Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic and Crystal Structures of 1,2,3-Triazole-Fused *p*-Benzoquinone Derivatives

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Table S1. Mulliken charge of HOMO and LUMO of molecule **1** using DFT calculation.

Atom label	Mulliken charge	HOMO			LUMO		
		$2p_x$	$2p_y$	$2p_z$	$2p_x$	$2p_y$	$2p_z$
1O	-0.528	-0.0049	-0.0003	-0.0491	-0.0008	0.0054	0.2907
2N	-0.651	0.0211	-0.0414	-0.2251	-0.0116	0.0124	0.0760
3N	-0.644	-0.0371	-0.0007	0.2204	-0.0205	0.0002	0.1391
4C	0.064	0.0007	0.0027	0.2573	-0.0005	-0.0015	-0.1218
5C	0.413	-0.0137	-0.0027	0.0304	-0.0004	0.0003	-0.2689
6C	0.135	0.0087	0.0057	-0.2116	0.0020	0.0033	-0.1918
11O	-0.528	0.0049	0.0003	0.0491	0.0008	-0.0054	-0.2907
12N	-0.651	-0.0211	0.0414	0.2250	0.0116	-0.0124	-0.0760
13N	-0.644	0.0371	0.0007	-0.2205	0.0205	-0.0002	-0.1391
14C	0.064	-0.0007	-0.0027	-0.2573	0.0005	0.0015	0.1218
15C	0.413	0.0137	0.0027	-0.0303	0.0004	-0.0003	0.2689
16C	0.135	-0.0087	-0.0057	0.2116	-0.0020	-0.0033	0.1918

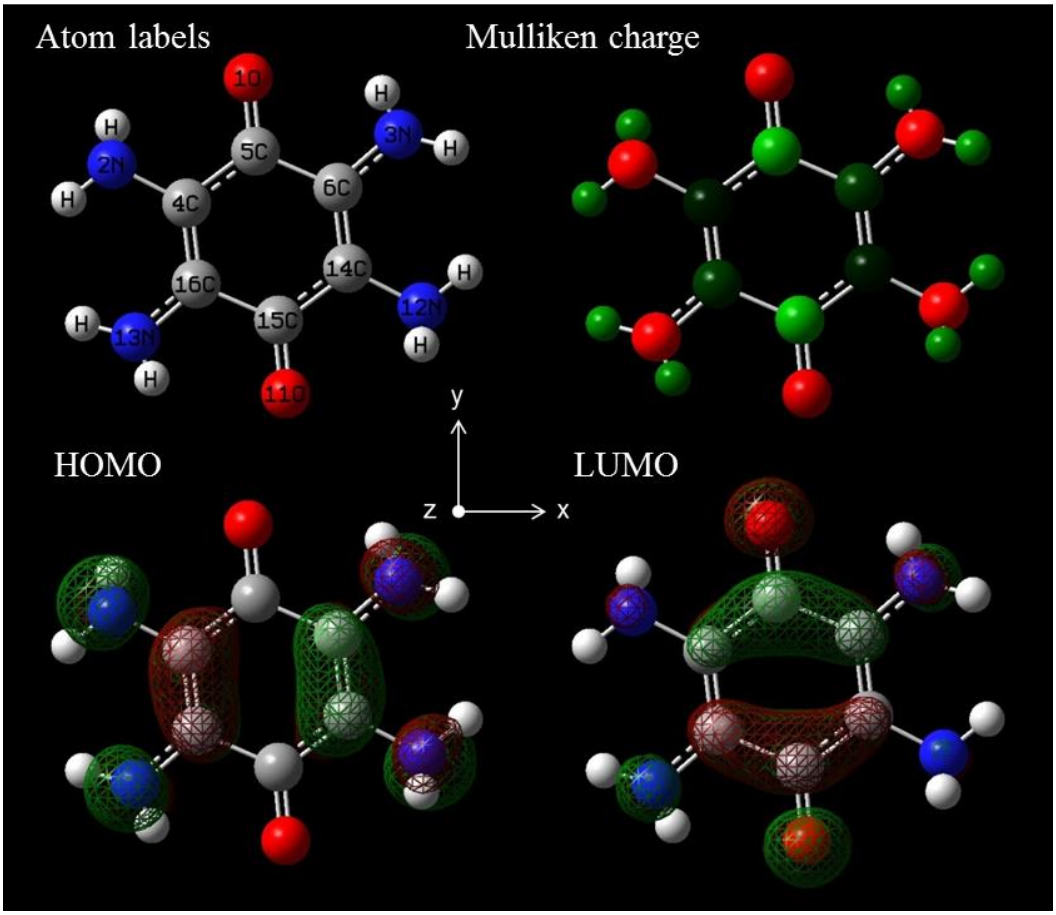


Figure S1. Atomic numbering scheme and Mulliken charge of HOMO and LUMO of molecule **1**.

Table S2. Mulliken charge of HOMO and LUMO of molecule **2** using DFT calculation.

Atom label	Mulliken charge	HOMO			LUMO		
		2px	2py	2pz	2px	2py	2pz
1O	-0.519	-0.0435	0.0212	-0.0744	0.0133	-0.0812	0.2606
2N	-0.510	0.1591	-0.1754	-0.1273	0.0037	0.0235	0.0204
3N	-0.501	0.0973	0.0843	0.1832	0.0486	0.0855	0.1525
4C	0.373	0.0750	-0.0284	0.0285	0.0014	0.0794	-0.2303
5C	0.253	-0.0305	0.0126	-0.1065	-0.0126	-0.0203	-0.2107
6C	0.096	-0.0395	-0.0209	0.2116	0.0034	-0.0261	-0.1061
23O	-0.519	0.0435	-0.0212	0.0745	-0.0134	0.0812	-0.2606
24N	-0.510	-0.1592	0.1754	0.1273	-0.0037	-0.0235	-0.0204
25N	-0.501	-0.0973	-0.0843	-0.1832	-0.0486	-0.0855	-0.1525
26C	0.373	-0.0750	0.0284	-0.0285	-0.0014	-0.0794	0.2303
27C	0.253	0.0305	-0.0126	0.1065	0.0126	0.0203	0.2107
28C	0.096	0.0395	0.0209	-0.2116	-0.0034	0.0261	0.1061

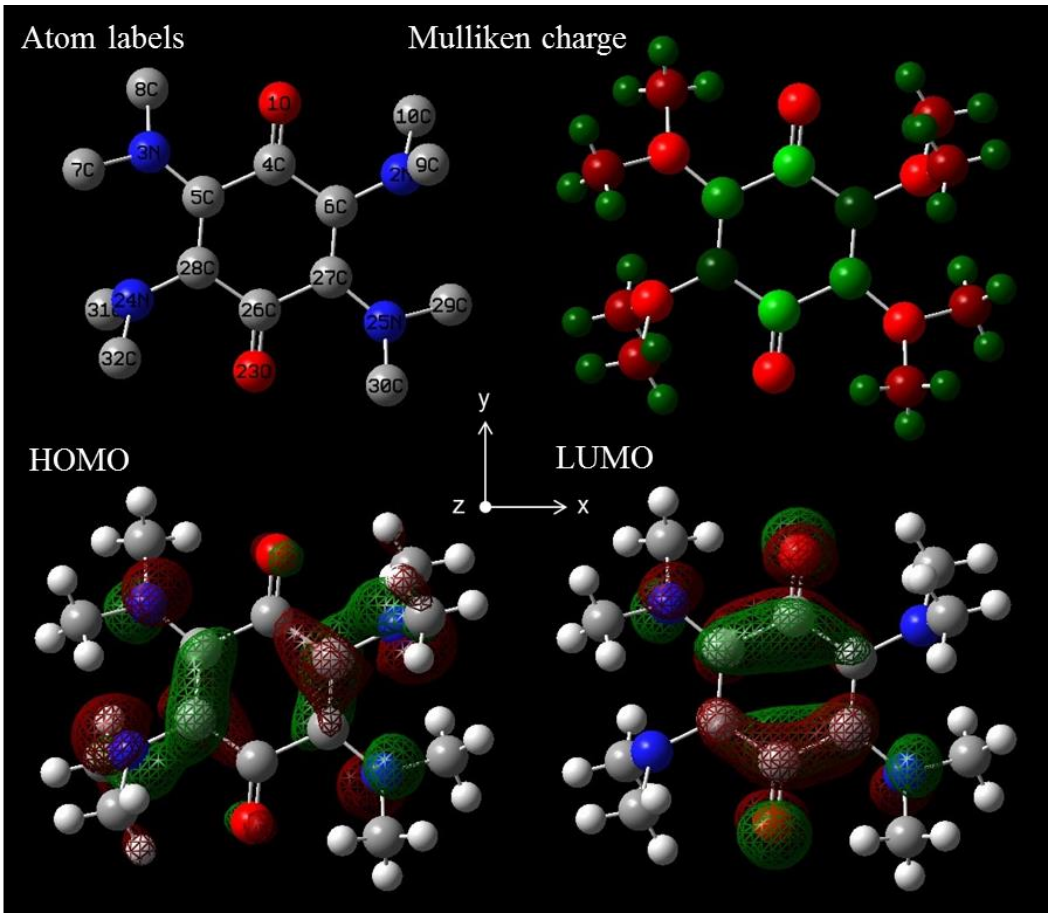
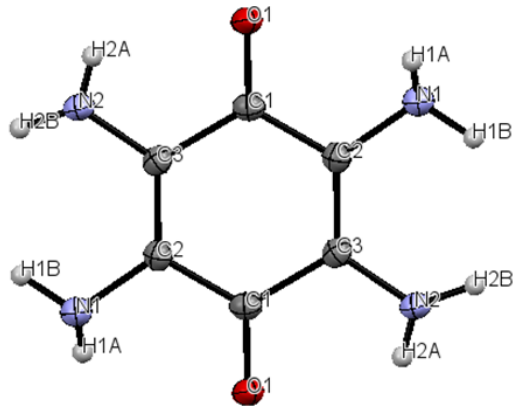
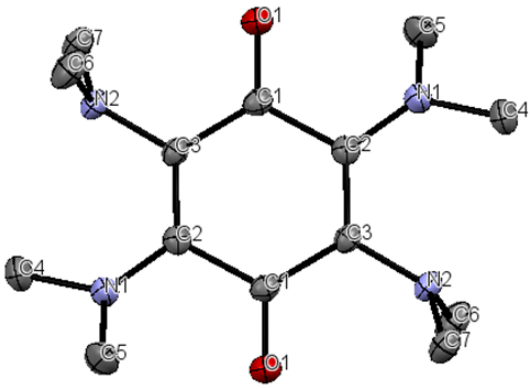


Figure S2. Atomic numbering scheme and Mulliken charge of HOMO and LUMO of molecule **2**.



atom	atom	length, Å
O1	C1	1.236(3)
C1	C2	1.443(3)
C1	C3	1.507(3)
C2	C3	1.362(3)
C2	N1	1.413(3)
C3	N2	1.352(3)



atom	atom	length, Å
O1	C1	1.230(2)
C1	C2	1.519(2)
C1	C3	1.460(2)
C2	C3	1.377(2)
C2	N1	1.362(2)
C3	N2	1.418(2)
N1	C4	1.459(2)
N1	C5	1.459(2)
N2	C6	1.453(2)
N2	C7	1.457(2)

Figure S3. Molecular structures and bond-lengths of molecules **1** (upper) and **2** (lower).

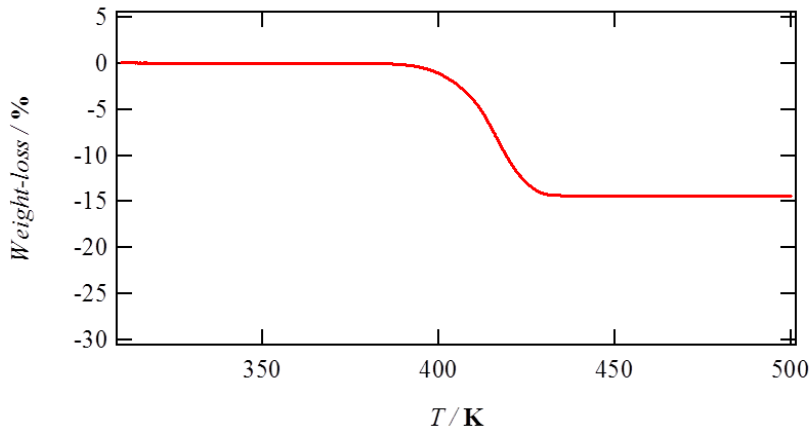
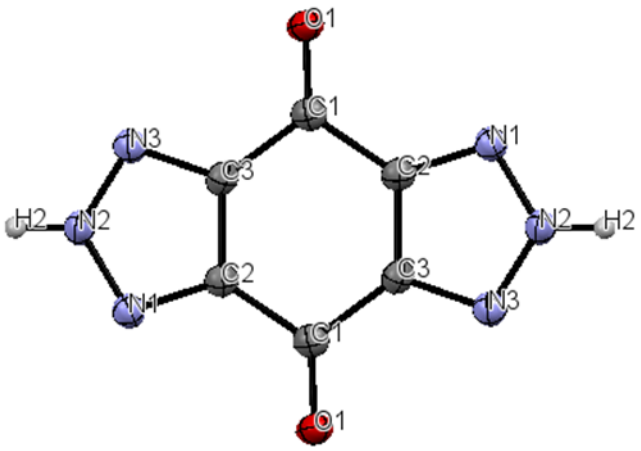
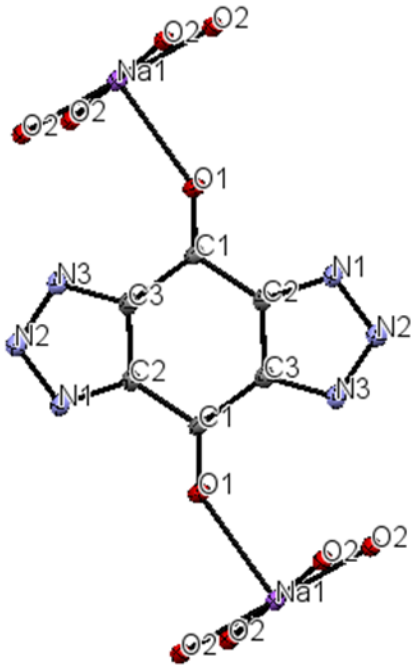


Figure S4. TG diagram of crystal **2**•$(H_2O)_2$.



atom	atom	length, Å
O1	C1	1.211(2)
N1	N2	1.326(2)
N1	C2	1.340(3)
N2	N3	1.321(2)
N3	C3	1.338(3)
C1	C2	1.479(2)
C1	C3	1.481(3)
C2	C3	1.403(3)

Figure S5. Molecular structures and bond-lengths of crystal **2**.



atom	atom	length, Å
Na1	O1	2.348(2)
Na1	O2	2.366(2)
O1	C1	1.216(4)
N1	N2	1.347(3)
N1	C2	1.352(3)
N2	N3	1.332(3)
N3	C3	1.353(3)
C1	C2	1.476(4)
C1	C3	1.480(3)
C2	C3	1.387(4)

Figure S6. Molecular structures and bond-lengths of crystal $Na^{+}(\mathbf{2}^{-})\bullet(H_2O)_2$.

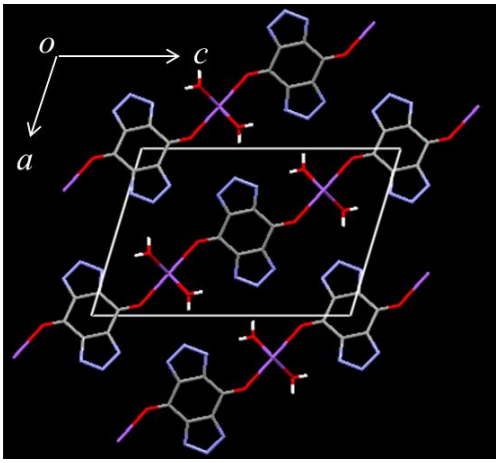
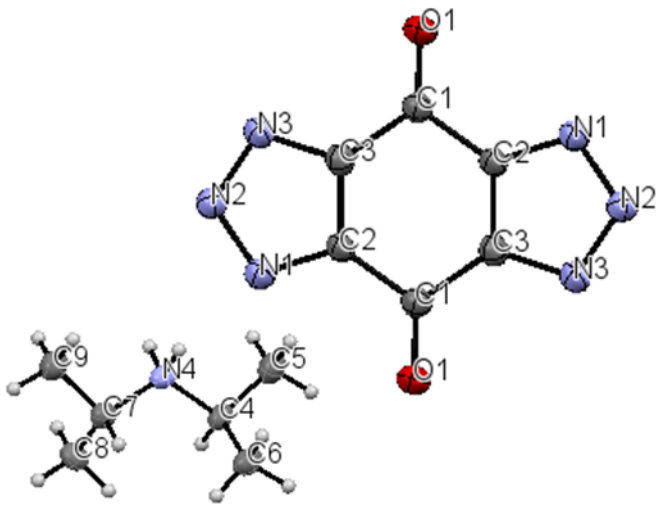


Figure S7. Packing structure of $Na^{+}(\mathbf{2}^{-})\bullet(H_2O)_2$ viewed along the *b* axis.



atom	atom	length, Å
O1	C1	1.224(3)
N1	N2	1.353(2)
N1	C2	1.343(2)
N2	N3	1.341(3)
N3	C3	1.357(2)
C1	C2	1.480(2)
C1	C3	1.474(3)
C2	C3	1.391(3)

Figure S8. Molecular structures and bond-lengths of crystal $(DIPA^{+})_2(\mathbf{2}^{2-})$.

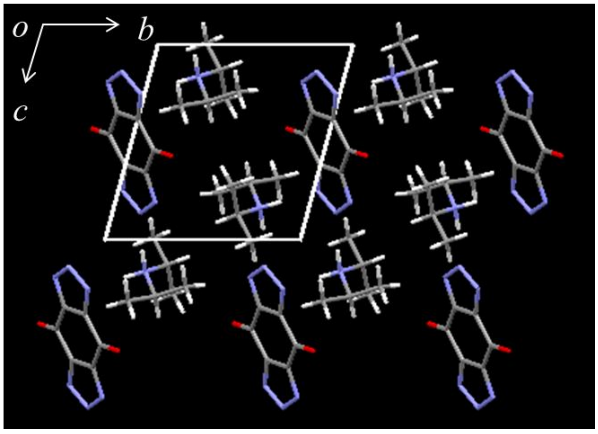


Figure S9. Packing structure of $(DIPA^{+})(\mathbf{2}^{-2})$ viewed along the *a* axis.

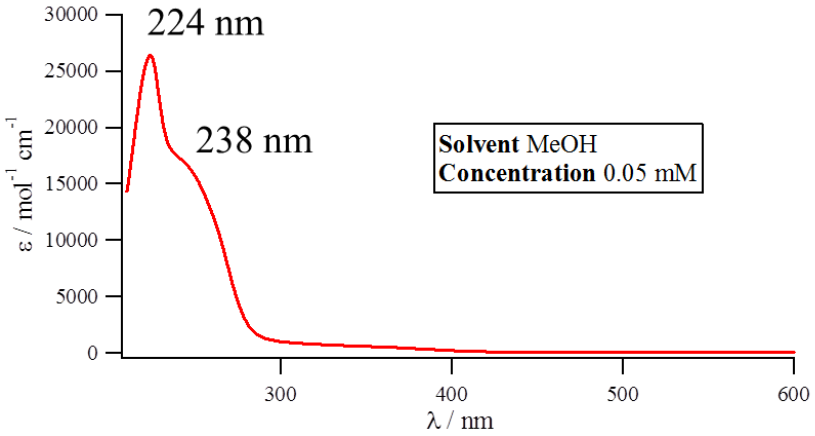


Figure S10. UV-vis spectra of **2** in CH_3OH (0.05 mM).

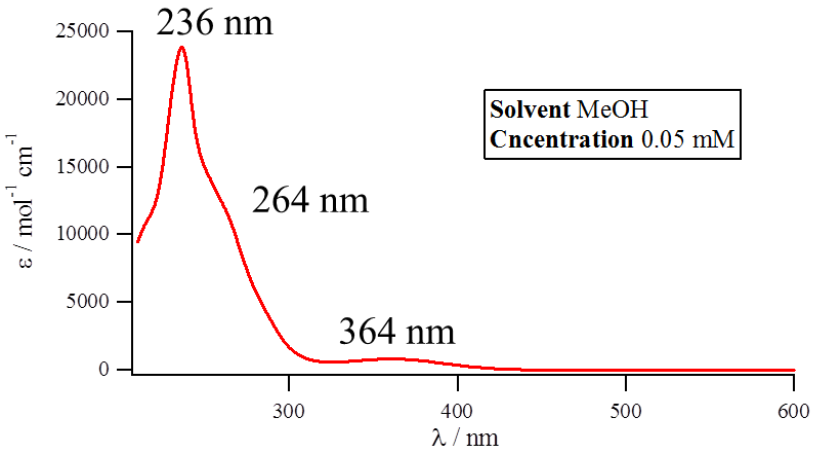


Figure S11. UV-vis spectra of $Na^+(\mathbf{2}^-)$ in CH_3OH (0.05 mM).

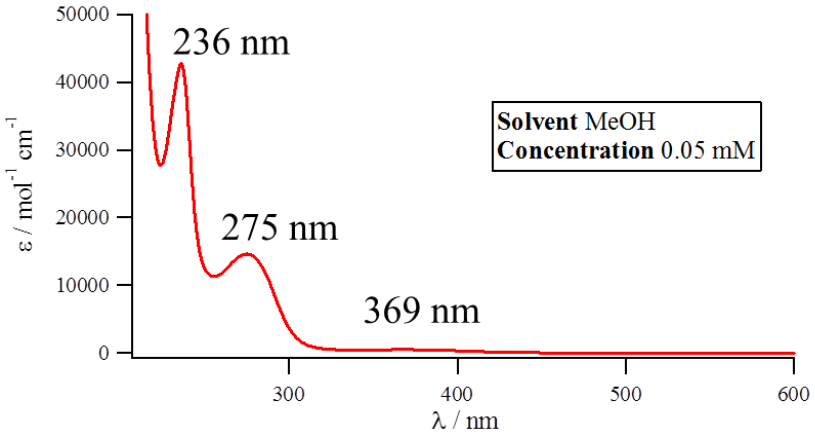
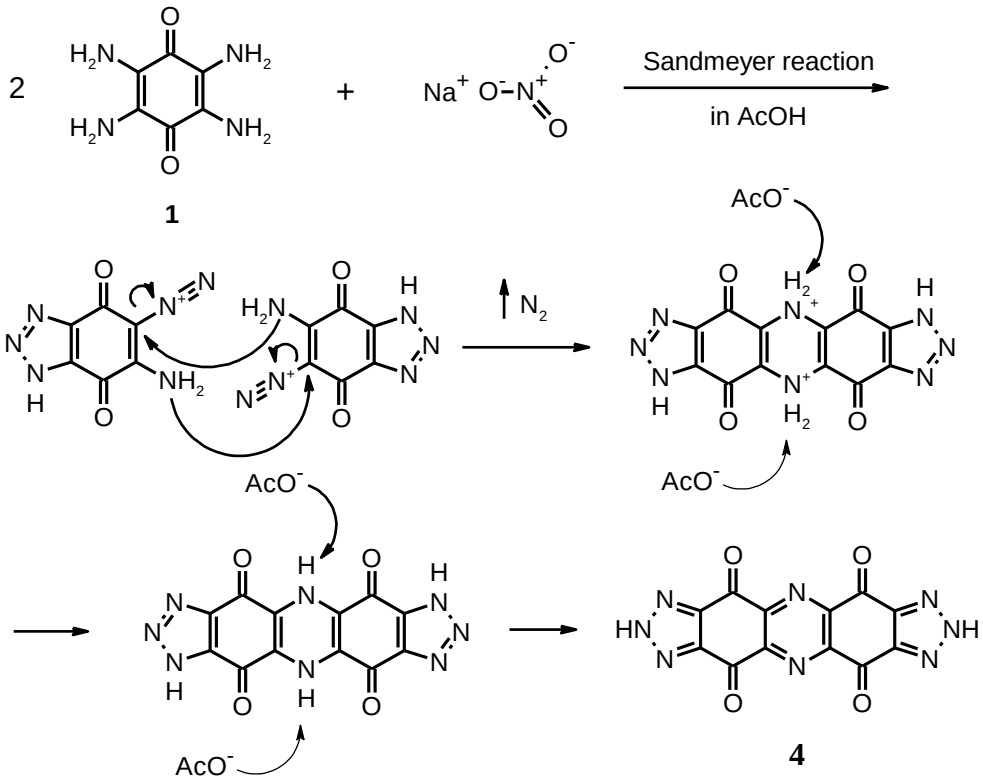
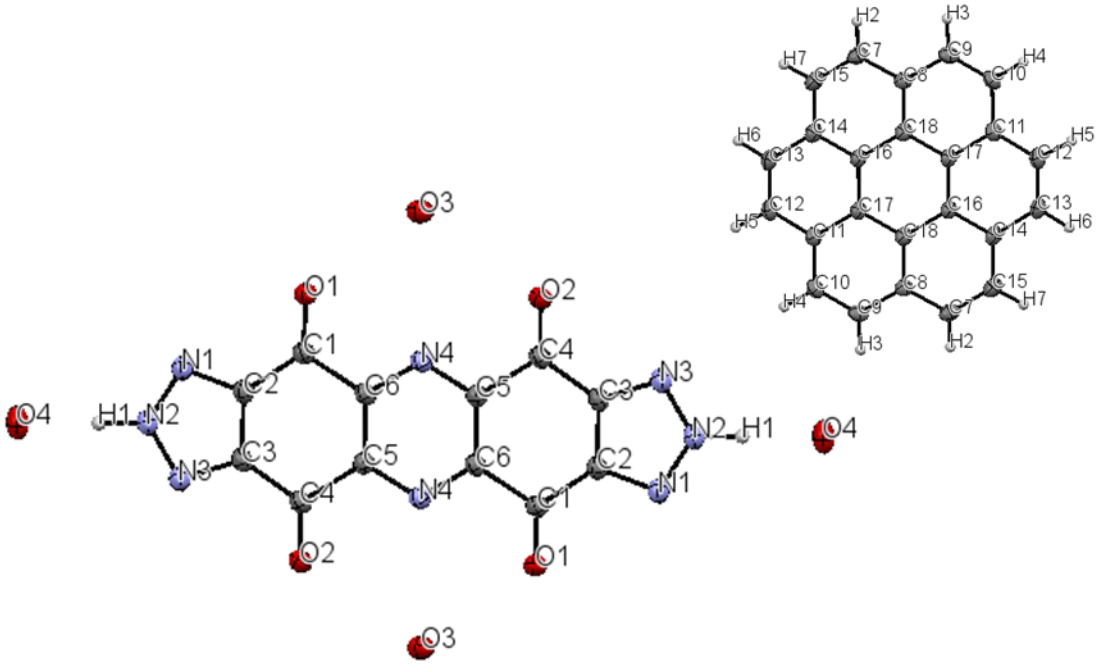


Figure S12. UV-vis spectra of $(DIPA^+)_2(\mathbf{2}^{2-})$ in CH_3OH (0.05 mM).

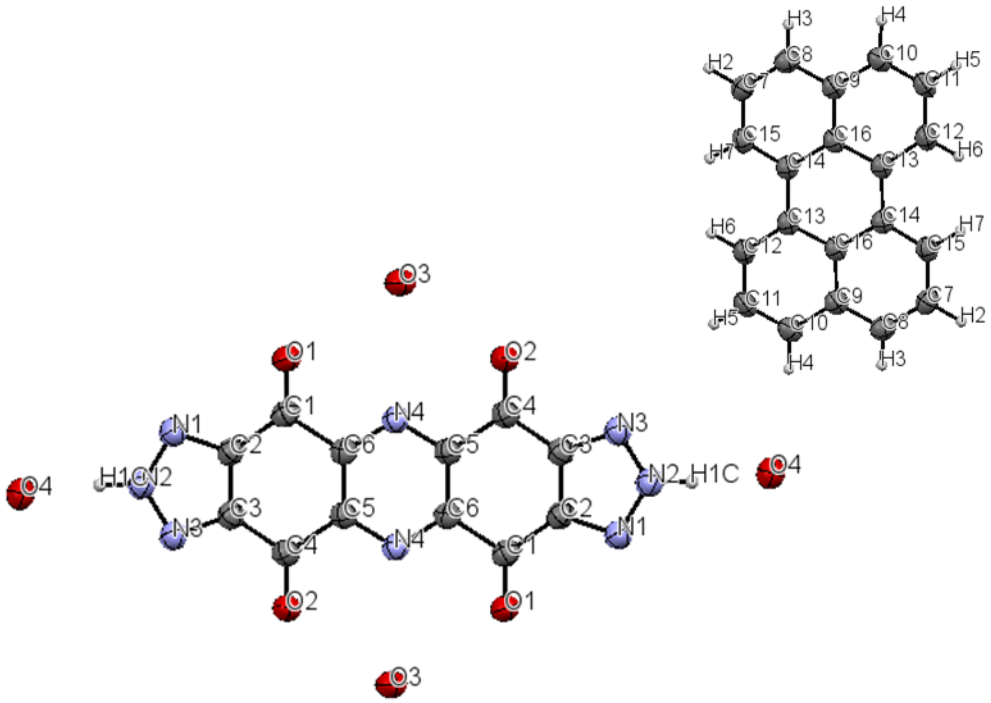


Scheme S1. Possible reaction scheme for the formation of compound **4**.



atom	atom	length, Å	atom	atom	length, Å
O1	C1	1.217(2)	N4	C5	1.330(2)
O2	C4	1.216(2)	C1	C2	1.466(3)
N1	N2	1.328(3)	C1	C6	1.510(3)
N1	C2	1.337(2)	C2	C3	1.399(3)
N2	N3	1.327(3)	C3	C4	1.469(3)
N3	C3	1.338(2)	C4	C5	1.516(3)
N4	C6	1.328(2)	C5	C6	1.418(3)

Figure S13. Molecular structures and bond-lengths of crystal (coronene)(**4**)•$(H_2O)_4$.



atom	atom	length, Å	atom	atom	length, Å
O1	C1	1.212(4)	N4	C5	1.341(4)
O2	C4	1.218(3)	C1	C2	1.461(4)
N1	N2	1.336(4)	C1	C6	1.526(4)
N1	C2	1.343(4)	C2	C3	1.397(4)
N2	N3	1.327(3)	C3	C4	1.465(4)
N3	C3	1.342(4)	C4	C5	1.508(4)
N4	C6	1.334(4)	C5	C6	1.398(4)

Figure S14. Molecular structures and bond-lengths of crystal (perylen)(**4**)•$(H_2O)_4$.

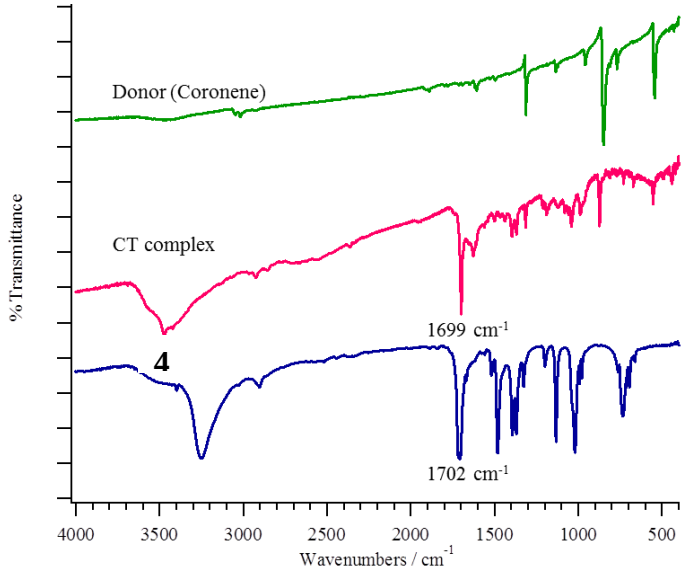


Figure S15. IR spectra of (perylen)(**4**)•$(H_2O)_4$ on KBr pellet.

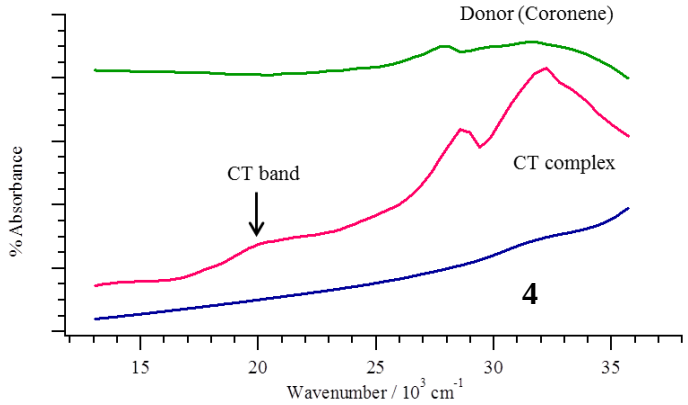


Figure S16. IR spectra of (coronene)(**4**)•$(H_2O)_4$ on KBr pellet.