SUPPORTING MATERIALS

3D High-Energy-Density Materials and Low Sensitivity: Synthesis, Structure and Physicochemical Property of An Azide-Cu(II) Complex with 3,5-Dinitrobenzoic Acid

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1. Apparatus and conditions of the calorimetric experiment.

The constant-volume combustion energy of the complex was determined with a precise rotating-bomb calorimeter (RBC-type II). The main experimental procedures were described previously [1]. The correct value of the heat exchange was calculated according to the Linio-Pyfengdelel-Wsava equation [2].

The energy equivalent of the calorimeter was calibrated with benzoic acid, which has an isothermal heat of combustion of (-26434 ± 3) J g^{-1} at 298.15 K. The analytical methods of the final products (gas, liquid, and solid) were as reported in Ref [1]. The amount of nitric acid was determined by using Devarda's alloy method [3]. Because the crucible in the rotating bomb was attached to the support, the final solid products were left in the crucible at the end of the experiment. Analytical data of the final products indicate that the combustion reaction was complete.

The constant-volume combustion energy is calculated by Eq. (1) [4, 5].

$$\Delta_c U = \frac{W\Delta T - aG - 5.97b}{m} \qquad (1)$$

where $\Delta_c U$ (complex, s) denotes the constant-volume combustion energy of the complex (in J g^{-1}), W is the energy equivalent of the rotating-bomb calorimeter (in J K^{-1}), a is the length of the actual Ni-Cr wire consumed (in cm). G is the combustion enthalpy of Ni-Cr wire for ignition (0.9 J cm^{-1}), 5.97 J·cm^{-3} is the formation enthalpy and solution enthalpy of nitric acid corresponding to 1 cm^3 of 0.1000 mol dm^{-3} NaOH, b is the volume (in cm^3) of consumed 0.1000 mol dm^{-3} NaOH and ΔT is the correct value of the temperature rise, m is the mass (in g) of the complex.

The constant-volume combustion energies of the complex were repeatedly measured for six times. Typical result is (-10971.11 ± 6.56) J g^{-1}. The relative atomic masses used in the calculation of all molar quantities were those recommended by the IUPAC Commission in 2005 [6].

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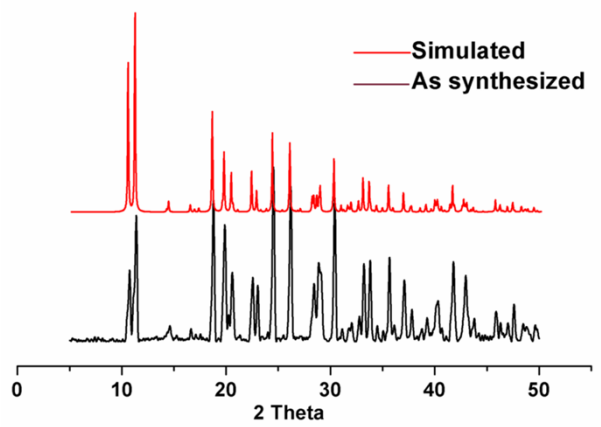

Fig. S1. XRPD diagrams for complex.

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

Cu(1)-O(1)	1.939(4)
Cu(1)-N(1)	1.990(5)
N(2)-N(3)	1.239(8)
N(1)-Cu(1)#1	1.967(5)
Cu(1)-N(1)#2	1.967(6)
N(2)-N(1)	1.145(8)
Cu(1)-O(2)#2	1.950(4)
Cu(1)-O(4)	2.609(6)
O(4)-N(5)	1.197(8)
Cu(1)-Cu(1A)	3.387(2)
O(3)-N(5)	1.236(7)
O(1)-Cu(1)-O(2)#2	164.8(2)
C(1)-O(2)-Cu(1)#1	129.1(4)
O(1)-Cu(1)-N(1)	94.1(2)
O(4)-N(5)-O(3)	123.9(6)
Cu(1)-N(1)-Cu(1A)#1	118.0(2)
N(3)-N(2)-N(1)	178.6(7)
O(6)-N(4)-O(5)	124.8(7)
N(2)-N(1)-Cu(1)#1	122.1(4)
O(1)-Cu(1)-N(1)#2	90.3(2)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+3/2,-z+1; #2 x-1/2,-y+3/2,-z+1