Supplementary Information

Discovery of Energetic Ionic Cocrystals via High-Throughput Virtual Screening

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1. Experimental Section

Chemicals and instruments

Ammonium dinitramide (ADN) was synthesized according to the method given in the literature [1]. 3,4-Diaminofurazan (OHD) and organic solvents used in this experiment were all purchased from Aladdin with a mass purity of > 98%.

The Cu-Kα radiation (λ = 1.5418 Å) was scanned over a diffraction angle range (2θ) of 5° to 50° under a scanning rate of 8 ° min^{-1} by powder X-ray diffraction (PXRD, D8 advance, Bruker). To investigate the desolvation and decomposition processes of ADN/OHD, a differential scanning calorimetry (Mettler-Toledo, DSC, Switzerland) and thermogravimetric analysis (Mettler-Toledo, TGA, Switzerland) were used and examined at a heating rate of 10 K/min while being shielded by nitrogen gas. Micrographs were taken by a polarized optical microscope (POM, Axio Scope. Al, Carl Zeiss) to observe the morphologies of all obtained cocrystals. The impact and friction sensitivity were analyzed using the Bundesanstalt für Materialprüfung (BAM) Fallhammer device.

Single-crystal X-ray diffraction (SCXRD)

Single crystal X-ray diffraction (SCXRD) was used to determine the crystal structures for ADN/OHD, collected on a Bruker SMART APEX II diffractometer equipped with a CCD detector (Mo Kα radiation, λ = 0.71073 Å). Integration and scaling of intensity data were performed using the APEX 4 software. The structure was solved with the SHELXT structure solution program [2] using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimization in Olex 2.1.2 software [3]. An extinction correction was applied during refinement.

Hygroscopicity measurement

Dynamic vapor sorption (DVS) experiments were performed using the Dynamic Vapor Sorption Analyzer (SMS-DVS Intrisic, Surface Measurement Systems). Sample mass was monitored from 5-90% relative humidity with a step size of 2%, where relative humidity was stepped once sample mass stabilized (<0.01% change for 2 minutes) with a maximum of 120 minutes equilibration time per step and starting from initial

masses of 10-12 mg.

Moisture content of samples was quantified using a METTLER TOLEDO-V20 Karl Fischer Titrator. Based on pre-experimental estimation, the target samples were expected to have moisture contents in the range of 0.01% to 10.00%, which is within the optimal detection range of the instrument. An aliquot of 10–15 mg was accurately weighed and introduced into the titration cell (sealed to prevent ambient moisture interference); Titration was performed with a 50 μL burette (precision: ±0.01 μL) using Hydranal®-Composite 5 reagent (c = 5 mg H_2O/mL); The endpoint was determined by a dual-platinum electrode (stabilization criterion: <5 mV drift over 30 seconds) to ensure accuracy; Each sample was analyzed in triplicate, and the mean value was reported as the final moisture content.

Preparation of ADN/OHD cocrystals

Preparation of single crystals. Single crystals of ADN/OHD were obtained via slow evaporation in acetonitrile at room temperature (25 ± 2°C). First, 0.62 g of ADN and 0.5 g of OHD (1:1 molar ratio) were dissolved in 10 mL of acetonitrile in a glass vial. After complete dissolution, the solution was filtered through a 0.22 μm membrane filter into a designated container to remove any undissolved particles. The filtrate was then left to evaporate slowly at room temperature. After approximately 2-4 hours, single crystals of ADN/OHD were obtained.

Cocrystal crystallization. The ADN/OHD cocrystals were produced using cooling crystallizations. ADN and OHD were dissolved at a stoichiometric ratio in 8 mL of an organic solvent at 70°C with magnetic stirring at 300 rpm. The solution was then gradually cooled to room temperature to induce crystallization.

Compatibility

The DSC was employed to investigate the compatibilities of ADN/OHD cocrystal with different contact components according to GJB 772A-97 standards (Chinese Military Standard). The cocrystals were mixed with other components at a mass ratio of 1:1, then both the individual components and the mixtures were under DSC testing. According to the evaluated standards of compatibility for energetic materials [4], we examined the change in the maximum exothermic peak temperature ($^{\Delta T_p}$) of the individual components and

the mixtures as the heating rate approaches 0 K and the change rate of apparent activation energy ($\Delta E/E_a$). The calculation formula is presented in equation S2:

$$T_p = T_{p0} + b\beta_i^2 + c\beta_i^2 + d\beta_i^2 \quad \text{(S1)}$$

where T_{pi} represents the maximum exothermic peak temperature of the single system as the heating rate approaches β_i K min^{-1}, and i=1, 2, 3 …….

$$\Delta T_p = T_{p1} - T_{p2} \quad \text{(S2)}$$

where T_{p1} represents the maximum exothermic peak temperature of the single system, and T_{p2} denotes the maximum exothermic peak temperature of the mixed system. The change rate of apparent activation energy ($\Delta E/E_a$) is calculated according to the following equation:

$$\frac{\Delta E}{E_a} = \left|\frac{E_a - E_b}{E_a}\right| \times 100\% \quad \text{(S3)}$$

where E_a and E_b represent the apparent activation energies (units: J·mol^{-1}) of the single-component system and mixed system respectively. Both E_a and E_b are determined through linear regression based on the Ozawa formula:

$$\lg \beta_i = lg\left[\frac{A_{a(arb)}E_{a(arb)}}{RF(a)}\right] - 2.315 - 0.4567\frac{E_{a(arb)}}{RT_i} \quad \text{(S4)}$$

Where $A_{a(arb)}$ denotes the apparent pre-exponential factor for either the single or blended system, $E_{a(arb)}$ is the apparent activation energy for the corresponding system, R is the molar gas constant (8.314 J·mol^{-1}·K^{-1}), $F(\alpha)$ represents the reaction model function, and i=1, 2, 3 ……..

Compatibility is evaluated according to the following standards:

1.$\Delta T_p < 2.0$°C, $\Delta E/E < 20\%$: Good compatibility, Class 1

2. $\Delta T_p < 2.0$°C, $\Delta E/E > 20\%$: Fair compatibility, Class 2

3. $\Delta T_p > 2.0$°C, $\Delta E/E < 20\%$: Poor compatibility, Class 3

4. $\Delta T_p > 2.0$°C with $\Delta E/E > 20\%$ or $\Delta T_p > 5$°C: Very poor compatibility, Class 4

2. Calculation Section

Crystal data extraction and automatic screening procedure

The workflow for extracting target data from the Cambridge Structural Database (CSD) begins with searching for single-component single crystal structure entries within the ConQuest application. Additional filters include "3D coordinates determined," "No error," "No polymeric," "no ions," "only single crystal structures," "only organics," and an extra filter of "Density > 1.6 g cm^{-3}" to focus on structures composed exclusively of C, H, O, N. After collecting Refcodes of qualified entries, individual molecules in corresponding CIF files are extracted, with any solvent or gas molecules removed to ensure purity. The processed structures are finally converted into SMI format files for subsequent automatic screening.

For automatic screening, the specified Python script is used to perform multi-stage conditional filtering on the compiled SMI files. First, initial validity filtering is conducted to exclude entries with invalid SMILES or abnormal structures that fail hydrogen addition. Then, descriptor-based filtering is carried out to retain molecules meeting criteria like positive oxygen balance and having both hydrogen bond acceptors and donors. Finally, duplicate SMILES are removed and center-symmetric molecules are identified, resulting in 51 molecules that meet all set conditions (Fig. S1). The automatic screening was used the following Python code:

```
from rdkit import Chem
from rdkit.Chem import AllChem, Descriptors, Draw, Lipinski, rdPartialCharges
from rdkit.ML.Descriptors import MoleculeDescriptors
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib.image as mpimg
from collections import defaultdict

def has_center_symmetry(mol, threshold=0.1):
    """Precisely detect if a molecule has center symmetry"""
    n_atoms = mol.GetNumAtoms()
    if n_atoms == 0:
        return False

    AllChem.Compute2DCoords(mol)
    conf = mol.GetConformer()
    pts = np.array([list(conf.GetAtomPosition(i)) for i in range(n_atoms)])

    centroid = pts.mean(axis=0)

    atom_type_map = defaultdict(list)
    for i in range(n_atoms):
        atom = mol.GetAtomWithIdx(i)
        atom_type_map[(atom.GetAtomicNum(), atom.GetDegree())].append(i)
```

```
    matched = [False] * n_atoms
    for atom_type, indices in atom_type_map.items():
        indices.sort(key=lambda i: np.linalg.norm(pts[i] - centroid), reverse=True)

        for i in indices:
            if matched[i]:
                continue

            sym_pos = 2 * centroid - pts[i]

            best_match = None
            best_dist = float('inf')

            for j in indices:
                if matched[j] or i == j:
                    continue

                dist = np.linalg.norm(pts[j] - sym_pos)
                if dist < best_dist and dist < threshold:
                    best_dist = dist
                    best_match = j

            if best_match is not None:
                matched[i] = True
                matched[best_match] = True
            else:
                dist_to_center = np.linalg.norm(pts[i] - centroid)
                if dist_to_center < threshold:
                    matched[i] = True
                else:
                    return False

    return all(matched)

def main():
    smi_path = "C:/Users/wangy/Desktop/ADN-ODH/cal/test5/search_1.6-1.smi"
    df = pd.read_csv(smi_path, header=None)
    df = df.iloc[:, 0].str.split('\t', expand=True)
    df.columns = ['smile', 'rfd']

    print(f"Initial molecules: {len(df)}")

    valid_mask = []
    for i, smile in enumerate(df['smile']):
        mol = Chem.MolFromSmiles(smile)
        if mol is None:
            valid_mask.append(False)
            print(f"Invalid SMILES: 5")
            continue

        try:
            Chem.AddHs(mol)
            valid_mask.append(True)
        except Exception as e:
            valid_mask.append(False)
            print(f"Failed to process molecule: {smile} - Error: {str(e)}")

    df = df[valid_mask].reset_index(drop=True)
    print(f"Valid molecules: {len(df)}")

    total_ob_list = []
    nAHB_01 = []
    nDHB_01 = []

    ADN_H = 8
    ADN_O = 8

    for smile in df['smile']:
```

```
    mol = Chem.MolFromSmiles(smile)
    mol = Chem.AddHs(mol)

    nH_comf = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 1)
    nC_comf = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 6)
    nO_comf = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 8)

    nH_total = nH_comf + ADN_H
    nO_total = nO_comf + ADN_O

    total_ob = 16 * (nO_total - nC_comf - nH_total/2)

    nAHB = Lipinski.NumHAcceptors(mol)
    nDHB = Lipinski.NumHDonors(mol)

    total_ob_list.append(total_ob)
    nAHB_01.append(nAHB)
    nDHB_01.append(nDHB)

df['total_OB'] = total_ob_list
df['nAHB_01'] = nAHB_01
df['nDHB_01'] = nDHB_01

df = df[df['total_OB'] > 0].reset_index(drop=True)
print(f"Molecules with positive oxygen balance: {len(df)}")

df = df[(df['nAHB_01'] > 0) & (df['nDHB_01'] > 0)].reset_index(drop=True)
print(f"After removing molecules without H-bond donors/acceptors: {len(df)}")

print(f"\nInitial molecules for symmetry detection: {len(df)}")
print(f"Unique SMILES count: {df['smile'].nunique()}")

duplicates = df[df.duplicated(subset=['smile'], keep=False)]
if not duplicates.empty:
    print(f"\nFound {len(duplicates)} duplicate SMILES:")
    print(duplicates[['smile', 'rfd']].head(10))
    if len(duplicates) > 10:
        print(f"... and {len(duplicates) - 10} more")
else:
    print("No duplicate SMILES found")

initial_count = len(df)
df = df.drop_duplicates(subset=['smile'], keep='first')
removed_count = initial_count - len(df)
print(f"\nRemoved {removed_count} duplicate molecules")
print(f"Unique molecules remaining: {len(df)}")

center_symmetry = []
print(f"\nDetecting molecular center symmetry for {len(df)} molecules...")

for i, smile in enumerate(df['smile']):
    mol = Chem.MolFromSmiles(smile)
    if mol is None:
        print(f"Molecule {i+1}/{len(df)}: Invalid SMILES - {smile}")
        center_symmetry.append(False)
        continue

    mol = Chem.AddHs(mol)

    is_center_sym = has_center_symmetry(mol)
    center_symmetry.append(is_center_sym)

    status = "Center symmetric" if is_center_sym else "Not center symmetric"
    print(f"Molecule {i+1}/{len(df)}: {status} - {smile}")

df['center_symmetry'] = center_symmetry

df_sym = df[df['center_symmetry']].copy()
```

```
    print("\nSymmetry detection results:")
    print(f"Total molecules: {len(df)}")
    print(f"Center-symmetric molecules: {len(df_sym)}")
    print(f"Percentage: {len(df_sym)/len(df)*100:.2f}%")

    output_file = 'final_CO.csv'
    df_sym.to_csv(output_file, index=False)
    print(f"\nCenter-symmetric molecules saved to {output_file}")
    print(f"Saved {len(df_sym)} center-symmetric molecules")

if __name__ == "__main__":
main()
```

Molecular interaction analysis

All molecule structures of the dimers were optimized using the DFT method through the Gaussian 09W software. All calculations were performed at the B3LYP/6-311+G (d,p) basis set. The wave function was recognized in Multiwfn 3.8 software [6], and the regions of interaction of the dimer were observed using the reduced density gradient (RDG) function [7]. The schematic diagram of RDG was drawn by VMD software [8].

Hirshfeld Surface (HS) analysis was conducted under Crystal Explorer, which was used to identify the interactions of the molecule with the neighboring molecules in ADN and ADN/OHD by Hirshfeld surface under B3LYP/6–31G (d).

Calculation on the enthalpy of formation

Combustion heat measurement. Combustion experiments were conducted in a ZDHW-HN7000C calorimeter (±0.8 mK thermal drift control). Samples (1000±20 mg, pressed into 12 mm pellets) were ignited in a 316L stainless steel bomb pressurized to 3.0 MPa O_2, submerged in 2.3 L thermostated water (298.150 ± 0.005 K). Temperature evolution was tracked via a 10 kΩ platinum resistance thermometer (PT-1000 Class AA) with 24-bit ADC resolution (effective δT = 2 μK). System calibration utilized NIST-certified benzoic acid (ΔH_c = -26434 ± 3 J·g^{-1}).

Determination of enthalpy of formation. The standard enthalpy of formation ($^{\Delta_f H_m^0}$) was calculated via Hessian thermochemical cycles based on combustion calorimetry data. Experimentally determined heats of combustion were acquired using a high-precision oxygen bomb calorimeter (ZDHW-HN7000C, Huaneng Instruments Co.). Standard molar combustion enthalpies ($^{\Delta_C H_m^\theta}$) can be obtained from the reaction heat ($^{\Delta_C U}$).

The standard molar enthalpy of formation ($^{\Delta_f H^{\theta}_m}$) can be obtained according to formula (S5). [CO_2(g): -393.51 kJ mol^{-1}; H_2O(l): -285.85 kJ mol^{-1}]

$$\Delta_f H^0_m(compound) = \Sigma\Delta_f H^O_m(products) - \Delta_c H^0_m(compound) \quad \text{(S5)}$$

The $\Delta_C U$ values of ADN and OHD are -3702, -8474.5 kJ kg^{-1}, and the $\Delta_C H^{\theta}_m$ values of these are -459.05, -1899.64 kJ mol^{-1}, respectively.

Table S1. Calculation of enthalpy of formation.

	ADN/OHD (kJ mol^{-1})
$\Sigma\Delta_f H^{\theta}_m(products)$	-2783.97
$\Delta_c H^{\theta}_m(compound)$	-2280.64
$\Delta_f H^{\theta}_m(compound)$	-503.33

Calculation of specific impulse

The specific impulse (I_{sp}) of the samples was calculated using NASA CEA software [9] based on the enthalpy of formation ($^{\Delta_f H^0_m}$) measured and calculated by a high-precision oxygen bomb calorimeter (ZDHW-HN7000C, Huaneng Instruments Co.), assuming ideal chemical equilibrium and isentropic expansion through a converging-diverging nozzle. The initial temperature of the system was set to 298.15 K, with a combustion chamber pressure of 6.98 MPa and a nozzle exit pressure of 0.1 MPa. The expansion ratio was adjusted to ensure that the nozzle exit pressure matched the specified external pressure.

3. Supporting Figures and Tables

Table S2 Performance comparison of all reported ADN cocrystals.

Compound	Density (298 K, g/cm³)	Oxygen balance (CO, %)	CRH [a] (%)	Specific impluse (I_{sp}, s)
ADN/18C6 [10, 11]	1.33	-66.59%	--	153 [c]
ADN/PDO [12]	1.78	0.00%	72.4%	259 [b]
ADN/Urea [13]	1.74	-13.11%	52.0%	--
ADN/ICM-102 [14]	1.69	0.00%	54.2%	236 [c]
ADN/DNBT [15]	1.85	10.13%	62.2%	258 [b]
ADN [15]	1.81	+25.80%	54.4%	202 [b]

[a] All CRH data above were measured under the same experimental conditions; [b] The specific impulse was calculated using Cheetah.7.0; [c] The specific impulse was calculated using NASA CEA.

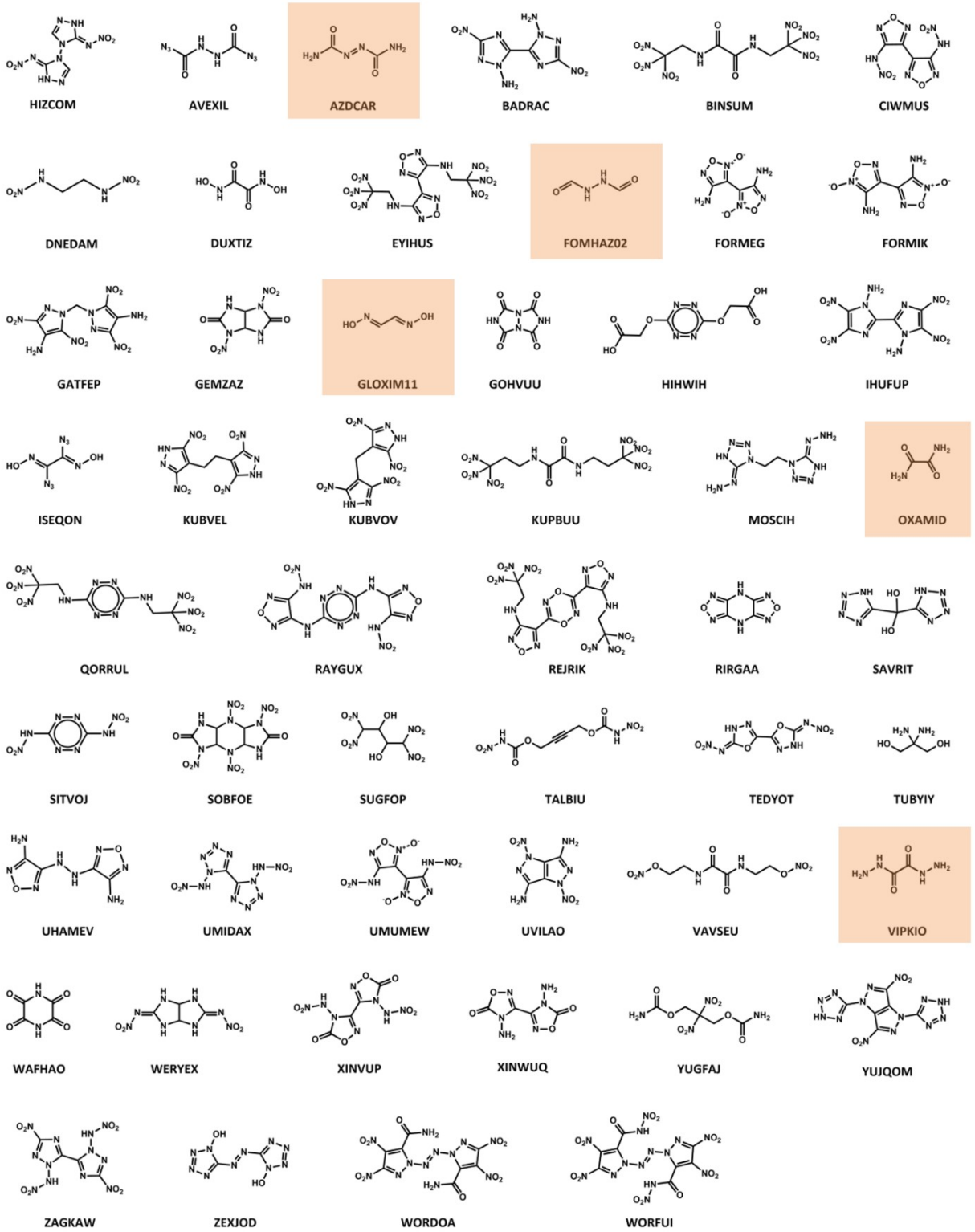

Fig. S1. Screening molecular formula of ADN cocrystal coformers. The molecules marked in orange are commercialized molecules.

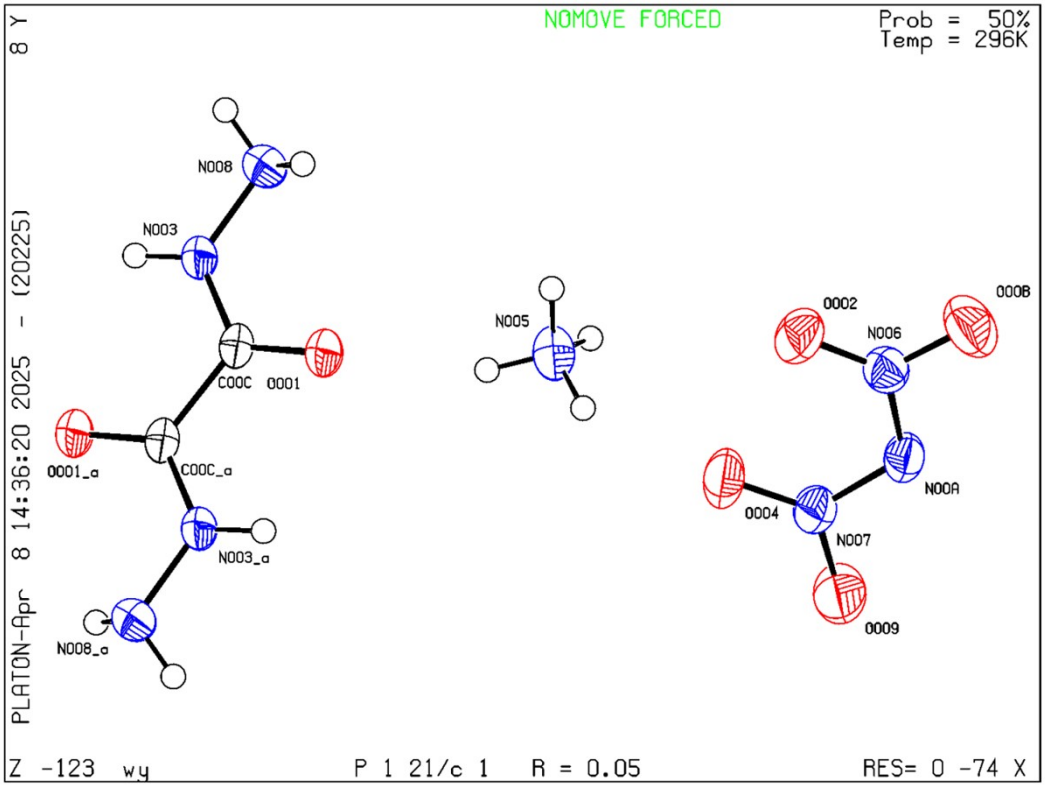

Fig. S2. Asymmetric unit of ADN/OHD. Anisotropic displacement parameters are drawn at 50% probability.

CCDC: 2456767.

Table S3. Crystal structure data.

	ADN/OHD	ADN/OHD (170 K)
empirical formula	$C_2H_{14}N_{12}O_{10}$	$C_2H_{14}N_{12}O_{10}$
space group	*P* 21/n	*P* 21/n
temperature (K)	296	170
a (Å)	7.9319(12)	7.9187(3)
b (Å)	6.6921(11)	6.5616(2)
c (Å)	13.836(2)	13.8804(4)
α (deg)	90	90
β (deg)	105.521(6)	105.586(1)
γ (deg)	90	90
Z	2	2
ρ_{calc} (g cm^{-3})	1.719	1.751
R_1	0.0449	0.0414
wR_2	0.1136(all data)	0.0995(all data)
S (goodness of fit)	1.049	1.117
data completeness	0.99	0.99
Deposition number	2456767	2456768

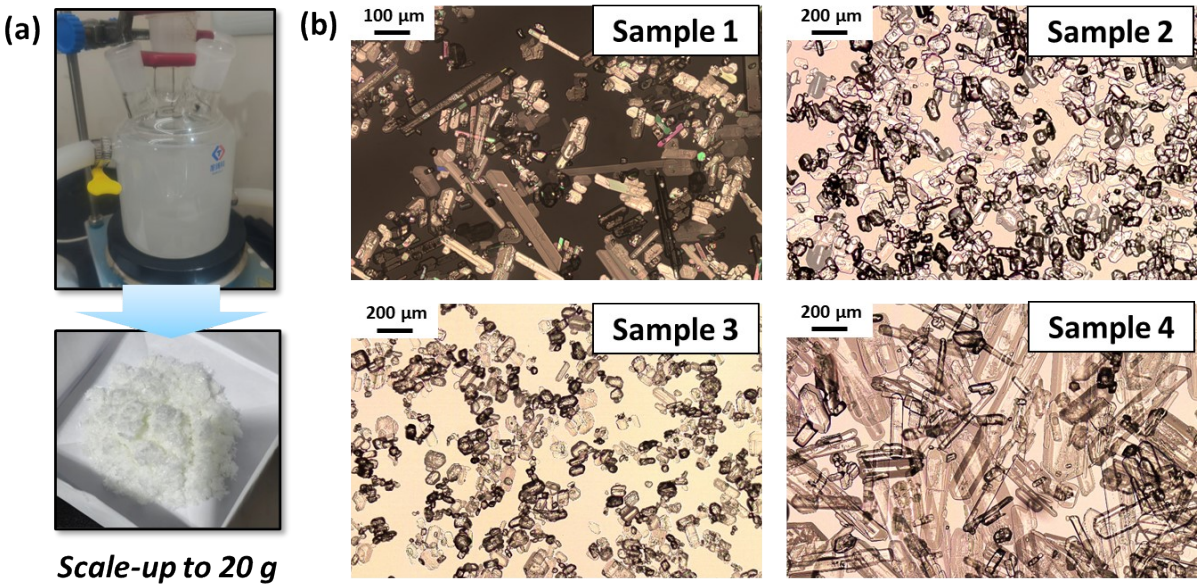

Fig. S3. (a) Scale-up preparation process and products of ADN/OHD cocrystal; (b) Crystal morphologies of the product obtained via different cooling crystallization conditions.

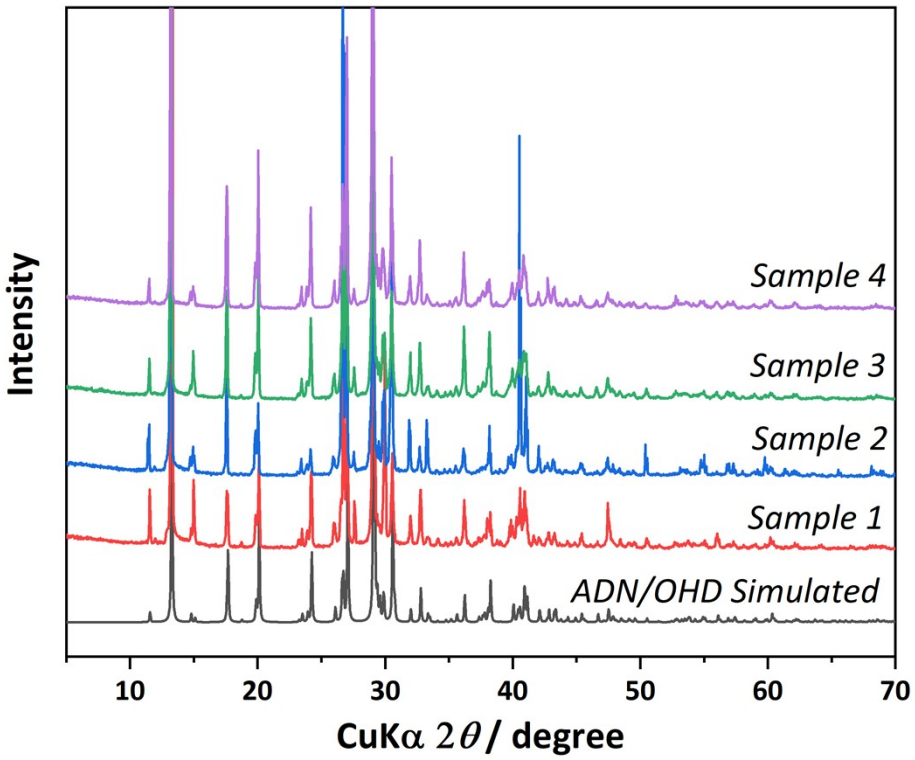

Fig. S4. The comparison of PXRD for the product obtained via different cooling crystallization conditions.

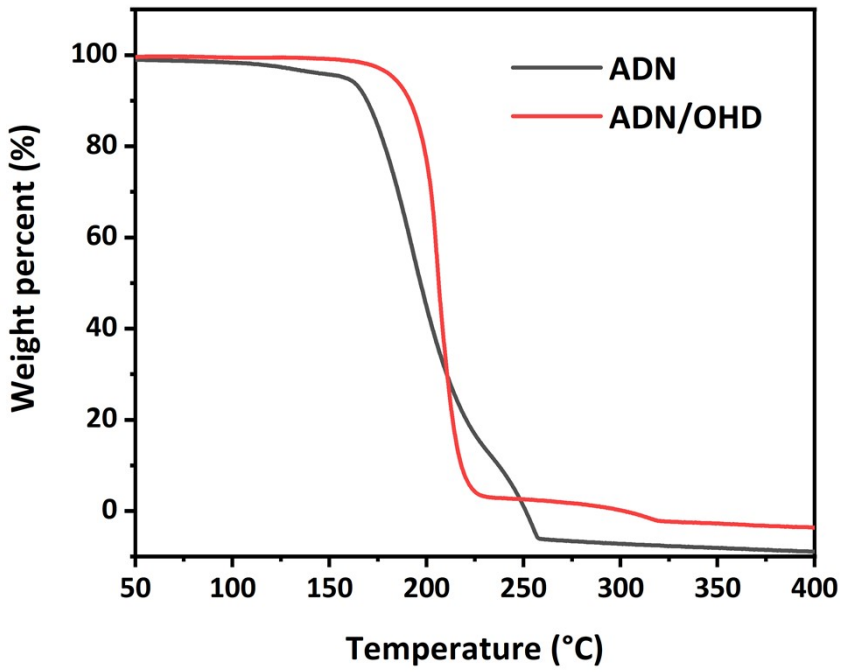

Fig. S5. TGA curves for ADN and ADN/OHD cocrystals.

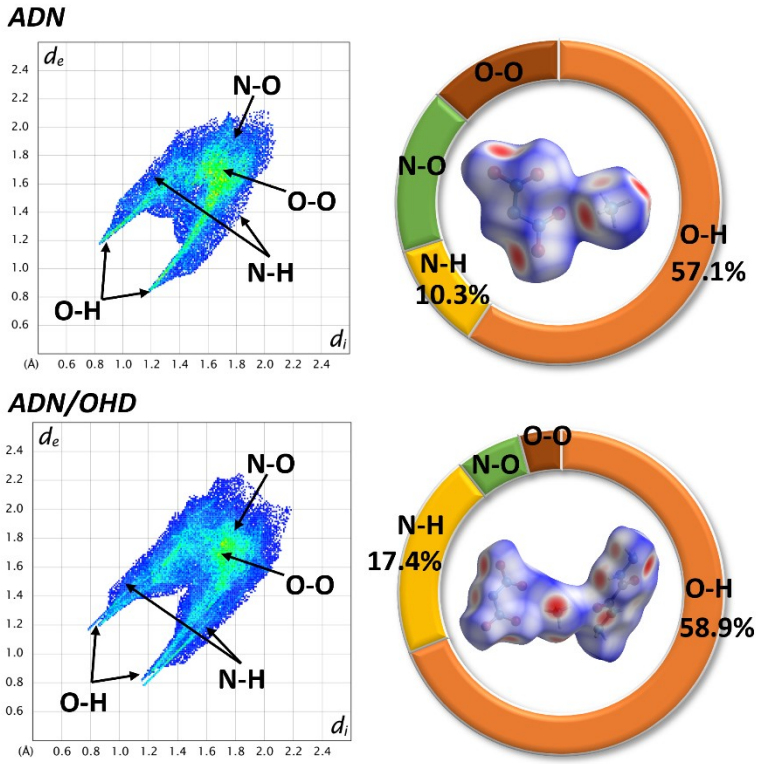

Fig. S6. 2D fingerprint plot generated by Hirshfeld surface and the main contributions of the intermolecular contacts to the Hirshfeld surface area in ADN and ADN/OHD.

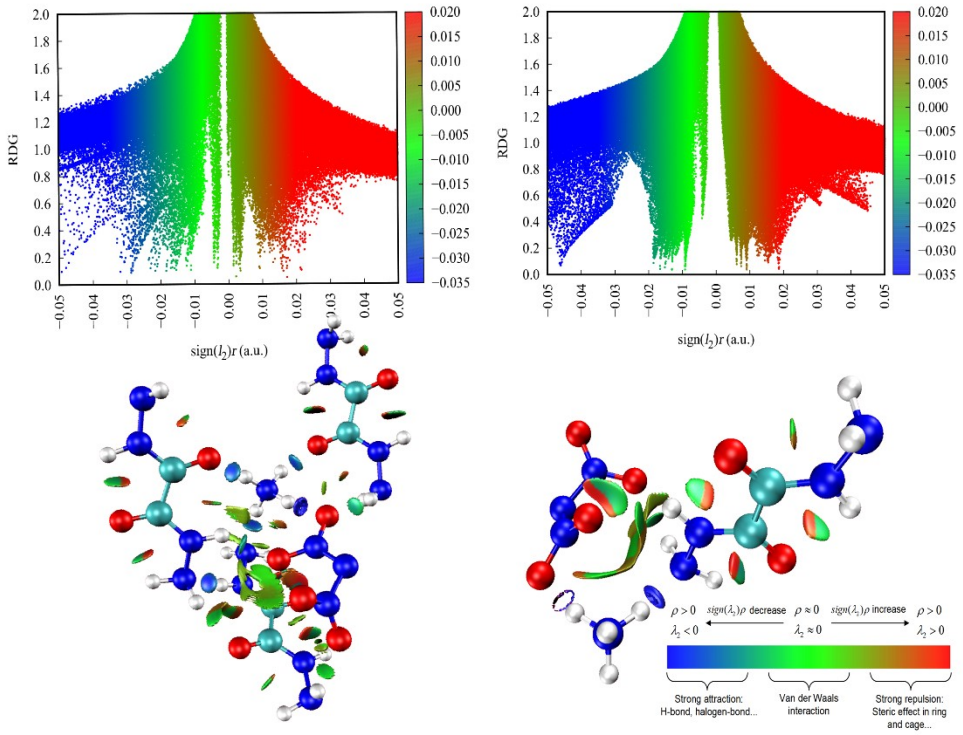

Fig. S7. Gradient isosurfaces and the reduced density gradient (RDG) versus effective density plots of ADN/OHD clusters around NH_4^+ (left) and N $(NO_2)_2^-$ (right).

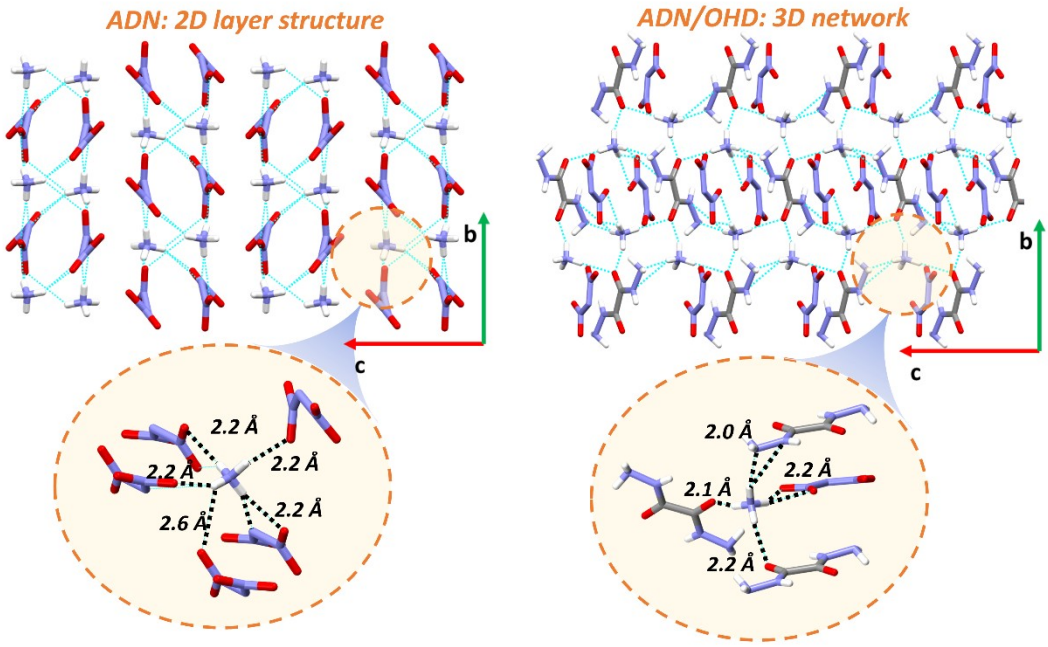

Fig. S8. Comparison of packing modes and hydrogen bonding interactions around ammonium ions of ADN and ADN/OHD.

Table S4. Parameters of DSC curves for the ADN/OHD cocrystal with different components.

System	Temperature				T_{P0}	ΔT_P
	5 K	10 K	15 K	20 K		
ADN/OHD	201.00	209.17	213.81	216.31	187.91	--
ADN/OHD+AP	201.03	209.14	213.83	218.22	186.38	**-1.53**
ADN/OHD+AL	199.15	206.89	211.85	215.18	187.48	**-0.43**
ADN/OHD+CL-20	199.86	206.40	211.38	216.86	189.70	**1.79**
ADN/OHD+HMX	201.67	209.54	214.02	217.64	187.88	**-0.03**
ADN/OHD+RDX	200.59	209.68	215.49	218.95	187.29	**-0.62**
ADN/OHD+GAP	200.59	209.68	215.49	218.95	187.29	**-0.62**

Table S5. The apparent activation energies and compatibility class for the ADN/OHD with different components.

Sample	E_a (kJ mol^{-1})	$\Delta E/E$ (%)	Class
ADN/OHD	163.32		
ADN/OHD +AP	86.23	47.2	**2**
ADN/OHD +AL	157.1	3.8	**1**
ADN/OHD +CL-20	150.54	7.82	**1**
ADN/OHD +HMX	160.69	1.61	**1**
ADN/OHD +RDX	152.37	6.70	**1**
ADN/OHD +HTPB	137.77	15.64	**1**
ADN/OHD +GAP	171.2	4.83	**1**

Table S6. Test conditions and test results of Electrostatic spark sensitivity.

Electrode gap	0.12 mm/0.25 mm/0.18 mm/0.50 mm	Polarity	Positive
Capacitance	10000 pF	Series resistance	0 Ω/100 kΩ
Number of tests	30	Charge per burst	25 mg
Experimental voltage	Upper limit: 10 kV	Experimental basis	GJB5891.27-2006 [16]
Environmental conditions	Temperature: 20°C, Humidity: 40%		
Experimental results	A 10000-pF capacitor was charged to 10.0 kV and subjected to 30 experiments under four different conditions: 0.12 mm with 0Ω, 0.25 mm with 0 Ω, 0.18 mm with 100 kΩ, and 0.50 mm with 100 kΩ. No ignition was observed in any of the experiments.		
Calculation results	50% ignition energy	E_{50} > 0.5 J	

The same test conditions were applied to both ADN and ADN/OHD, and the test results are consistent. 50% ignition energy is calculated according to formula (S6).

$$E_{50} = \frac{1}{2} C \hat{\mu}^2 \tag{S6}$$

E_{50}: value of 50% ignition energy, with units in Joules (J); C: measured value of the energy storage capacitor, with units in Farads (F); $\hat{\mu}$: value of the estimated mean ignition voltage, with units in Volts (V).

Table S7. Energetic performance of common oxidizers for solid propellants.

Sample	ρ [a] (g cm^{-3})	ΔH_f [b] (kJ mol^{-1})	I_{sp} [c] (s)	P_{cj} [d] (GPa)	D_v [e] (m s^{-1})
ADN/OHD	1.72	-503.33	251.28	29.50	8721.47
ADN	1.82	-150.00	202.34	28.90	8170.00
AP	1.95 [f]	-290.45 [f]	158.58	17.70 [g]	6430.00 [g]
AN	1.73 [f]	-365.56 [f]	160.64	21.30 [g]	7100.00 [g]

[a] Experimental crystal density (293 K). [b] Enthalpy of formation(calculated from heats of combustion). [c] Specific impulse (calculated). [d] Detonation pressure (calculated). [e] Detonation velocity (calculated). [f] Values are referred to Deyu Tian et. al. [17] [g] Values are referred to Matzger et. al. [12, 15]

4. References

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