Electronic Supplementary Information

Yu Shang[a], Bo Jin[a]*, Rufang Peng[a]*, Zhicheng Guo[b], Qiangqiang Liu[a], Jun Zhao[a], Qingchun Zhang[a]

[a] State Key Laboratory Cultivation Base for Nonmetal Composites and Functional Materials, Southwest University of Science and Technology, Mianyang 621010, China

[b]School of Nation Defence Science and Technology， Southwest University of Science and Technology, Mianyang 621010, China

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Table 1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
O001	3860.3(8)	1550.3(12)	6040.8(18)	49.0(4)
N002	4600.1(9)	1611.4(13)	5388.0(19)	37.4(4)
N003	2265.9(9)	4860.3(14)	7906.9(19)	41.1(4)
N004	3201.7(11)	3693.6(14)	6959(2)	43.1(4)
N005	5779.9(10)	1181.4(15)	4341(2)	43.9(5)
N006	4971.2(11)	2721.3(15)	5100(2)	46.9(4)
N007	5681.3(11)	2442.4(16)	4463(2)	49.7(5)
N008	2891.6(10)	5667.8(15)	7516(2)	49.2(5)
C009	5096.1(10)	664.7(16)	4930(2)	35.4(4)
C00A	2448.3(13)	3691.2(16)	7579(2)	41.7(5)
C00B	3453.1(13)	4919.5(17)	6943(3)	46.3(5)

Table 2. Bond Lengths [Å] and angles [°] for **2**.

bond	Length/Å	bond	Angle/°
O001-N002	1.3209(17)	O001-N002-N006	121.72(13)
N002-N006	1.334(2)	O001-N002-C009	129.10(14)
N002-C009	1.338(2)	N006-N002-C009	109.18(14)
N003-N008	1.3531(19)	C00A-N003-N008	111.43(14)
N003-C00A	1.296(2)	C00A-N004-C00B	105.81(14)
N004-C00A	1.325(3)	C009-N005-N007	105.95(14)
N004-C00B	1.346(2)	N007-N006-N002	105.93(14)
N005-N007	1.340(2)	N006-N007-N005	111.18(15)
N005-C009	1.330(2)	C00B-N008-N003	103.47(15)
N006-N007	1.304(2)	N002-C009-C009[1]	124.83(18)
N008-C00B	1.300(2)	N005-C009-N002	107.76(15)
C0090-C009[1]	1.437(3)	N005-C009-C009[1]	127.41(19)
		N003-C00A-N004	107.55(15)
		N008-C00B-N004	111.73(16)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O001	42.2(8)	34.8(7)	80.8(10)	-3.2(6)	39.5(7)	1.2(6)
N002	34.4(8)	32.5(8)	50.2(8)	-0.8(6)	20.9(6)	-0.8(6)
N003	36.4(8)	36.8(9)	55.5(9)	-1.8(6)	22.8(6)	2.3(6)

N004	40.7(8)	35.9(9)	57.5(9)	0.2(6)	21.4(7)	7.8(6)
N005	38.2(9)	41.1(9)	58.7(9)	-1.6(6)	25.2(7)	-3.4(6)
N006	47.5(9)	33.5(9)	66.8(10)	0.3(6)	28.6(7)	-4.0(6)
N007	47.1(9)	39.8(9)	69.7(11)	1.2(7)	30.2(8)	-6.4(7)
N008	47.9(10)	33.0(9)	73.0(11)	-0.4(7)	27.7(8)	-0.8(6)
C009	32.4(8)	36.2(10)	41.2(8)	-2.2(6)	16.6(6)	0.9(7)
C00A	39.6(10)	35.1(10)	55(1)	0.3(7)	20.6(7)	0.1(7)
C00B	40.4(9)	39.6(10)	64.9(12)	2.6(8)	25.5(8)	0.6(8)

Table 4. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **2**.

Atom	x	y	z	U(eq)
H00A	2112	2980	7747	50
H00B	3966	5198	6568	56
H003	1793(16)	5210(20)	8370(30)	71(7)
H004	3524(19)	2950(30)	6490(30)	93(8)

Table 5. Torsion Angles for **2**.

A-B-C-D	Angle/°	A-B-C-D	Angle/°
O001-N002-N006-N007	179.93(16)	N007-N005-C009-C009[1]	-179.8(2)
O001-N002-C009-N005	-179.87(17)	N008-N003-C00A-N004	0.0(2
O001-N002-C009-C009[1]	0.1(3)	C009-N002-N006-N007	0.4(2)
N002-N006-N007-N005	-0.3(2)	C009-N005-N007-N006	0.0(2)
N003-N008-C00B-N004	0.2(2)	C00A-N003-N008-C00B	-0.1(2)
N006-N002-C009-N005	-0.4(2)	C00A-N004-C00B-N008	-0.2(2)
N006-N002-C009-C009[1]	179.6(2)	C00B-N004-C00A-N003	0.1(2)
N007-N005-C009-N002	0.2(2)		

Table 6. Hydrogen bonds for **2**.

D-H...A	Symmetry	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C00A-H00A...N008	-x+1/2, y-1/2, -z+3/2	0.930	2.441	3.221	141.46
C00B-H00B...N007	-x+1, -y+1, -z+1	0.930	2.693	3.342	127.50
N003-H003...O001	-x+1/2, y+1/2, -z+3/2	0.940	1.830	2.701	152.78
N003-H003...N005	-x+1/2, y+1/2, -z+3/2	0.940	2.351	2.917	118.32
N004-H004...O001		1.027	1.616	2.620	164.43
N004-H004...N002		1.027	2.433	3.434	164.41
N004-H004...N006		1.027	2.642	3.442	134.69

Fig. S1 Crystal structures of salts **3·7H_2O**.

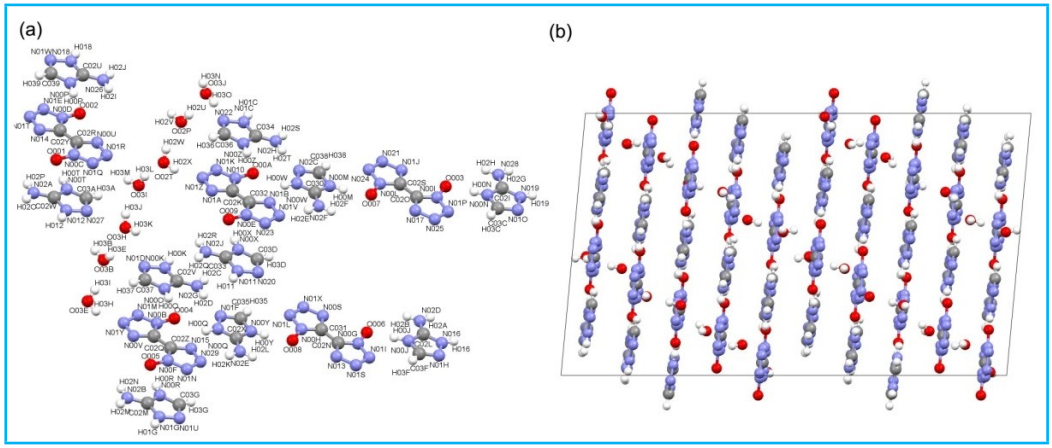

Figure 1. Molecular structure (a) and packing diagram in the unit cell (b) of **3·7H$_2$O**.

Bis-3-Amino-1, 2, 4-triazolium 1*H*,1*H*-5,5-Bitetrazole-1,1-diolate (**3**) crystallizes as a heptahydrate in the monoclinic space group $P2_1/c$ with a density of 1.670 g cm^{-3} and four molecular moieties in the unit cell. The unit cell has the dimensions a=19.0634(3) Å, b=11.83085(18) Å, c=32.1874(7) Å. It crystallizes with a cell volume of 7228.2(2) Å^3. Stronger hydrogen bonds between O007···N00M-H00M (1.808 Å), O003···N00N-H00N (1.806 Å), O004···N00O-H00O (1.832 Å), O005···N00R-H00R (1.829 Å), O001···N00T-H00T (1.828 Å), O009···N00X-H00X (1.815 Å), O00A···N00Z-H00Z (1.828 Å), O03J···O02P-H02U (1.99 Å), O02P···O02T-H02W (1.987 Å), O03B···O03E-H03I (1.97 Å), O02T···O03I-H03L (1.939 Å) , O002···N00P-H00P (1.774 Å) and O006···N00J-H00J (1.736 Å) are also observed.

Table 7. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **3·7H$_2$O**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
O001	1246.0(8)	9515.3(16)	2500.3(7)	41.6(5)
O002	3738.7(8)	11350.4(15)	2456.7(7)	40.6(5)
O003	9728.3(8)	-6009.1(15)	3478.4(7)	41.8(5)
O004	1738.7(8)	594.7(15)	498.9(7)	41.1(5)
O005	-762.2(8)	-1219.8(15)	535.5(7)	41.9(5)
O006	6723.7(8)	-6225.9(15)	466.6(7)	39.9(5)
O007	7242.2(8)	-4152.7(15)	3517.9(7)	41.9(5)
O008	4237.0(8)	-4377.5(15)	513.5(7)	42.2(5)
O009	2235.1(8)	-981.5(16)	3525.0(7)	44.7(5)
O00A	4737.1(8)	813.3(16)	3485.8(7)	44.4(5)
N00B	1082.9(10)	919.2(16)	483.4(7)	28.1(5)
N00C	1909.1(9)	9190.9(17)	2514.3(7)	28.3(5)
N00D	3078.3(10)	11669.1(17)	2459.5(7)	29.9(5)
N00E	2896.5(9)	-1308.7(18)	3531.9(7)	30.4(5)
N00F	-105.8(9)	-1542.5(17)	535.2(7)	29.4(5)
N00G	6056.1(9)	-6543.7(16)	463.8(7)	27.1(5)
N00H	4902.8(10)	-4058.6(16)	519.8(7)	29.1(5)
N00I	9067.1(9)	-6315.4(17)	3473.9(7)	28.8(5)

N00J	7513.9(10)	-8094.8(18)	513.3(8)	32.6(5)
N00K	3385.8(10)	3639.4(17)	506.6(7)	31.0(5)
N00L	7898.6(10)	-3840.7(17)	3520.5(7)	29.9(5)
N00M	6448.5(10)	-2292.8(17)	3481.2(7)	32.1(5)
N00N	10522.9(10)	-7865.8(18)	3518.3(7)	32.5(5)
N00O	2540.7(10)	2468.3(17)	528.4(7)	32.0(5)
N00P	4538.8(11)	13217.3(19)	2514.6(8)	35.2(5)
N00Q	2585.9(10)	-1341.3(17)	491.0(7)	32.3(5)
N00R	-1570.1(10)	-3084.7(18)	481.4(8)	33.4(5)
N00S	6034(1)	-4005.4(17)	513.9(8)	33.9(5)
N00T	461(1)	7626.5(17)	2472.7(7)	32.1(5)
N00U	3042(1)	9124.2(18)	2514.9(8)	33.3(5)
N00V	-53(1)	989.1(17)	477.6(8)	32.5(5)
N00W	5592.5(10)	-1125.2(18)	3489.9(7)	32.8(5)
N00X	1429(1)	-2834.3(18)	3478.6(8)	34.1(5)
N00Y	3452.5(10)	-2503.8(17)	480.3(7)	33.3(5)
N00Z	5542.9(10)	2680.5(18)	3521.3(8)	34.4(5)
N010	4075.8(9)	1143.4(17)	3471.2(7)	30.1(5)
N011	570.1(10)	-4015.1(18)	3492.3(8)	34.0(5)
N012	-391.3(10)	6461.8(18)	2494.1(8)	34.9(5)
N013	4922.9(10)	-6590.6(18)	477.5(8)	34.7(5)
N014	1949.1(10)	11714.9(18)	2480.3(8)	34.3(5)
N015	1027.8(10)	-1613.0(18)	521.0(8)	33.7(5)
N016	8380.8(10)	-9256.4(18)	512.3(8)	34.4(5)
N017	7932.1(10)	-6368.9(18)	3484.1(8)	34.8(5)
N018	5396.5(10)	14380.7(18)	2511.5(7)	33.5(5)
N019	11378.2(10)	-9026.7(18)	3513.8(8)	33.8(5)
N01A	2940.5(10)	1219.9(18)	3468.9(8)	35.1(5)
N01B	4030(1)	-1381.7(18)	3529.9(8)	35.8(5)
N01C	6395.9(10)	3856.2(18)	3503.9(8)	34.4(5)
N01D	2789.6(11)	4282.9(18)	543.5(8)	37.9(6)
N01E	2889.4(10)	12750.8(18)	2448.0(8)	34.5(5)
N01F	3192.4(11)	-695.0(17)	467.8(8)	36.9(6)
N01G	-2419(1)	-4251.9(18)	489.3(8)	35.7(5)
N01H	7781.7(11)	-9899.3(18)	538.6(8)	39.6(6)
N01I	5868.8(10)	-7630.0(18)	446.8(8)	37.3(6)
N01J	9034.7(10)	-3786.3(19)	3512.8(8)	35.7(5)
N01K	3896.8(10)	2236.4(18)	3443.5(8)	37.9(6)
N01L	5084.9(10)	-2974.9(18)	540.7(8)	36.7(6)
N01M	892.9(11)	2007.8(17)	456.5(8)	37.0(6)

N01N	84.8(11)	-2633.9(17)	546.9(8)	37.1(6)
N01O	10785.4(11)	-9674.5(19)	3536.3(8)	39.3(6)
N01P	8865.3(11)	-7414.3(18)	3457.0(8)	38.1(6)
N01Q	2088.9(11)	8109.6(19)	2538.2(8)	39.0(6)
N01R	2778.2(11)	8087.6(19)	2541.4(8)	39.0(6)
N01S	5185.1(11)	-7635.3(18)	454.4(8)	39.1(6)
N01T	2203.3(10)	12761.9(18)	2460.8(8)	37.3(6)
N01U	-1832.5(11)	-4886.7(19)	448.8(8)	40.4(6)
N01V	3760.8(11)	-2430.7(18)	3555.4(8)	39.4(6)
N01W	4799.8(11)	15027.2(18)	2548.2(8)	40.0(6)
N01X	5769.1(10)	-2956.7(18)	536.2(8)	37.4(6)
N01Y	202.8(10)	2035.6(18)	455.5(8)	37.2(6)
N01Z	3214.4(11)	2253.6(19)	3442.7(8)	39.5(6)
N020	1169.8(11)	-4654.1(19)	3447.1(8)	39.4(6)
N021	8785.1(11)	-2728.8(19)	3531.3(8)	39.3(6)
N022	5799.1(11)	4486.7(19)	3549.5(8)	39.1(6)
N023	3072.0(11)	-2398.6(19)	3557.3(8)	40.1(6)
N024	8094.9(10)	-2748.1(19)	3536.9(8)	36.6(5)
N025	8185.4(11)	-7418.7(19)	3464.3(9)	40.9(6)
N026	5671.6(12)	12425(2)	2460.1(9)	43.0(7)
N027	202.3(10)	5820.6(18)	2467.6(8)	37.5(6)
N028	11651.3(11)	-7068.9(19)	3488.1(9)	43.3(6)
N029	770.1(11)	-2651.4(18)	540.1(9)	41.2(6)
N02A	-674.7(11)	8417.8(19)	2509.6(9)	46.0(7)
N02B	-2693.5(11)	-2299.5(19)	543.2(9)	43.6(6)
N02C	6187.7(11)	-474.2(19)	3465.0(8)	40.2(6)
N02D	8648.5(11)	-7305.2(19)	474.2(9)	45.4(7)
N02E	2317.4(11)	-3300.0(19)	509.2(9)	47.6(7)
N02F	5317.1(11)	-3090.4(19)	3510.9(9)	45.2(7)
N02G	3666.7(11)	1690.7(18)	470.7(9)	46.3(7)
N02H	6670.4(11)	1903.2(19)	3450.4(9)	45.5(7)
C02I	11222.4(11)	-7932(2)	3502.8(8)	28.5(5)
N02J	304.0(11)	-2056.3(19)	3550.7(9)	46.5(7)
C02K	3492.6(11)	524(2)	3486.4(8)	26.3(5)
C02L	8214.1(12)	-8165(2)	497.1(9)	31.0(6)
C02M	-2263.9(11)	-3162(2)	508.5(9)	29.1(6)
C02N	5478.5(11)	-4693(2)	503.3(8)	26.9(5)
C02O	8481.5(11)	-4471(2)	3505.4(8)	26.2(5)
O02P	4070.1(17)	5252(2)	3859.4(11)	84.8(9)
C02Q	492.9(10)	293(2)	495.7(8)	25.9(5)

C02R	2493.6(11)	9817(2)	2501.6(8)	27.6(5)
C02S	8483.0(11)	-5678(2)	3487.8(8)	26.7(5)
O02T	3004.9(16)	4661(2)	3243.0(11)	85.1(9)
C02U	5241.5(12)	13295(2)	2492.4(9)	31.0(6)
C02V	3235.2(11)	2553(2)	498.5(9)	29.1(6)
C02W	-241.0(12)	7548(2)	2495.8(9)	31.3(6)
C02X	2750.2(12)	-2438(2)	496.4(9)	30.9(6)
C02Y	2500.8(11)	11027(2)	2480.0(8)	26.2(5)
C02Z	480.1(11)	-913.5(19)	518.8(8)	26.4(5)
C030	5750.1(12)	-2213(2)	3496.4(9)	29.5(6)
C031	5485.7(11)	-5906(2)	481.6(8)	27.3(5)
C032	3478.5(11)	-686(2)	3517.5(8)	29.4(6)
C033	732.5(12)	-2912(2)	3511.3(9)	30.3(6)
C034	6237.8(13)	2760(2)	3488.6(9)	32.7(6)
C035	3683.0(12)	-1438(2)	460.5(9)	36.0(6)
C036	5307.3(13)	3748(2)	3557.6(10)	37.8(7)
C037	2290.6(12)	3541(2)	554.5(10)	36.0(6)
C038	6688.5(13)	-1211(2)	3460.9(9)	36.0(6)
C039	4302.4(13)	14290(2)	2547.7(10)	39.4(7)
C03A	699.8(13)	6553(2)	2454.7(10)	39.0(7)
O03B	1169(2)	5161(3)	996.5(12)	106.7(12)
C03C	10279.2(13)	-8944(2)	3537(1)	40.0(7)
C03D	1661.1(12)	-3909(2)	3441.7(10)	38.1(7)
O03E	127.2(18)	4503(2)	375.8(15)	108.2(13)
C03F	7285.4(13)	-9167(2)	540.2(10)	39.2(7)
C03G	-1328.7(13)	-4156(2)	448.2(10)	38.1(7)
O03H	1687(2)	4784(3)	1828.2(14)	119.3(14)
O03I	2680(3)	5569(2)	2458.2(14)	125.7(15)
O03J	4536(3)	4578(3)	4682.2(13)	121.3(14)

Table 8. Bond Lengths [Å] and angles [°] for **3·7H_2O**.

bond	Length/Å	bond	Angle/°
O001-N00C	1.318(2)	O004-N00BN01M	122.58(19)
O002-N00D	1.315(2)	O004-N00BC02Q	129.44(19)
O003-N00I	1.310(2)	N01M-N00BC02Q	107.97(18)
O004-N00B	1.304(2)	O001-N00CN01Q	121.70(19)
O005-N00F	1.308(2)	O001-N00CC02R	129.4(2)
O006-N00G	1.326(2)	N01Q-N00CC02R	108.91(19)
O007-N00L	1.304(2)	O002-N00DN01E	122.20(19)
O008-N00H	1.322(2)	O002-N00DC02Y	128.8(2)

O009-N00H	1.317(2)	N01E-N00DC02Y	108.95(19)
O00A-N010	1.316(2)	O009-N00EN023	121.32(19)
N00B-N01M	1.338(3)	O009-N00EC032	129.3(2)
N00B-C02Q	1.350(3)	N023-N00EC032	109.33(19)
N00C-N01Q	1.325(3)	O005-N00FN01N	122.52(19)
N00C-C02R	1.342(3)	O005-N00FC02Z	129.4(2)
N00D-N01E	1.329(3)	N01N-N00FC02Z	108.04(18)
N00D-C02Y	1.344(3)	O006-N00GN01I	121.77(18)
N00E-N023	1.333(3)	O006-N00GC031	128.8(2)
N00E-C032	1.336(3)	C031-N00GN01I	109.38(18)
N00F-N01N	1.341(3)	O008-N00HN01L	121.48(18)
N00F-C02Z	1.347(3)	O008-N00HC02N	129.1(2)
N00G-N01I	1.334(3)	N01L-N00HC02N	109.42(19)
N00G-C031	1.329(3)	O003-N00IN01P	122.34(19)
N00H-N01L	1.328(3)	O003-N00IC02S	129.9(2)
N00H-C02N	1.335(3)	C02S-N00IN01P	107.76(18)
N00I-N01P	1.355(3)	C02L-N00JC03F	105.8(2)
N00I-C02S	1.349(3)	C02V-N00KN01D	111.09(19)
N00J-C02L	1.343(3)	O007-N00LN024	122.38(19)
N00J-C03F	1.346(3)	O007-N00LC02O	129.7(2)
N00K-N01D	1.382(3)	C02O-N00LN024	107.87(19)
N00K-C02V	1.317(3)	C030-N00MC038	106.0(2)
N00L-N024	1.345(3)	C02I-N00NC03C	106.9(2)
N00L-C02O	1.343(3)	C02V-N00OC037	106.8(2)
N00M-C030	1.340(3)	C02U-N00PC039	106.2(2)
N00M-C038	1.363(3)	C02X-N00QN01F	109.84(19)
N00N-C02I	1.341(3)	C02M-N00RC03G	106.6(2)
N00N-C03C	1.361(3)	C02N-N00SN01X	105.24(19)
N00O-C02V	1.340(3)	C02W-N00TC03A	106.1(2)
N00O-C037	1.362(3)	C02R-N00UN01R	105.70(19)
N00P-C02U	1.351(3)	C02Q-N00VN01Y	106.84(19)
N00P-C039	1.354(3)	C030-N00WN02C	110.96(19)
N00Q-N01F	1.394(3)	C033-N00XC03D	106.0(2)
N00Q-C02X	1.335(3)	C035-N00YC02X	106.23(19)
N00R-C02M	1.337(3)	C034-N00ZC036	106.3(2)
N00R-C03G	1.355(3)	O00A-N010N01K	121.77(19)
N00S-N01X	1.344(3)	O00A-N010C02K	129.3(2)
N00S-C02N	1.333(3)	C02K-N010N01K	108.93(19)
N00T-C02W	1.350(3)	C033-N011N020	110.21(19)
N00T-C03A	1.352(3)	C02W-N012N027	111.1(2)

N00U-N01R	1.331(3)	N01S-N013C031	104.80(18)
N00U-C02R	1.326(3)	C02Y-N014N01T	106.12(19)
N00V-N01Y	1.335(3)	N029-N015C02Z	106.39(19)
N00V-C02Q	1.324(3)	C02L-N016N01H	109.93(19)
N00W-N02C	1.380(3)	C02S-N017N025	106.43(19)
N00W-C030	1.322(3)	C02U-N018N01W	111.09(19)
N00X-C033	1.345(3)	C02I-N019N01O	111.26(19)
N00X-C03D	1.355(3)	C02K-N01AN01Z	104.85(19)
N00Y-C02X	1.347(3)	C032-N01BN01V	105.47(19)
N00Y-C035	1.339(3)	C034-N01CN022	110.2(2)
N00Z-C034	1.342(3)	C037-N01D-N00K	103.9(2)
N00Z-C036	1.349(3)	N01T-N01E-N00D	106.07(19)
N010-N01K	1.338(3)	C035-N01F-N00Q	103.5(2)
N010-C02K	1.336(3)	C02M-N01G-N01U	111.1(2)
N011-N020	1.389(3)	C03F-N01H-N016	104.0(2)
N011-C033	1.341(3)	N01S-N01I-N00G	105.53(18)
N012-N027	1.372(3)	C02O-N01J-N021	106.58(19)
N012-C02W	1.317(3)	N01Z-N01K-N010	105.31(19)
N013-N01S	1.338(3)	N01X-N01L-N00H	105.78(19)
N013-C031	1.343(3)	N01Y-N01M-N00B	106.8(2)
N014-N01T	1.334(3)	N029-N01N-N00F	106.44(19)
N014-C02Y	1.330(3)	C03C-N01O-N019	104.2(2)
N015-N029	1.327(3)	N025-N01P-N00I	106.5(2)
N015-C02Z	1.332(3)	N01R-N01Q-N00C	105.83(19)
N016-N01H	1.381(3)	N01Q-N01R-N00U	111.4(2)
N016-C02L	1.329(3)	N01I-N01S-N013	112.0(2)
N017-N025	1.336(3)	N01E-N01T-N014	111.08(19)
N017-C02S	1.330(3)	C03G-N01U-N01G	104.3(2)
N018-N01W	1.385(3)	N023-N01V-N01B	111.1(2)
N018-C02U	1.318(3)	C039-N01W-N018	103.7(2)
N019-N01O	1.373(3)	N01L-N01X-N00S	111.5(2)
N019-C02I	1.328(3)	N01M-N01Y-N00V	110.29(19)
N01A-N01Z	1.336(3)	N01K-N01Z-N01A	112.5(2)
N01A-C02K	1.333(3)	C03D-N020-N011	103.6(2)
N01B-N01V	1.348(3)	N024-N021-N01J	110.1(2)
N01B-C032	1.333(3)	C036-N022-N01C	104.2(2)
N01C-N022	1.380(3)	N01V-N023-N00E	105.8(2)
N01C-C034	1.331(3)	N021-N024-N00L	106.9(2)
N01D-C037	1.297(3)	N01P-N025-N017	111.3(2)
N01E-N01T	1.313(3)	C03A-N027-N012	104.1(2)

N01F-C035	1.285(3)	N01N-N029-N015	111.13(19)
N01G-N01U	1.363(3)	C038-N02C-N00W	103.6(2)
N01G-C02M	1.323(3)	N019-C02I-N00N	106.1(2)
N01H-C03F	1.283(3)	N028-C02I-N00N	125.5(2)
N01I-N01S	1.306(3)	N028-C02I-N019	128.4(2)
N01J-N021	1.342(3)	N010-C02K-C032	124.8(2)
N01J-C02O	1.328(3)	N01A-C02K-N010	108.4(2)
N01K-N01Z	1.301(3)	N01A-C02K-C032	126.8(2)
N01L-N01X	1.306(3)	N016-C02L-N00J	107.1(2)
N01M-N01Y	1.316(3)	N02D-C02L-N00J	125.9(2)
N01N-N029	1.309(3)	N02D-C02L-N016	127.0(2)
N01O-C03C	1.295(3)	N01G-C02M-N00R	106.4(2)
N01P-N025	1.298(3)	N02B-C02M-N00R	125.3(2)
N01Q-N01R	1.313(3)	N02B-C02M-N01G	128.3(2)
N01U-C03G	1.293(3)	N00H-C02N-C031	125.1(2)
N01V-N023	1.314(3)	N00S-C02N-N00H	108.1(2)
N01W-C039	1.288(3)	N00S-C02N-C031	126.8(2)
N020-C03D	1.287(3)	N00L-C02O-C02S	124.1(2)
N021-N024	1.318(3)	N01J-C02O-N00L	108.6(2)
N022-C036	1.284(3)	N01J-C02O-C02S	127.3(2)
N026-C02U	1.326(3)	N00B-C02Q-C02Z	124.58(19)
N027-C03A	1.289(3)	N00V-C02Q-N00B	108.1(2)
N028-C02I	1.312(3)	N00V-C02Q-C02Z	127.3(2)
N02A-C02W	1.323(3)	N00C-C02R-C02Y	124.4(2)
N02B-C02M	1.320(3)	N00U-C02R-N00C	108.2(2)
N02C-C038	1.294(3)	N00U-C02R-C02Y	127.5(2)
N02D-C02L	1.318(3)	N00I-C02S-C02O	124.4(2)
N02E-C02X	1.314(3)	N017-C02S-N00I	108.1(2)
N02F-C030	1.329(3)	N017-C02S-C02O	127.6(2)
N02G-C02V	1.319(3)	N018-C02U-N00P	106.4(2)
N02H-C034	1.320(3)	N018-C02U-N026	128.5(2)
N02J-C033	1.314(3)	N026-C02U-N00P	125.1(2)
C02K-C032	1.435(3)	N00K-C02V-N00O	106.7(2)
C02N-C031	1.437(3)	N00K-C02V-N02G	128.3(2)
C02O-C02S	1.430(3)	N02G-C02V-N00O	125.0(2)
C02Q-C02Z	1.430(3)	N012-C02W-N00T	106.5(2)
C02R-C02Y	1.433(3)	N012-C02W-N02A	128.5(2)
		N02A-C02W-N00T	125.0(2)
		N00Q-C02X-N00Y	106.7(2)
		N02E-C02X-N00Q	127.4(2)

	N02E-C02X-N00Y	125.9(2)
	N00D-C02Y-C02R	125.3(2)
	N014-C02Y-N00D	107.8(2)
	N014-C02Y-C02R	126.9(2)
	N00F-C02Z-C02Q	124.9(2)
	N015-C02Z-N00F	108.0(2)
	N015-C02Z-C02Q	127.1(2)
	N00W-C030-N00M	107.0(2)
	N00W-C030-N02F	128.3(2)
	N02F-C030-N00M	124.7(2)
	N00G-C031-N013	108.2(2)
	N00G-C031-C02N	125.5(2)
	N013-C031-C02N	126.3(2)
	N00E-C032-C02K	125.0(2)
	N01B-C032-N00E	108.3(2)
	N01B-C032-C02K	126.7(2)
	N011-C033-N00X	106.8(2)
	N02J-C033-N00X	125.6(2)
	N02J-C033-N011	127.7(2)
	N01C-C034-N00Z	106.7(2)
	N02H-C034-N00Z	125.7(2)
	N02H-C034-N01C	127.6(2)
	N01F-C035-N00Y	113.6(2)
	N022-C036-N00Z	112.7(2)
	N01D-C037-N00O	111.5(2)
	N02C-C038-N00M	112.4(2)
	N01W-C039-N00P	112.6(2)
	N027-C03A-N00T	112.3(2)
	N01O-C03C-N00N	111.6(2)
	N020-C03D-N00X	113.4(2)
	N01H-C03F-N00J	113.1(2)
	N01U-C03G-N00R	111.6(2)

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3·7H$_2$O**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O001	12.6(8)	30.4(10)	82.3(16)	-2.5(9)	6.6(8)	-1.0(7)
O002	12.6(8)	29.0(9)	80.5(15)	0.0(9)	5.4(8)	-1.3(7)
O003	9.6(7)	33.9(10)	82.3(16)	0.9(10)	6.5(8)	0.1(7)
O004	10.2(7)	28.6(9)	85.1(16)	-3.0(9)	7.7(8)	3.9(7)
O005	10.9(8)	30.1(9)	85.0(16)	-0.4(9)	6.2(8)	4.2(7)

O006	10.9(7)	29.8(9)	79.0(15)	2.7(9)	4.2(8)	2.6(7)
O007	12.9(8)	32(1)	81.2(16)	1.8(9)	6.8(8)	0.4(7)
O008	11.3(7)	29.9(9)	86.3(16)	4.8(9)	8.4(8)	5.0(7)
O009	11.3(8)	36.4(10)	86.6(16)	-3.5(10)	6.5(8)	0.0(7)
O00A	13.4(8)	34.7(10)	85.6(17)	-3(1)	6.4(9)	-0.4(7)
N00B	16.6(9)	19.5(10)	48.3(14)	-0.4(9)	2.1(8)	3.9(7)
N00C	12.8(9)	25.2(10)	47.0(14)	-3.0(9)	4.1(8)	0.4(7)
N00D	20.0(9)	24.8(10)	44.7(14)	0.0(9)	2.6(9)	-3.1(8)
N00E	11.3(9)	31.4(11)	48.6(14)	0.8(9)	2.7(8)	-2.3(8)
N00F	12.3(8)	26.4(10)	49.3(14)	1.7(9)	2.1(8)	4.5(8)
N00G	7.2(8)	26(1)	48.2(14)	2.6(9)	2.9(8)	2.9(7)
N00H	16.7(9)	22.1(10)	48.2(14)	2.4(9)	2.1(9)	9.2(8)
N00I	12.8(9)	27.1(10)	46.6(14)	2.9(9)	3.8(8)	-1.8(8)
N00J	14.2(9)	31.0(11)	53.2(15)	1.4(10)	6.3(9)	7.1(8)
N00K	11.8(9)	26.4(10)	55.4(15)	1.1(10)	5.9(9)	0.2(7)
N00L	14.1(9)	27.4(11)	48.0(14)	1.5(9)	2.3(8)	1.8(8)
N00M	20.5(10)	24.5(10)	51.7(15)	0.7(9)	5.4(9)	7.6(8)
N00N	18.1(9)	28.8(11)	51.1(15)	0.7(10)	5.9(9)	2.6(8)
N00O	20(1)	22.9(10)	53.2(15)	-0.1(9)	4.6(9)	-3.0(8)
N00P	21.4(10)	32.2(12)	52.1(16)	0(1)	4.3(10)	-7.2(9)
N00Q	16.6(9)	25.7(10)	54.7(15)	-0.1(10)	4.7(9)	9.2(8)
N00R	17.1(9)	28.7(11)	54.8(15)	0.1(10)	5.2(9)	-2.1(8)
N00S	20.8(10)	24.4(11)	56.4(16)	-3(1)	2.9(9)	3.9(8)
N00T	17.4(9)	27.1(11)	52.2(15)	2.3(9)	4.9(9)	-5.2(8)
N00U	18.2(9)	29.0(11)	52.6(15)	-1.1(10)	2.2(9)	1.5(8)
N00V	16.7(9)	25.4(10)	55.4(15)	0.1(9)	2.9(9)	8.9(8)
N00W	16.7(9)	28.8(11)	53.1(15)	1.4(10)	5.1(9)	1.7(8)
N00X	17.0(9)	30.1(11)	55.2(15)	0.3(10)	4.3(9)	-5.5(8)
N00Y	19.8(9)	26(1)	54.4(15)	1.2(10)	5.3(9)	12.4(8)
N00Z	18.8(10)	31.2(11)	54.0(15)	-0.4(10)	7.3(9)	-6.0(8)
N010	13.6(9)	29.2(11)	47.2(14)	-3.2(9)	1.4(9)	-0.8(8)
N011	15.0(9)	30.5(11)	56.7(15)	-0.1(10)	4.7(9)	-2.0(8)
N012	19.8(10)	31.0(12)	54.2(16)	2.6(10)	5.0(9)	-2.3(8)
N013	16.2(9)	28.5(11)	59.7(16)	-0.4(10)	5.0(9)	2.4(8)
N014	22.5(10)	26.7(11)	53.7(15)	1.8(10)	3.5(9)	1.4(8)
N015	13.3(9)	29.6(11)	58.4(16)	4.6(10)	4.3(9)	6.8(8)
N016	17.6(9)	29.3(11)	56.9(15)	4.7(10)	5.7(9)	9.2(8)
N017	14.0(9)	32.0(11)	59.0(16)	1.2(10)	6.3(9)	-2.5(8)
N018	14.3(9)	30.3(11)	55.8(15)	-1.1(10)	3.3(9)	-5.2(8)
N019	13.6(9)	31.4(11)	56.9(15)	0.6(10)	5.2(9)	5.1(8)

N01A	16.8(10)	32.6(12)	55.4(16)	0.8(10)	1.0(9)	2.3(8)
N01B	18.2(10)	31.5(11)	57.5(16)	4.9(10)	2.8(9)	-1.1(8)
N01C	17.5(10)	29.9(11)	56.2(15)	0.9(10)	5.7(9)	-6.3(8)
N01D	28.9(11)	22.8(11)	62.5(17)	2.9(10)	8(1)	6.1(9)
N01E	21.3(10)	24.7(11)	57.5(16)	2.3(10)	3.7(9)	1.8(8)
N01F	27.8(11)	21.3(10)	62.2(17)	0.7(10)	7.3(10)	2.1(8)
N01G	17.2(9)	31.8(11)	58.0(16)	-1(1)	3.9(9)	1.4(8)
N01H	21.5(10)	27.6(11)	70.4(18)	3.7(11)	7(1)	3.1(8)
N01I	21.9(10)	23.2(11)	67.4(17)	1.3(10)	7.2(10)	6.8(8)
N01J	17.5(10)	33.8(12)	55.7(16)	0.4(10)	3.4(9)	-4.7(8)
N01K	20.9(10)	27.7(11)	65.0(17)	0.8(10)	3.1(10)	-0.7(8)
N01L	18.6(10)	26.4(11)	65.7(17)	-0.4(10)	6.8(10)	5.1(8)
N01M	26.9(10)	20.6(10)	63.4(17)	-1.4(10)	4.1(10)	7.8(8)
N01N	25.3(10)	20.9(10)	65.0(17)	4.2(10)	4.7(10)	4.0(8)
N01O	24.4(11)	29.8(12)	64.0(17)	1.1(11)	5.2(10)	-0.7(9)
N01P	25.6(10)	24.0(11)	65.0(17)	4(1)	6.4(10)	-1.0(8)
N01Q	30.9(11)	24.7(11)	61.6(17)	-1.9(10)	5.2(11)	-3.4(9)
N01R	27.9(11)	28.0(11)	61.3(17)	0.6(11)	5.5(10)	6.5(9)
N01S	25.5(10)	24.0(11)	68.3(18)	-0.6(10)	7.4(10)	-0.6(8)
N01T	21.1(10)	26.8(11)	64.1(17)	0.9(10)	5.5(10)	2.3(8)
N01U	23.2(10)	30.6(12)	67.6(18)	-1.8(11)	4.5(10)	1.6(9)
N01V	21.7(10)	28.7(11)	68.2(17)	7.6(11)	5.5(10)	3.7(8)
N01W	32.1(11)	21.7(11)	66.6(17)	-4.5(10)	6.7(11)	-0.1(9)
N01X	21.2(10)	25.0(11)	66.5(17)	-0.7(10)	6.6(10)	0.7(8)
N01Y	20.5(10)	27.3(11)	63.7(17)	-1(1)	2.6(10)	6.3(8)
N01Z	22.5(10)	34.0(12)	62.0(17)	1.3(11)	4.1(10)	1.8(9)
N020	24.5(10)	31.6(12)	62.1(17)	-2.0(11)	4.1(10)	-1.8(9)
N021	22.3(10)	30.4(11)	65.4(17)	-2.1(11)	5.3(10)	-2.5(9)
N022	23.4(10)	29.6(11)	64.8(17)	1.0(11)	5.9(10)	0.6(9)
N023	21.1(10)	32.2(12)	67.3(18)	7.4(11)	5.4(10)	-1.8(9)
N024	23.5(10)	29.7(11)	56.8(16)	-0.6(10)	4.9(10)	-3.0(9)
N025	23(1)	32.7(12)	67.6(18)	2.0(11)	7.7(10)	-0.8(9)
N026	20.6(11)	29.2(13)	80(2)	-3.3(12)	7.4(11)	-3.7(9)
N027	22.7(10)	28.3(11)	61.7(17)	2.2(10)	5(1)	-0.3(8)
N028	22.5(10)	28.5(12)	79.7(19)	4.1(11)	8.7(11)	1.8(9)
N029	25.2(11)	25.7(11)	72.9(18)	5.5(11)	5.9(11)	7.1(9)
N02A	24.7(11)	25.3(11)	89(2)	0.2(12)	8.7(12)	-2.8(9)
N02B	20.6(10)	28.6(11)	82(2)	1.0(12)	6.7(11)	-1.3(9)
N02C	28.7(11)	29.5(12)	62.6(17)	0.7(11)	5.8(10)	3.3(9)
N02D	22.1(10)	30.3(12)	85(2)	4.5(12)	9.2(11)	8.0(9)

N02E	23.4(11)	24.1(11)	96(2)	5.2(12)	9.5(12)	7.3(9)
N02F	21.5(10)	28.2(12)	87(2)	2.9(12)	9.4(11)	-0.8(9)
N02G	23.4(11)	21.5(11)	95(2)	-8.6(12)	10.5(12)	0.4(9)
N02H	23.7(11)	28.6(12)	85(2)	-4.3(12)	8.7(11)	-3.7(9)
C02I	13.6(10)	30.3(13)	41.5(15)	2.3(11)	2.8(10)	4.1(9)
N02J	19.9(10)	31.6(12)	89(2)	-3.5(12)	9.1(11)	-1.2(9)
C02K	14.9(10)	24.8(12)	39.2(15)	-2.4(10)	2.5(9)	-2.3(9)
C02L	24.9(12)	28.2(13)	40.0(16)	1.8(11)	3.3(10)	9.3(10)
C02M	12.8(10)	32.3(13)	42.3(16)	1.5(11)	2.4(10)	-1.7(9)
C02N	12(1)	27.7(12)	40.8(15)	1.9(10)	1.4(9)	4.4(9)
C02O	13.8(10)	26.0(12)	38.4(15)	-0.1(10)	0.7(9)	0.0(9)
O02P	80.8(18)	44.7(15)	132(3)	-6.7(16)	28.3(19)	10.1(14)
C02Q	9.1(10)	29.3(12)	39.1(15)	0.9(10)	1.7(9)	3.0(8)
C02R	16.9(10)	27.2(12)	38.2(15)	-0.7(10)	0.2(10)	0.5(9)
C02S	12.4(10)	28.6(12)	39.2(15)	1.6(10)	3.3(9)	1.8(9)
O02T	76.3(19)	43.1(14)	138(3)	-11.8(16)	21.4(18)	9.8(13)
C02U	21.5(11)	30.5(13)	40.5(16)	1.2(11)	1.3(10)	-3.3(10)
C02V	15.8(10)	26.9(12)	44.5(16)	-1.7(11)	2.3(10)	1.6(9)
C02W	21.1(11)	29.5(13)	43.8(16)	0.1(11)	6(1)	-5.5(10)
C02X	24.8(12)	23.5(12)	44.4(16)	1.1(11)	3.0(11)	8(1)
C02Y	10.5(10)	32.1(13)	35.5(15)	-0.4(10)	0.1(9)	-0.7(9)
C02Z	17.0(11)	22.1(11)	40.2(15)	2.2(10)	2.3(10)	6.2(9)
C030	17.8(11)	27.9(12)	42.9(16)	-0.5(11)	3.8(10)	2.2(9)
C031	18.9(11)	22.4(12)	41.0(15)	1.3(10)	4.1(10)	5.6(9)
C032	14.7(10)	30.7(13)	42.5(16)	1.0(11)	1.5(10)	-1.8(9)
C033	20.4(11)	28.1(13)	42.3(16)	0.9(11)	2(1)	-6.5(9)
C034	26.8(12)	26.7(12)	44.8(16)	-0.3(11)	3.5(11)	-3.5(10)
C035	15.2(11)	34.3(14)	58.5(19)	-1.5(12)	3.8(11)	5.7(10)
C036	18.7(12)	36.1(14)	59(2)	-0.8(13)	4.8(12)	-3.3(10)
C037	17.5(11)	30.2(13)	60.5(19)	2.5(12)	5.1(11)	4.6(10)
C038	19.6(12)	33.3(14)	55.3(18)	-1.4(12)	4.7(11)	-4.6(10)
C039	19.1(12)	35.2(14)	64(2)	-3.4(13)	6.1(12)	-0.6(10)
C03A	26.1(13)	35.7(15)	55.8(19)	0.6(13)	7.6(12)	-1.4(11)
O03B	103(2)	54.9(18)	169(4)	6(2)	49(2)	20.3(18)
C03C	18.2(11)	38.2(15)	64(2)	2.1(13)	6.1(12)	0.2(10)
C03D	17.7(11)	38.9(15)	58.0(19)	1.0(13)	5.0(11)	-2.1(10)
O03E	102(2)	40.0(15)	187(4)	-8.5(19)	40(2)	10.3(16)
C03F	20.9(12)	33.4(14)	64(2)	3.7(13)	8.2(12)	8.1(10)
C03G	20.7(12)	32.7(14)	61(2)	-1.6(12)	4.0(12)	3.8(10)
O03H	144(4)	60.4(19)	160(4)	24(2)	48(3)	24(2)

O03I	177(4)	35.6(15)	173(4)	16.1(19)	60(4)	18(2)
O03J	183(4)	46.5(17)	139(4)	16.2(19)	41(3)	15(2)

Table 10. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **3·7H$_2$O**.

Atom	x	y	z	U(eq)
H00K	3800	3913	491	37
H00M	6695	-2902	3484	39
H00N	10276	-7258	3517	39
H00O	2300	1854	531	38
H00Q	2168	-1073	500	39
H00R	-1325	-2474	485	40
H00T	706	8236	2470	39
H00W	5175	-859	3500	39
H00X	1677	-2226	3481	41
H00Y	3703	-3109	482	40
H00Z	5297	2071	3519	41
H011	155	-4287	3506	41
H012	-807	6190	2508	42
H016	8800	-9523	506	41
H018	5813	14652	2502	40
H019	11796	-9295	3508	41
H01C	6810	4131	3488	41
H01G	-2835	-4524	501	43
H02G	12096	-7180	3484	52
H02H	11487	-6391	3482	52
H02O	-1119	8305	2519	55
H02P	-513	9096	2509	55
H02M	-3136	-2416	556	52
H02N	-2531	-1621	553	52
H02A	9092	-7424	468	55
H02B	8488	-6625	466	55
H02K	1873	-3185	515	57
H02L	2479	-3979	512	57
H02E	4872	-2981	3517	54
H02F	5482	-3767	3514	54
H02C	4109	1808	455	56
H02D	3506	1011	468	56
H02S	7111	2026	3432	55
H02T	6511	1222	3444	55
H02Q	-137	-2176	3568	56
H02R	465	-1377	3560	56

H02U	4172	4977	4101	127
H02V	4079	5970	3873	127
H02W	3242	4954	3452	128
H02X	3029	3944	3261	128
H035	4153	-1253	443	43
H037	1821	3720	577	43
H038	7159	-1024	3446	43
H03A	1169	6366	2435	47
H03B	1198	5864	1049	160
H03E	1127	4799	1221	160
H03C	9808	-9134	3549	48
H03D	2129	-4091	3415	46
H03H	77	3803	321	162
H03I	496	4602	541	162
H03F	6816	-9357	558	47
H03G	-859	-4341	428	46
H03J	1928	5210	2000	179
H03K	1692	4112	1923	179
H03L	2782	5435	2716	189
H03M	2647	6277	2419	189
H03N	4465	4815	4924	182
H03O	4444	3876	4665	182
H036	4813(17)	3870(30)	3592(11)	67(11)
H00P	4265(17)	12590(30)	2495(11)	64(11)
H039	3834(17)	14480(30)	2592(10)	62(10)
H02I	5504(14)	11800(20)	2459(8)	26(7)
H02J	6126(16)	12580(30)	2425(10)	50(9)
H00J	7228(15)	-7450(30)	516(9)	44(8)

Table 11. Torsion Angles for **3·7H_2O**.

A-B-C-D	Angle/°	A-B-C-D	Angle/°
O001-N00C-N01Q-N01R	179.3(2)	N01R-N00U-C02R-C02Y	178.8(3)
O001-N00C-C02R-N00U	-178.6(3)	N01S-N013-C031-N00G	-0.3(3)
O001-N00C-C02R-C02Y	1.8(4)	N01S-N013-C031-C02N	179.9(3)
O002-N00D-N01E-N01T	-179.1(2)	N01T-N014-C02Y-N00D	-0.1(3)
O002-N00D-C02Y-N014	179.1(3)	N01T-N014-C02Y-C02R	179.3(3)
O002-N00D-C02Y-C02R	-0.3(4)	N01U-N01G-C02M-N00R	-0.2(3)
O003-N00I-N01P-N025	179.0(2)	N01U-N01G-C02M-N02B	179.2(3)
O003-N00I-C02S-N017	-178.7(3)	N01V-N01B-C032-N00E	-0.5(3)
O003-N00I-C02S-C02O	1.0(4)	N01V-N01B-C032-C02K	-179.4(3)
O004-N00B-N01M-N01Y	-178.8(2)	N01W-N018-C02U-N00P	0.2(3)

O004-N00B-C02Q-N00V	179.0(3)	N01W-N018-C02U-N026	-179.4(3)
O004-N00B-C02Q-C02Z	-1.8(4)	N01X-N00S-C02N-N00H	-0.1(3)
O005-N00F-N01N-N029	179.6(2)	N01X-N00S-C02N-C031	-179.6(3)
O005-N00F-C02Z-N015	-179.3(3)	N01Y-N00V-C02Q-N00B	-0.2(3)
O005-N00F-C02Z-C02Q	-0.3(5)	N01Y-N00V-C02Q-C02Z	-179.4(3)
O006-N00G-N01I-N01S	179.2(2)	N01Z-N01A-C02K-N010	0.1(3)
O006-N00G-C031-N013	-178.9(2)	N01Z-N01A-C02K-C032	179.9(3)
O006-N00G-C031-C02N	0.8(5)	N020-N011-C033-N00X	0.0(3)
O007-N00L-N024-N021	-179.5(2)	N020-N011-C033-N02J	179.5(3)
O007-N00L-C02O-N01J	179.6(3)	N021-N01J-C02O-N00L	-0.2(3)
O007-N00L-C02O-C02S	-0.9(4)	N021-N01J-C02O-C02S	-179.7(3)
O008-N00H-N01L-N01X	-179.2(2)	N022-N01C-C034-N00Z	0.4(3)
O008-N00H-C02N-N00S	179.3(3)	N022-N01C-C034-N02H	-179.4(3)
O008-N00H-C02N-C031	-1.2(5)	N023-N00E-C032-N01B	0.6(3)
O009-N00E-N023-N01V	179.7(2)	N023-N00E-C032-C02K	179.6(2)
O009-N00E-C032-N01B	-179.6(3)	N024-N00L-C02O-N01J	0.1(3)
O009-N00E-C032-C02K	-0.6(5)	N024-N00L-C02O-C02S	179.6(2)
O00A-N010-N01K-N01Z	-179.0(2)	N025-N017-C02S-N00I	-0.5(3)
O00A-N010-C02K-N01A	178.9(3)	N025-N017-C02S-C02O	179.8(3)
O00A-N010-C02K-C032	-1.0(4)	N027-N012-C02W-N00T	-0.4(3)
N00B-N01M-N01Y-N00V	-0.5(3)	N027-N012-C02W-N02A	178.5(3)
N00B-C02Q-C02Z-N00F	179.3(3)	N029-N015-C02Z-N00F	-0.2(3)
N00B-C02Q-C02Z-N015	-1.9(5)	N029-N015-C02Z-C02Q	-179.2(3)
N00C-N01Q-N01R-N00U	-0.8(3)	N02C-N00W-C030-N00M	0.8(3)
N00C-C02R-C02Y-N00D	-178.7(2)	N02C-N00W-C030-N02F	-178.6(3)
N00C-C02R-C02Y-N014	1.9(5)	C02I-N00N-C03C-N01O	0.3(4)
N00D-N01E-N01T-N014	0.0(3)	C02I-N019-N01O-C03C	0.2(3)
N00F-N01N-N029-N015	-0.5(3)	C02K-N010-N01K-N01Z	0.0(3)
N00G-N01I-N01S-N013	-0.2(3)	C02K-N01A-N01Z-N01K	-0.1(3)
N00H-N01L-N01X-N00S	-0.2(3)	C02L-N00J-C03F-N01H	-0.6(4)
N00H-C02N-C031-N00G	179.8(3)	C02L-N016-N01H-C03F	-0.3(3)
N00H-C02N-C031-N013	-0.5(5)	C02M-N00R-C03G-N01U	0.7(4)
N00I-N01P-N025-N017	0.2(3)	C02M-N01G-N01U-C03G	0.5(3)
N00K-N01D-C037-N00O	0.3(3)	C02N-N00H-N01L-N01X	0.1(3)
N00L-C02O-C02S-N00I	-179.8(3)	C02N-N00S-N01X-N01L	0.2(3)
N00L-C02O-C02S-N017	-0.1(4)	C02O-N00L-N024-N021	0.0(3)
N00Q-N01F-C035-N00Y	-0.5(3)	C02O-N01J-N021-N024	0.2(3)
N00S-C02N-C031-N00G	-0.8(5)	C02Q-N00B-N01M-N01Y	0.4(3)
N00S-C02N-C031-N013	178.9(3)	C02Q-N00V-N01Y-N01M	0.4(3)
N00U-C02R-C02Y-N00D	1.7(5)	C02R-N00C-N01Q-N01R	0.2(3)

N00U-C02R-C02Y-N014	-177.7(3)	C02R-N00U-N01R-N01Q	1.0(3)
N00V-C02Q-C02Z-N00F	-1.6(5)	C02S-N00I-N01P-N025	-0.5(3)
N00V-C02Q-C02Z-N015	177.2(3)	C02S-N017-N025-N01P	0.2(3)
N00W-N02C-C038-N00M	0.1(3)	C02U-N00P-C039-N01W	-0.1(4)
N010-N01K-N01Z-N01A	0.0(3)	C02U-N018-N01W-C039	-0.3(3)
N010-C02K-C032-N00E	-179.8(3)	C02V-N00K-N01D-C037	-0.3(3)
N010-C02K-C032-N01B	-1.0(4)	C02V-N00O-C037-N01D	-0.1(3)
N011-N020-C03D-N00X	-0.2(3)	C02W-N00T-C03A-N027	-0.4(4)
N012-N027-C03A-N00T	0.2(3)	C02W-N012-N027-C03A	0.1(3)
N016-N01H-C03F-N00J	0.5(4)	C02X-N00Q-N01F-C035	0.0(3)
N018-N01W-C039-N00P	0.2(4)	C02X-N00Y-C035-N01F	0.8(4)
N019-N01O-C03C-N00N	-0.3(3)	C02Y-N00D-N01E-N01T	-0.1(3)
N01A-C02K-C032-N00E	0.3(4)	C02Y-N014-N01T-N01E	0.1(3)
N01A-C02K-C032-N01B	179.1(3)	C02Z-N00F-N01N-N029	0.4(3)
N01B-N01V-N023-N00E	0.1(3)	C02Z-N015-N029-N01N	0.5(3)
N01C-N022-C036-N00Z	0.1(3)	C030-N00M-C038-N02C	0.4(3)
N01D-N00K-C02V-N00O	0.2(3)	C030-N00W-N02C-C038	-0.5(3)
N01D-N00K-C02V-N02G	-179.2(3)	C031-N00G-N01I-N01S	0.0(3)
N01E-N00D-C02Y-N014	0.1(3)	C031-N013-N01S-N01I	0.4(3)
N01E-N00D-C02Y-C02R	-179.3(2)	C032-N00E-N023-N01V	-0.4(3)
N01F-N00Q-C02X-N00Y	0.5(3)	C032-N01B-N01V-N023	0.2(3)
N01F-N00Q-C02X-N02E	-178.7(3)	C033-N00X-C03D-N020	0.2(4)
N01G-N01U-C03G-N00R	-0.7(3)	C033-N011-N020-C03D	0.1(3)
N01H-N016-C02L-N00J	0.0(3)	C034-N00Z-C036-N022	0.1(4)
N01H-N016-C02L-N02D	179.4(3)	C034-N01C-N022-C036	-0.3(3)
N01I-N00G-C031-N013	0.2(3)	C035-N00Y-C02X-N00Q	-0.8(3)
N01I-N00G-C031-C02N	180.0(3)	C035-N00Y-C02X-N02E	178.4(3)
N01J-N021-N024-N00L	-0.2(3)	C036-N00Z-C034-N01C	-0.3(3)
N01J-C02O-C02S-N00I	-0.3(4)	C036-N00Z-C034-N02H	179.5(3)
N01J-C02O-C02S-N017	179.3(3)	C037-N00O-C02V-N00K	-0.1(3)
N01K-N010-C02K-N01A	0.0(3)	C037-N00O-C02V-N02G	179.4(3)
N01K-N010-C02K-C032	-179.9(2)	C038-N00M-C030-N00W	-0.7(3)
N01L-N00H-C02N-N00S	0.0(3)	C038-N00M-C030-N02F	178.8(3)
N01L-N00H-C02N-C031	179.5(3)	C039-N00P-C02U-N018	-0.1(3)
N01M-N00B-C02Q-N00V	-0.2(3)	C039-N00P-C02U-N026	179.5(3)
N01M-N00B-C02Q-C02Z	179.1(2)	C03A-N00T-C02W-N012	0.5(3)
N01N-N00F-C02Z-N015	-0.1(3)	C03A-N00T-C02W-N02A	-178.5(3)
N01N-N00F-C02Z-C02Q	178.9(3)	C03C-N00N-C02I-N019	-0.2(3)
N01O-N019-C02I-N00N	0.0(3)	C03C-N00N-C02I-N028	-179.0(3)
N01O-N019-C02I-N028	178.8(3)	C03D-N00X-C033-N011	-0.1(3)

N01P-N00I-C02S-N017	0.6(3)	C03D-N00X-C033-N02J	-179.7(3)
N01P-N00I-C02S-C02O	-179.6(2)	C03F-N00J-C02L-N016	0.3(3)
N01Q-N00C-C02R-N00U	0.4(3)	C03F-N00J-C02L-N02D	-179.1(3)
N01Q-N00C-C02R-C02Y	-179.3(3)	C03G-N00R-C02M-N01G	-0.3(3)
N01R-N00U-C02R-N00C	-0.9(3)	C03G-N00R-C02M-N02B	-179.7(3)

Table 12. Hydrogen bonds for **3·7H$_2$O**.

D-H...A	Symmetry	d(D-H)	d(H...A)	d(D...A)	<(DHA
N00K-H00K...O008	x, y+1, z	0.86	2.186	2.852	134.04
N00K-H00K...N013	x, y+1, z	0.86	2.225	2.953	142.32
N00M-H00M...O007		0.86	1.808	2.667	176.54
N00M-H00M...N00L		0.86	2.542	3.309	148.93
N00M-H00M...N024		0.86	2.665	3.173	119.1
N00N-H00N...O003		0.86	1.806	2.665	176.05
N00N-H00N...N00I		0.86	2.551	3.319	149.05
N00N-H00N...N01P		0.86	2.684	3.193	119.19
N00O-H00O...O004		0.86	1.832	2.69	175.26
N00O-H00O...N00B		0.86	2.561	3.321	147.8
N00O-H00O...N01M		0.86	2.676	3.176	118.31
N00Q-H00Q...O004		0.86	2.136	2.804	134.13
N00Q-H00Q...N015		0.86	2.273	2.998	142.05
N00R-H00R...O005		0.86	1.829	2.687	174.86
N00R-H00R...N00F		0.86	2.563	3.326	148.3
N00R-H00R...N01N		0.86	2.682	3.187	118.8
N00T-H00T...O001		0.86	1.828	2.686	176.27
N00T-H00T...N00C		0.86	2.548	3.316	149.18
N00T-H00T...N01Q		0.86	2.628	3.143	119.59
N00W-H00W...O00A		0.86	2.146	2.813	134.2
N00W-H00W...N01B		0.86	2.279	3.009	142.72
N00X-H00X...O009		0.86	1.815	2.673	175.36
N00X-H00X...N00E		0.86	2.558	3.32	148.28
N00X-H00X...N023		0.86	2.656	3.161	118.74
N00Y-H00Y...O008		0.86	1.811	2.671	177.26
N00Y-H00Y...N00H		0.86	2.542	3.313	149.84
N00Y-H00Y...N01L		0.86	2.629	3.15	120.12
N00Z-H00Z...O00A		0.86	1.828	2.687	176.18
N00Z-H00Z...N010		0.86	2.565	3.327	148.26
N00Z-H00Z...N01K		0.86	2.665	3.169	118.68
N011-H011...O003	x-1, y, z	0.86	2.192	2.851	133.31
N011-H011...N01J	x-1, y, z	0.86	2.218	2.946	142.39
N012-H012...O001	-x, y,-z+1/2	0.86	2.15	2.822	134.7

N012-H012...N014	-x, y-1/2, -z+1/2	0.86	2.268	2.993	142.1
N016-H016...O005	x+1, y-1, z	0.86	2.174	2.837	133.74
N016-H016...N00V	x+1, y-1, z	0.86	2.28	3.012	143.1
N018-H018...O002	-x+1, y+1/2, -z+1	0.86	2.183	2.851	134.35
N018-H018...N00U	-x+1, y+1/2, -z+1	0.86	2.275	3.001	142.16
N019-H019...O009	x+1, y-1, z	0.86	2.162	2.83	134.19
N019-H019...N01A	x+1, y-1, z	0.86	2.279	3.009	142.81
N01C-H01C...O007	x, y+1, z	0.86	2.19	2.853	133.8
N01C-H01C...N017	x, y+1, z	0.86	2.221	2.947	142.15
N01G-H01G...O006	x-1, y, z	0.86	2.181	2.848	134.13
N01G-H01G...N00S	x-1, y, z	0.86	2.246	2.972	142.13
N028-H02G...N01A	x+1, y-1, z	0.86	2.488	3.189	139.28
N028-H02G...N01Z	x+1, y-1, z	0.86	2.25	3.102	171.08
N028-H02H...N020	x+1, y, z	0.86	2.143	3	174.65
N02A-H02O...N014	-x, y-1/2, -z+1/2	0.86	2.459	3.159	139.02
N02A-H02O...N01T	-x, y-1/2, -z+1/2	0.86	2.172	3.026	171.76
N02A-H02P...N027	-x, y+1/2, -z+1/2	0.86	2.124	2.981	174.52
N02B-H02M...N00S	x-1, y, z	0.86	2.453	3.15	138.63
N02B-H02M...N01X	x-1, y, z	0.86	2.178	3.03	170.92
N02B-H02N...N01H	x-1, y+1, z	0.86	2.124	2.981	174.37
N02D-H02A...N00V	x+1, y-1, z	0.86	2.484	3.193	140.25
N02D-H02A...N01Y	x+1, y-1, z	0.86	2.215	3.07	172.61
N02D-H02B...N01U	x+1, y, z	0.86	2.145	3.003	175.72
N02E-H02K...N015		0.86	2.462	3.17	140.08
N02E-H02K...N029		0.86	2.204	3.058	172.46
N02E-H02L...N01D	x, y-1, z	0.86	2.14	2.997	174.5
N02F-H02E...N01B		0.86	2.484	3.184	139.07
N02F-H02E...N01V		0.86	2.231	3.084	171.52
N02F-H02F...N022	x, y-1, z	0.86	2.153	3.009	174.18
N02G-H02C...N013	x, y+1, z	0.86	2.446	3.14	138.21
N02G-H02C...N01S	x, y+1, z	0.86	2.155	3.008	170.88
N02G-H02D...N01F		0.86	2.105	2.964	175.68
N02H-H02S...N017	x, y+1, z	0.86	2.457	3.151	138.22
N02H-H02S...N025	x, y+1, z	0.86	2.144	2.994	169.48
N02H-H02T...N02C		0.86	2.103	2.961	175.4
N02J-H02Q...N01J	x-1, y, z	0.86	2.47	3.163	138.14
N02J-H02Q...N021	x-1, y, z	0.86	2.148	2.998	169.35
N02J-H02R...N01O	x-1, y+1, z	0.86	2.108	2.965	174.59
O02P-H02U...O03J		0.849	1.99	2.829	169.2
O02P-H02V...N01V	x, y+1, z	0.85	2.209	2.952	146

O02T-H02W...O02P		0.85	1.987	2.793	158.01
O02T-H02X...N01K		0.851	2.643	3.366	143.62
O02T-H02X...N01Z		0.851	2.105	2.939	166.51
C037-H037...N01M		0.93	2.694	3.215	116.22
C037-H037...O03B		0.93	2.565	3.292	135.24
C038-H038...O03H	-x+1, y-1/2, -z+1	0.93	2.625	3.518	161.29
O03B-H03B...N01P	-x+1, y+3/2, -z+1	0.85	2.593	3.369	152.24
O03B-H03B...N029	x, y+1, z	0.85	2.487	3.038	123.29
O03B-H03E...O03H		0.85	2.138	2.802	134.7
C03C-H03C...O03B	-x+1, y-3/2, -z+1	0.93	2.609	3.429	147.36
C03D-H03D...O02T	x, y-1, z	0.93	2.333	3.184	151.89
O03E-H03H...N01M		0.85	2.644	3.293	134.12
O03E-H03H...N01Y		0.85	2.144	2.933	154.25
O03E-H03I...O03B		0.849	1.97	2.794	162.92
C03G-H03G...O03E	x, y-1, z	0.93	2.343	3.224	157.94
O03H-H03J...O03I		0.851	2.005	2.802	155.5
O03H-H03K...N01T	x, y-1, z	0.851	2.487	3.235	147.17
O03I-H03L...O02T		0.851	1.939	2.762	162.46
O03I-H03M...N01Q		0.849	2.46	3.229	151.01
O03I-H03M...N01R		0.849	2.188	2.996	159.09
O03J-H03N...O03J	-x+1, -y+1, -z+1	0.851	2.302	2.765	114.4
O03J-H03O...N01L	-x+1, y+1/2, -z+1	0.85	2.48	3.203	143.39
O03J-H03O...N01X	-x+1, y+1/2, -z+1	0.85	2.288	3.123	167.15
C036-H036...N01K		0.97	2.62	3.222	120.4
C036-H036...O02P		0.97	2.375	3.178	139.77
N00P-H00P...O002		0.907	1.774	2.681	179.28
N00P-H00P...N00D		0.907	2.504	3.324	150.61
N00P-H00P...N01E		0.907	2.619	3.18	120.73
C039-H039...O03I	x, y+1, z	0.946	2.549	3.431	155.31
N026-H02I...N01W	-x+1, y-1/2, -z+1	0.801	2.18	2.975	171.83
N026-H02J...N00U	-x+1, y+1/2, -z+1	0.902	2.414	3.166	140.95
N026-H02J...N01R	-x+1, y+1/2, -z+1	0.902	2.167	3.058	169.17
N00J-H00J...O006		0.939	1.736	2.672	173.9
N00J-H00J...N00G		0.939	2.469	3.322	150.98
N00J-H00J...N01I		0.939	2.589	3.172	120.58

Table 13. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
O(1)	925(2)	597(1)	7437(1)	19(1)
N(1)	2093(2)	1156(1)	6536(1)	14(1)

N(2)	4489(2)	2410(1)	6749(1)	18(1)
N(3)	5078(2)	2649(1)	5656(1)	20(1)
N(4)	3118(2)	1586(1)	4739(1)	17(1)
N(5)	3322(2)	6645(1)	8848(1)	17(1)
N(6)	5873(2)	7879(1)	7660(1)	17(1)
C(1)	1248(2)	653(1)	5294(1)	14(1)
C(2)	7288(2)	8378(2)	8827(1)	21(1)
C(3)	5684(2)	7609(2)	9576(1)	20(1)
C(4)	3482(2)	6815(1)	7686(1)	15(1)
C(5)	1403(2)	5979(2)	6607(1)	19(1)
O(2)	1176(2)	6485(1)	1280(1)	20(1)

Table 14. Bond Lengths [Å] and angles [°] for **6**.

bond	**Length/Å**	**bond**	**Angle/°**
O(1)-N(1)	1.3099(11)	O(1)-N(1)-N(2)	122.38(8)
N(1)-N(2)	1.3458(13)	O(1)-N(1)-C(1)	129.41(9)
N(1)-C(1)	1.3507(12)	N(2)-N(1)-C(1)	108.20(8)
N(2)-N(3)	1.3152(12)	N(3)-N(2)-N(1)	106.81(8)
N(3)-N(4)	1.3443(12)	N(2)-N(3)-N(4)	110.63(8)
N(4)-C(1)	1.3405(13)	C(1)-N(4)-N(3)	106.29(8)
N(5)-C(4)	1.3361(13)	C(4)-N(5)-C(3)	109.34(9)
N(5)- C(3)	1.3823(14)	C(4)-N(5)-H(5)	123.0(9)
N(5)-H(5)	0.899(9)	C(3)-N(5)-H(5)	127.6(9)
N(6)-C(4)	1.3303(14)	C(4)-N(6)-C(2)	109.40(9)
N(6)-C(2)	1.3820(13)	C(4)-N(6)-H(6)	122.1(9)
N(6)- H(6)	0.890(8)	C(2)-N(6)-H(6)	128.5(9)
C(1)-C(1)#1	1.4393(19)	N(4)-C(1)-N(1)	108.07(9)
C(2)-C(3)	1.3522(15)	N(4)-C(1)-C(1)#1	127.32(11)
C(2)-H(2)	0.9500	N(1)-C(1)-C(1)#1	124.61(11)
C(3)-H(3)	0.9500	C(3)-C(2)-N(6)	106.92(9)
C(4)-C(5)	1.4823(14)	C(3)-C(2)-H(2)	126.5
C(5)-H(5A)	0.9800	N(6)-C(2)-H(2)	126.5
C(5)-H(5B)	0.9800	C(2)-C(3)-N(5)	106.71(9)
C(5)-H(5C)	0.9800	C(2)-C(3)-H(3)	126.6
O(2)-H(2A)	0.877(9)	N(5)-C(3)-H(3)	126.6
O(2)-H(2B)	0.877(9)	N(6)-C(4)-N(5)	107.62(9)
		N(6)-C(4)-C(5)	125.41(9)
		N(5)-C(4)-C(5)	126.98(9)
		C(4)-C(5)-H(5A)	109.5
		C(4)-C(5)-H(5B)	109.5

	H(5A)-C(5)-H(5B)	109.5
	C(4)-C(5)-H(5C)	109.5
	H(5A)-C(5)-H(5C)	109.5
	H(5B)-C(5)-H(5C)	109.5
	H(2A)-O(2)-H(2B)	108.1(11)

Table 15. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	22(1)	23(1)	12(1)	7(1)	5(1)	3(1)
N(1)	14(1)	16(1)	12(1)	4(1)	2(1)	3(1)
N(2)	14(1)	20(1)	17(1)	5(1)	0(1)	1(1)
N(3)	16(1)	22(1)	17(1)	5(1)	1(1)	0(1)
N(4)	15(1)	20(1)	15(1)	5(1)	2(1)	1(1)
N(5)	16(1)	19(1)	17(1)	8(1)	5(1)	2(1)
N(6)	15(1)	20(1)	13(1)	6(1)	3(1)	1(1)
C(1)	15(1)	15(1)	11(1)	4(1)	2(1)	3(1)
C(2)	17(1)	26(1)	15(1)	6(1)	0(1)	0(1)
C(3)	19(1)	26(1)	14(1)	7(1)	2(1)	3(1)
C(4)	16(1)	15(1)	15(1)	5(1)	3(1)	4(1)
C(5)	16(1)	21(1)	18(1)	6(1)	0(1)	2(1)
O(2)	18(1)	23(1)	16(1)	4(1)	1(1)	2(1)

Table 16. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **6**.

Atom	x	y	z	U(eq)
H(5)	1880(20)	5953(18)	9076(13)	21
H(6)	6380(30)	8170(20)	6968(10)	20
H(2)	9051	9120	9059	25
H(3)	6101	7711	10435	24
H(5A)	531	6995	6567	29
H(5B)	150	4820	6721	29
H(5C)	2154	5568	5820	29
H(2A)	2540(20)	6590(20)	1784(13)	41(4)
H(2B)	450(30)	7420(20)	1653(14)	47(5)

Table 17. Torsion Angles for **6**.

A-B-C-D	Angle/°	A-B-C-D	Angle/°
O(1)-N(1)-N(2)-N(3)	179.73(8)	N(2)-N(1)-C(1)-C(1)#1	-179.41(11)
C(1)-N(1)-N(2)-N(3)	-0.29(11)	C(4)-N(6)-C(2)-C(3)	-0.75(12)
N(1)-N(2)-N(3)-N(4)	0.21(11)	N(6)-C(2)-C(3)-N(5)	0.31(12)

N(2)-N(3)-N(4)-C(1)	-0.04(11)	C(4)-N(5)-C(3)-C(2)	0.23(12)
N(3)-N(4)-C(1)-N(1)	-0.14(11)	C(2)-N(6)-C(4)-N(5)	0.89(12)
N(3)-N(4)-C(1)-C(1)#1	179.53(12)	C(2)-N(6)-C(4)-C(5)	-178.99(10)
O(1)-N(1)-C(1)-N(4)	-179.75(9)	C(3)-N(5)-C(4)-N(6)	-0.70(11)
N(2)-N(1)-C(1)-N(4)	0.27(11)	C(3)-N(5)-C(4)-C(5)	179.18(10)
O(1)-N(1)-C(1)-C(1)#1	0.57(18)		

Table 18. Hydrogen bonds for **6**.

D-H...A	Symmetry	d(D-H)	d(H...A)	d(D...A)	<(DHA
O(2)-H(2A)...N(2)	-x+1,-y+1,-z+1	0.877(9)	2.071(10)	2.9220(12)	163.5(14)
N(6)-H(6)...N(4)	-x+1,-y+1,-z+1	0.890(8)	1.978(9)	2.8553(12)	168.6(13)
N(5)-H(5)...O(2)	x,y,z+1	0.899(9)	2.432(12)	3.0035(12)	121.7(11)
N(6)-H(6)...O(1)	x+1,y+1,z	0.890(8)	2.562(13)	2.9980(12)	111.0(10)
N(5)-H(5)...O(2)	-x,-y+1,-z+1	0.899(9)	2.022(10)	2.8409(12)	150.7(12)
O(2)-H(2B)...O(1)	-x,-y+1,-z+1	0.877(9)	1.855(9)	2.7300(11)	175.3(15)
O(2)-H(2B)...N(1)	-x,-y+1,-z+1	0.877(9)	2.604(12)	3.3857(12)	149.0(15)

Table 19. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
O(1)	4708(1)	4099(1)	7156(1)	22(1)
O(2)	5140(1)	7619(1)	9862(1)	22(1)
N(1)	5631(1)	4791(1)	7312(2)	19(1)
N(2)	6895(1)	4631(1)	6986(2)	23(1)
N(3)	7534(1)	5452(1)	7338(2)	24(1)
N(4)	6702(1)	6134(1)	7890(2)	21(1)
N(5)	4144(1)	7005(1)	9131(2)	19(1)
N(6)	2867(1)	7154(1)	9391(2)	23(1)
N(7)	2217(1)	6384(1)	8699(2)	25(1)
N(8)	3061(1)	5730(1)	8034(2)	21(1)
N(9)	1982(1)	3822(1)	7196(2)	22(1)
N(10)	1844(1)	2867(1)	6916(2)	22(1)
C(1)	5509(1)	5714(1)	7867(2)	18(1)
C(2)	4269(1)	6130(1)	8316(2)	18(1)
C(3)	763(1)	4213(1)	7101(2)	26(1)
C(4)	-190(1)	3490(1)	6754(2)	29(1)
C(5)	537(1)	2647(1)	6655(2)	26(1)

Table 20. Bond Lengths [Å] and angles [°] for **8**.

bond	Length/Å	bond	Angle/°

O(1)-N(1)	1.3288(12)	N(5)-O(2)-H(2)	107.4(12)
O(2)-N(5)	1.3526(13)	O(1)-N(1)-N(2)	122.38(9)
O(2)-H(2)	0.860(9)	O(1)-N(1)-C(1)	128.36(10)
N(1)-N(2)	1.3368(15)	N(2)-N(1)-C(1)	109.21(10)
N(1)-C(1)	1.3448(14)	N(3)-N(2)-N(1)	106.18(10)
N(2)-N(3)	1.3126(15)	N(2)-N(3)-N(4)	110.62(10)
N(3)-N(4)	1.3492(15)	C(1)-N(4)-N(3)	106.32(10)
N(4)-C(1)	1.3311(15)	N(6)-N(5)-C(2)	109.89(10)
N(5)-N(6)	1.3344(15)	N(6)-N(5)-O(2)	121.96(10)
N(5)-C(2)	1.3438(15)	C(2)-N(5)-O(2)	127.61(10)
N(6)-N(7)	1.3027(15)	N(7)-N(6)-N(5)	105.59(10)
N(7)-N(8)	1.3594(15)	N(6)-N(7)-N(8)	111.09(10)
N(8)-C(2)	1.3235(16)	C(2)-N(8)-N(7)	105.94(10)
N(9)-C(3)	1.3322(17)	C(3)-N(9)-N(10)	108.65(10)
N(9)-N(10)	1.3439(14)	C(3)-N(9)-H(9)	130.6(11)
N(9)-H(9)	0.895(9)	N(10)-N(9)-H(9)	120.7(11)
N(10)-C(5)	1.3347(17)	C(5)-N(10)-N(9)	108.87(10)
N(10)-H(10)	0.892(9)	C(5)-N(10)-H(10)	129.5(11)
C(1)-C(2)	1.4426(17)	N(9)-N(10)-H(10)	121.5(11)
C(3)-C(4)	1.3840(18)	N(4)-C(1)-N(1)	107.67(10)
C(3)-H(3)	0.9500	N(4)-C(1)-C(2)	128.64(11)
C(4)-C(5)	1.3854(18)	N(1)-C(1)-C(2)	123.68(11)
C(4)-H(4)	0.9500	N(8)-C(2)-N(5)	107.47(10)
C(5)-H(5)	0.9500	N(8)-C(2)-C(1)	127.11(11)
		N(5)-C(2)-C(1)	125.41(11)
		N(9)-C(3)-C(4)	108.74(11)
		N(9)-C(3)-H(3)	125.6
		C(4)-C(3)-H(3)	125.6
		C(3)-C(4)-C(5)	105.31(12)
		C(3)-C(4)-H(4)	127.3
		C(5)-C(4)-H(4)	127.3
		N(10)-C(5)-C(4)	108.43(11)
		N(10)-C(5)-H(5)	125.8
		C(4)-C(5)-H(5)	125.8

Table 21. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
O(1)	23(1)	8(1)	36(1)	-2(1)	6(1)	-3(1)
O(2)	28(1)	8(1)	30(1)	-1(1)	1(1)	-4(1)

N(1)	21(1)	9(1)	25(1)	0(1)	3(1)	1(1)
N(2)	22(1)	14(1)	32(1)	0(1)	6(1)	2(1)
N(3)	23(1)	15(1)	34(1)	1(1)	5(1)	2(1)
N(4)	21(1)	12(1)	30(1)	0(1)	3(1)	1(1)
N(5)	23(1)	8(1)	26(1)	0(1)	4(1)	0(1)
N(6)	25(1)	13(1)	32(1)	1(1)	7(1)	2(1)
N(7)	25(1)	13(1)	37(1)	0(1)	7(1)	2(1)
N(8)	21(1)	12(1)	32(1)	0(1)	5(1)	1(1)
N(9)	23(1)	12(1)	33(1)	-1(1)	3(1)	-2(1)
N(10)	23(1)	11(1)	33(1)	0(1)	5(1)	2(1)
C(1)	22(1)	9(1)	23(1)	1(1)	3(1)	0(1)
C(2)	23(1)	8(1)	24(1)	1(1)	3(1)	0(1)
C(3)	26(1)	13(1)	39(1)	-1(1)	4(1)	2(1)
C(4)	22(1)	20(1)	46(1)	-3(1)	5(1)	0(1)
C(5)	26(1)	14(1)	39(1)	-2(1)	6(1)	-3(1)

Table 22. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **8**.

Atom	x	y	z	U(eq)
H(2)	5038(17)	8134(9)	9140(20)	27
H(9)	2798(11)	4094(12)	7380(30)	27
H(10)	2557(13)	2478(11)	6990(30)	27
H(3)	579	4879	7247	32
H(4)	-1140	3557	6613	35
H(5)	167	2020	6439	32

Table 23. Torsion Angles for **8**.

A-B-C-D	Angle/°	A-B-C-D	Angle/°
O(1)-N(1)-N(2)-N(3)	-177.78(10)	N(7)-N(8)-C(2)-N(5)	-0.04(13)
C(1)-N(1)-N(2)-N(3)	-0.14(13)	N(7)-N(8)-C(2)-C(1)	179.24(12)
N(1)-N(2)-N(3)-N(4)	0.23(13)	N(6)-N(5)-C(2)-N(8)	0.83(13)
N(2)-N(3)-N(4)-C(1)	-0.23(13)	O(2)-N(5)-C(2)-N(8)	172.38(11)
C(2)-N(5)-N(6)-N(7)	-1.29(13)	N(6)-N(5)-C(2)-C(1)	-178.47(11)
O(2)-N(5)-N(6)-N(7)	-173.41(10)	O(2)-N(5)-C(2)-C(1)	-6.92(19)
N(5)-N(6)-N(7)-N(8)	1.27(14)	N(4)-C(1)-C(2)-N(8)	170.65(12)
N(6)-N(7)-N(8)-C(2)	-0.79(14)	N(1)-C(1)-C(2)-N(8)	-8.6(2)
C(3)-N(9)-N(10)-C(5)	-0.40(15)	N(4)-C(1)-C(2)-N(5)	-10.2(2)
N(3)-N(4)-C(1)-N(1)	0.13(13)	N(1)-C(1)-C(2)-N(5)	170.56(11)
N(3)-N(4)-C(1)-C(2)	-179.22(12)	N(10)-N(9)-C(3)-C(4)	0.14(16)
O(1)-N(1)-C(1)-N(4)	177.46(10)	N(9)-C(3)-C(4)-C(5)	0.16(17)
N(2)-N(1)-C(1)-N(4)	0.00(13)	N(9)-N(10)-C(5)-C(4)	0.51(16)

O(1)-N(1)-C(1)-C(2)	-3.15(19)	C(3)-C(4)-C(5)-N(10)	-0.41(17)
N(2)-N(1)-C(1)-C(2)	179.39(11)		

Table 24. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **8**.

D-H...A	Symmetry	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)	-x+1,y+1/2,-z+3/2	0.860(9)	1.637(10)	2.4760(12)	164.4(17)
O(2)-H(2)...N(1)	-x+1,y+1/2,-z+3/2	0.860(9)	2.551(10)	3.3895(14)	165.3(15)
N(9)-H(9)...O(1)		0.895(9)	1.945(11)	2.7679(15)	152.2(16)
N(9)-H(9)...N(8)		0.895(9)	2.321(16)	2.8871(15)	121.1(14)
N(10)-H(10)...N(4)	-x+1,y-1/2,-z+3/2	0.892(9)	2.005(12)	2.8065(15)	148.7(15)

Fig. S2. Crystal structures of salts **10·4H$_2$O**.

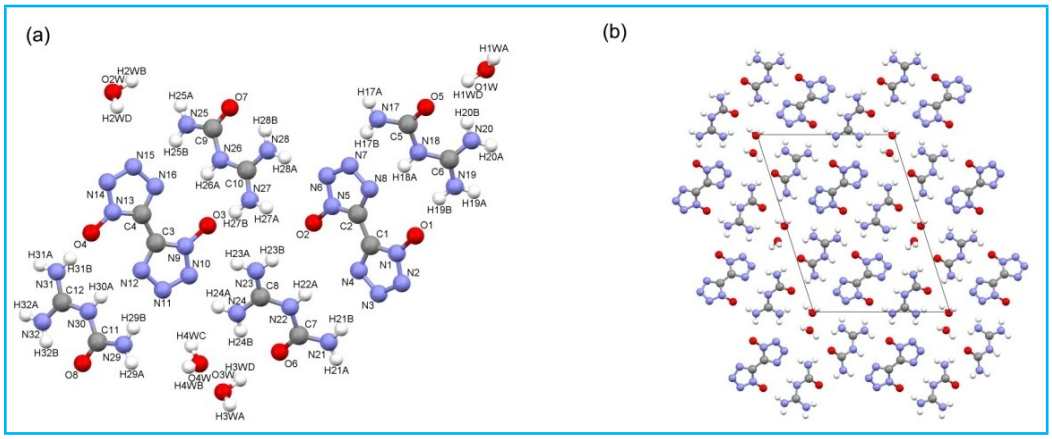

Figure 2. Molecular structure (a) and packing diagram in the unit cell (b) of **10·4 H$_2$O**.

Bis-dicyandiamidine 1*H*,1*H*-5,5-Bitetrazole-1,1-diolate (**10·4 H$_2$O**) crystallizes as a tetrahydrate in the triclinic space group *P1* with a density of 1.688 g cm^{-3} and two molecular moieties in the unit cell. The unit cell has the dimensions a=3.5356(14) Å, b=13.300(5) Å, c=18.164(7) Å. It crystallizes with a cell volume of 811.3(6) Å ^{3}. Stronger hydrogen bonds between O5···N21-H21A (1.957 Å) , O6···N24-H24B (1.969 Å), O8···N25-H25A (1.955 Å), O2···N27-H27A (1.988 Å) , O3···N27-H27B (1.988 Å), O7···N28-H28B (1.999 Å) and O1···N31-H31A (1.968 Å) are also observed.

Table 25. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **10·4H$_2$O**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
O(1)	4831(11)	4888(3)	1633(2)	21(1)
O(1W)	7560(30)	-711(8)	1034(7)	124(4)
O(2)	10765(11)	4536(3)	4297(2)	22(1)
O(2W)	12670(40)	-101(5)	10054(4)	112(4)
O(3)	6338(11)	4404(3)	6773(2)	19(1)
O(3W)	-3070(80)	9881(10)	5155(7)	230(11)
O(4)	-673(12)	4339(3)	9425(2)	22(1)

O(4W)	1680(40)	9030(9)	5996(5)	145(5)
O(5)	3440(13)	413(3)	2180(2)	25(1)
O(6)	1715(11)	8691(3)	4123(2)	19(1)
O(7)	5896(13)	332(3)	6984(2)	25(1)
O(8)	89(13)	8866(3)	8809(2)	26(1)
N(1)	6040(14)	5514(3)	1991(3)	16(1)
N(2)	6074(14)	6558(4)	1682(3)	20(1)
N(3)	7365(15)	6937(4)	2198(3)	22(1)
N(4)	8247(14)	6144(4)	2845(3)	20(1)
N(5)	9365(13)	3931(3)	3931(3)	15(1)
N(6)	9337(15)	2878(4)	4247(3)	23(1)
N(7)	7931(16)	2506(4)	3736(3)	24(1)
N(8)	7030(14)	3299(4)	3091(3)	18(1)
N(9)	5163(14)	5059(3)	7166(3)	18(1)
N(10)	5763(15)	6093(4)	6895(3)	20(1)
N(11)	4351(14)	6524(4)	7415(3)	20(1)
N(12)	2960(14)	5794(4)	8029(3)	21(1)
N(13)	683(13)	3681(3)	9062(2)	15(1)
N(14)	366(15)	2628(4)	9376(3)	20(1)
N(15)	1972(15)	2169(4)	8877(3)	22(1)
N(16)	3271(14)	2911(4)	8245(3)	20(1)
N(17)	4422(17)	805(4)	3288(3)	25(1)
N(18)	5580(14)	2025(4)	2111(3)	17(1)
N(19)	7745(14)	3299(4)	1050(3)	19(1)
N(20)	6556(15)	1696(4)	917(3)	20(1)
N(21)	978(15)	8368(4)	2980(3)	21(1)
N(22)	-324(13)	7081(3)	4122(3)	15(1)
N(23)	-2508(14)	5740(4)	5142(3)	19(1)
N(24)	-764(14)	7244(4)	5361(3)	20(1)
N(25)	7491(15)	931(4)	7950(3)	22(1)
N(26)	5051(14)	2101(4)	6862(3)	18(1)
N(27)	2791(15)	3442(3)	5847(3)	18(1)
N(28)	3229(15)	1766(4)	5736(3)	22(1)
N(29)	-1793(16)	8197(4)	7895(3)	24(1)
N(30)	597(14)	7088(4)	9012(3)	18(1)
N(31)	2666(15)	5756(4)	10073(3)	20(1)
N(32)	2534(15)	7467(4)	10095(3)	21(1)
C(1)	7399(16)	5256(4)	2709(3)	16(1)
C(2)	7924(17)	4181(4)	3231(3)	16(1)
C(3)	3456(16)	4867(4)	7865(3)	20(1)

C(4)	2472(17)	3836(4)	8376(3)	18(1)
C(5)	4364(17)	1012(4)	2520(3)	17(1)
C(6)	6612(16)	2330(4)	1333(3)	15(1)
C(7)	829(16)	8107(4)	3748(3)	17(1)
C(8)	-1198(15)	6683(4)	4893(3)	16(1)
C(9)	6142(15)	1044(4)	7270(3)	14(1)
C(10)	3647(15)	2436(4)	6130(3)	16(1)
C(11)	-381(16)	8123(4)	8576(3)	19(1)
C(12)	1939(16)	6791(4)	9736(3)	17(1)

Table 26. Bond Lengths [Å] and angles [°] for **10·4H$_2$O**.

bond	Length/Å	bond	Angle/°
O(1)-N(1)	1.304(6)	H(1WD)-O(1W)-H(1WA)	109.5
O(1W)-H(1WD)	0.9601	H(2WD)-O(2W)-H(2WB)	109.4
O(1W)-H(1WA)	0.9601	H(3WD)-O(3W)-H(3WA)	109.5
O(2)-N(5)	1.320(6)	H(4WB)-O(4W)-H(4WC)	109.5
O(2W)-H(2WD)	0.96	O(1)-N(1)-N(2)	123.5(4)
O(2W)-H(2WB)	0.96	O(1)-N(1)-C(1)	128.3(4)
O(3)-N(9)	1.321(6)	N(2)-N(1)-C(1)	108.2(5)
O(3W)-H(3WD)	0.9601	N(3)-N(2)-N(1)	107.5(4)
O(3W)-H(3WA)	0.96	N(2)-N(3)-N(4)	110.3(4)
O(4)-N(13)	1.303(6)	C(1)-N(4)-N(3)	105.8(5)
O(4W)-H(4WB)	0.96	O(2)-N(5)-C(2)	130.4(4)
O(4W)-H(4WC)	0.96	O(2)-N(5)-N(6)	121.4(4)
O(5)-C(5)	1.215(7)	C(2)-N(5)-N(6)	108.2(5)
O(6)-C(7)	1.241(7)	N(7)-N(6)-N(5)	106.7(4)
O(7)-C(9)	1.221(7)	N(6)-N(7)-N(8)	110.6(5)
O(8)-C(11)	1.211(7)	C(2)-N(8)-N(7)	105.4(5)
N(1)-N(2)	1.330(6)	O(3)-N(9)-C(3)	130.3(4)
N(1)-C(1)	1.348(7)	O(3)-N(9)-N(10)	121.3(4)
N(2)-N(3)	1.303(7)	C(3)-N(9)-N(10)	108.3(5)
N(3)-N(4)	1.352(7)	N(11)-N(10)-N(9)	107.0(4)
N(4)-C(1)	1.334(8)	N(10)-N(11)-N(12)	110.9(5)
N(5)-C(2)	1.331(7)	N(11)-N(12)-C(3)	105.8(5)
N(5)-N(6)	1.343(6)	O(4)-N(13)-C(4)	131.7(4)
N(6)-N(7)	1.307(7)	O(4)-N(13)-N(14)	121.0(4)
N(7)-N(8)	1.351(6)	C(4)-N(13)-N(14)	107.3(4)
N(8)-C(2)	1.333(8)	N(15)-N(14)-N(13)	107.2(4)
N(9)-C(3)	1.338(8)	N(14)-N(15)-N(16)	109.8(4)
N(9)-N(10)	1.338(6)	C(4)-N(16)-N(15)	105.9(5)

N(10)-N(11)	1.311(7)	C(5)-N(17)-H(17A)	120
N(11)-N(12)	1.332(7)	C(5)-N(17)-H(17B)	120
N(12)-C(3)	1.354(8)	H(17A)-N(17)-H(17B)	120
N(13)-C(4)	1.334(7)	C(6)-N(18)-C(5)	123.6(5)
N(13)-N(14)	1.351(6)	C(6)-N(18)-H(18A)	118.2
N(14)-N(15)	1.326(7)	C(5)-N(18)-H(18A)	118.2
N(15)-N(16)	1.348(7)	C(6)-N(19)-H(19A)	120
N(16)-C(4)	1.334(8)	C(6)-N(19)-H(19B)	120
N(17)-C(5)	1.337(7)	H(19A)-N(19)-H(19B)	120
N(17)-H(17A)	0.88	C(6)-N(20)-H(20A)	120
N(17)-H(17B)	0.88	C(6)-N(20)-H(20B)	120
N(18)-C(6)	1.384(7)	H(20A)-N(20)-H(20B)	120
N(18)-C(5)	1.409(7)	C(7)-N(21)-H(21A)	120
N(18)-H(18A)	0.88	C(7)-N(21)-H(21B)	120
N(19)-C(6)	1.314(7)	H(21A)-N(21)-H(21B)	120
N(19)-H(19A)	0.88	C(8)-N(22)-C(7)	125.5(5)
N(19)-H(19B)	0.88	C(8)-N(22)-H(22A)	117.3
N(20)-C(6)	1.295(8)	C(7)-N(22)-H(22A)	117.3
N(20)-H(20A)	0.88	C(8)-N(23)-H(23A)	120
N(20)-H(20B)	0.88	C(8)-N(23)-H(23B)	120
N(21)-C(7)	1.331(7)	H(23A)-N(23)-H(23B)	120
N(21)-H(21A)	0.88	C(8)-N(24)-H(24A)	120
N(21)-H(21B)	0.88	C(8)-N(24)-H(24B)	120
N(22)-C(8)	1.364(7)	H(24A)-N(24)-H(24B)	120
N(22)-C(7)	1.402(7)	C(9)-N(25)-H(25A)	120
N(22)-H(22A)	0.88	C(9)-N(25)-H(25B)	120
N(23)-C(8)	1.303(7)	H(25A)-N(25)-H(25B)	120
N(23)-H(23A)	0.88	C(10)-N(26)-C(9)	125.2(5)
N(23)-H(23B)	0.88	C(10)-N(26)-H(26A)	117.4
N(24)-C(8)	1.311(8)	C(9)-N(26)-H(26A)	117.4
N(24)-H(24A)	0.88	C(10)-N(27)-H(27A)	120
N(24)-H(24B)	0.88	C(10)-N(27)-H(27B)	120
N(25)-C(9)	1.307(8)	H(27A)-N(27)-H(27B)	120
N(25)-H(25A)	0.88	C(10)-N(28)-H(28A)	120
N(25)-H(25B)	0.88	C(10)-N(28)-H(28B)	120
N(26)-C(10)	1.374(7)	H(28A)-N(28)-H(28B)	120
N(26)-C(9)	1.413(7)	C(11)-N(29)-H(29A)	120
N(26)-H(26A)	0.88	C(11)-N(29)-H(29B)	120
N(27)-C(10)	1.300(7)	H(29A)-N(29)-H(29B)	120
N(27)-H(27A)	0.88	C(12)-N(30)-C(11)	125.4(5)

N(27)-H(27B)	0.88	C(12)-N(30)-H(30A)	117.3
N(28)-C(10)	1.320(8)	C(11)-N(30)-H(30A)	117.3
N(28)-H(28A)	0.88	C(12)-N(31)-H(31A)	120
N(28)-H(28B)	0.88	C(12)-N(31)-H(31B)	120
N(29)-C(11)	1.329(8)	H(31A)-N(31)-H(31B)	120
N(29)-H(29A)	0.88	C(12)-N(32)-H(32A)	120
N(29)-H(29B)	0.88	C(12)-N(32)-H(32B)	120
N(30)-C(12)	1.353(8)	H(32A)-N(32)-H(32B)	120
N(30)-C(11)	1.393(7)	N(4)-C(1)-N(1)	108.2(5)
N(30)-H(30A)	0.88	N(4)-C(1)-C(2)	126.7(5)
N(31)-C(12)	1.338(7)	N(1)-C(1)-C(2)	125.1(5)
N(31)-H(31A)	0.88	N(5)-C(2)-N(8)	109.1(5)
N(31)-H(31B)	0.88	N(5)-C(2)-C(1)	124.8(5)
N(32)-C(12)	1.294(8)	N(8)-C(2)-C(1)	126.1(5)
N(32)-H(32A)	0.88	N(9)-C(3)-N(12)	108.0(5)
N(32)-H(32B)	0.88	N(9)-C(3)-C(4)	126.1(5)
C(1)-C(2)	1.460(7)	N(12)-C(3)-C(4)	125.9(5)
C(3)-C(4)	1.454(8)	N(16)-C(4)-N(13)	109.8(5)
		N(16)-C(4)-C(3)	126.0(5)
		N(13)-C(4)-C(3)	124.2(5)
		O(5)-C(5)-N(17)	126.0(5)
		O(5)-C(5)-N(18)	120.9(5)
		N(17)-C(5)-N(18)	113.1(5)
		N(20)-C(6)-N(19)	122.2(5)
		N(20)-C(6)-N(18)	122.4(5)
		N(19)-C(6)-N(18)	115.4(5)
		O(6)-C(7)-N(21)	124.5(5)
		O(6)-C(7)-N(22)	121.0(5)
		N(21)-C(7)-N(22)	114.5(5)
		N(23)-C(8)-N(24)	121.6(5)
		N(23)-C(8)-N(22)	118.0(5)
		N(24)-C(8)-N(22)	120.4(5)
		O(7)-C(9)-N(25)	125.2(5)
		O(7)-C(9)-N(26)	121.2(5)
		N(25)-C(9)-N(26)	113.6(5)
		N(27)-C(10)-N(28)	122.2(5)
		N(27)-C(10)-N(26)	116.5(5)
		N(28)-C(10)-N(26)	121.3(5)
		O(8)-C(11)-N(29)	124.9(5)
		O(8)-C(11)-N(30)	121.7(5)

	N(29)-C(11)-N(30)	113.4(5)
	N(32)-C(12)-N(31)	120.5(5)
	N(32)-C(12)-N(30)	122.3(5)
	N(31)-C(12)-N(30)	117.2(5)

Table 27. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10·4H$_2$O**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	25(2)	20(2)	18(2)	-5(2)	-16(2)	4(2)
O(1W)	110(8)	107(7)	142(9)	-17(7)	-55(7)	18(6)
O(2)	28(2)	23(2)	16(2)	-9(2)	-3(2)	0(2)
O(2W)	264(14)	34(3)	32(3)	-4(3)	3(5)	-1(5)
O(3)	23(2)	20(2)	15(2)	-5(2)	1(2)	-3(2)
O(3W)	450(30)	110(9)	103(9)	-14(8)	37(14)	36(15)
O(4)	29(2)	18(2)	19(2)	-8(2)	12(2)	1(2)
O(4W)	224(13)	162(8)	73(5)	-63(5)	34(6)	-94(8)
O(5)	40(3)	18(2)	19(2)	-5(2)	-2(2)	-7(2)
O(6)	22(2)	22(2)	11(2)	-3(2)	-4(2)	-2(2)
O(7)	37(2)	16(2)	21(2)	-4(2)	-9(2)	5(2)
O(8)	32(2)	17(2)	28(2)	-6(2)	-13(2)	-1(2)
N(1)	20(2)	15(2)	13(2)	-2(2)	3(2)	-3(2)
N(2)	20(2)	16(2)	19(2)	0(2)	-4(2)	5(2)
N(3)	24(3)	21(2)	23(2)	-11(2)	-1(2)	-3(2)
N(4)	20(2)	16(2)	21(2)	-3(2)	-8(2)	2(2)
N(5)	14(1)	15(1)	14(1)	-4(1)	-1(1)	1(1)
N(6)	27(3)	17(2)	26(3)	-5(2)	-3(2)	-7(2)
N(7)	30(3)	20(2)	18(2)	-2(2)	-10(2)	7(2)
N(8)	16(2)	21(2)	12(2)	-1(2)	-2(2)	2(2)
N(9)	29(3)	9(2)	11(2)	2(2)	2(2)	-3(2)
N(10)	26(3)	19(2)	14(2)	-4(2)	3(2)	0(2)
N(11)	18(2)	20(2)	24(2)	-12(2)	0(2)	-2(2)
N(12)	19(2)	19(2)	21(2)	0(2)	-1(2)	2(2)
N(13)	15(2)	16(2)	12(2)	-2(2)	-8(2)	1(2)
N(14)	27(3)	16(2)	14(2)	-1(2)	-6(2)	-3(2)
N(15)	23(3)	20(2)	20(2)	-3(2)	-5(2)	-1(2)
N(16)	16(2)	24(2)	23(2)	-12(2)	3(2)	-5(2)
N(17)	39(3)	19(2)	14(2)	-2(2)	5(2)	-7(2)
N(18)	23(2)	14(2)	14(2)	-4(2)	1(2)	-1(2)
N(19)	17(2)	21(2)	17(2)	-6(2)	2(2)	-2(2)
N(20)	25(3)	20(2)	12(2)	0(2)	0(2)	-6(2)

N(21)	29(3)	16(2)	17(2)	-1(2)	-6(2)	-7(2)
N(22)	16(2)	14(2)	14(2)	-3(2)	-2(2)	1(2)
N(23)	20(2)	19(2)	16(2)	-3(2)	3(2)	-3(2)
N(24)	24(3)	15(2)	17(2)	-1(2)	6(2)	-1(2)
N(25)	29(3)	15(2)	19(2)	-2(2)	-5(2)	1(2)
N(26)	21(2)	17(2)	17(2)	-7(2)	-7(2)	6(2)
N(27)	26(2)	13(2)	16(2)	-7(2)	-6(2)	-2(2)
N(28)	24(3)	20(2)	19(2)	-3(2)	-9(2)	11(2)
N(29)	34(3)	14(2)	24(2)	-5(2)	-3(2)	0(2)
N(30)	21(2)	14(2)	20(2)	-6(2)	-5(2)	8(2)
N(31)	29(3)	17(2)	10(2)	-1(2)	-10(2)	9(2)
N(32)	31(3)	14(2)	19(2)	-5(2)	-6(2)	-3(2)
C(1)	10(2)	22(3)	15(2)	-3(2)	-8(2)	0(2)
C(2)	13(2)	26(3)	10(2)	-8(2)	-7(2)	5(2)
C(3)	17(3)	18(3)	24(3)	-6(2)	0(2)	-5(2)
C(4)	18(3)	21(3)	17(3)	-8(2)	3(2)	-5(2)
C(5)	18(3)	15(3)	13(2)	5(2)	-2(2)	0(2)
C(6)	15(3)	13(2)	11(2)	6(2)	7(2)	0(2)
C(7)	16(3)	18(3)	12(2)	3(2)	-1(2)	-5(2)
C(8)	12(3)	18(2)	16(3)	-2(2)	-5(2)	1(2)
C(9)	14(3)	11(2)	17(2)	-5(2)	-11(2)	9(2)
C(10)	7(2)	17(3)	24(3)	-5(2)	-1(2)	1(2)
C(11)	13(3)	21(3)	22(3)	-7(2)	1(2)	1(2)
C(12)	16(3)	14(2)	19(3)	-2(2)	-2(2)	3(2)

Table 28. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **10·4H$_2$O**.

Atom	x	y	z	U(eq)
H(1WD)	6311	-373	1383	148
H(1WA)	5814	-1137	890	185
H(2WD)	10549	350	9821	134
H(2WB)	13845	-430	9692	168
H(3WD)	-1617	9518	4845	276
H(3WA)	-5185	10272	4868	345
H(4WB)	-888	9052	6193	217
H(4WC)	3098	8451	6339	217
H(17A)	3748	187	3594	30
H(17B)	5133	1286	3486	30
H(18A)	5690	2490	2365	20
H(19A)	8501	3536	562	22
H(19B)	7749	3710	1349	22

H(20A)	7294	1909	426	24
H(20B)	5781	1051	1124	24
H(21A)	1745	8991	2703	25
H(21B)	308	7917	2748	25
H(22A)	-498	6660	3836	18
H(23A)	-3124	5466	5635	23
H(23B)	-2775	5378	4817	23
H(24A)	-1362	6986	5856	24
H(24B)	125	7879	5180	24
H(25A)	8312	303	8239	26
H(25B)	7578	1484	8117	26
H(26A)	5289	2583	7095	21
H(27A)	1900	3697	5379	21
H(27B)	3102	3868	6125	21
H(28A)	2345	1997	5266	27
H(28B)	3835	1089	5943	27
H(29A)	-2464	8821	7577	29
H(29B)	-2058	7622	7763	29
H(30A)	319	6587	8799	22
H(31A)	3557	5530	10542	23
H(31B)	2255	5301	9825	23
H(32A)	3424	7248	10565	25
H(32B)	2048	8147	9870	25

Table 29. Torsion Angles for **10·4H_2O**.

A-B-C-D	Angle/°	A-B-C-D	Angle/°
O(1)-N(1)-N(2)-N(3)	178.6(5)	O(3)-N(9)-C(3)-N(12)	177.4(5)
C(1)-N(1)-N(2)-N(3)	-0.9(6)	N(10)-N(9)-C(3)-N(12)	0.5(7)
N(1)-N(2)-N(3)-N(4)	1.0(6)	O(3)-N(9)-C(3)-C(4)	0.2(10)
N(2)-N(3)-N(4)-C(1)	-0.7(6)	N(10)-N(9)-C(3)-C(4)	-176.8(5)
O(2)-N(5)-N(6)-N(7)	-177.5(5)	N(11)-N(12)-C(3)-N(9)	0.8(6)
C(2)-N(5)-N(6)-N(7)	0.7(6)	N(11)-N(12)-C(3)-C(4)	178.0(5)
N(5)-N(6)-N(7)-N(8)	-0.1(7)	N(15)-N(16)-C(4)-N(13)	-0.8(6)
N(6)-N(7)-N(8)-C(2)	-0.4(7)	N(15)-N(16)-C(4)-C(3)	177.7(5)
O(3)-N(9)-N(10)-N(11)	-178.8(5)	O(4)-N(13)-C(4)-N(16)	-178.9(5)
C(3)-N(9)-N(10)-N(11)	-1.5(6)	N(14)-N(13)-C(4)-N(16)	0.4(6)
N(9)-N(10)-N(11)-N(12)	2.1(6)	O(4)-N(13)-C(4)-C(3)	2.5(9)
N(10)-N(11)-N(12)-C(3)	-1.8(6)	N(14)-N(13)-C(4)-C(3)	-178.2(5)
O(4)-N(13)-N(14)-N(15)	179.6(5)	N(9)-C(3)-C(4)-N(16)	3.3(10)
C(4)-N(13)-N(14)-N(15)	0.2(6)	N(12)-C(3)-C(4)-N(16)	-173.4(6)

N(13)-N(14)-N(15)-N(16)	-0.7(6)	N(9)-C(3)-C(4)-N(13)	-178.3(6)
N(14)-N(15)-N(16)-C(4)	1.0(6)	N(12)-C(3)-C(4)-N(13)	5.0(9)
N(3)-N(4)-C(1)-N(1)	0.1(6)	C(6)-N(18)-C(5)-O(5)	-14.7(9)
N(3)-N(4)-C(1)-C(2)	178.6(5)	C(6)-N(18)-C(5)-N(17)	164.3(5)
O(1)-N(1)-C(1)-N(4)	-179.0(5)	C(5)-N(18)-C(6)-N(20)	-0.4(9)
N(2)-N(1)-C(1)-N(4)	0.4(6)	C(5)-N(18)-C(6)-N(19)	-178.7(5)
O(1)-N(1)-C(1)-C(2)	2.5(9)	C(8)-N(22)-C(7)-O(6)	11.4(8)
N(2)-N(1)-C(1)-C(2)	-178.1(5)	C(8)-N(22)-C(7)-N(21)	-170.4(5)
O(2)-N(5)-C(2)-N(8)	177.0(5)	C(7)-N(22)-C(8)-N(23)	174.8(5)
N(6)-N(5)-C(2)-N(8)	-1.0(6)	C(7)-N(22)-C(8)-N(24)	-4.4(8)
O(2)-N(5)-C(2)-C(1)	-3.5(9)	C(10)-N(26)-C(9)-O(7)	0.1(9)
N(6)-N(5)-C(2)-C(1)	178.6(5)	C(10)-N(26)-C(9)-N(25)	178.2(5)
N(7)-N(8)-C(2)-N(5)	0.9(6)	C(9)-N(26)-C(10)-N(27)	179.9(5)
N(7)-N(8)-C(2)-C(1)	-178.7(5)	C(9)-N(26)-C(10)-N(28)	-0.6(9)
N(4)-C(1)-C(2)-N(5)	-0.2(9)	C(12)-N(30)-C(11)-O(8)	3.8(9)
N(1)-C(1)-C(2)-N(5)	178.0(6)	C(12)-N(30)-C(11)-N(29)	-177.1(6)
N(4)-C(1)-C(2)-N(8)	179.3(6)	C(11)-N(30)-C(12)-N(32)	-1.6(9)
N(1)-C(1)-C(2)-N(8)	-2.5(9)	C(11)-N(30)-C(12)-N(31)	178.8(5)

Table 30. Hydrogen bonds for **10·4H_2O**.

D-H...A	Symmetry	d(D-H)	d(H...A)	d(D...A)	<(DHA
O1W-H1WD...O5		2.204	3.165	179.64	2.204
O1W-H1WD...N20		2.626	3.14	113.93	2.626
O2W-H2WD...N15	x+1, y, z	2.566	3.124	117.23	2.566
O2W-H2WB...O8	x+1, y-1, z	2.549	3.177	123.2	2.549
O3W-H3WD...O6		2.209	3.169	179.57	2.209
N17-H17A...O6	x, y-1, z	2.086	2.954	168.69	2.086
N17-H17B...N7		2.126	2.985	165.32	2.126
N17-H17B...N8		2.673	3.409	141.98	2.673
N18-H18A...N8		2.028	2.889	165.2	2.028
N18-H18A...N7		2.657	3.358	137.32	2.657
N19-H19A...O4	x+1, y, z-1	2.031	2.896	167.28	2.031
N19-H19B...O1		2.006	2.763	143.5	2.006
N20-H20A...N14	x+1, y, z-1	2.133	2.985	162.78	2.133
N20-H20B...O5		2.006	2.645	128.41	2.006
N20-H20B...O1W		2.439	3.14	136.93	2.439
N21-H21A...O5	x, y+1, z	1.957	2.835	174.52	1.957
N21-H21B...N3	x-1, y, z	2.203	3.067	167.35	2.203
N21-H21B...N4	x-1, y, z	2.464	3.25	149	2.464
N22-H22A...N4	x-1, y, z	2.185	3.024	159.39	2.185

N23-H23A...O3	x-1, y, z	2.125	2.976	162.69	2.125
N23-H23A...N10	x-1, y, z	2.669	3.379	138.56	2.669
N23-H23B...O2	x-1, y, z	2.016	2.711	135.07	2.016
N24-H24A...N10	x-1, y, z	2.146	2.986	159.69	2.146
N24-H24B...O6		1.969	2.628	130.76	1.969
N24-H24B...O4W		2.533	3.122	125.05	2.533
N25-H25A...O8	x+1, y-1, z	1.955	2.832	175.28	1.955
N25-H25B...N16		2.416	3.119	137.06	2.416
N25-H25B...N15	x+1, y, z	2.511	3.217	137.65	2.511
N26-H26A...N16		2.331	3.047	138.54	2.331
N26-H26A...O3		2.362	3.081	139	2.362
N27-H27A...O2	x-1, y, z	1.988	2.85	166.35	1.988
N27-H27B...O3		1.988	2.786	150.15	1.988
N28-H28A...N6	x-1, y, z	2.153	3.008	163.94	2.153
N28-H28B...O7		1.999	2.646	129.43	1.999
N28-H28B...O3W	x+1, y-1, z	2.618	3.188	123.43	2.618
N29-H29A...O7	x-1, y+1, z	2.031	2.903	171.51	2.031
N29-H29B...N11	x-1, y, z	2.242	3.044	151.33	2.242
N30-H30A...N12		2.14	2.897	143.66	2.14
N31-H31A...O1	x, y, z+1	1.968	2.838	170.83	1.968
N31-H31B...O4		2.012	2.848	158.09	2.012
N32-H32A...N2	x, y, z+1	2.186	3.061	172.83	2.186
N32-H32B...O8		2.007	2.647	128.56	2.007
N32-H32B...O2W	x-1, y+1, z	2.479	3.216	141.69	2.479

2 Differential scanning calorimetry (DSC) curves of compounds 2-11

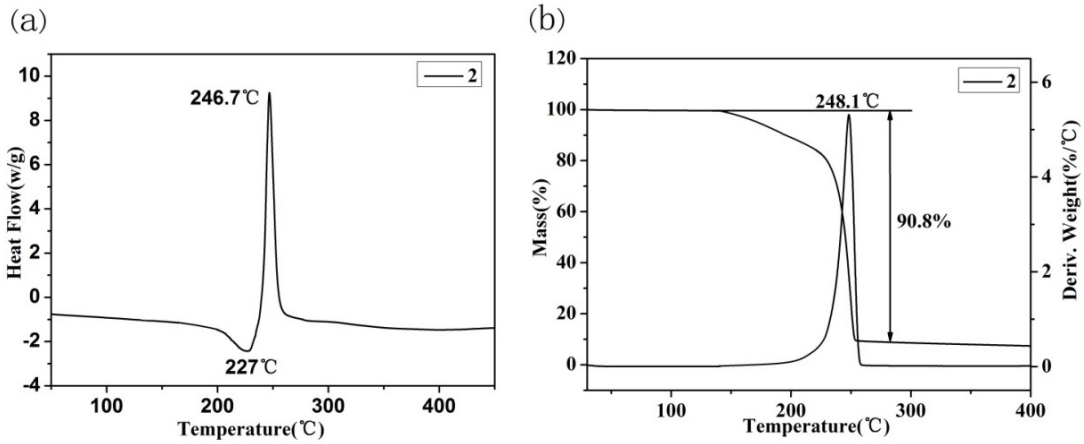

Fig. S3 DSC (a) and TG-DTG (b) curves of **2** under nitrogen with a heating rate of 10℃ min^{-1}.

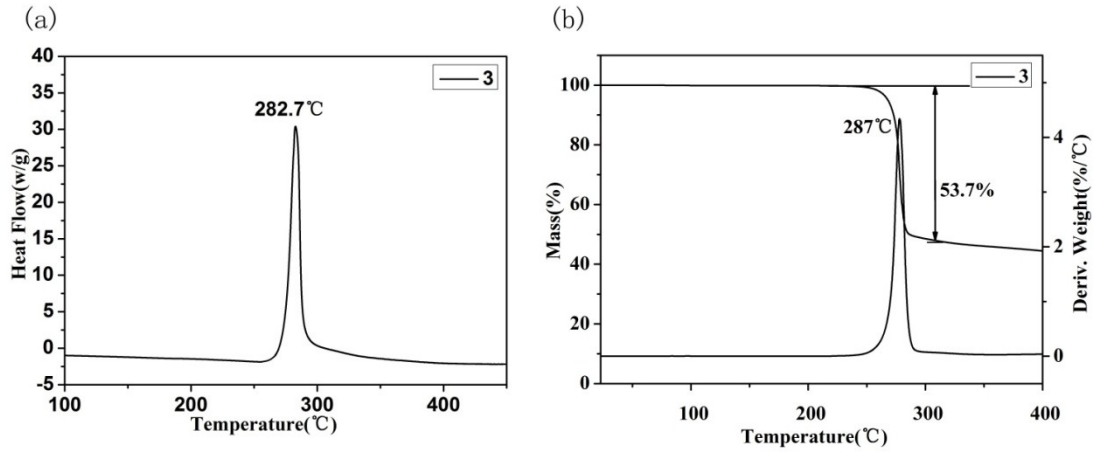

Fig. S4 DSC (a) and TG-DTG (b) curves of **3** under nitrogen with a heating rate of 10℃ min^{-1}.

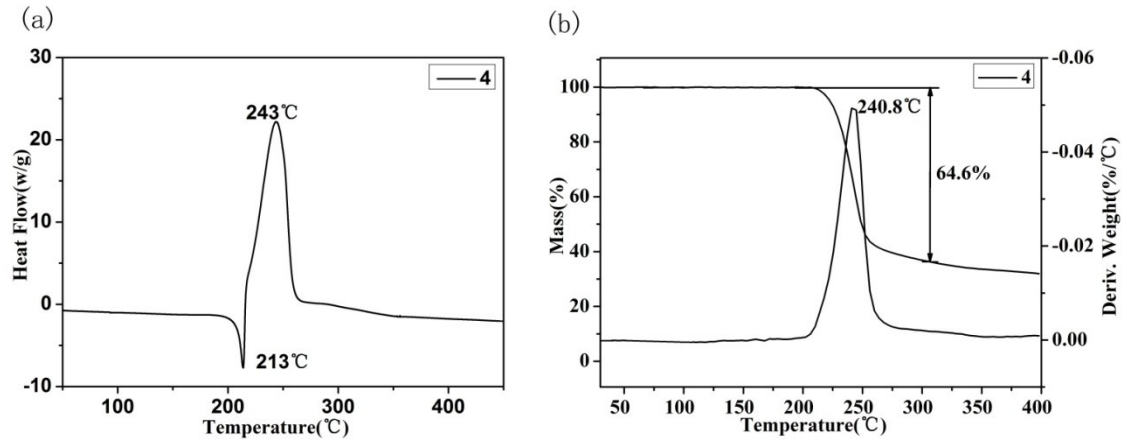

Fig. S5 DSC (a) and TG-DTG (b) curves of **4** under nitrogen with a heating rate of 10℃ min^{-1}.

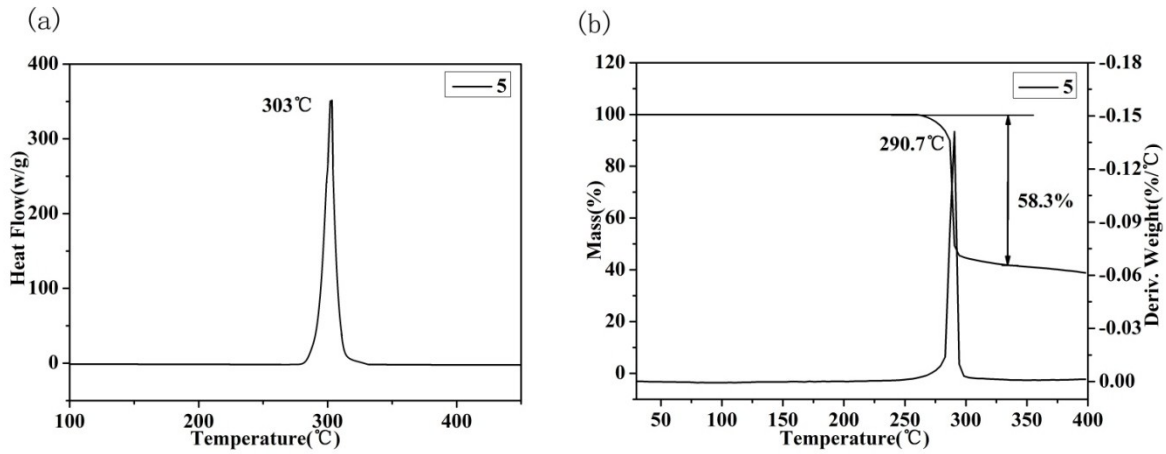

Fig. S6 DSC (a) and TG-DTG (b) curves of **5** under nitrogen with a heating rate of 10℃ min^{-1}.

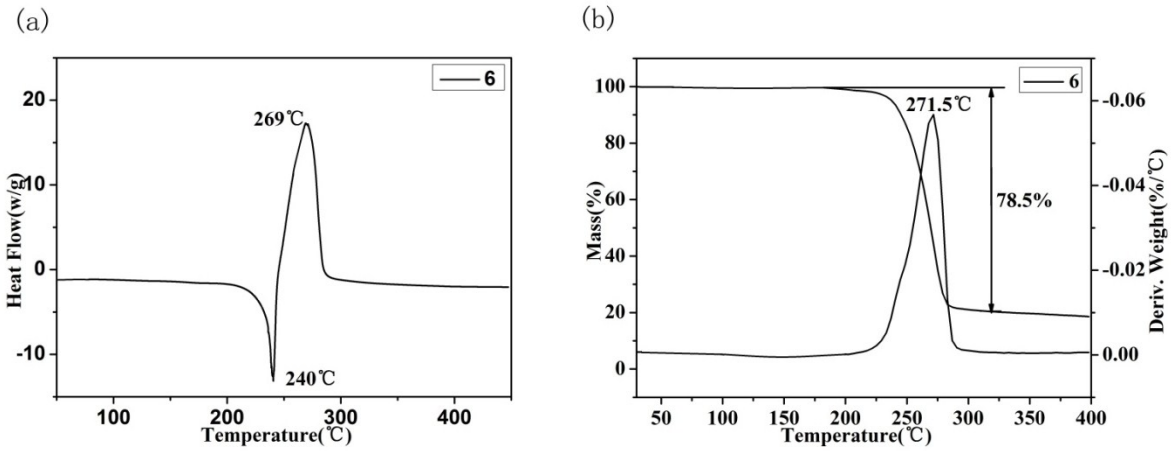

Fig. S7 DSC (a) and TG-DTG (b) curves of **6** under nitrogen with a heating rate of 10℃ min^{-1}.

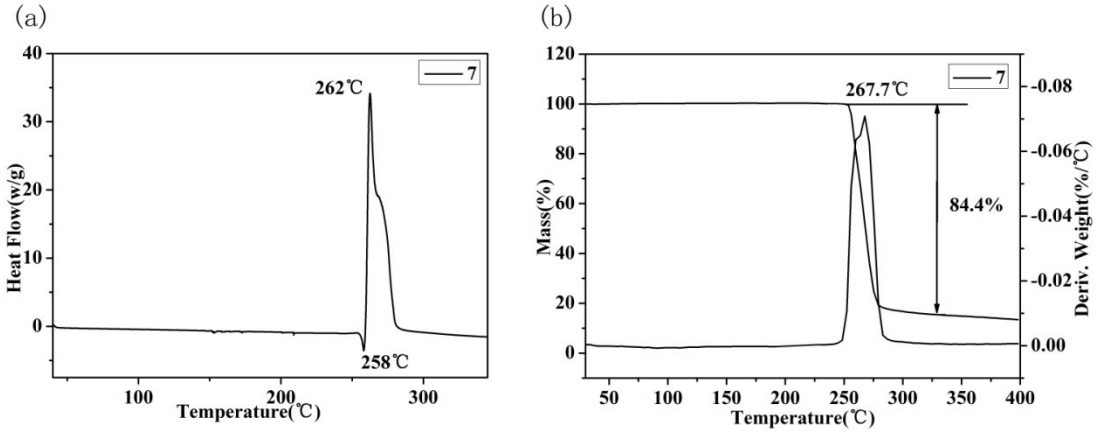

Fig. S8 DSC (a) and TG-DTG (b) curves of **7** under nitrogen with a heating rate of 10℃ min^{-1}.

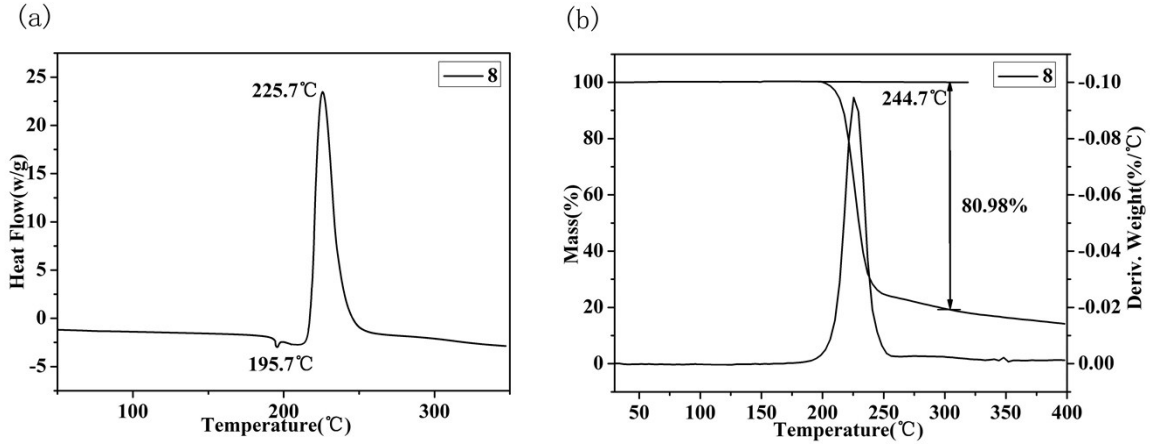

Fig. S9 DSC (a) and TG-DTG (b) curves of **8** under nitrogen with a heating rate of 10℃ min^{-1}.

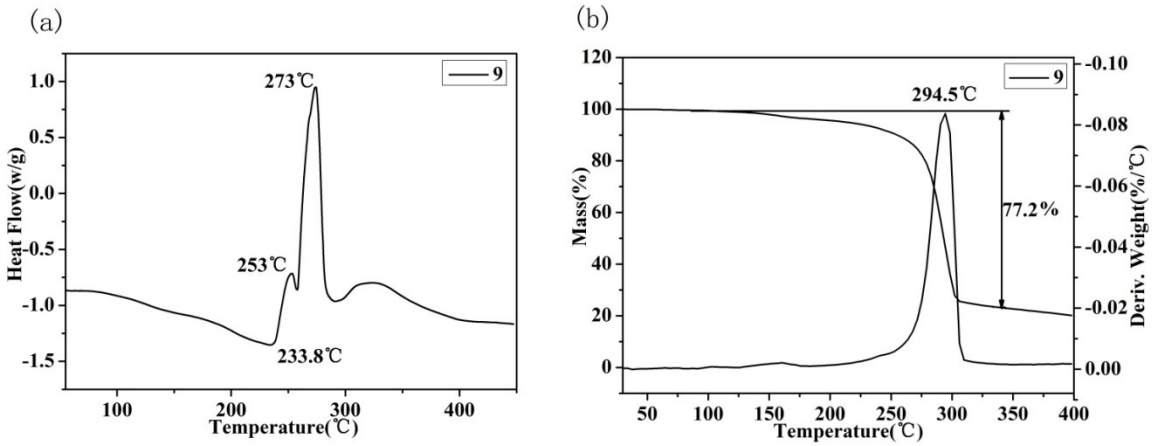

Fig. S10 DSC (a) and TG-DTG (b) curves of **9** under nitrogen with a heating rate of 10℃ min^{-1}.

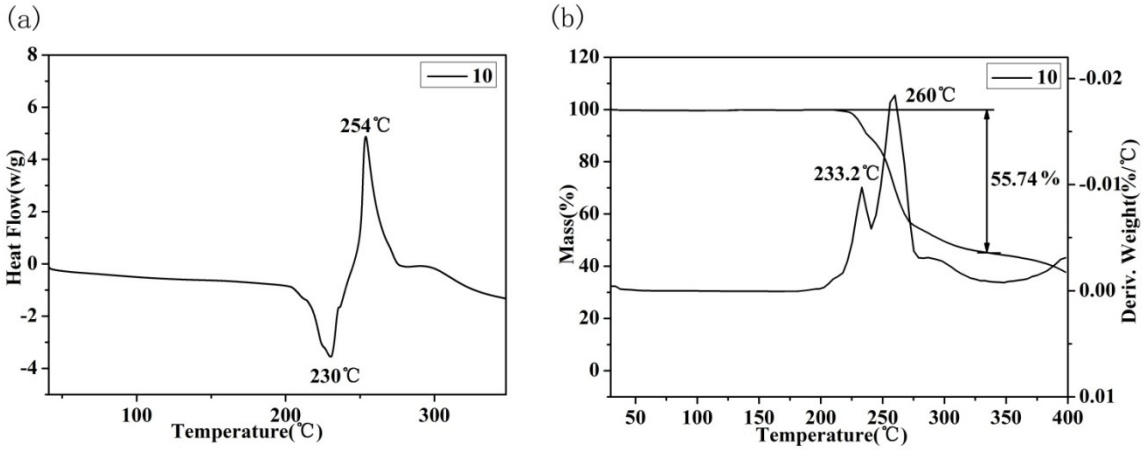

Fig. S11 DSC (a) and TG-DTG (b) curves of **10** under nitrogen with a heating rate of 10℃ min^{-1}.

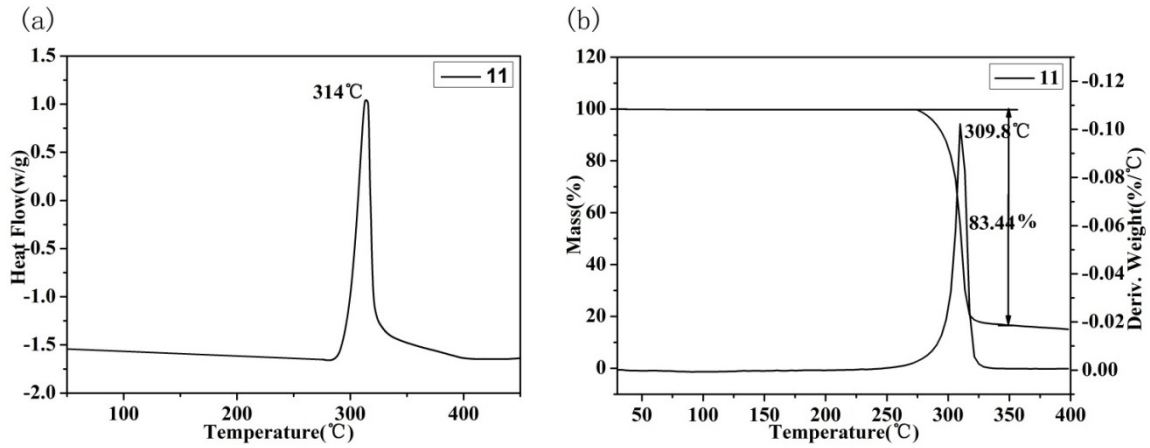

Fig. S12 DSC (a) and TG-DTG (b) curves of **11** under nitrogen with a heating rate of 10℃ min^{-1}.

Table 31. Calculated (B3LYP/6–31++G**//MP2/6–311++G**) total energy (E_0), zero-point energy (ZPE), values of thermal correction (H_T), and heats of formation (HOF) of the selected cations.

Name	E_0 (hartree)	ZPE (hartree)	H_T (hartree)	HOF (KJ/mol)
2-Methylimidazolium	−265. 88394	0. 112643	0. 00656	672. 4

3-Amino-5-hydroxypyrazole	−356. 2904875	0. 103155	0. 007978	1010. 7
2,4-Diamino-6-methyl-1,3,5-triazolium	−429. 7455464	0. 139818	0. 009678	648. 0
Imidazolium	−226. 569963	0. 076644	0. 005204	723.0
Pyrazolium	−225. 9694035	0.084265	0. 004987	821. 5
triazine	−279. 666076	0.065360	0. 005066	225.9[1]
CH_4	−40. 3796274	0. 047228	0. 003798	-74.6[2]
NH_3	−56. 4154673	0.034381	0. 003817	-45.9[2]
NH_4^+	−56. 7556705	0.049701	0. 003796	626.4[3]
CH_3CH_3	−79. 5716379	0. 074594	0. 004429	-84.7[2]
CH_3NH_2	−95. 5938475	0.064013	0. 004374	-23.0[2]
CH_3OH	−115. 4432398	0.051674	0. 003898	201.5[4]

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