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Polymorphism Dependent Charge Transport Property of 9, 10-Bis ((E)-2-(pyrid-2-yl) vinyl) anthracene: A Theoretical Study

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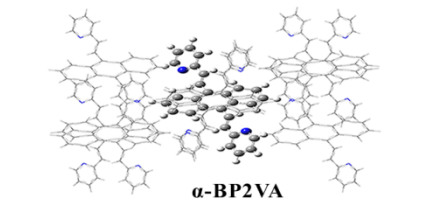
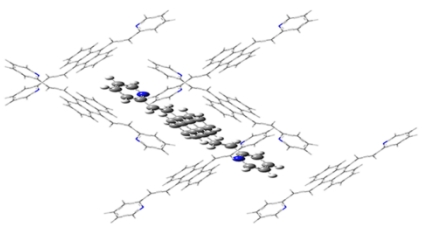
Table S1.Selected Bond Lengths (Ang) Angles (Deg) and Torsion (Deg) of different crystal structure in the Neutral and Ionic States, together with Experimental Values for α-, β- and γ-BP2VA. separately.

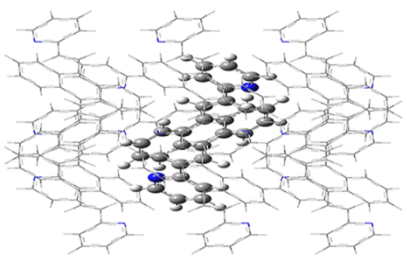
Parameters(α)	Neutral(N)	Cationic(C)	Anionic(A)	Crystal	Δ(C-N)	Δ(A-N)
R(N1-C2)/ R(N1'-C2')	1.33	1.33	1.33	1.33	0	0
R(C6-N1) /R(C6'-N1')	1.35	1.35	1.36	1.34	0	0.01
R(C7-C8)/ R(C7'-C8')	1.35	1.36	1.38	1.32	0.01	0.03
R(C8-C9) /R(C8'-C9')	1.47	1.45	1.44	1.48	-0.02	-0.03
θ(N1-C2-C3)/ θ(N1'-C2'-C3')	124.0	123.6	124.9	124.3	-0.4	0.9
θ(C5-C6-N1)/θ(C5'-C6'-N1')	121.7	122.5	120.2	121.8	0.8	-1.5
θ(N1-C6-C7-C8)/θ(N1'-C6'-C7'-C8')	1.6	2.7	5.8	8.2	1.1	4.2
θ(C7-C8-C9-C10)/θ(C7'-C8'-C9'-C10')	52.4	41.6	30.5	59.5	-10.8	-21.9
Parameters(β)	Neutral(N)	Cationic(C)	Anionic(A)	Crystal	Δ(C-N)	Δ(A-N)
R(N1-C2)/ R(N1'-C2')	1.34	1.33	1.33	1.32	-0.01	-0.01
R(C6-N1) /R(C6'-N1')	1.35	1.35	1.37	1.32	0	0.02
R(C7-C8)/ R(C7'-C8')	1.35	1.36	1.37	1.27	0.01	0.02
R(C8-C9) /R(C8'-C9')	1.48	1.45	1.44	1.49	-0.03	-0.04
θ(N1-C2-C3)/ θ(N1'-C2'-C3')	123.9	123.5	124.8	124.9	-0.4	0.9
θ(C5-C6-N1)/θ(C5'-C6'-N1')	121.6	122.3	120.2	122.0	0.7	-1.4
θ(N1-C6-C7-C8)/θ(N1'-C6'-C7'-C8')	172.2	173.2	169.1	176.7	1	-3.1
θ(C7-C8-C9-C10)/θ(C7'-C8'-C9'-C10')	128.3	136.7	148.3	116.8	8.4	20
Parameters(γ)	Neutral(N)	Cationic(C)	Anionic(A)	Crystal	Δ(C-N)	Δ(A-N)
R(N1-C2)/ R(N1'-C2')	1.33	1.33	1.33	1.34/1.32	0	0
R(C6-N1) /R(C6'-N1')	1.35	1.35	1.36	1.35/1.34	0	0.01
R(C7-C8)/ R(C7'-C8')	1.35	1.36	1.38	1.30/1.33	0.01	0.03
R(C8-C9) /R(C8'-C9')	1.47	1.45	1.44	1.50/1.47	-0.02	-0.03
θ(N1-C2-C3)/ θ(N1'-C2'-C3')	124.0	123.6	124.9	123.7/124.4	-0.4	0.9
θ(C5-C6-N1)/θ(C5'-C6'-N1')	121.7	122.5	120.2	121.6/121.7	0.8	-1.5
θ(N1-C6-C7-C8)/θ(N1'-C6'-C7'-C8')	1.6	2.7	5.9	14.1/6.7	1.1	4.3
θ(C7-C8-C9-C10)/θ(C7'-C8'-C9'-C10')	52.4	41.8	30.9	51.2/53.4	-10.6	-21.5



α-BP2VA



β- BP2VA



γ-BP2VA

Figure S1.The central molecule surrounded by the nearest-neighbouring (NN) molecules used to calculate the reorganization energy. The ball and stick model represents the region treated with QM method, and the wire model represents the region treated with MM method.