Electronic Supplementary Material (ESI) for CrystEngComm.

Supramolecular Zwitterions Based on a Novel Boronic Acid-Squarate Dianion Synthon

ELECTRONIC SUPPLEMENTARY INFORMATION

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Content:

CRYSTAL DATA AND REFINEMENT DETAILS

TABLE ESI-1. Crystallographic data for [SQ(**1**BAH)$_2$]·2H$_2$O, [SQ(**2**BAH)$_2$]·H$_2$O, [SQ(**3**BAH)$_2$]·2H$_2$O, and [SQ(4pyBAH)$_2$]·bpy.

	[SQ(1BAH)$_2$]·2H$_2$O	**[SQ(2BAH)$_2$]· H$_2$O**	**[SQ(3BAH)$_2$]·2H$_2$O**	**[SQ(1BAH)$_2$]·bpy**
Empirical formula	$C_{14}H_{18}B_2N_2O_{10}$	$C_{14}H_{16}B_2N_2O_9$	$C_{26}H_{26}B_2N_2O_{10}$	$C_{24}H_{22}B_2N_4O_8$
Formula weight	395.92	377.91	548.11	516.07
Temperature/K	250	300	300	300
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	I2/m	$P2_1/c$	$P2_1/c$	C2/m
a/Å	3.7455(3)	10.5211(5)	3.9208(4)	12.3874(6)
b/Å	10.5330(6)	21.0309(9)	10.4450(9)	10.7643(4)
c/Å	21.5313(12)	7.6551(4)	29.717(3)	8.7610(4)
α/°	90	90	90	90
β/°	94.556(6)	99.368(5)	90.340(9)	98.765(5)
γ/°	90	90	90	90
Volume/Å^3	846.75(10)	1671.24(14)	1216.97(19)	1154.56(9)
Z	2	4	2	2
ρ_{calc}g/cm^3	1.553	1.502	1.496	1.484
μ/mm^{-1}	0.130	0.123	0.114	0.111
F(000)	412.0	784.0	572.0	536.0
Crystal size/mm^3	0.5 × 0.2 × 0.1	0.2 × 0.2 × 0.05	0.2 × 0.2 × 0.03	0.2 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.884 to 52.002	6.432 to 58.442	6.73 to 58.354	6.54 to 58.042
Reflections collected	2893	6685	4924	2546
Independent reflections	884 [R_{int} = 0.0169, R_{sigma} = 0.0161]	3735 [R_{int} = 0.0270, R_{sigma} = 0.0549]	2712 [R_{int} = 0.0287, R_{sigma} = 0.0476]	1388 [R_{int} = 0.0189, R_{sigma} = 0.0324]
Data/restraints/parameters	884/0/73	3735/0/251	2712/0/186	1388/0/95
Goodness-of-fit on F^2	1.079	1.014	1.014	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0375, wR_2 = 0.1024	R_1 = 0.0514, wR_2 = 0.1082	R_1 = 0.0574, wR_2 = 0.1387	R_1 = 0.0463, wR_2 = 0.1125
Final R indexes [all data]	R_1 = 0.0415, wR_2 = 0.1059	R_1 = 0.0960, wR_2 = 0.1298	R_1 = 0.0895, wR_2 = 0.1677	R_1 = 0.0601, wR_2 = 0.1199
Largest diff. peak/hole / e Å^{-3}	0.24/-0.23	0.22/-0.23	0.26/-0.27	0.32/-0.23

ORTEP DRAWINGS AND NUMBERING SCHEMES

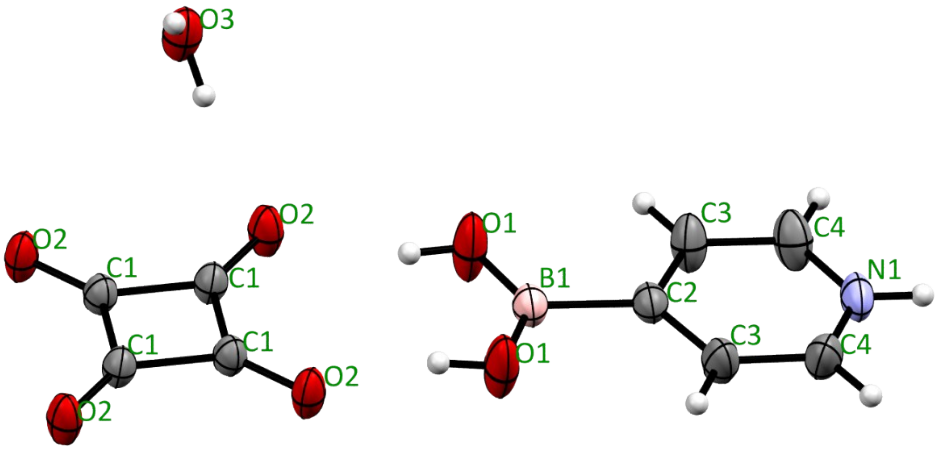

FIGURE ESI-1. Ortep drawing of [SQ(**1**BAH)$_2$]·2H$_2$O (ellipsoids drawn at 50% probability)

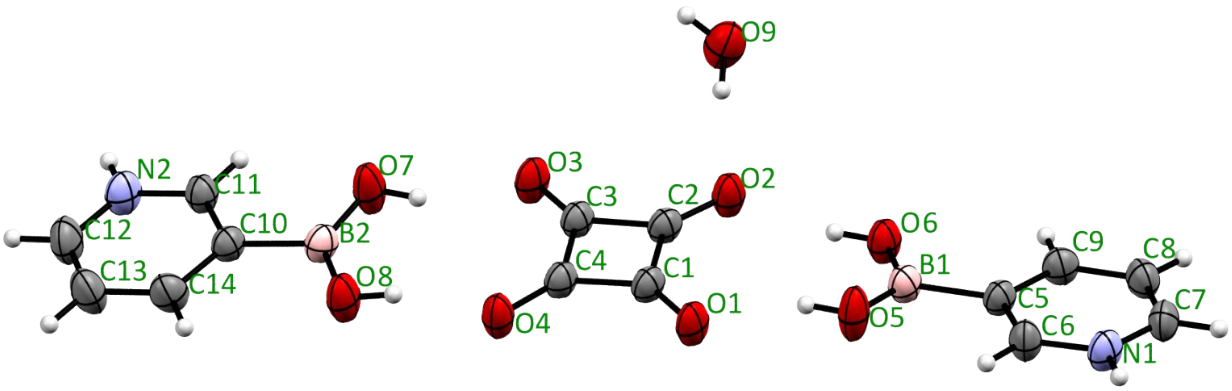

FIGURE ESI-2. Ortep drawing of [SQ(**2**BAH)$_2$]· H$_2$O (ellipsoids drawn at 50% probability)

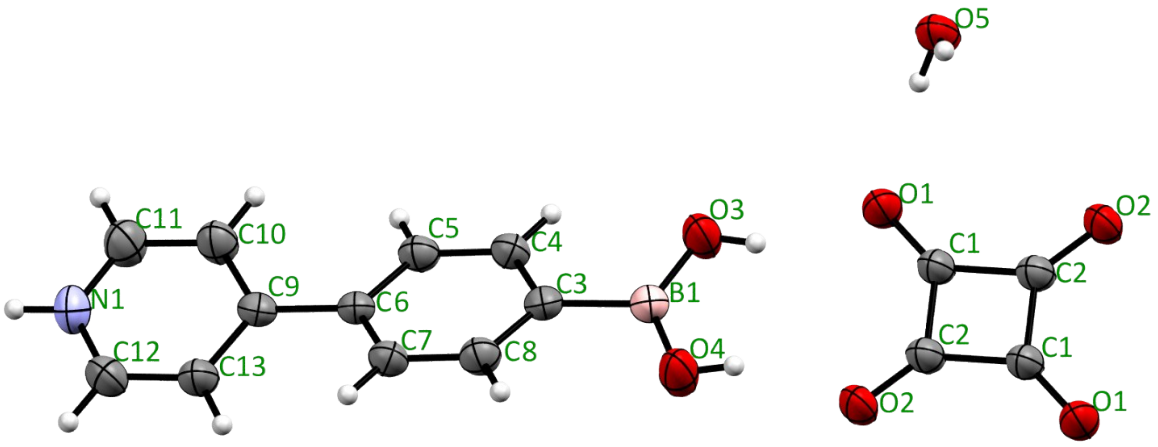

FIGURE ESI-3. Ortep drawing of [SQ(**3**BAH)$_2$]·2H$_2$O (ellipsoids drawn at 50% probability)

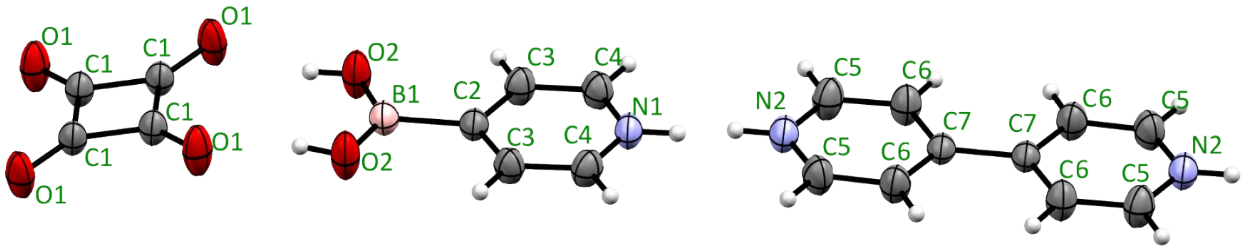

FIGURE ESI-4. Ortep drawing of [SQ(**1**BAH)$_2$]·bpy (ellipsoids drawn at 50% probability)

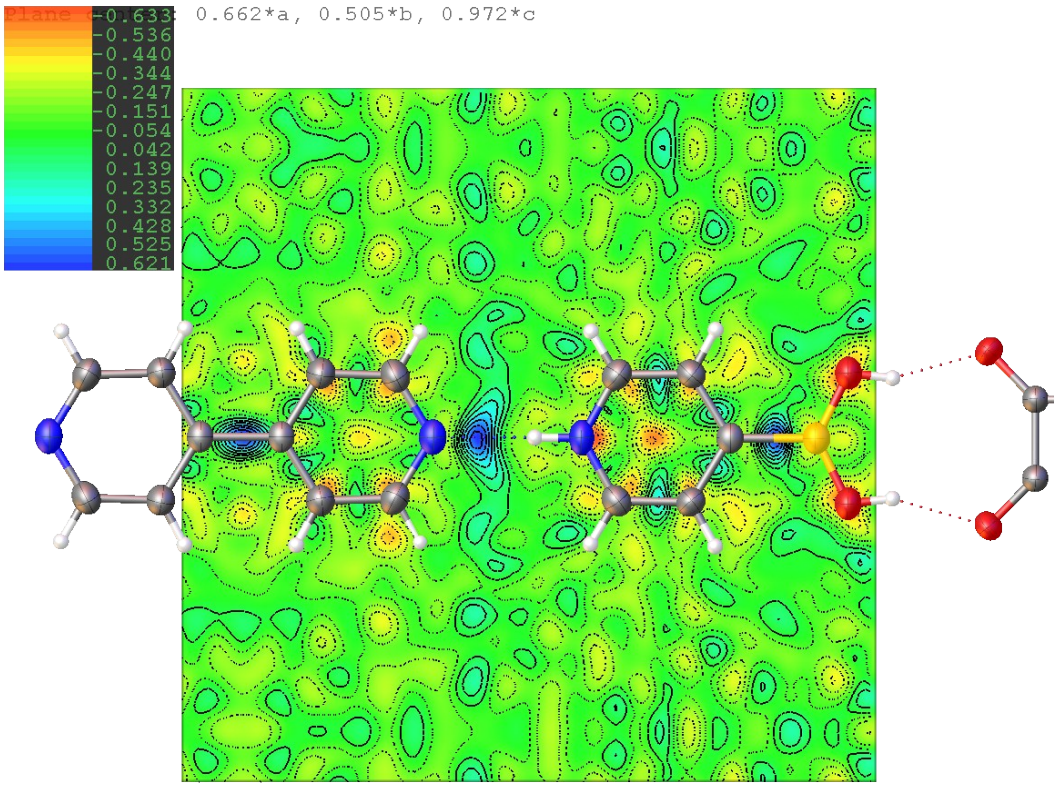

Figure ESI-5. Electron density difference map of [SQ(**1**BAH)$_2$]·bpy.

X-RAY POWDER DIFFRACTION PATTERNS

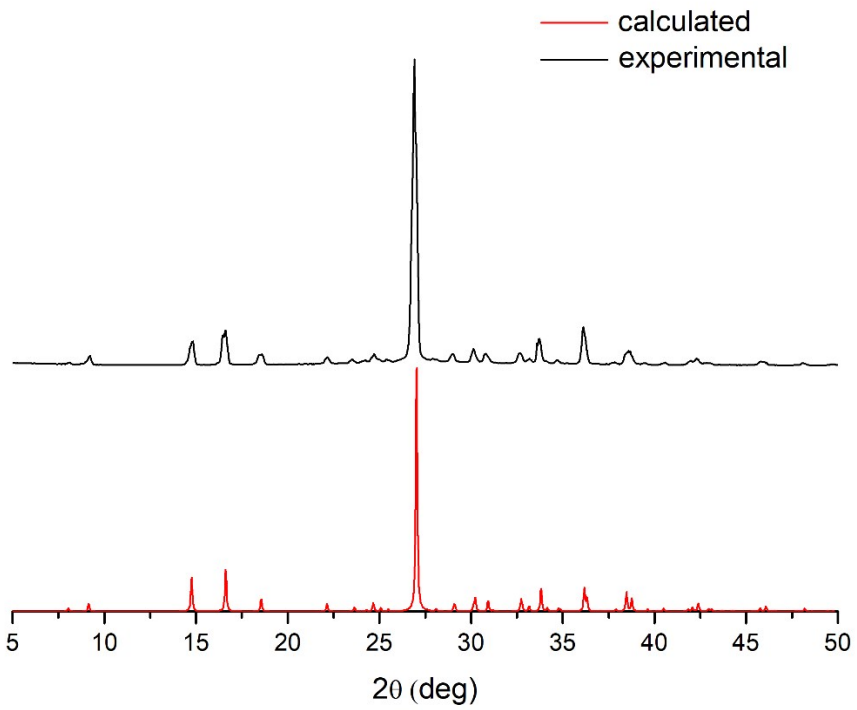

FIGURE ESI-6. Comparison between the experimental (black-line) and calculated (red-line) diffraction pattern of [SQ(**1**BAH)$_2$]·2H$_2$O.

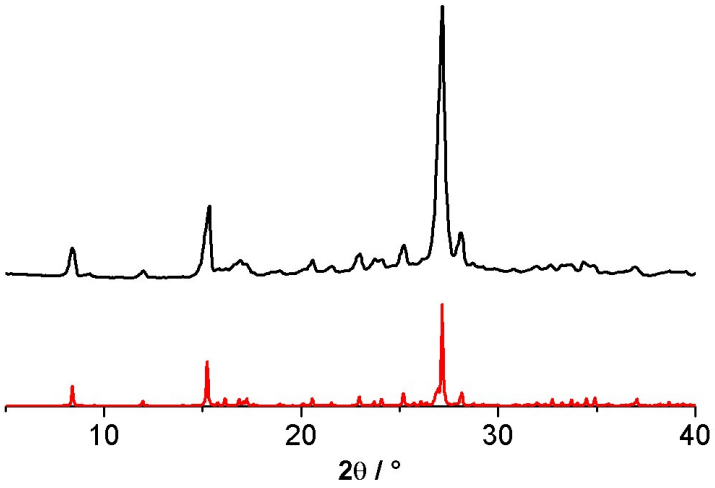

FIGURE ESI-7. Comparison between the experimental (black-line) and calculated (red-line) diffraction pattern of [SQ(**2**BAH)$_2$]· H$_2$O.

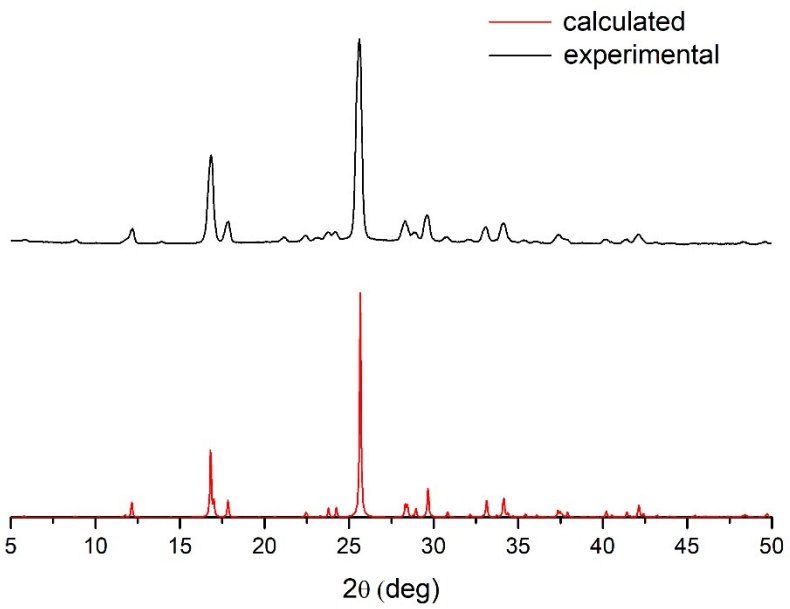

FIGURE ESI-8. Comparison between the experimental and calculated diffraction pattern of [SQ(**3**BAH)$_2$]·H$_2$O.

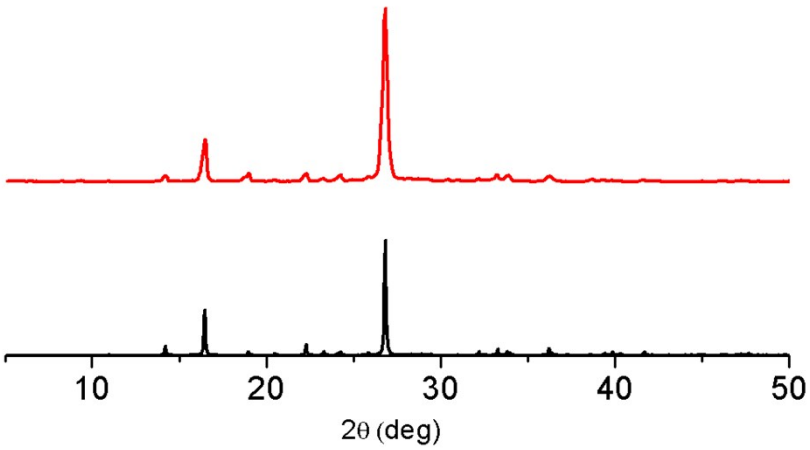

FIGURE ESI-9. Comparison between the experimental (red-line) and calculated (black-line) diffraction pattern of [SQ(**1**BAH)$_2$]·bpy.

ATR-FTIR SPECTRA

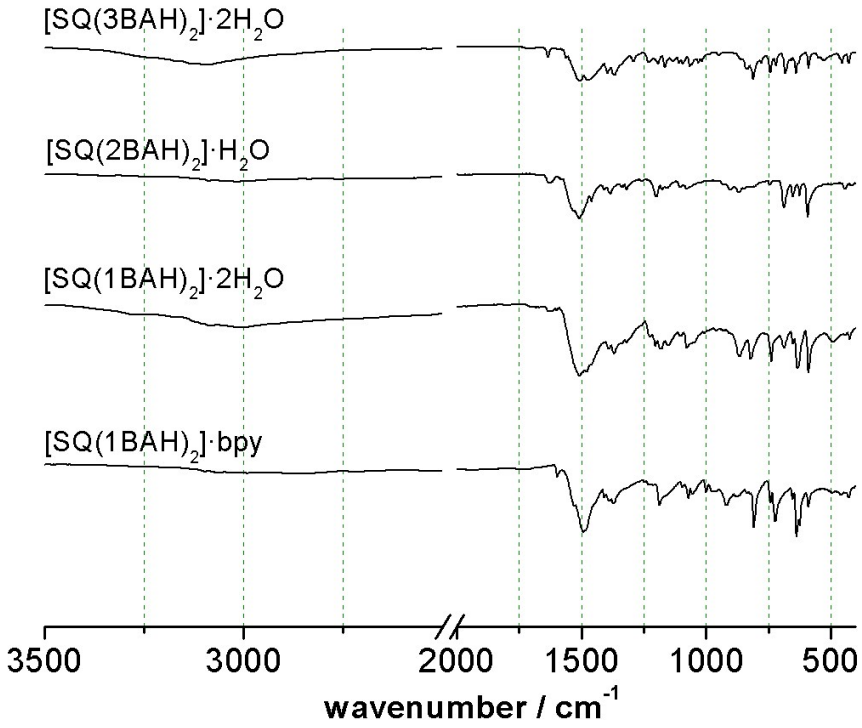

Figure ESI-10. ATR-FTIR spectra of compounds [SQ(**1**BAH)$_2$]·bpy, [SQ(**1**BAH)$_2$]·2H$_2$O, [SQ(**2**BAH)$_2$]·H$_2$O, and [SQ(**3**BAH)$_2$]·2H$_2$O.