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Positions of Amino Groups in Ammonium Salts Turn the Conformations of Crown Ethers: Crystal Structure, Hirshfeld Surfaces and Spectroscopic Studies

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Table S1 Crystal data and structure refinement for complexes **1-6**

Compound	**1**	**2**	**3**	**4**	**5**	**6**
Formula	$C_{22}H_{38}Cl_2N_4O_{14}$	$C_{17}H_{29}Cl_2N_2O_{10}$	$C_{48}H_{96}B_4F_{16}N_6O_{24}$	$C_{22}H_{34}BF_4NO_6$	$C_{16}H_{27}BF_4NO_5$	$C_{19}H_{30}BF_2NO_8$
Formula weight	653.46	492.32	1488.55	495.31	400.2	449.25
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P-1*	*P 21/c*	*P 21/c*	P 21/c	P 21/c	P 21
b/ Å	10.346(2)	14.090(3)	8.8817(18)	15.408(3)	14.503(3)	14.330(3)
c/ Å	10.659(2)	17.098(6)	23.870(5)	13.991(3)	16.888(5)	9.2084(18)
α/°	62.22(3)	90	90	90	90	90
β/°	83.15(3)	126.958(19)	97.56(3)	90.28(3)	112.47(3)	103.72(3)
γ/°	79.28(3)	90	90	90	90	90
T/K	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)
μ (mm^{-1})	0.278	0.329	0.129	0.11	0.12	0.113
Cryst dimensions	0.3×0.25×0.15	0.25×0.2×0.15	0.3×0.25×0.12	0.3×0.25×0.15	0.3×0.25×0.12	0.3×0.25×0.12
No. of reflns collected	2825	5377	6445	5820	3643	5073
No. of unique reflns	1887	3568	3664	2962	1784	3229
No. of params	213	282	463	335	245	280
Goodness-of-fit on F^2	1.037	1.037	1.022	1.047	1.089	1.009
R_1 ,wR_2 ((I>2σ(I))	0.0697, 0.1933	0.0727, 0.1820	0.1097, 0.2924	0.0845, 0.2301	0.0988, 0.2814	0.0514, 0.0995
R1 ,wR2 (all data)	0.1055, 0.2251	0.1052, 0.2035	0.1665, 0.3425	0.1561, 0.2725	0.1694, 0.3353	0.0928, 0.1146
CCDC No	946957	946960	946964	956958	946957	946963