Supporting Information

Dynamic pedal motion and thermal expansion in an ionic co-crystal with 1,2-bis(4-pyridyl) ethylene

Yuchen Zhang,[a] Yijia Jiao,[a] Yan Guo,[*a] Peipei Cen,[*b] Zhenyi Zhang[c] and Xiangyu Liu[*a]

[a] State Key Laboratory of High-Efficiency Utilization of Coal and Green Chemical Engineering, College of Chemistry and Chemical Engineering, School of Civiland Hydraulic Engineering, Ningxia University, Yinchuan 750021, China. E-mail: xiangyuliu432@126.com

[b] College of Public Health, Key Laboratory of Environmental Factors and Chronic Disease Control, Ningxia Medical University, Yinchuan 750004, China. E-mail: 13895400691@163.com

[c] Bruker Scientific Instruments (shanghai) Co., Ltd

***Corresponding author**

Prof. Xiangyu Liu

E-mail: xiangyuliu432@126.com

***Corresponding author**

Dr. Yan Guo

E-mail: gy2020054@163.com

***Corresponding author**

Dr. Peipei Cen

E-mail: 13895400691@163.com

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Table S1. Crystallographic parameters for **Bpe-BPh$_4$** at variable temperatures.

	Bpe-BPh$_4$			
Empirical formula	$C_{36}H_{31}BN_2$	$C_{36}H_{31}BN_2$	$C_{36}H_{31}BN_2$	$C_{36}H_{31}BN_2$
Formula weight	502.44	502.44	502.44	502.44
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$
Temperature(K)	140	170	200	230
a (Å)	11.4237(12)	11.4488(8)	11.4651(9)	11.4902(8)
b (Å)	10.4916(12)	10.5125(9)	10.5281(11)	10.566(7)
c (Å)	23.34(3)	23.383(2)	23.44(2)	23.4778(15)
α (°)	90	90	90	90
β (°)	101.622(8)	101.810(6)	102.0019(7)	102.2836(5)
γ (°)	90	90	90	90
V (Å^3)	2740.1(5)	2754.7(4)	2767.455(4)	2785.1(3)
Z	4	4	4	4
μ (mm^{-1})	0.532	0.529	0.527	0.523
Unique reflections	4955	4854	4837	4885
Observed	15965	17263	17027	16809
R_{int}	0.1062	0.1366	0.1688	0.1506
R_1, wR_2 [$I > 2\sigma(I)$]	0.0707, 0.1758	0.0671, 0.1704	0.0757, 0.1768	0.0766, 0.1828
R_1, wR_2 (all data)	0.1330, 0.2487	0.1363, 0.2218	0.1688, 0.2317	0.1643, 0.2324

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Formula weight	502.44	502.44	502.44
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
Temperature(K)	260	290	320
a (Å)	11.5246(6)	11.5542(8)	11.5947(9)
b (Å)	10.5868(6)	10.6145(9)	10.6548(9)
c (Å)	23.5275(13)	23.5906(17)	23.6679(17)
α (°)	90	90	90
β (°)	102.595(4)	102.906(5)	103.405(5)
γ (°)	90	90	90
V (Å^3)	2801.5(3)	2820.1(4)	2844.3(4)
Z	4	4	4
μ (mm^{-1})	0.52	0.517	0.513
Unique reflections	4935	4959	4955
Observed	17671	17694	18823
R_{int}	0.1601	0.1582	0.1125
R_1, wR_2 [$I > 2\sigma(I)$]	0.0656, 0.1632	0.0705, 0.1738	0.0855, 0.2112
R_1, wR_2 (all data)	0.1574, 0.2223	0.1673, 0.2431	0.1907, 0.3020

Table S2. Unit cell parameters and disorder for **Bpe-BPh$_4$** at variable temperatures

Temperature/K	**Disorder ratio**	***a*/Å**	***b*/Å**	***c*/Å**	***α*/°**	***β*/°**	***γ*/°**	**Volume/Å^3**
140	0.50247	11.4237	10.4916	23.34	90	101.622	90	2740.1
170	0.555	11.4488	10.5125	23.383	90	101.810	90	2754.7
200	0.60144	11.4651	10.5281	23.44	90	102.0019	90	2767.455
230	0.63628	11.4902	10.566	23.4778	90	102.2836	90	2785.1
260	0.67163	11.5246	10.5868	23.5275	90	102.5968	90	2801.5
290	0.69577	11.5542	10.6145	23.5906	90	102.906	90	2820.1
320	0.72256	11.5947	10.6548	23.6679	90	103.405	90	2844.273

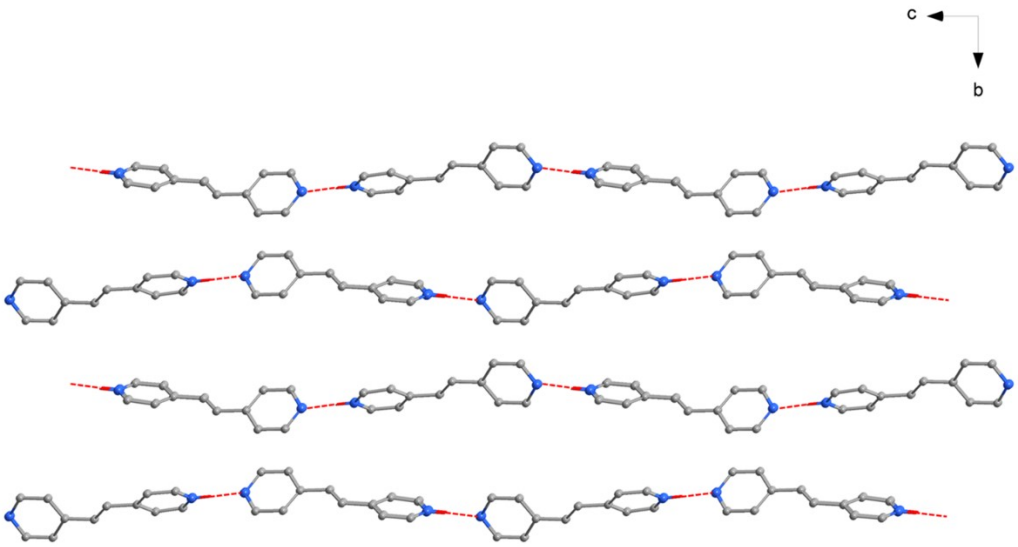

Fig. S1 Hydrogen bond accumulation for conformation **A**. The hydrogen atoms on the carbon and all counterions are omitted.

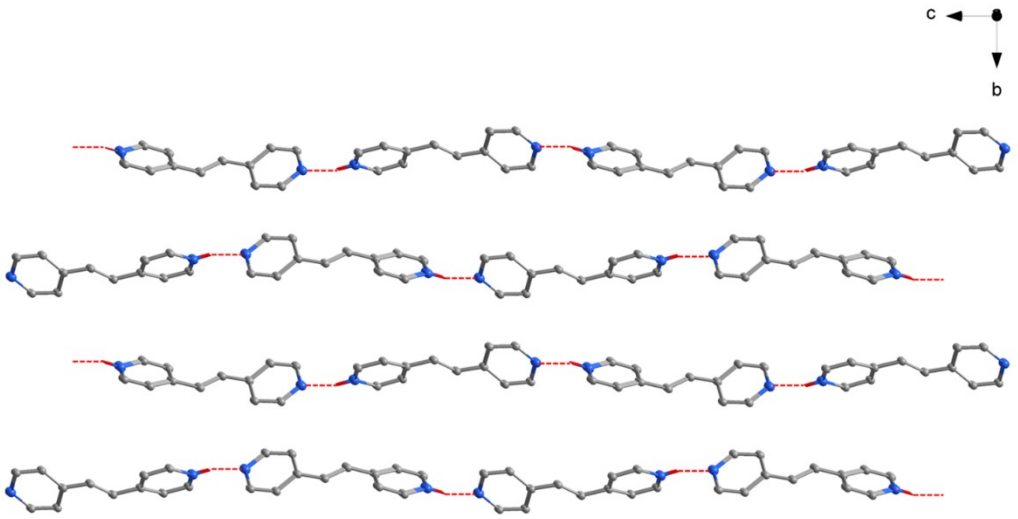

Fig. S2 Hydrogen bond accumulation for conformation **B**. The hydrogen atoms on the carbon and all counterions are omitted.

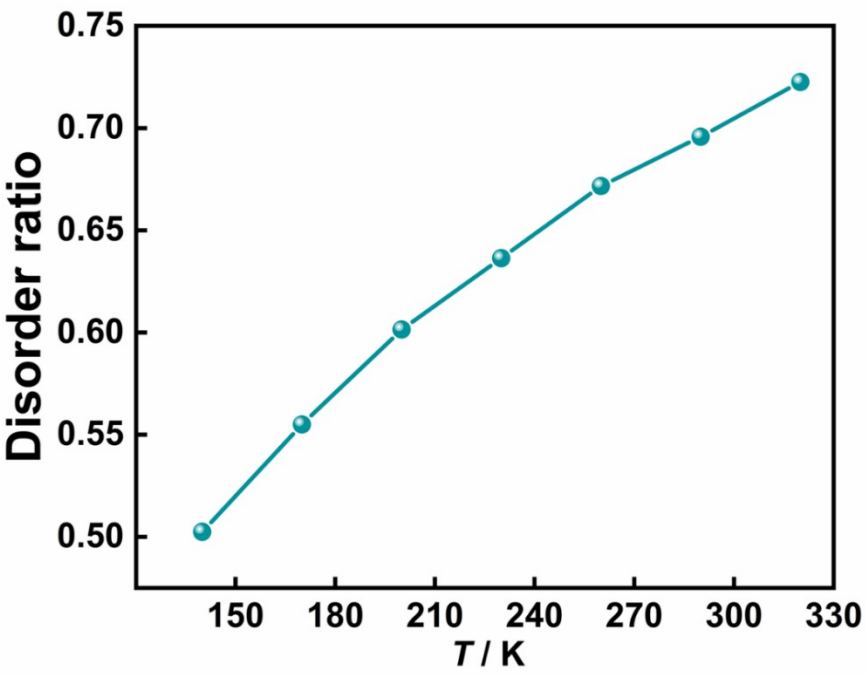

Fig. S3 Occupation change diagram of C=C crystal positions.

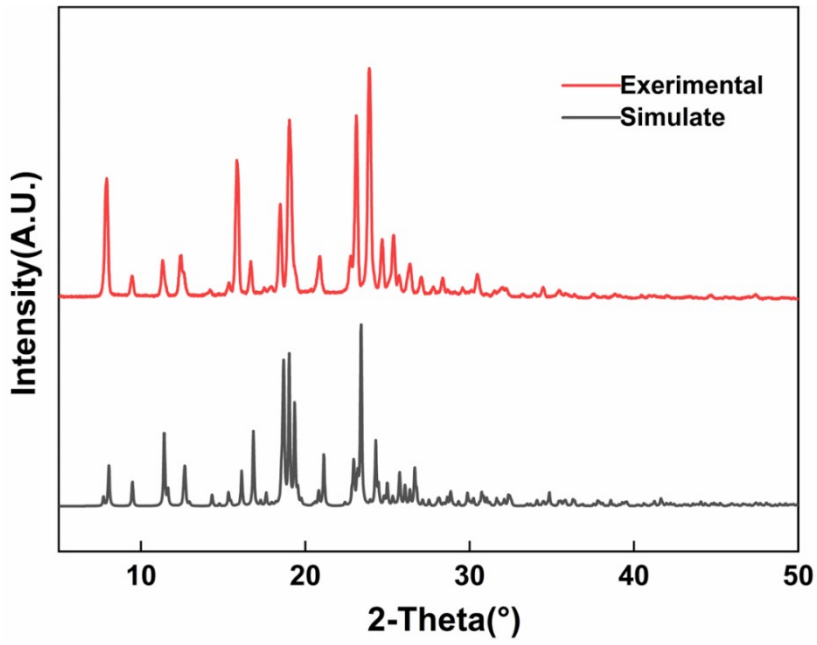

Fig. S4 P-XRD curves of **Bpe-BPh$_4$**.

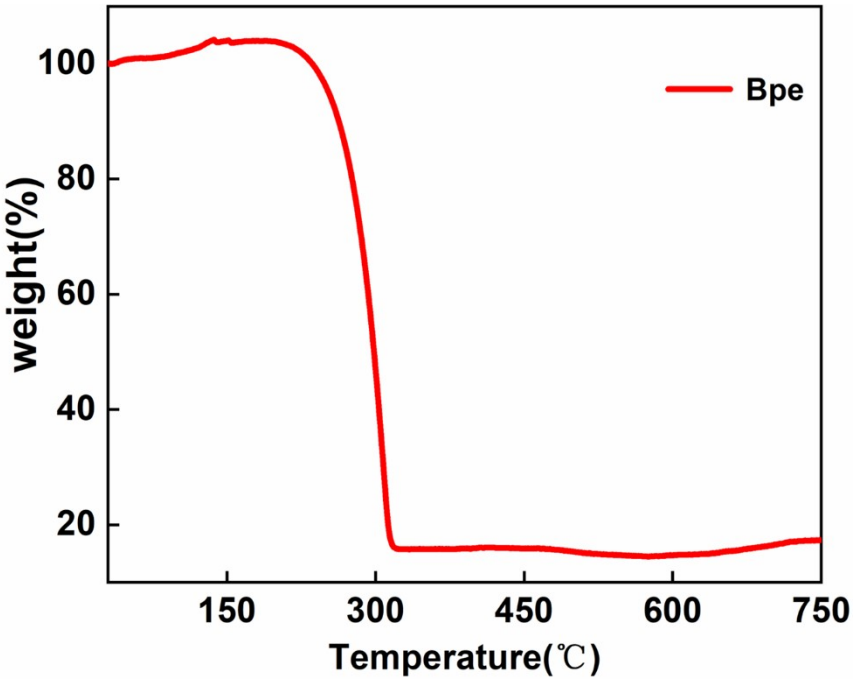

Fig. S5 TG curve of **Bpe**.

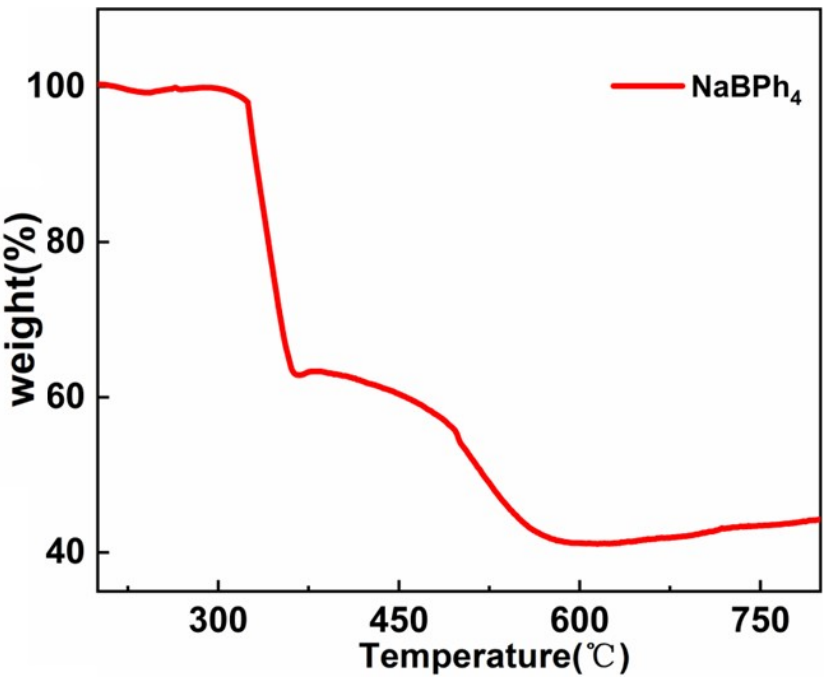

Fig. S6 TG curve of **$NaBPh_4$**.

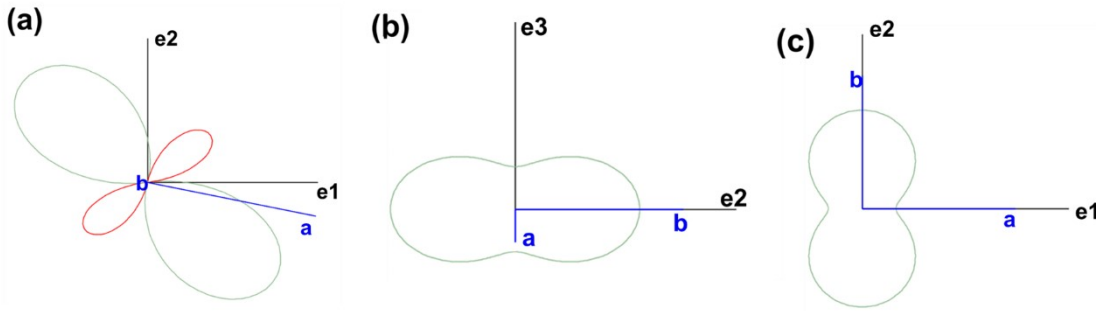

Fig. S7 Three default (a–c) sections through the 3-D representation surface for **Bpe-BPh_4** at 320 K.

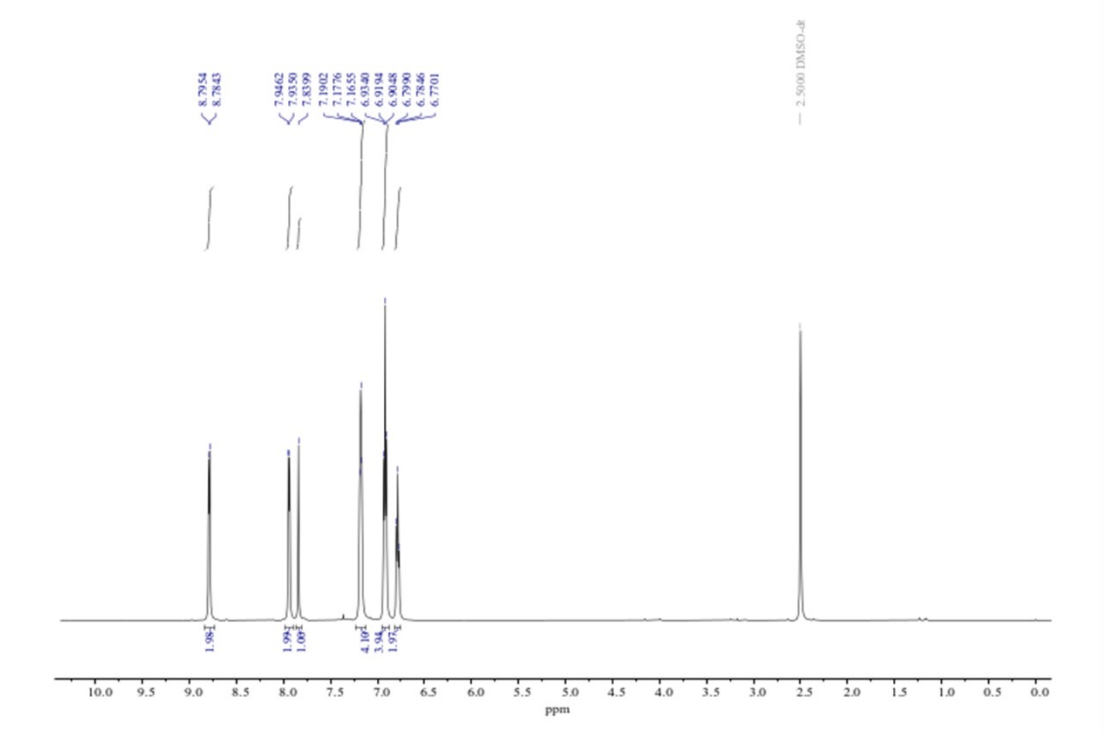

Fig. S8 ^{1}H NMR curve of **Bpe-BPh_4**.

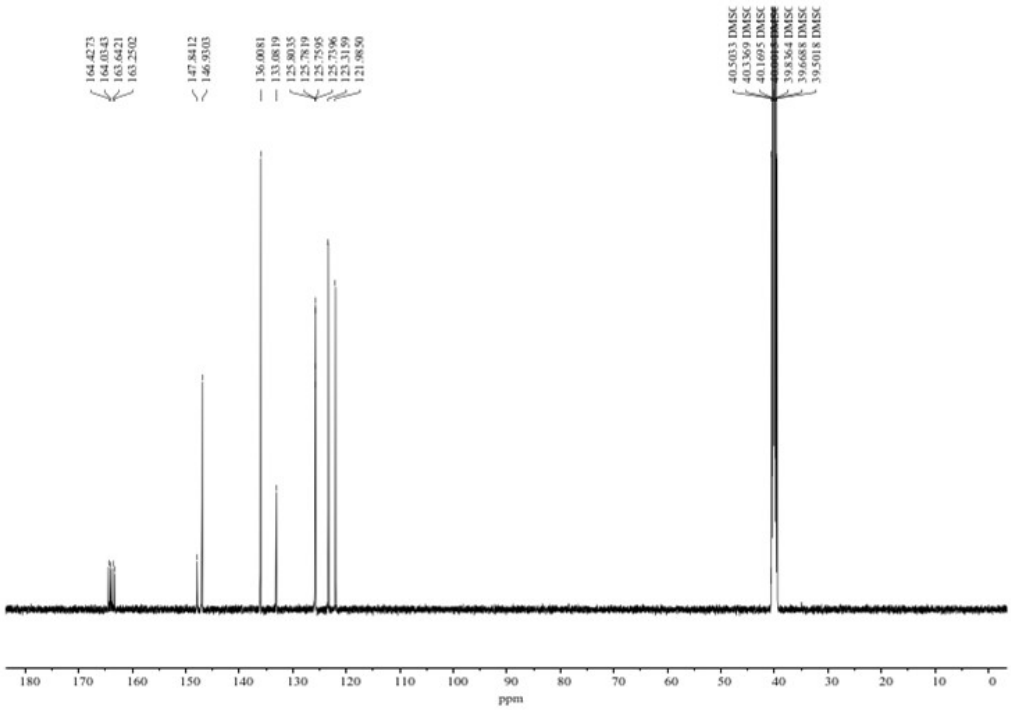

Fig. S9 ^{13}C NMR curve of **Bpe-BPh$_4$**.