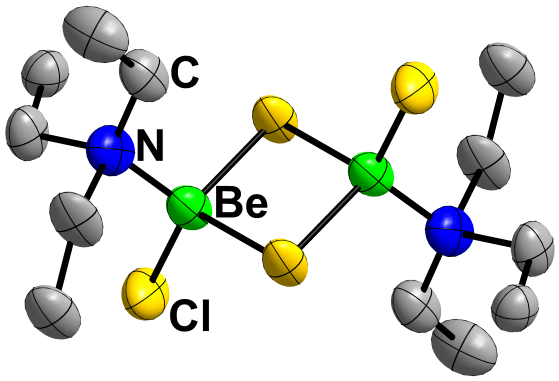

Figure S1 Molecular structure of **1a** in the solid state. Ellipsoids are depicted at 70 % probability at 100 K. Hydrogen atoms are omitted for clarity.

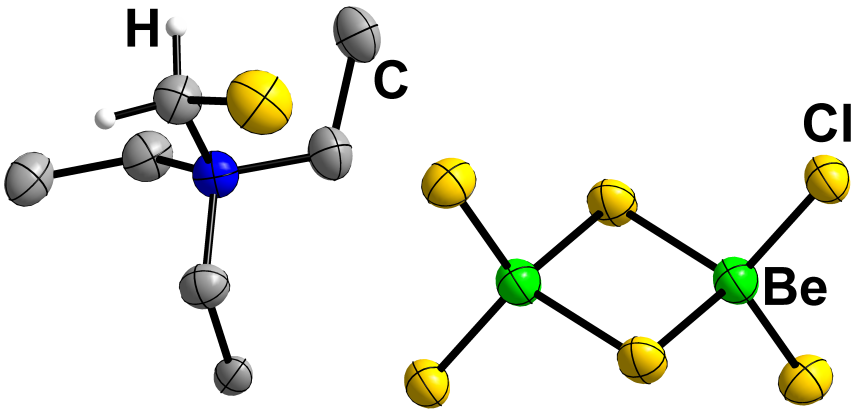

Figure S2 Molecular structure of the cations (left) and anions (right) of **3a** in the solid state. Ellipsoids are depicted at 70 % probability at 100 K. Hydrogen atoms are depicted with arbitrary radii and ethyl hydrogen atoms are omitted for clarity.

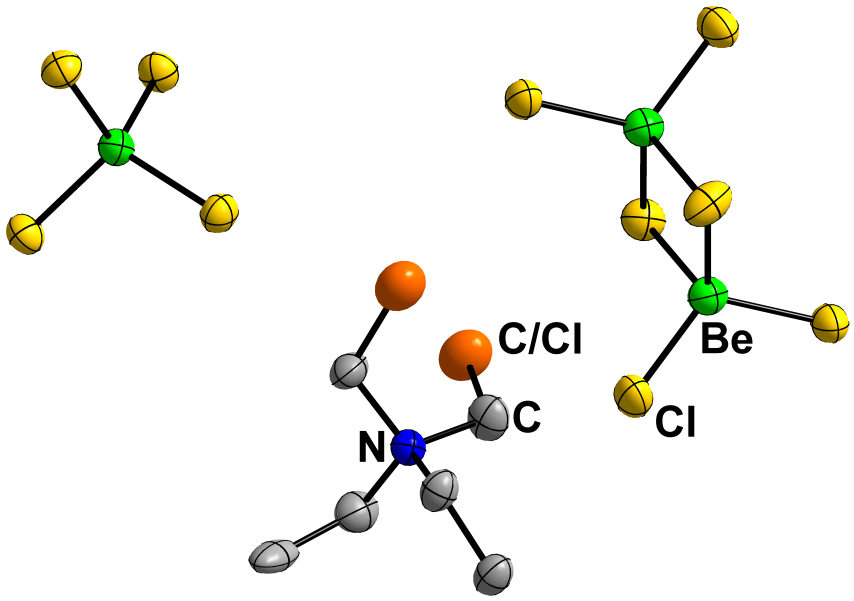

Figure S3 Molecular structure of the cations and anions in co-crystallized **3a** and **3b** in the solid state. Ellipsoids are depicted at 70 % probability at 100 K. Hydrogen atoms are omitted for clarity.

4 NMR Data

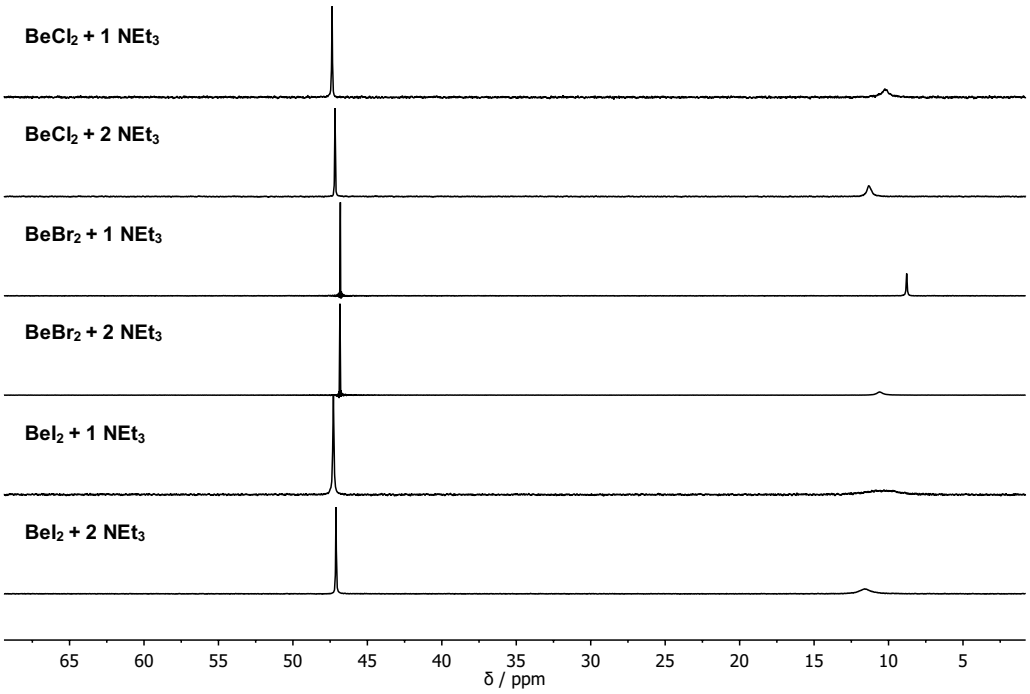

Figure S4 ^{13}C NMR spectra of BeX_2 (X = Cl, Br, I) with 1 and 2 eq. NEt_3 in C_6D_6.

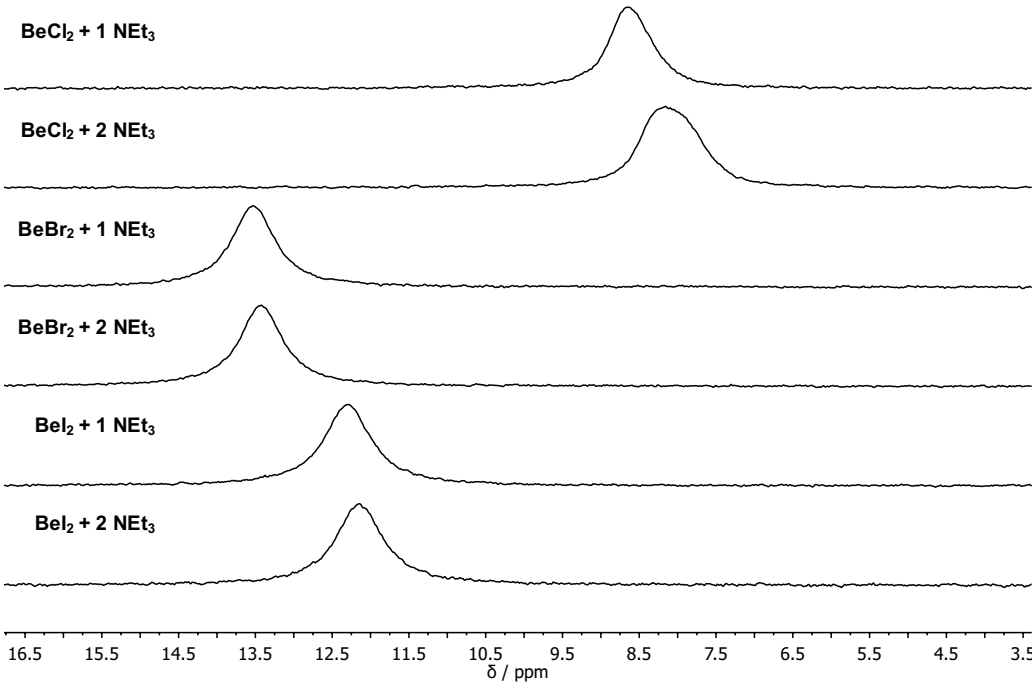

Figure S5 ^{9}Be NMR spectra of BeX_2 (X = Cl, Br, I) with 1 and 2 eq. NEt_3 in $CDCl_3$.

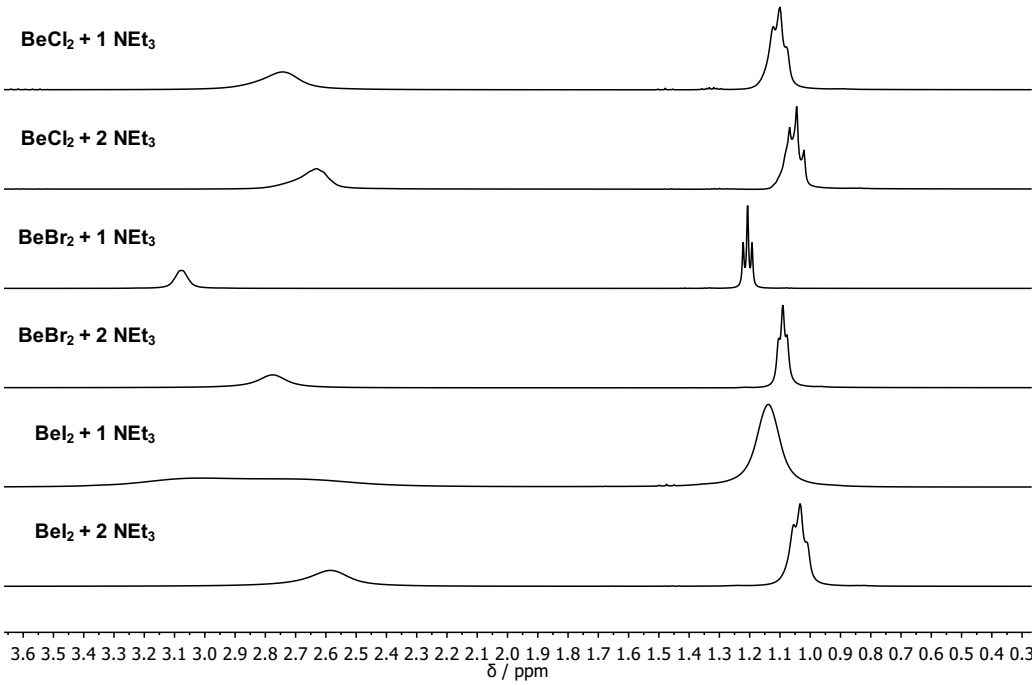

Figure S6 ^{1}H NMR spectra of BeX_2 (X = Cl, Br, I) with 1 and 2 eq. NEt_3 in $CDCl_3$.

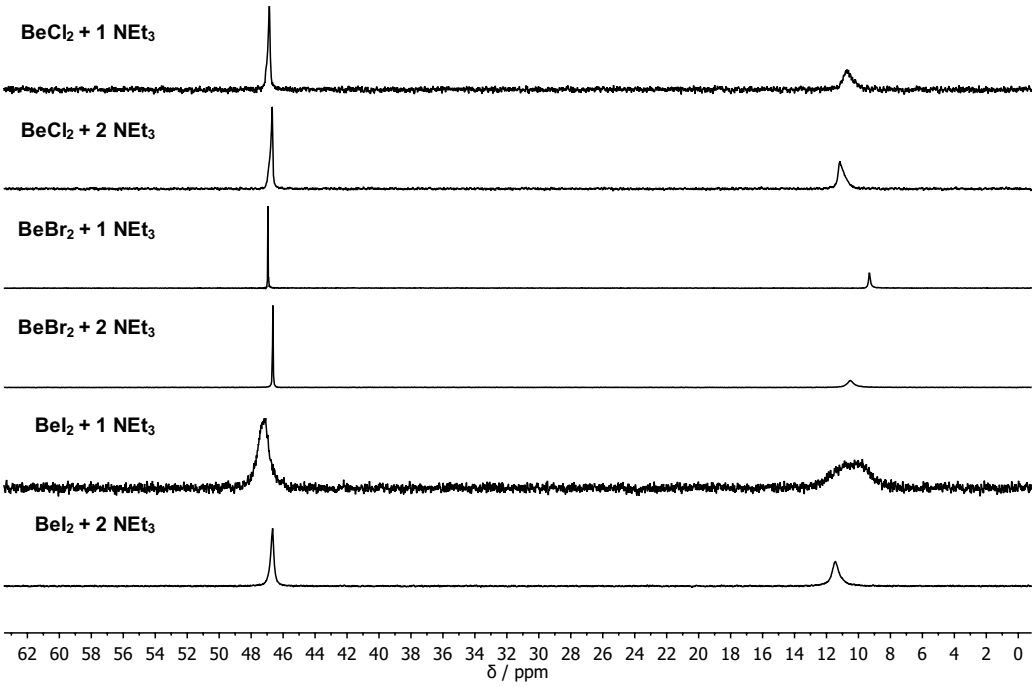

Figure S7 ^{13}C NMR spectra of BeX_2 (X = Cl, Br, I) with 1 and 2 eq. NEt_3 in $CDCl_3$.

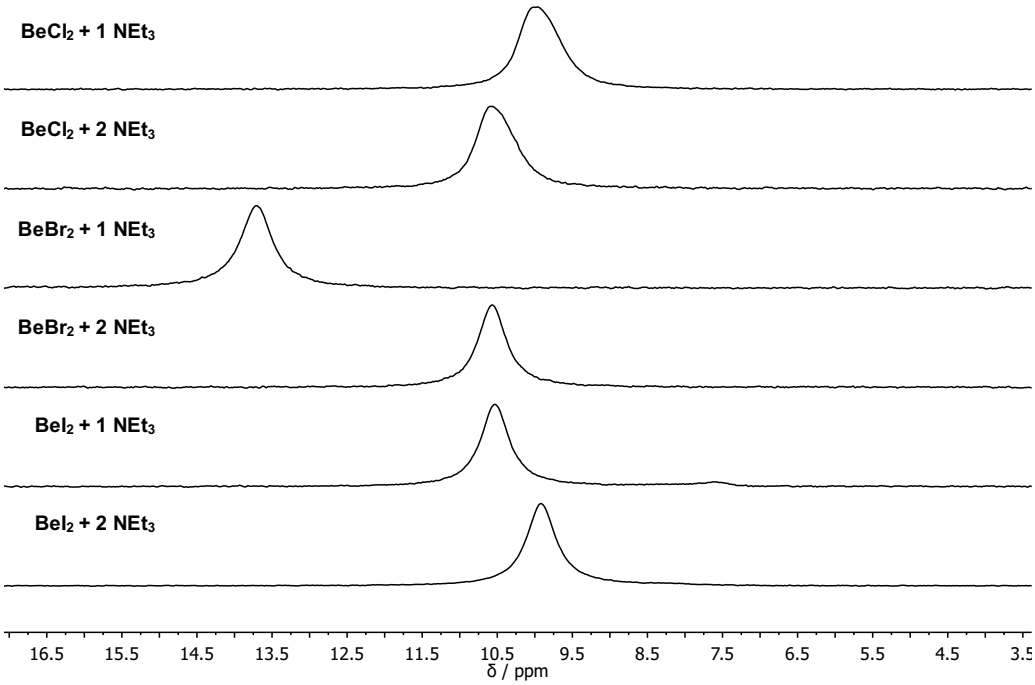

Figure S8 ^{9}Be NMR spectra of BeX_2 (X = Cl, Br, I) with 1 and 2 eq. NEt_3 in CD_2Cl_2.

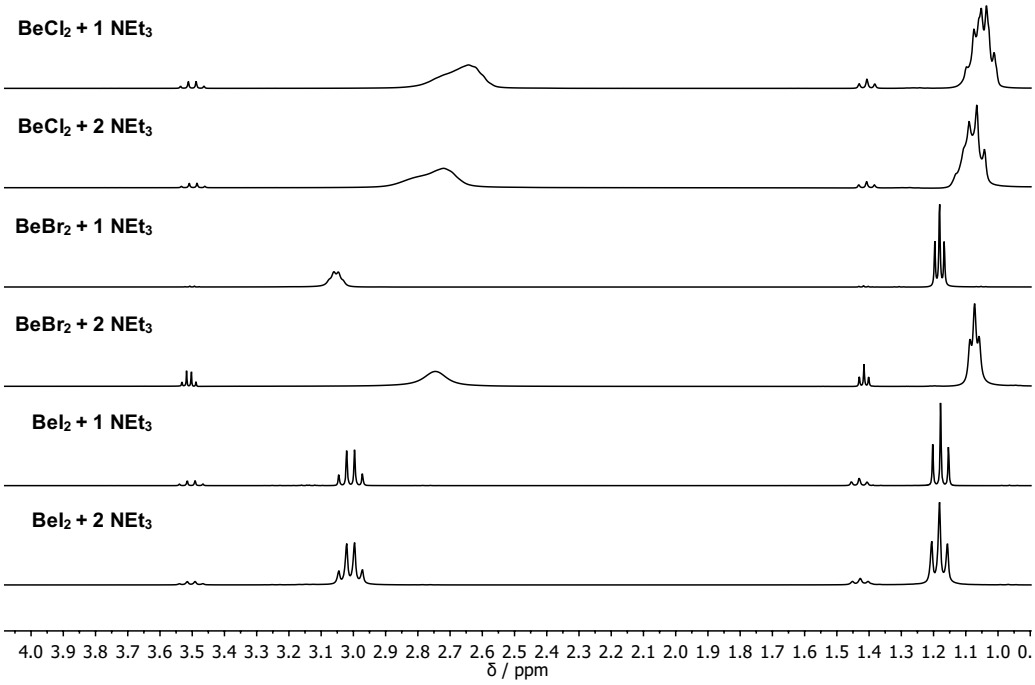

Figure S9 ^{1}H NMR spectra of BeX_2 (X = Cl, Br, I) with 1 and 2 eq. NEt_3 in CD_2Cl_2.

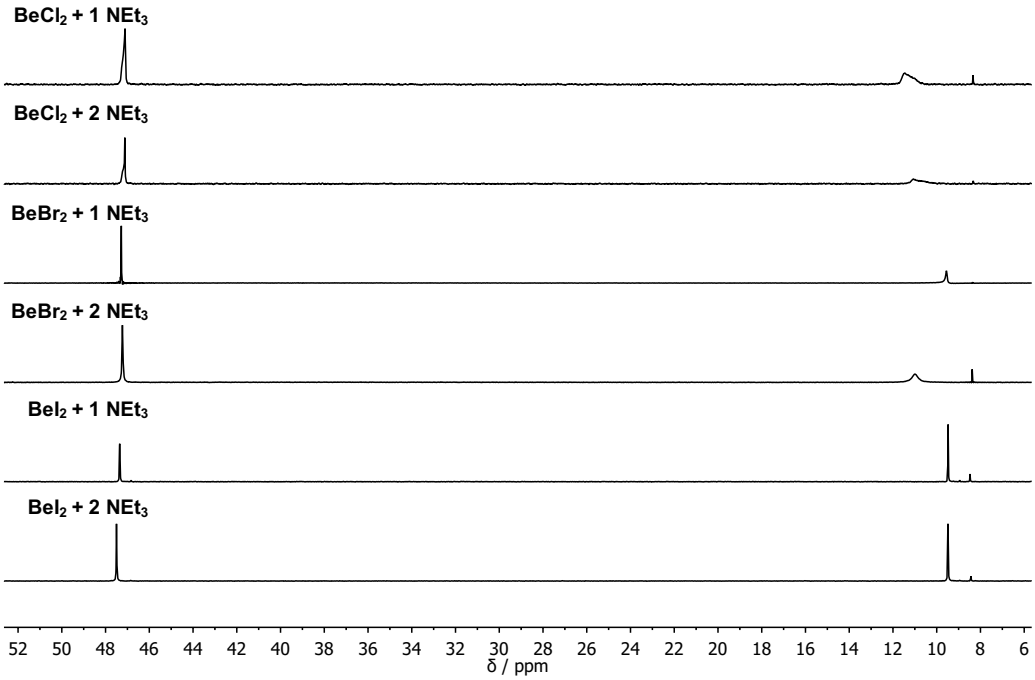

Figure S10 ^{13}C NMR spectra of BeX_2 (X = Cl, Br, I) with 1 and 2 eq. NEt_3 in CD_2Cl_2.

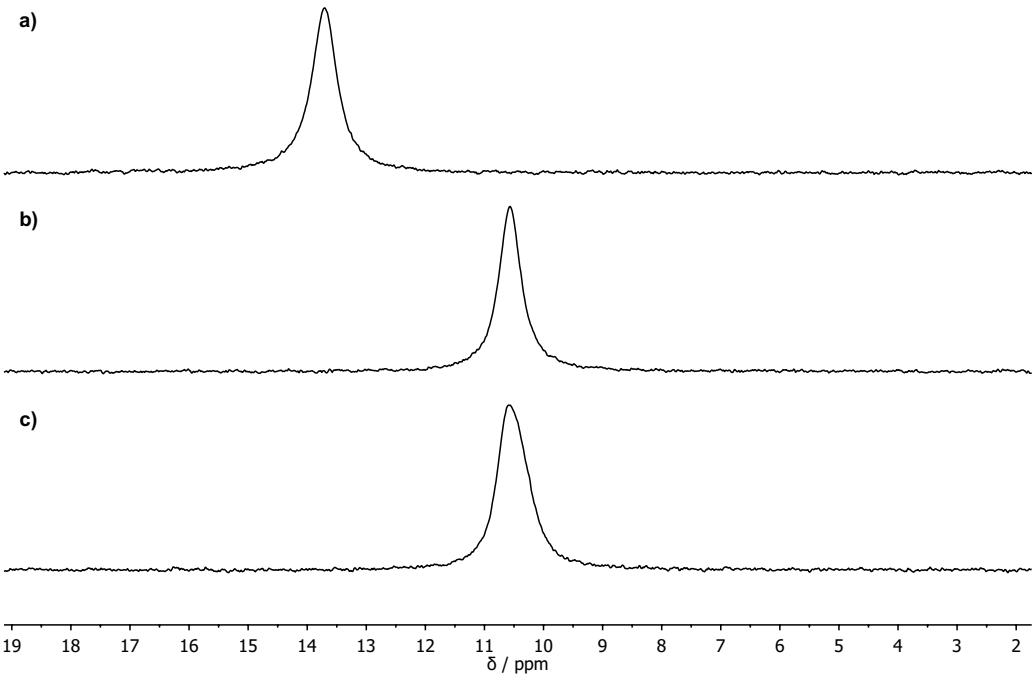

Figure S11 ^{9}Be NMR spectra of $BeBr_2$ with a) 1 and b) 2 eq. NEt_3 and c) $BeCl_2$ with 2 eq. NEt_3 in CD_2Cl_2.

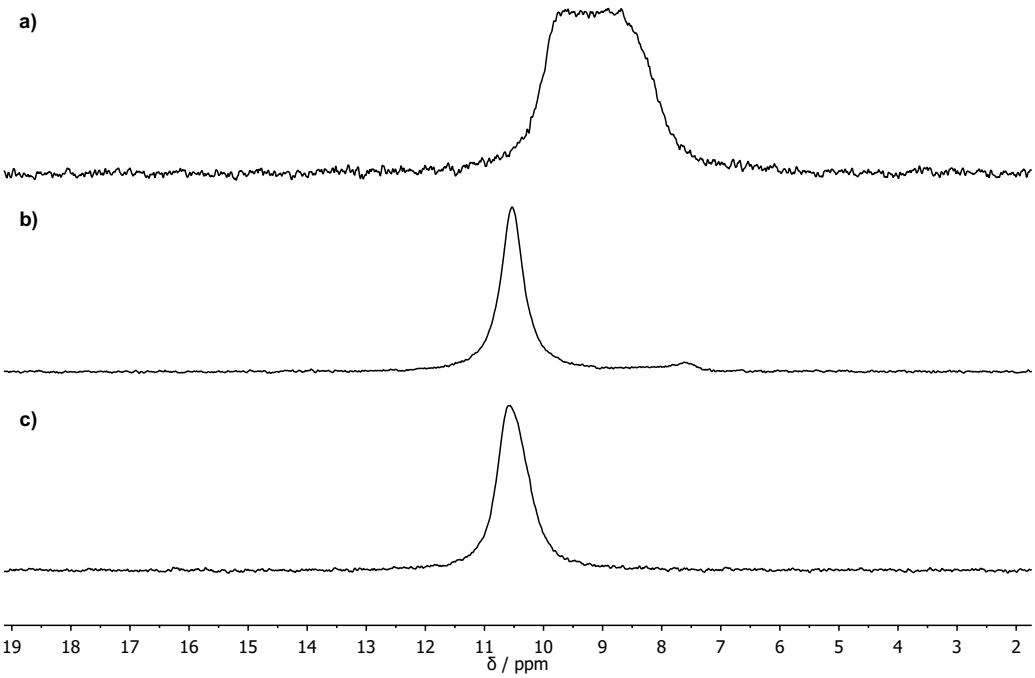

Figure S12 ^{9}Be NMR spectra of BeI_2 a) directly after addition of 1 eq. NEt_3, b) after 14 days and c) $BeCl_2$ with 2 eq. NEt_3 in CD_2Cl_2.

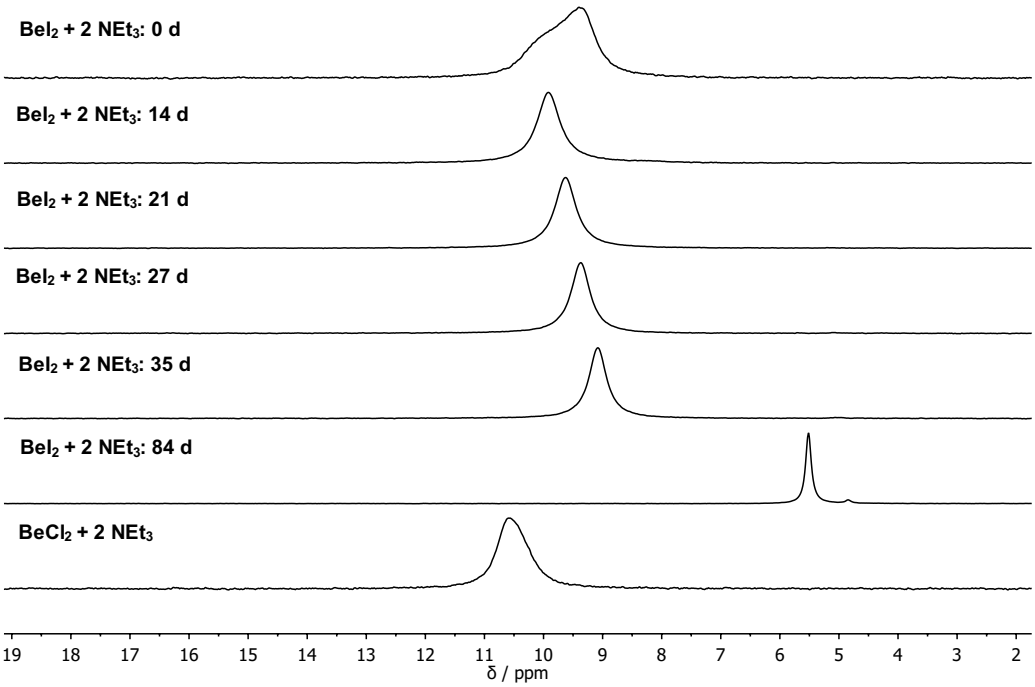

Figure S13 ^{9}Be NMR spectra of the reaction of BeI_2 with 2 eq. NEt_3 and of $BeCl_2$ with 2 eq. NEt_3 in CD_2Cl_2.

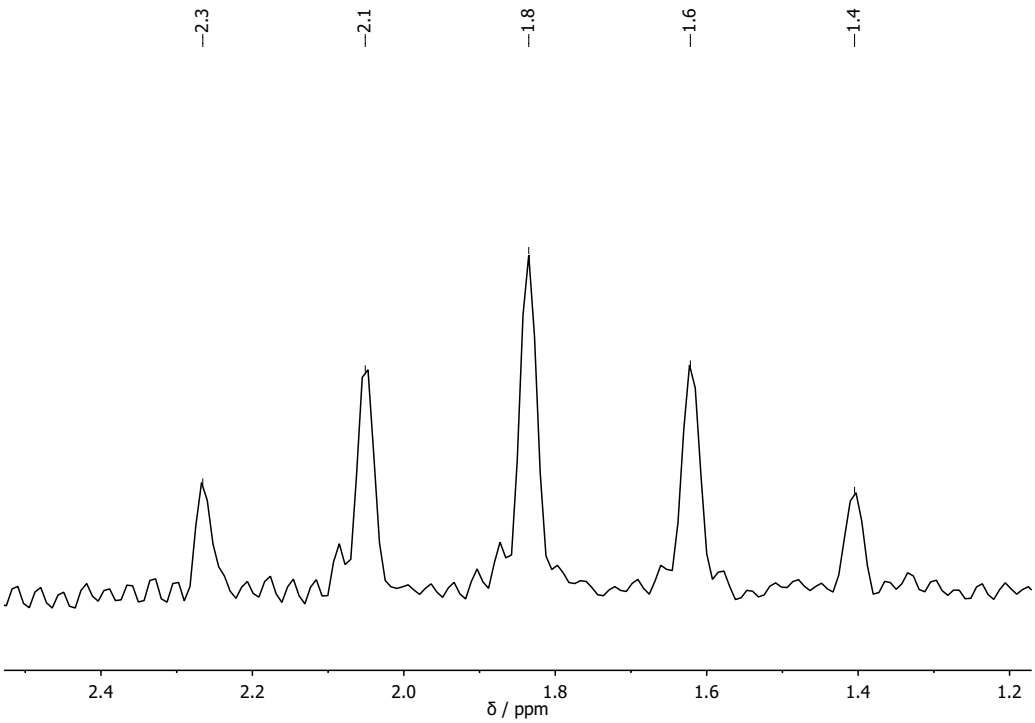

Figure S14 ^{13}C NMR spectrum of CD_2ICl in CD_2Cl_2.

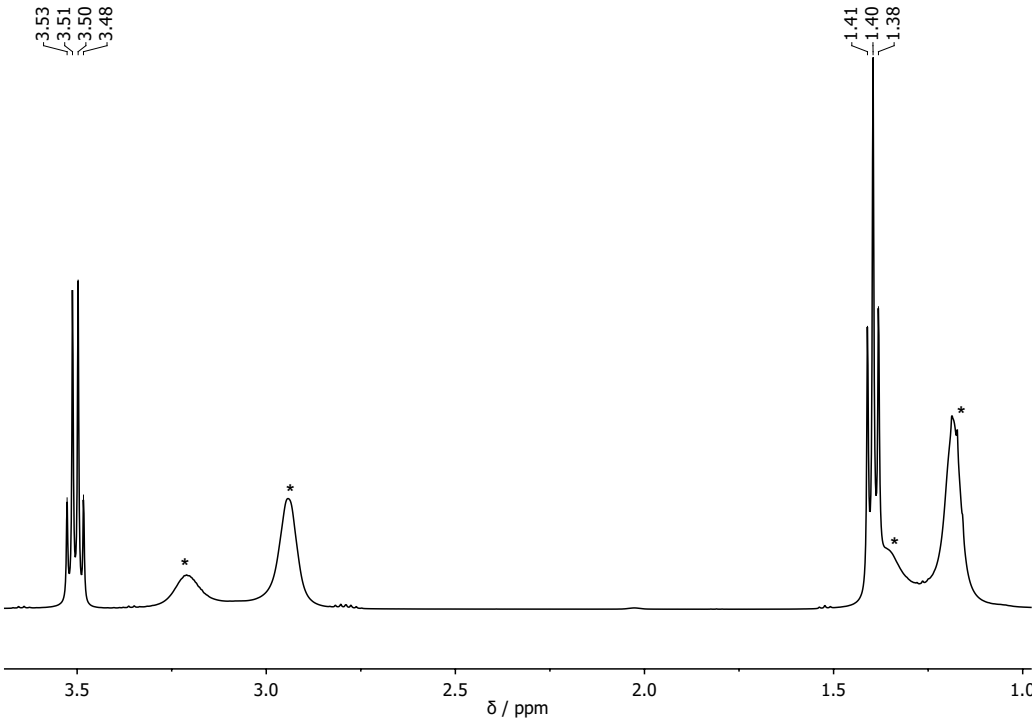

Figure S15 ^1H NMR spectrum of $[Et_3N(CD_2Cl)]^+$ in CD_2Cl_2. The signals marked with an asterisk are caused by free and coordinated NEt_3.

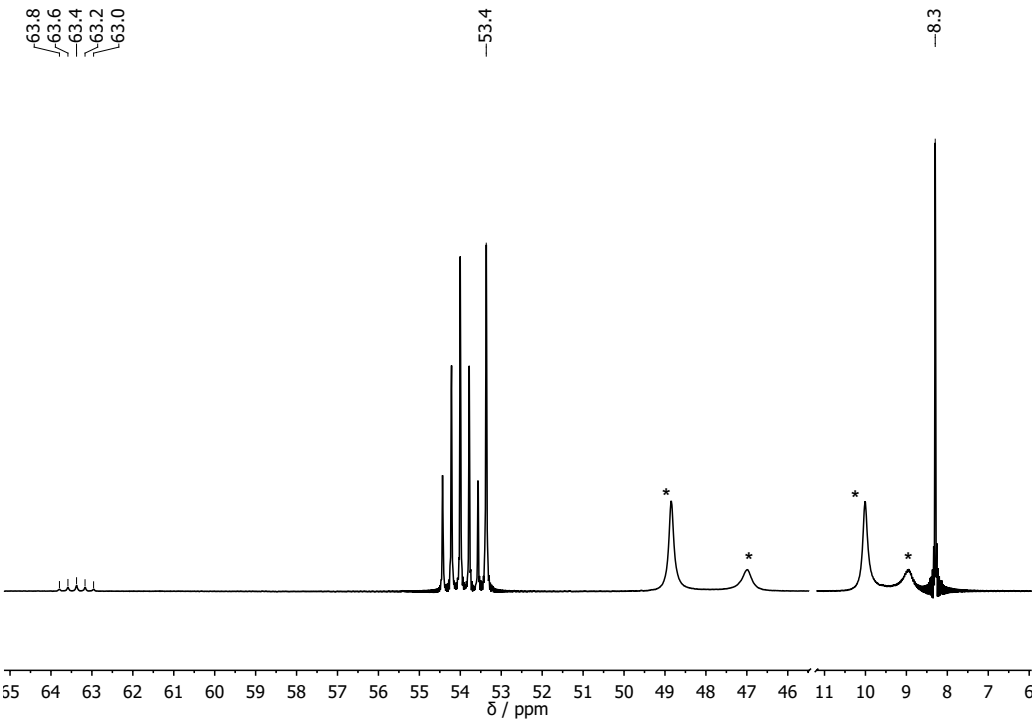

Figure S16 ^{13}C NMR spectrum of $[Et_3N(CD_2Cl)]^+$ in CD_2Cl_2. The signals marked with an asterisk are caused by free and coordinated NEt_3.

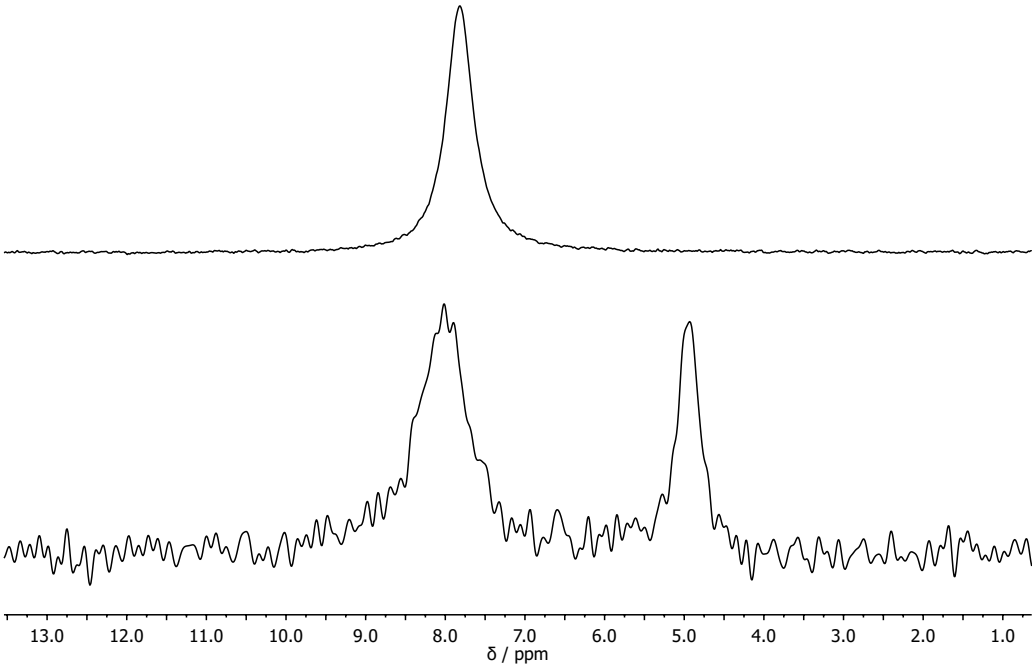

Figure S17 ^{9}Be NMR spectra of $BeCl_2$ with 1 eq. NEt_3 in C_6D_6 (top) and after H_2O addition (bottom).

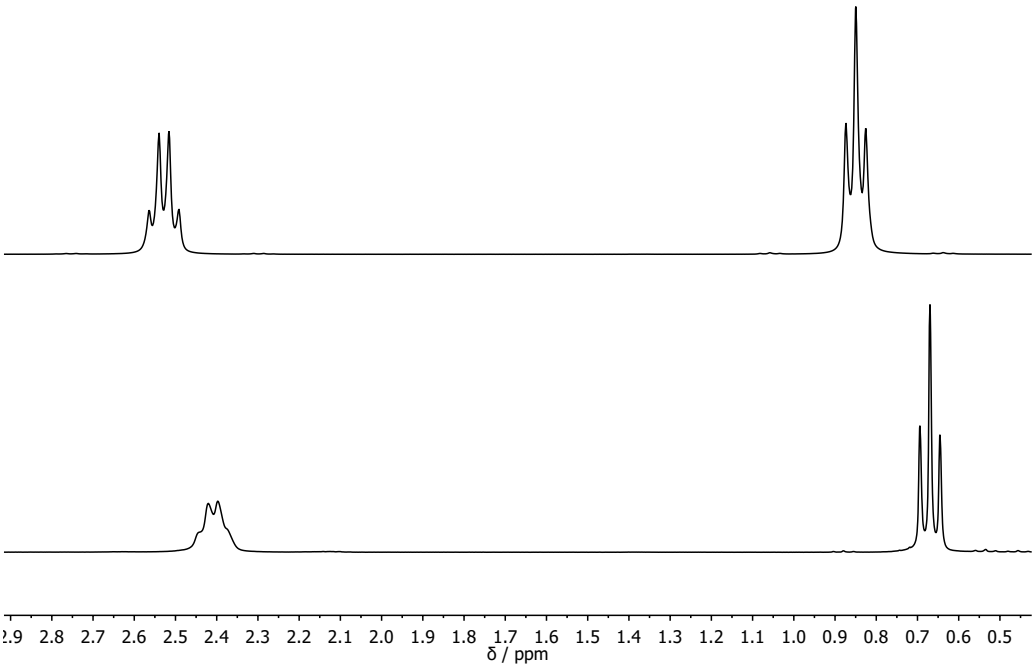

Figure S18 ^{1}H NMR spectra of $BeCl_2$ with 1 eq. NEt_3 in C_6D_6 (top) and after H_2O addition (bottom).

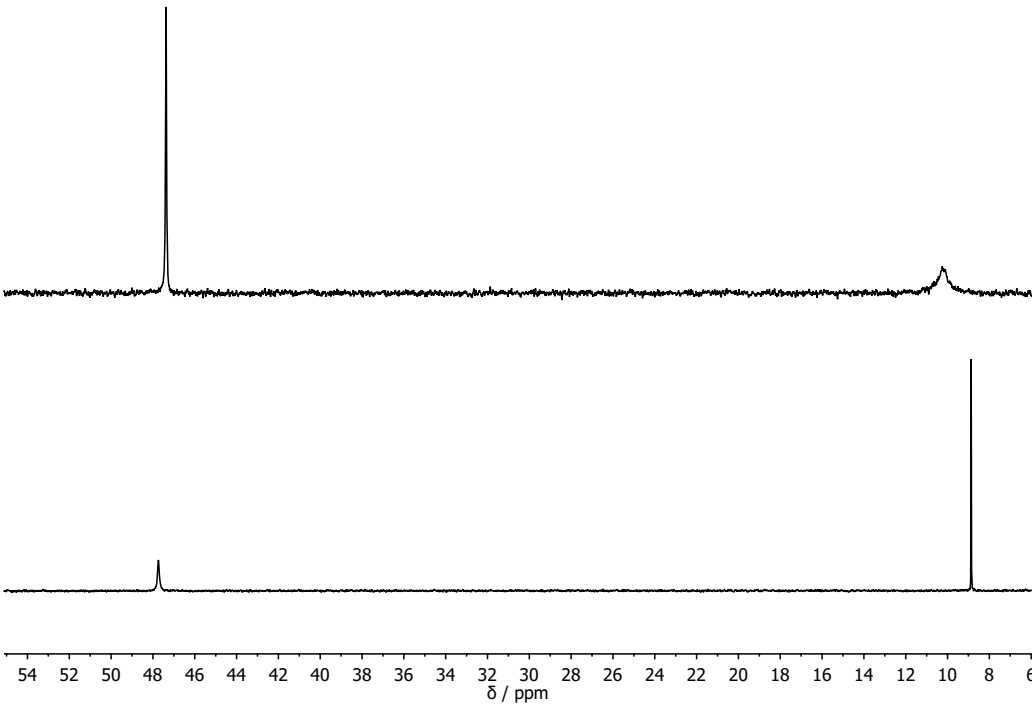

Figure S19 ^{13}C NMR spectra of $BeCl_2$ with 1 eq. NEt_3 in C_6D_6 (top) and after H_2O addition (bottom).

Table S3 NMR spectroscopic data of **1a**, **2b** and **2c**.

			NEt_3 [10]	**1a**		**2b**		**2c**	
nucleus	group	solvent	δ / ppm	δ / ppm ($\omega_{1/2}$ / Hz)	$\Delta\delta^a$ / ppm	δ / ppm ($\omega_{1/2}$ / Hz)	$\Delta\delta^a$ / ppm	δ / ppm ($\omega_{1/2}$ / Hz)	$\Delta\delta^a$ / ppm
^{9}Be		C_6D_6	–	8.0 (16.8)	–	13.5 (25.0)	–	12.7 (27.9)	–
		$CDCl_3$	–	8.0 (16.8)	–	13.5 (27.9)	–	12.3 (28.9)	–
		CD_2Cl_2	–	10.0 (30.1)	–	13.7 (21.5)	–	–	–
^{1}H	CH_3	C_6D_6	0.96	0.85	−0.11	0.58	−0.38	0.72	−0.24
		$CDCl_3$	1.03	1.10	0.07	1.21	0.18	1.14	0.11
		CD_2Cl_2	0.99	1.04	0.05	1.18	0.19	–	–
	CH_2	C_6D_6	2.40	2.53	0.13	2.45	0.05	2.45	0.05
		$CDCl_3$	2.53	2.74	0.21	3.08	0.55	2.45–3.36	0.38
		CD_2Cl_2	2.48	2.55–2.79	0.19	3.05	0.57	–	–
^{13}C	CH_3	C_6D_6	12.4	10.3 (40.4)	−1.9	8.8 (8.4)	−3.6	10.3 (137.7)	−2.1
		$CDCl_3$	11.6	10.6 (45.1)	−1.0	9.3 (15.9)	−2.3	10.3 (167.1)	−1.3
		CD_2Cl_2	12.1	11.3 (47.6)	−0.8	9.6 (10.4)	−1.7	–	–
	CH_2	C_6D_6	46.8	47.4 (4.6)	0.6	46.8 (3.7)	0.0	47.3 (3.9)	0.5
		$CDCl_3$	46.3	46.9 (8.4)	0.6	47.0 (3.3)	0.7	47.2 (52.0)	0.9
		CD_2Cl_2	46.8	47.1 (3.9)	0.3	47.3 (3.2)	0.5	–	–

a) $\Delta\delta = \delta_{compound} - \delta_{NEt_3}$

5 IR Spectra

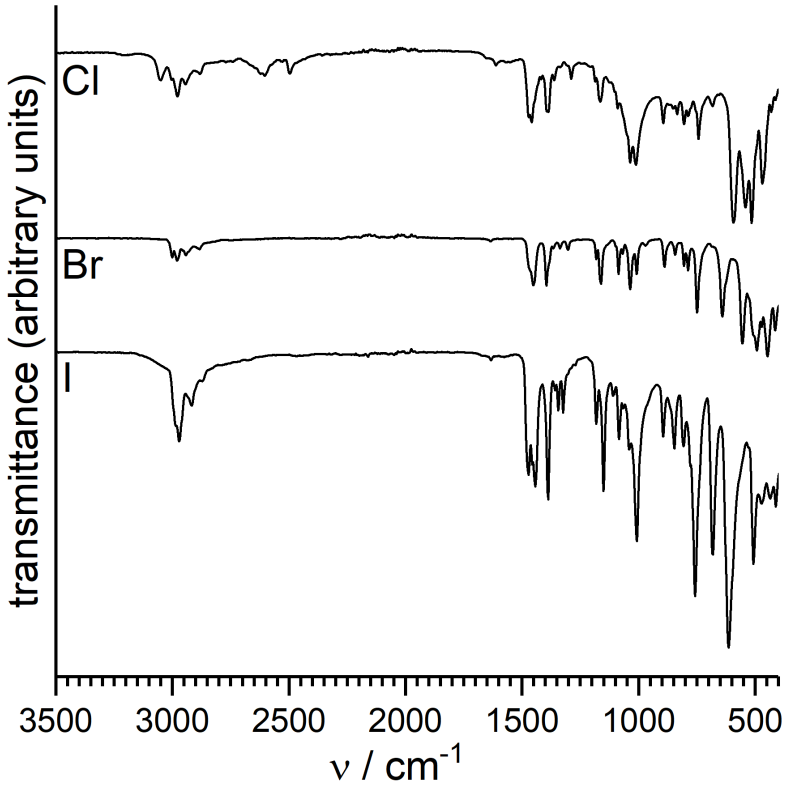

Figure S20 IR spectra of $[(NEt_3)BeCl_2]_2$ (**1a**), $[(NEt_3)BeBr_2]_2$ (**1b**) and $(NEt_3)BeI_2$ (**2c**).

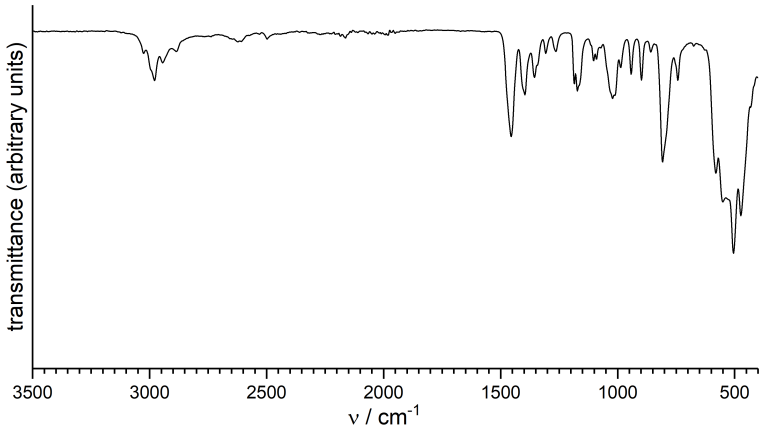

Figure S21 IR spectrum of co-crystallized $[Et_3N(CD_2Cl)]_2[Be_2Cl_6]$ (**3a**) and $[Et_3N(CD_2Cl)]_2[BeCl_4]$ (**3b**)

6 Computational Details

Quantum chemical calculations were carried out with the TURBOMOLE program package,[11,12] using the hybrid density functional TPSS method (DFT-TPSS) and a triple-ζ-valence + polarization quality basis set (def2-TZVP).[13–15] The beryllium complexes were fully optimized and they were confirmed to be true local minima by means of harmonic frequency calculations. The optimized atom coordinates are given in tables S4–**??**.

Partial charges at the atoms were determined with Mulliken population analysis[16], Natural Population Analysis (NPA)[17], Population Analysis Based On Occupation Numbers (PABOON)[18] and the Intrinsic Atomic Orbital method (IAO).[19,20] However, for the investigated molecules only NPA and IAO yielded reasonable values, which are given in tables S10–**??**. For completeness the Mulliken population analysis and PABOON results are given in tables S16–**??**.

Table S4 Coordinates of the optimized structure of **1a** (DFT-TPSS/def2-TZVP level of theory) in XYZ format and Ångström units.

	gas phase			COSMO C_6H_6			COSMO CH_2Cl_2			COSMO $CHCl_3$		
atom	x	y	z	x	y	z	x	y	z	x	y	z
1 Cl	2.107336	2.328318	5.906560	2.114299	2.327993	5.902297	2.122676	2.327900	5.896766	2.119612	2.328120	5.898815
2 Be	3.432434	3.530635	6.669119	3.451808	3.526016	6.677498	3.472188	3.521724	6.686839	3.465038	3.523271	6.683578
3 Cl	2.657519	5.106516	7.832411	2.655146	5.102550	7.827947	2.651844	5.097744	7.822774	2.653226	5.099600	7.824705
4 Be	3.474115	6.360393	6.315120	3.454367	6.364125	6.306530	3.433623	6.367396	6.296795	3.441005	6.366411	6.300237
5 N	4.722532	2.746833	7.639750	4.730718	2.738767	7.642782	4.740011	2.730487	7.646644	4.736687	2.733363	7.645250
6 C	5.095868	1.412843	7.036213	5.105650	1.402717	7.040888	5.116211	1.392395	7.046073	5.112427	1.395982	7.044209
7 C	4.244358	2.506632	9.058846	4.253659	2.498046	9.063883	4.263657	2.488953	9.069622	4.260111	2.492114	9.067580
8 C	5.916790	3.680676	7.710695	5.929628	3.668491	7.715345	5.943755	3.655750	7.721211	5.938766	3.660165	7.719118
9 C	5.690432	1.491926	5.634629	5.703569	1.480934	5.640814	5.716027	1.469970	5.646951	5.711748	1.473779	5.644822
10 C	7.117829	3.197973	8.525388	7.126532	3.180539	8.532311	7.136125	3.161962	8.540587	7.132726	3.168384	8.537640
11 C	2.922876	1.757623	9.201243	2.929116	1.755167	9.206724	2.936157	1.751972	9.211944	2.933656	1.753051	9.210142
12 H	5.790581	0.912920	7.724076	5.799757	0.905885	7.730180	5.810247	0.898477	7.736111	5.806399	0.901019	7.734052
13 H	4.173125	0.832323	6.999078	4.184864	0.819211	7.006010	4.197246	0.806065	7.014255	4.192818	0.810660	7.011223
14 H	6.649484	2.017073	5.610633	6.665289	2.001188	5.620855	6.680018	1.985879	5.629931	6.675013	1.991095	5.626920
15 H	5.860586	0.470991	5.277002	5.869300	0.459406	5.283059	5.878131	0.447974	5.289212	5.874981	0.451935	5.287035
16 H	5.001191	1.978831	4.940120	5.020134	1.972657	4.943377	5.037171	1.965959	4.947354	5.031465	1.968395	4.945903
17 H	6.221310	3.879703	6.683711	6.237603	3.864783	6.688791	6.255252	3.849350	6.695096	6.249049	3.854708	6.692859
18 H	5.536206	4.623448	8.113266	5.551483	4.611566	8.119391	5.568115	4.599271	8.126685	5.562281	4.603512	8.124141
19 H	7.532534	2.259212	8.144988	7.536129	2.239388	8.152814	7.540545	2.218597	8.161765	7.538925	2.225773	8.158573
20 H	7.901043	3.958918	8.444484	7.913230	3.937877	8.450399	7.926564	3.915438	8.458389	7.921874	3.923196	8.455503
21 H	6.892525	3.074479	9.588108	6.897661	3.059835	9.594455	6.903293	3.043378	9.601928	6.901289	3.049110	9.599276
22 H	5.036290	1.955586	9.580134	5.043187	1.940997	9.580653	5.050464	1.925979	9.582343	5.047906	1.931222	9.581674
23 H	4.160385	3.494608	9.518602	4.177155	3.484665	9.527574	4.194123	3.474164	9.537148	4.188161	3.477814	9.533784
24 H	2.704703	1.669407	10.271471	2.717029	1.659289	10.277355	2.728550	1.649896	10.282671	2.724592	1.653035	10.280856
25 H	2.097378	2.287756	8.722504	2.102828	2.294972	8.739556	2.109747	2.300183	8.753852	2.107217	2.298392	8.749076
26 H	2.965326	0.747830	8.785672	2.964476	0.748723	8.782353	2.965918	0.748153	8.780852	2.965289	0.748372	8.781235
27 Cl	4.249434	4.784533	5.152073	4.250817	4.787552	5.156058	4.253013	4.791239	5.160500	4.252288	4.790003	5.158956
28 Cl	4.798972	7.563182	7.077318	4.791918	7.561956	7.081885	4.783569	7.560209	7.087455	4.786618	7.561025	7.085386
29 N	2.183729	7.143671	5.344455	2.175487	7.151574	5.341319	2.166151	7.159681	5.337290	2.169521	7.156891	5.338747
30 C	1.810284	8.477785	5.947622	1.800678	8.487602	5.943340	1.790611	8.497689	5.938445	1.794132	8.494207	5.940138
31 C	0.989606	6.209630	5.274069	0.976487	6.221982	5.268665	0.961928	6.235117	5.262270	0.967180	6.230473	5.264626
32 C	2.661625	7.383454	3.925210	2.652566	7.392357	3.920226	2.642628	7.401559	3.914400	2.646162	7.398339	3.916462
33 C	1.215863	8.399057	7.349287	1.202794	8.409307	7.343427	1.190755	8.419786	7.337538	1.194781	8.416186	7.339504
34 H	1.115455	8.977435	5.259677	1.106591	8.984561	5.254116	1.096827	8.992284	5.248637	1.100298	8.989558	5.250434
35 H	2.732956	9.058426	5.984509	2.721522	9.071019	5.978240	2.709882	9.083522	5.970519	2.713907	9.079259	5.973281
36 C	−0.211670	6.691804	4.459407	−0.220471	6.710219	4.451950	−0.230538	6.730261	4.443852	−0.226927	6.723085	4.446823
37 H	0.685292	6.010953	6.301178	0.668597	6.025575	6.295214	0.650714	6.040816	6.288323	0.657153	6.035457	6.290861
38 H	1.370253	5.266751	4.871801	1.354485	5.278937	4.864414	1.336925	5.291762	4.855821	1.343262	5.287252	4.858944
39 C	3.983107	8.132377	3.782345	3.977119	8.135219	3.777432	3.970379	8.138120	3.772329	3.972720	8.137235	3.774036
40 H	1.869619	7.934396	3.403924	1.863059	7.949432	3.403455	1.856041	7.964964	3.401819	1.858468	7.959422	3.402425
41 H	2.745462	6.395356	3.465703	2.729059	6.405749	3.456505	2.711829	6.416476	3.446551	2.717980	6.412704	3.450095
42 H	0.256883	7.873795	7.373542	0.241091	7.889017	7.363403	0.226686	7.904007	7.354420	0.231513	7.898862	7.357328
43 H	1.045611	9.420082	7.706617	1.037015	9.430813	7.701223	1.028752	9.441695	7.695568	1.031508	9.437967	7.697449
44 H	1.905242	7.912465	8.043873	1.886284	7.917605	8.040824	1.869563	7.923540	8.036994	1.875080	7.921493	8.038353
45 H	−0.626302	7.630780	4.839351	−0.630094	7.651189	4.831867	−0.634703	7.673148	4.824131	−0.633076	7.665280	4.826976
46 H	−0.994845	5.930887	4.540984	−1.007128	5.952807	4.533575	−1.021111	5.976824	4.525131	−1.016041	5.968166	4.528285
47 H	0.013335	6.814660	3.396551	0.008347	6.831395	3.389851	0.002075	6.850347	3.382639	0.004322	6.843520	3.385282
48 H	4.201280	8.219927	2.712061	4.189229	8.231132	2.706809	4.178015	8.240524	2.701638	4.181802	8.237432	2.703342
49 H	4.808608	7.602550	4.261411	4.803393	7.595401	4.244612	4.796598	7.589459	4.230223	4.799083	7.591704	4.235015
50 H	3.940657	9.142432	4.197280	3.941750	9.141657	4.201822	3.940963	9.141799	4.203779	3.941219	9.141845	4.203121

Table S5 Coordinates of the optimized structure of **1b** (DFT-TPSS/def2-TZVP level of theory) in XYZ format and Ångström units.

	gas phase			COSMO C_6H_6			COSMO CH_2Cl_2			COSMO $CHCl_3$		
atom	x	y	z	x	y	z	x	y	z	x	y	z
1 Br	1.9459094	2.2097762	5.9547457	2.0146980	2.1290287	5.8517596	2.0217014	2.1299960	5.8427515	2.0190100	2.1297123	5.8458355
2 Be	3.4609416	3.4522090	6.7427233	3.4775647	3.4103703	6.7139718	3.4995807	3.4059924	6.7232396	3.4917486	3.4073669	6.7199052
3 Br	2.6478724	5.1661261	7.9621412	2.5949599	5.1125536	7.9434126	2.5900632	5.1066253	7.9362681	2.5917604	5.1086217	7.9387875
4 Be	3.4455392	6.4384486	6.2414818	3.4285738	6.4797045	6.2699791	3.4058057	6.4826648	6.2604039	3.4138081	6.4816581	6.2638298
5 N	4.7437433	2.6742425	7.6673446	4.7640521	2.639502	7.6766584	4.7737724	2.6309277	7.6800455	4.7702909	2.6338977	7.6787494
6 C	5.1322599	1.3394849	7.0691548	5.1559130	1.3016481	7.0842875	5.1663216	1.2907306	7.0893587	5.1626847	1.2945126	7.0875425
7 C	4.3028616	2.4209997	9.0960131	4.3012379	2.3990336	9.1048159	4.3112611	2.3910481	9.1101304	4.3077661	2.3938802	9.1082028
8 C	5.9384073	3.6082725	7.7287349	5.9564566	3.5820156	7.7426370	5.9712413	3.5690508	7.7471852	5.9659636	3.5736092	7.7454078
9 C	5.7586321	1.4160995	5.6836919	5.7560081	1.3734525	5.6854321	5.7681160	1.3616820	5.6913548	5.7640686	1.3657463	5.6893139
10 C	7.1155460	3.1418685	8.5916363	7.1547106	3.1163107	8.5700151	7.1644266	3.0980532	8.5781291	7.1609276	3.1046304	8.5751988
11 C	3.0041128	1.6387558	9.2685627	2.9903707	1.6371135	9.2650677	2.9982107	1.6334183	9.2694501	2.9955834	1.6345933	9.2679932
12 H	5.7666582	0.8814622	7.7144273	5.8543870	0.8210207	7.7801686	5.8645437	0.8128764	7.7859401	5.8609356	0.8157399	7.7839723
13 H	4.2576912	0.7620653	7.0327670	4.2421258	0.7064774	7.0542092	4.2541692	0.6931370	7.0626592	4.2499989	0.6977134	7.0595762
14 H	6.6827189	1.8836511	5.6780825	6.7107601	1.9059757	5.6616820	6.7255148	1.8893111	5.6705884	6.7205838	1.8950317	5.6676596
15 H	5.9154052	0.4451748	5.3319909	5.9354529	0.3502427	5.3394811	5.9433235	0.3378604	5.3453871	5.9406795	0.3421311	5.3433224
16 H	5.1464623	1.8761328	4.9916134	5.0674196	1.8474409	4.9804834	5.0843153	1.8405459	4.9843489	5.0787482	1.8429790	4.9829335
17 H	6.2716730	3.7217998	6.7602134	6.2668100	3.7675727	6.7149886	6.2855657	3.7503094	6.7198905	6.2789517	3.7562486	6.7179884
18 H	5.6001472	4.5133646	8.0808473	5.5674036	4.5264144	8.1337361	5.5848280	4.5146709	8.1380511	5.5786011	4.5188201	8.1362575
19 H	7.4722779	2.2191733	8.2991182	7.5697678	2.1698535	8.2105262	7.5732316	2.1481231	8.2214590	7.5719022	2.1558129	8.2177557
20 H	7.8824592	3.8261741	8.4504212	7.9366426	3.8764519	8.4705281	7.9510319	3.8532025	8.4766609	7.9458923	3.8615111	8.4742016
21 H	6.8782084	3.0793536	9.5892812	6.9274805	3.0183588	9.6346437	6.9331508	3.0048278	9.6421210	6.9310811	3.0100419	9.6394493
22 H	5.0602299	1.9114005	9.5512612	5.1048740	1.8564604	9.6142862	5.1125277	1.8442796	9.6169869	5.1099722	1.8487351	9.6159628
23 H	4.2377693	3.3427504	9.5696001	4.2159797	3.3870154	9.5642090	4.2313055	3.3783075	9.5717294	4.2258682	3.3814151	9.5689650
24 H	2.8408516	1.4790020	10.2751066	2.7913899	1.5448949	10.3385197	2.8013598	1.5385854	10.3428401	2.7980735	1.540684	10.3414223
25 H	2.1992909	2.1320033	8.8655371	2.1502415	2.1618469	8.8049623	2.1581677	2.1635962	8.8143804	2.1553974	2.1627643	8.8112613
26 H	3.0528859	0.7289605	8.8083587	3.0360648	0.6289431	8.8461132	3.0410593	0.6262721	8.8476466	3.0394806	0.6270955	8.8471703
27 Br	4.2588387	4.7245053	5.0226057	4.3106310	4.7774066	5.0403163	4.3138805	4.7817201	5.0467488	4.3126475	4.7801662	5.0444468
28 Br	4.9604208	7.6808666	7.0296097	4.8915495	7.7606375	7.1324494	4.8842878	7.7569325	7.1419347	4.8870409	7.7579500	7.1387106
29 N	2.1623640	7.2162726	5.3172519	2.1421276	7.2507922	5.3073932	2.1322645	7.2592464	5.3039073	2.1357754	7.2563297	5.3052334
30 C	1.7737067	8.5506835	5.9153049	1.7504106	8.5886571	5.8998597	1.7408376	8.5994984	5.8952356	1.7442784	8.5957647	5.8969411
31 C	0.9679539	6.2817788	5.2558608	0.9496313	6.3084126	5.2414496	0.9339974	6.3222507	5.2362709	0.9394706	6.3175048	5.2382014
32 C	2.6032887	7.4692473	3.8882634	2.6049154	7.4912578	3.8792177	2.5950906	7.4993760	3.8739560	2.5985430	7.4965281	3.8758800
33 C	1.1472793	8.4743781	7.3004081	1.1509415	8.5168969	7.2989895	1.1386298	8.5283428	7.2930574	1.1426017	8.5243892	7.2950412
34 H	1.1397328	9.0089145	5.2693776	1.0515797	9.0691761	5.2042635	1.0432321	9.0783975	5.1987577	1.0464981	9.0753524	5.2006036
35 H	2.6483086	9.1286777	5.9510293	2.6641669	9.1838950	5.9294782	2.6535665	9.1961755	5.9224708	2.6574201	9.1918393	5.9252984
36 C	−0.2091060	6.7481220	4.3925831	−0.2487358	6.7742943	4.4143404	−0.2589492	6.7948254	4.4058905	−0.2553462	6.7877528	4.4089256
37 H	0.6345128	6.1687772	6.2242945	0.6394325	6.1227987	6.2691266	0.6196813	6.1406494	6.2634913	0.6265358	6.1345501	6.2655674
38 H	1.3064187	5.3771022	4.9035592	1.3385812	5.3640281	4.8502134	1.3196035	5.3765599	4.8447819	1.3261870	5.3722571	4.8468040
39 C	3.9018412	8.2519177	3.7156004	3.9155329	8.2536012	3.7189445	3.9088580	8.2558558	3.7151102	3.9113292	8.2548441	3.7164580
40 H	1.8459210	7.9790739	3.4330114	1.8011197	8.0334919	3.3696413	1.7943849	8.0471296	3.3672815	1.7968002	8.0424965	3.3682774
41 H	2.6687596	6.5477752	3.4144264	2.6905281	6.5032476	3.4199532	2.6741414	6.5122518	3.4119185	2.6796687	6.5090948	3.4147676
42 H	0.2234893	8.0065493	7.3059800	0.1963597	7.9840861	7.3232658	0.1808091	8.0014464	7.3133413	0.1857636	7.9956626	7.3163529
43 H	0.9903472	9.4452166	7.6517347	0.9713190	9.5401073	7.6448447	0.9640862	9.5521314	7.6394528	0.9665009	9.5479834	7.6413507
44 H	1.7596153	8.0143714	7.9923550	1.8399990	8.0432549	8.0037104	1.8218978	8.0486460	8.0000066	1.8275322	8.0465312	8.0013717
45 H	−0.5663297	7.6705630	4.6846341	−0.6636857	7.7206975	4.7740913	−0.6671236	7.7446064	4.7636717	−0.6657768	7.7364647	4.7672679
46 H	−0.9758916	6.0633791	4.5336284	−1.0306878	6.0141733	4.5138101	−1.0460176	6.0400579	4.5065810	−1.0406907	6.0311936	4.5093596
47 H	0.0278689	6.810526	3.3947714	−0.0216706	6.8724512	3.3497003	−0.0276835	6.8891116	3.3419982	−0.0255699	6.8831724	3.3447414
48 H	4.0652176	8.4114383	2.7089497	4.1146268	8.3456061	2.6454950	4.1059553	8.3508996	2.6417837	4.1090379	8.3489021	2.6430781
49 H	4.7070445	7.7590347	4.1185735	4.7557853	7.7293005	4.1793194	4.7483365	7.7247495	4.1701417	4.7510426	7.7259022	4.1731686
50 H	3.8530531	9.1619171	4.1754005	3.8694069	9.2618671	4.1376221	3.8668479	9.2628849	4.1372735	3.8681417	9.2622556	4.1375581

Table S6 Coordinates of the optimized structure of **1c** (DFT-TPSS/def2-TZVP level of theory) in XYZ format and Ångström units.

	gas phase			COSMO C_6H_6			COSMO CH_2Cl_2			COSMO $CHCl_3$		
atom	x	y	z	x	y	z	x	y	z	x	y	z
1 I	1.8903943	1.8451724	5.7964088	1.8966596	1.8494919	5.7944857	1.9079387	1.8525351	5.7873743	1.9044432	1.8514162	5.7892529
2 Be	3.5037759	3.2568254	6.7599052	3.5278146	3.2549151	6.7715270	3.5550980	3.2542891	6.7821837	3.5456660	3.2543661	6.7781728
3 I	2.5169725	5.1318450	8.1036079	2.5153365	5.1292114	8.0976443	2.5105643	5.1232720	8.0899561	2.5119666	5.1248744	8.0925072
4 Be	3.4024148	6.6336836	6.2242598	3.3781820	6.6351203	6.2124818	3.3509420	6.6354391	6.2014691	3.3603771	6.6354373	6.2055734
5 N	4.8127158	2.5064974	7.7283230	4.8232345	2.4986550	7.7333666	4.8356023	2.4908692	7.7384786	4.8313328	2.4935373	7.7365623
6 C	5.2223407	1.1691657	7.1452916	5.2321885	1.1595556	7.1501871	5.2427723	1.1492814	7.1559579	5.2390926	1.1527282	7.1539995
7 C	4.3659585	2.2660280	9.1618897	4.3754174	2.2579137	9.1681451	4.3859280	2.2507770	9.1744474	4.3822667	2.2534177	9.1721336
8 C	5.9920446	3.4668196	7.7836817	6.0079367	3.4541594	7.7908425	6.0267803	3.4401696	7.7981335	6.0203242	3.4449330	7.7953620
9 C	5.8249962	1.2344973	5.7478958	5.8361251	1.2255875	5.7535118	5.8480574	1.2151078	5.7600164	5.8441434	1.2185003	5.7578889
10 C	7.1976882	3.0309502	8.6168051	7.2090334	3.0107319	8.6257903	7.2224301	2.9876538	8.6352828	7.2178152	2.9956609	8.6318953
11 C	3.0715238	1.4818288	9.3422793	3.0779212	1.4787941	9.3459575	3.0848364	1.4774749	9.3486544	3.0824295	1.4780640	9.3476122
12 H	5.9240714	0.7021132	7.8481392	5.9334083	0.6937274	7.8529521	5.9431131	0.6841415	7.8587151	5.9396392	0.6873448	7.8568787
13 H	4.3140107	0.5645099	7.1156714	4.3250667	0.5533828	7.1233179	4.3361829	0.5425118	7.1320354	4.3322882	0.5462178	7.1289481
14 H	6.7717317	1.7810526	5.7187489	6.7861043	1.7664710	5.7279389	6.8017978	1.7492679	5.7379020	6.7967678	1.7546940	5.7347642
15 H	6.0198234	0.2103220	5.4129603	6.0252072	0.2010221	5.4167909	6.0308258	0.1900858	5.4215893	6.0287616	0.1936135	5.4199285
16 H	5.1286702	1.6883998	5.0372648	5.1448872	1.6862745	5.0416877	5.1622938	1.6832291	5.0471085	5.1567564	1.6843378	5.0452958
17 H	6.2993361	3.6444831	6.7535615	6.3186335	3.6294913	6.7612786	6.3411049	3.6125265	6.7691266	6.3334625	3.6181125	6.7661648
18 H	5.5884955	4.4114519	8.1606588	5.6078086	4.3994464	8.1697797	5.6310455	4.3866446	8.1787110	5.6231267	4.3910842	8.1751782
19 H	7.6240050	2.0824975	8.2755879	7.6289033	2.0596782	8.2844147	7.6347310	2.0337122	8.2936342	7.6326802	2.0426168	8.2905224
20 H	7.9703260	3.7980161	8.5001971	7.9862486	3.7732278	8.5091289	8.0052290	3.7445316	8.5192370	7.9987186	3.7544272	8.5155279
21 H	6.9764402	2.9520157	9.6842722	6.9840531	2.9334691	9.6924883	6.9930169	2.9117499	9.7009165	6.9898574	2.9195238	9.6978971
22 H	5.1859323	1.7422203	9.6660661	5.1923912	1.7290156	9.6701004	5.1990248	1.7161970	9.6749356	5.1967151	1.7208814	9.6732274
23 H	4.2674623	3.2560488	9.6155994	4.2825592	3.2470451	9.6246179	4.2990061	3.2391744	9.6333023	4.2932568	3.2421216	9.6300479
24 H	2.8868448	1.3916816	10.4186929	2.8948662	1.3846094	10.4221007	2.9013355	1.3811906	10.424306	2.8989634	1.3826395	10.4234291
25 H	2.2169370	1.9889882	8.8890583	2.2240417	1.9929378	8.8983871	2.2328005	1.9978313	8.9037762	2.2297773	1.9961658	8.9016798
26 H	3.1277341	0.4728283	8.9269515	3.1302762	0.4713967	8.9259681	3.1343680	0.4709221	8.9262727	3.1329929	0.4711858	8.9261620
27 I	4.3893798	4.7586901	4.8806581	4.3905504	4.7608301	4.8863113	4.3950040	4.7663124	4.8934379	4.3936677	4.7648220	4.8910119
28 I	5.0156573	8.0455159	7.1877129	5.0096233	8.0402086	7.1893580	4.9987566	8.0364733	7.1960626	5.0021743	8.0377746	7.1943228
29 N	2.0934605	7.3839003	5.2558000	2.0828474	7.3916852	5.2507748	2.0704516	7.3994143	5.2455077	2.0747427	7.3967608	5.2474648
30 C	1.6836889	8.7211936	5.8388164	1.6741769	8.7307935	5.8341227	1.6639138	8.7410445	5.8283444	1.6675210	8.7376070	5.8302973
31 C	0.9142278	6.4234703	5.2003490	0.8979047	6.4364641	5.1931908	0.8788983	6.4506079	5.1859454	0.8854255	6.4457900	5.1887262
32 C	2.5402887	7.6244497	3.8222757	2.5306511	7.6324977	3.8159934	2.5199109	7.6395434	3.8094698	2.5236387	7.6369152	3.8118370
33 C	1.0812013	8.6558691	7.2362871	1.0706666	8.6647500	7.2309811	1.0593625	8.6752333	7.2246084	1.0630758	8.6718504	7.2266742
34 H	0.9817918	9.1880956	5.1360317	0.9727496	9.1966826	5.1316082	0.9632921	9.2064201	5.1260215	0.9667473	9.2031987	5.1277814
35 H	2.5919216	9.3260084	5.8682909	2.5813493	9.3369014	5.8607181	2.5706566	9.3475891	5.8518248	2.5744611	9.3439197	5.8549876
36 C	−0.2914928	6.8593451	4.3673404	−0.3030824	6.8802491	4.3582721	−0.3169472	6.9039490	4.3495109	−0.3121928	6.8957470	4.3527342
37 H	0.6069845	6.2456143	6.2304506	0.5871612	6.2611138	6.2227349	0.5648655	6.2779540	6.2149914	0.5724976	6.2723947	6.2179510
38 H	1.3178492	5.4789361	4.8232082	1.2978201	5.4911233	4.8141634	1.2741768	5.5041442	4.8048676	1.2822312	5.4996316	4.8085212
39 C	3.8347906	8.4085792	3.6420409	3.8283838	8.4112139	3.6381704	3.8213511	8.4122097	3.6350439	3.8237650	8.4117449	3.6361841
40 H	1.7203872	8.1483720	3.3181012	1.7138132	8.1617254	3.3141641	1.7069823	8.1746163	3.3092410	1.7093290	8.1698597	3.3109566
41 H	2.6387318	6.6344635	3.3684814	2.6231466	6.6433944	3.3593789	2.6062116	6.6511819	3.3504325	2.6121364	6.6482390	3.3537725
42 H	0.1345453	8.1091830	7.2655755	0.1208899	8.1235302	7.2569291	0.1058845	8.1406346	7.2473489	0.1106705	8.1352929	7.2503210
43 H	0.8862585	9.6800400	7.5711688	0.8813261	9.6892977	7.5676134	0.8763220	9.7002242	7.5629681	0.8782311	9.6967117	7.5645757
44 H	1.7776655	8.2021160	7.9468761	1.7622988	8.2044233	7.9426505	1.7457547	8.2075578	7.9371930	1.7509816	8.2063853	7.9390012
45 H	−0.7178758	7.8077135	4.7087120	−0.7230607	7.8311049	4.7000611	−0.7291141	7.8575386	4.6922989	−0.7269183	7.8485411	4.6949726
46 H	−1.0640528	6.0921898	4.4838796	−1.0802832	6.1176616	4.4744159	−1.0997570	6.1469898	4.4650031	−1.0931441	6.1369581	4.4686680
47 H	−0.0703116	6.9384481	3.2998719	−0.0779255	6.9580760	3.2916532	−0.0878884	6.9809553	3.2838892	−0.0844994	6.9727284	3.2867440
48 H	4.0195153	8.4988483	2.5656445	4.0113400	8.5055153	2.5620198	4.0045058	8.5087160	2.5593510	4.0069531	8.5073476	2.5603339
49 H	4.6893302	7.9013188	4.0952357	4.6821396	7.8967078	4.0855619	4.6732819	7.8912823	4.0794533	4.6763293	7.8931730	4.0817383
50 H	3.7786216	9.4175368	4.0574833	3.7764183	9.4185589	4.0583312	3.7725085	9.4186625	4.0577322	3.7737643	9.4185445	4.0578805

Table S7 Coordinates of the optimized structure of **2a** (DFT-TPSS/def2-TZVP level of theory) in XYZ format and Ångström units.

	gas phase			COSMO C_6H_6			COSMO CH_2Cl_2			COSMO $CHCl_3$		
atom	x	y	z	x	y	z	x	y	z	x	y	z
1 Cl	1.2219528	10.3321666	7.7683978	1.2042366	10.3118488	7.7580560	1.1861184	10.2922386	7.7494119	1.1920294	10.2983665	7.7518184
2 Be	2.1481310	8.9036454	8.6231359	2.1615223	8.9043327	8.6304919	2.1744685	8.9059178	8.6390515	2.1704299	8.9053361	8.6361666
3 Cl	1.6792189	7.0676298	8.6448737	1.6629528	7.0665282	8.6332421	1.6456501	7.0667132	8.6241131	1.6510996	7.0666159	8.6267488
4 N	3.6038211	9.4086213	9.4807265	3.6034185	9.4080233	9.4808655	3.6043235	9.4077046	9.4815284	3.6038773	9.4077445	9.4812769
5 C	3.1813543	10.4317632	10.5086160	3.1827762	10.4318234	10.5118143	3.1847444	10.4319002	10.5153222	3.1840367	10.4318460	10.5141625
6 C	4.4926639	10.1083103	8.4797189	4.4960843	10.1078190	8.4801474	4.5002073	10.1075835	8.4808373	4.4988001	10.1076173	8.4806234
7 C	4.2974229	8.2270194	10.1173420	4.3007731	8.2265445	10.1198517	4.3051000	8.2261417	10.1226176	4.3035788	8.2262404	10.1217174
8 C	2.1815432	9.8898386	11.5252018	2.1783404	9.8903970	11.5234962	2.1738195	9.8904723	11.5200012	2.1754296	9.8904920	11.5213402
9 C	5.5744482	8.5395698	10.8960547	5.5769107	8.5440179	10.8969093	5.5805591	8.5483987	10.8976693	5.5792685	8.5470014	10.8973840
10 C	4.8926759	9.2212663	7.3053181	4.8891036	9.2217837	7.3031084	4.8849904	9.2222454	7.3010255	4.8864046	9.2221372	7.3017175
11 H	2.7236146	11.2436847	9.9379762	2.7336648	11.2505023	9.9441813	2.7453362	11.2574535	9.9502218	2.7413923	11.2551618	9.9482653
12 H	4.0776404	10.8250110	11.0037343	4.0801093	10.8167141	11.0093854	4.0821817	10.8078451	11.0174484	4.0815614	10.8107461	11.0145820
13 H	1.8232115	10.7188840	12.1430297	1.8241262	10.7189752	12.1441329	1.8223951	10.7179826	12.1433792	1.8232219	10.7184257	12.1438107
14 H	2.6201414	9.1417838	12.1919164	2.6120177	9.1366330	12.1867467	2.6014334	9.1307336	12.1800884	2.6051528	9.1327612	12.1824620
15 H	1.3112844	9.4445007	11.0296419	1.3049501	9.4524777	11.0256578	1.2984075	9.4600156	11.0177163	1.3005715	9.4575487	11.0207589
16 H	4.4984615	7.5176037	9.3136056	4.5061263	7.5178885	9.3164968	4.5139878	7.5180514	9.3195767	4.5113657	7.5179762	9.3185913
17 H	3.5594966	7.7461070	10.7611363	3.5652945	7.7471559	10.7676385	3.5719198	7.7481980	10.7741603	3.5696992	7.7478952	10.7721262
18 H	5.9699184	7.5995912	11.2944044	5.9726029	7.6040184	11.2949333	5.9766091	7.6087373	11.2959199	5.9751762	7.6072055	11.2955579
19 H	5.3971255	9.2059542	11.7456114	5.3975635	9.2105065	11.7457387	5.3993118	9.2156561	11.7452118	5.3986735	9.2140043	11.7453623
20 H	6.3542585	8.9811339	10.2678385	6.3548853	8.9859846	10.2670211	6.3563382	8.9904911	10.2655495	6.3557973	8.9890142	10.2659982
21 H	5.3748017	10.4978132	9.0021919	5.3799297	10.4882213	9.0043579	5.3864196	10.4788546	9.0056483	5.3841607	10.4818720	9.0053827
22 H	3.9082063	10.9575227	8.1169511	3.9193622	10.9644857	8.1228669	3.9307443	10.9714859	8.1295094	3.9270128	10.9691939	8.1273275
23 H	5.4166292	9.8320211	6.5637046	5.4171374	9.8318962	6.5639785	5.4164931	9.8310538	6.5635451	5.4168390	9.8314512	6.5637947
24 H	4.0118293	8.7894817	6.8157326	4.0057506	8.7974752	6.8101661	3.9982630	8.8052454	6.8063010	4.0008680	8.8027975	6.8073824
25 H	5.5603886	8.4063662	7.5990398	5.5506010	8.4012367	7.5946153	5.5404182	8.3961699	7.5900457	5.5437932	8.3978392	7.5915423

Table S8 Coordinates of the optimized structure of **2b** (DFT-TPSS/def2-TZVP level of theory) in XYZ format and Ångström units.

	gas phase			COSMO C_6H_6			COSMO CH_2Cl_2			COSMO $CHCl_3$		
atom	x	y	z	x	y	z	x	y	z	x	y	z
1 Br	1.1295114	10.4314944	7.6860833	1.1074459	10.4134628	7.6816493	1.0826241	10.3952511	7.6796686	1.0908494	10.4010994	7.6801517
2 Be	2.1541285	8.9016070	8.6257261	2.1668863	8.9043209	8.6348774	2.1793214	8.9074499	8.6440113	2.1754401	8.9065025	8.6411477
3 Br	1.6141467	6.9189444	8.6285879	1.5986746	6.9197985	8.6160387	1.5855906	6.9196965	8.6020438	1.5896469	6.9197908	8.6068973
4 N	3.6055612	9.4078665	9.4820354	3.6061754	9.4079539	9.4826316	3.6072787	9.4083802	9.4834665	3.6068655	9.4082085	9.4831447
5 C	3.1868530	10.4317869	10.5134051	3.1888716	10.4321138	10.5170392	3.1915970	10.4327891	10.5208923	3.1907254	10.4325203	10.5196753
6 C	4.4996348	10.1093535	8.4840684	4.5030386	10.1090878	8.4840916	4.5069973	10.1089394	8.4843148	4.5057062	10.1089619	8.4842074
7 C	4.3036822	8.2274961	10.1208102	4.3074815	8.2272521	10.1232006	4.3115795	8.2270628	10.1259704	4.3102765	8.2271033	10.1250201
8 C	2.1888650	9.8919688	11.5323888	2.1844082	9.8922681	11.5291302	2.1795702	9.8928149	11.5247679	2.1810682	9.8926337	11.5261603
9 C	5.5797385	8.5440279	10.8989995	5.5831947	8.5479857	10.8991764	5.5869559	8.5519427	10.8995957	5.5857097	8.5507277	10.8994756
10 C	4.9006424	9.2261725	7.3075293	4.8979456	9.2255182	7.3061695	4.8944982	9.2247407	7.3048829	4.8956152	9.2249654	7.3052685
11 H	2.7305301	11.2461002	9.9446255	2.7423627	11.2536579	9.9512230	2.7560117	11.2619604	9.9579261	2.7517225	11.2593572	9.9558611
12 H	4.0868601	10.8203736	11.0048469	4.0892398	10.8116275	11.0126746	4.0920055	10.8023656	11.0218414	4.0911713	10.8051769	11.0189294
13 H	1.8380669	10.7215107	12.1538531	1.8363531	10.7209729	12.1530468	1.8334137	10.7200701	12.1513671	1.8345034	10.7203137	12.1520596
14 H	2.6258417	9.1393859	12.1949648	2.6154097	9.1337535	12.1885727	2.6037828	9.1281301	12.1812053	2.6073163	9.1296945	12.1834002
15 H	1.3136774	9.4534981	11.0392167	1.3070470	9.4613141	11.0318748	1.3007832	9.4694219	11.0219295	1.3025896	9.4671043	11.0251449
16 H	4.5066317	7.5180113	9.3175790	4.5139714	7.5185621	9.3201258	4.5210791	7.5189386	9.3231275	4.5189667	7.5188669	9.3220971
17 H	3.5670057	7.7455116	10.7652810	3.5733164	7.7471165	10.7719867	3.5795649	7.7490812	10.7788598	3.5776085	7.7483982	10.7765872
18 H	5.9756395	7.6043016	11.2974774	5.9790259	7.6080441	11.2971399	5.9830403	7.6120751	11.2972705	5.9818678	7.6108306	11.2970626
19 H	5.4014379	9.2100329	11.7485130	5.4034437	9.2142228	11.7479723	5.4057960	9.2186162	11.7474676	5.4048595	9.2170792	11.7477577
20 H	6.3593535	8.9856687	10.2707867	6.3606961	8.9897267	10.2687469	6.3621547	8.9938459	10.2668359	6.3615630	8.9928327	10.2675340
21 H	5.3802884	10.4929827	9.0127832	5.3851407	10.4856059	9.0134908	5.3911281	10.4777082	9.0138822	5.3891647	10.4802135	9.0137658
22 H	3.9189034	10.9623397	8.1236767	3.9288969	10.9681960	8.1281341	3.9397086	10.9745136	8.1332451	3.9362621	10.9724980	8.1315653
23 H	5.4317708	9.8384156	6.5722895	5.4316535	9.8366739	6.5720455	5.4309608	9.8339396	6.5713740	5.4309765	9.8348304	6.5714384
24 H	4.0196905	8.8029014	6.8104214	4.0150560	8.8069502	6.8071467	4.0087876	8.8114800	6.8048111	4.0108596	8.8098023	6.8056280
25 H	5.5617787	8.4055381	7.5999511	5.5545047	8.4011040	7.5977149	5.5460100	8.3960763	7.5951428	5.5489056	8.3977781	7.5959202

Table S9 Coordinates of the optimized structure of **2c** (DFT-TPSS/def2-TZVP level of theory) in XYZ format and Ångström units.

	gas phase			COSMO C_6H_6			COSMO CH_2Cl_2			COSMO $CHCl_3$		
atom	x	y	z	x	y	z	x	y	z	x	y	z
1 Br	0.9193054	10.5902401	7.6664652	0.9070884	10.5667554	7.6450794	0.8996255	10.5412932	7.6184021	0.9022154	10.5497389	7.6267174
2 Be	2.1493113	8.9033477	8.6224797	2.1656899	8.9040840	8.6289139	2.1836162	8.9049216	8.6366586	2.1770618	8.9046049	8.6339706
3 Br	1.5824718	6.6981373	8.4787379	1.5657455	6.6970922	8.4735545	1.5449263	6.6968092	8.4782155	1.5512578	6.6972036	8.4772276
4 N	3.6015930	9.4084170	9.4825891	3.6034796	9.4083832	9.4830553	3.6071901	9.4088461	9.4845369	3.6056075	9.4086189	9.4838763
5 C	3.2004275	10.4381296	10.5174540	3.2016918	10.4387262	10.5195834	3.2035769	10.4390679	10.5229430	3.2026857	10.4388563	10.5217379
6 C	4.5015371	10.1060884	8.4837163	4.5072785	10.1058991	8.4848987	4.5141823	10.1064707	8.4868191	4.5115931	10.1063707	8.4861848
7 C	4.3017879	8.2289505	10.1258772	4.3057497	8.2285619	10.1291975	4.3117557	8.2282556	10.1328512	4.3094886	8.2283510	10.1314253
8 C	2.2093707	9.9090277	11.5476730	2.2084485	9.9082432	11.5464852	2.2046341	9.9066007	11.5427174	2.2060600	9.9070942	11.5443253
9 C	5.5780588	8.5481979	10.9027805	5.5792046	8.5519106	10.9078410	5.5825419	8.5556775	10.9127387	5.5814097	8.5543380	10.9105976
10 C	4.9279750	9.2154865	7.3221981	4.9197308	9.2182065	7.3166451	4.9091739	9.2218962	7.3107861	4.9133678	9.2207323	7.3130534
11 H	2.7463752	11.2567667	9.9528511	2.7532784	11.2614740	9.9567634	2.7633825	11.2671351	9.9616208	2.7594762	11.2650453	9.9600022
12 H	4.1103707	10.8173741	10.9973607	4.1114318	10.8137221	11.0011600	4.1120679	10.8081924	11.0092427	4.1117125	10.8100834	11.0061296
13 H	1.8708887	10.7436720	12.1690916	1.8703821	10.7421646	12.1689737	1.8667478	10.7388953	12.1672436	1.8683991	10.7400439	12.1681871
14 H	2.6468227	9.1553822	12.2085831	2.6449433	9.1526333	12.2056182	2.6370735	9.1468976	12.1995802	2.6401051	9.1488895	12.2019140
15 H	1.3255162	9.4777359	11.0634393	1.3236831	9.4783442	11.0613746	1.3196025	9.4805133	11.0530220	1.3208945	9.4796916	11.0567209
16 H	4.5042079	7.5165306	9.3252470	4.5147196	7.5179505	9.3285820	4.5265385	7.5197034	9.3318194	4.5221177	7.5189753	9.3306180
17 H	3.5656733	7.7497005	10.7735204	3.5703835	7.7500397	10.7782747	3.5771699	7.7502425	10.7832637	3.5747755	7.7503131	10.7816191
18 H	5.9746484	7.6080663	11.2996254	5.9751693	7.6116946	11.3050456	5.9780277	7.6153676	11.3100349	5.9768539	7.6140306	11.3079922
19 H	5.4004381	9.2127667	11.7533295	5.3971260	9.2163568	11.7574033	5.3962238	9.2198729	11.7613381	5.3968936	9.2188226	11.7594312
20 H	6.3566356	8.9905604	10.2739885	6.3574154	8.9950935	10.2794011	6.3600216	8.9998501	10.2844306	6.3591597	8.9977962	10.2820315
21 H	5.3711585	10.5028150	9.0207342	5.3817093	10.4889280	9.0221615	5.3946747	10.4741147	9.0229503	5.3896820	10.4796183	9.0230442
22 H	3.9183170	10.9520113	8.1089701	3.9336912	10.9620641	8.1193368	3.9506482	10.9737323	8.1324760	3.9445247	10.9696455	8.1276720
23 H	5.4618483	9.8273102	6.5886153	5.4613104	9.8283738	6.5874841	5.4563588	9.8299834	6.5843092	5.4589865	9.8295940	6.5859717
24 H	4.0601608	8.7740242	6.8181369	4.0455190	8.7929707	6.8081758	4.0268059	8.8131136	6.8008740	4.0342367	8.8061394	6.8030499
25 H	5.5953401	8.4065514	7.6324360	5.5753703	8.3976180	7.6208910	5.5536740	8.3898370	7.6070259	5.5616749	8.3926923	7.6124004

Table S10 NPA and IAO results for **1a** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	NPA	IAO	NPA	IAO	NPA	IAO	NPA	IAO
1 Cl	−0.77147	−0.79152	−0.78055	−0.79813	−0.78957	−0.80473	−0.78645	−0.80244
2 Be	1.46672	1.44046	1.47175	1.44106	1.47674	1.44158	1.47502	1.44141
3 Cl	−0.71883	−0.72799	−0.72081	−0.7301	−0.72274	−0.73213	−0.72208	−0.73144
4 Be	1.46672	1.44046	1.47175	1.44105	1.47672	1.44157	1.47501	1.4414
5 N	−0.60667	−0.38053	−0.61282	−0.38641	−0.61924	−0.39247	−0.61698	−0.39035
6 C	−0.22385	−0.14588	−0.22429	−0.14674	−0.22481	−0.14761	−0.22462	−0.14731
7 C	−0.21433	−0.14503	−0.21574	−0.14642	−0.21716	−0.14776	−0.21666	−0.1473
8 C	−0.23	−0.15542	−0.22809	−0.15484	−0.22603	−0.15403	−0.22676	−0.15431
9 C	−0.5988	−0.4089	−0.60157	−0.41076	−0.60396	−0.41227	−0.60317	−0.41177
10 C	−0.61041	−0.41733	−0.61366	−0.41917	−0.61655	−0.42086	−0.61559	−0.4203
11 C	−0.59834	−0.4086	−0.60041	−0.41012	−0.60218	−0.41136	−0.60159	−0.41095
12 H	0.17459	0.11635	0.18153	0.12311	0.18935	0.13068	0.18654	0.12797
13 H	0.22197	0.15480	0.22015	0.15388	0.21799	0.15266	0.21877	0.15311
14 H	0.19450	0.13239	0.19803	0.13547	0.20169	0.13868	0.20041	0.13755
15 H	0.21392	0.14928	0.21813	0.15299	0.22235	0.15671	0.22089	0.15542
16 H	0.22267	0.15272	0.21758	0.14799	0.21168	0.14245	0.21381	0.14445
17 H	0.21568	0.15013	0.21509	0.14996	0.21416	0.14942	0.21452	0.14964
18 H	0.22330	0.15500	0.21988	0.15236	0.21593	0.14918	0.21736	0.15033
19 H	0.19550	0.13228	0.19883	0.13533	0.20271	0.13895	0.20130	0.13764
20 H	0.22139	0.15554	0.22337	0.15715	0.22478	0.15832	0.22435	0.15796
21 H	0.19873	0.13601	0.20184	0.13884	0.20518	0.14194	0.20400	0.14084
22 H	0.17797	0.12061	0.18458	0.12715	0.19205	0.13445	0.18937	0.13183
23 H	0.21034	0.14767	0.21069	0.14866	0.21066	0.1493	0.21071	0.14911
24 H	0.20914	0.14471	0.21392	0.14895	0.21899	0.15348	0.21721	0.15189
25 H	0.22527	0.15440	0.21949	0.14924	0.21304	0.14335	0.21533	0.14545
26 H	0.20102	0.13886	0.20306	0.14053	0.20487	0.14202	0.20426	0.14152
27 Cl	−0.71884	−0.72799	−0.72077	−0.73007	−0.72266	−0.73208	−0.72202	−0.7314
28 Cl	−0.77147	−0.79153	−0.78053	−0.79811	−0.78951	−0.80466	−0.78642	−0.80241
29 N	−0.60667	−0.38052	−0.61282	−0.3864	−0.61921	−0.39245	−0.61696	−0.39034
30 C	−0.22385	−0.14589	−0.22428	−0.14674	−0.22481	−0.1476	−0.22461	−0.1473
31 C	−0.23001	−0.15542	−0.22804	−0.15481	−0.22593	−0.15398	−0.22668	−0.15426
32 C	−0.21433	−0.14503	−0.21574	−0.14642	−0.21716	−0.14777	−0.21667	−0.14731
33 C	−0.5988	−0.4089	−0.60156	−0.41075	−0.60394	−0.41226	−0.60316	−0.41176
34 H	0.17459	0.11635	0.18153	0.12312	0.18937	0.1307	0.18656	0.12799
35 H	0.22198	0.15481	0.22013	0.15387	0.21797	0.15264	0.21875	0.15309
36 C	−0.61041	−0.41733	−0.61366	−0.41917	−0.61655	−0.42085	−0.61559	−0.4203
37 H	0.21568	0.15012	0.21500	0.14988	0.21399	0.14926	0.21438	0.14951
38 H	0.22331	0.15500	0.21989	0.15237	0.21591	0.1492	0.21735	0.15035
39 C	−0.59834	−0.4086	−0.60041	−0.41012	−0.60217	−0.41135	−0.60159	−0.41096
40 H	0.17797	0.12061	0.18460	0.12717	0.19209	0.13448	0.18940	0.13186
41 H	0.21034	0.14768	0.21068	0.14865	0.21063	0.14928	0.21070	0.1491
42 H	0.19450	0.13239	0.19801	0.13545	0.20165	0.13864	0.20038	0.13753
43 H	0.21392	0.14928	0.21814	0.153	0.22237	0.15672	0.22091	0.15543
44 H	0.22267	0.15272	0.21758	0.14799	0.21169	0.14246	0.21382	0.14446
45 H	0.19550	0.13227	0.19882	0.13533	0.20271	0.13896	0.20130	0.13763
46 H	0.22139	0.15553	0.22338	0.15717	0.22479	0.15832	0.22437	0.15798
47 H	0.19874	0.13601	0.20185	0.13885	0.20522	0.14198	0.20402	0.14087
48 H	0.20914	0.14471	0.21393	0.14896	0.21902	0.15351	0.21723	0.15191
49 H	0.22527	0.15439	0.21949	0.14923	0.21301	0.14333	0.21532	0.14544
50 H	0.12297	0.13886	0.20305	0.14052	0.20487	0.14202	0.20426	0.14152

Table S11 NPA and IAO results for **1b** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	NPA	IAO	NPA	IAO	NPA	IAO	NPA	IAO
1 Br	−0.73676	−0.77157	−0.74155	−0.77972	−0.75327	−0.78814	−0.74919	−0.7852
2 Be	1.38134	1.4028	1.38755	1.4041	1.39438	1.4054	1.39201	1.4049
3 Br	−0.66665	−0.70696	−0.66816	−0.70931	−0.67025	−0.7114	−0.66956	−0.71071
4 Be	1.38135	1.4028	1.38754	1.4041	1.39436	1.4054	1.39199	1.4049
5 N	−0.60829	−0.38748	−0.62772	−0.39358	−0.63473	−0.40006	−0.63226	−0.39779
6 C	−0.20571	−0.14582	−0.22553	−0.14668	−0.2259	−0.14756	−0.22576	−0.14725
7 C	−0.19636	−0.14524	−0.21708	−0.14659	−0.21845	−0.14791	−0.21797	−0.14745
8 C	−0.20529	−0.15477	−0.22946	−0.15406	−0.22731	−0.15326	−0.22806	−0.15354
9 C	−0.58548	−0.40894	−0.6029	−0.41083	−0.60518	−0.41242	−0.60443	−0.4119
10 C	−0.59341	−0.41802	−0.61421	−0.41993	−0.61709	−0.42161	−0.61613	−0.42105
11 C	−0.57975	−0.40827	−0.60241	−0.4099	−0.60414	−0.41124	−0.60358	−0.41081
12 H	0.16793	0.1178	0.18327	0.1248	0.19141	0.1327	0.18850	0.1299
13 H	0.21337	0.1543	0.22081	0.1534	0.21858	0.1523	0.21938	0.1527
14 H	0.19067	0.1335	0.19914	0.1367	0.20284	0.1400	0.20153	0.1388
15 H	0.21045	0.1507	0.22020	0.1545	0.22445	0.1583	0.22298	0.1569
16 H	0.21520	0.1509	0.21708	0.1462	0.21116	0.1407	0.21330	0.1427
17 H	0.20327	0.1488	0.21608	0.1488	0.21520	0.1484	0.21553	0.1486
18 H	0.21284	0.1542	0.21999	0.1516	0.21627	0.1484	0.21761	0.1496
19 H	0.18858	0.1331	0.19953	0.1363	0.20361	0.1401	0.20213	0.1387
20 H	0.21503	0.1571	0.22480	0.1588	0.22609	0.1598	0.22572	0.1595
21 H	0.19270	0.1369	0.20279	0.1399	0.20619	0.1431	0.20499	0.1420
22 H	0.16952	0.1218	0.18657	0.1285	0.19430	0.1361	0.19153	0.1334
23 H	0.20086	0.1469	0.21182	0.1480	0.21182	0.1488	0.21186	0.1485
24 H	0.20341	0.1463	0.21595	0.1507	0.22120	0.1555	0.21936	0.1538
25 H	0.21682	0.1519	0.21888	0.1468	0.21241	0.1410	0.21474	0.1431
26 H	0.19566	0.1401	0.20455	0.1416	0.20632	0.1431	0.20571	0.1426
27 Br	−0.6666	−0.70697	−0.66811	−0.70926	−0.67013	−0.71131	−0.66946	−0.71064
28 Br	−0.73676	−0.77158	−0.7415	−0.77967	−0.75318	−0.78804	−0.74912	−0.78512
29 N	−0.60831	−0.38748	−0.62772	−0.39358	−0.63471	−0.40003	−0.63224	−0.39777
30 C	−0.20579	−0.14582	−0.22552	−0.14667	−0.22589	−0.14755	−0.22575	−0.14725
31 C	−0.20518	−0.15477	−0.22937	−0.154	−0.22708	−0.15312	−0.22788	−0.15343
32 C	−0.19634	−0.14524	−0.2171	−0.1466	−0.21845	−0.14792	−0.21798	−0.14747
33 C	−0.58545	−0.40894	−0.6029	−0.41083	−0.60517	−0.41241	−0.60442	−0.41189
34 H	0.16792	0.1178	0.18327	0.1248	0.19142	0.1327	0.18850	0.1299
35 H	0.21339	0.1543	0.22079	0.1534	0.21858	0.1523	0.21938	0.1527
36 C	−0.59347	−0.41802	−0.61422	−0.41993	−0.61709	−0.42162	−0.61613	−0.42106
37 H	0.20326	0.1488	0.21598	0.1487	0.21501	0.1483	0.21538	0.1485
38 H	0.21280	0.1542	0.21990	0.1515	0.21606	0.1483	0.21745	0.1495
39 C	−0.5798	−0.40827	−0.60242	−0.4099	−0.60414	−0.41124	−0.60358	−0.41081
40 H	0.16955	0.1218	0.18658	0.1285	0.19432	0.1361	0.19156	0.1334
41 H	0.20088	0.1469	0.21183	0.1480	0.21181	0.1488	0.21185	0.1485
42 H	0.19067	0.1335	0.19913	0.1367	0.20281	0.1399	0.20151	0.1388
43 H	0.21047	0.1507	0.22021	0.1545	0.22447	0.1583	0.22300	0.1570
44 H	0.21521	0.1509	0.21710	0.1462	0.21117	0.1407	0.21331	0.1427
45 H	0.18860	0.1331	0.19954	0.1363	0.20361	0.1401	0.20212	0.1387
46 H	0.21503	0.1571	0.22482	0.1588	0.22613	0.1599	0.22575	0.1595
47 H	0.19271	0.1369	0.20281	0.1399	0.20624	0.1432	0.20503	0.1420
48 H	0.20342	0.1463	0.21596	0.1507	0.22121	0.1555	0.21936	0.1538
49 H	0.21682	0.1519	0.21889	0.1468	0.21241	0.1410	0.21473	0.1431
50 H	0.19566	0.1401	0.20454	0.1416	0.20632	0.1431	0.20571	0.1426

Table S12 NPA and IAO results for **1c** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	NPA	IAO	NPA	IAO	NPA	IAO	NPA	IAO
1 I	−0.66793	−0.73866	−0.68311	−0.74937	−0.69914	−0.7608	−0.6935	−0.75676
2 Be	1.25513	1.3466	1.26405	1.3490	1.27324	1.3514	1.27001	1.3506
3 I	−0.58713	−0.67579	−0.589	−0.67772	−0.59022	−0.67898	−0.58986	−0.67862
4 Be	1.25513	1.3466	1.26405	1.3490	1.27322	1.3514	1.27000	1.3506
5 N	−0.63626	−0.39309	−0.64307	−0.39929	−0.65025	−0.40573	−0.64771	−0.40346
6 C	−0.22734	−0.14608	−0.22743	−0.14693	−0.22772	−0.1478	−0.22761	−0.14749
7 C	−0.21732	−0.14497	−0.21855	−0.14628	−0.21985	−0.14758	−0.21939	−0.14713
8 C	−0.23398	−0.15434	−0.23162	−0.15376	−0.22916	−0.1532	−0.22999	−0.15339
9 C	−0.60261	−0.4095	−0.60515	−0.41131	−0.60733	−0.41283	−0.60661	−0.41234
10 C	−0.61169	−0.41811	−0.61483	−0.41979	−0.61757	−0.42121	−0.61666	−0.42075
11 C	−0.60303	−0.4093	−0.60494	−0.41067	−0.60648	−0.41178	−0.60598	−0.41143
12 H	0.17766	0.1192	0.18512	0.1264	0.19348	0.1344	0.19049	0.1315
13 H	0.22312	0.1527	0.22118	0.1518	0.21901	0.1507	0.21980	0.1511
14 H	0.19666	0.1339	0.20026	0.1372	0.20403	0.1406	0.20270	0.1394
15 H	0.21849	0.1530	0.22264	0.1566	0.22673	0.1602	0.22533	0.1590
16 H	0.22126	0.1484	0.21623	0.1438	0.2104	0.1385	0.21250	0.1404
17 H	0.21679	0.1468	0.21617	0.1469	0.21528	0.1467	0.21561	0.1468
18 H	0.22240	0.1520	0.21917	0.1496	0.21551	0.1469	0.21680	0.1479
19 H	0.19675	0.1338	0.20035	0.1371	0.20454	0.1410	0.20302	0.1396
20 H	0.22433	0.1588	0.22621	0.1603	0.22741	0.1612	0.22706	0.1609
21 H	0.20069	0.1378	0.20385	0.1406	0.20725	0.1438	0.20605	0.1427
22 H	0.18154	0.1233	0.18858	0.1301	0.19648	0.1378	0.19366	0.1350
23 H	0.21153	0.1452	0.21182	0.1463	0.21187	0.1473	0.21188	0.1470
24 H	0.21314	0.1482	0.21812	0.1526	0.22337	0.1573	0.22153	0.1557
25 H	0.22315	0.1493	0.21762	0.1443	0.21126	0.1384	0.21355	0.1405
26 H	0.20465	0.1412	0.20633	0.1425	0.20787	0.1438	0.20734	0.1434
27 I	−0.58713	−0.67579	−0.58903	−0.67774	−0.59027	−0.67902	−0.5899	−0.67866
28 I	−0.66793	−0.73866	−0.6831	−0.74936	−0.69909	−0.76075	−0.69346	−0.75673
29 N	−0.63627	−0.39309	−0.64307	−0.39928	−0.65023	−0.40571	−0.64769	−0.40344
30 C	−0.22733	−0.14607	−0.22743	−0.14692	−0.22772	−0.1478	−0.22761	−0.14749
31 C	−0.23398	−0.15434	−0.2316	−0.15375	−0.22914	−0.15319	−0.22998	−0.15339
32 C	−0.21732	−0.14497	−0.21855	−0.14628	−0.21985	−0.14759	−0.21939	−0.14713
33 C	−0.60262	−0.4095	−0.60511	−0.41128	−0.60725	−0.41279	−0.60655	−0.4123
34 H	0.17767	0.1192	0.18512	0.1264	0.19349	0.1344	0.19050	0.1315
35 H	0.22311	0.1527	0.22118	0.1518	0.21902	0.1507	0.21980	0.1511
36 C	−0.61169	−0.41811	−0.61484	−0.41979	−0.61756	−0.42121	−0.61665	−0.42074
37 H	0.21679	0.1468	0.21618	0.1469	0.21531	0.1467	0.21563	0.1468
38 H	0.22240	0.1520	0.21912	0.1496	0.2154	0.1469	0.21673	0.1478
39 C	−0.60303	−0.40929	−0.60493	−0.41067	−0.60646	−0.41176	−0.60596	−0.41141
40 H	0.18154	0.1233	0.18859	0.1301	0.1965	0.1378	0.19367	0.1350
41 H	0.21153	0.1452	0.21181	0.1463	0.21186	0.1473	0.21188	0.1470
42 H	0.19666	0.1339	0.20028	0.1372	0.20406	0.1406	0.20273	0.1394
43 H	0.21849	0.1530	0.22265	0.1566	0.22676	0.1603	0.22535	0.1590
44 H	0.22126	0.1484	0.21615	0.1438	0.21023	0.1384	0.21236	0.1403
45 H	0.19675	0.1338	0.20035	0.1371	0.20452	0.1410	0.20301	0.1396
46 H	0.22433	0.1588	0.22623	0.1603	0.22741	0.1612	0.22706	0.1609
47 H	0.20069	0.1378	0.20387	0.1407	0.20728	0.1438	0.20608	0.1427
48 H	0.21313	0.1482	0.21811	0.1526	0.22335	0.1573	0.22151	0.1556
49 H	0.22315	0.1493	0.21762	0.1443	0.21125	0.1384	0.21354	0.1405
50 H	0.20465	0.1412	0.20633	0.1425	0.20788	0.1438	0.20735	0.1434

Table S13 NPA and IAO results for **2a** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	NPA	IAO	NPA	IAO	NPA	IAO	NPA	IAO
1 Cl	−0.75576	−0.77879	−0.7655	−0.78633	−0.77451	−0.79307	−0.77174	−0.79099
2 Be	1.47973	1.4680	1.48828	1.4687	1.49626	1.4692	1.49379	1.4691
3 Cl	−0.75183	−0.78078	−0.76155	−0.78714	−0.77072	−0.79301	−0.76787	−0.79118
4 N	−0.60586	−0.3829	−0.61514	−0.39201	−0.62453	−0.40086	−0.62154	−0.39805
5 C	−0.22298	−0.15162	−0.22323	−0.15244	−0.22377	−0.1533	−0.22357	−0.153
6 C	−0.22357	−0.15079	−0.22383	−0.15158	−0.22429	−0.15244	−0.22413	−0.15216
7 C	−0.223	−0.15183	−0.22239	−0.15226	−0.22181	−0.15265	−0.22199	−0.15252
8 C	−0.60044	−0.41111	−0.60363	−0.41311	−0.60606	−0.41454	−0.60536	−0.41412
9 C	−0.61234	−0.41978	−0.61523	−0.42127	−0.61758	−0.4224	−0.61689	−0.42208
10 C	−0.60131	−0.41064	−0.60473	−0.41272	−0.60726	−0.41421	−0.30355	−0.4138
11 H	0.22166	0.1575	0.21954	0.1568	0.21759	0.1561	0.21819	0.1563
12 H	0.18070	0.1233	0.18871	0.1310	0.19724	0.1391	0.19448	0.1365
13 H	0.22002	0.1553	0.22460	0.1594	0.22904	0.1632	0.22765	0.1620
14 H	0.19867	0.1373	0.20286	0.1410	0.20707	0.1447	0.20573	0.1435
15 H	0.21304	0.1457	0.20884	0.1414	0.20334	0.1359	0.20522	0.1378
16 H	0.21495	0.1533	0.21463	0.1534	0.21407	0.1532	0.21427	0.1533
17 H	0.21586	0.1536	0.21535	0.1536	0.21465	0.1533	0.21488	0.1534
18 H	0.22089	0.1554	0.22405	0.1583	0.22672	0.1607	0.22593	0.1600
19 H	0.19799	0.1355	0.20105	0.1384	0.20425	0.1414	0.20323	0.1404
20 H	0.19806	0.1354	0.20118	0.1383	0.20446	0.1414	0.20341	0.1404
21 H	0.18078	0.1234	0.18850	0.1312	0.19741	0.1393	0.19464	0.1367
22 H	0.22229	0.1571	0.22007	0.1563	0.21800	0.1556	0.21863	0.1558
23 H	0.22049	0.1555	0.22513	0.1595	0.22961	0.1634	0.22821	0.1621
24 H	0.21302	0.1451	0.20888	0.1408	0.20341	0.1355	0.20527	0.1373
25 H	0.19893	0.1371	0.20321	0.1408	0.20744	0.1445	0.20611	0.1433

Table S14 NPA and IAO results for **2b** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	NPA	IAO	NPA	IAO	NPA	IAO	NPA	IAO
1 Br	−0.71172	−0.75527	−0.72331	−0.76394	−0.73426	−0.77197	−0.73085	−0.76948
2 Be	1.39646	1.4244	1.40757	1.4264	1.41837	1.4281	1.41500	1.4275
3 Br	−0.70658	−0.75697	−0.71806	−0.76422	−0.72915	−0.77125	−0.72568	−0.76904
4 N	−0.61871	−0.38993	−0.62786	−0.39846	−0.63726	−0.40714	−0.63429	−0.4044
5 C	−0.22447	−0.15112	−0.22451	−0.1524	−0.22481	−0.15365	−0.22469	−0.15327
6 C	−0.22535	−0.15076	−0.22529	−0.152	−0.2255	−0.15323	−0.2254	−0.15284
7 C	−0.22538	−0.15208	−0.22441	−0.15234	−0.22352	−0.15253	−0.22379	−0.15247
8 C	−0.60122	−0.41093	−0.60436	−0.41308	−0.60678	−0.41477	−0.60607	−0.41429
9 C	−0.61279	−0.41973	−0.61562	−0.42133	−0.61794	−0.42256	−0.61726	−0.42222
10 C	−0.60218	−0.41096	−0.60543	−0.41308	−0.60787	−0.41466	−0.60718	−0.41422
11 H	0.22277	0.1560	0.22046	0.1555	0.21834	0.1550	0.21899	0.1551
12 H	0.18200	0.1244	0.19019	0.1324	0.19888	0.1409	0.19608	0.1381
13 H	0.22109	0.1563	0.22576	0.1603	0.23025	0.1643	0.22885	0.1630
14 H	0.19929	0.1374	0.20355	0.1414	0.20791	0.1454	0.20648	0.1441
15 H	0.21383	0.1452	0.20950	0.1409	0.20389	0.1355	0.20582	0.1373
16 H	0.21612	0.1533	0.21573	0.1534	0.21520	0.1533	0.21539	0.1534
17 H	0.21707	0.1536	0.21643	0.1536	0.21561	0.1533	0.21588	0.1534
18 H	0.22197	0.1565	0.22513	0.1593	0.22782	0.1617	0.22702	0.1610
19 H	0.19853	0.1359	0.20163	0.1389	0.20489	0.1420	0.20385	0.1410
20 H	0.19857	0.1358	0.20175	0.1388	0.20510	0.1419	0.20402	0.1409
21 H	0.18211	0.1242	0.19033	0.1322	0.19905	0.1407	0.19623	0.1379
22 H	0.22363	0.1562	0.22114	0.1555	0.21882	0.1550	0.21953	0.1551
23 H	0.22163	0.1564	0.22629	0.1604	0.23080	0.1643	0.22938	0.1631
24 H	0.21377	0.1448	0.20947	0.1406	0.20394	0.1352	0.20582	0.1371
25 H	0.19957	0.1374	0.20391	0.1414	0.20822	0.1453	0.20686	0.1441

Table S15 NPA and IAO results for **2c** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	NPA	IAO	NPA	IAO	NPA	IAO	NPA	IAO
1 I	−0.64472	−0.7187	−0.65866	−0.72885	−0.67279	−0.73893	−0.66791	−0.73549
2 Be	1.27242	1.3573	1.28676	1.3607	1.30180	1.3644	1.29540	1.3632
3 I	−0.63791	−0.7195	−0.65153	−0.72795	−0.66556	−0.73663	−0.66068	−0.73364
4 N	−0.6319	−0.39634	−0.641	−0.4049	−0.65072	−0.41387	−0.64727	−0.41072
5 C	−0.2264	−0.15171	−0.22592	−0.1524	−0.22577	−0.15312	−0.22576	−0.15288
6 C	−0.22743	−0.15211	−0.22718	−0.15291	−0.22723	−0.15365	−0.60685	−0.15341
7 C	−0.2286	−0.15242	−0.22735	−0.15269	−0.22618	−0.15314	−0.61784	−0.15298
8 C	−0.60226	−0.41139	−0.60524	−0.41334	−0.60756	−0.4149	−0.60685	−0.41444
9 C	−0.61353	−0.41971	−0.61627	−0.42114	−0.6186	−0.42228	−0.61784	−0.42193
10 C	−0.60339	−0.41202	−0.60647	−0.41402	−0.60889	−0.41553	−0.60813	−0.41508
11 H	0.22388	0.1550	0.22121	0.1542	0.21858	0.1535	0.21945	0.1537
12 H	0.18288	0.1254	0.19116	0.1334	0.20045	0.1423	0.19712	0.1391
13 H	0.22254	0.1575	0.22697	0.1614	0.23142	0.1653	0.22987	0.1639
14 H	0.19945	0.1376	0.20382	0.1415	0.20842	0.1457	0.20681	0.1442
15 H	0.21388	0.1442	0.20970	0.1401	0.20403	0.1345	0.20619	0.1366
16 H	0.21851	0.1533	0.21762	0.1531	0.21656	0.1529	0.21693	0.1530
17 H	0.21652	0.1525	0.21634	0.1529	0.21591	0.1529	0.21610	0.1530
18 H	0.22311	0.1574	0.22627	0.1602	0.22904	0.1627	0.22814	0.1619
19 H	0.19918	0.1365	0.20230	0.1394	0.20574	0.1427	0.20451	0.1415
20 H	0.19926	0.1363	0.20244	0.1394	0.20597	0.1428	0.20471	0.1416
21 H	0.18363	0.1261	0.19195	0.1340	0.20127	0.1428	0.19792	0.1396
22 H	0.22319	0.1546	0.22085	0.1541	0.21867	0.1537	0.21940	0.1539
23 H	0.22241	0.1572	0.22722	0.1613	0.23213	0.1656	0.23042	0.1641
24 H	0.21470	0.1449	0.21018	0.1404	0.20400	0.1343	0.20634	0.1366
25 H	0.20060	0.1383	0.20484	0.1421	0.20930	0.1461	0.20771	0.1447

Table S16 Mulliken population analysis and PABOON results for **1a** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON
1 Cl	−0.35220	−0.7222	−0.38371	−0.7549	−0.41563	−0.7874	−0.40450	−0.7762
2 Be	0.11248	0.3618	0.11400	0.3651	0.11553	0.3686	0.11500	0.3674
3 Cl	−0.25919	−0.6172	−0.26286	−0.5971	−0.26586	−0.5745	−0.26491	−0.5826
4 Be	0.11246	0.3618	0.11418	0.3651	0.11582	0.3686	0.11532	0.3674
5 N	0.07293	0.1870	0.07893	0.1891	0.08511	0.1919	0.08296	0.1908
6 C	−0.16408	0.0491	−0.16356	0.0455	−0.16269	0.0422	−0.16305	0.0433
7 C	−0.15225	0.0389	−0.15174	0.0383	−0.15012	0.0382	−0.15079	0.0382
8 C	−0.19747	0.0297	−0.19278	0.0316	−0.18851	0.0334	−0.18999	0.0328
9 C	−0.35573	−0.1244	−0.37073	−0.1316	−0.38357	−0.1382	−0.37935	−0.1360
10 C	−0.37053	−0.1414	−0.38429	−0.1458	−0.39515	−0.1492	−0.39167	−0.1482
11 C	−0.35495	−0.1212	−0.36722	−0.1285	−0.37798	−0.1351	−0.37437	−0.1329
12 H	0.11162	0.0441	0.12419	0.0505	0.13809	0.0574	0.13313	0.0550
13 H	0.13993	0.0780	0.13902	0.0775	0.13687	0.0764	0.13775	0.0769
14 H	0.11996	0.0641	0.12896	0.0680	0.13775	0.0717	0.13473	0.0704
15 H	0.11988	0.0636	0.12995	0.0694	0.13962	0.0747	0.13631	0.0729
16 H	0.16167	0.0908	0.15613	0.0862	0.14868	0.0804	0.15147	0.0825
17 H	0.15610	0.0805	0.15733	0.0806	0.15757	0.0800	0.15761	0.0803
18 H	0.16031	0.0920	0.15432	0.0888	0.14704	0.0845	0.14972	0.0861
19 H	0.12343	0.0637	0.13076	0.0676	0.13854	0.0718	0.13580	0.0703
20 H	0.13742	0.0790	0.14203	0.0809	0.14504	0.0820	0.14416	0.0817
21 H	0.13372	0.0666	0.14112	0.0704	0.14843	0.0741	0.14591	0.0728
22 H	0.11206	0.0466	0.12367	0.0527	0.13631	0.0592	0.13182	0.0569
23 H	0.14341	0.0703	0.14558	0.0717	0.14670	0.0725	0.14641	0.0723
24 H	0.11726	0.0614	0.12777	0.0677	0.13829	0.0736	0.13465	0.0716
25 H	0.16122	0.0908	0.15304	0.0851	0.14345	0.0784	0.14686	0.0808
26 H	0.12299	0.0682	0.12999	0.0712	0.13622	0.0736	0.13414	0.0729
27 Cl	−0.25917	−0.6171	−0.26271	−0.5971	−0.26555	−0.5747	−0.26468	−0.5828
28 Cl	−0.35219	−0.7222	−0.3837	−0.7549	−0.41550	−0.7873	−0.40448	−0.7762
29 N	0.07288	0.1869	0.07896	0.1891	0.08538	0.1919	0.08312	0.1908
30 C	−0.16407	0.0491	−0.16361	0.0455	−0.16283	0.0422	−0.16313	0.0433
31 C	−0.19744	0.0297	−0.19252	0.0317	−0.18823	0.0336	−0.18963	0.0330
32 C	−0.15223	0.0389	−0.15183	0.0383	−0.15029	0.0382	−0.15097	0.0381
33 C	−0.35572	−0.1244	−0.37065	−0.1316	−0.38337	−0.1382	−0.37919	−0.1360
34 H	0.11161	0.0441	0.12421	0.0505	0.13813	0.0575	0.13316	0.0550
35 H	0.13993	0.0780	0.13896	0.0775	0.13674	0.0763	0.13762	0.0768
36 C	−0.37054	−0.1414	−0.38430	−0.1458	−0.39507	−0.1491	−0.39167	−0.1481
37 H	0.15608	0.0805	0.15693	0.0805	0.15686	0.0797	0.15698	0.0801
38 H	0.16032	0.0920	0.15439	0.0888	0.14716	0.0845	0.14981	0.0861
39 C	−0.35494	−0.1212	−0.36723	−0.1285	−0.37793	−0.1351	−0.37437	−0.1329
40 H	0.11207	0.0466	0.12376	0.0528	0.13648	0.0593	0.13196	0.0570
41 H	0.14342	0.0703	0.14553	0.0717	0.14656	0.0724	0.14635	0.0722
42 H	0.11995	0.0641	0.12894	0.0680	0.13770	0.0716	0.13469	0.0704
43 H	0.11989	0.0636	0.12996	0.0694	0.13965	0.0748	0.13633	0.0730
44 H	0.16166	0.0908	0.15609	0.0861	0.14861	0.0804	0.15141	0.0825
45 H	0.12343	0.0637	0.13075	0.0676	0.13850	0.0717	0.13577	0.0703
46 H	0.13741	0.0790	0.14205	0.0809	0.14504	0.0820	0.14419	0.0817
47 H	0.13372	0.0666	0.14115	0.0704	0.14851	0.0741	0.14596	0.0728
48 H	0.11726	0.0614	0.12781	0.0677	0.13836	0.0737	0.13471	0.0716
49 H	0.16123	0.0908	0.15302	0.0851	0.14331	0.0784	0.14680	0.0808
50 H	0.12297	0.0682	0.12998	0.0712	0.13622	0.0736	0.13413	0.0728

Table S17 Mulliken population analysis and PABOON results for **1b** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON
1 Br	−0.38809	−0.7558	−0.41164	−0.7757	−0.44823	−0.8134	−0.43543	−0.7997
2 Be	0.06686	0.3203	0.07482	0.3714	0.07467	0.3904	0.07470	0.3828
3 Br	−0.24199	−0.5332	−0.25227	−0.5075	−0.25315	−0.4673	−0.25297	−0.4837
4 Be	0.06682	0.3204	0.07500	0.3713	0.07475	0.3903	0.07473	0.3827
5 N	0.09625	0.1885	0.08788	0.1778	0.09446	0.1788	0.09216	0.1786
6 C	−0.16364	0.0510	−0.16352	0.0419	−0.16343	0.0372	−0.16352	0.0390
7 C	−0.17669	0.0353	−0.16257	0.0328	−0.16019	0.0319	−0.16118	0.0321
8 C	−0.19899	0.0396	−0.19518	0.0241	−0.19211	0.0233	−0.19311	0.0237
9 C	−0.37770	−0.1217	−0.37419	−0.1360	−0.38657	−0.1436	−0.38253	−0.1410
10 C	−0.37851	−0.1275	−0.38794	−0.1486	−0.39800	−0.1532	−0.39484	−0.1516
11 C	−0.35507	−0.1095	−0.36539	−0.1306	−0.37694	−0.1383	−0.37312	−0.1356
12 H	0.12607	0.0634	0.12686	0.0481	0.14119	0.0541	0.13611	0.0521
13 H	0.14646	0.0819	0.14836	0.0742	0.14695	0.0714	0.14757	0.0725
14 H	0.12793	0.0748	0.13187	0.0663	0.14052	0.0688	0.13752	0.0680
15 H	0.12287	0.0768	0.13153	0.0675	0.14117	0.0717	0.13789	0.0704
16 H	0.16771	0.0962	0.16240	0.0828	0.15539	0.0759	0.15804	0.0785
17 H	0.15822	0.0835	0.16427	0.0759	0.16533	0.0741	0.16505	0.0749
18 H	0.17252	0.0975	0.16068	0.0840	0.15477	0.0781	0.15695	0.0804
19 H	0.12541	0.0732	0.13190	0.0655	0.13986	0.0686	0.13704	0.0676
20 H	0.13954	0.0877	0.14369	0.0802	0.14635	0.0799	0.14562	0.0803
21 H	0.13703	0.0735	0.14300	0.0684	0.15031	0.0710	0.14779	0.0702
22 H	0.12512	0.0647	0.12687	0.0521	0.13977	0.0573	0.13521	0.0556
23 H	0.15396	0.0729	0.15563	0.0669	0.15701	0.0663	0.15666	0.0667
24 H	0.12155	0.0715	0.12978	0.0656	0.14037	0.0705	0.13671	0.0690
25 H	0.16657	0.0984	0.16065	0.0830	0.15158	0.0751	0.15492	0.0780
26 H	0.12648	0.0822	0.13244	0.0697	0.13866	0.0708	0.13656	0.0706
27 Br	−0.24182	−0.5333	−0.25213	−0.5078	−0.25279	−0.4664	−0.25267	−0.4832
28 Br	−0.38803	−0.7557	−0.41159	−0.7755	−0.44799	−0.8129	−0.43522	−0.7993
29 N	0.09630	0.1885	0.08787	0.1778	0.09461	0.1789	0.09228	0.1787
30 C	−0.16372	0.0508	−0.16354	0.0420	−0.16339	0.0373	−0.16348	0.0391
31 C	−0.19864	0.0398	−0.19449	0.0244	−0.19095	0.0239	−0.19221	0.0242
32 C	−0.17679	0.0353	−0.16272	0.0328	−0.16032	0.0319	−0.16130	0.0321
33 C	−0.37753	−0.1215	−0.37408	−0.1360	−0.38635	−0.1436	−0.38235	−0.1409
34 H	0.12600	0.0633	0.12686	0.0481	0.14116	0.0541	0.13606	0.0521
35 H	0.14641	0.0818	0.14829	0.0742	0.14681	0.0713	0.14745	0.0725
36 C	−0.37881	−0.1277	−0.38798	−0.1486	−0.39790	−0.1530	−0.39472	−0.1515
37 H	0.15821	0.0835	0.16386	0.0758	0.16456	0.0739	0.16442	0.0747
38 H	0.17249	0.0976	0.16027	0.0839	0.15390	0.0778	0.15626	0.0802
39 C	−0.35519	−0.1096	−0.36541	−0.1306	−0.37687	−0.1383	−0.37306	−0.1356
40 H	0.12513	0.0647	0.12694	0.0522	0.13988	0.0573	0.13532	0.0556
41 H	0.15404	0.0729	0.15565	0.0669	0.15696	0.0663	0.15661	0.0667
42 H	0.12792	0.0748	0.13186	0.0663	0.14051	0.0688	0.13753	0.0681
43 H	0.12288	0.0768	0.13154	0.0675	0.14117	0.0717	0.13788	0.0704
44 H	0.16771	0.0962	0.16236	0.0828	0.15531	0.0759	0.15797	0.0785
45 H	0.12551	0.0732	0.13189	0.0655	0.13981	0.0685	0.13698	0.0676
46 H	0.13953	0.0876	0.14372	0.0802	0.14642	0.0800	0.14568	0.0803
47 H	0.13704	0.0735	0.14302	0.0685	0.15039	0.0710	0.14785	0.0703
48 H	0.12155	0.0716	0.12980	0.0656	0.14040	0.0705	0.13674	0.0690
49 H	0.16657	0.0983	0.16067	0.0831	0.15157	0.0751	0.15491	0.0780
50 H	0.12650	0.0822	0.13243	0.0697	0.13863	0.0708	0.13653	0.0705

Table S18 Mulliken population analysis and PABOON results for **1c** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON
1 I	−0.36346	−0.4718	−0.40017	−0.5197	−0.43943	−0.5871	−0.42557	−0.5611
2 Be	0.00508	0.3141	0.00196	0.3146	−0.00076	0.3161	0.00011	0.3150
3 I	−0.21527	−0.6554	−0.21775	−0.6419	−0.21808	−0.6113	−0.21814	−0.6245
4 Be	0.00505	0.3142	0.00204	0.3144	−0.00059	0.3160	0.00024	0.3149
5 N	0.06864	0.1435	0.07404	0.1497	0.08012	0.1569	0.07793	0.1542
6 C	−0.17007	0.0315	−0.17075	0.0306	−0.17166	0.0305	−0.17142	0.0304
7 C	−0.18639	0.0151	−0.18563	0.0154	−0.18422	0.0162	−0.18491	0.0159
8 C	−0.18784	0.0205	−0.18421	0.0228	−0.18117	0.0246	−0.18210	0.0242
9 C	−0.36247	−0.1322	−0.37672	−0.1383	−0.38819	−0.1434	−0.38442	−0.1417
10 C	−0.37647	−0.1463	−0.38907	−0.1498	−0.39889	−0.1518	−0.39578	−0.1512
11 C	−0.34835	−0.1284	−0.36069	−0.1343	−0.37130	−0.1392	−0.36780	−0.1376
12 H	0.11615	0.0390	0.12952	0.0468	0.14418	0.0552	0.13895	0.0523
13 H	0.15693	0.0741	0.15791	0.0742	0.15801	0.0740	0.15812	0.0741
14 H	0.12841	0.0624	0.13720	0.0673	0.14578	0.0721	0.14281	0.0705
15 H	0.12309	0.0615	0.13296	0.0682	0.14225	0.0746	0.13910	0.0724
16 H	0.16947	0.0859	0.16512	0.0821	0.15870	0.0773	0.16114	0.0791
17 H	0.16464	0.0749	0.16796	0.0760	0.17038	0.0764	0.16962	0.0764
18 H	0.16954	0.0862	0.16475	0.0839	0.15915	0.0807	0.16117	0.0819
19 H	0.1256	0.0608	0.13308	0.0657	0.14108	0.0712	0.13825	0.0693
20 H	0.14092	0.0784	0.14521	0.0811	0.14768	0.0829	0.14702	0.0824
21 H	0.13722	0.0642	0.14458	0.0689	0.15187	0.0738	0.14936	0.0721
22 H	0.11855	0.0446	0.13042	0.0514	0.14325	0.0587	0.13870	0.0561
23 H	0.16457	0.0651	0.16845	0.0676	0.17145	0.0697	0.17056	0.0691
24 H	0.12085	0.0597	0.13146	0.0669	0.14198	0.0740	0.13835	0.0716
25 H	0.16773	0.0844	0.16100	0.0794	0.15256	0.0734	0.15567	0.0756
26 H	0.13296	0.0681	0.13938	0.0716	0.14524	0.0747	0.14327	0.0737
27 I	−0.21527	−0.6554	−0.21783	−0.6419	−0.21821	−0.6115	−0.21824	−0.6246
28 I	−0.36345	−0.4717	−0.40011	−0.5199	−0.43925	−0.5872	−0.42544	−0.5613
29 N	0.06864	0.1435	0.07407	0.14980	0.08017	0.1569	0.07798	0.1542
30 C	−0.17009	0.0315	−0.17066	0.0306	−0.17152	0.0306	−0.17130	0.0305
31 C	−0.18784	0.0205	−0.18419	0.0229	−0.18119	0.0247	−0.18214	0.0242
32 C	−0.18636	0.0151	−0.18566	0.0154	−0.18427	0.0162	−0.18495	0.0159
33 C	−0.36245	−0.1322	−0.37651	−0.1382	−0.38776	−0.1432	−0.38407	−0.1415
34 H	0.11615	0.0390	0.12951	0.0468	0.14417	0.0552	0.13896	0.0523
35 H	0.15692	0.0741	0.15785	0.0741	0.15788	0.0740	0.15801	0.0741
36 C	−0.37646	−0.1463	−0.38909	−0.1497	−0.39872	−0.1518	−0.39564	−0.1512
37 H	0.16464	0.0749	0.16800	0.0760	0.17051	0.0765	0.16973	0.0764
38 H	0.16953	0.0862	0.16460	0.0838	0.15873	0.0805	0.16088	0.0818
39 C	−0.34834	−0.1284	−0.36060	−0.1342	−0.37111	−0.1392	−0.36764	−0.1376
40 H	0.11854	0.0446	0.13045	0.0514	0.14329	0.0587	0.13874	0.0561
41 H	0.16456	0.0651	0.16843	0.0676	0.17142	0.0697	0.17052	0.0691
42 H	0.12841	0.0624	0.13726	0.0673	0.14588	0.0722	0.14289	0.0705
43 H	0.12309	0.0615	0.13298	0.0682	0.14230	0.0746	0.13913	0.0724
44 H	0.16947	0.0859	0.16478	0.0819	0.15804	0.0771	0.16058	0.0789
45 H	0.12559	0.0608	0.13306	0.0657	0.14101	0.0711	0.13819	0.0692
46 H	0.14092	0.0784	0.14525	0.0811	0.14766	0.0829	0.14699	0.0824
47 H	0.13721	0.0642	0.14460	0.0689	0.15193	0.0738	0.14941	0.0722
48 H	0.12085	0.0597	0.13143	0.0669	0.14193	0.0740	0.13831	0.0716
49 H	0.16772	0.0844	0.16097	0.0794	0.15250	0.0734	0.15563	0.0756
50 H	0.13296	0.0681	0.13936	0.0716	0.14521	0.0747	0.14325	0.0737

Table S19 Mulliken population analysis and PABOON results for **2a** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON
1 Cl	−0.29938	−0.6170	−0.32515	−0.6206	−0.34912	−0.6214	−0.34172	−0.6214
2 Be	0.09119	0.3321	0.09451	0.3304	0.09588	0.3300	0.09563	0.3300
3 Cl	−0.30292	−0.6826	−0.33195	−0.7021	−0.35927	−0.7218	−0.35078	−0.7155
4 N	0.04518	0.1998	0.05274	0.2036	0.06022	0.2070	0.05786	0.2060
5 C	−0.14320	0.0395	−0.14356	0.0379	−0.14342	0.0367	−0.14351	0.0370
6 C	−0.13272	0.0390	−0.13533	0.0370	−0.13732	0.0352	−0.13676	0.0357
7 C	−0.19413	0.0260	−0.18959	0.0237	−0.18581	0.0215	−0.18691	0.0222
8 C	−0.34122	−0.1271	−0.35601	−0.1336	−0.36748	−0.1389	−0.36415	−0.1373
9 C	−0.36941	−0.1428	−0.38518	−0.1462	−0.39724	−0.1485	−0.39380	−0.1479
10 C	−0.36215	−0.1335	−0.37757	−0.1405	−0.38970	−0.1461	−0.38616	−0.1445
11 H	0.13846	0.0822	0.13908	0.0818	0.13925	0.0813	0.13924	0.0815
12 H	0.11478	0.0464	0.12844	0.0540	0.14238	0.0616	0.13792	0.0592
13 H	0.12598	0.0708	0.13525	0.0764	0.14379	0.0815	0.14115	0.0799
14 H	0.12234	0.0646	0.13221	0.0698	0.14168	0.0747	0.13871	0.0732
15 H	0.15487	0.0841	0.15242	0.0810	0.14714	0.0762	0.14910	0.0779
16 H	0.14603	0.0785	0.14847	0.0793	0.15014	0.0793	0.14969	0.0794
17 H	0.14880	0.0802	0.15063	0.0808	0.15174	0.0806	0.15143	0.0807
18 H	0.13626	0.0788	0.14229	0.0822	0.14673	0.0848	0.14548	0.0841
19 H	0.12714	0.0650	0.13420	0.0694	0.14087	0.0735	0.13881	0.0722
20 H	0.12801	0.0650	0.13510	0.0693	0.14185	0.0735	0.13975	0.0722
21 H	0.11271	0.0451	0.12667	0.0525	0.14104	0.0601	0.13644	0.0577
22 H	0.13976	0.0833	0.14102	0.0832	0.14182	0.0828	0.14161	0.0830
23 H	0.12996	0.0718	0.13934	0.0773	0.14797	0.0823	0.14531	0.0808
24 H	0.15866	0.0854	0.15683	0.0826	0.15199	0.0781	0.15382	0.0797
25 H	0.12499	0.0654	0.13514	0.0708	0.14486	0.0757	0.14183	0.0742

Table S20 Mulliken population analysis and PABOON results for **2b** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON
1 Br	−0.30914	−0.7520	−0.33650	−0.7373	−0.36255	−0.7189	−0.35440	−0.7249
2 Be	0.08520	0.3756	0.09295	0.3575	0.09964	0.3450	0.09760	0.3482
3 Br	−0.30146	−0.4765	−0.33235	−0.5376	−0.36233	−0.5941	−0.35298	−0.5769
4 N	0.04617	0.2225	0.05448	0.2299	0.06249	0.2356	0.06005	0.2340
5 C	−0.15303	0.0277	−0.15476	0.0280	−0.15578	0.0283	−0.15554	0.0282
6 C	−0.14690	0.0268	−0.14928	0.0269	−0.15097	0.0268	−0.15050	0.0269
7 C	−0.20159	0.0115	−0.19866	0.0122	−0.19637	0.0125	−0.19715	0.0124
8 C	−0.33807	−0.1345	−0.35250	−0.1394	−0.36402	−0.1436	−0.36057	−0.1423
9 C	−0.36916	−0.1490	−0.38465	−0.1507	−0.39650	−0.1516	−0.39308	−0.1514
10 C	−0.35702	−0.1403	−0.37260	−0.1457	−0.38490	−0.1502	−0.38133	−0.1488
11 H	0.14603	0.0737	0.14679	0.0747	0.14712	0.0751	0.14705	0.0750
12 H	0.11642	0.0408	0.13037	0.0501	0.14468	0.0591	0.14014	0.0563
13 H	0.12665	0.0664	0.13596	0.0737	0.14450	0.0799	0.14187	0.0781
14 H	0.12330	0.0599	0.13327	0.0670	0.14310	0.0733	0.13989	0.0713
15 H	0.15498	0.0801	0.15253	0.0786	0.14732	0.0751	0.14929	0.0764
16 H	0.15076	0.0727	0.15337	0.0750	0.15529	0.0761	0.15478	0.0759
17 H	0.15375	0.0743	0.15560	0.0762	0.15675	0.0771	0.15646	0.0769
18 H	0.13745	0.0751	0.14338	0.0803	0.14773	0.0841	0.14652	0.0830
19 H	0.12813	0.0606	0.13521	0.0666	0.14192	0.0720	0.13984	0.0703
20 H	0.12895	0.0605	0.13607	0.0665	0.14287	0.0720	0.14074	0.0703
21 H	0.11444	0.0392	0.12871	0.0486	0.14337	0.0576	0.13867	0.0548
22 H	0.14885	0.0753	0.14967	0.0764	0.15012	0.0769	0.15005	0.0768
23 H	0.13058	0.0674	0.14006	0.0747	0.14875	0.0809	0.14605	0.0791
24 H	0.15862	0.0814	0.15651	0.0800	0.15158	0.0767	0.15345	0.0780
25 H	0.12611	0.0609	0.13636	0.0680	0.14617	0.0743	0.14311	0.0724

Table S21 Mulliken population analysis and PABOON results for **2c** (DFT-TPSS/def2-TZVP level of theory).

	gas phase		COSMO C_6H_6		COSMO CH_2Cl_2		COSMO $CHCl_3$	
atom	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON	Mulliken	PABOON
1 I	−0.31467	−0.6533	−0.34499	−0.6470	−0.37575	−0.6406	−0.36504	−0.6430
2 Be	0.09238	0.3178	0.10239	0.3118	0.11215	0.3067	0.10878	0.3084
3 I	−0.30539	−0.4701	−0.33844	−0.5056	−0.37215	−0.5395	−0.36036	−0.5277
4 N	0.03362	0.2277	0.04507	0.2326	0.05615	0.2368	0.05241	0.2353
5 C	−0.16942	0.0193	−0.18140	0.0188	−0.17241	0.0191	−0.17216	0.0189
6 C	−0.15631	0.0186	−0.16198	0.0182	−0.16679	0.0182	−0.16529	0.0181
7 C	−0.20677	0.0019	−0.20682	0.0018	−0.20718	0.0017	−0.20701	0.0017
8 C	−0.33092	−0.1379	−0.34671	−0.14410	−0.35958	−0.1493	−0.35548	−0.1476
9 C	−0.37290	−0.1511	−0.38727	−0.15410	−0.39867	−0.1561	−0.39506	−0.1554
10 C	−0.35590	−0.1444	−0.36968	−0.15060	−0.38069	−0.1558	−0.37720	−0.1541
11 H	0.15159	0.0711	0.15353	0.0706	0.15500	0.0699	0.15452	0.0702
12 H	0.11876	0.0388	0.13290	0.0467	0.14808	0.0551	0.14273	0.0521
13 H	0.12758	0.0656	0.13692	0.0715	0.14571	0.0769	0.14282	0.0751
14 H	0.12476	0.0584	0.13481	0.0642	0.14489	0.0698	0.14140	0.0678
15 H	0.15520	0.0795	0.15332	0.0766	0.14846	0.0719	0.15052	0.0737
16 H	0.15857	0.0725	0.16115	0.0729	0.16322	0.0726	0.16255	0.0728
17 H	0.15844	0.0722	0.16209	0.0733	0.16493	0.0735	0.16402	0.0735
18 H	0.13884	0.0751	0.14468	0.0788	0.14906	0.0818	0.14771	0.0808
19 H	0.12944	0.0598	0.13642	0.0645	0.14337	0.0691	0.14096	0.0675
20 H	0.13015	0.0599	0.13716	0.0645	0.14420	0.0691	0.14176	0.0675
21 H	0.11608	0.0378	0.13075	0.0457	0.14661	0.0541	0.14101	0.0511
22 H	0.15553	0.0727	0.15764	0.0725	0.15933	0.0722	0.15879	0.0723
23 H	0.13168	0.0666	0.14107	0.0725	0.15006	0.0781	0.11470	0.0762
24 H	0.16104	0.0812	0.15881	0.0782	0.15342	0.0733	0.15564	0.0752
25 H	0.12862	0.0602	0.13857	0.0659	0.14858	0.0715	0.14508	0.0695

Table S22 Atom (*X* or N / Be) contribution to the Intrinsic Bond Orbitals (IBO) in % (DFT-TPSS/def2-TZVP level of theory).

	gas phase			COSMO C_6H_6			COSMO $CHCl_3$			COSMO CH_2Cl_2		
	X−Be	μ_2-*X*−Be	N−Be	*X*−Be	μ_2-*X*−Be	N−Be	*X*−Be	μ_2-*X*−Be	N−Be	*X*−Be	μ_2-*X*−Be	N−Be
$[(Et_3N)BeCl_2]_2$ (**1a**)	90 / 9	93 / 6	90 / 7	91 / 9	93 / 6	90 / 7	91 / 9	93 / 6	90 / 7	91 / 9	93 / 6	90 / 7
$[(Et_3N)BeBr_2]_2$ (**1b**)	89 / 10	93 / 6–7	90 / 7	90 / 10	93 / 6–7	90 / 7	90 / 9	93 / 6–7	90 / 7	90 / 9	93 / 6–7	90 / 7
$[(Et_3N)BeI_2]_2$ (**1c**)	88 / 12	92 / 7	90 / 7	88 / 11	92 / 7	90 / 7	88 / 11	92 / 7	90 / 7	88 / 11	92 / 7	90 / 7
$(Et_3N)BeCl_2$ (**2a**)	89–90 / 10	–	90 / 6	90 / 9–10	–	90 / 7	90 / 9–10	–	90 / 7	90 / 9–10	–	90 / 7
$(Et_3N)BeBr_2$ (**2b**)	88–89 / 11	–	90 / 7	88–89 / 10–11	–	90 / 7	89 / 10–11	–	90 / 7	89 / 10–11	–	90 / 7
$(Et_3N)BeI_2$ (**2c**)	86–87 / 12–13	–	90 / 7	87 / 12–13	–	90 / 7	87 / 12	–	90 / 7	87 / 12	–	90 / 7

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