Supporting Information

2-Imidazolidone metal complexes: increase hydrogen bond and fused ring ligand ratio to be insensitive

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Index:

1. Experimental details

The analytical grade reagents used in the experiment were bought from Aladdin and Azov and utilized without additional purification. The analytical grade reagents used in the experiment were bought from Aladdin and Azov and utilized without additional purification.

Differential scanning calorimetry (TGA/DSC2, METTLER TOLEDO) was used to study the thermal behavior of synthesized compound under a nitrogen environment and a heating rate of 5 $^{\circ}C \cdot min^{-1}$.

Infrared (IR) spectra were measured on a Nicolet Is10 spectrometer with a measurement range of 4000 - 400 cm^{-1}. On an elemental analyzer (Vario EL Cube, Germany), elemental analyses (C, H, N or C, H, N, O) were performed.

By using a BAM DFH-10 device with a weight drop of 5 kg, the standard step approach of the drop weight device was used to assess the mechanical sensitivities of the material, including impact sensitivity and friction sensitivity.

The experimental density is obtained by the powder densitometer test (Micromeritics AccuPyc II 1340). And the experimental density is directly imported.

The process of flame test is that 5 mg ECCs was dispersed on the operating table in a powdered state. And using an alcohol lamp to slowly heat a metal spoon or heating the ECCs directly by open flame while recording the deflagration process of the compound with a high-speed camera.

The detonation performance of novel ECCs was calculated by using EXPLO5 6.02, and the heat of formation was performed based on its definition. The enthalpy change associated with the formation of one mole of a compound from its elemental constituents in their standard states is defined as the standard molar enthalpy of formation of the compound. Taking the compound $C_aH_bN_cO_dM_e$ as an example (M is metal), the corresponding general equation for its formation reaction is as follows:

$$aC + \frac{b}{2}H_2 + \frac{c}{2}N_2 + \frac{d}{2}O_2 + eM \rightarrow C_aH_bN_cO_dM_e \quad \textbf{(S1)}$$

By definition, the enthalpy of formation is the reaction enthalpy of the above Equation **(S1)**. The enthalpy of reaction is determined by calculating the difference between the enthalpy of the products and the enthalpy of the reactants. To calculate the enthalpy of each species involved in the reaction, Gaussian package was used. Carbon and Metal are solids at room temperature, but the enthalpy value obtained from quantum chemistry computational programs corresponds to its formation in the gaseous state. Subtracting the sublimation enthalpy (H_{sub}) from the enthalpy value (H) obtained from quantum chemistry computational programs is necessary to determine the enthalpy of carbon in its stable phase (solid).In summary, the formula for calculating the enthalpy of formation using the definition method is as follows:

$$\Delta_f H_m^\theta = \Delta_r H_m^\theta = H(C_aH_bN_cO_dM_e) - a[H(C) - H_{sub}(C)] - \frac{b}{2}H(H_2) - \frac{c}{2}H(N_2) - \frac{d}{2}H(O_2) - e[H(M) - H_{sub}(M)] \quad \textbf{(S2)}$$

The enthalpy values above correspond to the stable phase at 298 K. The calculated enthalpy of formation is also determined at this temperature. Based on the previously optimized structures, we conducted single-point calculations at the PBE0 def2S level of theory to obtain high-precision single-point energies. These high-precision single-point energies, when combined with the zero-point energy (corrected with a factor of 0.9819) and the enthalpy correction term Hcor obtained from the earlier vibrational analysis, allowed us to calculate the enthalpy values for each compound. Using the aforementioned methods, we ultimately calculated their enthalpy of formation.

2. Tables

Table S1. Selected bond distances (Å) and bond angles (°).

ECCs-1			
Cu(1)–O(1)	1.917(5)	Cl(1)–O(3)	1.380(11)
Cu(1)–O(2)	1.940(5)	Cl(1)–O(4)	1.39(3)
Cu(1)–O(5)	2.587(12)	Cl(1)–O(6)	1.50(2)
Cu(1)–O(4)	2.72(3)	C(1)–O(1)	1.243(9)
C(1)–N(1)	1.299(11)	C(3)–N(7)	1.462(12)
O(1)–Cu(1)–O(2)	94.6(2)	O(6)–Cl(1)–O(7)	122.1(10)
O(1)–Cu(1)–O(5)	83.2(3)	O(6)–Cl(1)–O(8)	124.3(12)
O(1)–Cu(1)–O(4)	85.6(6)	O(5)–Cl(2)–O(9)	94.3(11)
Cu(1)–O(1) –C(1)	131.9(5)	Cu(1)–O(4) –Cl(1)	140.1(18)
Cu(1)–O(2) –C(4)	131.7(5)	Cu(1)–O(5) –Cl(1)	156.6(9)

Table S2. Selected bond distances (Å) and bond angles (°).

ECCs-2			
Co(1)–O(1)	2.097(3)	Cl(1)–O(7)	1.411(15)

Co(1)–O(2)	2.083(4)	Cl(1)–O(8)	1.404(14)
Co(1)–O(3)	2.057(3)	Cl(2)–O(9)	1.382(18)
C(1)–O(1)	1.242(6)	C(1)–N(1)	1.304(7)
C(1)–N(2)	1.304(7)	N(1)–H(1)	0.8600
O(1)–Co(1)–O(2)	90.56(13)	O(5)–Cl(1)–O(7)	109.0(10)
O(1)–Co(1)–O(3)	93.84(12)	Co(1)–O(3) –C(3)	132.4(3)
O(2)–Co(1)–O(5)	180.00	N(1)–C(1)–N(2)	107.8(5)
Co(1)–O(1) –C(1)	129.9(3)	O(1)–C(1)–N(2)	127.9(5)
Co(1)–O(2) –C(2)	130.7(3)	N(1)–C(1)–H(1)	111.00

3. Graphics

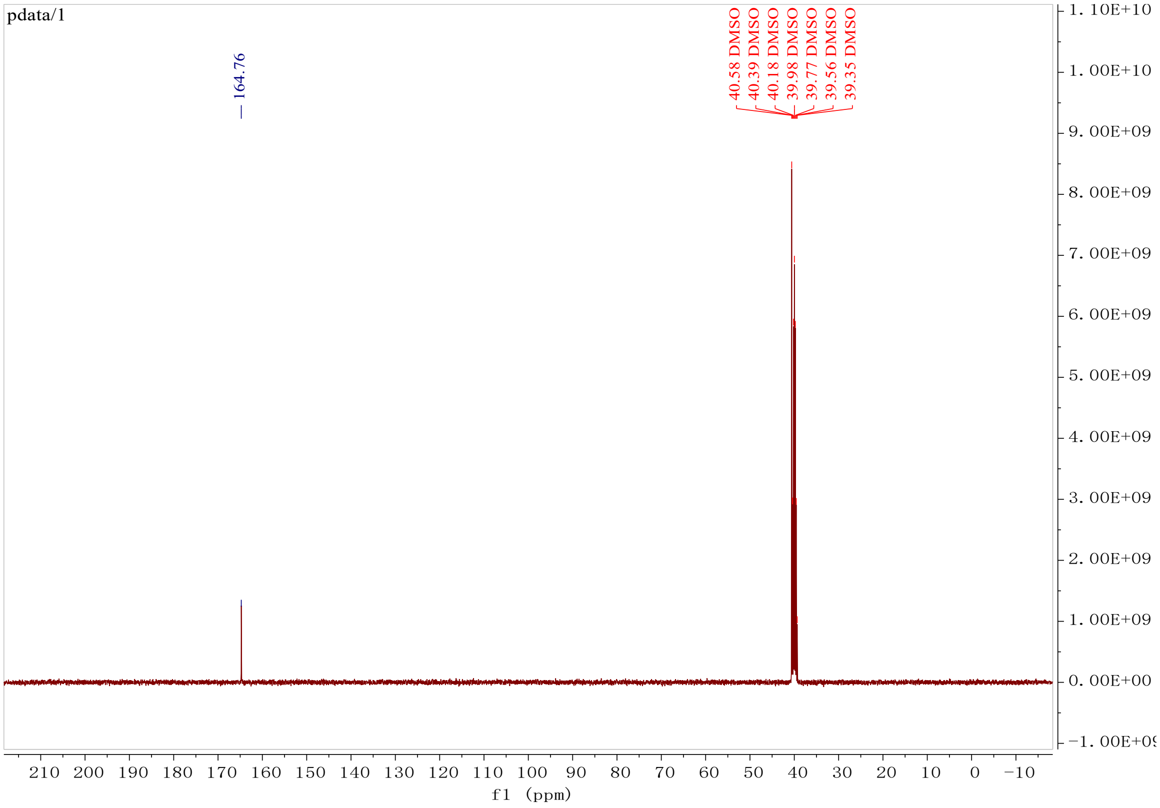

Figure S1. ^{13}C NMR of 2-IMTO.

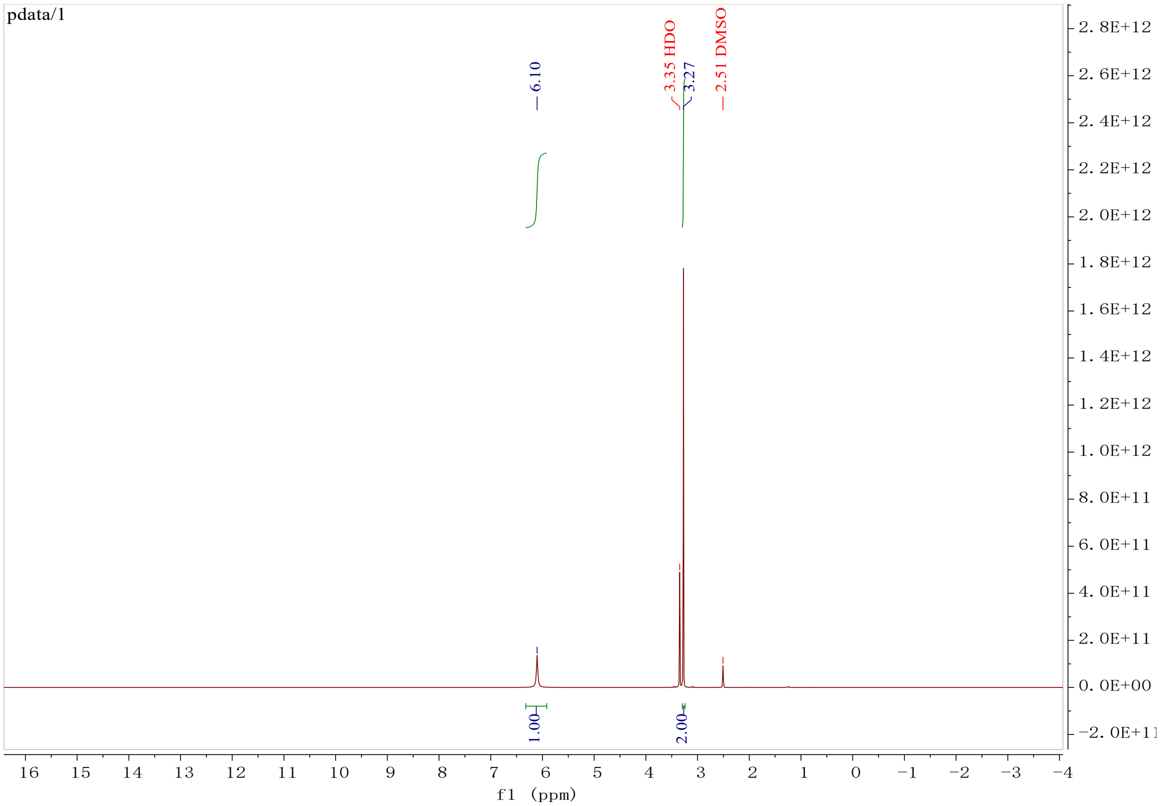

Figure S2. ^{1}H NMR of 2-IMTO.

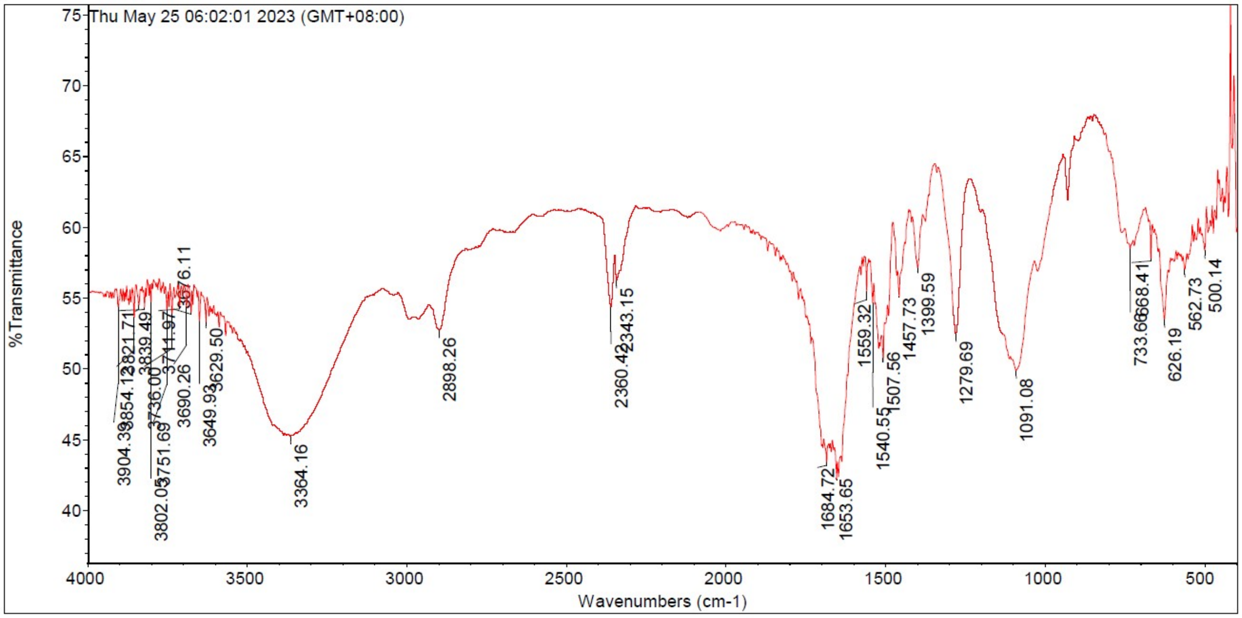

Figure S3. The IR spectra of **ECCs-1**.

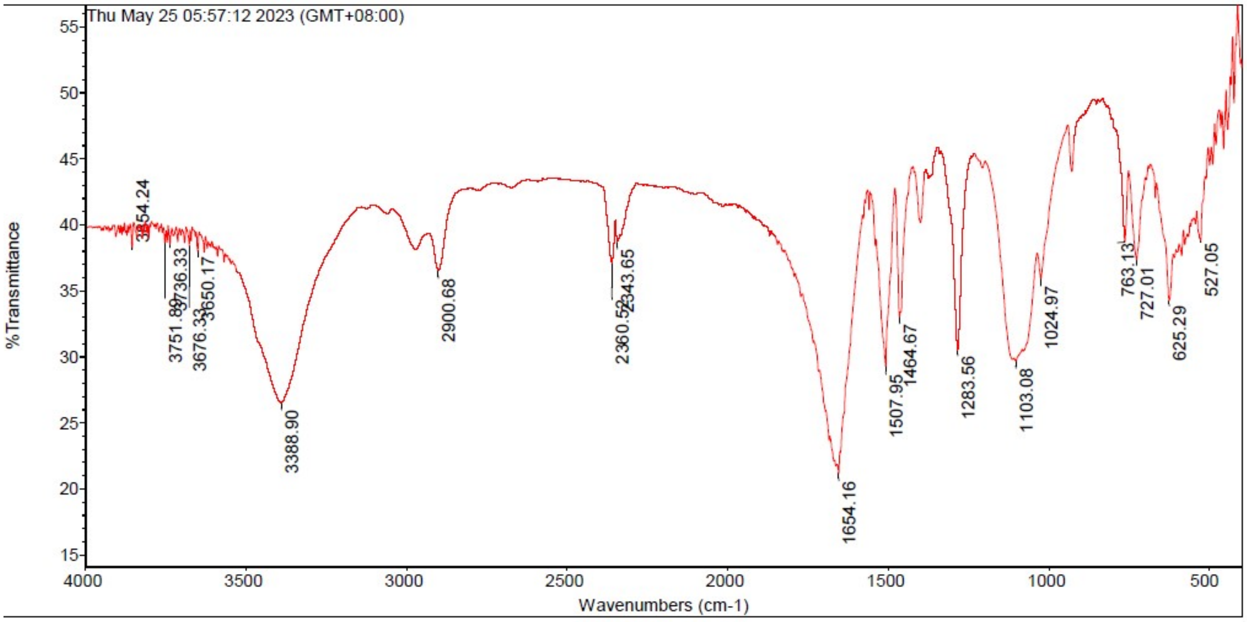

Figure S4. The IR spectra of **ECCs-2**.