Supporting Information

Direct Transformation of Nitriles to Cyanide Using Chloride Anion as Catalyst

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1. Experimental Section

1) General Information

Acetonitrile, propionitrile, butyronitrile, *N,N'*-dimethyl-formamide and chloroform were freshly distilled over CaH_2. Other commercial liquid nitriles were distilled over P_2O_5 before use. Tetrahydrofuran, 1,4-dioxane and diethyl ether were distilled over sodium under N_2. Solid nitriles were used as received. IR spectra were recorded on Bruker Vertex 70. HR-MS (ESI) spectra were obtained using a Bruker Impact II quardrupole time off light mass spectrometer. Elemental analysis of C, H and N was carried out on a Vario EL III CHNOS elemental analyzer. X-ray diffraction data were collected on an Oxford Diffraction Supernova dual diffractometer equipped with an Oxford Cryostream 700 low-temperature apparatus. Cu K\a radiation source ($\lambda = 1.54184$ Å) was used for the data collection.

2) General Methods for the Synthesis of $(Et_4N)_2[Zn(CN)_4]$ (2) with the Starting Materials of Nitriles Shown in Table S3.

***Method 1** with the starting material **1a**.* $ZnCl_2$ (13.6 mg, 0.1 mmol), Et_4NCl (66 mg, 0.4 mmol), NaOH (40 mg, 1.0 mmol) and MeCN (4 mL) were mixed in a 50 mL Schlenk tube under N_2 atmosphere. The mixture was vigorously stirred at 80 °C for 5 hours with the diffusion of air into the solution through the knob of outlet. A second portion of $ZnCl_2$ (13.6 mg, 0.1 mmol) was added, and the mixture was stirred for the other 7 hours. The resultant suspension was cooled, diluted with MeCN (20 mL), stirred for 20 minutes, and filtered. Solvent was removed and the residue was washed with THF/$CHCl_3$ (1 mL/3 mL). The remaining solid was dissolved in MeCN (10 mL) and filtered. The filtrate was added with THF (30 mL) to deposit the product as white solid (25.8 mg, 30%). The single crystal suitable for X-ray crystallography was obtained by diffusion of Et_2O into the solution of compound **2** in DMF. IR (KBr): v_{CN} 2132 cm^{-1}. Anal. Calcd. for $C_{20}H_{40}N_6Zn$: C, 55.87; H, 9.38; N, 19.55. Found: C, 56.05; H, 9.32; N, 16.46.

***Method 2** with the starting materials **1b** – **1i**, **1l**, **1p**, **1s**, **1t**, **1u** and **1v**.* $ZnCl_2$ (13.6 mg, 0.1 mmol), Et_4NCl (66 mg, 0.4 mmol), NaOH (40 mg, 1.0 mmol) and nitrile (4 mL) were mixed in a 50 mL Schlenk tube under N_2 atmosphere. The mixture was vigorously stirred at 80 °C for 5 hours with the diffusion of air into the solution through the knob of outlet. A second portion of $ZnCl_2$ (13.6 mg, 0.1 mmol) was added, and the mixture was stirred for the other 7 hours. The resultant suspension was cooled, added with THF (20 mL), and stirred for 15 minutes. The precipitate was collected, treated with MeCN (12 mL), and filtered. Solvent was removed and the residue was washed with THF/$CHCl_3$ (1 mL/3 mL). The remaining solid was dissolved in MeCN (10 mL) and filtered. The filtrate was added with THF (30 mL) to deposit the product as white solid. The yields of products are shown in Table S3.

***Method 3** with the starting materials **1j**, **1k**, **1m** – **1o**, **1q**, **1r**, **1w** – **1z**, **1aa**, and **1ab**.* $ZnCl_2$ (13.6 mg, 0.1 mmol), Et_4NCl (66 mg, 0.4 mmol), NaOH (40 mg, 1.0 mmol), nitrile (1.0 mmol), and 1,4-dioxane (3 mL) were mixed in a 50 mL Schlenk tube under N_2 atmosphere. The mixture was vigorously stirred at 80 °C for 5 hours with the diffusion of air into the solution through the knob of outlet. A second portion of $ZnCl_2$ (13.6 mg, 0.1 mmol) was added, and the mixture was stirred for the other 7 hours. The resultant suspension was cooled, added with THF (20 mL), and stirred for 15 minutes. The precipitate was collected by filter, treated with MeCN (12 mL), and filtered. Solvent was removed and the residue was washed with THF/$CHCl_3$ (1 mL/3 mL). The remaining solid was dissolved in MeCN (10 mL) and filtered. The filtrate was added with THF (30 mL) to deposit the product as white solid. The yields of products are shown in Table S3.

3) The Synthetic Procedure for the Reactions Shown in Figure 2.

a) **(Et$_4$N)$_2$[Ni(CN)$_4$] (3)**. NiCl$_2$ (25.9 mg, 0.2 mmol), Et$_4$NCl (66 mg, 0.4 mmol), NaOH (40 mg, 1.0 mmol) and MeCN (4 mL) were mixed in a 50 mL Schlenk tube under N$_2$ atmosphere. The mixture was vigorously stirred at 80 °C for 12 hours with the diffusion of air into the solution through the knob of outlet. The resultant suspension was cooled, diluted with MeCN (20 mL), stirred for 20 minutes, and filtered. Solvent was removed and the residue was washed with THF/CHCl$_3$ (1 mL/3 mL). The remaining solid was dissolved in MeCN (10 mL) and filtered. The filtrate was added with THF (30 mL) to deposit the product as pale white solid (18.6 mg, 22%). The structure of this compound was checked by X-ray crystallography with a fast data collection (20.0920, 20.0920, 19.6418; 90 90 90; v = 7929.2, space group C2/m), and the single crystal suitable for X-ray crystallography was obtained by diffusion of Et$_2$O into the solution of compound **3** in MeCN. IR (KBr): v_{CN} 2126 cm^{-1}. Anal. Calcd. for C$_{20}$H$_{40}$N$_6$Ni: C, 56.75; H, 9.53; N, 19.86. Found: C, 56.95; H, 9.60; N, 19.76.

b) **(Et$_4$N)$_2$[Zn(CN)$_4$] (2)**. Et$_4$NCl (66 mg, 0.4 mmol), NaOH (40 g, 1.0 mmol) and MeCN (4 mL) were mixed in a 50 mL Schlenk tube under N$_2$ atmosphere. The mixture was vigorously stirred at 80 °C for 12 h with the diffusion of air into the solution through the knob of outlet. Solvent was removed in *vacuo* to leave an organe-yellow solid, which was stirred with ZnCl$_2$ (27.2 mg, 0.2 mmol) in degassed MeCN (15 mL) for 10 hours under N$_2$ atmosphere. The mixture was filtered, and solvent was removed by rotary evaporator. The residue was washed with THF/CHCl$_3$ (1 mL/3 mL), dissolved in MeCN (10 mL), and filtered. The filtrate was added with THF (25 mL) to leave the compound **2** as white solid (20 mg, 23%).

c) **(Et$_4$N)$_2$[M(CN)$_4$] (M = Zn (2), Ni (3))**. A mixture of MCl$_2$ (0.2 mmol), Et$_4$NCl (66 mg, 0.4 mmol), NaOH (40 g, 1.0 mmol) and MeCN (4 mL) was packed in a 50 mL Schlenk tube under N$_2$ atmosphere. The tube was sealed and the mixture was vigorously stirred at 80 °C for 12 h to give an orange suspension, which was cooled to room temperature spontaneously. The suspension was opened to air and diluted with MeCN (20 mL). The mixture was stirred for 20 min, and filtered to remove some white precipitate. Solvent was removed by rotary evaporator to leave a little amount of solid residue, which is completely dissolved in THF/CHCl$_3$ (1 mL/3 mL). No product could be obtained.

d) **(Et$_4$N)$_2$[M(CN)$_4$] (M = Zn (2), Ni (3))**. MCl$_2$ (0.1 mmol), Et$_4$NCl (66 mg, 0.4 mmol), NaOH (40 g, 1.0 mmol), MeCN (4 mL) and water (10 μL) were mixed in a 50 mL Schlenk tube under N$_2$ atmosphere. The mixture was vigorously stirred at 80 °C for 4 h with the diffusion of air into the solution through the knob of outlet. A second portion of MCl$_2$ (0.1 mmol) was added, and the mixture was stirred for the other 8 h to give an orange suspension. The suspension was cooled, diluted with MeCN (20 mL), stirred for 20 min, and filtered. Solvent was removed by rotary evaporator, and the residue was washed with THF/CHCl$_3$ (1 mL/3 mL). The remaining solid was treated with MeCN (12 mL) and filtered. The filtrate was added with THF (25 mL) to deposit the product as white solid in 22% yield (19 mg for **2**, 18.6 mg for **3**).

e) **(Et₄N)₂[M(CN)₄] (M = Zn (2), Ni (3)).** MCl_2 (1.0 mmol), Et_4NCl (3.31 g, 20 mmol), NaOH (2.0 g, 50 mmol), and MeCN (200 mL) were mixed in a 500 mL Schlenk flask under N_2 atmosphere. The mixture was vigorously stirred at 80 °C for 8 h with the diffusion of air into the solution through the knob of outlet. After that, a total nine portions of MCl_2 were added successively, each 1.0 mmol for 8 h. The resultant mixture was cooled and diluted with MeCN (200 mL). The mixture were stirred for 1 h, and filtered to remove some white precipitate. Solvent was removed by rotary evaporator, and the residue was stirred with $THF/CHCl_3$ (50 mL/300 mL) for 30 min. The solid was collected, dissolved in MeCN (300 mL), and filtered. The filtrate was added with THF (750 mL) to deposit the product as white solid (0.77 g, 18% for **2**; 0.72 g, 17% for **3**).

2. X-ray Structure Determinations

Diffraction data were collected on an Oxford Diffraction Supernova dual diffractometer equipped with an Oxford Cryostream 700 low-temperature apparatus. Cu K\a radiation source (λ = 1.54184 Å) was used for the data collection. Single crystals were coated with Paratone-N oil and mounted on a Nylon loop for diffraction at 100 K. The data reduction and cell refinement were processed using CrysAlisPro software.[1] Structures were solved by direct methods using the SHELXTL program packages.[2] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were added geometrically. Crystal data and refinement details are given in Tables S1.
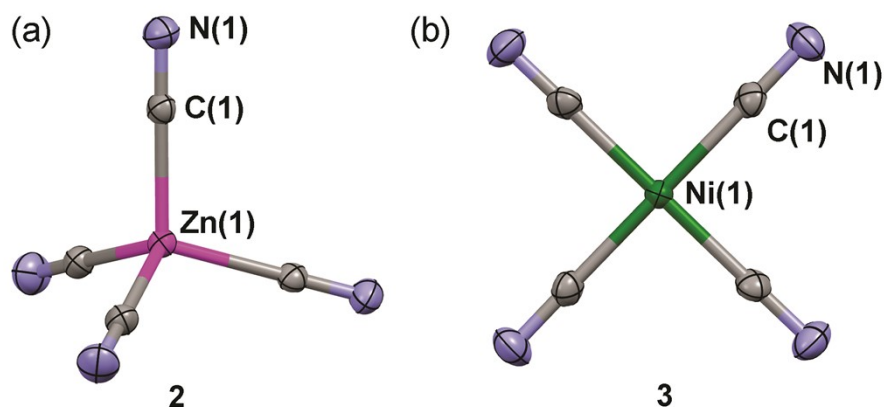
Fig. S1 Crystal structures of compounds $(Et_4N)_2[Zn(CN)_4]$ (**2**) and $(Et_4N)_2[Ni(CN)_4]$ (**3**), showing the thermal ellipsoids of 50% probability surfaces. The reported structure of compound **3** is shown here for comparison.

3. Crystallographic Data of Compound 2

Table S1. Crystallographic Data[a] for $(Et_4N)_2[Zn(CN)_4]$ (**2**)

	2
formula	$C_{20}H_{40}N_6Zn$
M	429.95
crystal system	monoclinic
space group	C2/c
a, Å	15.4081(3)
b, Å	10.2686(2)
c, Å	15.6427(3)
α, deg	90
β, deg	99.301(2)
γ, deg	90
V, Å^3	2442.44(8)
Z	4
μ, mm^{-1}	1.499
independent data	2363
refined parameters	123
$R_1{}^b$, $wR_2{}^c$ ($I > 2\sigma(I)$)	0.0223, 0.0601
R_1, wR_2 (all data)	0.0232, 0.0608

[a]T = 100(2) K, Cu Kα radiation (λ = 1.54184 Å). [b]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [c]$wR_2 = \{\Sigma[w(F_o{}^2 - F_c{}^2)^2/(F_o{}^2)^2]\}^{1/2}$.

4. Optimization of the Formation of Compound 2 (Table S2).[a]

$$\text{R−CN} + \text{Et}_4\text{NCl} + \text{ZnCl}_2 \xrightarrow[\text{80 °C, 12 h}]{\text{NaOH, air}} (\text{Et}_4\text{N})_2[\text{Zn(CN)}_4]$$
1 **2**

En	Zinc Salts	TEMA Salts	Base	Temp (°C)	Adding Mode	Nitrile Agents	Yields of **2**[b]	CN$^-$ Yields[c]
1	**ZnCl₂**	**Et₄NCl**	**NaOH**	**80**	**one portion**	**MeCN**	**24%**	**96%**
2	ZnBr₂	**Et₄NBr**	NaOH	80	one portion	MeCN	None	None
3	ZnI₂	**Et₄NI**	NaOH	80	one portion	MeCN	None	None
4	Zn(OTf)₂	**Et₄NOTf**	NaOH	80	one portion	MeCN	None	None
5	Zn(BF₄)₂	**Et₄NBF₄**	NaOH	80	one portion	MeCN	None	None
6	ZnCl₂	**NaCl**	NaOH	80	one portion	MeCN	None	trace
7	ZnCl₂	**None**	NaOH	80	one portion	MeCN	None	trace
8	ZnCl₂	Et₄NCl	**KOH**	80	one portion	MeCN	12%	48%
9	ZnCl₂	Et₄NCl	**K₂CO₃**	80	one portion	MeCN	10%	40%
10	ZnCl₂	Et₄NCl	**None**	80	one portion	MeCN	None	None
11	ZnCl₂	Et₄NCl	NaOH	**60**	one portion	MeCN	22%	88%
12	ZnCl₂	Et₄NCl	NaOH	**40**	one portion	MeCN	8%	32%
13	ZnCl₂	Et₄NCl	NaOH	80	**two portions**	**MeCN**	**30%**	**120%**
14	ZnCl₂	Et₄NCl	NaOH	80	**two portions**	**PhCH₂CN**	**36%**	**144%**
15	ZnCl₂	Et₄NCl	NaOH	80	**two portions**	**PhCN**	None	None
16	ZnCl₂	Et₄NCl	NaOH	80	**two portions**	**PhCH(Me)CN**	None	None

[a]Reaction conditions: zinc salt (0.2 mmol), TEMA salt (0.4 mmol), nitrile (4 mL), base (1.0 mmol), 80 °C; [b]Isolated yields based on zinc salts. [c]The CN$^-$ yields are four times the yields of compound **2**.

5. IR Spectra for Detecting the Generated $[Zn(CN)_4]^{2-}$ Moiety
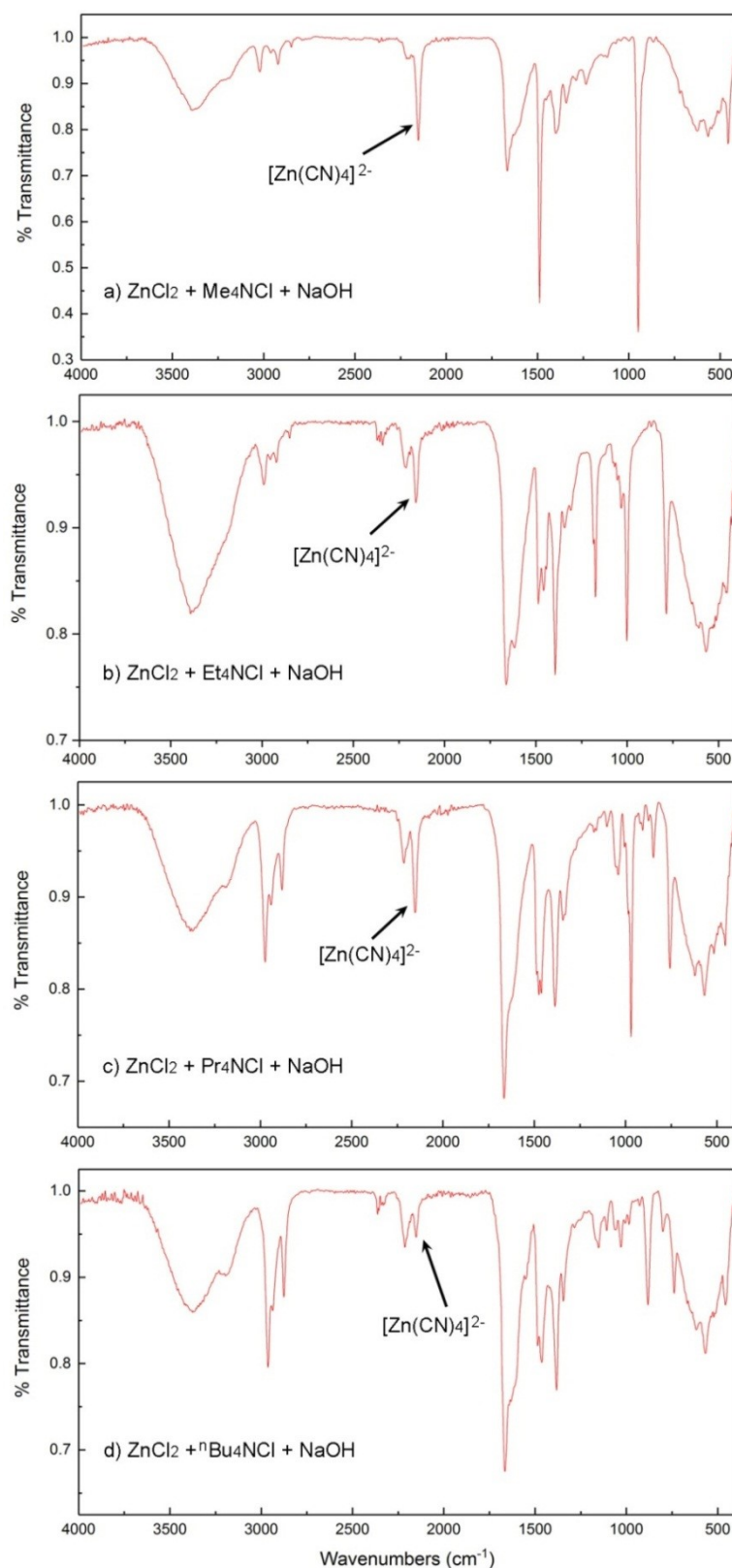
Fig. S2 IR spectra for detecting the generated $[Zn(CN)_4]^{2-}$ moiety with various cations. The reactions were conducted under the standard conditions by changing the chloride salts. Note: the PPNCl salt (bis(triphenylphosphine)iminium chloride) did not work in our reaction, for unknown reasons.

6. Scope of Nitriles 1 with Respect to Compound 2 (Table S3)[a,e]

$$ZnCl_2 \ + \ Et_4NCl \ + \ R-CN \xrightarrow[80\ ^oC,\ 12\ h]{NaOH,\ air} (Et_4N)_2[Zn(CN)_4]$$

1   **2**

MeCN **1a** (30%)   **1b** (13%)   **1c** (3%)   Ph—CN **1d** (2%)

1e (6%)   Cl—CN **1f** (12%)   **1g** (10%)   NC—CN **1h** (10%)

R—CN

R = 4-H (**1i**, 36%)
    4-OMe (**1j**, 10%)[b]
    4-^{i}Bu (**1k**, 6%)[b]
    4-Me (**1l**, 31%)
    4-Ph (**1m**, 20%)[b]
   4-Br (**1n**, 18%)[b]
    4-Cl (**1o**, 24%)[b]

4-F (**1p**, 26%)
4-CF$_3$ (**1q**, 12%)[b]
4-CN (**1r,** 5%)[b]
3-Me (**1s,** 27%)
3-F (**1t**, 21%)
2-Me (**1u,** 22%)
2-F (**1v**, 19%)
3,4-OMe (**1w,** 8%)[b]
3,5-Me (**1x,** 26%)[b]
3,6-Me (**1y**, 22%)[b]
4,6-F (**1z**, 20%)[b]

1aa (5%)[b]

1ab (7%)[b]
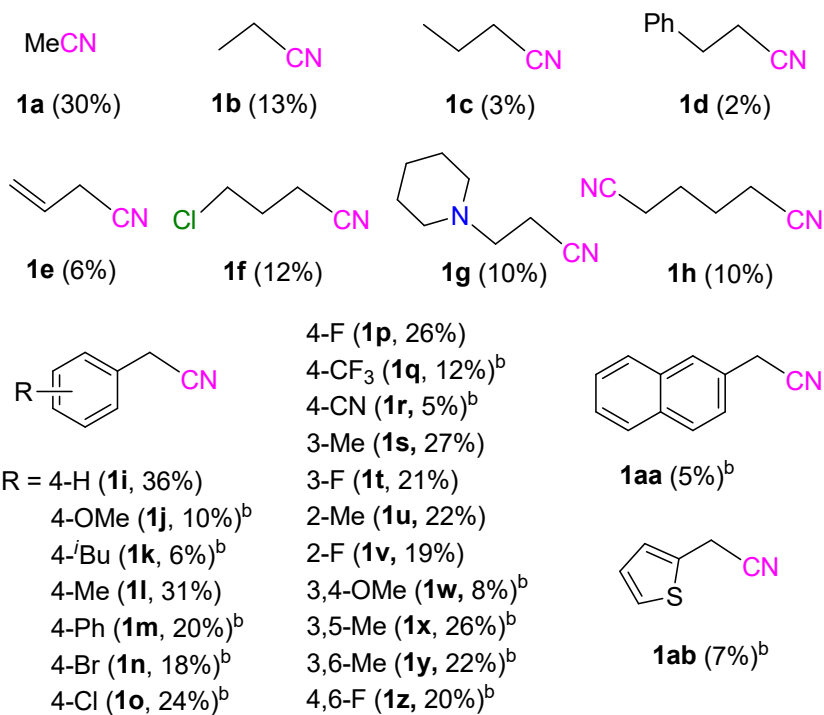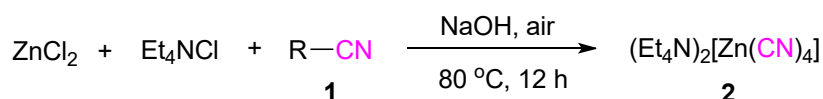
[a]Conditions: ZnCl$_2$ (0.2 mmol), Et$_4$NCl (0.4 mmol), NaOH (1.0 mmol), nitrile (4 mL), 80 °C, 12 h; [b]Conditions: ZnCl$_2$ (0.2 mmol), Et$_4$NCl (0.4 mmol), NaOH (1.0 mmol), nitrile (1.0 mmol), 1,4-dioxane (3 mL), 80 °C, 12 h; [c]Isolated yields; [d]The CN$^-$ yields are four times the yields of compound **2**. [e]ZnCl$_2$ was added in two portions.

    As the optimal reaction condition was determined, we set out to explore the scope of **1** for the generation of **2** (Table S3). When the alkyl-chain of nitriles increased, the yields decreased dramatically (**1b-1d**). Addition of functional groups to the alkyl nitriles might help to increase the production of the target compound (**1e-1h**). The phenylacetonitriles worked better than the alkyl nitriles (**1i-1z**). The steric effect on the reaction was studied by employing the methyl groups and the fluoro groups on the different positions of the phenyl rings of phenylacetonitriles (**1l, 1s, 1u; 1p, 1t, 1v**). It showed that the yields of reactions decreased with the increase of the steric hindrance from *para*-position to *ortho*-position. This result was consistent with that of the reactions, in which the yields of the reaction of the di-substituted nitriles were generally lower than those of the mono-substituted nitriles (**1w-1z**). In addition, the reactions of 1-naphthyl acetonitrile (**1aa**) and 2-thiopheneacetonitrile (**1ab**) afforded the same product. It seemed that the production of **2** in our system would be influenced by the polarity and thermal stability of nitriles, and the level of difficulty of the deprotonation of the α-H of nitriles.
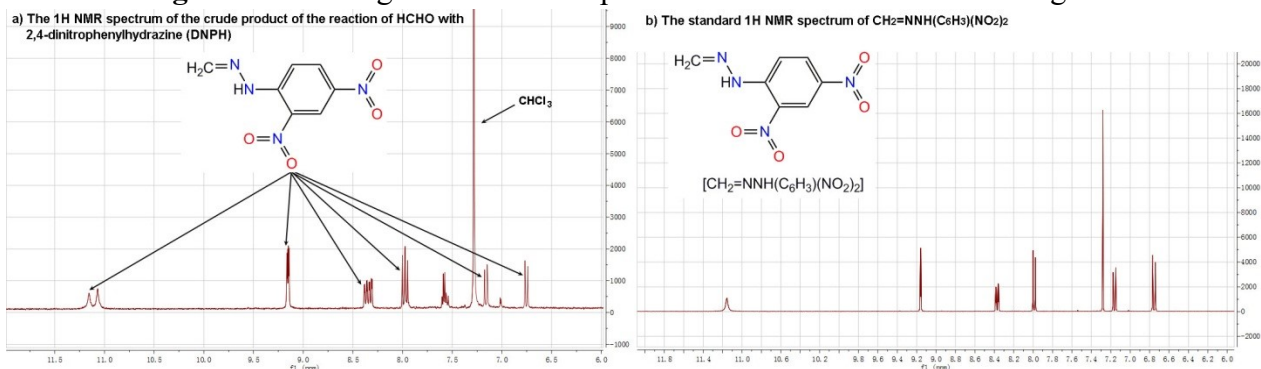
7. Experiment for Detecting the Generated Formaldehyde
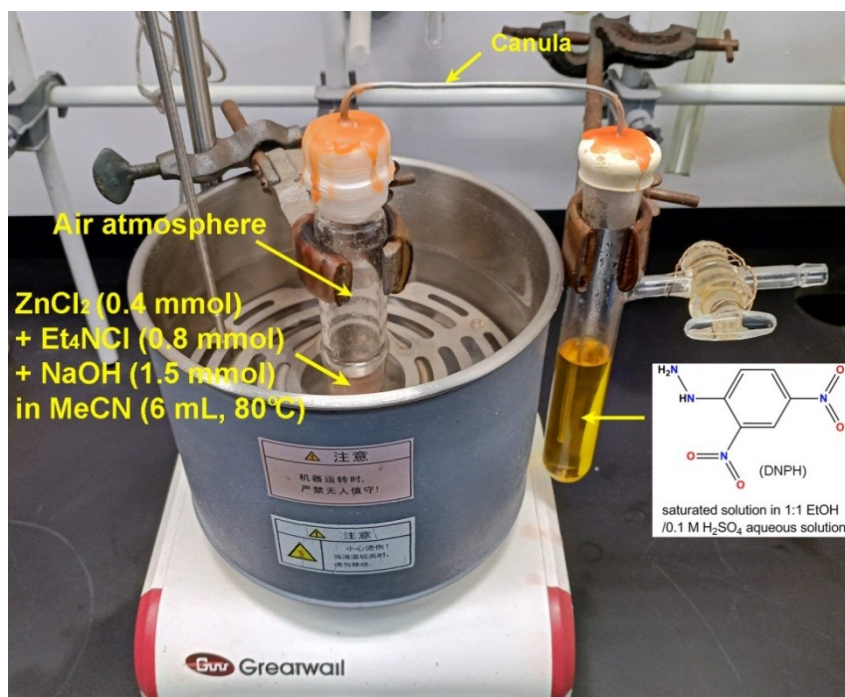
Fig. S3 Experiment for detecting the generated formaldehyde in the scission of CH_3–CN bond by the reaction $HCHO + NH_2NH(C_6H_3)(NO_2)_2 \rightarrow CH_2=NNH(C_6H_3)(NO_2)_2$.
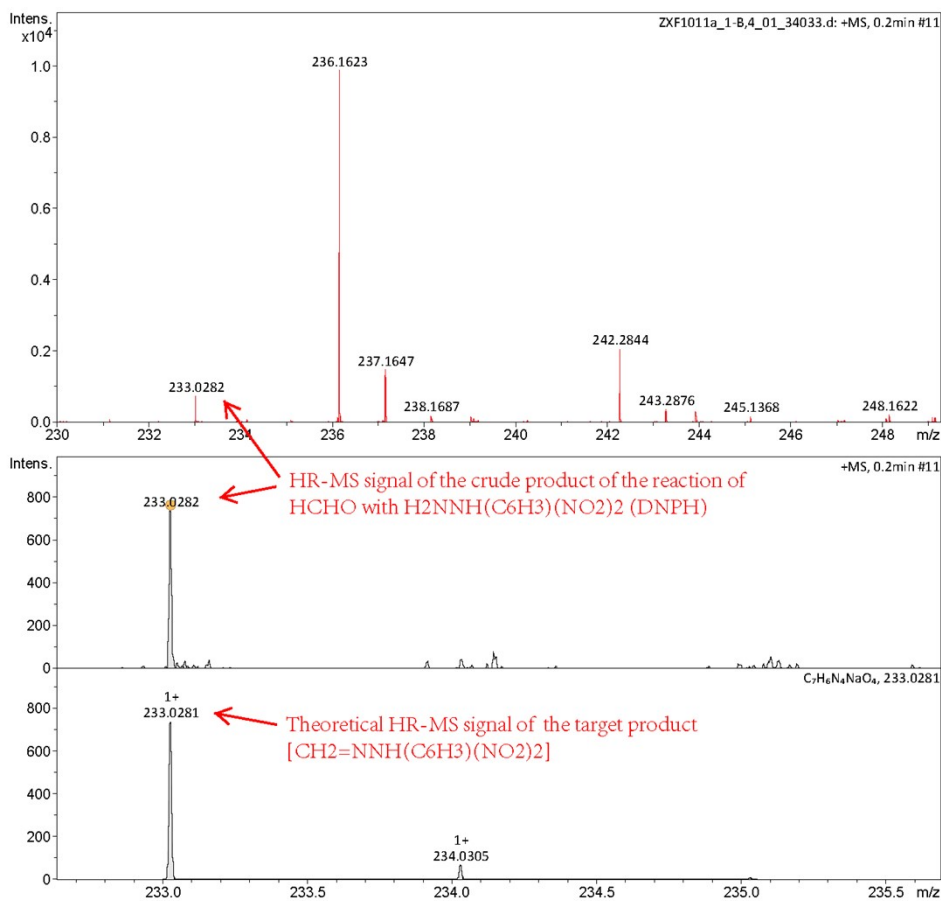
Fig. S5 ^{1}H NMR signal of the crude product of the reaction shown in Fig. S3.

8. Quantum Chemical Calculations

Density functional theory (DFT) geometry optimization of the states of (**a**)–(**h**) were performed using the B3LYP[3] functional implemented in the Gaussian 09 program package.[4] A basis set of 6-311++G** was used for all the ligand atoms (C, H, N, O and Cl). The B3LYP/6-311++G** Gibbs free energy profile are provided in Fig. 3. The calculated free energies are listed in Table S4. The calculated bond lengths and bond angles of (**a**)–(**h**) are listed in Table S5. The optimized geometry coordinates of intermediates are given in Table S6.

The computed reaction begins with the chloride anion approaching to the CN group of CH_3CN (a) from the reactants at infinite separation. The induction of the carbon atom leads to one pair electrons transfer from the C≡N bond to the terminal nitrogen atom, accompanying with the change of the bond angle C···C···N from 179.89° to 121.54°. One of hydrogen of CH_3 is induced by the pair electrons of the nitrogen atom and shifts from the carbon atom to the nitrogen atom to form a weakly associated precursor complex (b). From (b), the reaction proceeds with the release of chloride anion to give an imine complex (c). Two intermediate (c) molecules approach to one dioxygen molecule with the C=C bond heading to either one of oxygen atoms from the side direction. The closest contact occurs in the intermediate (d) between the C=C bonds and the oxygen atoms at distances close to the van der Waals separation (2.5–3.0 Å). The immediate product from (d) is the ethylene oxide imine complex (e) with the C_2ON unit locating at an approximate mirror plane. This product geometry can rearrange to the more stable COCN open conformation (f) by electron transfer from the C-C bond to the C-O bond. Further electron transfer from the C-O bond to the O-C bond leads to the elongation of the C-O bond in (g), from which the final products formaldehyde and cyanide anion were obtained depending on a large-scale decrease of free energy compared to the start (-76.7 kcal/mol). We note that our computational models do not include solvation effects, and hydrogen bonding is not addressed. These interactions may be contributors to the overall solution thermochemistry.

Table S4. Calculated free energies of (**a**)–(**h**) with B3LYP/6-311++G** method ($\Delta G = G_x - G_0$).

G_0 (a.u.)	G_x (a.u.)		ΔG (a.u.)	ΔG (Kcal/mol)
[(**a**) + Cl⁻ + OH⁻ + ½O₂]	[(**b**) + OH⁻ + ½O₂]	-743.9470	+0.0405	+25.41
	[(**c**) + Cl⁻ + OH⁻ + ½O₂]	-743.9512	+0.0363	+22.78
	[½(**d**) + Cl⁻ + OH⁻]	-743.9413	+0.0462	+28.99
-743.9875	[(**e**) + Cl⁻ + OH⁻]	-744.0088	-0.0213	-13.37
	[(**f**) + Cl⁻ + H₂O]	- 744.0479	-0.0604	-37.90

| | [(g) + Cl⁻ + H_2O] | -744.0123 | -0.0248 | -15.56 |
| | [(h) + Cl⁻ + H_2O] | -744.1097 | -0.1222 | -76.68 |

Table S5. Calculated bond lengths (Å) and bond angles (deg) of the structures of (**a**)–(**h**) with B3LYP/6-311++G** method.

(a)		(b)		(c)	
N(1)–C(1)	1.153	N(1)–C(1)	1.233	N(1)–C(1)	1.222
C(1)–C(2)	1.457	C(1)–C(2)	1.492	C(1)–C(2)	1.309
N(1)–C(1)–C(2)	179.89	Cl(1)···C(1)	2.010	N(1)–H(1)	1.020
		N(1)···H(1)	1.350	H(1)–N(1)–C(1)	116.46
		C(2)···H(1)	1.556	N(1)–C(1)–C(2)	174.23
		N(1)–C(1)–C(2)	121.54		
		N(1)···H(1)···C(2)	109.85		

(d)		(e)		(f)	
N(1)–C(1)	1.218	N(1)–C(1)	1.250	N(1)–C(1)	1.171
C(1)–C(2)	1.311	C(1)–C(2)	1.448	C(1)···C(2)	2.470
O(1)···C(1)	2.893	O(1)–C(1)	1.336	O(1)–C(1)	1.254
O(1)···C(2)	2.945	O(1)–C(2)	1.503	O(1)···C(2)	1.644
O(1)–O(1A)	1.224	N(1)–H(1)	1.018	N(1)–C(1)–C(2)	148.00
N(1)–H(1)	1.019	N(1)–C(1)–C(2)	159.08	N(1)–C(1)–O(1)	175.38
N(1)–C(1)–C(2)	171.70	N(1)–C(1)–O(1)	135.74	C(1)–O(1)–C(2)	116.31
O(1)–C(1)–C(2)	79.24	C(1)–O(1)–C(2)	61.00	O(1)–C(2)–C(1)	27.08
O(1)–C(2)–C(1)	74.83	O(1)–C(2)–C(1)	53.81	C(2)–C(1)–O(1)	36.62

(g)		(h)	
N(1)–C(1)	1.175	N(1)–C(1)	1.175
C(1)···C(2)	2.624		
O(1)···C(1)	1.539	O(1)–C(2)	1.202
O(1)–C(2)	1.362		
N(1)–C(1)–C(2)	169.79		
N(1)–C(1)–O(1)	146.17		
C(1)–O(1)–C(2)	129.46		
O(1)–C(2)–C(1)	26.92		
C(2)–C(1)–O(1)	23.62		
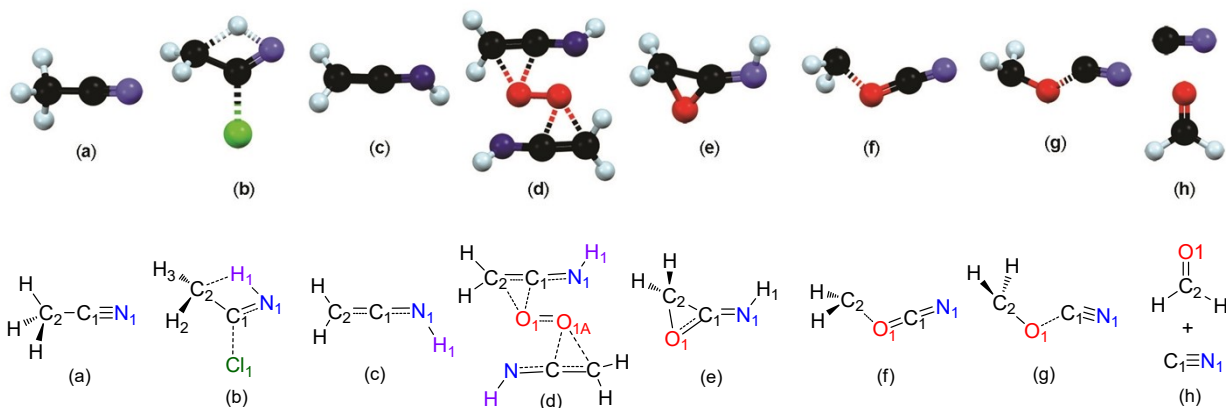
The structures showing the labels of atoms for the calculated bond lengths and bond angles

Table S6. Optimized geometry coordinates of calculated intermediates

Geometry optimized coordinates for (a)			
N	-1.433150	-0.000025	-0.000390
C	-0.280520	-0.000069	0.000863
C	1.176208	0.000060	-0.000200
H	1.552496	-0.537788	-0.872650
H	1.551865	1.024810	-0.029850
H	1.553528	-0.486793	0.901215

Geometry optimized coordinates for (b)			
Cl	-1.418578	-0.078920	0.000030
N	1.054660	1.322603	-0.000005
C	0.574148	0.187423	-0.000056
C	1.440924	-1.026924	-0.000134
H	2.046185	0.406055	-0.000533
H	1.297357	-1.643650	-0.894300
H	1.299222	-1.641978	0.895492

Geometry optimized coordinates for (c)			
N	-0.00017	1.239387	0.0377
C	0	0.053271	-0.0203
C	0.000165	-1.268	0
H	0.935397	-1.80877	0.0029
H	-0.93494	-1.809	0.0029
H	-0.00026	2.23046	-0.2871

Geometry optimized coordinates for (d)			
N	2.884964	-1.27068	0.042161
C	2.986715	-0.05106	0.056992
C	2.938546	1.255584	0.006945
H	3.322949	1.780223	-0.91008
H	2.517166	1.822416	0.877196
H	3.706047	-1.80043	0.432053
O	0.054043	0.515596	-0.14381
O	-0.2256	-0.67571	-0.16426
C	-2.93353	0.11638	0.061163
C	-3.05538	-1.18967	0.011859
H	-3.08914	-1.7719	0.926317
H	-3.16196	-1.69345	-0.93811
N	-2.6229	1.287599	0.096846
H	-3.35476	1.997385	0.149747

Geometry optimized coordinates for (e)			
O	-0.686298	0.851268	0.000000
N	1.552243	-0.001945	-0.000003

Geometry optimized coordinates for (f)			
O	-0.403751	0.576217	0.000317
N	1.860291	-0.286658	-0.000202

C	0.303337	-0.046561	-0.000001	C	0.750024	0.084282	0.000075
C	-1.029872	-0.611613	0.000003	C	-1.651677	-0.493419	-0.000607
H	-1.483365	-0.954388	0.924309	H	-2.189999	-0.076189	0.872870
H	-1.483370	-0.954390	-0.924300	H	-2.192115	-0.072123	-0.870799
H	1.950628	-0.938701	-0.000003				

Geometry optimized coordinates for (g)

O	0.541914	0.458441	-0.000074
N	-2.004693	-0.055819	-0.000058
C	-0.841027	-0.215959	0.000164
C	1.780789	-0.107185	-0.000041
H	2.029351	-0.669301	-0.909968
H	2.029616	-0.668628	0.910231

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