Supporting Information

A comparative study of the structures, thermal stabilities and energetic performances of two energetic regioisomers: 3(4)-(4-aminofurazan-3-yl)-4(3)-(4-nitrofurazan-3-yl)furoxan

Jiarong Zhang[a, c], Fuqiang Bi[b, c *], Lianjie Zhai[c], Huan Huo[c], Bozhou Wang[c *]

[a]. School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing, 100081, PR China

[b]. Key Laboratory of Applied Surface and Colloid Chemistry, MOE / School of Chemistry and Chemical Engineering, Shaanxi Normal University, Xi'an 710062, PR China

[c]. Xi'an Modern Chemistry Research Institute, Xi'an 710065, PR China

Corresponding authors

Prof. Bozhou Wang

E-mail address: wbz600@163.com

Dr. Fuqiang Bi

E-mail address: bifuqiang@gmail.com

NMR spectra

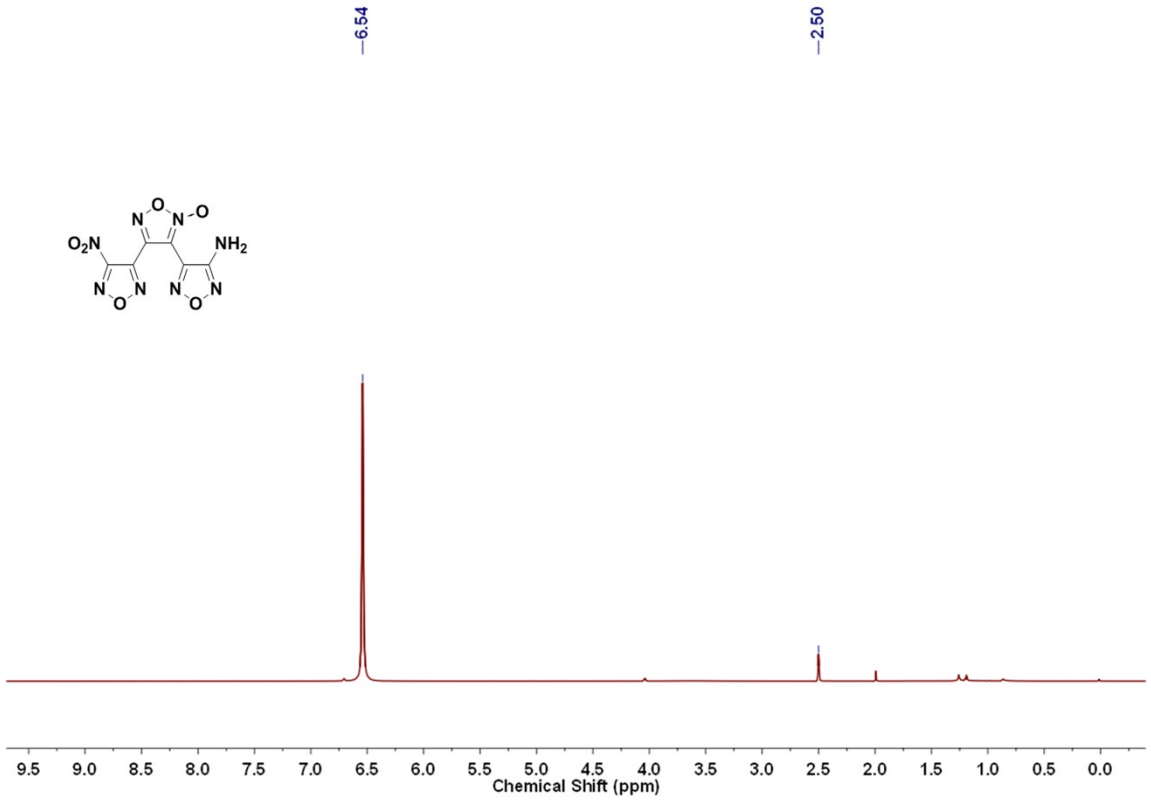

Figure S1. ^{1}H NMR spectrum of ANFF-34

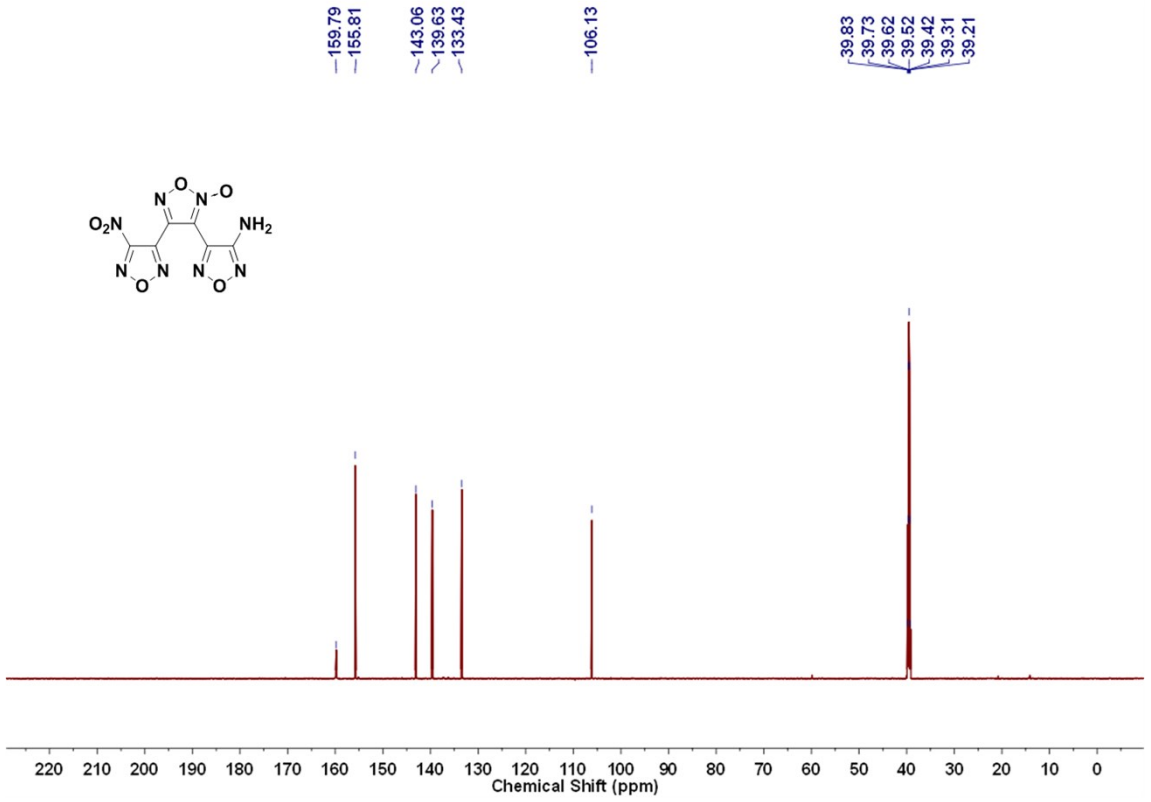

Figure S2. ^{13}C NMR spectrum of ANFF-34

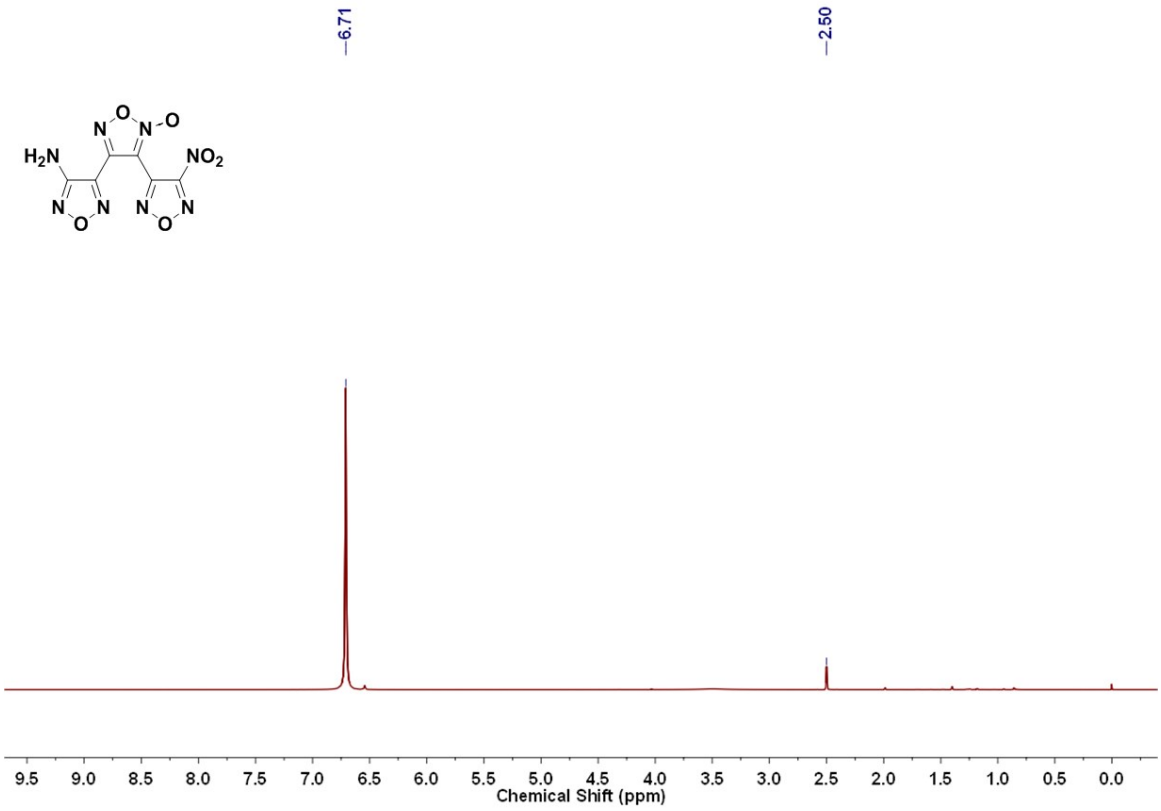

Figure S3. ^{1}H NMR spectrum of ANFF-43

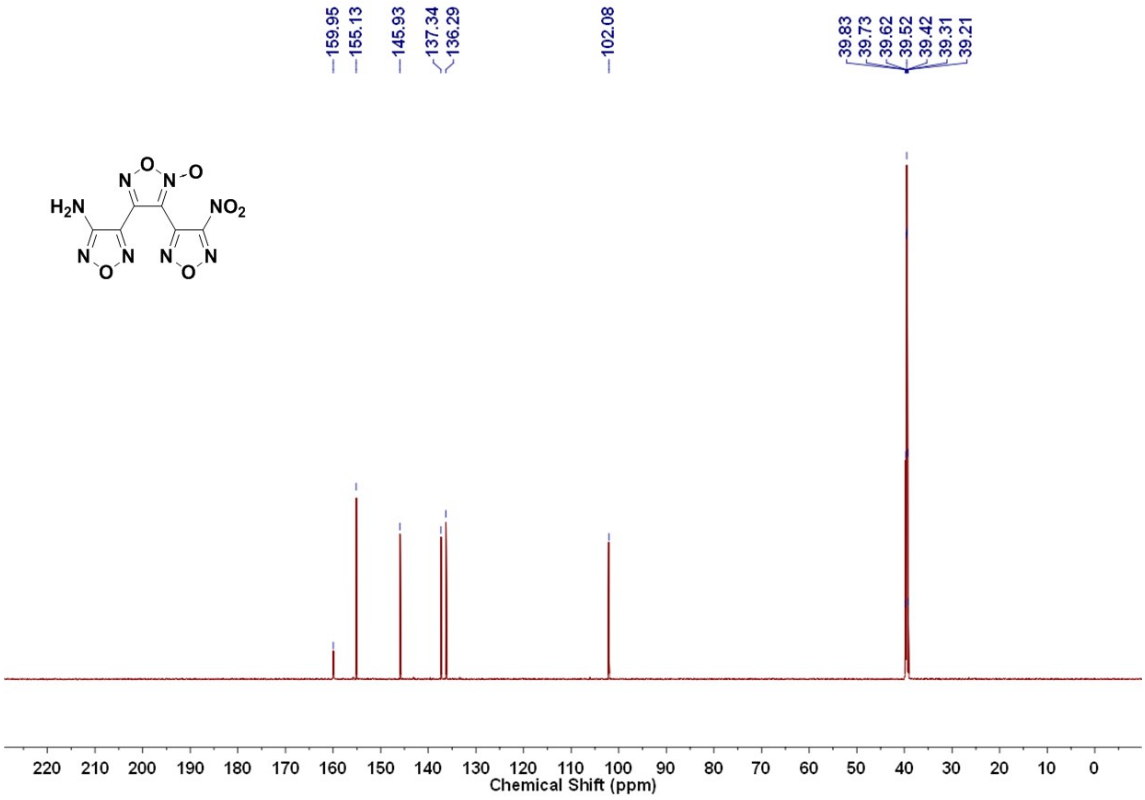

Figure S4. ^{13}C NMR spectrum of ANFF-43

Crystallographic data

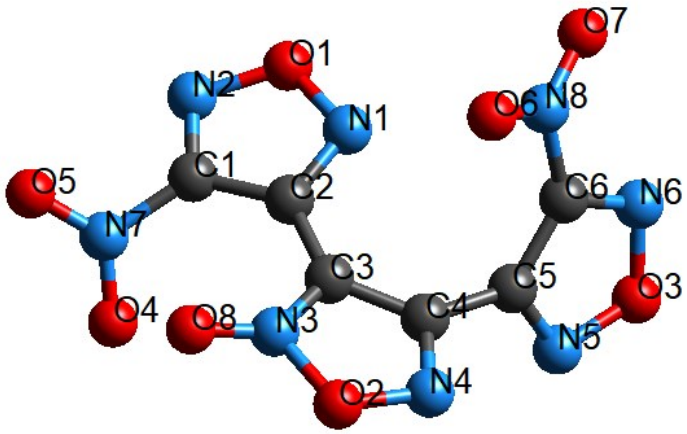

Figure S5. Single-crystal X-ray structures of DNTF

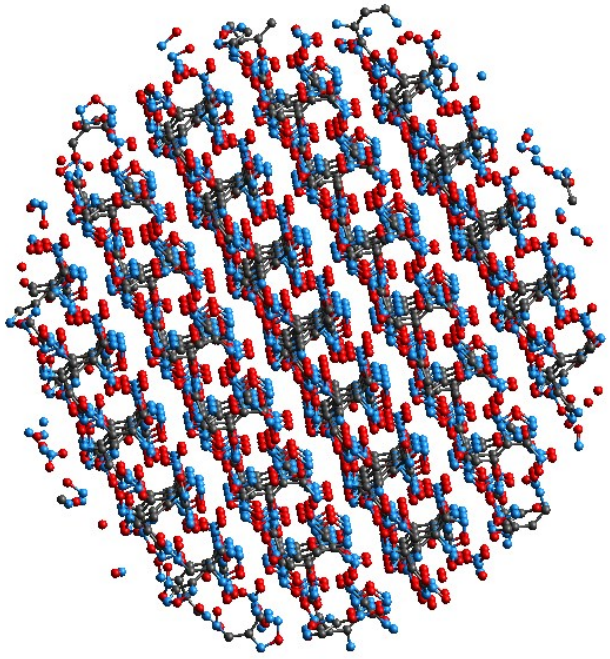

Figure S6. Crystal packing diagram of DNTF

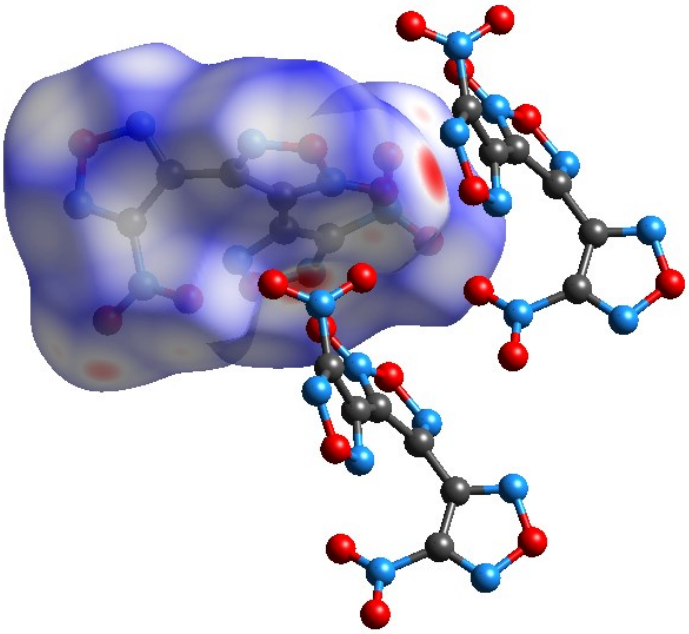

Figure S7. Hirshfeld surface of DNTF

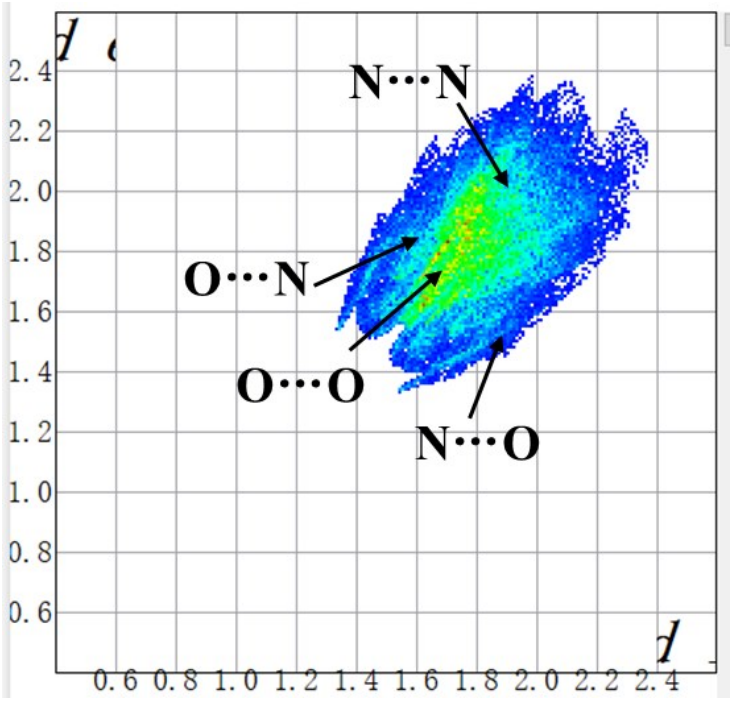

Figure S8. 2D fingerprint plot of DNTF

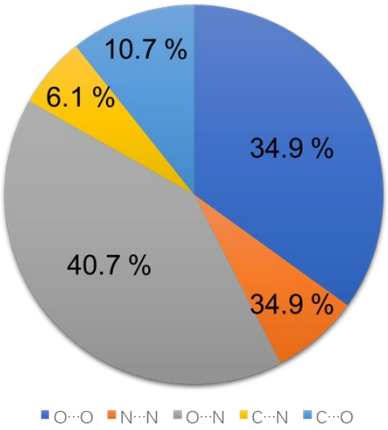

Figure S9. The contents of close interactions in DNTF

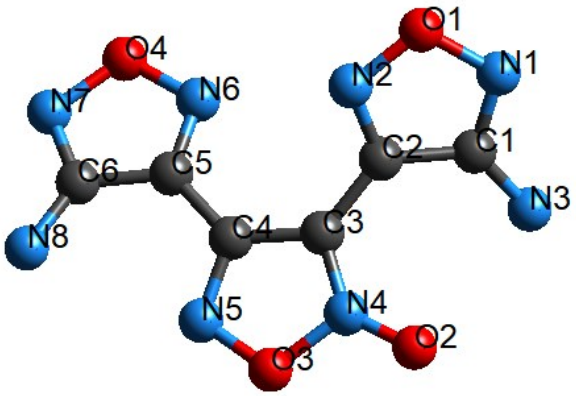

Figure S10. Single-crystal X-ray structures of DAFF

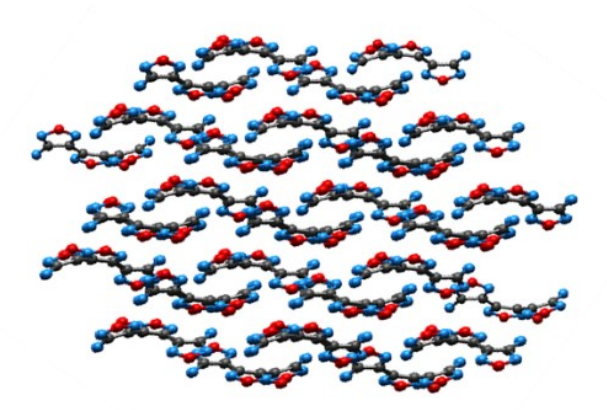

Figure S11. Crystal packing diagram of DAFF

IR spectra

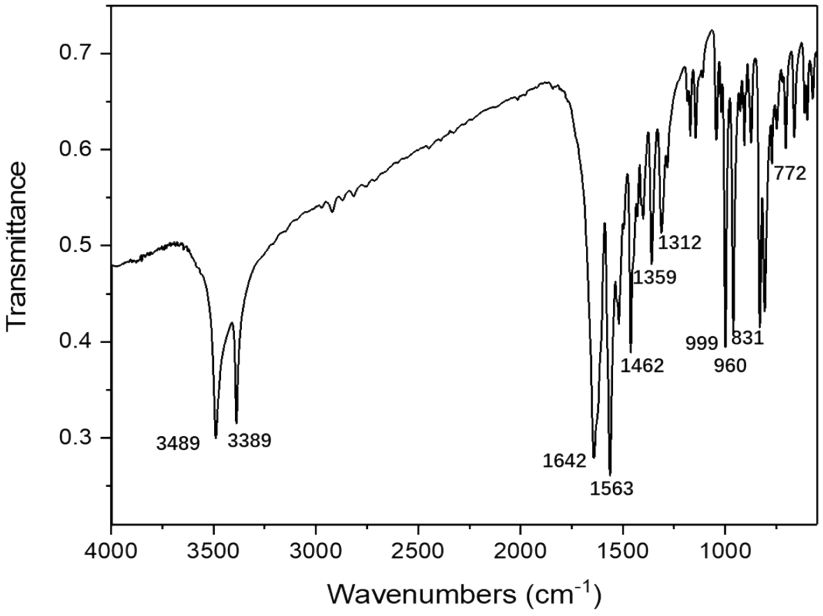

Figure S12. IR spectrum of ANFF-34

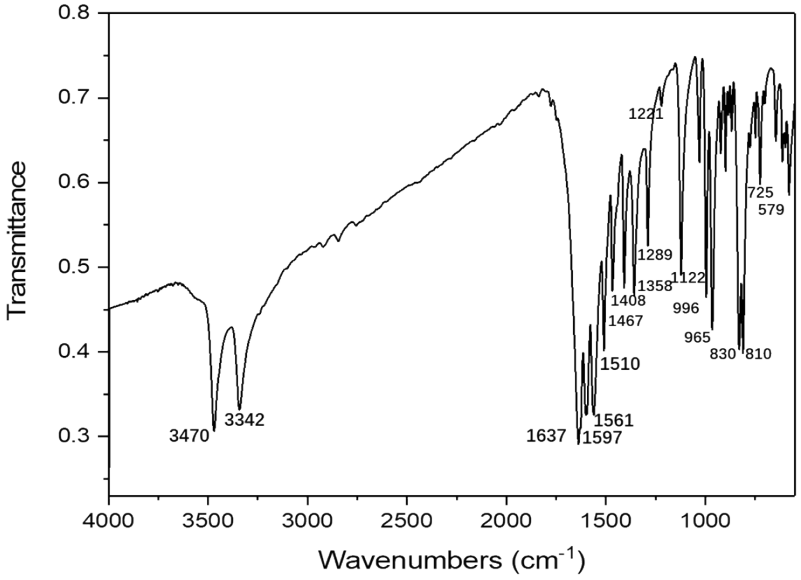

Figure S13. IR spectrum of ANFF-43

The apparatus and conditions of crystal structure determination

A single crystal of ANFF-34 suitable for X-ray diffraction analysis was prepared by slow evaporation of ethyl acetate and petroleum ether solvent at room temperature. A colorless crystal with dimension of 0.35 x 0.29 x 0.15 mm was selected for X-ray single crystal diffraction analysis. The diffraction data were collected on a BRUKER SMART Apex Ⅱ CCD X-ray diffractometer equipped with a Mo *K*α radiation (λ=0.71073 A) using an *ω*-*θ* scan mode at 296(2) K. A total of 5129 reflections were obtained in the range of 2.53≤θ≤25.09° , of which 1855 were independent (*R* int =0.0210) were considered to be observed and used for the refinement. The structure was solved by direct methods and refined by full-matrix least-squares techniques on F^2 using SHELES-97 and SHELXL-97 programs. A full-matrix least-squares refinement gave the final R_1= 0.0371 and ωR_2= 0.0883 (ω=1/[$\sigma^2(F_0^2)$ + (0.0270 P)^2 + 0.0000 P], where P =(F_0^2+2F_c^2)/3). The goodness-of-fit on F^2 is 1.027. The largest difference peak and hole were 0.166 and -0.159 e/Å^3.

A single crystal of ANFF-43 suitable for X-ray diffraction analysis was prepared by slow evaporation of ethyl acetate and petroleum ether solvent at room temperature. A colorless crystal with dimension of 0.36 x 0.30 x 0.16 mm was selected for X-ray single crystal diffraction analysis. The diffraction data were collected on a BRUKER SMART Apex Ⅱ CCD X-ray diffractometer equipped with a Mo *K*α radiation (λ=0.71073 A) using an *ω*-*θ* scan mode at 296(2) K. A total of 2650 reflections were obtained in the range of 2.08≤θ≤25.10° , of which 1911 were independent (*R* int =0.0273) were considered to be observed and used for the refinement. The structure was solved by direct methods and refined by full-matrix least-squares techniques on F^2 using SHELES-97 and SHELXL-97 programs. A full-matrix least-squares refinement gave the final R_1= 0.0630 and ωR_2= 0.2010 (ω=1/[$\sigma^2(F_0^2)$ + (0.0270 P)^2 +

0.0000 P], where P =(F_0^2+2F_c^2)/3). The goodness-of-fit on F^2 is 1.024. The largest difference peak and hole were 0.358 and -0.386 e/Å^3.

Table S1. Crystallographic data and structure refinement details for ANFF-34

compound	ANFF-34
Chemical formula	C6 H2 N8 O6
Crystal system	Monoclinic
Space group	P2(1) / n
a/ Å	7.7624(12)
b/ Å	13.253(2)
c/ Å	10.4256(16)
α/°	90
β/°	104.100(2)
γ/°	90
Volume/ Å^3	1040.2(3)
Z	4
Density/ g·cm^3	1.802
Temperature/K	296(2) K
Wavelength/ Å	0.71073 A
F(000)	568
No. of reflections measured	5129
No. of independent reflections	1855
R(int)	0.0210
R_1 (I>2σ(I))	0.0319
ωR(F^2) (I>2σ(I))	0.0837
R_1 (all reflections)	0.0371
Goodness-of-fit on F^2	1.027
CCDC number	2012930

Table S2. Crystallographic data and structure refinement details for ANFF-43

compound	ANFF-43
Chemical formula	C6 H2 N8 O6
Crystal system	Triclinic
Space group	P-1
a/ Å	6.188(8)
b/ Å	9.187(11)
c/ Å	10.300(13)
α/°	71.902(18)
β/°	84.505(18)
γ/°	82.972(19)
Volume/ Å^3	551.3(12)
Z	2
Density/ g·cm^3	1.700
Temperature/K	296(2) K

Wavelength/ Å	0.71073 A
F(000)	284
No. of reflections measured	2650
No. of independent reflections	1911
R(int)	0.0273
R_1 ($I>2\sigma(I)$)	0.0630
$\omega R(F^2)$ ($I>2\sigma(I)$)	0.2010
R_1 (all reflections)	0.0668
Goodness-of-fit on F^2	1.024
CCDC number	2012931

Table S3. Selected bond lengths (Å) and bond angles (°) of compound ANFF-34

Bond	Dist. (Å)	Bond	Dist. (Å)
N(1)-O(1)	1.2035(18)	N(1)-O(2)	1.2195(17)
N(1)-C(1)	1.441(2)	N(2)-C(1)	1.288(2)
N(2)-O(3)	1.366(2)	N(3)-C(2)	1.301(2)
N(3)-O(3)	1.389(2)	N(4)-C(3)	1.304(2)
N(4)-O(4)	1.364(2)	N(5)-O(5)	1.2224(18)
N(5)-C(4)	1.323(2)	N(5)-O(4)	1.4519(18)
N(6)-C(5)	1.296(2)	N(6)-O(6)	1.3594(17)
N(7)-C(6)	1.305(2)	N(7)-O(6)	1.3955(19)
N(8)-C(6)	1.337(2)	N(8)-H(8A)	0.86
N(8)-H(8B)	0.86	C(1)-C(2)	1.413(2)
C(2)-C(3)	1.470(2)	C(4)-C(5)	1.452(2)
C(5)-C(6)	1.441(2)		
Angle	(°)	Angle	(°)
O(2)-N(1)-O(1)	126.01	O(2)-N(1)-C(1)	118.19
O(2)-N(1)-C(1)	115.80	O(3)-N(2)-C(1)	109.78
O(3)-N(3)-C(2)	105.49	O(4)-N(4)-C(3)	106.87
C(4)-N(5)-O(5)	136.33	O(4)-N(5)-O(5)	116.80
O(4)-N(5)-C(4)	106.86	O(6)-N(6)-C(5)	106.38
O(6)-N(7)-C(6)	105.60	H(8A)-N(8)-C(6)	120.0
H(8B)-N(8)-C(6)	120	H(8B)-N(8)- H(8A)	120
N(3)-O(3)-N(2)	111.62	N(5)-O(4)-N(4)	107.96
N(7)-O(6)-N(6)	110.91	C(2)-C(1)-N(2)	111.94
N(1)-C(1)-N(2)	120.05	N(1)-C(1)-C(2)	127.97
C(3)-C(2)-C(1)	107.17	C(3)-C(2)-N(3)	121.00
C(3)-C(2)-C(1)	131.74	C(4)-C(3)-N(4)	111.96
C(2)-C(3)-N(4)	119.01	C(2)-C(3)-C(4)	129.03
C(3)-C(4)-N(5)	106.35	C(5)-C(4)-N(5)	125.30
C(5)-C(3)-C(3)	128.31	C(6)-C(5)-N(6)	109.09
C(4)-C(5)-N(6)	117.23	C(4)-C(5)-C(6)	133.68
N(8)-C(6)-N(7)	123.01	C(5)-C(6)-N(7)	108.02
C(5)-C(6)-N(8)	128.92		

Table S4. Hydrogen bond lengths (Å) and bond angles (°) of ANFF-34

D-H···A	d(D-H) (Å)	d(H…A) (Å)	d(D…A) (Å)	∠DHA(°)
N8-H8A···O2	0.860	2.290	3.137	168.50
N8-H8B···O5	0.860	2.122	2.872	145.41
N8-H8B···N3	0.860	2.559	3.070	119.04

Table S5. Selected bond lengths (Å) and bond angles(°) of compound ANFF-43

Bond	Dist. (Å)	Bond	Dist. (Å)
N(1)-O(1)	1.221(4)	N(1)-O(2)	1.225(4)
N(1)-C(1)	1.462(4)	N(2)-C(1)	1.297(4)
N(2)-O(3)	1.380(5)	N(3)-C(2)	1.305(4)
N(3)-O(3)	1.396(4)	N(4)-O(4)	1.237(3)
N(4)-C(3)	1.332(4)	N(4)-O(5)	1.456(3)
N(5)-C(4)	1.317(4)	N(5)-O(5)	1.380(4)
N(6)-C(5)	1.308(4)	N(6)-O(6)	1.370(3)
N(7)-C(6)	1.316(4)	N(8)-C(6)	1.358(4)
N(8)-H(8A)	0.86	N(8)-H(8B)	0.86
C(1)-C(2)	1.437(4)	C(2)-C(3)	1.472(4)
C(3)-C(4)	1.424(4)	C(4)-C(5)	1.465(4)
C(5)-C(6)	1.455(4)		
Angle	(°)	Angle	(°)
O(2)-N(1)-O(1)	126.64	C(1)-N(1)-O(1)	116.33
C(1)-N(1)-O(2)	117.04	O(3)-N(2)-C(1)	104.57
O(3)-N(3)-C(2)	105.28	C(3)-N(4)-O(4)	134.90
O(5)-N(4)-O(4)	118.39	O(5)-N(4)-C(3)	106.70
O(5)-N(5)-C(4)	106.77	O(6)-N(6)-C(5)	106.01
O(6)-N(7)-C(6)	105.64	H(8A)-N(8)-C(6)	120.0
H(8B)-N(8)-C(6)	120.0	H(8B)-N(8)- H(8A))	120.0
N(3)-O(3)-N(2)	111.60	N(4)-O(5)-N(5)	108.06
N(7)-O(6)-N(6)	111.03	C(2)-C(1)-N(2)	110.50
N(1)-C(1)-N(2)	121.32	N(1)-C(1)-C(2)	128.14
C(1)-C(2)-N(3)	108.05	C(3)-C(2)-N(3)	121.02
C(3)-C(2)-C(1)	130.92	C(4)-C(3)-N(4)	106.91
C(2)-C(3)-N(4)	121.20	C(2)-C(3)-C(4)	131.89
C(3)-C(4)-N(5)	111.52	C(5)-C(4)-N(5)	120.76
C(5)-C(4)-C(3)	127.52	C(6)-C(5)-N(6)	109.61
C(4)-C(5)-N(6)	120.59	C(6)-C(5)-C(6)	129.66
N(8)-C(6)-N(7)	124.92	C(5)-C(6)-N(7)	107.69
C(5)-C(6)-N(8)	127.36		

Table S6. Hydrogen bond lengths (Å) and bond angles (°) of ANFF-43

D-H⋯A	d(D-H) (Å)	d(H…A) (Å)	d(D…A) (Å)	∠DHA(°)
N8-H8A⋯N7	0.860	2.365	3.171	156.29
N8-H8B⋯N5	0.860	2.521	3.076	123.10

Table S7. Selected bond lengths (Å) and bond angles (°) of compound DNTF

Bond	Dist. (Å)	Bond	Dist. (Å)
N(1)-O(1)	1.377(3)	N(2)-O(1)	1.371(3)
N(4)-O(2)	1.371(3)	N(3)-O(2)	1.440(3)
N(6)-O(3)	1.369(3)	N(5)-O(3)	1.380(3)
N(3)-O(8)	1.199(3)	N(7)-O(5)	1.205(3)
N(7)-O(4)	1.211(3)	N(8)-O(7)	1.223(3)
N(8)-O(8)	1.220(3)	N(1)-C(2)	1.311(3)
N(2)-C(2)	1.288(3)	N(3)-C(3)	1.339(3)
N(4)-C(4)	1.306(3)	N(5)-C(5)	1.299(3)
N(6)-C(6)	1.296(3)	N(7)-C(1)	1.460(4)
N(8)-C(6)	1.455(3)	C(1)-C(2)	1.427(3)
C(2)-C(3)	1.445(3)	C(3)-C(4)	1.416(3)
C(4)-C(5)	1.472(4)	C(5)-C(6)	1.413(3)

Table S8. Selected bond lengths (Å) and bond angles (°) of compound DAFF

Bond	Dist. (Å)	Bond	Dist. (Å)
N(1)-O(1)	1.410(3)	N(2)-O(1)	1.374(3)
N(4)-O(3)	1.483(3)	N(5)-O(3)	1.361(3)
N(4)-O(2)	1.212(3)	N(6)-O(4)	1.367(3)
N(7)-O(4)	1.413(3)	N(1)-C(1)	1.310(3)
N(2)-C(2)	1.294(3)	N(4)-C(3)	1.318(3)
N(5)-C(4)	1.341(3)	N(6)-C(5)	1.293(3)
N(7)-C(6)	1.306(3)	N(3)-C(1)	1.346(4)
N(8)-C(6)	1.327 (3)	C(1)-C(2)	1.443(3)
C(2)-C(3)	1.450(3)	C(3)-C(4)	1.432(3)
C(4)-C(5)	1.449(4)	C(5)-C(6)	1.439(3)