

Electronic Supplementary Information

Why can't *cyclo*-pentazolate anion in Oxone solution be *N*-oxidized?

Ze Xu,[‡] Shuaijie Jiang,[‡] Tianyang Hou, Xiaopeng Zhang, Ming Lu* and Yuangang Xu*

School of Chemistry and Chemical Engineering, Nanjing University of Science and
Technology, Nanjing 210094, Jiangsu, China

[‡] These authors contributed equally.

E-mail: luming@njust.edu.cn; yuangangxu@163.com

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1. Single-crystal X-ray diffraction analysis

Table S1. Crystal data, data collection, and refinement for compound **1**

$C_4H_7N_5Na_2O_4$	$Z = 2$
$M_r = 235.13$	$F(000) = 240$
Triclinic, $P\bar{1}$	$D_x = 1.709 \text{ Mg m}^{-3}$
$a = 6.8450 (7) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 7.2316 (7) \text{ \AA}$	Cell parameters from 3422 reflections
$c = 10.2686 (10) \text{ \AA}$	$\theta = 3.0\text{--}27.5^\circ$
$\alpha = 71.886 (4)^\circ$	$\mu = 0.22 \text{ mm}^{-1}$
$\beta = 71.147 (4)^\circ$	$T = 100 \text{ K}$
$\gamma = 82.079 (4)^\circ$	Plate, colourless
$V = 456.80 (8) \text{ \AA}^3$	$0.12 \times 0.05 \times 0.04 \text{ mm}$
Bruker APEX-II CCD diffractometer	1818 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.0^\circ$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(\text{int})$ was 0.0690 before and 0.0456 after correction. The Ratio of minimum to maximum transmission is 0.9149. The $\lambda/2$ correction factor is Not present.	$h = -8?8$
$T_{\min} = 0.849$, $T_{\max} = 0.928$	$k = -9?9$
2047 measured reflections	$l = -9?13$
2047 independent reflections	
Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 0.6514P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{\max} < 0.001$
2047 reflections	$\Delta\rho_{\max} = 0.34 \text{ e \AA}^{-3}$
140 parameters	$\Delta\rho_{\min} = -0.36 \text{ e \AA}^{-3}$
0 restraints	

Table S2. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for compound **1**

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Na2	1.03809 (13)	0.80008 (12)	0.84582 (9)	0.0136 (2)
Na1	0.87369 (13)	0.78441 (12)	0.55587 (9)	0.0141 (2)
O2	0.1927 (2)	0.8741 (2)	0.57720 (16)	0.0149 (3)
O3	0.7198 (2)	0.8052 (2)	0.80269 (16)	0.0175 (3)
O1	0.5075 (2)	0.7556 (2)	0.59000 (16)	0.0173 (3)
O4	0.3885 (2)	0.7630 (3)	0.83878 (17)	0.0204 (4)
H4	0.433535	0.757480	0.753611	0.031*
N2	0.9590 (3)	0.8367 (3)	0.19393 (19)	0.0154 (4)
N3	0.9538 (3)	0.7272 (3)	0.11261 (19)	0.0155 (4)
N1	0.9759 (3)	0.7184 (3)	0.31793 (19)	0.0152 (4)
N4	0.9667 (3)	0.5424 (3)	0.18661 (19)	0.0167 (4)
N5	0.9824 (3)	0.5373 (3)	0.3133 (2)	0.0173 (4)
C1	0.3666 (3)	0.8029 (3)	0.5258 (2)	0.0135 (4)
C3	0.5418 (3)	0.7757 (3)	0.8832 (2)	0.0156 (4)
C2	0.4247 (4)	0.7627 (3)	0.3829 (2)	0.0188 (5)
H2A	0.435008	0.621688	0.397075	0.028*
H2B	0.558266	0.818614	0.323217	0.028*
H2C	0.318938	0.821468	0.335222	0.028*
C4	0.4870 (4)	0.7491 (4)	1.0416 (2)	0.0243 (5)
H4A	0.607323	0.774423	1.064569	0.036*
H4B	0.445420	0.615311	1.094138	0.036*
H4C	0.372622	0.840265	1.069613	0.036*

Table S3. Atomic displacement parameters (\AA^2) for compound **1**

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na2	0.0139 (4)	0.0157 (4)	0.0112 (4)	-0.0013 (3)	-0.0037 (3)	-0.0034 (3)
Na1	0.0154 (4)	0.0153 (4)	0.0116 (4)	-0.0002 (3)	-0.0046 (3)	-0.0033 (3)
O2	0.0138 (8)	0.0163 (8)	0.0131 (7)	-0.0008 (6)	-0.0031 (6)	-0.0030 (6)
O3	0.0158 (8)	0.0220 (8)	0.0154 (7)	-0.0001 (6)	-0.0052 (6)	-0.0059 (6)
O1	0.0151 (8)	0.0231 (8)	0.0151 (7)	-0.0002 (6)	-0.0063 (6)	-0.0059 (6)
O4	0.0156 (8)	0.0332 (10)	0.0134 (7)	-0.0017 (7)	-0.0041 (6)	-0.0080 (7)

N2	0.0150 (9)	0.0178 (9)	0.0128 (8)	-0.0007 (7)	-0.0037 (7)	-0.0041 (7)
N3	0.0155 (9)	0.0177 (9)	0.0129 (8)	-0.0012 (7)	-0.0048 (7)	-0.0032 (7)
N1	0.0157 (9)	0.0155 (9)	0.0135 (8)	-0.0015 (7)	-0.0033 (7)	-0.0035 (7)
N4	0.0199 (10)	0.0174 (9)	0.0136 (9)	-0.0001 (7)	-0.0075 (7)	-0.0035 (7)
N5	0.0209 (10)	0.0172 (9)	0.0145 (9)	-0.0025 (7)	-0.0064 (7)	-0.0035 (7)
C1	0.0173 (11)	0.0104 (9)	0.0118 (9)	-0.0036 (8)	-0.0044 (8)	-0.0002 (8)
C3	0.0154 (11)	0.0183 (11)	0.0143 (10)	0.0027 (8)	-0.0055 (8)	-0.0064 (8)
C2	0.0187 (12)	0.0248 (12)	0.0145 (10)	-0.0002 (9)	-0.0056 (9)	-0.0070 (9)
C4	0.0225 (12)	0.0360 (14)	0.0145 (11)	-0.0022 (10)	-0.0049 (9)	-0.0076 (10)

Table S4. Geometric parameters (Å, °) for compound **1**

Na2—Na1	3.5432 (12)	O1—C1	1.289 (3)
Na2—Na1 ⁱ	4.1941 (12)	O4—H4	0.8400
Na2—O2 ⁱⁱ	2.5232 (17)	O4—C3	1.296 (3)
Na2—O3	2.3526 (18)	N2—N3	1.328 (3)
Na2—O4 ⁱⁱ	2.3565 (18)	N2—N1	1.325 (3)
Na2—N2 ⁱ	2.532 (2)	N3—N4	1.323 (3)
Na2—N3 ⁱⁱⁱ	2.506 (2)	N1—N5	1.320 (3)
Na2—N4 ^{iv}	2.605 (2)	N4—N5	1.328 (3)
Na1—Na1 ⁱ	3.4653 (17)	C1—C2	1.500 (3)
Na1—O2 ⁱⁱ	2.4546 (18)	C3—C4	1.502 (3)
Na1—O2 ^v	2.4829 (17)	C2—H2A	0.9800
Na1—O3	2.4544 (18)	C2—H2B	0.9800
Na1—O1	2.4454 (18)	C2—H2C	0.9800
Na1—N1	2.493 (2)	C4—H4A	0.9800
Na1—N5 ^{iv}		C4—H4B	0.9800
O2—C1	1.247 (3)	C4—H4C	0.9800
O3—C3	1.235 (3)		
Na1—Na2—Na1 ⁱ	52.39 (3)	O1—Na1—N1	91.89 (6)
O2 ⁱⁱ —Na2—Na1 ⁱ	32.79 (4)	O1—Na1—N5 ^{iv}	109.31 (7)
O2 ⁱⁱ —Na2—Na1	43.85 (4)	N1—Na1—Na2	146.29 (6)
O2 ⁱⁱ —Na2—N2 ⁱ	85.87 (6)	N1—Na1—Na2 ⁱ	53.38 (5)
O2 ⁱⁱ —Na2—N4 ^{iv}	79.68 (6)	N1—Na1—Na1 ⁱ	97.39 (6)
O3—Na2—Na1 ⁱ	77.83 (5)	N1—Na1—N5 ^{iv}	96.15 (7)

O3—Na2—Na1	43.64 (4)	N5 ^{iv} —Na1—Na2	64.85 (5)
O3—Na2—O2 ⁱⁱ	85.51 (6)	N5 ^{iv} —Na1—Na2 ⁱ	143.14 (5)
O3—Na2—O4 ⁱⁱ	165.49 (7)	N5 ^{iv} —Na1—Na1 ⁱ	122.26 (6)
O3—Na2—N2 ⁱ	96.12 (6)	Na1 ^v —O2—Na2 ^{vi}	113.82 (6)
O3—Na2—N3 ⁱⁱⁱ	105.37 (7)	Na1 ^{vi} —O2—Na2 ^{vi}	90.75 (6)
O3—Na2—N4 ^{iv}	76.35 (6)	Na1 ^{vi} —O2—Na1 ^v	89.15 (6)
O4 ⁱⁱ —Na2—Na1 ⁱ	95.94 (5)	C1—O2—Na2 ^{vi}	119.84 (13)
O4 ⁱⁱ —Na2—Na1	122.45 (5)	C1—O2—Na1 ^{vi}	123.08 (14)
O4 ⁱⁱ —Na2—O2 ⁱⁱ	82.39 (6)	C1—O2—Na1 ^v	114.60 (13)
O4 ⁱⁱ —Na2—N2 ⁱ	90.98 (7)	Na2—O3—Na1	94.94 (6)
O4 ⁱⁱ —Na2—N3 ⁱⁱⁱ	86.82 (6)	C3—O3—Na2	132.68 (14)
O4 ⁱⁱ —Na2—N4 ^{iv}	93.56 (7)	C3—O3—Na1	129.90 (14)
N2 ⁱ —Na2—Na1	101.58 (5)	C1—O1—Na1	143.36 (14)
N2 ⁱ —Na2—Na1 ⁱ	55.86 (4)	Na2 ^{vi} —O4—H4	95.1
N2 ⁱ —Na2—N4 ^{iv}	164.13 (7)	C3—O4—Na2 ^{vi}	153.78 (14)
N3 ⁱⁱⁱ —Na2—Na1	146.53 (6)	C3—O4—H4	109.5
N3 ⁱⁱⁱ —Na2—Na1 ⁱ	148.64 (5)	N3—N2—Na2 ⁱ	134.03 (14)
N3 ⁱⁱⁱ —Na2—O2 ⁱⁱ	169.12 (7)	N1—N2—Na2 ⁱ	118.16 (14)
N3 ⁱⁱⁱ —Na2—N2 ⁱ	92.95 (6)	N1—N2—N3	107.72 (17)
N3 ⁱⁱⁱ —Na2—N4 ^{iv}	102.48 (7)	N2—N3—Na2 ^{vii}	131.33 (14)
N4 ^{iv} —Na2—Na1	63.29 (5)	N4—N3—Na2 ^{vii}	117.06 (13)
N4 ^{iv} —Na2—Na1 ⁱ	108.48 (5)	N4—N3—N2	108.07 (17)
Na2—Na1—Na2 ⁱ	127.61 (3)	N2—N1—Na1	128.45 (14)
Na1 ⁱ —Na1—Na2 ⁱ	54.10 (3)	N5—N1—Na1	119.09 (13)
Na1 ⁱ —Na1—Na2	73.51 (3)	N5—N1—N2	108.31 (17)
O2 ^v —Na1—Na2	107.33 (5)	N3—N4—Na2 ^{iv}	138.11 (14)
O2 ⁱⁱ —Na1—Na2	45.40 (4)	N3—N4—N5	107.94 (17)
O2 ^v —Na1—Na2 ⁱ	33.39 (4)	N5—N4—Na2 ^{iv}	113.94 (13)
O2 ⁱⁱ —Na1—Na2 ⁱ	90.96 (4)	N1—N5—Na1 ^{iv}	133.89 (14)
O2 ^v —Na1—Na1 ⁱ	45.10 (4)	N1—N5—N4	107.95 (17)
O2 ⁱⁱ —Na1—Na1 ⁱ	45.76 (4)	N4—N5—Na1 ^{iv}	114.57 (14)
O2 ⁱⁱ —Na1—O2 ^v	90.85 (6)	O2—C1—O1	123.64 (19)
O2 ^v —Na1—N1	85.48 (6)	O2—C1—C2	121.33 (19)
O2 ⁱⁱ —Na1—N1	105.15 (6)	O1—C1—C2	115.03 (19)

O2 ⁱⁱ —Na1—N5 ^{iv}	76.52 (6)	O3—C3—O4	123.1 (2)
O2 ^v —Na1—N5 ^{iv}	167.28 (7)	O3—C3—C4	122.2 (2)
O3—Na1—Na2 ⁱ	132.76 (5)	O4—C3—C4	114.7 (2)
O3—Na1—Na2	41.42 (4)	C1—C2—H2A	109.5
O3—Na1—Na1 ⁱ	93.15 (5)	C1—C2—H2B	109.5
O3—Na1—O2 ^v	99.51 (6)	C1—C2—H2C	109.5
O3—Na1—O2 ⁱⁱ	84.87 (6)	H2A—C2—H2B	109.5
O3—Na1—N1	168.84 (7)	H2A—C2—H2C	109.5
O3—Na1—N5 ^{iv}	81.20 (6)	H2B—C2—H2C	109.5
O1—Na1—Na2	120.03 (5)	C3—C4—H4A	109.5
O1—Na1—Na2 ⁱ	93.56 (4)	C3—C4—H4B	109.5
O1—Na1—Na1 ⁱ	125.93 (6)	C3—C4—H4C	109.5
O1—Na1—O2 ⁱⁱ	161.49 (6)	H4A—C4—H4B	109.5
O1—Na1—O2 ^v	83.20 (6)	H4A—C4—H4C	109.5
O1—Na1—O3	78.90 (6)	H4B—C4—H4C	109.5
Na2 ^{vi} —O2—C1—O1	-27.3 (3)	Na1 ^{vi} —O2—C1—C2	38.6 (3)
Na2 ^{vi} —O2—C1—C2	151.63 (16)	Na1—O3—C3—O4	-14.0 (3)
Na2—O3—C3—O4	-171.51 (15)	Na1—O3—C3—C4	165.19 (16)
Na2—O3—C3—C4	7.7 (3)	Na1—O1—C1—O2	-132.4 (2)
Na2 ^{vi} —O4—C3—O3	-148.8 (3)	Na1—O1—C1—C2	48.7 (3)
Na2 ^{vi} —O4—C3—C4	32.0 (4)	Na1—N1—N5—Na1 ^{iv}	-45.2 (2)
Na2 ⁱ —N2—N3—Na2 ^{vii}	19.0 (3)	Na1—N1—N5—N4	158.18 (14)
Na2 ⁱ —N2—N3—N4	176.55 (15)	N2—N3—N4—Na2 ^{iv}	177.67 (16)
Na2 ⁱ —N2—N1—Na1	26.9 (2)	N2—N3—N4—N5	-0.7 (2)
Na2 ⁱ —N2—N1—N5	-176.62 (13)	N2—N1—N5—Na1 ^{iv}	155.81 (16)
Na2 ^{vii} —N3—N4—Na2 ^{iv}	-21.1 (3)	N2—N1—N5—N4	-0.8 (2)
Na2 ^{vii} —N3—N4—N5	160.47 (14)	N3—N2—N1—Na1	-156.07 (14)
Na2 ^{iv} —N4—N5—Na1 ^{iv}	20.44 (18)	N3—N2—N1—N5	0.4 (2)
Na2 ^{iv} —N4—N5—N1	-177.86 (13)	N3—N4—N5—Na1 ^{iv}	-160.73 (14)
Na1 ^{vi} —O2—C1—O1	-140.31 (17)	N3—N4—N5—N1	1.0 (2)
Na1 ^v —O2—C1—O1	113.51 (19)	N1—N2—N3—Na2 ^{vii}	-157.32 (15)
Na1 ^v —O2—C1—C2	-67.6 (2)	N1—N2—N3—N4	0.2 (2)

Symmetry codes: (i) -x+2, -y+2, -z+1; (ii) x+1, y, z; (iii) x, y, z+1; (iv) -x+2, -y+1, -z+1; (v) -x+1, -y+2, -z+1; (vi) x-1, y, z; (vii) x, y, z-1.

Table S5. Hydrogen bonds (Å, °) for compound **1**

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4 \cdots O1	0.84	1.59	2.433 (2)	177
C4—H4A \cdots N3	0.98	2.53	3.473 (4)	161

Symmetry code: (ii) $-x, -x+y, -z+5/3$.

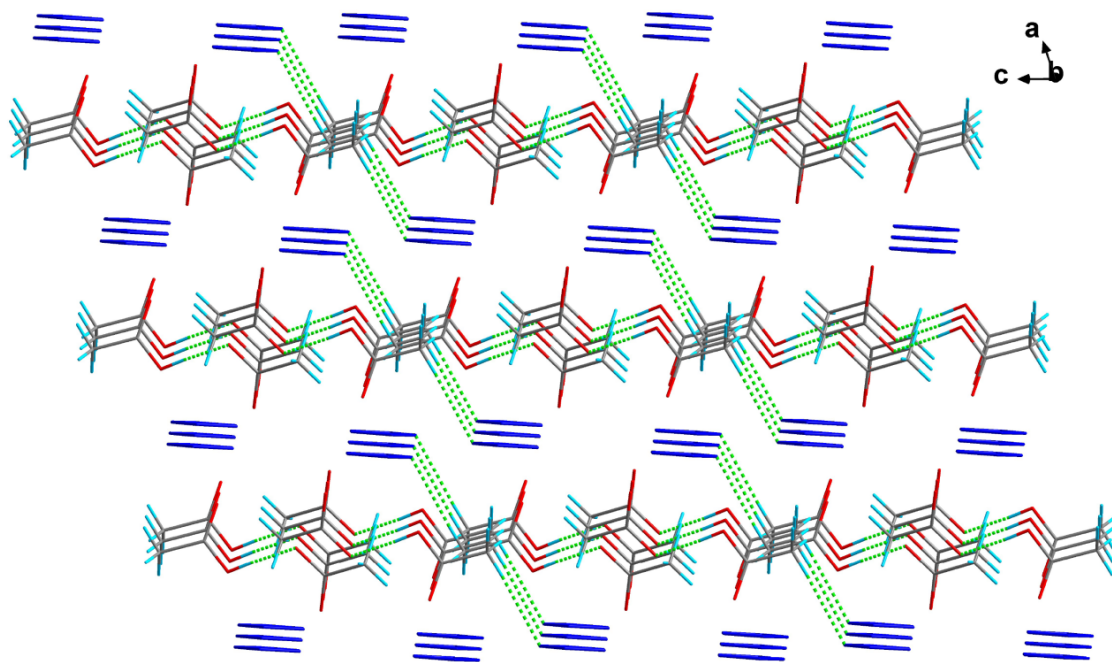


Fig. S1 Stacking diagram of **1**. Dashed lines indicate hydrogen bonding.

2. Mass spectra

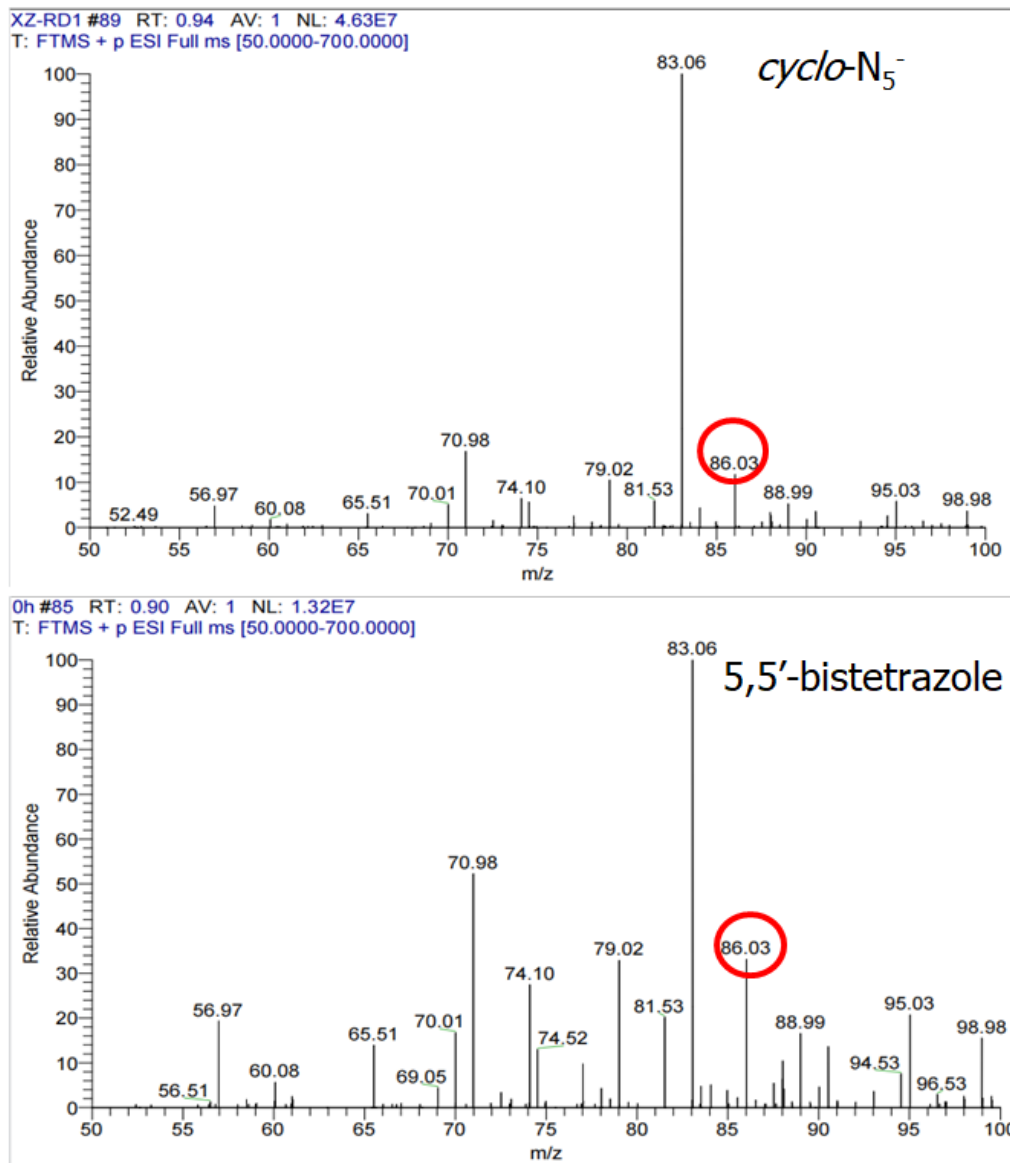


Fig. S2 The mass spectra of compound **1** and 5,5'-bistetrazole.

3. IR spectrum

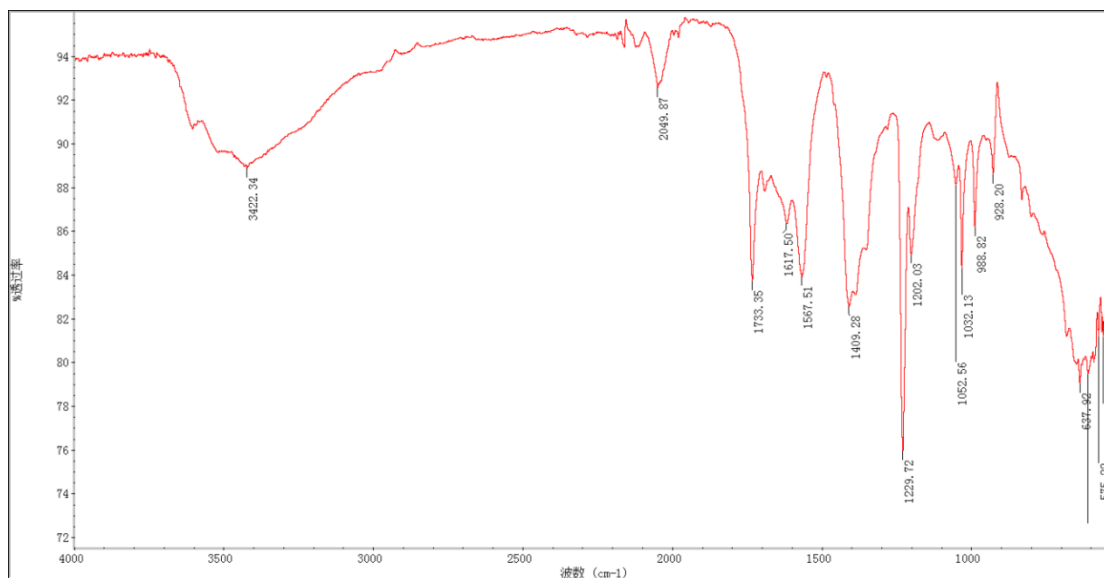


Fig. S3 The IR spectrum of compound **1**.

4. Hirshfeld surface and two-dimensional fingerprint plot

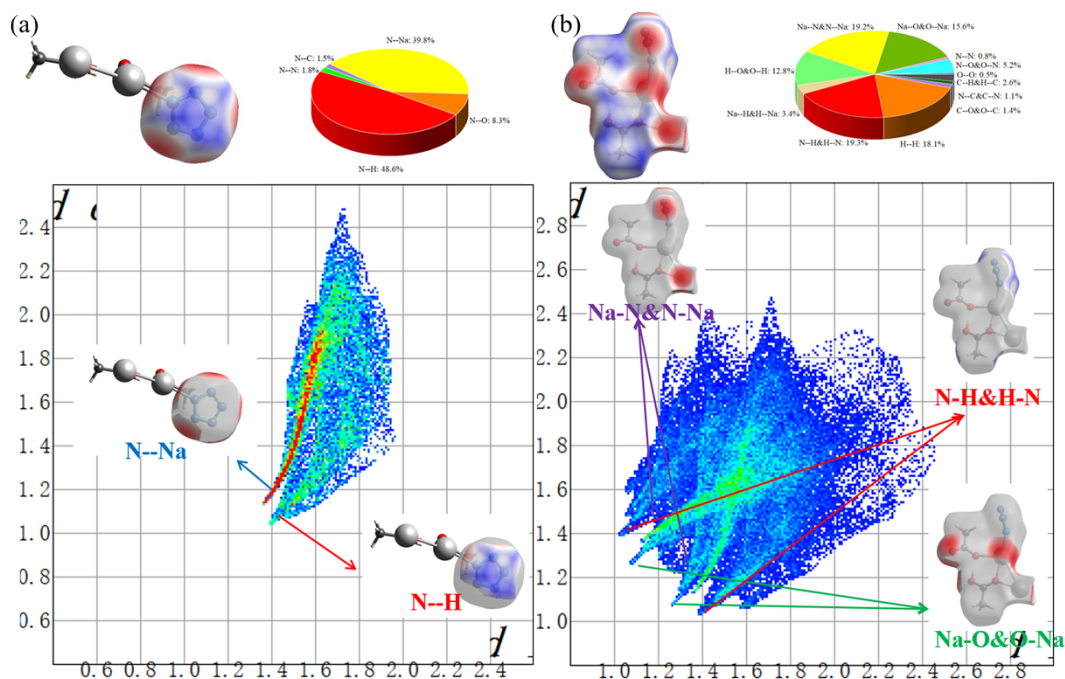


Fig. S4 (a) Hirshfeld surfaces of *cyclo-N₅⁻* in **1**, pie graph for individual atomic contacts percentage contribution to the Hirshfeld surface and two-dimensional fingerprint plot in crystal stacking for *cyclo-N₅⁻*. (b) Hirshfeld surfaces of **1**, pie graph for individual atomic contacts percentage contribution to the Hirshfeld surface and two-dimensional fingerprint plot in crystal stacking for **1**.

5. Surface electrostatic potential

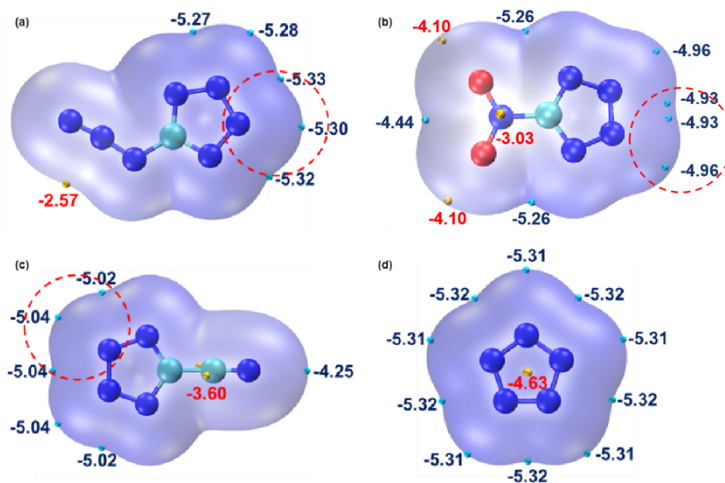


Fig. S5 Surface electrostatic potential of 5-azidotetrazolate (a), 5-nitrotetrazolate (b), 5-cyanotetrazolate (c), and *cyclo-N₅⁻* anion (d).

6. DSC curve

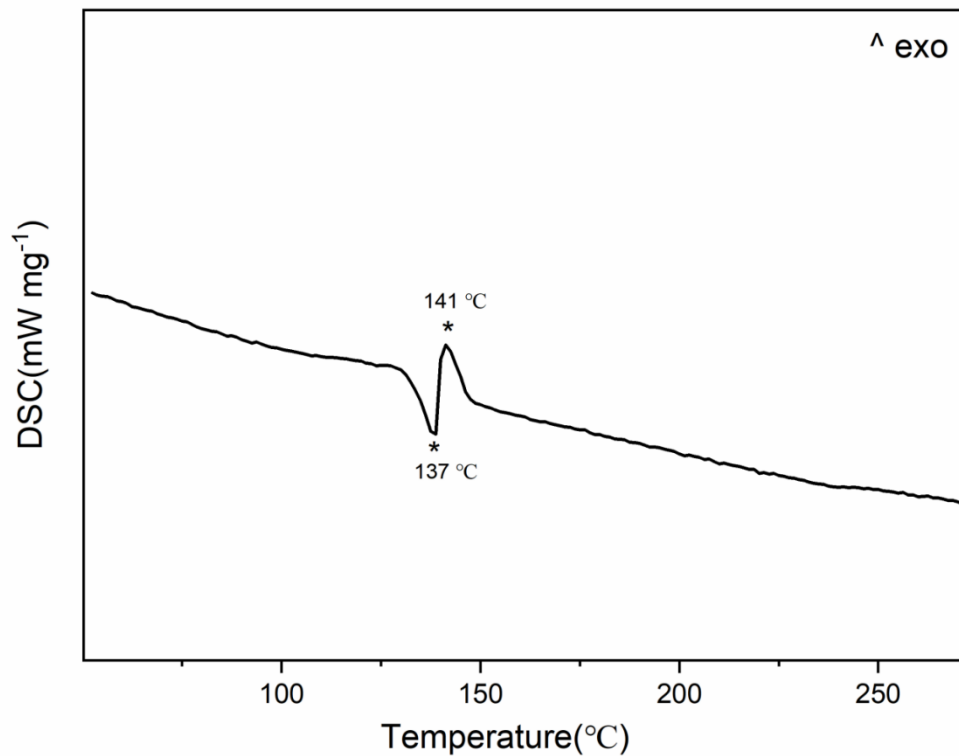


Fig. S6 The DSC curve of **1** with a heating rate of 5 K min⁻¹.

7. Experimental section

7.1 Caution

Although no explosion or hazards were observed during the preparation and handling of these energetic compounds, all the materials investigated are potentially energetic materials. Small-scale syntheses are strongly encouraged. Manipulations must be carried out in a hood behind a safety shield. Eye protection and leather gloves must be worn at all times.

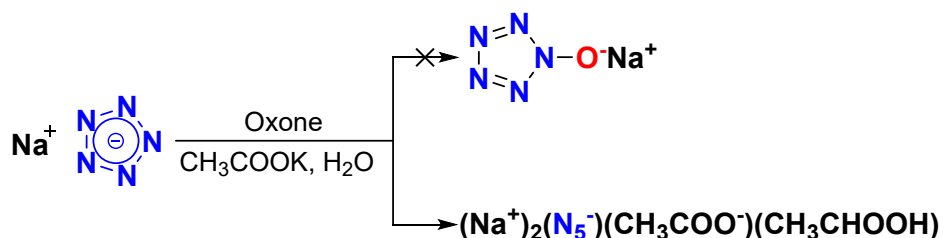
7.2 General methods

All reagents were purchased from Energy chemical in analytical grade and were used as supplied, if not stated otherwise. The decomposition (onset) points were obtained on a differential scanning calorimeter (NETZSCH DSC 204 F1 Phoenix) at a scan rate of $5\text{ }^{\circ}\text{C min}^{-1}$ in closed Al containers with a high-purity nitrogen flow of 50 mL min^{-1} . IR spectra were recorded on a Thermo Nicolet iS10 spectrometer equipped with a Thermo Scientific Smart iTR diamond ATR accessory. Elemental analyses were carried out on a vario EL III CHNOS elemental analyzer.

7.3 X-ray crystallography

A colourless needle crystal of dimensions $0.08 \times 0.05 \times 0.04\text{ mm}^3$ was mounted on a Bruker Smart Apex-II diffractometer using Mo-K α radiation ($\lambda = 0.71073\text{ \AA}$) with a graphite monochromator at 100 K. An Oxford Cobra low-temperature device was used to maintain the low temperature. Integration and scaling of intensity data was accomplished using the SAINT program¹. The structures were solved by intrinsic using SHELXT2015² and refinement was carried out by a full-matrix least-squares technique using SHELXL2014³. The hydrogen atoms were refined isotropically, and the heavy atoms were refined anisotropically. N-H and O-H hydrogens were located from different electron density maps. Data were corrected for the effects of absorption using SADABS⁴. Relevant crystal data and refinement results are summarized in Table S1.

7.4 Synthesis procedures



Scheme. S1 The oxidation of cyclo-N₅⁻.

Na(H₂O)(N₅)·2H₂O was synthesized according to our previously published procedures.⁵

Na(H₂O)(N₅)·2H₂O (0.147 g, 1 mmol) was dissolved in 5 mL of distilled water, and potassium acetate (0.86 g, 8.75 mmol) was added. The solution was stirred at room temperature, and Oxone (3.87 g, 6.3 mmol) was added slowly. After stirring of the

suspension for 20 h at 40 °C, the solution was poured into 60 mL of acetone and the precipitated salts were filtered off. After evaporation of the solvent under reduced pressure, the remaining solid was dissolved in ethanol. The insoluble residues were filtered off, and the filtrate was left for crystallization give colorless crystals of **1** 0.054 g, Yield 46 %. T_d : 139 °C. IR (ATR): 3429, 2049, 1733, 1617, 1567, 1229, 1032, 637 cm^{-1} . Elem anal. Calcd (%) for $\text{C}_4\text{H}_7\text{Na}_2\text{N}_5\text{O}_4$ (MW = 235.11): C 20.43, N 29.79, H 3.00; Found: C 20.35, N 29.86, H 2.92.

8. Computational methods

8.1 Geometric optimization and energy evaluation

All initial geometries involved in this study were optimized using the M06-2X density functional method⁶ with Grimme's DFT-D3 dispersion correction⁷, in combination with the def2-SVP basis set⁸. The thermodynamic correction energies for all configurations were obtained by harmonic frequency calculations at M06-2X-D3/def2-SVP based on the geometry optimized at the same level and at the experimental temperature 40 °C. Solvent effects were implicitly taken into account by means of solvation model based on density (SMD) method⁹ with water. The zero-point energies were scaled by a factor of 0.9700 to reduce the systematic error and account for the anharmonic effect. The reactant (R1) and product (P1) configurations having no imaginary frequency, and transition state (TS1) having one imaginary mode. Above calculations were performed using Gaussian 09 suite of program¹⁰. The energy of all the optimized configurations was evaluated using the double-hybrid functional PWPB95¹¹ in conjunction with a very large basis set, def2-QZVPP⁸, and SMD method with water were employed. The accuracy of the PWPB95-D3(BJ)/def2-QZVPP level is very close to the well-recognized gold standard CCSD(T)/CBS.¹² Therefore, ORCA 5.0.1¹³ was used to perform PWPB95-D3(BJ) calculations, and to reduce the computational time, the resolution-of-identity (RI) technique¹⁴ was used to accelerate both the self-consistent field (SCF) process and second-order perturbative correction part. The loss of accuracy owing to the RI was negligible.¹²

8.2 Wavefunction analyses

Atomic charges (ADCH), surface electrostatic potential (ESP), HOMO-LUMO orbitals, and orbital-weighted dual descriptor analyses for 5-azidotetrazolate, 5-nitrotetrazolate, 5-cyanotetrazolate, and *cyclo*-N₅⁻ anions were completed using Multiwfn 3.8¹⁵. Unless otherwise specified, default settings were used throughout the calculations. All isosurface maps were rendered by the VMD 1.9.3 program¹⁶ based on the outputs of Multiwfn. The wavefunctions used in all analyses were produced at the M062X/6-31+G(d,p) level.

8.3 Compound coordinates

Reactant

E = -1048.7530 a.u. G = -1048.8153 a.u.

S	1.98687300	-0.10901300	0.30848900
O	0.99563500	-0.89039200	1.05374700
O	2.60382900	0.99289500	1.04701300
O	2.90810300	-0.91789400	-0.49243700
O	1.09244500	0.77238500	-0.79877600
O	0.35528300	-0.11779600	-1.60714900
N	-1.96688700	-0.03673400	-0.29590200
N	-2.89990000	0.83770600	-0.56871000
N	-3.88346600	0.63014700	0.26232500
N	-3.55441000	-0.37165100	1.04422100
N	-2.36666500	-0.78514700	0.69898700

H -0.52789900 -0.14094300 -1.11803400

Transition state

E = -1048.7167 a.u. G = -1048.7591 a.u.

S	2.32195826	0.08634138	0.05524144
O	1.35484423	0.71402628	1.02055979
O	2.81637618	1.06342365	-0.93238695
O	3.40743002	-0.63534998	0.74330405
O	1.45833469	-0.99252986	-0.69698394
O	-0.26016435	-0.61972662	-0.42594402
N	-2.00764190	-0.15293325	-0.02835459
N	-2.51937644	1.03971016	-0.09862383
N	-3.80994027	0.89071265	0.02009916
N	-4.06852010	-0.39128570	0.15163134
N	-2.93999841	-1.04473402	0.11773412
H	0.05244141	-0.01049886	0.31034208

Product

cyclo-N₅O⁻

E = -348.9492 a.u. G = -348.9799 a.u.

O	1.91249063	-0.00000870	0.00003407
N	0.65243332	-0.00000039	-0.00011238
N	-0.09195240	1.08411167	0.00004983
N	-1.32710095	0.65188725	-0.00001938
N	-1.32711448	-0.65188185	0.00000251
N	-0.09196907	-1.08410672	0.00004048

HSO₄⁻

E = -699.8448 a.u. G = -699.8773 a.u.

S	-0.13022826	-0.02086473	0.00004705
O	1.44490753	0.42466784	-0.00127590
O	-0.80697076	1.27789148	-0.00037952
O	-0.31438531	-0.80786177	-1.22727398
O	-0.31266247	-0.80598650	1.22886851
H	1.99654025	-0.37585280	-0.00026566

References

- 1 Bruker, *SAINT v8.34A*, Bruker AXS Inc., Madison, Wisconsin, USA, 2013.
- 2 G. M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3-8.
- 3 G. M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3-8.
- 4 Bruker, *SADABS v2014/5*, Bruker AXS Inc., Madison, Wisconsin, USA, 2014.
- 5 Y. Xu, Q. Wang, C. Shen, Q. Lin, P. Wang and M. Lu, *Nature*, 2017, **549**, 78-81.
- 6 Y. Zhao and D. G. Truhlar, *Theor. Chem. Account.*, 2008, **120**, 215-241.
- 7 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
- 8 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.
- 9 A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B.*, 2009, **113**, 6378– 6396.
- 10 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision E.01*, Gaussian, Inc., Wallingford CT, 2013.
- 11 L. Goerigk and S. Grimme, *J. Chem. Theory Comput.*, 2011, **7**, 291-309.
- 12 L. Goerigk and S. Grimme, *Phys. Chem. Chem. Phys.*, 2011, **13**, 6670-6688.
- 13 F. Neese, F. Wennmohs, U. Becker and C. Riplinger, *J. Chem. Phys.*, 2020, **152**, 224108.
- 14 F. Weigend, *Phys. Chem. Chem. Phys.*, 2002, **4**, 4285-4291.
- 15 T. Lu, F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.
- 16 W. Humphrey, A. Dalke and K. Schulten, *J. Mol. Graph.*, 1996, **14**, 33-38.