Supplementary Information (SI) for CrystEngComm.

Supporting Information

Noncovalent Synergistic-Directed Crystallization (NSDC): A Halogen Engineering Strategy for Multifunctional Energetic Crystals

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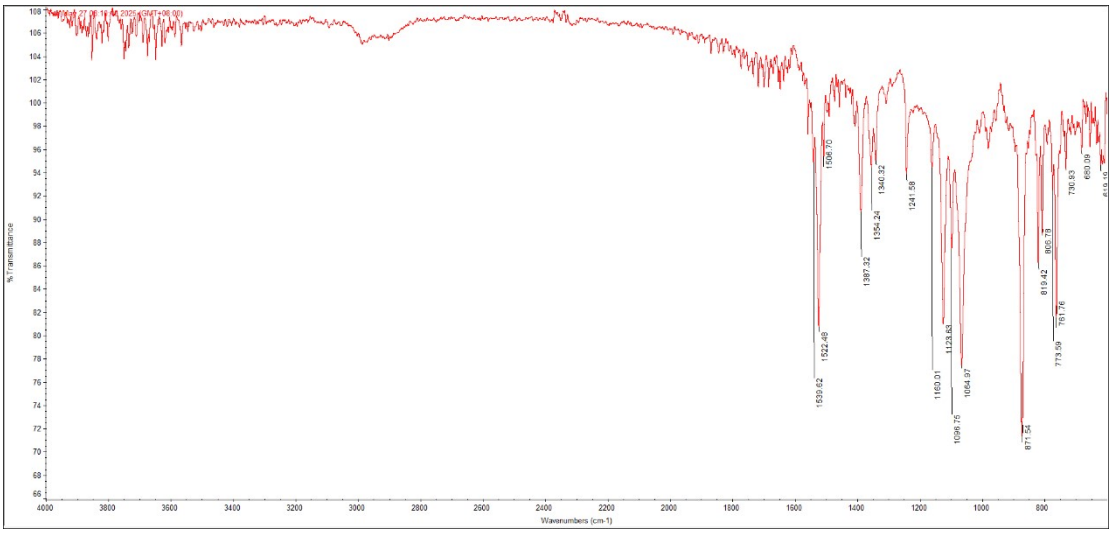
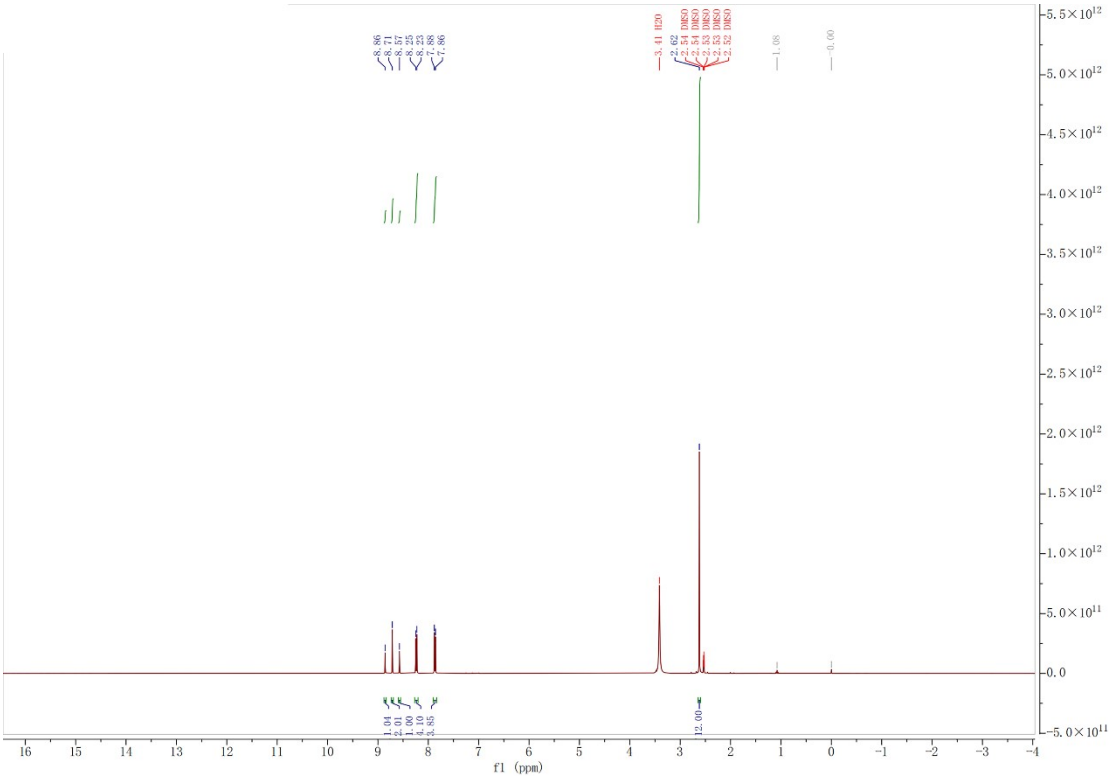
Content

1. Spectral data of DFMNBT and INP





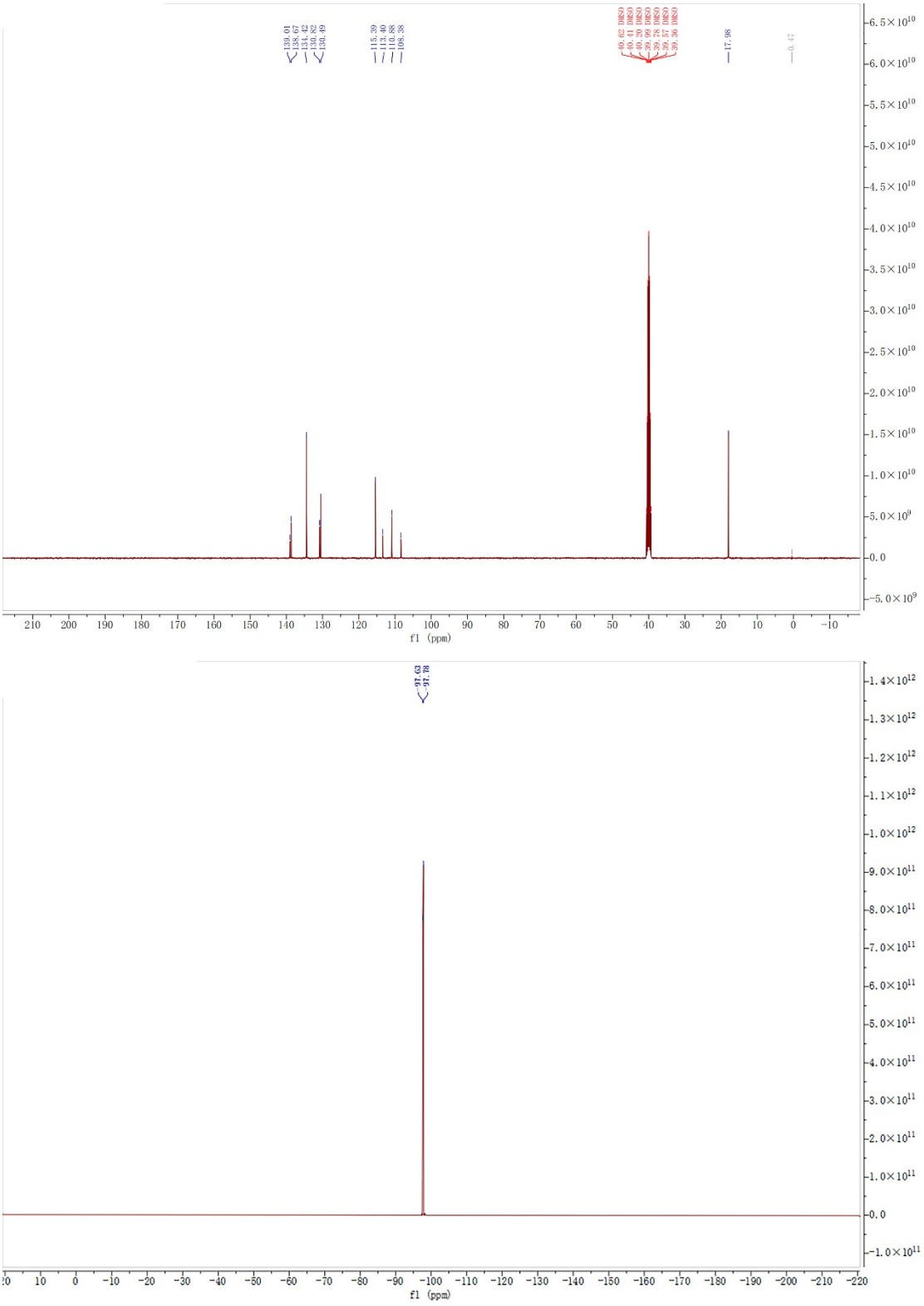
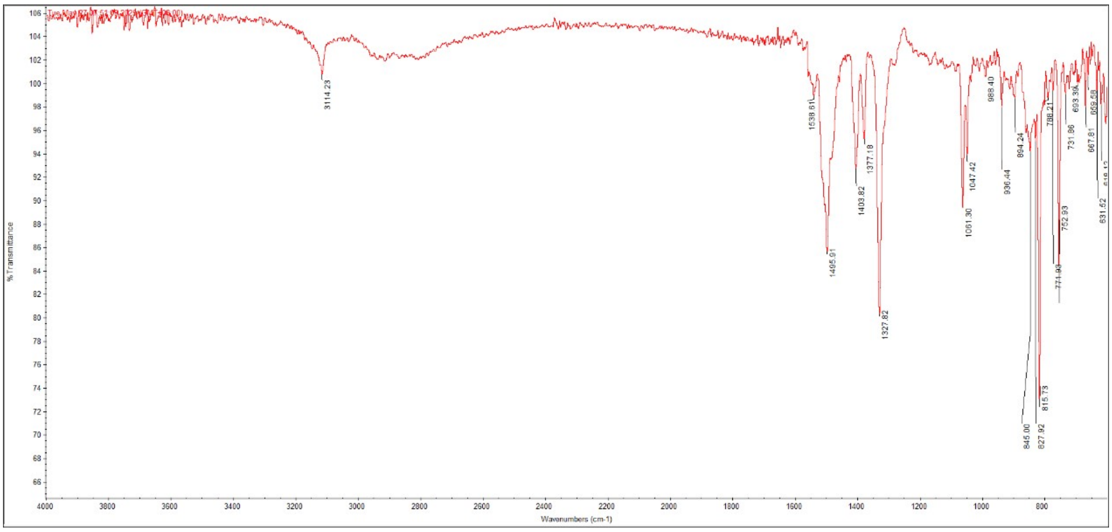
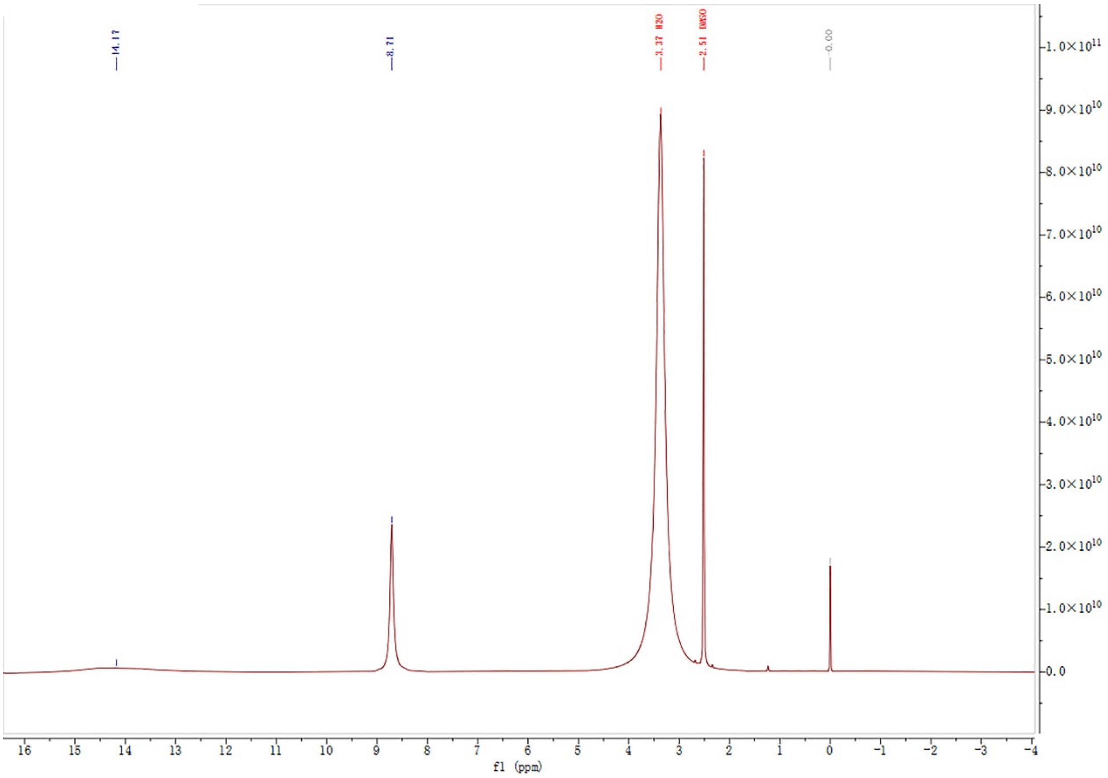


Fig. S1 Infrared spectrum, ^{1}H spectrum, ^{13}C spectrum and ^{19}F spectrum of DFMNBT



% Transmittance
Wavenumbers (cm-1)
3114.23
1539.61
1495.91
1403.82
1377.18
1327.82
1061.30
1047.42
988.40
936.44
894.24
845.00
827.92
815.73
788.21
771.93
752.93
731.86
693.39
667.81
631.62



14.17
8.71
3.37 H2O
2.51 DMSO
0.00
f1 (ppm)

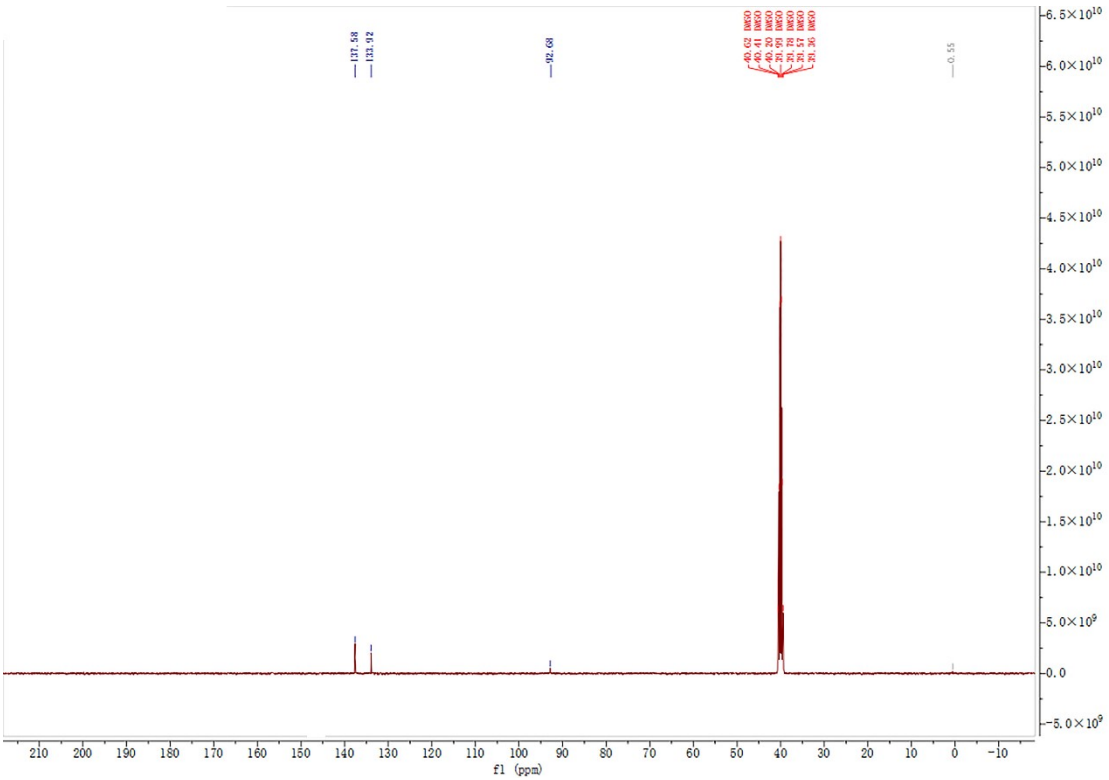


Fig. S2 Infrared spectrum, ^{1}H spectrum, and ^{13}C spectrum of INP

2. Crystallographic data

Table S1. Crystallographic data for DFMNBT and INP.

Comp.	DFMNBT	INP
Formular	$C_8H_6F_2N_4O_2$	$C_3H_2IN_3O_2$
M_W	228.17	238.98
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	P_{-1}
a [Å]	6.8400(3)	8.9073(6)
b [Å]	189.3788(8)	16.8666(11)
c [Å]	7.3602(4)	20.2753(13)
α [°]	90.00	67.857
β [°]	99.490	87.035
γ [°]	90.00	77.872
V [$Å^3$]	912.60(8)	2757.2(3)
Z	4	18
T [K]	100.00(10)	117.95(10)
ρ [g cm^{-3}]	1.661	2.591
μ [mm^{-1}]	1.323	5.151
F (000)	464	1980
θ range [°]	9.624 to 141.026	5.84 to 52
Index ranges	$-8 \le h \le 5$ $-22 \le k \le 19$ $-7 \le l \le 8$	$-10 \le h \le 10$ $-19 \le k \le 20$ $-22 \le l \le 24$
Data/restraints/parameters	1696/0/146	10575/432/730
GOF on F^2	1.024	1.037
R_1 [$F^2 > 2\sigma(F^2)$]	0.0351	0.0632
wR_2 (F^2)	0.0941	0.0943