

Figure 2.

(A)  $C(2)_3^+ s^-$ ; (B)  $C(2)_3^+ s^-$ ; (C)  $C(2)_3^+ s^-$ ; (D)  $C(2)_3^+ s^-$ ; (E)  $C(2)_3^+ s^-$ ; (F)  $C(2)_3^+ s^-$ ; (G)  $C(2)_3^+ s^-$ ; (H)  $C(2)_3^+ s^-$ .

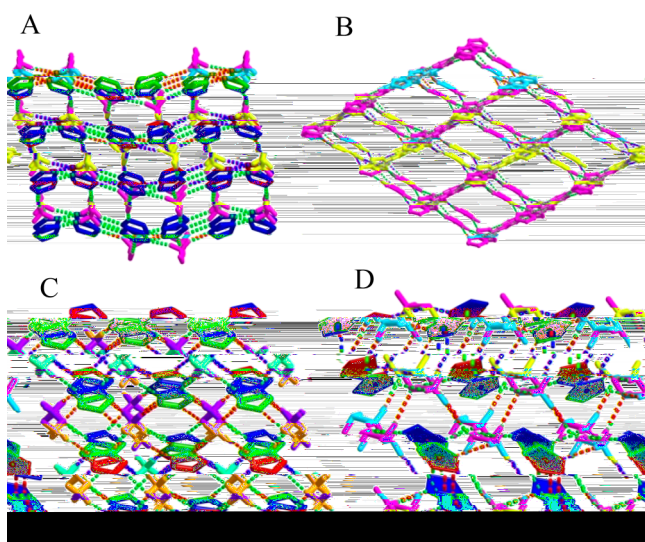


Figure 3. 3D  $C(2)_3^+ s^-$ ; (A)  $C(2)_3^+ s^-$ ; (B)  $C(2)_3^+ s^-$ ; (C)  $C(2)_3^+ s^-$ ; (D)  $C(2)_3^+ s^-$ .

$C_2^2(7)$ ,  $(39)$ . A  $C(2)_3^+ s^-$ ;  $\pi-\pi$   $C(2)_3^+ s^-$ ;  $\pi-\pi$   $C(2)_3^+ s^-$ .

40, 41).  
2.3. Thermal Behavior.

$(C_2)_3^+ s^-$ ,  $(C_3)_4^+ s^-$ ,  $(C_4)_5^+ s^-$ ,  $(C_5)_6^+ s^-$ ,  $(C_6)_7^+ s^-$ ,  $(C_7)_8^+ s^-$ ,  $(C_8)_9^+ s^-$ ,  $(C_9)_{10}^+ s^-$ ,  $(C_{10})_{11}^+ s^-$ ,  $(C_{11})_{12}^+ s^-$ ,  $(C_{12})_{13}^+ s^-$ ,  $(C_{13})_{14}^+ s^-$ ,  $(C_{14})_{15}^+ s^-$ ,  $(C_{15})_{16}^+ s^-$ ,  $(C_{16})_{17}^+ s^-$ ,  $(C_{17})_{18}^+ s^-$ ,  $(C_{18})_{19}^+ s^-$ ,  $(C_{19})_{20}^+ s^-$ ,  $(C_{20})_{21}^+ s^-$ ,  $(C_{21})_{22}^+ s^-$ ,  $(C_{22})_{23}^+ s^-$ ,  $(C_{23})_{24}^+ s^-$ ,  $(C_{24})_{25}^+ s^-$ ,  $(C_{25})_{26}^+ s^-$ ,  $(C_{26})_{27}^+ s^-$ ,  $(C_{27})_{28}^+ s^-$ ,  $(C_{28})_{29}^+ s^-$ ,  $(C_{29})_{30}^+ s^-$ ,  $(C_{30})_{31}^+ s^-$ ,  $(C_{31})_{32}^+ s^-$ ,  $(C_{32})_{33}^+ s^-$ ,  $(C_{33})_{34}^+ s^-$ ,  $(C_{34})_{35}^+ s^-$ ,  $(C_{35})_{36}^+ s^-$ ,  $(C_{36})_{37}^+ s^-$ ,  $(C_{37})_{38}^+ s^-$ ,  $(C_{38})_{39}^+ s^-$ ,  $(C_{39})_{40}^+ s^-$ ,  $(C_{40})_{41}^+ s^-$ ,  $(C_{41})_{42}^+ s^-$ ,  $(C_{42})_{43}^+ s^-$ ,  $(C_{43})_{44}^+ s^-$ ,  $(C_{44})_{45}^+ s^-$ ,  $(C_{45})_{46}^+ s^-$ ,  $(C_{46})_{47}^+ s^-$ ,  $(C_{47})_{48}^+ s^-$ ,  $(C_{48})_{49}^+ s^-$ ,  $(C_{49})_{50}^+ s^-$ ,  $(C_{50})_{51}^+ s^-$ ,  $(C_{51})_{52}^+ s^-$ ,  $(C_{52})_{53}^+ s^-$ ,  $(C_{53})_{54}^+ s^-$ ,  $(C_{54})_{55}^+ s^-$ ,  $(C_{55})_{56}^+ s^-$ ,  $(C_{56})_{57}^+ s^-$ ,  $(C_{57})_{58}^+ s^-$ ,  $(C_{58})_{59}^+ s^-$ ,  $(C_{59})_{60}^+ s^-$ ,  $(C_{60})_{61}^+ s^-$ ,  $(C_{61})_{62}^+ s^-$ ,  $(C_{62})_{63}^+ s^-$ ,  $(C_{63})_{64}^+ s^-$ ,  $(C_{64})_{65}^+ s^-$ ,  $(C_{65})_{66}^+ s^-$ ,  $(C_{66})_{67}^+ s^-$ ,  $(C_{67})_{68}^+ s^-$ ,  $(C_{68})_{69}^+ s^-$ ,  $(C_{69})_{70}^+ s^-$ ,  $(C_{70})_{71}^+ s^-$ ,  $(C_{71})_{72}^+ s^-$ ,  $(C_{72})_{73}^+ s^-$ ,  $(C_{73})_{74}^+ s^-$ ,  $(C_{74})_{75}^+ s^-$ ,  $(C_{75})_{76}^+ s^-$ ,  $(C_{76})_{77}^+ s^-$ ,  $(C_{77})_{78}^+ s^-$ ,  $(C_{78})_{79}^+ s^-$ ,  $(C_{79})_{80}^+ s^-$ ,  $(C_{80})_{81}^+ s^-$ ,  $(C_{81})_{82}^+ s^-$ ,  $(C_{82})_{83}^+ s^-$ ,  $(C_{83})_{84}^+ s^-$ ,  $(C_{84})_{85}^+ s^-$ ,  $(C_{85})_{86}^+ s^-$ ,  $(C_{86})_{87}^+ s^-$ ,  $(C_{87})_{88}^+ s^-$ ,  $(C_{88})_{89}^+ s^-$ ,  $(C_{89})_{90}^+ s^-$ ,  $(C_{90})_{91}^+ s^-$ ,  $(C_{91})_{92}^+ s^-$ ,  $(C_{92})_{93}^+ s^-$ ,  $(C_{93})_{94}^+ s^-$ ,  $(C_{94})_{95}^+ s^-$ ,  $(C_{95})_{96}^+ s^-$ ,  $(C_{96})_{97}^+ s^-$ ,  $(C_{97})_{98}^+ s^-$ ,  $(C_{98})_{99}^+ s^-$ ,  $(C_{99})_{100}^+ s^-$ .

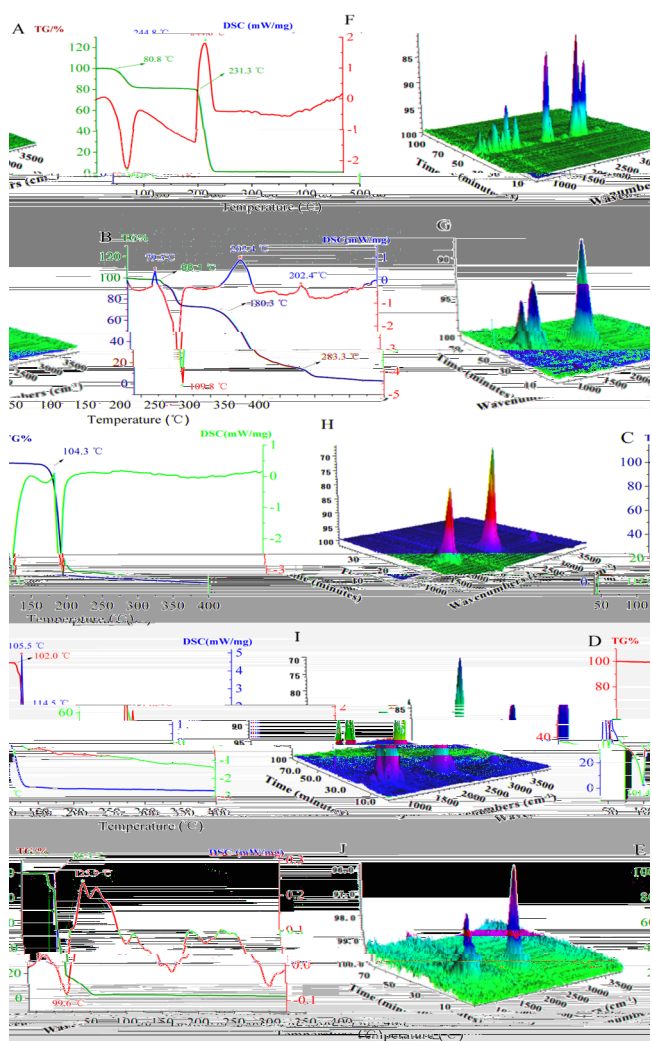


Figure 4.

(A)  $C(2)_3^+ s^-$ ; (B)  $C(2)_3^+ s^-$ ; (C)  $C(2)_3^+ s^-$ ; (D)  $C(2)_3^+ s^-$ ; (E)  $C(2)_3^+ s^-$ ; (F)  $C(2)_3^+ s^-$ ; (G)  $C(2)_3^+ s^-$ ; (H)  $C(2)_3^+ s^-$ ; (I)  $C(2)_3^+ s^-$ ; (J)  $C(2)_3^+ s^-$ ; (K)  $C(2)_3^+ s^-$ ; (L)  $C(2)_3^+ s^-$ ; (M)  $C(2)_3^+ s^-$ ; (N)  $C(2)_3^+ s^-$ ; (O)  $C(2)_3^+ s^-$ ; (P)  $C(2)_3^+ s^-$ ; (Q)  $C(2)_3^+ s^-$ ; (R)  $C(2)_3^+ s^-$ ; (S)  $C(2)_3^+ s^-$ ; (T)  $C(2)_3^+ s^-$ ; (U)  $C(2)_3^+ s^-$ ; (V)  $C(2)_3^+ s^-$ ; (W)  $C(2)_3^+ s^-$ ; (X)  $C(2)_3^+ s^-$ ; (Y)  $C(2)_3^+ s^-$ ; (Z)  $C(2)_3^+ s^-$ .

$$\frac{1}{5} \cdot \frac{3}{3} \cdot \frac{27}{2}$$

$$85 \text{ } ^\circ\text{C}, \quad \frac{(C_3)_4^+ \cdot 5^-}{80.8 \text{ } ^\circ\text{C}}$$

$$40 \text{ } ^\circ\text{C} \quad 300 \text{ } ^\circ\text{C}. \quad B \quad C \left( \frac{2}{3} \right)_3^+ \cdot 5^- \quad \left( \frac{C_3 \right)_4^+ \cdot 5^-$$

$$\frac{fi}{4} \cdot \frac{11,12}{2} \cdot \left( \frac{5}{6} \right)_3 \cdot \left( \frac{4}{3} \right)_3 \cdot C \quad C \left( \frac{2}{4} \right)_4 \cdot \left( \frac{5}{2} \right)_2$$

$$\left( \frac{27}{3} \right)^+ \cdot 5^-, \quad \left( \frac{28}{4} \right)^+ \cdot 5^-, \quad \left( \frac{2}{2} \right)^+ \cdot 5^-$$

$$100\% \quad D \quad C \quad 90 \quad 125 \text{ } ^\circ\text{C} \quad 112$$

$$^\circ\text{C}, 101 \text{ } ^\circ\text{C}, \quad 100 \text{ } ^\circ\text{C} \quad \left( \frac{3}{3} \right)^+ \cdot 5^-, \quad \left( \frac{4}{4} \right)^+ \cdot 5^-,$$

$$\left( \frac{2}{2} \right)^+ \cdot 5^-,$$

30 °C.  
2.4. Spectral Properties.

$$\left( \frac{15}{5} \right)^+ \cdot 5^- \quad \left( \frac{12-22}{15} \right)^+ \cdot 5^- \quad -5.40 \quad -4.98$$

$$\left( \frac{C_3 \right)_4^+ \cdot 5^- \quad -6.5 \quad B \quad 28$$

$$\frac{15}{5} \quad -5 \quad -6$$

$$C \quad 29 \quad B \quad 30 \quad D_5$$

$$(3 - 6) = 9 \quad fi$$

$$A_1' + 1' + 2' + 2'' \quad A_1' \quad 2' \quad 2'' \quad 1' \quad fi$$

$$(5). B \quad fi \quad D_5 \quad 31$$

$$\frac{4}{32} \cdot \left( \frac{C_3 \right)_4^+ \cdot 5^- \quad 2-11$$

$$B \quad 33 \quad \left( \frac{5}{6} \right)_3 \cdot \left( \frac{4}{4} \right)_4 \cdot C^{11} \quad 1224 \quad -1$$

$$1 \quad 20 \quad -1 \quad \left( \frac{C_3 \right)_4^+ \quad fi \quad C- \dots \pi$$

2.5. Physical Properties.

$$ff \quad 15 \quad 2. \quad 1.25-1.64 / 3^3$$

$$fi \quad fi \quad (3.4355 / 8^3)$$

$$C \quad 7.0 \quad 2$$

Table 1. Calculated and Observed Vibrational Spectra of  $\text{N}_5^-$  in Space Group  $D_{5h}$ 

Vib. Mode	$D_{5h}$		$D_{5d}$		$D_{5h}$		$D_{5d}$		Obs. (cm <sup>-1</sup> )
	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	
$A_1'$ $\nu_1$ (A)	1189.7	38.6	1141	47.8	1187	1176	1153	1170	1176
$A_1'$ $\nu_2$ (A)	1243.7	(17.5)	1202	(13.6)	1222	1221	1202	1218	1221
$A_1'$ $\nu_3$ (A)	1106.5	0.3	1078	1.8	1120	1112		1137	1105
$A_1'$ $\nu_4$ (A)	1016.6	2.4	1001	1.5	1005	1010	1006		1020
$A_1'$ $\nu_5$ (A)	769.5		739						

Table 2. Physical Properties of Five  $\text{N}_5^-$ -Pentazolate Compounds and Three Azide Compounds and Their Comparison with RDX and HMX

Compound	$\rho$ (g/cm <sup>3</sup> )	$\Delta H_f$ (kJ/mol)	$\Delta H_c$ (kJ/mol)	$\Delta H_{exp}$ (kJ/mol)	$\Delta H_{cal}$ (kJ/mol)	$\Delta H_{cal} - \Delta H_{exp}$ (kJ/mol)	$\Delta H_{cal} - \Delta H_{exp}$ (kJ/mol)	$\Delta H_{cal} - \Delta H_{exp}$ (kJ/mol)	$\Delta H_{cal} - \Delta H_{exp}$ (kJ/mol)	$\Delta H_{cal} - \Delta H_{exp}$ (kJ/mol)
$(C_3)_4^+ (S_5)^-$	1.245		80.8	58.29	297.2	5.88	10.08	197.7	35	>360
$C(2)_3^+ (S_5)^-$	1.515	-5.40	88.1	86.12	312.3	7.96	20.14	201.5	24	>360
$(C_3)_3^+ (S_5)^-$	1.636	-5.03	104.3	80.70	371.7	9.93	35.80	281.7	6	60
$(C_4)^+ (S_5)^-$	1.520	-4.98	102.0	95.42	308.1	9.28	27.29	238.0	13	140
$(C_2)_5^+ (S_5)^-$	1.620	-5.33	85.3	95.11	471.3	10.40	37.00	266.3	6	100
$(C_3)_4^+ (S_3)^-$	1.156			48.28	222.3	5.50	8.10	200.7		
$(C_4)^+ (S_3)^-$	1.346		400	93.33	112.1	8.81	21.70	242.7	>118	
$(C_2)_5^+ (S_3)^-$	1.40			93.33	383.4	9.63	27.85	282.2		
RDX	1.816		230	37.84	70.03	8.84	35.84	259.8	7.4(7.5)	120(120)
HMX	1.905		277	37.84	75.03	9.16	41.18	258.8	7.4	120

$(C_3)_4^+$   $(S_5)^-$   $(C_3)_3^+$   $(S_5)^-$   $(C_4)^+$   $(S_5)^-$   $(C_2)_5^+$   $(S_5)^-$   $(C_3)_4^+$   $(S_3)^-$   $(C_4)^+$   $(S_3)^-$   $(C_2)_5^+$   $(S_3)^-$   $(C_3)_4^+$   $(S_3)^-$   $(C_4)^+$   $(S_3)^-$   $(C_2)_5^+$   $(S_3)^-$

## ASSOCIATED CONTENT

### Supporting Information

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## Notes

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