

## Supplementary Data File

**Table S1.** The vibrational frequency of the selected bonds in **[BTAD][A1-8]<sub>2</sub>**, (BTAD= [C<sub>6</sub>H<sub>4</sub>N<sub>6</sub>O<sub>2</sub>]<sup>2+</sup> and A1-8 = [CH<sub>3</sub>CO<sub>2</sub>]<sup>-</sup>, [CF<sub>3</sub>CO<sub>2</sub>]<sup>-</sup>, [N(CN)<sub>2</sub>]<sup>-</sup>, [CF<sub>3</sub>SO<sub>3</sub>]<sup>-</sup>, [ClO<sub>4</sub>]<sup>-</sup>, [BF<sub>4</sub>]<sup>-</sup>, [NTf<sub>2</sub>]<sup>-</sup> and [PF<sub>6</sub>]<sup>-</sup>) DCILs and corresponding isolated dication at M06–2X/6-31++G(d,p) level of theory.

v/cm <sup>-1</sup>	[BTAD] <sup>2+</sup>	[BTAD][A1] <sub>2</sub>	[BTAD][A2] <sub>2</sub>	[BTAD][A3] <sub>2</sub>	[BTAD][A4] <sub>2</sub>
N2–H5	3494.4	3441.1	3529.90	3484.3	3548.6
N2'–H5'	3494.4	3441.1	3529.90	3484.3	3548.6
v/cm <sup>-1</sup>	[BTAD][A5] <sub>2</sub>	[BTAD][A6] <sub>2</sub>	[BTAD][A7] <sub>2</sub>	[BTAD][A8] <sub>2</sub>	
N1–H4	3509.9	-	-	-	3377.9
N1'–H4'	3509.9	-	-	-	3377.9
N2–H5		3571.2	3526.4	3484.9	2013.9
N2'–H5'		3571.2	3526.4	3484.9	2013.9