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Electronic Supplementary Information

Organic matrix-induced formation of a discrete cyclic $[Cl_2(H_2O)_2]^{2-}$cluster

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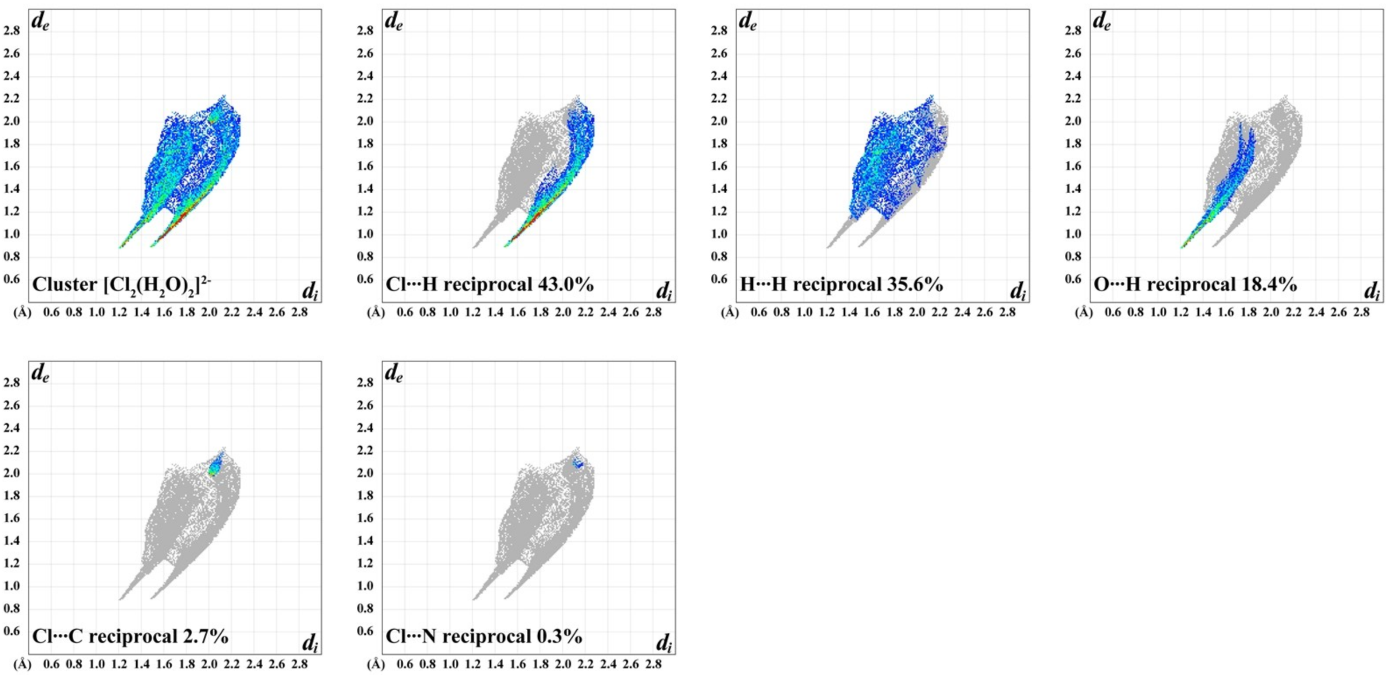

Fig. S1 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for the $[Cl_2(H_2O)_2]^{2-}$ cluster in the structure of **1**.

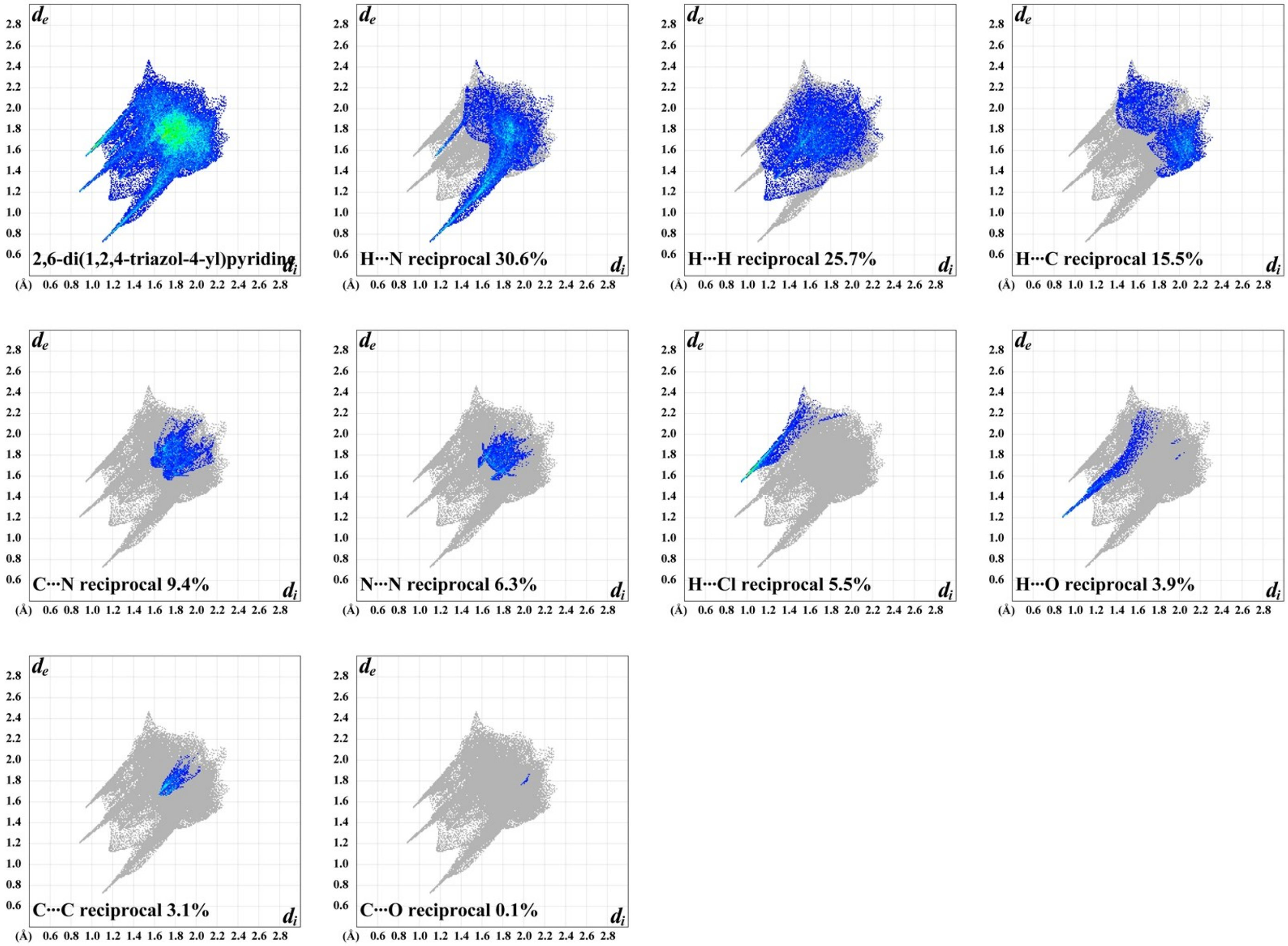

Fig. S2 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for the 2,6-di(4*H*-1,2,4-triazol-4-yl)pyridine in the structure of **1**.

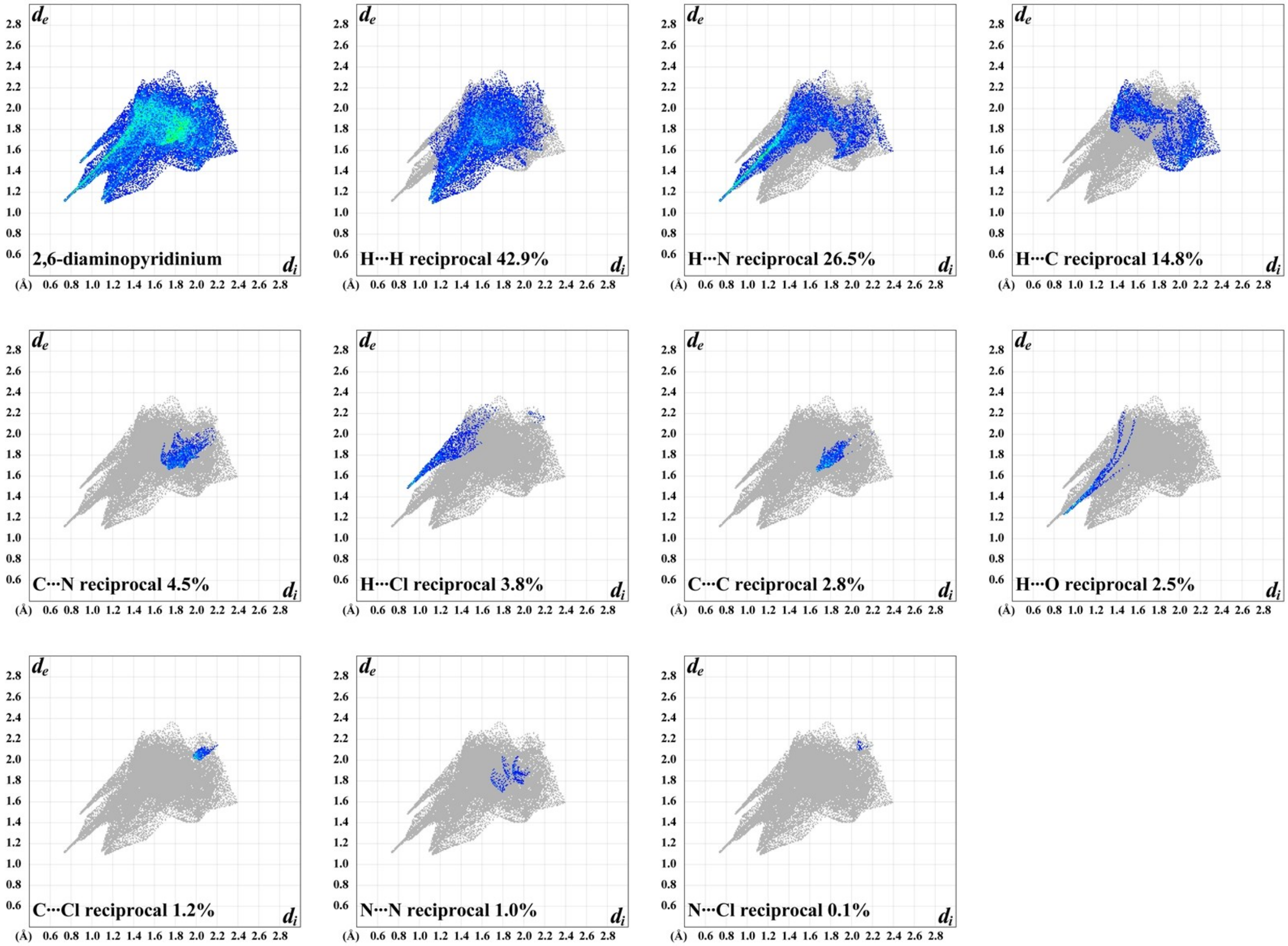

Fig. S3 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for the 2,6-diaminopyridinium in the structure of **1**.

Table S1 Selected bond lengths (Å) and angles (°) for **1**

Bond lengths					
N(2)–C(3)	1.329(3)	N(13)–C(14)	1.365(3)	N(21)–C(22)	1.363(3)
N(2)–C(7)	1.332(3)	N(13)–C(17)	1.363(3)	N(21)–C(26)	1.365(3)
N(8)–C(3)	1.429(3)	N(15)–N(16)	1.393(3)	N(27)–C(22)	1.348(3)
N(8)–C(9)	1.367(3)	N(15)–C(14)	1.315(3)	N(28)–C(26)	1.338(3)
N(8)–C(12)	1.359(3)	N(16)–C(17)	1.307(3)	C(22)–C(23)	1.387(4)
N(10)–N(11)	1.388(3)	C(3)–C(4)	1.380(3)	C(23)–C(24)	1.375(4)
N(10)–C(9)	1.301(3)	C(4)–C(5)	1.382(3)	C(24)–C(25)	1.367(4)
N(11)–C(12)	1.311(3)	C(5)–C(6)	1.387(3)	C(25)–C(26)	1.391(3)
N(13)–C(7)	1.425(3)	C(6)–C(7)	1.369(3)		
Bond angles					
C(3)–N(2)–C(7)	116.76(19)	N(2)–C(3)–C(4)	124.5(2)	N(13)–C(17)–N(16)	110.1(2)
C(3)–N(8)–C(9)	127.0(2)	N(8)–C(3)–C(4)	122.0(2)	C(22)–N(21)–C(26)	122.9(2)
C(3)–N(8)–C(12)	128.90(19)	C(3)–C(4)–C(5)	116.9(2)	N(21)–C(22)–N(27)	117.1(2)
C(9)–N(8)–C(12)	104.08(19)	C(4)–C(5)–C(6)	120.2(2)	N(21)–C(22)–C(23)	119.0(2)
N(11)–N(10)–C(9)	107.4(2)	C(5)–C(6)–C(7)	117.4(2)	N(27)–C(22)–C(23)	123.9(2)
N(10)–N(11)–C(12)	106.5(2)	N(2)–C(7)–N(13)	113.03(18)	C(22)–C(23)–C(24)	118.3(2)
C(7)–N(13)–C(14)	129.91(18)	N(2)–C(7)–C(6)	124.3(2)	C(23)–C(24)–C(25)	122.7(2)
C(7)–N(13)–C(17)	125.41(18)	N(13)–C(7)–C(6)	122.6(2)	C(24)–C(25)–C(26)	118.6(2)
C(14)–N(13)–C(17)	104.68(18)	N(8)–C(9)–N(10)	110.8(2)	N(21)–C(26)–N(28)	117.9(2)
N(16)–N(15)–C(14)	105.80(18)	N(8)–C(12)–N(11)	111.2(2)	N(21)–C(26)–C(25)	118.6(2)
N(15)–N(16)–C(17)	108.21(19)	N(13)–C(14)–N(15)	111.21(19)	N(28)–C(26)–C(25)	123.5(2)
N(2)–C(3)–N(8)	113.52(19)				
Torsion angles					
C(7)–N(2)–C(3)–N(8)	–178.99(18)	N(10)–N(11)–C(12)–N(8)	0.1(3)	C(3)–C(4)–C(5)–C(6)	–0.6(4)
C(7)–N(2)–C(3)–C(4)	0.4(3)	C(14)–N(13)–C(7)–N(2)	172.2(2)	C(4)–C(5)–C(6)–C(7)	0.4(4)
C(3)–N(2)–C(7)–N(13)	179.49(18)	C(14)–N(13)–C(7)–C(6)	–7.7(4)	C(5)–C(6)–C(7)–N(2)	0.3(4)
C(3)–N(2)–C(7)–C(6)	–0.7(3)	C(17)–N(13)–C(7)–N(2)	–7.2(3)	C(5)–C(6)–C(7)–N(13)	–179.9(2)
C(9)–N(8)–C(3)–N(2)	3.2(3)	C(17)–N(13)–C(7)–C(6)	172.9(3)	C(26)–N(21)–C(22)–N(27)	179.7(3)
C(9)–N(8)–C(3)–C(4)	–176.3(3)	C(7)–N(13)–C(14)–N(15)	–179.6(2)	C(26)–N(21)–C(22)–C(23)	0.0(4)
C(12)–N(8)–C(3)–N(2)	–174.0(2)	C(17)–N(13)–C(14)–N(15)	–0.1(3)	C(22)–N(21)–C(26)–N(28)	178.9(2)
C(12)–N(8)–C(3)–C(4)	6.6(4)	C(7)–N(13)–C(17)–N(16)	179.2(2)	C(22)–N(21)–C(26)–C(25)	–0.3(4)
C(3)–N(8)–C(9)–N(10)	–178.7(2)	C(14)–N(13)–C(17)–N(16)	–0.3(3)	N(21)–C(22)–C(23)–C(24)	0.1(4)
C(12)–N(8)–C(9)–N(10)	–0.9(3)	C(14)–N(15)–N(16)–C(17)	–0.7(3)	N(27)–C(22)–C(23)–C(24)	–179.6(3)
C(3)–N(8)–C(12)–N(11)	178.2(2)	N(16)–N(15)–C(14)–N(13)	0.5(3)	C(22)–C(23)–C(24)–C(25)	0.1(5)
C(9)–N(8)–C(12)–N(11)	0.5(3)	N(15)–N(16)–C(17)–N(13)	0.6(3)	C(23)–C(24)–C(25)–C(26)	–0.4(5)
C(9)–N(10)–N(11)–C(12)	–0.7(3)	N(2)–C(3)–C(4)–C(5)	0.2(4)	C(24)–C(25)–C(26)–N(21)	0.4(4)
N(11)–N(10)–C(9)–N(8)	1.0(3)	N(8)–C(3)–C(4)–C(5)	179.6(2)	C(24)–C(25)–C(26)–N(28)	–178.7(3)