Inorganica Chimica Acta 466 (2017) 405-409

Contents lists available at ScienceDirect

Inorganica Chimica Acta

journal homepage: www.elsevier.com/locate/ica



Chelates with π -stacking and hydrogen-bonding interactions as safer and structurally reinforced energetic materials



Inorganica Chimica Acta

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ARTICLE INFO

Article history: Received 17 March 2017 Received in revised form 31 May 2017 Accepted 28 June 2017 Available online 29 June 2017

Keywords: Energetic Chelate Semicarbazide Crystal Property

ABSTRACT

Three chelating energetic materials (CEM), $[Co(SCZ)_2(H_2O)_2](TNR)(H_2O)_2$ (1), $[Ni(SCZ)_2(H_2O)_2](TNR)(H_2O)_2$ (2) and $[Zn(SCZ)_2(H_2O)_2](TNR)(H_2O)_2$ (3, SCZ = semicarbazide, H_2TNR = styphnic acid), were synthesized and characterized by elemental analysis, FTIR spectroscopy and single-crystal X-ray diffraction analysis. Single-crystal X-ray diffraction analysis revealed that 1 mainly exhibits swathe construction, whereas 2 and 3 manifest grating structure. Thermal decomposition behaviors of 1–3 were studied by differential scanning calorimetry (DSC). The critical temperature of thermal explosion, the entropy of activation (ΔS^{\neq}), the enthalpy of activation (ΔH^{\neq}), and the free energy of activation (ΔG^{\neq}) were also calculated. Sensitivity tests revealed that 1–3 are insensitive to mechanical stimuli, and that the grating structure (2 and 3) shows better shock resistance and flame retardant property than the swathe construction (1) at the molecular level.

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1. Introduction

Nowadays, insensitive high-energy-density materials (HEDMs) remain to be the overriding theme in the field of energetic materials [1–7]. The development of insensitive HEDMs continues to focus on coordination energetic materials [8–14]. Linear ligands usually can be obtained commercially with inexpensive price, so research on linear ligands start early and many achievements have turned into applications. For instance, zinc tri(carbohydrazide) per-chlorate, cadmium tri(carbohydrazide) perchlorate and nickel hydrazine nitrate are all widely used as lead-free primary explosives in industrial detonators [15–17]. Among the linear ligands, azotic and oxygenic ligand carbohydrazide, 3-amino-1-nitroguanidine and SCZ have attracted researcher's attention, because they can coordinate to central metal ion to form five-member rings and the chelate effect can enhance their structural stability definitely.

SCZ based coordination chelates were reported extensively [18–21], but its energetic characteristics didn't arouse attention until recently [22,23]. Hydrogen bonding, as an interesting interaction between hydrogen and other atoms, has been found as an effective methodology for the construction of HEDMs [24–26]. The amino groups in SCZ can form vast hydrogen bond with counterions

 $(NO_3^-, N(NO_2)_2^-, ClO_4^-, N_3^-, and TNR^{2-})$ in the coordination complexes. Inter- and intramolecular interactions in the molecule give rise to compact and stable packing, which are conducive to increasing the density of these energetic materials. In addition, π -stacking in benzene or nitrogen heterocyclic compounds can also enhance the structural reinforcement and will definitely strengthen the thermal stability of the complex.

In pursuit of safer and structurally reinforced energetic material, we report herein the syntheses, structures and properties of three CEMs with transition metal as the central ion, SCZ as the ligand, and TNR^{2–} as the outside counterion.

2. Experimental section

2.1. Materials and physical techniques

All reagents (analytic grade) were obtained from commercial sources and used without further purification. Elemental analyses were performed with a Flash EA 1112 full automatic trace element analyzer. The FT-IR spectra were recorded with a Bruker Equinox 55 infrared spectrometer (KBr pellets) in the range of 4000–400 cm⁻¹ with a resolution of 4 cm⁻¹. DSC measurement were performed with a Pyris-1 differential scanning calorimeter in a dry nitrogen atmosphere with flowing rate of 20 mL·min⁻¹. The conditions for the thermal analyses were as follow: the crystal sample was powdered and sealed in the aluminum pans with a linear heating rate of 10 °C·min⁻¹ from 50 °C to 500 °C.



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2.2. Synthesis of SCZ (aq.)

Semicarbazide hydrochloride (30 mmol, 3.33 g) was dissolved in distilled water. Using solid Na₂CO₃ adjusted the solution pH value to 6–7.

2.3. Synthesis of $[Co(SCZ)_2(H_2O)_2](TNR)(H_2O)_2(1)$

Cobalt carbonate (10 mmol, 1.19 g) was added to a solution of 2,4,6-trinitroresorcinol (10 mmol, 2.45 g) in deionized water (40 mL), and the mixture was stirred at 60–65 °C until a clear solution resulted. A solution containing SCZ (30 mmol) in deionized water (30 mL) was added and the mixture was kept at 60–65 °C for 15 min. Then the solution was cooled to room temperature. The precipitate was collected by filtration, washed with ethanol, and dried under vacuum in an explosion-proof water-bath dryer. Yield: 71% (3.72 g). Orange prism single crystals suitable for X-ray measurements were obtained by recrystallization of the products from deionized water at room temperature over half month. Anal. Calcd. (%) for C₈H₁₉CON₉O₁₄: C, 18.33; H, 3.65; N, 24.07. Found (%): C, 18.26; H, 3.59; N, 23.99. IR (KBr): 3434, 3375, 3320, 1658, 1578, 1491, 1437, 1345, 1307, 1236, 1182, 1088, 1051, 774, 703, 516 cm⁻¹.

2.4. Synthesis of $[Ni(SCZ)_2(H_2O)_2](TNR)(H_2O)_2(2)$

Nickel carbonate (10 mmol, 1.25 g) was added to a solution of 2,4,6-trinitroresorcinol (10 mmol, 2.45 g) in deionized water (40 mL), and the mixture was stirred at 60–65 °C until a clear solution resulted. A solution containing SCZ (30 mmol) in deionized water (30 mL) was added and the mixture was kept at 60–65 °C for 15 min. Then the solution was cooled to room temperature. The precipitate was collected by filtration, washed with ethanol, and dried under vacuum in an explosion-proof water-bath dryer. Yield: 68% (3,56 g). Yellow prism single crystals suitable for X-ray measurements were obtained by recrystallization of the products from deionized water at room temperature over half month. Anal. Calcd. (%) for C₈H₁₉N₉NiO₁₄: C, 18.34; H, 3.65; N, 24.06. Found (%): C, 18.26; H, 3.57; N, 23.98. IR (KBr): 3830, 3745, 3463, 3323, 3239, 2423, 1633, 1534, 1387, 1303, 1165, 1086, 932, 787, 746, 688, 632, 515 cm⁻¹.

2.5. Synthesis of $[Zn(SCZ)_2(H_2O)_2](TNR)(H_2O)_2(3)$

Zinc carbonate (10 mmol, 1.14 g) was added to a solution of 2,4,6-trinitroresorcinol (10 mmol, 2.45 g) in deionized water (40 mL), and the mixture was stirred at 60–65 °C until a clear solution resulted. A solution containing SCZ (30 mmol) in deionized water (30 mL) was added and the mixture was kept at 60–65 °C for 15 min. Then the solution was cooled to room temperature. The precipitate was collected by filtration, washed with ethanol, and dried under vacuum in an explosion-proof water-bath dryer. Yield: 54% (2.84 g). Brown prism single crystals suitable for X-ray measurements were obtained by recrystallization of the products from deionized water at room temperature over half month. Anal. Calcd. (%) for C₈H₁₉N₉ZnO₁₄: C, 18.11; H, 3.61; N, 23.75. Found (%): C, 18.06; H, 3.50; N, 23.88. IR (KBr): 3430, 3185, 2925, 1635, 1501, 1392, 1325, 1200, 1089, 933, 779, 710, 533 cm⁻¹.

2.6. X-ray data collection and structure refinement

The X-ray diffraction data collection was performed with a Rigaku AFC-10/Saturn724⁺CCD detector diffractometer with graphite monochromated Mo-K α radiation (λ = 0.71073) with φ and ω modes at 153(2) K. The structure was solved by direct methods using SHELXS-97 and refined with SHELXL-97 [27,28]. All non-

hydrogen atoms were obtained from the difference Fourier map and subjected to anisotropic refinement by full-matrix least squares on F². Detailed information concerning crystallographic data collection and structure refinement are summarized in Table 1.

3. Results and discussion

3.1. Structure description

The molecular structures of **1–3** are illustrated in Figs. **1–3**. In all of these compounds, SCZ exhibits typical bidentate coordination, which is coordinated with central ion via the carbonyl oxygen and the terminal nitrogen of hydrazine. Compounds **1–3** all contain one central metal cation, one TNR^{2-} , two SCZ groups and four water molecules. These TNR^{2-} based compounds all contain two formula units in the unit cell. Compound **1** is structurally more symmetrical, which crystallized in the monoclinic space group *Cm*, while the other two are crystallizing isotypically with a triclinic unit cell in the space group *P*-1. The central ions are hexacoordinated with two SCZ and two water molecules, composing an octahedral structure. These selected bond angles obviously deviate from the ideal angle of 180° and bond lengths mostly are different from each other, which demonstrate that the central ion is coordinated to form a considerable distorted octahedral configuration.

In all of these compounds, amino groups from SCZ, nitro groups from TNR^{2-} and H_2O molecules play an important role to construct intermolecular and intramolecular hydrogen bonds, which are conducive to increasing the molecular density and stability. Selected hydrogen bonds are shown in Tables S1–S3. In **1**, the benzene ring and the Co-O-C-N-N five-member ring are almost in the same plane (A or B), linked by N2–H2…O5, N2–H2…O6, N3–H3 A…O5 and other hydrogen bonds. Plane A is 7.174x – 0.093y + 2.823z = -1.8433 (mean deviation 0.2109 Å). Plane B is 7.296x – 0.053y + 2.778z = 1.7118 (mean deviation 0.1829 Å). Obviously, plane A and plane B are almost parallel to each other

Table	1			
Crysta	llographic	data	of	1-3.

1–3	1	2	3
CCDC	1010968	1010970	1013946
Empirical formula	C ₈ H ₁₉ CoN ₉ O ₁₄	C ₈ H ₁₉ N ₉ NiO ₁₄	C ₈ H ₁₉ N ₉ ZnO ₁₄
Formula weight	524.25	524.03	527.67
T/K	153(2)	153(2)	153(2)
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	Ст	P-1	P-1
a/nm	1.2723(4)	0.7032(3)	0.7034(2)
b/nm	1.5900(5)	0.9727(5)	0.9730(3)
c/nm	0.47442(16)	1.5154(7)	1.5115(3)
α/(°)	90.00	108.346(6)	108.302(7)
β/(°)	109.162(4)	90.760(4)	90.755(3)
γ/(°)	90.00	108.039(4)	108.084(14)
V/nm ³	0.9066(5)	0.9283(7)	0.9265(4)
Ζ	2	2	2
$D_c/(g \cdot cm^{-3})$	1.921	1.875	1.891
θ/(°)	2.56-31.51	$2.34\sim29.11$	$2.34\sim 27.99$
h, k, l	-18-18, -22-	-9-9, -13-	-9-9,
	23,	13,	$-12\sim12$,
	-6-6	-20-20	-19-19
Reflections	2849	4949	3839
collections			
R _{int}	0.0252	0.0554	0.0392
S	1.000	1.001	0.998
$R_1, wR_2[I > 2\sigma(I)]$	0.0306, 0.0659	0.1454,	0.0898, 0.2373
		0.3710	
R_1 , w R_2 (all data)	0.0380, 0.0906	0.1617,	0.0968, 0.2405
		0.3780	
μ(MoKα)/mm ⁻¹	1.047	1.143	1.423
F(000)	538	540	538



Fig. 1. Molecular moiety of **1**. Selected coordination distances (nm): Co1–O1 0.2085(2), Co1–O2 0.2090(3), Co1–O3 0.2071(3), Co1–N1 0.2156(3); angles (deg): O1–Co1–O2 92.44(9), O1–Co1–N1 77.04(9), O3–Co1–O1 92.27(9), O3–Co1–N1 89.92(10), O3–Co1–O2 173.12(13), O2–Co1–N1 86.25(9). Symmetry codes: (i) x, –y, z; (ii) x + 1/2, y + 1/2, z; (iii) x + 1/2, -y + 1/2, z.



Fig. 2. Molecular moiety of **2**. Selected coordination distances (nm): Ni1–O1 0.2077 (8), Ni1–O2 0.2066(9), Ni1–O3 0.2183(7), Ni1–O4 0.2232(9), Ni1–N1 0.2114(9), Ni1–N4 0.2107(10); angles (deg): O1–Ni1–O3 90.6(3), O1–Ni1–N1 80.0(3), O3–Ni1–O4 176.6(3), O3–Ni1–N1 89.0(3). Symmetry codes: (i) –x, –y, –z.



Fig. 3. Molecular moiety of **3.** Selected coordination distances (nm): Zn1–O1 0.2068(5), Zn1–O2 0.2076(5), Zn1–O3 0.2181(5), Zn1–O4 0.2229(6), Zn1–N1 0.2098(6), Zn1–N4 0.2116(6); angles (deg): O1–Zn1–O3 89.4(2), O1–Zn1–N1 80.5 (2), O3–Zn1–O4 175.6(2), O3–Zn1–N1 91.4(2). Symmetry codes: (i) –x, –y, –z.

with plane angle 0.7° . And thus, complex **1** is extended into a swathe structure (Fig. 4). In **2**, in one unit cell nickel connected five-member rings are almost in the same plane (A or B), and the two planes are almost parallel. The planes (C and D) of benzene rings are parallel to each other, but vertical to plane A (or B), which constitutes a grating structure. The coordinating environment of compound **3** is similar with **2**. Beside, π -stacking in these parallel benzene rings can further enhance their structural stability. The crystal densities of **1–3** are 1.921 g cm⁻³, 1.875 g cm⁻³ and

 $1.891 \,\mathrm{g} \,\mathrm{cm}^{-3}$, so swathe construction is more compact than the grating structure.

3.2. Thermal decomposition and non-isothermal kinetics analysis

The thermal behavior of **1–3** were investigated by using differential scanning calorimetry with a linear heating rate of 10 °- C·min⁻¹ (Fig. 5). In the DSC curves of all the three compounds, there is one endothermic and multiple exothermic processes, which manifest that these compounds have the similar response to the influence of heat. The DSC curves manifest that, owing to π -stacking and hydrogen-bonding interactions, these chelates are all thermally stable with first exothermic peak temperatures above 200 °C. The sensitivity order is as follows: $T_{p2}(246.8 \text{ °C}) > T_{p3}(241.8 \text{ °C}) > T_{p1}(222.9 \text{ °C})$, which indicates that strong structural reinforcement of the grating structure in complexes **2** and **3** is thermally more stable than the swathe construction of chelate **1**.

In the present works, Kissinger's method and Ozawa-Doyle's method are widely used to determine the apparent activation energy (E) and the pre-exponential factor (A) [29–31]. The Kissinger and Ozawa-Doyle equations are as follows, respectively.

$$\ln \beta / T_p^2 \nu = \ln[RA/E] - E/(RT_p) \tag{1}$$

$$\lg \beta = \lg[AE/RG(\alpha)] - 2.315 - 0.4567E/RT_p$$
(2)

where T_p is the peak temperature (°C), R is the gas constant (8.314 J °C⁻¹ mol⁻¹), β is the linear heating rate (°C min⁻¹), and $G(\alpha)$ is the reaction mechanism function.

Based on the first exothermic peak temperatures measured at four different heating rates of 5, 10, 15 and 20 °C min⁻¹, Kissinger's method and Ozawa-Doyle's method were applied to study the kinetics parameters of **1**–**3**. From the original data, the apparent activation energy *E*, pre-exponential factor *A*, linear coefficient *R*c and standard deviations *S* were determined and shown in Table 2.

So, the Arrhenius equations of 1-3 can be expressed as follows: (E is the average of E_k and E_o):

$$\ln \kappa = 52.39 - 231.1 \times 10^3 / (RT) \tag{3}$$

$$\ln \kappa = 67.90 - 307.3 \times 10^3 / (RT) \tag{4}$$

$$\ln \kappa = 92.46 - 406.0 \times 10^3 / (RT) \tag{5}$$

The equations can be used to estimate the rate constants of the initial thermal decomposition process of these compounds.

3.3. Calculation of critical temperatures of thermal explosion, ΔS^{\neq} , ΔH^{\neq} and ΔG^{\neq}

The values of the peak temperature corresponding to $\beta \rightarrow 0$ obtained according to the following Eq. (6)[32,33] are shown in Table 3, where *a*, *b* and *c* are coefficients.

$$T_{pi} = T_{p0} + \alpha\beta + b\beta^2 + c\beta^3 \tag{6}$$

The corresponding critical temperatures of thermal explosion (T_b) obtained by the following Eq. (7) [32,33] are shown in Table 3.

$$T_{\rm b} = (E - \sqrt{E^2 - 4ERT_{P0}})/2R \tag{7}$$

The entropies of activation (ΔS^{\neq}) , enthalpies of activation (ΔH^{\neq}) , and free energies of activation (ΔG^{\neq}) of the decomposition reaction corresponding to $T = T_{p0}$, $E_a = E_K$ and $A = A_K$, obtained by the following Eqs. (8)(10)[32,33] are shown in Table 3.

$$A = (k_B T/h)(e^{\Delta S^{\neq}/R})$$
(8)



Fig. 4. Hydrogen bonds, planes and topologies of 1 (top), 2 (middle), and 3 (bottom).



Fig. 5. DSC curve for **1** with $\beta = 10 \circ C \cdot min^{-1}$ in a nitrogen atmosphere.

$$\Delta H^{\neq} = E_a - RT \tag{9}$$

$$\Delta G^{\neq} = \Delta H^{\neq} - T \Delta S^{\neq} \tag{10}$$

where $k_{\rm B}$ is the Boltzmann constant (1.381 × 10⁻²³ J/K) and *h* is the Planck constant (6.626 × 10⁻³⁴ J·s).

3.4. Sensitivity test

Impact sensitivity was determined by a fall hammer apparatus. The compound (20 mg) was placed between two steel poles and was hit by a 5.0 kg drop hammer. The tests showed that the 50% firing heights (h_{50}) was 30.0 cm (=15 J) for **1** and the firing rate was 0% for the other two at 80 cm height (>40 J). The testing results were shown in Table 4. So the grating structure possesses better shock resistance than the swathe construction.

Friction sensitivity was determined using 20 mg sample, which was placed on a Julius Peter's machine. 25 tests were done. An explosion or non-explosion was recorded. The tested compounds did not fire, which demonstrate that these compounds are structurally abrasion-resistance.

According to the method of flame sensitivity test [34], 20 mg of **1** was compacted to a copper cap under the press of 39.2 MPa and was ignited by black powder pellet. The test result demonstrated that the height for 50% explosion probability (h_{50}) of **1** was 6 cm and less than 6 cm (testing minimum height) for the other two, which indicate that the grating structure exhibits good flame retardant property.

4. Conclusions

Three insensitive CEMs with π -stacking and hydrogen-bonding interactions were synthesized and characterized. Despite all the three compounds were prepared by the similar reaction route, single-crystal X-ray diffraction analysis revealed that complex **1** crystallizes in the monoclinic space group *Cm* exhibiting swathe construction, whereas the crystal structures of both **2** and **3** belong

 Table 2

 Peak temperatures of the first exotherm at different heating rates and the chemical kinetics parameters.

β (°C min ⁻¹) T _p (°C)			Parameter	Kissinger's method			Ozawa's method			
	1	2	3		1	2	3	1	2	3
5	218.1	243.3	239.8	$E(kJ mol^{-1})$	232.8	310.8	412.0	229.3	303.8	400.0
10	222.4	247.6	242.3	lgA	22.78	29.52	40.2	1	/	/
15	226.5	250.5	244.4	R _c	-0.9892	-0.9965	-0.9771	-0.9900	-0.9967	-0.978
20	229.8	253.2	247.1	S	0.1041	0.0597	0.1537	0.0452	0.0259	0.0667

Table 3	
Calculation of $T_{\rm b}$, ΔS^{\neq} , ΔH^{\neq} and ΔG^{\neq} .	

Compounds	T_{p0} (°C)	$T_{\rm b}$ (°C)	$\Delta S^{\neq} (\mathbf{J} \cdot (\mathbf{K} \cdot \mathbf{mol}^{-1}))$	$\Delta H^{\neq} (\text{kJ} \cdot \text{mol}^{-1})$	$\Delta G^{\neq} (kJ \cdot mol^{-1})$
1	214.2	216.5	192.9	231.0	143.4
2	236.4	237.9	321.1	308.8	248.1
3	235.9	237.1	530.4	410.0	433.7

Table 4

Physicochemical properties of compounds 1-3.

Compd	$T_{\rm m}^{[a]}$ (°C)	$T_{\text{dec.}}^{[b]}$ (°C)	$D^{[c]}(g \ cm^{-3})$	N ^[d] (%)	N + O ^[e] (%)	IS ^[f] (J)	FS ^[g] (N)	FlS ^[h] (cm)
1	128	200	1.86	24.07	66.80	15	>360	6
2	99	232	1.90	24.06	66.81	>40	>360	<6
3	108	231	1.87	23.75	65.96	>40	>360	<6

^[a] Melting point/DSC endothermic peak.

^[b] Thermal decomposition temperature (onset) (DSC, 10 °C min⁻¹).

[c] Measured density

^[d] Nitrogen content.

[e] Nitrogen and oxygen content.

^[f] Impact sensitivity, h_{50} (BAM drophammer).

[g] Friction sensitivity.

^[h] Flame sensitivity, h₅₀.

to triclinic P-1 space group manifesting grating structure. DSC analyses showed that they are thermally stable with onset decomposition temperatures all above 200 °C. Non-isothermal kinetics analyses reveal that the Arrhenius equations of 1-3 can be expressed as follows: $\ln k = 52.39 - 231.1 \times 10^3 / (RT).$ $\ln k = 67.90 - 307.3 \times 10^3 / (RT)$ and $\ln k = 92.46 - 406.0 \times 10^3 / (RT)$. The critical temperature of thermal explosion $(T_{\rm b})$, entropy of activation (ΔS^{\neq}), enthalpy of activation (ΔH^{\neq}), and free energy of activation (ΔG^{\neq}) of the decomposition reaction are 216.5 °C, 192.9 J·K⁻¹·mol⁻¹, 231.0 kJ·mol⁻¹, 143.4 kJ·mol⁻¹ for **1**, 237.9 °C, 321.1 $[K^{-1} \text{ mol}^{-1}, 308.8 \text{ k}] \text{ mol}^{-1}, 248.1 \text{ k}] \text{ mol}^{-1}$ for **2** and 237.1 °C, 530.4 $|K^{-1} \text{ mol}^{-1}$, 410.0 k $|\text{ mol}^{-1}$, 433.7 k $|\text{ mol}^{-1}$ for **3**. Sensitivity tests indicated that they are all insensitive to mechanical stimuli. In addition, the lightweight grating structure (2 and 3) shows good thermal stability, shock resistance and flame retardant property comparing with the swathe construction (1) in a molecular level. Therefore, chelates with π -stacking and hydrogen-bonding interactions as a package of strategy for designing insensitive energetic materials is emerging, and the research on safe yet powerful chelates is on the way.

Acknowledgements

We gratefully acknowledge financial support from the State Key Laboratory of Explosion Science and Technology (No. YB2016-16) and the National Natural Science Foundation of China (No. 11672040).

Appendix A. Supplementary data

CCDC 1010968, 1010970 and 1013946 contains the supplementary crystallographic data for compounds 1-3. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving. html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk. Supplementary data associated with this article can be found, in the online version, at http:// dx.doi.org/10.1016/j.ica.2017.06.071.

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