Electronic Supplementary Information

Strategic Modular Assembly of Trifluoromethylated Energetics via Triazine-Based Scaffolds

Jiyuan Yu [a], Xiangyan Miao [a], and Yuchuan Li [a,*]

a. School of Materials Science & Engineering, Beijing Institute of Technology, Beijing 100081, China.

E-mail: liyuchuan@bit.edu.cn

Table of Contents

1. X-ray crystallograph

X-ray of all single crystals were carried out at 170 K on a Bruker D8 VENTURE diffractometer using Mo-Kα radiation (λ = 0.71073Å). Integration and scaling of intensity data was performed using the SAINT program. Data were corrected for the effects of absorption using SADABS. The structures were solved by direct methods and refined with full-matrix least-squares technique using SHELX-2014 software. Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were places in calculated positions and refined with riding model.

Table S1 Crystal data of **4**.

Compound	**4**	**5**
CCDC	2525729	2530986
Empirical formula	C29H0.50Cl4F12N48O18.20	C7H18F3N13O8
Formula weight	1682.35	469.34
Temperature	170.00 K	100 K
Crystal system	Triclinic	Triclinic
Spance group	*P-1*	*P-1*
Unit cell dimensions	a = 13.619(2) Å α = 69.224(6)° b = 15.295(3) Å β = 69.711(6)° c = 17.404(2) Å γ = 83.327(7)°	a = 8.1025(10) Å α = 93.339(5)° b = 8.1837(11) Å β =97.166(5)° c = 14.7785(16) Å γ =99.686(6)°
Volume	3179.2(9) Å^3	955.3(2) Å^3
Z	2	2
Density(calculated)	1.757 g cm^{-3}	1.632 g cm^{-3}

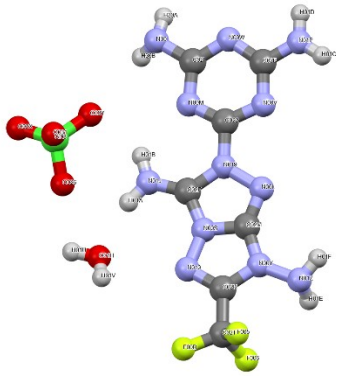


Figure S1. Single-crystal X-ray structures of **4**.

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **4**. *Ueq* is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	**x**	**y**	**z**	***U(eq)***
Cl(01)	17102(2)	1266(2)	-10437(1)	44(1)
Cl(02)	15653(2)	2322(2)	-5227(2)	49(1)
Cl(03)	10585(2)	4694(2)	-6272(2)	58(1)
Cl(00)	18854(3)	5196(3)	-8808(3)	97(1)

F(005)	13326(4)	293(4)	-2123(3)	57(2)
F(006)	12067(4)	-571(4)	-1921(3)	57(2)
F(007)	15524(4)	2691(4)	-12897(3)	66(2)
F(008)	14228(5)	2087(5)	-12964(3)	67(2)
F(009)	14145(6)	3492(4)	-12952(4)	75(2)
F(00A)	7532(5)	5695(4)	-6242(4)	67(2)
F(00B)	6179(5)	4892(4)	-5847(4)	74(2)
O(00C)	12714(5)	6223(5)	-7732(4)	46(2)
F(00D)	11782(5)	824(4)	-1899(4)	79(2)
F(00E)	20754(5)	1520(5)	-10023(4)	78(2)
F(00F)	21054(4)	2524(5)	-11278(4)	79(2)
N(00G)	10188(5)	823(5)	-4389(4)	34(2)
N(00H)	13056(5)	1413(5)	-9056(4)	33(2)
N(00I)	9180(5)	833(5)	-2966(4)	35(2)
N(00J)	13249(5)	2201(5)	-10376(4)	36(2)
N(00K)	11430(5)	-322(5)	-4505(4)	39(2)
N(00L)	13772(5)	879(5)	-5414(4)	39(2)
N(00M)	13211(5)	2885(5)	-7079(4)	37(2)
F(00N)	6400(6)	5512(5)	-5000(4)	82(2)
N(00O)	16920(5)	3966(5)	-9245(4)	37(2)
N(00P)	13227(5)	320(5)	-7795(4)	38(2)
N(00Q)	18963(5)	3258(5)	-10742(4)	37(2)
N(00R)	18212(5)	3037(5)	-9374(4)	36(2)
N(00S)	12603(5)	1476(5)	-4480(4)	38(2)
N(00T)	13793(5)	913(5)	-9539(4)	38(2)
N(00U)	7340(5)	3938(5)	-4361(4)	37(2)
N(00V)	14471(5)	1671(5)	-7140(4)	38(2)
N(00W)	14382(5)	2855(5)	-8449(4)	36(2)
N(00X)	8024(5)	3688(5)	-5646(4)	36(2)
N(00Y)	13311(5)	250(5)	-3799(4)	38(2)
N(00Z)	8877(5)	1910(5)	-4150(4)	36(2)
N(010)	12179(5)	1419(5)	-3619(4)	42(2)
N(011)	14364(5)	1467(5)	-11163(4)	39(2)
N(012)	8950(5)	2236(5)	-5049(4)	40(2)
N(013)	10494(5)	-322(5)	-3134(4)	36(2)
N(014)	7961(5)	3139(5)	-4315(4)	36(2)
N(015)	12016(5)	1580(5)	-7758(4)	34(2)
N(016)	13380(6)	2762(5)	-11226(4)	42(2)
N(017)	15923(5)	5311(5)	-9500(4)	38(2)
N(018)	15726(5)	4248(5)	-8062(4)	37(2)
N(019)	13310(5)	1712(5)	-5837(4)	36(2)
N(01A)	19017(5)	2393(5)	-9413(5)	41(2)
N(01B)	12142(5)	443(5)	-6433(4)	37(2)
F(01C)	19993(5)	1415(6)	-10885(6)	95(3)

N(01D)	14728(6)	5653(5)	-8266(4)	42(2)
N(01E)	7966(6)	2333(6)	-2865(5)	47(2)
O(01F)	16030(6)	2731(6)	-4780(5)	70(2)
N(01G)	17184(6)	2908(5)	-7906(4)	43(2)
O(01H)	10608(6)	2906(5)	-3828(5)	62(2)
N(01I)	10956(6)	1669(5)	-6421(5)	42(2)
N(01J)	12047(6)	2833(5)	-5404(5)	47(2)
N(01K)	14905(6)	6626(5)	-9647(5)	46(2)
N(01L)	15056(6)	838(6)	-11511(5)	47(2)
N(01M)	17410(5)	4177(5)	-10154(4)	40(2)
O(01N)	11394(7)	-2057(5)	-2873(6)	71(2)
N(01O)	13386(6)	-711(5)	-6532(5)	48(2)
N(01P)	15617(6)	1716(6)	-8445(5)	49(2)
N(01Q)	14584(6)	4609(5)	-6885(5)	45(2)
N(01R)	9516(6)	-254(5)	-1776(4)	44(2)
N(01T)	12071(6)	2855(5)	-9360(5)	49(2)
N(01U)	19162(6)	3484(6)	-11634(5)	49(2)
O(01V)	17996(6)	1122(6)	-11094(4)	73(2)
O(01W)	17278(6)	2017(6)	-10180(5)	78(2)
O(01X)	16258(6)	1537(6)	-10767(6)	73(2)
C(01Y)	9467(6)	1135(5)	-3824(5)	32(2)
N(01Z)	13917(6)	-536(6)	-3518(5)	52(2)
O(020)	16820(7)	438(6)	-9693(5)	76(2)
C(021)	11722(6)	1208(6)	-6873(5)	34(2)
C(022)	13692(6)	2123(6)	-6748(5)	33(2)
C(023)	8251(6)	2440(6)	-3698(5)	34(2)
C(024)	13855(6)	1412(6)	-10317(5)	34(2)
C(025)	12742(6)	1088(6)	-8138(5)	33(2)
O(026)	10152(6)	4053(5)	-5409(5)	72(2)
C(027)	9741(6)	86(6)	-2638(5)	36(2)
C(028)	10669(6)	50(6)	-3993(5)	36(2)
N(029)	8197(7)	3799(6)	-6523(5)	57(2)
C(02A)	16151(6)	4543(6)	-8926(6)	37(2)
C(02B)	12891(6)	43(6)	-6917(5)	34(2)
C(02C)	18156(7)	3577(6)	-10169(5)	35(2)
C(02D)	8383(6)	2961(6)	-5078(5)	36(2)
C(02E)	14806(6)	2086(6)	-7997(5)	36(2)
C(02F)	12600(7)	2097(6)	-5267(5)	39(2)
C(02G)	15188(7)	5845(6)	-9123(5)	38(2)
C(02H)	12642(6)	658(6)	-3240(5)	37(2)
C(02I)	13596(7)	3224(6)	-7957(6)	38(2)
C(02J)	15012(6)	4846(6)	-7751(6)	38(2)
C(02K)	17404(7)	3277(6)	-8757(6)	39(2)
C(02L)	19409(6)	2545(6)	-10234(5)	36(2)

C(02M)	13315(6)	792(6)	-4607(5)	34(2)
C(02N)	14041(7)	2310(6)	-11652(5)	39(2)
C(02O)	12724(6)	2205(6)	-9560(5)	35(2)
O(02P)	10453(7)	3342(7)	-7924(6)	92(3)
C(02Q)	7420(7)	4232(6)	-5180(5)	40(2)
C(02R)	6881(7)	5093(7)	-5562(6)	46(2)
C(02S)	14489(8)	2646(7)	-12633(6)	50(3)
C(02T)	12427(8)	283(7)	-2273(6)	50(2)
C(02U)	20303(7)	1997(7)	-10614(6)	49(3)
O(02V)	19365(9)	5230(8)	-8242(7)	73(4)
O(02W)	16006(10)	2921(8)	-6119(7)	70(3)
O(02X)	9868(14)	5325(13)	-6508(11)	67(3)
O(02Y)	11075(14)	4238(12)	-6882(11)	68(3)
O(02Z)	19200(70)	4380(40)	-8220(50)	80(4)
O(030)	19000(30)	5970(30)	-9580(30)	76(4)
O(031)	11388(13)	5061(13)	-6155(11)	77(3)
O(1)	15979(10)	1417(8)	-5150(8)	68(2)
O(2)	14524(8)	2419(8)	-4941(7)	65(2)
O(3)	17728(14)	5080(20)	-8281(17)	59(4)
N(30)	13150(6)	4018(5)	-8357(5)	45(2)
O(5)	15251(19)	1385(16)	-4637(16)	61(3)
O(4)	16570(20)	1770(18)	-5545(17)	67(3)
O(10)	15240(20)	2664(17)	-5885(15)	64(3)
O(33)	17890(20)	5480(30)	-8980(30)	76(4)
C(1)	10133(12)	4125(12)	-8566(13)	133(7)
O(7)	11596(13)	4414(11)	-6726(11)	72(3)
O(9)	9839(13)	4898(14)	-6701(12)	77(3)
O(8)	10777(13)	5619(11)	-6307(10)	73(3)
O(6)	19236(14)	4344(11)	-9007(12)	72(3)
O(11)	19100(130)	6230(120)	-9350(120)	79(5)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U11**	**U22**	**U33**	**U23**	**U13**	**U12**
Cl(01)	45(1)	55(1)	32(1)	-20(1)	-6(1)	-4(1)
Cl(02)	54(1)	56(1)	39(1)	-13(1)	-20(1)	-2(1)
Cl(03)	51(1)	60(2)	53(2)	-11(1)	-17(1)	3(1)
Cl(00)	110(3)	74(2)	109(3)	-7(2)	-60(2)	-7(2)
F(005)	70(4)	66(4)	38(3)	-14(3)	-24(3)	-1(3)
F(006)	58(3)	53(3)	44(3)	0(3)	-13(3)	-7(3)
F(007)	51(4)	86(4)	38(3)	-4(3)	-2(3)	-12(3)
F(008)	88(4)	84(4)	32(3)	-17(3)	-18(3)	-21(4)

F(009)	111(5)	56(4)	38(3)	3(3)	-25(3)	17(4)
F(00A)	64(4)	47(3)	64(4)	9(3)	-18(3)	-5(3)
F(00B)	71(4)	62(4)	86(5)	-7(3)	-47(4)	13(3)
O(00C)	53(4)	48(4)	39(4)	-17(3)	-16(3)	9(3)
F(00D)	109(5)	79(4)	34(3)	-25(3)	-12(3)	38(4)
F(00E)	73(4)	96(5)	48(4)	-17(3)	-22(3)	45(4)
F(00F)	47(3)	89(5)	72(4)	-10(4)	-6(3)	17(3)
N(00G)	38(4)	40(4)	24(3)	-11(3)	-11(3)	6(3)
N(00H)	33(3)	38(4)	27(4)	-13(3)	-9(3)	6(3)
N(00I)	34(4)	43(4)	22(3)	-7(3)	-6(3)	0(3)
N(00J)	36(4)	38(4)	30(4)	-9(3)	-12(3)	7(3)
N(00K)	41(4)	43(4)	29(4)	-13(3)	-10(3)	10(3)
N(00L)	36(4)	44(4)	35(4)	-14(3)	-14(3)	15(3)
F(00N)	108(5)	73(4)	53(4)	-24(3)	-25(4)	52(4)
N(00O)	43(4)	40(4)	32(4)	-15(3)	-17(3)	11(3)
N(00P)	38(4)	46(4)	24(4)	-8(3)	-10(3)	5(3)
N(00Q)	41(4)	39(4)	27(4)	-8(3)	-11(3)	5(3)
N(00R)	41(4)	38(4)	28(4)	-12(3)	-11(3)	6(3)
N(00S)	42(4)	48(4)	22(4)	-11(3)	-11(3)	7(3)
N(00T)	42(4)	39(4)	23(4)	-5(3)	-6(3)	8(3)
N(00U)	36(4)	44(4)	32(4)	-16(3)	-11(3)	11(3)
N(00V)	41(4)	42(4)	31(4)	-12(3)	-12(3)	6(3)
N(00W)	36(4)	40(4)	34(4)	-13(3)	-12(3)	4(3)
N(00X)	43(4)	41(4)	23(3)	-9(3)	-13(3)	5(3)
N(00Y)	39(4)	46(4)	28(4)	-9(3)	-13(3)	5(3)
N(00Z)	35(4)	46(4)	23(3)	-10(3)	-9(3)	10(3)
N(010)	40(4)	51(5)	29(4)	-17(3)	-4(3)	7(3)
N(011)	44(4)	42(4)	24(4)	-6(3)	-10(3)	8(3)
N(012)	48(4)	51(5)	17(3)	-12(3)	-10(3)	15(4)
N(013)	41(4)	41(4)	18(3)	-6(3)	-5(3)	4(3)
N(014)	39(4)	38(4)	26(4)	-10(3)	-10(3)	10(3)
N(015)	34(4)	37(4)	28(4)	-13(3)	-5(3)	2(3)
N(016)	53(5)	38(4)	28(4)	-5(3)	-15(3)	7(4)
N(017)	43(4)	40(4)	25(4)	-9(3)	-10(3)	8(3)
N(018)	46(4)	39(4)	24(4)	-10(3)	-11(3)	4(3)
N(019)	38(4)	38(4)	31(4)	-14(3)	-14(3)	12(3)
N(01A)	42(4)	42(4)	38(4)	-10(3)	-18(3)	8(3)
F(01C)	67(4)	114(6)	146(7)	-103(6)	-31(4)	22(4)
N(01D)	50(4)	46(4)	30(4)	-14(3)	-14(3)	9(4)
N(01E)	48(4)	65(5)	28(4)	-20(4)	-10(3)	12(4)
O(01F)	76(5)	82(5)	58(5)	-25(4)	-20(4)	-28(4)
N(01G)	60(5)	38(4)	23(4)	-5(3)	-11(3)	6(3)
O(01H)	69(5)	64(5)	44(4)	-16(4)	-15(4)	16(4)
N(01I)	41(4)	49(4)	36(4)	-18(3)	-8(3)	0(3)

N(01J)	56(5)	46(5)	34(4)	-14(3)	-13(4)	16(4)
N(01K)	58(5)	46(4)	28(4)	-10(3)	-14(3)	19(4)
N(01L)	53(5)	60(5)	24(4)	-17(3)	-9(3)	12(4)
N(01M)	50(4)	44(4)	21(3)	-6(3)	-15(3)	7(4)
O(01N)	94(6)	62(5)	77(6)	-26(4)	-60(5)	36(4)
N(01O)	60(5)	47(5)	32(4)	-6(3)	-18(4)	7(4)
N(01P)	42(4)	57(5)	37(4)	-11(4)	-11(3)	18(4)
N(01Q)	49(4)	48(5)	35(4)	-15(3)	-9(3)	3(4)
N(01R)	52(4)	55(5)	22(4)	-13(3)	-14(3)	14(4)
N(01T)	58(5)	49(5)	43(5)	-20(4)	-21(4)	20(4)
N(01U)	48(5)	62(5)	35(4)	-17(4)	-13(3)	13(4)
O(01V)	59(4)	108(6)	33(4)	-23(4)	-2(3)	32(4)
O(01W)	86(6)	85(6)	68(5)	-43(4)	-2(4)	-33(5)
O(01X)	56(4)	81(5)	96(6)	-40(5)	-37(4)	14(4)
N(01Z)	50(5)	57(5)	32(4)	-7(4)	-10(3)	28(4)
O(020)	105(6)	70(5)	43(4)	-12(4)	-14(4)	-15(5)
C(021)	29(4)	44(5)	25(4)	-10(4)	-4(3)	-6(4)
C(023)	33(4)	40(5)	26(4)	-10(4)	-9(3)	4(4)
C(024)	36(4)	37(5)	27(4)	-9(4)	-9(3)	1(4)
C(025)	33(4)	36(5)	30(4)	-9(4)	-10(3)	-4(4)
O(026)	75(5)	70(5)	55(5)	-2(4)	-22(4)	5(4)
C(027)	33(4)	43(5)	34(5)	-12(4)	-16(4)	2(4)
C(028)	34(4)	40(5)	33(4)	-10(4)	-11(4)	-5(4)
N(029)	80(6)	59(5)	38(5)	-17(4)	-31(4)	19(5)
C(02A)	38(5)	44(5)	37(5)	-18(4)	-17(4)	3(4)
C(02B)	30(4)	45(5)	25(4)	-11(4)	-8(3)	0(4)
C(02C)	39(5)	33(5)	30(4)	-7(3)	-10(4)	1(4)
C(02D)	37(4)	47(5)	23(4)	-13(4)	-7(3)	3(4)
C(02E)	40(5)	37(5)	28(4)	-6(4)	-14(4)	1(4)
C(02F)	47(5)	43(5)	27(4)	-11(4)	-12(4)	2(4)
C(02G)	41(5)	45(5)	33(5)	-15(4)	-16(4)	3(4)
C(02H)	38(5)	35(5)	34(5)	-13(4)	-7(4)	9(4)
C(02I)	43(5)	38(5)	39(5)	-18(4)	-16(4)	1(4)
C(02K)	40(5)	38(5)	36(5)	-15(4)	-9(4)	9(4)
C(02L)	33(4)	37(5)	30(5)	-4(4)	-7(3)	1(4)
C(02M)	32(4)	44(5)	23(4)	-7(4)	-10(3)	5(4)
C(02N)	41(5)	43(5)	28(4)	-4(4)	-13(4)	2(4)
C(02O)	36(4)	40(5)	26(4)	-7(4)	-12(3)	6(4)
O(02P)	66(6)	99(7)	76(6)	-8(5)	-10(4)	26(5)
C(02Q)	43(5)	44(5)	32(5)	-9(4)	-18(4)	7(4)
C(02R)	41(5)	49(6)	46(6)	-12(5)	-17(4)	6(4)
C(02S)	52(6)	61(7)	27(5)	-1(4)	-14(4)	4(5)
C(02T)	51(6)	61(7)	40(5)	-20(5)	-17(4)	13(5)
C(02U)	32(5)	62(6)	32(5)	-7(5)	-1(4)	11(4)

O(02V)	88(7)	76(7)	68(7)	-2(5)	-56(5)	-23(5)
O(02W)	77(5)	81(5)	39(4)	-8(3)	-14(4)	0(5)
O(02X)	68(5)	59(5)	63(6)	-18(5)	-18(4)	16(4)
O(02Y)	57(6)	69(5)	64(5)	-22(4)	-7(5)	12(5)
O(02Z)	92(7)	74(6)	87(7)	-9(5)	-58(6)	-15(6)
O(030)	101(7)	64(6)	81(6)	-5(5)	-73(6)	4(6)
O(031)	66(5)	83(6)	70(5)	-11(5)	-17(4)	-19(5)
O(1)	74(5)	62(4)	66(5)	-15(4)	-28(4)	4(4)
O(2)	51(3)	77(5)	72(5)	-26(4)	-21(3)	-12(4)
O(3)	86(5)	44(7)	87(7)	-17(6)	-78(5)	-7(6)
N(30)	52(5)	47(5)	33(4)	-11(3)	-16(3)	8(4)
O(5)	63(5)	63(5)	57(5)	-12(4)	-24(4)	-12(5)
O(4)	68(5)	67(5)	56(5)	-17(5)	-14(4)	4(4)
O(10)	69(5)	77(6)	54(5)	-14(5)	-34(4)	-10(5)
O(33)	106(5)	60(6)	90(6)	-15(6)	-72(5)	-8(5)
C(1)	78(10)	90(12)	178(18)	-67(12)	45(11)	-9(9)
O(7)	58(4)	65(5)	66(6)	-13(5)	-2(4)	10(5)
O(9)	62(5)	82(6)	70(6)	-2(5)	-26(4)	-1(5)
O(8)	73(6)	60(4)	70(5)	-22(4)	-3(5)	-2(4)
O(6)	83(6)	69(5)	84(7)	-15(5)	-58(6)	-14(5)
O(11)	103(7)	68(5)	89(7)	-11(5)	-73(7)	-6(6)

Table S4 Bond Lengths for **4**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Cl(01)	O(01V)	1.411(7)	N(00Y)	C(02M)	1.355(10)
Cl(01)	O(01W)	1.441(8)	N(00Z)	N(012)	1.434(9)
Cl(01)	O(01X)	1.415(7)	N(00Z)	C(01Y)	1.411(10)
Cl(01)	O(020)	1.425(8)	N(00Z)	C(023)	1.353(10)
Cl(02)	O(01F)	1.399(7)	N(010)	H(010)	0.88
Cl(02)	O(02W)	1.434(10)	N(010)	C(02H)	1.327(10)
Cl(02)	O(1)	1.377(12)	N(011)	N(01L)	1.410(10)
Cl(02)	O(2)	1.451(10)	N(011)	C(024)	1.368(10)
Cl(02)	O(5)	1.47(2)	N(011)	C(02N)	1.389(10)
Cl(02)	O(4)	1.48(3)	N(012)	H(012)	0.88
Cl(02)	O(10)	1.36(2)	N(012)	C(02D)	1.271(11)
Cl(03)	O(026)	1.429(7)	N(013)	C(027)	1.343(10)
Cl(03)	O(02X)	1.352(17)	N(013)	C(028)	1.340(10)
Cl(03)	O(02Y)	1.408(17)	N(014)	C(023)	1.354(10)
Cl(03)	O(031)	1.390(17)	N(014)	C(02D)	1.364(10)
Cl(03)	O(7)	1.432(15)	N(015)	C(021)	1.364(10)
Cl(03)	O(9)	1.404(17)	N(015)	C(025)	1.306(10)
Cl(03)	O(8)	1.445(16)	N(016)	C(02N)	1.263(11)

Cl(00)	O(02V)	1.406(10)	N(017)	H(017)	0.88
Cl(00)	O(02Z)	1.45(2)	N(017)	C(02A)	1.331(10)
Cl(00)	O(030)	1.416(15)	N(017)	C(02G)	1.355(11)
Cl(00)	O(3)	1.482(18)	N(018)	C(02A)	1.332(10)
Cl(00)	O(33)	1.435(18)	N(018)	C(02J)	1.362(11)
Cl(00)	O(6)	1.458(15)	N(019)	C(022)	1.405(10)
Cl(00)	O(11)	1.53(11)	N(019)	C(02F)	1.373(11)
F(005)	C(02T)	1.340(11)	N(01A)	H(01G)	0.88
F(006)	C(02T)	1.302(12)	N(01A)	C(02L)	1.283(10)
F(007)	C(02S)	1.324(11)	N(01B)	C(021)	1.340(10)
F(008)	C(02S)	1.323(12)	N(01B)	C(02B)	1.323(10)
F(009)	C(02S)	1.317(11)	F(01C)	C(02U)	1.312(12)
F(00A)	C(02R)	1.313(10)	N(01D)	C(02G)	1.336(11)
F(00B)	C(02R)	1.326(11)	N(01D)	C(02J)	1.350(11)
O(00C)	H(00C)	0.87	N(01E)	C(023)	1.316(10)
O(00C)	H(00D)	0.87	N(01G)	C(02K)	1.320(10)
F(00D)	C(02T)	1.303(11)	O(01H)	H(01U)	0.87
F(00E)	C(02U)	1.330(11)	O(01H)	H(01V)	0.87
F(00F)	C(02U)	1.320(10)	N(01I)	H(01Q)	0.8847
N(00G)	C(01Y)	1.308(10)	N(01I)	H(01R)	0.8848
N(00G)	C(028)	1.363(10)	N(01I)	C(021)	1.363(10)
N(00H)	N(00T)	1.411(9)	N(01J)	H(01A)	0.88
N(00H)	C(025)	1.412(10)	N(01J)	H(01B)	0.88
N(00H)	C(02O)	1.355(10)	N(01J)	C(02F)	1.276(11)
N(00I)	C(01Y)	1.321(10)	N(01K)	H(01H)	0.88
N(00I)	C(027)	1.360(10)	N(01K)	H(01I)	0.88
N(00J)	N(016)	1.382(9)	N(01K)	C(02G)	1.331(11)
N(00J)	C(024)	1.374(11)	N(01L)	H(01S)	0.8808
N(00J)	C(02O)	1.352(10)	N(01L)	H(01T)	0.8808
N(00K)	H(00A)	0.88	N(01M)	H(01M)	0.88
N(00K)	H(00B)	0.88	N(01M)	C(02C)	1.286(11)
N(00K)	C(028)	1.333(10)	O(01N)	H(01W)	0.87
N(00L)	H(00L)	0.88	O(01N)	H(01X)	0.87
N(00L)	N(019)	1.425(9)	N(01O)	C(02B)	1.348(11)
N(00L)	C(02M)	1.288(10)	N(01P)	H(01C)	0.88
N(00M)	C(022)	1.314(10)	N(01P)	H(01D)	0.88
N(00M)	C(02I)	1.350(10)	N(01P)	C(02E)	1.310(11)
F(00N)	C(02R)	1.302(11)	N(01Q)	H(01J)	0.8816
N(00O)	N(01M)	1.418(9)	N(01Q)	H(01K)	0.8817
N(00O)	C(02A)	1.383(11)	N(01Q)	C(02J)	1.340(10)
N(00O)	C(02K)	1.363(10)	N(01R)	H(01O)	0.88
N(00P)	C(025)	1.329(10)	N(01R)	H(01P)	0.88
N(00P)	C(02B)	1.351(10)	N(01R)	C(027)	1.335(10)
N(00Q)	N(01U)	1.396(9)	N(01T)	C(02O)	1.314(11)

N(00Q)	C(02C)	1.379(11)	N(01U)	H(01L)	0.8803
N(00Q)	C(02L)	1.369(10)	N(01U)	H(01N)	0.8803
N(00R)	N(01A)	1.386(10)	N(01Z)	H(01E)	0.8811
N(00R)	C(02C)	1.360(10)	N(01Z)	H(01F)	0.881
N(00R)	C(02K)	1.366(10)	N(029)	H(02A)	0.8839
N(00S)	N(010)	1.380(9)	N(029)	H(02B)	0.8841
N(00S)	C(02F)	1.363(10)	C(02H)	C(02T)	1.504(12)
N(00S)	C(02M)	1.365(11)	C(02I)	N(30)	1.360(11)
N(00T)	H(00T)	0.88	C(02L)	C(02U)	1.489(12)
N(00T)	C(024)	1.275(10)	C(02N)	C(02S)	1.510(12)
N(00U)	H(00U)	0.88	O(02P)	H(02P)	0.84
N(00U)	N(014)	1.397(9)	O(02P)	C(1)	1.46(2)
N(00U)	C(02Q)	1.301(10)	C(02Q)	C(02R)	1.486(12)
N(00V)	C(022)	1.316(10)	O(02V)	O(02Z)	1.33(8)
N(00V)	C(02E)	1.326(10)	O(02Z)	C(1)#1	1.28(9)
N(00W)	C(02E)	1.356(10)	N(30)	H(30A)	0.8816
N(00W)	C(02I)	1.329(10)	N(30)	H(30B)	0.8817
N(00X)	N(029)	1.412(9)	C(1)	H(1A)	0.98
N(00X)	C(02D)	1.372(10)	C(1)	H(1B)	0.981
N(00X)	C(02Q)	1.372(11)	C(1)	H(1C)	0.9801
N(00Y)	N(01Z)	1.413(9)	C(1)	O(6)#2	1.60(3)
N(00Y)	C(02H)	1.360(10)			

Table S5 Bond Angles for **4**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O(01V)	Cl(01)	O(01W)	110.8(5)	C(02E)	N(01P)	H(01C)	120
O(01V)	Cl(01)	O(01X)	109.2(5)	C(02E)	N(01P)	H(01D)	120
O(01V)	Cl(01)	O(020)	111.3(5)	H(01J)	N(01Q)	H(01K)	109.2
O(01X)	Cl(01)	O(01W)	106.9(5)	C(02J)	N(01Q)	H(01J)	109.5
O(01X)	Cl(01)	O(020)	109.3(5)	C(02J)	N(01Q)	H(01K)	109.5
O(020)	Cl(01)	O(01W)	109.3(5)	H(01O)	N(01R)	H(01P)	120
O(01F)	Cl(02)	O(02W)	105.5(6)	C(027)	N(01R)	H(01O)	119.9
O(01F)	Cl(02)	O(2)	106.8(6)	C(027)	N(01R)	H(01P)	120.1
O(01F)	Cl(02)	O(5)	108.0(10)	N(00Q)	N(01U)	H(01L)	109.3
O(01F)	Cl(02)	O(4)	100.8(11)	N(00Q)	N(01U)	H(01N)	109.1
O(02W)	Cl(02)	O(2)	105.1(7)	H(01L)	N(01U)	H(01N)	109.4
O(1)	Cl(02)	O(01F)	114.3(6)	N(00G)	C(01Y)	N(00Z)	117.6(7)
O(1)	Cl(02)	O(02W)	110.9(7)	N(00I)	C(01Y)	N(00G)	130.0(7)
O(1)	Cl(02)	O(2)	113.5(7)	N(00I)	C(01Y)	N(00Z)	112.4(7)
O(5)	Cl(02)	O(4)	81.5(14)	N(00Y)	N(01Z)	H(01E)	110
O(10)	Cl(02)	O(01F)	134.1(11)	N(00Y)	N(01Z)	H(01F)	108.5
O(10)	Cl(02)	O(5)	112.6(14)	H(01E)	N(01Z)	H(01F)	109.2

O(10)	Cl(02)	O(4)	105.5(15)	N(01B)	C(021)	N(015)	124.6(7)
O(026)	Cl(03)	O(8)	113.9(8)	N(01B)	C(021)	N(01I)	119.1(7)
O(02X)	Cl(03)	O(026)	111.5(8)	N(01I)	C(021)	N(015)	116.4(7)
O(02X)	Cl(03)	O(02Y)	112.6(10)	N(00M)	C(022)	N(00V)	129.8(8)
O(02X)	Cl(03)	O(031)	114.8(12)	N(00M)	C(022)	N(019)	115.7(7)
O(02Y)	Cl(03)	O(026)	112.5(8)	N(00V)	C(022)	N(019)	114.5(7)
O(031)	Cl(03)	O(026)	98.6(8)	N(014)	C(023)	N(00Z)	103.0(7)
O(031)	Cl(03)	O(02Y)	105.9(11)	N(01E)	C(023)	N(00Z)	130.4(8)
O(7)	Cl(03)	O(026)	112.4(7)	N(01E)	C(023)	N(014)	126.5(8)
O(7)	Cl(03)	O(8)	103.1(10)	N(00T)	C(024)	N(00J)	113.7(7)
O(9)	Cl(03)	O(026)	109.9(8)	N(00T)	C(024)	N(011)	141.8(8)
O(9)	Cl(03)	O(7)	116.5(11)	N(011)	C(024)	N(00J)	104.4(7)
O(9)	Cl(03)	O(8)	100.3(11)	N(00P)	C(025)	N(00H)	114.6(7)
O(02V)	Cl(00)	O(02Z)	55(3)	N(015)	C(025)	N(00H)	115.3(7)
O(02V)	Cl(00)	O(030)	117(2)	N(015)	C(025)	N(00P)	130.1(7)
O(02V)	Cl(00)	O(3)	105.2(12)	N(013)	C(027)	N(00I)	123.5(7)
O(02Z)	Cl(00)	O(3)	96(4)	N(01R)	C(027)	N(00I)	117.4(7)
O(030)	Cl(00)	O(02Z)	154(4)	N(01R)	C(027)	N(013)	119.1(7)
O(030)	Cl(00)	O(3)	109.9(19)	N(00K)	C(028)	N(00G)	117.2(7)
O(33)	Cl(00)	O(6)	110.7(19)	N(013)	C(028)	N(00G)	125.2(8)
O(33)	Cl(00)	O(11)	80(7)	N(013)	C(028)	N(00K)	117.3(7)
O(6)	Cl(00)	O(11)	131(10)	N(00X)	N(029)	H(02A)	109
H(00C)	O(00C)	H(00D)	104.5	N(00X)	N(029)	H(02B)	110
C(01Y)	N(00G)	C(028)	111.9(7)	H(02A)	N(029)	H(02B)	108.9
N(00T)	N(00H)	C(025)	120.7(6)	N(017)	C(02A)	N(00O)	117.6(7)
C(02O)	N(00H)	N(00T)	113.3(6)	N(018)	C(02A)	N(00O)	114.4(7)
C(02O)	N(00H)	C(025)	126.0(7)	N(018)	C(02A)	N(017)	128.0(8)
C(01Y)	N(00I)	C(027)	113.4(7)	N(01B)	C(02B)	N(00P)	125.7(7)
C(024)	N(00J)	N(016)	112.8(7)	N(01B)	C(02B)	N(01O)	119.8(7)
C(02O)	N(00J)	N(016)	139.0(7)	N(01O)	C(02B)	N(00P)	114.5(7)
C(02O)	N(00J)	C(024)	108.2(6)	N(00R)	C(02C)	N(00Q)	103.8(7)
H(00A)	N(00K)	H(00B)	120	N(01M)	C(02C)	N(00Q)	141.2(8)
C(028)	N(00K)	H(00A)	120	N(01M)	C(02C)	N(00R)	114.9(7)
C(028)	N(00K)	H(00B)	120	N(012)	C(02D)	N(00X)	141.4(8)
N(019)	N(00L)	H(00L)	129.1	N(012)	C(02D)	N(014)	115.7(7)
C(02M)	N(00L)	H(00L)	129.2	N(014)	C(02D)	N(00X)	102.9(7)
C(02M)	N(00L)	N(019)	101.7(6)	N(00V)	C(02E)	N(00W)	125.7(8)
C(022)	N(00M)	C(02I)	112.5(7)	N(01P)	C(02E)	N(00V)	117.0(7)
C(02A)	N(00O)	N(01M)	120.4(7)	N(01P)	C(02E)	N(00W)	117.3(7)
C(02K)	N(00O)	N(01M)	113.6(6)	N(00S)	C(02F)	N(019)	102.3(7)
C(02K)	N(00O)	C(02A)	124.9(7)	N(01J)	C(02F)	N(00S)	127.0(8)
C(025)	N(00P)	C(02B)	111.8(7)	N(01J)	C(02F)	N(019)	130.8(8)
C(02C)	N(00Q)	N(01U)	127.3(7)	N(01D)	C(02G)	N(017)	125.3(8)
C(02L)	N(00Q)	N(01U)	126.2(7)	N(01K)	C(02G)	N(017)	117.4(7)

C(02L)	N(00Q)	C(02C)	105.5(6)	N(01K)	C(02G)	N(01D)	117.4(8)
C(02C)	N(00R)	N(01A)	113.5(7)	N(00Y)	C(02H)	C(02T)	123.5(7)
C(02C)	N(00R)	C(02K)	108.0(7)	N(010)	C(02H)	N(00Y)	114.3(7)
C(02K)	N(00R)	N(01A)	138.5(7)	N(010)	C(02H)	C(02T)	122.2(7)
C(02F)	N(00S)	N(010)	137.1(7)	N(00M)	C(02I)	N(30)	116.6(8)
C(02F)	N(00S)	C(02M)	109.3(7)	N(00W)	C(02I)	N(00M)	125.1(8)
C(02M)	N(00S)	N(010)	113.1(6)	N(00W)	C(02I)	N(30)	118.3(8)
N(00H)	N(00T)	H(00T)	129.1	N(01D)	C(02J)	N(018)	123.5(8)
C(024)	N(00T)	N(00H)	101.7(6)	N(01Q)	C(02J)	N(018)	117.2(7)
C(024)	N(00T)	H(00T)	129.1	N(01Q)	C(02J)	N(01D)	119.3(8)
N(014)	N(00U)	H(00U)	129.8	N(00O)	C(02K)	N(00R)	102.7(7)
C(02Q)	N(00U)	H(00U)	129.8	N(01G)	C(02K)	N(00O)	130.8(8)
C(02Q)	N(00U)	N(014)	100.4(7)	N(01G)	C(02K)	N(00R)	126.6(8)
C(022)	N(00V)	C(02E)	112.3(7)	N(00Q)	C(02L)	C(02U)	122.0(7)
C(02I)	N(00W)	C(02E)	114.4(7)	N(01A)	C(02L)	N(00Q)	115.5(8)
C(02D)	N(00X)	N(029)	125.3(7)	N(01A)	C(02L)	C(02U)	122.5(8)
C(02Q)	N(00X)	N(029)	127.7(7)	N(00L)	C(02M)	N(00S)	113.7(7)
C(02Q)	N(00X)	C(02D)	106.8(6)	N(00L)	C(02M)	N(00Y)	141.4(8)
C(02H)	N(00Y)	N(01Z)	122.1(7)	N(00Y)	C(02M)	N(00S)	104.9(7)
C(02H)	N(00Y)	C(02M)	106.4(7)	N(011)	C(02N)	C(02S)	120.2(8)
C(02M)	N(00Y)	N(01Z)	131.2(7)	N(016)	C(02N)	N(011)	116.0(7)
C(01Y)	N(00Z)	N(012)	120.4(6)	N(016)	C(02N)	C(02S)	123.7(8)
C(023)	N(00Z)	N(012)	113.5(6)	N(00H)	C(02O)	N(00J)	103.0(7)
C(023)	N(00Z)	C(01Y)	126.1(7)	N(01T)	C(02O)	N(00H)	131.5(8)
N(00S)	N(010)	H(010)	129.4	N(01T)	C(02O)	N(00J)	125.4(7)
C(02H)	N(010)	N(00S)	101.2(7)	C(1)	O(02P)	H(02P)	109
C(02H)	N(010)	H(010)	129.4	N(00U)	C(02Q)	N(00X)	115.1(7)
C(024)	N(011)	N(01L)	130.5(7)	N(00U)	C(02Q)	C(02R)	121.2(8)
C(024)	N(011)	C(02N)	104.5(7)	N(00X)	C(02Q)	C(02R)	123.6(8)
C(02N)	N(011)	N(01L)	125.0(7)	F(00A)	C(02R)	C(02Q)	112.0(7)
N(00Z)	N(012)	H(012)	130	F(00B)	C(02R)	F(00A)	105.7(8)
C(02D)	N(012)	N(00Z)	100.0(6)	F(00B)	C(02R)	C(02Q)	110.6(8)
C(02D)	N(012)	H(012)	130	F(00N)	C(02R)	F(00A)	108.1(8)
C(028)	N(013)	C(027)	115.8(7)	F(00N)	C(02R)	F(00B)	108.0(8)
C(023)	N(014)	N(00U)	137.5(7)	F(00N)	C(02R)	C(02Q)	112.1(8)
C(023)	N(014)	C(02D)	107.7(7)	F(007)	C(02S)	C(02N)	110.9(8)
C(02D)	N(014)	N(00U)	114.7(7)	F(008)	C(02S)	F(007)	107.9(9)
C(025)	N(015)	C(021)	112.3(7)	F(008)	C(02S)	F(009)	108.8(8)
C(02N)	N(016)	N(00J)	102.2(6)	F(008)	C(02S)	C(02N)	112.0(8)
C(02A)	N(017)	H(017)	123.4	F(009)	C(02S)	F(007)	107.6(8)
C(02A)	N(017)	C(02G)	113.1(7)	F(009)	C(02S)	C(02N)	109.6(8)
C(02G)	N(017)	H(017)	123.5	F(005)	C(02T)	C(02H)	108.4(8)
C(02A)	N(018)	C(02J)	114.0(7)	F(006)	C(02T)	F(005)	108.4(8)
C(022)	N(019)	N(00L)	120.1(6)	F(006)	C(02T)	F(00D)	110.1(8)

C(02F)	N(019)	N(00L)	113.1(6)	F(006)	C(02T)	C(02H)	112.4(8)
C(02F)	N(019)	C(022)	126.2(7)	F(00D)	C(02T)	F(005)	106.7(9)
N(00R)	N(01A)	H(01G)	129.2	F(00D)	C(02T)	C(02H)	110.7(8)
C(02L)	N(01A)	N(00R)	101.6(7)	F(00E)	C(02U)	C(02L)	110.0(8)
C(02L)	N(01A)	H(01G)	129.2	F(00F)	C(02U)	F(00E)	105.4(8)
C(02B)	N(01B)	C(021)	115.5(7)	F(00F)	C(02U)	F(01C)	107.4(9)
C(02G)	N(01D)	C(02J)	116.0(7)	F(00F)	C(02U)	C(02L)	113.4(8)
H(01U)	O(01H)	H(01V)	104.5	F(01C)	C(02U)	F(00E)	109.3(9)
H(01Q)	N(01I)	H(01R)	108.9	F(01C)	C(02U)	C(02L)	111.2(8)
C(021)	N(01I)	H(01Q)	109.7	Cl(00)	O(02V)	O(02Z)	64.1(19)
C(021)	N(01I)	H(01R)	109.7	C(02I)	N(30)	H(30A)	109
H(01A)	N(01J)	H(01B)	120	C(02I)	N(30)	H(30B)	109.4
C(02F)	N(01J)	H(01A)	120	H(30A)	N(30)	H(30B)	109.2
C(02F)	N(01J)	H(01B)	120	O(02P)	C(1)	H(1A)	108.4
H(01H)	N(01K)	H(01I)	120	O(02P)	C(1)	H(1B)	111
C(02G)	N(01K)	H(01H)	119.9	O(02P)	C(1)	H(1C)	110.4
C(02G)	N(01K)	H(01I)	120.1	O(02P)	C(1)	O(6)#2	137.7(14)
N(011)	N(01L)	H(01S)	109.2	O(02Z)#2	C(1)	O(02P)	110(2)
N(011)	N(01L)	H(01T)	109.3	O(02Z)#2	C(1)	O(6)#2	55(4)
H(01S)	N(01L)	H(01T)	109.4	H(1A)	C(1)	H(1B)	108.9
N(00O)	N(01M)	H(01M)	129.6	H(1A)	C(1)	H(1C)	109.2
C(02C)	N(01M)	N(00O)	100.7(6)	H(1B)	C(1)	H(1C)	108.8
C(02C)	N(01M)	H(01M)	129.6	O(6)#2	C(1)	H(1A)	112.5
H(01W)	O(01N)	H(01X)	109.5	O(6)#2	C(1)	H(1B)	45
H(01C)	N(01P)	H(01D)	120	O(6)#2	C(1)	H(1C)	65.4

Table S6 Torsion Angles for **4**.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
N(00H)	N(00T)	C(024)	N(00J)	1.9(9)	C(023)	N(00Z)	N(012)	C(02D)	2.0(9)
N(00H)	N(00T)	C(024)	N(011)	178.3(11)	C(023)	N(00Z)	C(01Y)	N(00G)	-166.3(8)
N(00J)	N(016)	C(02N)	N(011)	1.3(10)	C(023)	N(00Z)	C(01Y)	N(00I)	14.0(12)
N(00J)	N(016)	C(02N)	C(02S)	-177.8(8)	C(023)	N(014)	C(02D)	N(00X)	178.5(6)
N(00L)	N(019)	C(022)	N(00M)	179.5(7)	C(023)	N(014)	C(02D)	N(012)	-2.0(11)
N(00L)	N(019)	C(022)	N(00V)	0.5(11)	C(024)	N(00J)	N(016)	C(02N)	0.3(9)
N(00L)	N(019)	C(02F)	N(00S)	-1.7(9)	C(024)	N(00J)	C(02O)	N(00H)	0.4(9)
N(00L)	N(019)	C(02F)	N(01J)	179.4(9)	C(024)	N(00J)	C(02O)	N(01T)	179.7(9)
N(00O)	N(01M)	C(02C)	N(00Q)	176.5(11)	C(024)	N(011)	C(02N)	N(016)	-2.3(11)
N(00O)	N(01M)	C(02C)	N(00R)	-2.2(9)	C(024)	N(011)	C(02N)	C(02S)	176.7(8)
N(00Q)	C(02L)	C(02U)	F(00E)	164.4(8)	C(025)	N(00H)	N(00T)	C(024)	179.3(7)

N(00Q)	C(02L)	C(02U)	F(00F)	46.8(13)	C(025)	N(00H)	C(02O)	N(00J)	179.7(7)
N(00Q)	C(02L)	C(02U)	F(01C)	-74.4(11)	C(025)	N(00H)	C(02O)	N(01T)	0.4(15)
N(00R)	N(01A)	C(02L)	N(00Q)	2.7(10)	C(025)	N(00P)	C(02B)	N(01B)	2.7(12)
N(00R)	N(01A)	C(02L)	C(02U)	-178.5(8)	C(025)	N(00P)	C(02B)	N(01O)	-177.4(7)
N(00S)	N(010)	C(02H)	N(00Y)	0.0(10)	C(025)	N(015)	C(021)	N(01B)	1.8(12)
N(00S)	N(010)	C(02H)	C(02T)	-179.4(8)	C(025)	N(015)	C(021)	N(01I)	-179.1(7)
N(00T)	N(00H)	C(025)	N(00P)	2.8(11)	C(027)	N(00I)	C(01Y)	N(00G)	0.5(13)
N(00T)	N(00H)	C(025)	N(015)	-176.5(7)	C(027)	N(00I)	C(01Y)	N(00Z)	-179.9(7)
N(00T)	N(00H)	C(02O)	N(00J)	0.8(9)	C(027)	N(013)	C(028)	N(00G)	3.7(12)
N(00T)	N(00H)	C(02O)	N(01T)	-178.5(9)	C(027)	N(013)	C(028)	N(00K)	178.3(7)
N(00U)	N(014)	C(023)	N(00Z)	-180.0(9)	C(028)	N(00G)	C(01Y)	N(00I)	2.3(12)
N(00U)	N(014)	C(023)	N(01E)	0.2(16)	C(028)	N(00G)	C(01Y)	N(00Z)	-177.3(7)
N(00U)	N(014)	C(02D)	N(00X)	0.7(9)	C(028)	N(013)	C(027)	N(00I)	-0.3(12)
N(00U)	N(014)	C(02D)	N(012)	-179.8(7)	C(028)	N(013)	C(027)	N(01R)	179.2(8)
N(00U)	C(02Q)	C(02R)	F(00A)	125.5(10)	N(029)	N(00X)	C(02D)	N(012)	4.5(18)
N(00U)	C(02Q)	C(02R)	F(00B)	-116.9(10)	N(029)	N(00X)	C(02D)	N(014)	-176.2(8)
N(00U)	C(02Q)	C(02R)	F(00N)	3.7(13)	N(029)	N(00X)	C(02Q)	N(00U)	175.6(8)
N(00X)	C(02Q)	C(02R)	F(00A)	-55.0(12)	N(029)	N(00X)	C(02Q)	C(02R)	-3.9(14)
N(00X)	C(02Q)	C(02R)	F(00B)	62.6(11)	C(02A)	N(00O)	N(01M)	C(02C)	170.7(8)
N(00X)	C(02Q)	C(02R)	F(00N)	-176.7(8)	C(02A)	N(00O)	C(02K)	N(00R)	-169.1(8)
N(00Y)	C(02H)	C(02T)	F(005)	61.4(12)	C(02A)	N(00O)	C(02K)	N(01G)	10.8(15)
N(00Y)	C(02H)	C(02T)	F(006)	-58.3(12)	C(02A)	N(017)	C(02G)	N(01D)	0.6(12)
N(00Y)	C(02H)	C(02T)	F(00D)	178.1(8)	C(02A)	N(017)	C(02G)	N(01K)	-179.6(8)
N(00Z)	N(012)	C(02D)	N(00X)	179.3(11)	C(02A)	N(018)	C(02J)	N(01D)	2.2(12)
N(00Z)	N(012)	C(02D)	N(014)	0.1(10)	C(02A)	N(018)	C(02J)	N(01Q)	-177.4(7)
N(010)	N(00S)	C(02F)	N(019)	172.8(9)	C(02B)	N(00P)	C(025)	N(00H)	-179.7(7)
N(010)	N(00S)	C(02F)	N(01J)	-8.2(17)	C(02B)	N(00P)	C(025)	N(015)	-0.5(13)
N(010)	N(00S)	C(02M)	N(00L)	-175.2(7)	C(02B)	N(01B)	C(021)	N(015)	0.0(12)
N(010)	N(00S)	C(02M)	N(00Y)	3.0(9)	C(02B)	N(01B)	C(021)	N(01I)	-179.1(7)
N(010)	C(02H)	C(02T)	F(005)	-119.2(9)	C(02C)	N(00Q)	C(02L)	N(01A)	-2.7(10)
N(010)	C(02H)	C(02T)	F(006)	121.1(9)	C(02C)	N(00Q)	C(02L)	C(02U)	178.5(8)
N(010)	C(02H)	C(02T)	F(00D)	-2.5(13)	C(02C)	N(00R)	N(01A)	C(02L)	-1.8(9)
N(011)	C(02N)	C(02S)	F(007)	-55.7(12)	C(02C)	N(00R)	C(02K)	N(00O)	-0.5(9)
N(011)	C(02N)	C(02S)	F(008)	64.9(11)	C(02C)	N(00R)	C(02K)	N(01G)	179.5(9)
N(011)	C(02N)	C(02S)	F(009)	-174.2(8)	C(02D)	N(00X)	C(02Q)	N(00U)	-0.2(10)

N(012)	N(00Z)	C(01Y)	N(00G)	10.3(11)	C(02D)	N(00X)	C(02Q)	C(02R)	-179.8(8)
N(012)	N(00Z)	C(01Y)	N(00I)	-169.4(7)	C(02D)	N(014)	C(023)	N(00Z)	3.0(9)
N(012)	N(00Z)	C(023)	N(014)	-3.1(9)	C(02D)	N(014)	C(023)	N(01E)	-176.9(8)
N(012)	N(00Z)	C(023)	N(01E)	176.7(9)	C(02E)	N(00V)	C(022)	N(00M)	1.4(13)
N(014)	N(00U)	C(02Q)	N(00X)	0.6(9)	C(02E)	N(00V)	C(022)	N(019)	-179.8(7)
N(014)	N(00U)	C(02Q)	C(02R)	-179.9(8)	C(02E)	N(00W)	C(02I)	N(00M)	-0.9(12)
N(016)	N(00J)	C(024)	N(00T)	176.0(7)	C(02E)	N(00W)	C(02I)	N(30)	177.6(8)
N(016)	N(00J)	C(024)	N(011)	-1.7(9)	C(02F)	N(00S)	N(010)	C(02H)	-172.3(10)
N(016)	N(00J)	C(02O)	N(00H)	-176.3(9)	C(02F)	N(00S)	C(02M)	N(00L)	-2.1(10)
N(016)	N(00J)	C(02O)	N(01T)	3.1(17)	C(02F)	N(00S)	C(02M)	N(00Y)	176.1(7)
N(016)	C(02N)	C(02S)	F(007)	123.3(10)	C(02F)	N(019)	C(022)	N(00M)	-9.8(12)
N(016)	C(02N)	C(02S)	F(008)	-116.1(10)	C(02F)	N(019)	C(022)	N(00V)	171.2(8)
N(016)	C(02N)	C(02S)	F(009)	4.8(14)	C(02G)	N(017)	C(02A)	N(00O)	-177.8(7)
N(019)	N(00L)	C(02M)	N(00S)	0.9(9)	C(02G)	N(017)	C(02A)	N(018)	2.3(13)
N(019)	N(00L)	C(02M)	N(00Y)	-176.3(11)	C(02G)	N(01D)	C(02J)	N(018)	0.2(13)
N(01A)	N(00R)	C(02C)	N(00Q)	0.3(9)	C(02G)	N(01D)	C(02J)	N(01Q)	179.8(8)
N(01A)	N(00R)	C(02C)	N(01M)	179.5(7)	C(02H)	N(00Y)	C(02M)	N(00L)	174.6(12)
N(01A)	N(00R)	C(02K)	N(00O)	-177.2(9)	C(02H)	N(00Y)	C(02M)	N(00S)	-2.8(9)
N(01A)	N(00R)	C(02K)	N(01G)	2.9(17)	C(02I)	N(00M)	C(022)	N(00V)	0.7(13)
N(01A)	C(02L)	C(02U)	F(00E)	-14.3(13)	C(02I)	N(00M)	C(022)	N(019)	-178.1(7)
N(01A)	C(02L)	C(02U)	F(00F)	-132.0(9)	C(02I)	N(00W)	C(02E)	N(00V)	3.5(12)
N(01A)	C(02L)	C(02U)	F(01C)	106.9(11)	C(02I)	N(00W)	C(02E)	N(01P)	-176.8(8)
N(01L)	N(011)	C(024)	N(00J)	-176.9(8)	C(02J)	N(018)	C(02A)	N(00O)	176.4(7)
N(01L)	N(011)	C(024)	N(00T)	6.6(19)	C(02J)	N(018)	C(02A)	N(017)	-3.7(13)
N(01L)	N(011)	C(02N)	N(016)	176.8(8)	C(02J)	N(01D)	C(02G)	N(017)	-1.7(13)
N(01L)	N(011)	C(02N)	C(02S)	-4.1(13)	C(02J)	N(01D)	C(02G)	N(01K)	178.5(8)
N(01M)	N(00O)	C(02A)	N(017)	-2.4(12)	C(02K)	N(00O)	N(01M)	C(02C)	1.9(9)
N(01M)	N(00O)	C(02A)	N(018)	177.5(7)	C(02K)	N(00O)	C(02A)	N(017)	165.1(8)
N(01M)	N(00O)	C(02K)	N(00R)	-0.8(9)	C(02K)	N(00O)	C(02A)	N(018)	-15.0(12)
N(01M)	N(00O)	C(02K)	N(01G)	179.1(9)	C(02K)	N(00R)	N(01A)	C(02L)	174.7(10)
N(01U)	N(00Q)	C(02C)	N(00R)	170.2(8)	C(02K)	N(00R)	C(02C)	N(00Q)	-177.3(7)
N(01U)	N(00Q)	C(02C)	N(01M)	-8.6(18)	C(02K)	N(00R)	C(02C)	N(01M)	1.9(10)
N(01U)	N(00Q)	C(02L)	N(01A)	-171.8(8)	C(02L)	N(00Q)	C(02C)	N(00R)	1.3(9)
N(01U)	N(00Q)	C(02L)	C(02U)	9.4(14)	C(02L)	N(00Q)	C(02C)	N(01M)	-177.6(11)
C(01Y)	N(00G)	C(028)	N(00K)	-179.1(7)	C(02M)	N(00L)	N(019)	C(022)	172.4(7)

C(01Y)	N(00G)	C(028)	N(013)	-4.5(12)	C(02M)	N(00L)	N(019)	C(02F)	0.5(9)
C(01Y)	N(00I)	C(027)	N(013)	-1.6(12)	C(02M)	N(00S)	N(010)	C(02H)	-1.9(9)
C(01Y)	N(00I)	C(027)	N(01R)	178.8(7)	C(02M)	N(00S)	C(02F)	N(019)	2.1(9)
C(01Y)	N(00Z)	N(012)	C(02D)	-175.0(7)	C(02M)	N(00S)	C(02F)	N(01J)	-178.9(9)
C(01Y)	N(00Z)	C(023)	N(014)	173.7(7)	C(02M)	N(00Y)	C(02H)	N(010)	1.8(10)
C(01Y)	N(00Z)	C(023)	N(01E)	-6.5(15)	C(02M)	N(00Y)	C(02H)	C(02T)	-178.8(8)
N(01Z)	N(00Y)	C(02H)	N(010)	176.4(8)	C(02N)	N(011)	C(024)	N(00J)	2.2(9)
N(01Z)	N(00Y)	C(02H)	C(02T)	-4.2(13)	C(02N)	N(011)	C(024)	N(00T)	-174.3(11)
N(01Z)	N(00Y)	C(02M)	N(00L)	0.7(18)	C(02O)	N(00H)	N(00T)	C(024)	-1.7(9)
N(01Z)	N(00Y)	C(02M)	N(00S)	-176.7(8)	C(02O)	N(00H)	C(025)	N(00P)	-176.0(7)
C(021)	N(015)	C(025)	N(00H)	177.7(7)	C(02O)	N(00H)	C(025)	N(015)	4.7(12)
C(021)	N(015)	C(025)	N(00P)	-1.5(13)	C(02O)	N(00J)	N(016)	C(02N)	176.8(10)
C(021)	N(01B)	C(02B)	N(00P)	-2.5(12)	C(02O)	N(00J)	C(024)	N(00T)	-1.6(10)
C(021)	N(01B)	C(02B)	N(01O)	177.6(8)	C(02O)	N(00J)	C(024)	N(011)	-179.3(7)
C(022)	N(00M)	C(02I)	N(00W)	-1.0(12)	C(02Q)	N(00U)	N(014)	C(023)	-177.7(10)
C(022)	N(00M)	C(02I)	N(30)	-179.5(7)	C(02Q)	N(00U)	N(014)	C(02D)	-0.8(9)
C(022)	N(00V)	C(02E)	N(00W)	-3.7(12)	C(02Q)	N(00X)	C(02D)	N(012)	-179.6(12)
C(022)	N(00V)	C(02E)	N(01P)	176.6(8)	C(02Q)	N(00X)	C(02D)	N(014)	-0.3(9)
C(022)	N(019)	C(02F)	N(00S)	-172.9(8)	O(030)	Cl(00)	O(02V)	O(02Z)	-151(5)
C(022)	N(019)	C(02F)	N(01J)	8.1(15)	O(3)	Cl(00)	O(02V)	O(02Z)	86(5)

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4**.

Atom	**x**	**y**	**z**	***U(eq)***
H(00C)	12432	6615	-7458	70
H(00D)	12555	5675	-7334	70
H(00A)	11794	-793	-4276	46
H(00B)	11568	-97	-5073	46
H(00L)	14246	519	-5644	47
H(00T)	14123	393	-9353	46
H(00U)	6992	4176	-3952	45
H(010)	11724	1787	-3384	50
H(012)	9289	2001	-5462	48
H(017)	16219	5456	-10067	45
H(01G)	19209	1987	-8986	49
H(01U)	10298	3445	-3885	93
H(01V)	10748	2765	-3347	93

H(01Q)	10772	2173	-6789	51
H(01R)	10402	1300	-6102	51
H(01A)	11610	2984	-4962	57
H(01B)	12102	3190	-5940	57
H(01H)	14432	6992	-9426	55
H(01I)	15192	6776	-10215	55
H(01S)	14843	261	-11182	56
H(01T)	15059	939	-12042	56
H(01M)	17249	4601	-10589	47
H(01W)	11476	-2174	-2372	107
H(01X)	11596	-1487	-3202	107
H(01C)	15913	1215	-8176	59
H(01D)	15865	1969	-9015	59
H(01J)	13951	4848	-6755	54
H(01K)	14539	3995	-6647	54
H(01O)	9859	-740	-1539	53
H(01P)	9024	6	-1443	53
H(01L)	19177	2968	-11752	59
H(01N)	18660	3848	-11781	59
H(01E)	13513	-1036	-3217	63
H(01F)	14388	-626	-3979	63
H(02A)	8711	3428	-6691	69
H(02B)	7624	3644	-6577	69
H(02P)	10750	3548	-7673	138
H(30A)	13268	4057	-8899	54
H(30B)	12469	3996	-8083	54
H(1A)	10478	4699	-8660	199
H(1B)	9372	4197	-8352	199
H(1C)	10336	4001	-9116	199

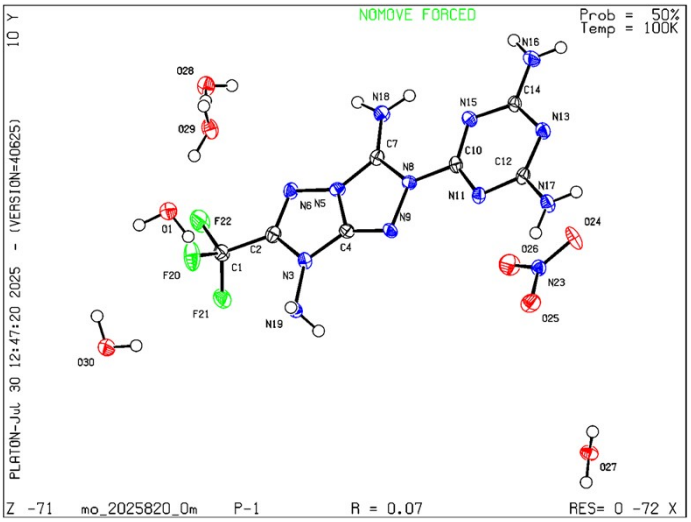


Figure S2. Single-crystal X-ray structures of 5.

Table S8 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **5**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	*U(eq)*
F(21)	1375(3)	2201(3)	1710(1)	27(1)
F(22)	3157(3)	1866(3)	785(1)	39(1)
F(20)	2942(3)	4321(3)	1300(2)	36(1)
O(27)	1951(3)	-13(3)	8674(2)	19(1)
O(29)	7402(3)	5453(3)	1034(2)	22(1)
O(28)	7427(4)	2434(3)	162(2)	22(1)
O(1)	5184(3)	7701(3)	1213(2)	22(1)
O(30)	235(3)	7827(3)	994(2)	24(1)
O(24)	8293(3)	746(3)	7226(2)	31(1)
O(26)	6203(4)	68(3)	6141(2)	30(1)
O(25)	6221(4)	2136(3)	7116(2)	27(1)
N(5)	6472(4)	2285(3)	3066(2)	16(1)
N(9)	6612(4)	3548(3)	4467(2)	16(1)
N(19)	3035(4)	4311(4)	3417(2)	19(1)
N(11)	9159(4)	3746(3)	5835(2)	16(1)
N(23)	6936(4)	983(3)	6833(2)	17(1)
N(3)	4328(4)	3505(3)	3156(2)	16(1)
N(8)	8014(4)	2738(3)	4362(2)	15(1)
N(17)	10435(4)	4767(3)	7272(2)	19(1)
N(6)	5542(4)	1939(3)	2201(2)	17(1)
N(15)	10619(4)	2134(3)	4915(2)	17(1)
N(13)	11850(4)	3130(4)	6450(2)	18(1)
N(18)	8960(4)	1112(3)	3168(2)	19(1)
N(16)	13185(4)	1591(4)	5535(2)	23(1)
C(1)	2920(5)	2761(4)	1518(2)	19(1)
C(4)	5769(4)	3220(4)	3654(2)	15(1)
C(10)	9350(4)	2879(4)	5091(2)	15(1)
C(14)	11865(5)	2311(4)	5643(2)	16(1)
C(12)	10484(5)	3849(4)	6506(2)	17(1)
C(2)	4270(5)	2695(4)	2296(2)	18(1)
C(7)	7925(4)	1958(4)	3505(2)	15(1)

Table S9 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **5**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	x	y	z	*U(eq)*
F(21)	18(1)	34(1)	27(1)	6(1)
F(22)	38(2)	61(2)	19(1)	-14(1)
F(20)	46(2)	25(1)	33(1)	14(1)
O(27)	17(1)	18(1)	22(1)	-2(1)
O(29)	26(2)	17(1)	24(1)	2(1)
O(28)	30(2)	16(1)	22(1)	2(1)

O(1)	22(2)	25(1)	21(1)	2(1)
O(30)	23(2)	29(2)	21(1)	2(1)
O(24)	25(2)	34(2)	34(2)	7(1)
O(26)	29(2)	32(2)	27(1)	-7(1)
O(25)	37(2)	23(1)	27(1)	4(1)
N(5)	18(2)	16(2)	14(1)	-3(1)
N(9)	17(2)	18(2)	17(1)	2(1)
N(19)	22(2)	21(2)	18(2)	-1(1)
N(11)	21(2)	15(1)	13(1)	2(1)
N(23)	18(2)	16(2)	17(2)	4(1)
N(3)	18(2)	14(1)	14(1)	0(1)
N(8)	18(2)	16(2)	15(1)	1(1)
N(17)	22(2)	19(2)	17(2)	-1(1)
N(6)	20(2)	19(2)	13(1)	-1(1)
N(15)	18(2)	16(2)	19(2)	4(1)
N(13)	20(2)	18(2)	18(2)	3(1)
N(18)	21(2)	21(2)	15(1)	-4(1)
N(16)	22(2)	31(2)	20(2)	1(1)
C(1)	20(2)	20(2)	16(2)	-3(1)
C(4)	17(2)	13(2)	17(2)	1(1)
C(10)	17(2)	12(2)	16(2)	4(1)
C(14)	18(2)	15(2)	17(2)	6(1)
C(12)	22(2)	12(2)	16(2)	6(1)
C(2)	20(2)	18(2)	16(2)	1(1)
C(7)	19(2)	13(2)	14(2)	1(1)

Table S10 Bond Lengths for **5**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
F(21)	C(1)	1.330(4)	N(19)	H(19B)	0.874(19)
F(22)	C(1)	1.324(4)	N(11)	C(10)	1.314(4)
F(20)	C(1)	1.333(4)	N(11)	C(12)	1.355(5)
O(27)	H(27A)	0.87	N(3)	C(4)	1.362(4)
O(27)	H(27B)	0.87	N(3)	C(2)	1.390(4)
O(29)	H(29A)	0.87	N(8)	C(10)	1.414(4)
O(29)	H(29B)	0.87	N(8)	C(7)	1.372(4)
O(28)	H(28A)	0.87	N(17)	H(17A)	0.88
O(28)	H(28B)	0.77(5)	N(17)	H(17B)	0.88
O(1)	H(1A)	0.87	N(17)	C(12)	1.330(4)
O(1)	H(1B)	0.87	N(6)	C(2)	1.306(4)
O(30)	H(30A)	0.87	N(15)	C(10)	1.325(4)
O(30)	H(30B)	0.87	N(15)	C(14)	1.363(4)
O(24)	N(23)	1.228(4)	N(13)	C(14)	1.336(4)
O(26)	N(23)	1.252(4)	N(13)	C(12)	1.347(5)
O(25)	N(23)	1.264(4)	N(18)	H(18A)	0.88

N(5)	N(6)	1.389(4)	N(18)	H(18B)	0.88
N(5)	C(4)	1.363(4)	N(18)	C(7)	1.300(4)
N(5)	C(7)	1.347(4)	N(16)	H(16A)	0.88
N(9)	N(8)	1.428(4)	N(16)	H(16B)	0.88
N(9)	C(4)	1.296(4)	N(16)	C(14)	1.326(4)
N(19)	H(19A)	0.8827	C(1)	C(2)	1.495(5)
N(19)	N(3)	1.409(4)	N(19)	H(19B)	0.874(19)

Table S11 Bond Angles for **5**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
H(27A)	O(27)	H(27B)	104.5	C(7)	N(18)	H(18A)	120
H(29A)	O(29)	H(29B)	104.5	C(7)	N(18)	H(18B)	120
H(28A)	O(28)	H(28B)	116.5	H(16A)	N(16)	H(16B)	120
H(1A)	O(1)	H(1B)	104.5	C(14)	N(16)	H(16A)	120
H(30A)	O(30)	H(30B)	104.5	C(14)	N(16)	H(16B)	120
C(4)	N(5)	N(6)	113.9(3)	F(21)	C(1)	F(20)	106.7(3)
C(7)	N(5)	N(6)	137.5(3)	F(21)	C(1)	C(2)	112.9(3)
C(7)	N(5)	C(4)	108.6(3)	F(22)	C(1)	F(21)	108.0(3)
C(4)	N(9)	N(8)	100.2(3)	F(22)	C(1)	F(20)	108.0(3)
H(19A)	N(19)	H(19B)	113.1	F(22)	C(1)	C(2)	110.5(3)
N(3)	N(19)	H(19A)	109.9	F(20)	C(1)	C(2)	110.6(3)
N(3)	N(19)	H(19B)	108(3)	N(9)	C(4)	N(5)	114.8(3)
C(10)	N(11)	C(12)	112.6(3)	N(9)	C(4)	N(3)	140.4(3)
O(24)	N(23)	O(26)	120.6(3)	N(3)	C(4)	N(5)	104.7(3)
O(24)	N(23)	O(25)	121.6(3)	N(11)	C(10)	N(8)	115.3(3)
O(26)	N(23)	O(25)	117.8(3)	N(11)	C(10)	N(15)	129.8(3)
C(4)	N(3)	N(19)	130.5(3)	N(15)	C(10)	N(8)	114.9(3)
C(4)	N(3)	C(2)	105.5(3)	N(13)	C(14)	N(15)	125.3(3)
C(2)	N(3)	N(19)	123.8(3)	N(16)	C(14)	N(15)	116.7(3)
C(10)	N(8)	N(9)	119.5(3)	N(16)	C(14)	N(13)	118.0(3)
C(7)	N(8)	N(9)	113.3(3)	N(17)	C(12)	N(11)	116.8(3)
C(7)	N(8)	C(10)	127.1(3)	N(17)	C(12)	N(13)	117.9(3)
H(17A)	N(17)	H(17B)	120	N(13)	C(12)	N(11)	125.3(3)
C(12)	N(17)	H(17A)	120	N(3)	C(2)	C(1)	123.1(3)
C(12)	N(17)	H(17B)	120	N(6)	C(2)	N(3)	114.8(3)
C(2)	N(6)	N(5)	101.1(3)	N(6)	C(2)	C(1)	122.0(3)
C(10)	N(15)	C(14)	112.2(3)	N(5)	C(7)	N(8)	103.0(3)
C(14)	N(13)	C(12)	114.7(3)	N(18)	C(7)	N(5)	126.8(3)
H(18A)	N(18)	H(18B)	120	N(18)	C(7)	N(8)	130.2(3)

Table S12 Torsion Angles for **5**.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
F(21)	C(1)	C(2)	N(3)	-58.1(4)	C(4)	N(9)	N(8)	C(10)	175.8(3)

F(21)	C(1)	C(2)	N(6)	125.7(4)	C(4)	N(9)	N(8)	C(7)	-0.8(4)
F(22)	C(1)	C(2)	N(3)	-179.2(3)	C(4)	N(3)	C(2)	N(6)	-0.6(4)
F(22)	C(1)	C(2)	N(6)	4.6(5)	C(4)	N(3)	C(2)	C(1)	-177.0(3)
F(20)	C(1)	C(2)	N(3)	61.3(4)	C(10)	N(11)	C(12)	N(17)	177.1(3)
F(20)	C(1)	C(2)	N(6)	-114.9(4)	C(10)	N(11)	C(12)	N(13)	-1.3(5)
N(5)	N(6)	C(2)	N(3)	0.4(4)	C(10)	N(8)	C(7)	N(5)	-175.9(3)
N(5)	N(6)	C(2)	C(1)	176.9(3)	C(10)	N(8)	C(7)	N(18)	3.7(6)
N(9)	N(8)	C(10)	N(11)	1.4(4)	C(10)	N(15)	C(14)	N(13)	0.0(5)
N(9)	N(8)	C(10)	N(15)	-177.7(3)	C(10)	N(15)	C(14)	N(16)	179.4(3)
N(9)	N(8)	C(7)	N(5)	0.4(3)	C(14)	N(15)	C(10)	N(11)	1.2(5)
N(9)	N(8)	C(7)	N(18)	180.0(3)	C(14)	N(15)	C(10)	N(8)	-179.9(3)
N(19)	N(3)	C(4)	N(5)	175.6(3)	C(14)	N(13)	C(12)	N(11)	2.3(5)
N(19)	N(3)	C(4)	N(9)	-4.1(7)	C(14)	N(13)	C(12)	N(17)	-176.1(3)
N(19)	N(3)	C(2)	N(6)	-176.2(3)	C(12)	N(11)	C(10)	N(8)	-179.5(3)
N(19)	N(3)	C(2)	C(1)	7.4(5)	C(12)	N(11)	C(10)	N(15)	-0.6(5)
N(8)	N(9)	C(4)	N(5)	0.9(4)	C(12)	N(13)	C(14)	N(15)	-1.6(5)
N(8)	N(9)	C(4)	N(3)	-179.3(4)	C(12)	N(13)	C(14)	N(16)	179.1(3)
N(6)	N(5)	C(4)	N(9)	179.6(3)	C(2)	N(3)	C(4)	N(5)	0.4(3)
N(6)	N(5)	C(4)	N(3)	-0.2(4)	C(2)	N(3)	C(4)	N(9)	-179.3(4)
N(6)	N(5)	C(7)	N(8)	179.6(3)	C(7)	N(5)	N(6)	C(2)	-179.5(4)
N(6)	N(5)	C(7)	N(18)	0.0(6)	C(7)	N(5)	C(4)	N(9)	-0.8(4)
C(4)	N(5)	N(6)	C(2)	-0.1(4)	C(7)	N(5)	C(4)	N(3)	179.4(3)
C(4)	N(5)	C(7)	N(8)	0.2(3)	C(7)	N(8)	C(10)	N(11)	177.4(3)
C(4)	N(5)	C(7)	N(18)	-179.4(3)	C(7)	N(8)	C(10)	N(15)	-1.6(5)

Table S13 Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **5**.

Atom	**x**	**y**	**z**	***U(eq)***
H(27A)	2899	687	8728	29
H(27B)	1255	544	8903	29
H(29A)	6568	6000	1023	34
H(29B)	8249	6174	914	34
H(28A)	7360	3401	418	34
H(1A)	4338	7787	805	34
H(1B)	4796	7792	1733	34
H(30A)	962	7729	617	36
H(30B)	840	8009	1531	36
H(19A)	2626	3848	3885	23
H(17A)	11279	4889	7721	23
H(17B)	9559	5253	7329	23
H(18A)	8737	685	2597	22
H(18B)	9883	965	3512	22

H(16A)	14016	1662	5987	28
H(16B)	13229	1043	5011	28
H(28B)	7600(60)	1760(60)	490(30)	36(14)
H(19B)	3450(60)	5370(30)	3530(30)	50(15)

2. Experimental

Caution! Proper safety precautions should be taken during the preparation, characterization, and handling of energetic materials. Lab personnel should be properly grounded. All the reactions and performance testing of the prepared materials were conducted in a protected fume hood and behind a safety shield. Face shields and leather gloves must be used.

General methods

All reagents were purchased from Energy Chemical or Aladdin in analytical grade. ^{1}H and ^{13}C NMR spectra were recorded on Bruker AVANCE 400 nuclear magnetic resonance spectrometer. DMSO-d_6 was employed as a solvent and locking solvent. The onset decomposition temperature was measured using a TA Instruments DSC25 differential scanning calorimeter at a heating rate of 10 °C min^{-1} under dry nitrogen atmosphere. Infrared (IR) spectra were recorded on an FT-IR spectrometer (Thermo Nicolet AVATAR 370). Elemental analyses (C, H, N) were performed on a Vario Micro cube Elementar Analyzer. Impact and friction sensitivity measurements were made using a standard BAM Fallhammer and a BAM friction tester.

6-(Trifluoromethyl)-7H-[1,2,4]triazolo[4,3-b][1,2,4]triazole-3,7-diamine (2): Compound **2** was synthesized according to the literature method.[1]

6-(7-Amino-3-imino-6-(trifluoromethyl)-3H-[1,2,4]triazolo[4,3-b][1,2,4]triazol-2(7H)-yl)-1,3,5-triazine-2,4-diamine (3): 2-Chloro-4,6-diamino-1,3,5-triazine (0.146 g, 1.0 mmol) and compound **2** (0.207 g, 1.0 mmol) were charged into a 25 mL three-necked flask, followed by DMF (5 mL). The mixture was heated to reflux at 120 °C for 12 h under a condenser. Reaction progress was monitored by TLC. After completion of the reaction, the mixture turned orange–red, and a white precipitate formed. The mixture was allowed to cool to room temperature, and the solid was collected by filtration, washed with cold water, and dried to afford compound **3** as a white solid

(87.3% yield). T_d (onset): 253.48 °C. ^{1}H NMR (400 MHz, DMSO-*d*6) δ = 8.42(s, 1H), 7.03 (d, 2H), 6.81 (d, 2H), 6.10 (s, 2H); ^{13}C NMR (DMSO-d_6) δ = 167.38, 163.96, 143.26, 109.46 ppm; ^{19}F NMR (DMSO-d_6) δ = -64.41 ppm; IR (KBr): ṽ = 3341(s), 3132(s), 2926(s), 1690(m), 1605(s), 1538(s), 1487(w), 1414(s), 1332(s), 1093(s), 1016(w), 975(m), 852(w), 821(s), 746(w), 720(s), 714(s) cm^{-1}; Anal. calcd. for $C_7H_7F_3N_{12}$: C 26.59; H 2.23; N 53.16; found: C 26.68; H 2.10; N 53.09.

7-Amino-2-(4,6-diamino-1,3,5-triazin-2-yl)-6-(trifluoromethyl)-2,7-dihydro-3H-[1,2,4]triazolo[4,3-b][1,2,4]triazol-3-iminium perchlorate (4): Compound **3** (0.417 g, 1.0 mmol) was dispersed in water (5 mL) in a 25 mL three-necked flask. Aqueous $HClO_4$ (70%) was added dropwise with stirring until the suspension became clear and transparent, indicating complete salt formation. The resulting solution was then subjected to recrystallization to afford compound **4** as a white solid (72.2% yield). T_d (onset): 241.38 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.46 (d, 1H), 7.39 (d, 1H), 6.62 (s, 1H), 4.51 (s, 4H); ^{13}C NMR (DMSO-d_6) δ = 167.18, 162.76, 148.36, 111.57 ppm; ^{19}F NMR (DMSO-d_6) δ = -64.41, -65.53, ppm; IR (KBr): ṽ = 3436(s), 3330(s), 3192(s), 1664(m), 1608(s), 1542(s), 1479(w), 1413(s), 1336(m), 1262(s), 1188(s), 1096(vs), 1032(m), 972(w), 826(s), 626(vs) cm^{-1}; Anal. calcd. for $C_7H_8ClF_3N_{12}O_4$: C 20.18; H 1.94; N 40.34; found: C 20.04; H 2.07; N 40.26.

7-Amino-2-(4,6-diamino-1,3,5-triazin-2-yl)-6-(trifluoromethyl)-2,7-dihydro-3H-[1,2,4]triazolo[4,3-b][1,2,4]triazol-3-iminium nitrate (5): Compound 3 (0.417 g, 1.0 mmol) was dissolved in methanol (5 mL), followed by dropwise addition of 68% nitric acid. The mixture was stirred at room temperature for 12 h and then left undisturbed to give compound **5** as a white solid in 79.1% yield. T_d (onset): 241.21 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.65 (d, 1H), 7.48 (d, 1H), 6.65 (s, 1H), 5.79 (s, 2H); ^{19}F NMR (DMSO-d_6) δ = -64.47, -64.88 ppm; IR (KBr): ṽ = 3447(m), 3337(m), 3281(m), 3210(m), 1701(s), 1679(s), 1638(m), 1553(s), 1485(w), 1466(w), 1424(m), 1379(vs), 1274(m), 1220(m), 1186(s), 1164(s), 1114(s), 838(w), 800(s), 777(w), 728(m) cm^{-1}; Anal. calcd. for $C_7H_8F_3N_{13}O_3$: C, 22.17; H, 2.13; N, 48.02; found: C 21.09; H 2.17; N 47,89.

2,2'-(6-Amino-1,3,5-triazine-2,4-diyl)bis(3-imino-6-(trifluoromethyl)-2,3-dihydro-7H-[1,2,4]triazolo[4,3-b][1,2,4]triazol-7-amine) (6): 4,6-Dichloro-1,3,5-triazine-2-amine (0.165 g, 1.0 mmol) and compound **2** (0.414 g, 2.0 mmol) were added sequentially to a 25 mL three-necked flask, followed by DMF (8 mL). The reaction mixture was heated at 120 °C under reflux for 12 h. Reaction progress was monitored by TLC, and after completion of the reaction, the solution turned orange-red

with the formation of a light-yellow precipitate. After cooling to room temperature, the solid was collected by filtration, washed with cold water, and dried to afford compound **6** as a pale yellow solid (78.6% yield). T_d (onset): 233.95 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 8.53 (d, 2H), 8.37 (d, 2H), 6.67(d, 4H) ^{19}F NMR (DMSO-d_6) δ = -64.17 ppm; IR (KBr): ṽ = 3193(s), 3079(m), 1696(s), 1539(s), 1425(s), 1297(m), 1257(s), 1223(s), 1163(s), 1100(vs), 1034(m), 986(w), 838(m), 796(w), 729(w), 648(vs) cm^{-1}; Anal. calcd. for $C_{11}H_8F_6N_{18}$: C 26.10; H 1.59; N 49.80. found: C 26.33; H 1.87; N 49.65.

3. Theoretical calculations

The calculations of the heats of formation were carried out using Gaussian 09 (Revision D.01) suite of programs. All the compounds were determined using isodesmic reactions (Scheme S1). The geometry optimization and frequency analyses of the structures were calculated using B3LYP/6-31+G** level. Gas phase heats of formation of the title compounds were computed based on an isodesmic reaction. The enthalpy of reaction was carried out by combining the M062X/6-311++G** energy difference for the reactions, the scaled zero-point energies (*ZPE*), values of thermal correction (HT), and other thermal factors.[2,3] The solid-state heats of formation were obtained by employing Trouton's rule according to equation 1 (*T* represents either melting point or decomposition temperature when no melting occurs prior to decomposition).

$$\Delta H_{sub} = 188\ /J\ mol^{-1}\ K^{-1} \times T \quad (1)$$

For energetic salts, the solid-phase heat of formation is calculated on basis of a Born-Haber energy cycle (Scheme S2). The number is simplified by equation 2:

$$\Delta H_f(\text{salt, 298 K}) = \Delta H_f(\text{cation, 298K}) + \Delta H_f(\text{anion, 298K}) - \Delta H_L \quad (2)$$

in which ΔH_L can be predicted by using the formula suggested by Jenkins, etal.(equation 3):

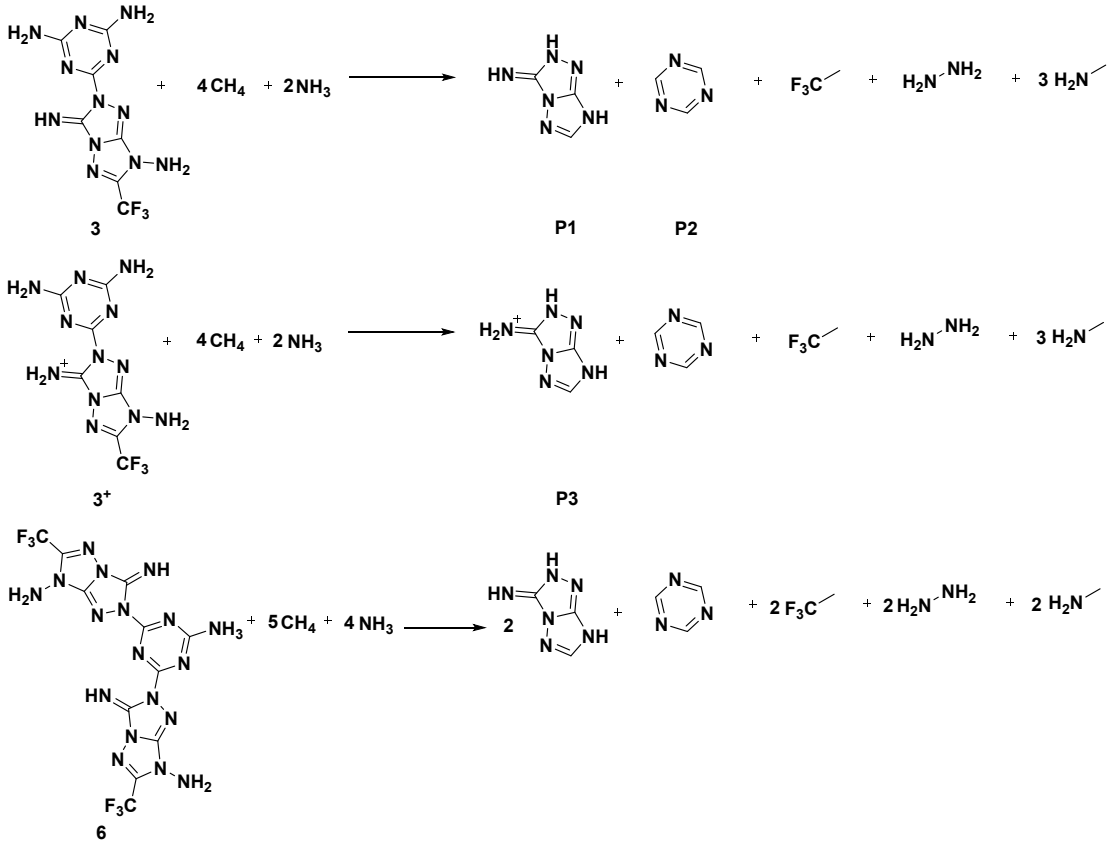
$$\Delta H_L = U_{pot} + [p(n_M/2 - 2) + q(n_X/2 - 2)]RT \quad (3)$$

In this equation, n_M and n_X depend on the nature of the ions Mp^+ and Xq^-, respectively.

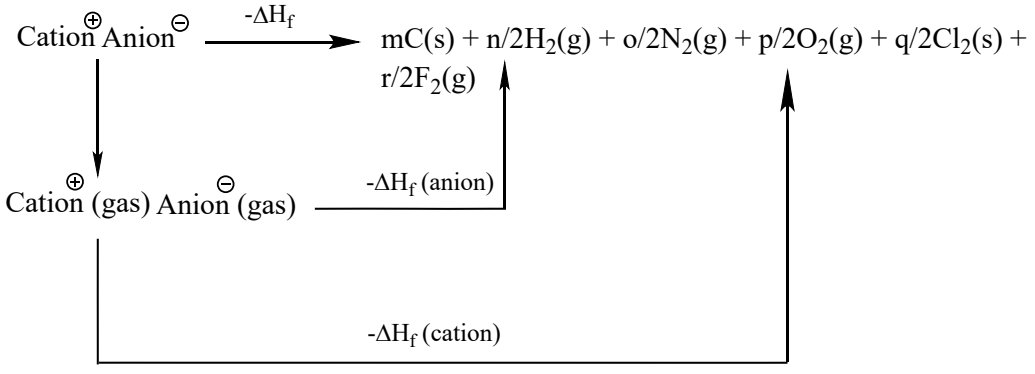
The equation for lattice potential energy U_{pot}(equation 4) has the form:

$$U_{POT}\ [kJ\ mol^{-1}] = \gamma(\rho m/Mm)^{1/3} + \delta \quad (4)$$

where ρ_m [g cm^{-3}] is the density of the salt, Mm is the chemical formula mass of the ionic material, and values for g and the coefficients γ (kJ mol^{-1} cm) and δ (kJ mol^{-1}) are assigned literature values.[4]



Scheme S1. Isodesmic reactions.



Scheme S2. Born−Haber Cycle for the formation of energetic salts.

Table S8 The scaled zero point energies (*ZPE*), values of thermal correction (H_{corr}), total energy (E_0) and heats of formation (*HOF*).

Species	*ZEP*	H^{corr}	E_0	*Corrected* E_0	*HOF(kJ mol^{-1})*
3	0.194332	0.21419	-1227.490152	-1227.28374	- 5.7345196
3$^+$	0.203501	0.224309	-1228.046598	-1227.83043	137.1672365
6	0.271964	0.302576	-2008.466028	-2008.17433	20.8292104
P1	0.092964	0.100651	-445.1702301	-445.07330	500.3913449
P2	0.065605	0.070658	-280.3783907	-280.31036	225.87
P3	0.103242	0.111548	-445.7222398	-445.61482	609.2133248
CH_4	0.045214	0.049022	-40.5203022	-40.47309	-74.6
NH_3	0.034534	0.038337	-56.5491671	-56.51221	-45.90
CH_3CF_3	0.052891	0.058625	-377.5614376	-377.50493	-772.0207611
NH_2NH_2	0.053494	0.057694	-111.859798	-111.80424	95.35
CH_3NH_2	0.064435	0.068758	-95.8575523	-95.79137	-23.5

Table S9 Calculated heat of formation for energetic salts.

Compound	ΔH_L*(kJ mol^{-1})*	ΔH_f^{cation}*(kJ mol^{-1})*	ΔH_f^{anion}*(kJ mol^{-1})*	ΔH_f^{298}*(kJ mol^{-1})*
4	431.2132625	137.2	307.7135581	13.66753209
5	442.3251163	137.2	-314.39	-619.5478798

Table S10 Cartesian coordinates of compound **3**.

Atom	**X**	**Y**	**Z**
C	0.2026	3.7556	0.1989
N	0.5527	2.4702	0.2075
C	-0.472	1.6312	0.0629
N	-1.7518	1.9721	-0.0818
C	-1.9638	3.2873	-0.0731
N	-1.0342	4.2318	0.0629
N	-0.2045	0.3938	0.0629
C	-1.2011	-0.7181	0.0629
N	-0.4349	-1.8707	0.4711
C	0.8748	-1.4323	0.3023
N	1.0857	-0.1736	0.0629
N	-0.6065	-3.1913	0.0538
C	0.6407	-3.5876	-0.0595
N	1.5661	-2.6	0.1649
N	1.1325	4.6043	0.3326
N	-3.1613	3.6761	-0.2065
N	-2.4262	-0.6628	-0.2263
N	2.9074	-2.7547	0.2362
C	1.0192	-4.9945	-0.4034
F	2.4061	-5.1044	-0.4498

F	0.4863	-5.3272	-1.6456
F	0.5176	-5.8597	0.5647
H	0.9106	5.6306	0.3326
H	2.1256	4.2819	0.4433
H	-3.3831	4.7024	-0.2064
H	-3.9325	2.9722	-0.3172
H	-2.6828	0.2937	-0.4791
H	3.5055	-1.9466	0.4084
H	3.3211	-3.6795	0.1178

Table S11 Cartesian coordinates of compound **3**$^{+}$.

Atom	**X**	**Y**	**Z**
C	-5.2408	-2.0879	-0.4128
N	-3.9468	-1.7714	-0.393
C	-3.7091	-0.4901	-0.1164
N	-4.6272	0.4439	0.1281
C	-5.8803	-0.0051	0.0772
N	-6.2563	-1.2556	-0.187
N	-2.4972	-0.1257	-0.0828
C	-2.0077	1.2776	0.0601
N	-0.6295	1.209	-0.3618
C	-0.3776	-0.1592	-0.3338
N	-1.3755	-0.9744	-0.1738
N	0.4438	1.9526	0.1308
C	1.3953	1.0473	0.1484
N	0.9793	-0.2113	-0.2054
N	-5.5328	-3.2926	-0.6702
N	-6.8004	0.8353	0.3008
N	-2.6693	2.319	0.4694
N	1.7645	-1.2962	-0.3913
C	2.8105	1.3614	0.522
F	3.579	0.2032	0.4468
F	2.8472	1.8583	1.8217
F	3.321	2.3144	-0.3549
H	-6.538	-3.5947	-0.6981
H	-4.7698	-3.9896	-0.8558
H	-7.8056	0.5331	0.2729
H	-6.5582	1.8344	0.5142
H	-3.6723	2.2249	0.7469
H	-2.198	3.2503	0.5209
H	1.3471	-2.1887	-0.655
H	2.7743	-1.2221	-0.2679

Table S12 Cartesian coordinates of compound **6**.

Atom	X	Y	Z
C	-2.0579	1.2617	0.3183
N	-3.3477	1.7635	0.7265
C	-4.1667	0.6513	0.5577
N	-3.615	-0.4994	0.3183
N	-3.9673	2.9423	0.3092
C	-5.2153	2.5489	0.1959
N	-5.404	1.2086	0.4203
N	-1.0241	1.9213	0.029
N	-6.5899	0.5634	0.4916
N	-1.6578	-2.3551	0.4629
C	-1.3024	-1.0793	0.3183
N	-0.0596	-0.6218	0.1736
C	0.8706	-1.5754	0.1823
N	0.6537	-2.8828	0.3183
C	-0.6318	-3.205	0.4543
N	-0.9041	-4.4341	0.5879
N	-2.2332	-0.2211	0.3183
N	2.0737	-1.2044	0.0489
C	3.2827	-2.0382	0.3177
N	4.3528	-1.0755	0.4182
C	3.7799	0.065	-0.1361
N	2.5044	0.0676	-0.3793
N	5.6809	-1.243	0.0236
C	5.9451	-0.064	-0.4916
N	4.8687	0.7858	-0.5303
N	3.3523	-3.2912	0.4307
N	4.8842	2.0888	-0.8904
C	-6.3344	3.4817	-0.1481
F	-7.532	2.7736	-0.1944
F	-6.09	4.0605	-1.3902
F	-6.422	4.4781	0.8201
C	7.3026	0.3192	-0.993
F	7.268	1.6238	-1.4772
F	7.6794	-0.5453	-2.017
F	8.2224	0.2353	0.0485
H	-0.2638	1.2867	-0.2237
H	-6.6142	-0.4416	0.6638
H	-7.4604	1.0817	0.3732
H	-0.1321	-5.1458	0.588
H	-1.9018	-4.7418	0.6987

H	2.4257	-3.7051	0.3098
H	4.0199	2.6304	-0.8828
H	5.7603	2.5304	-1.1696

4. DSC spectra of all products

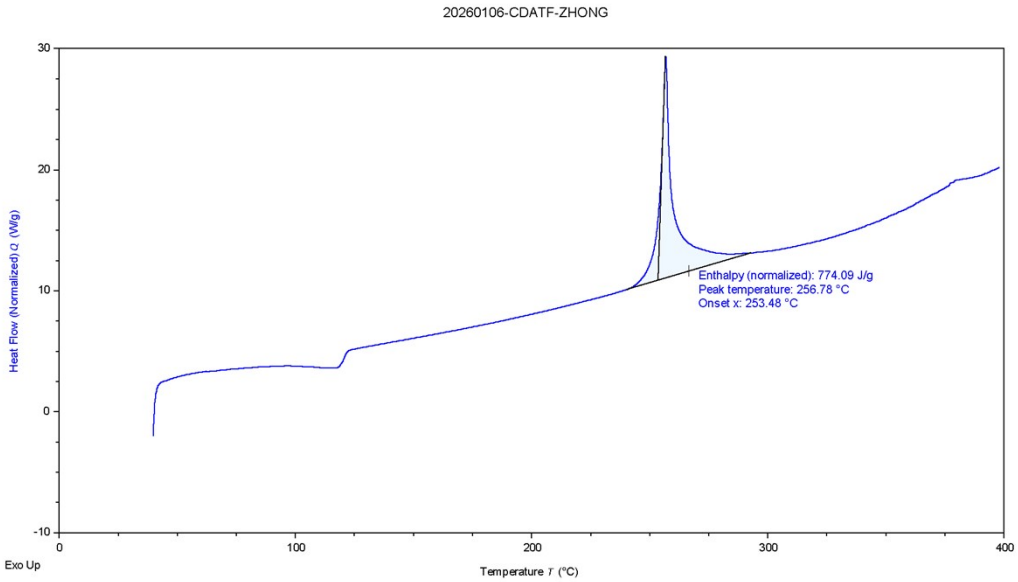


Figure S3. DSC curve of **3**.

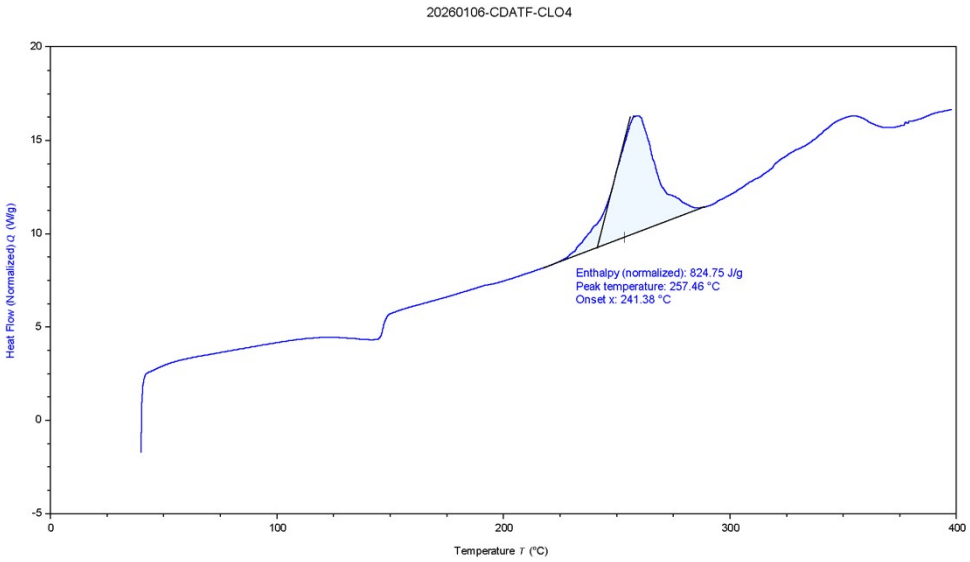


Figure S4. DSC curve of **4**.

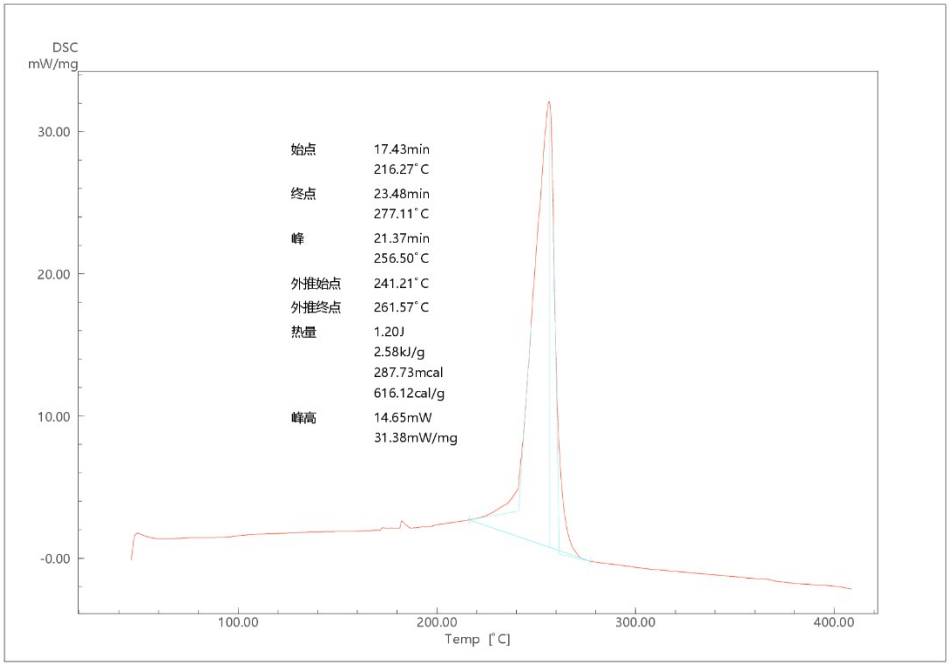


Figure S5. DSC curve of **5**.

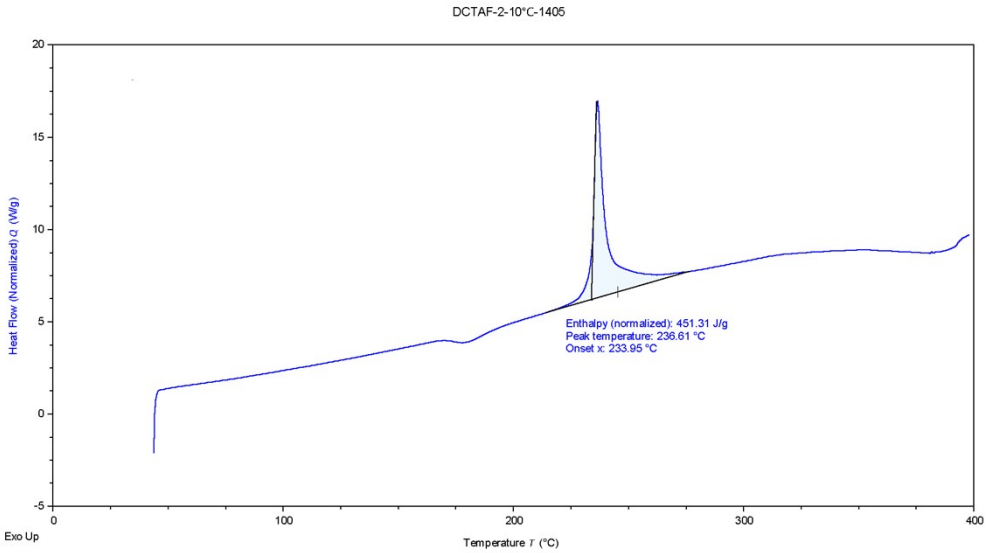


Figure S6. DSC curve of **5**.

5. ^{1}H, ^{19}F and ^{13}C NMR spectra of all products

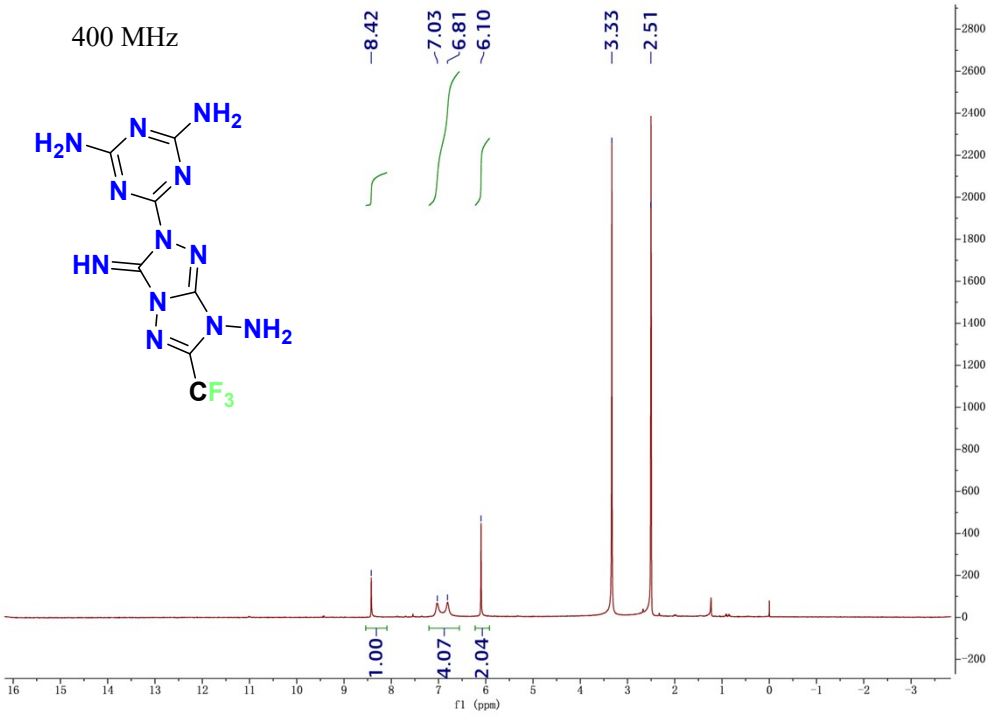


Figure S7. ^{1}H NMR of **3** in DMSO-d_6.

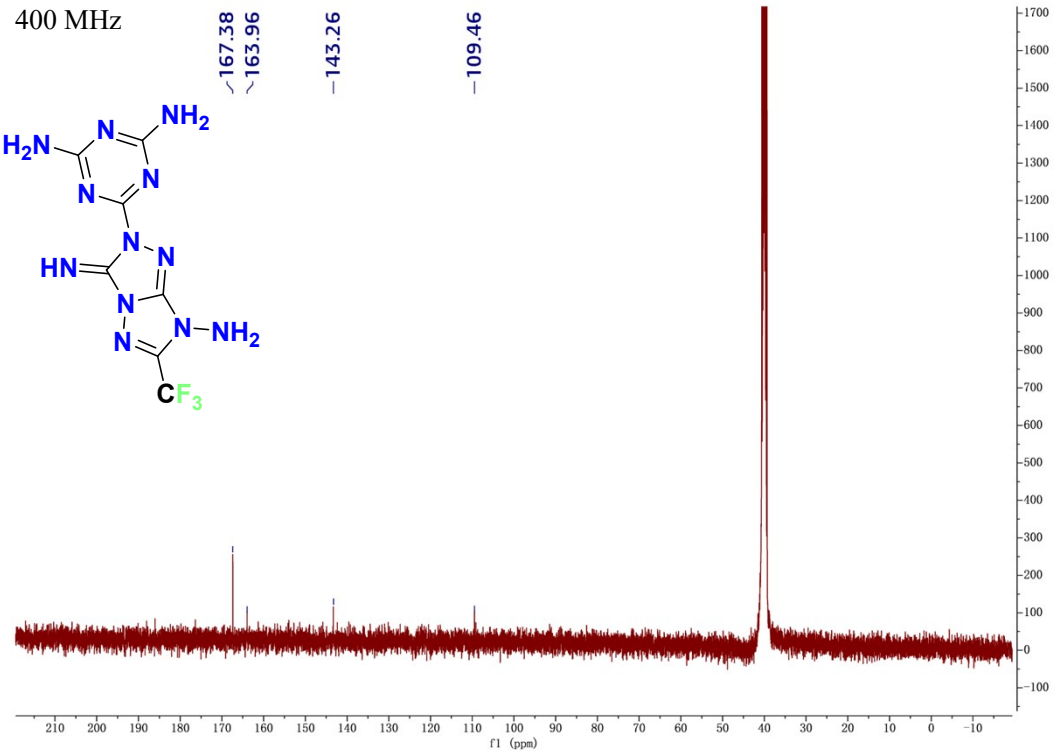


Figure S8. ^{13}C NMR of **3** in DMSO-d_6.

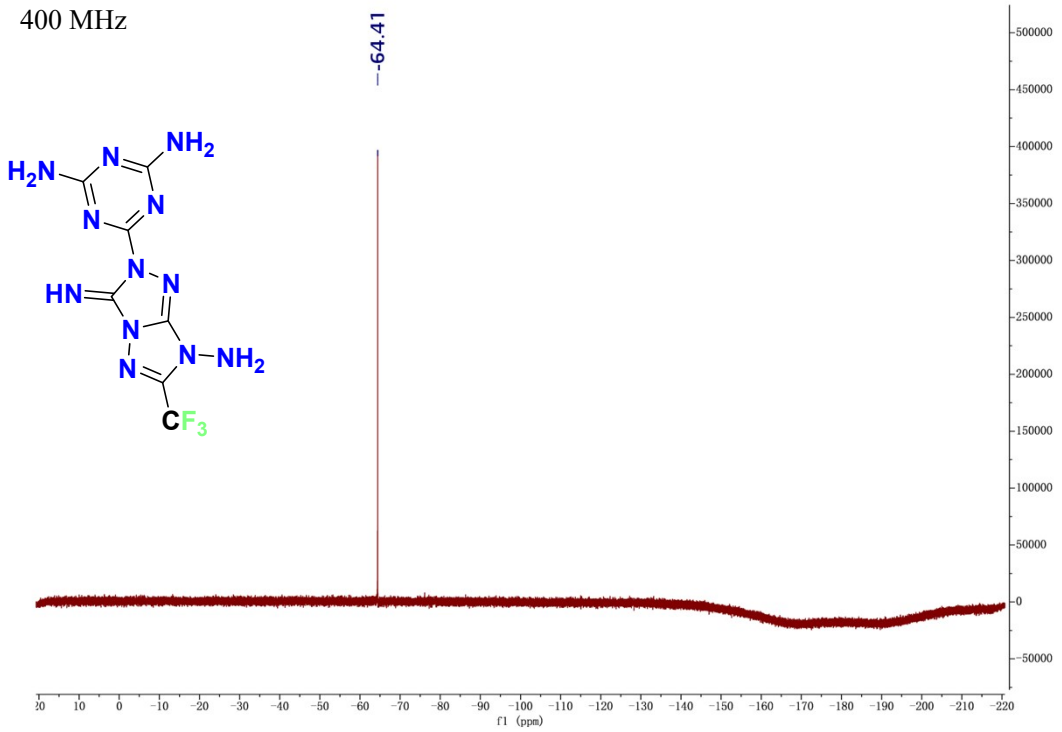


Figure S9. ^{19}F NMR of **3** in DMSO-d_6.

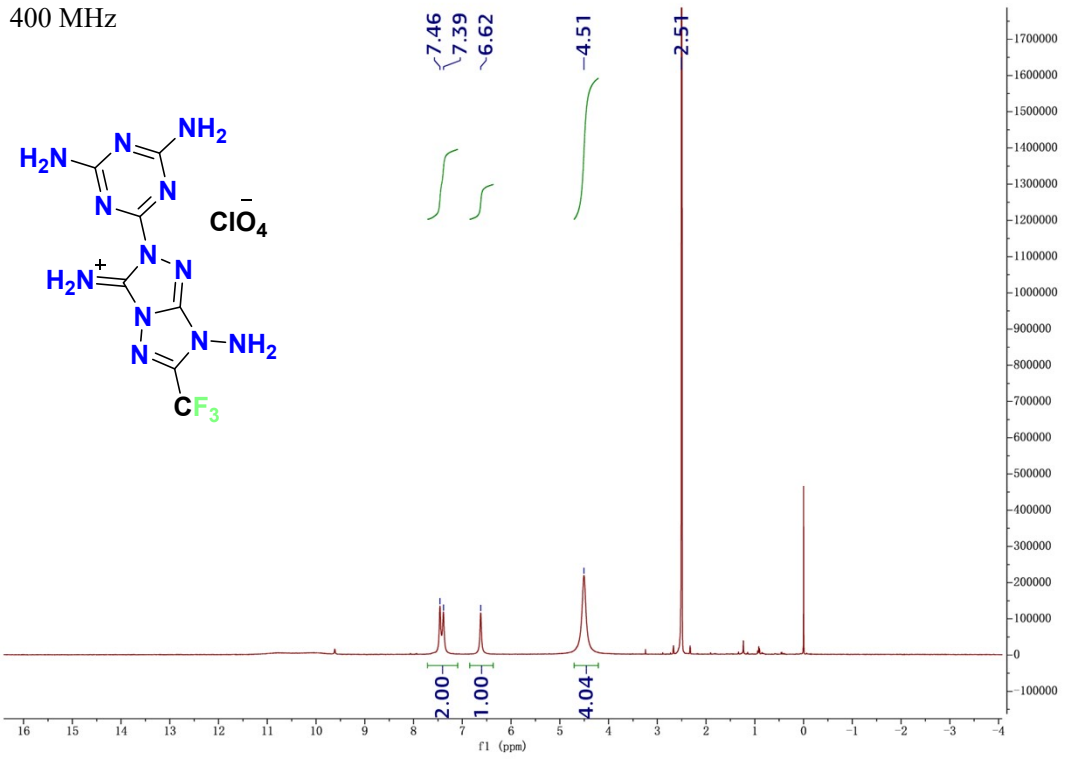


Figure S10. ^{1}H NMR of **4** in DMSO-d_6.

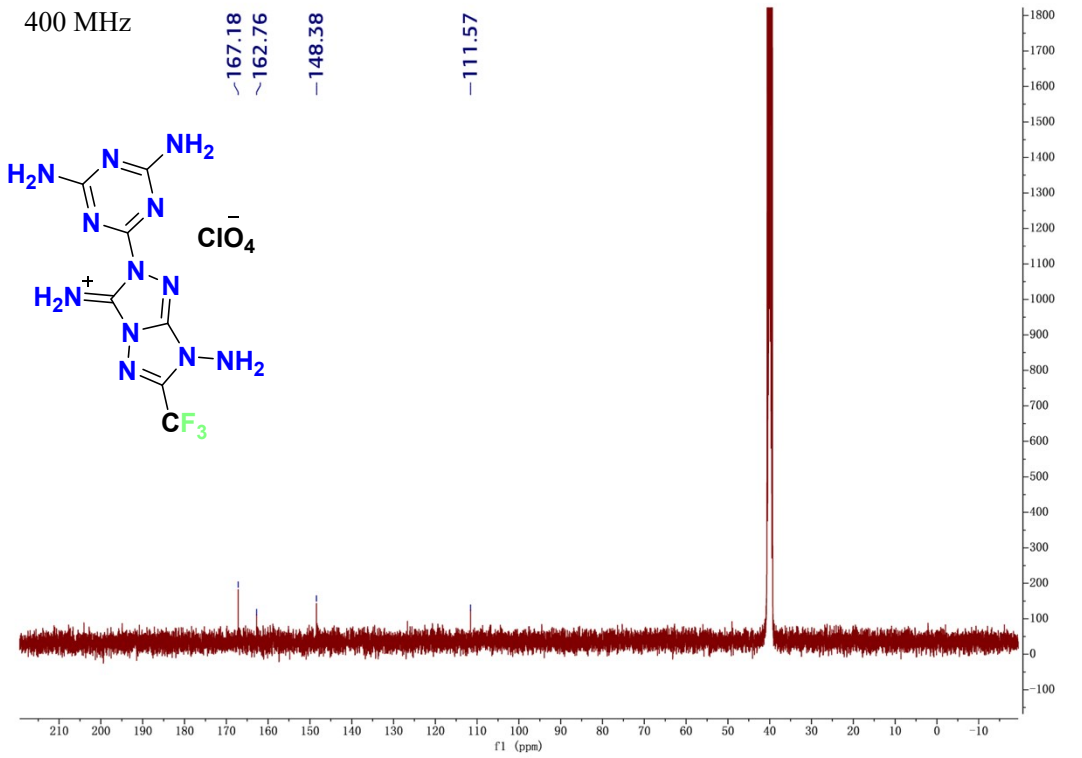


Figure S11. ^{13}C NMR of **4** in DMSO-d_6.

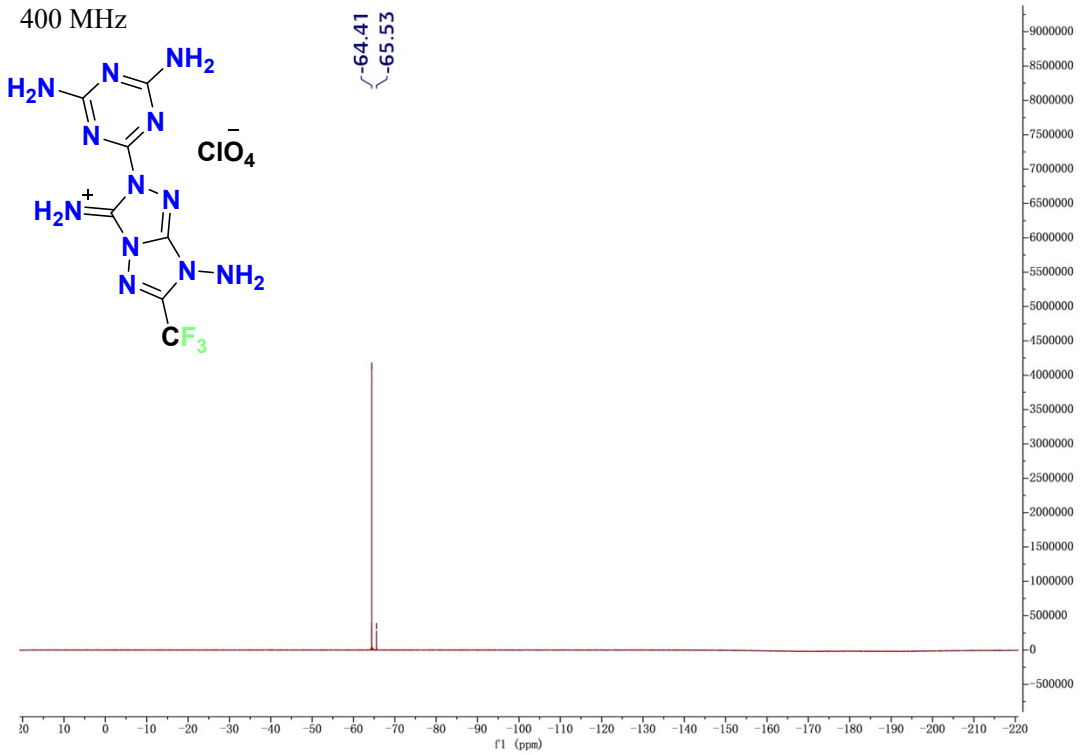


Figure S12. ^{19}F NMR of **4** in DMSO-d_6.

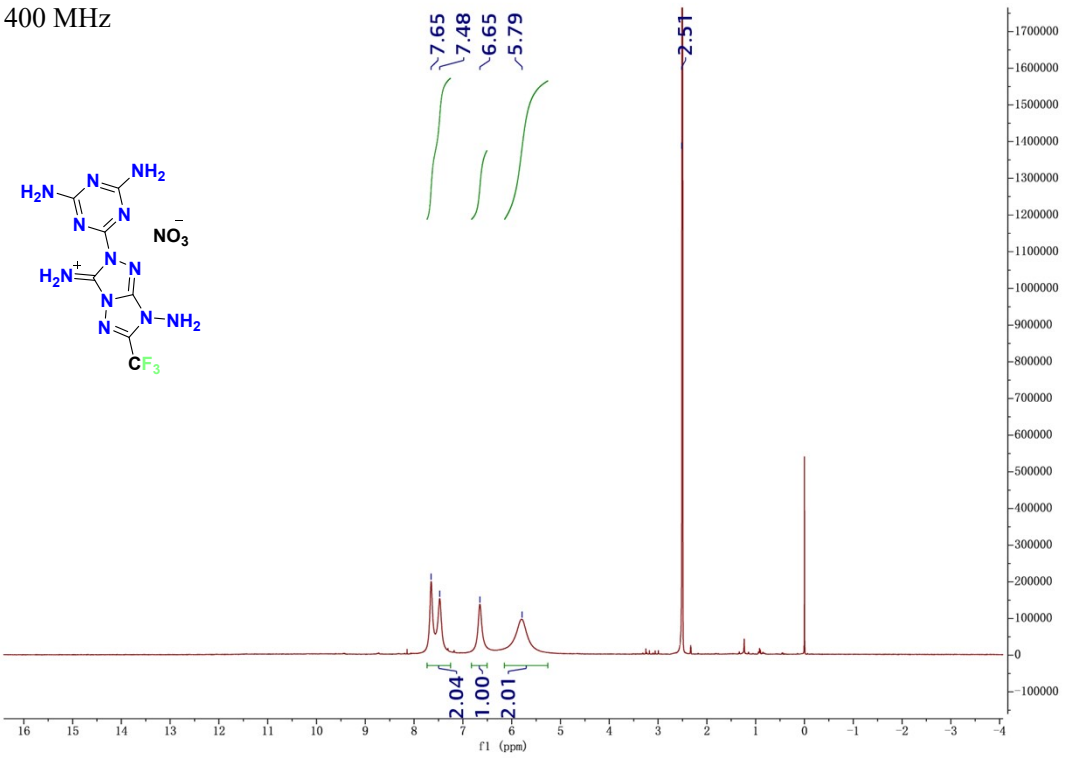


Figure S13. ^{1}H NMR of **5** in DMSO-d_6.

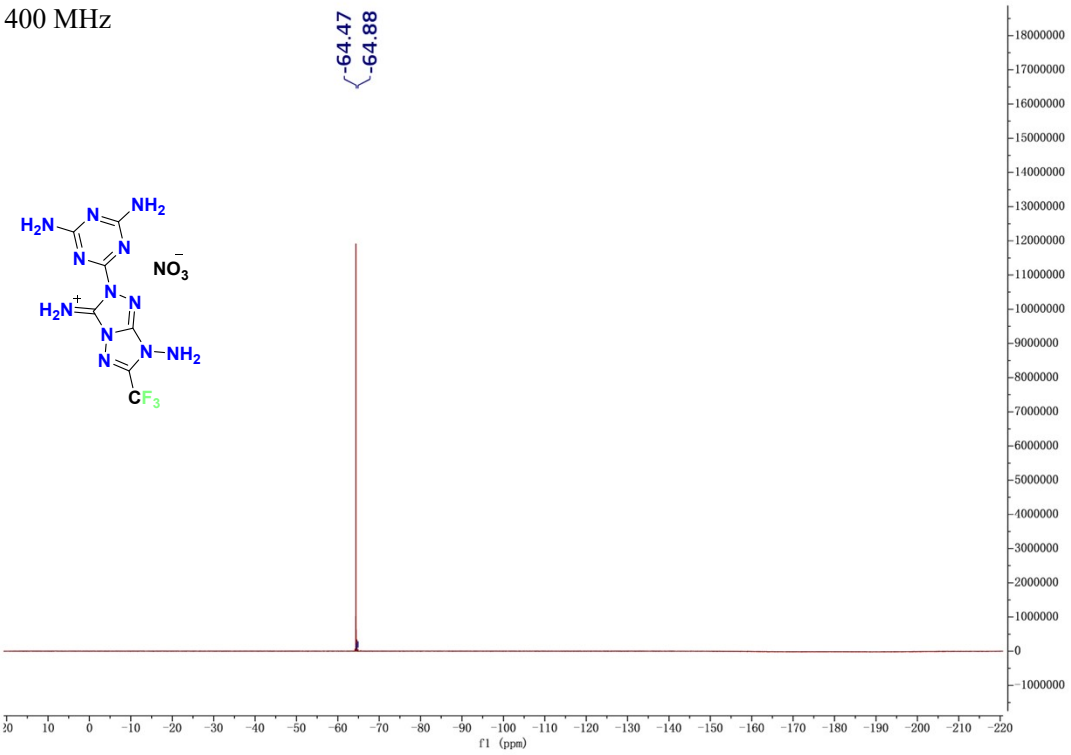


Figure S14. ^{19}F NMR of **5** in DMSO-d_6.

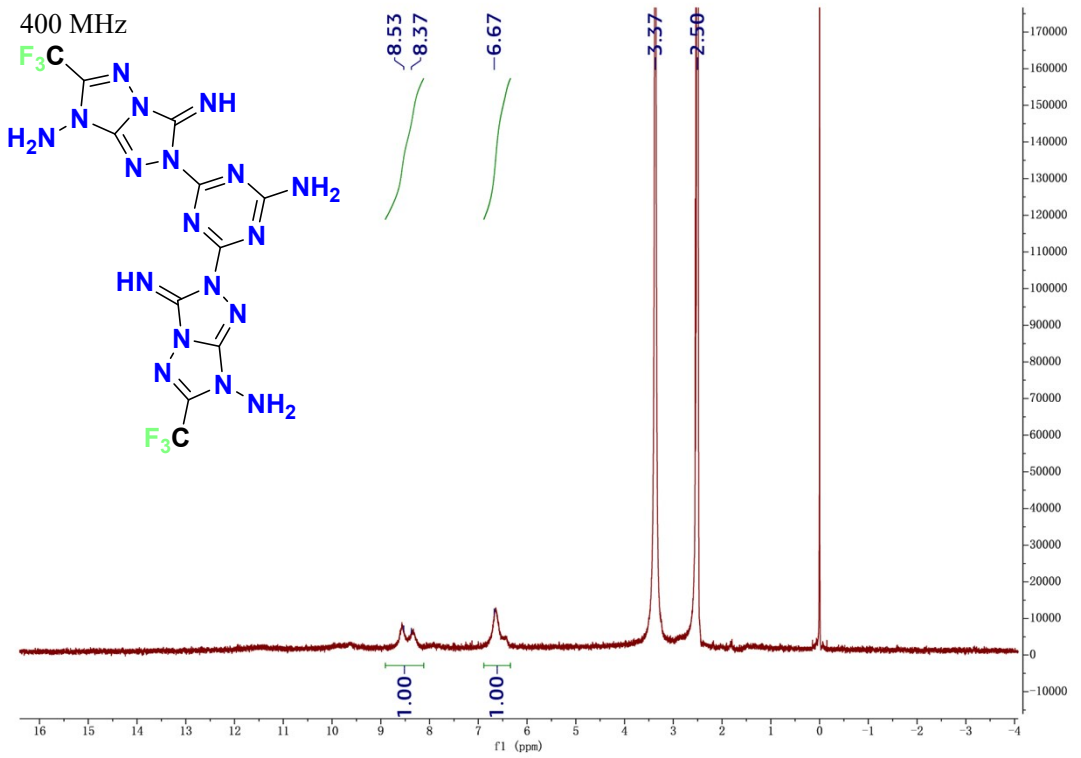


Figure S15. ^{1}H NMR of **6** in DMSO-d_6.

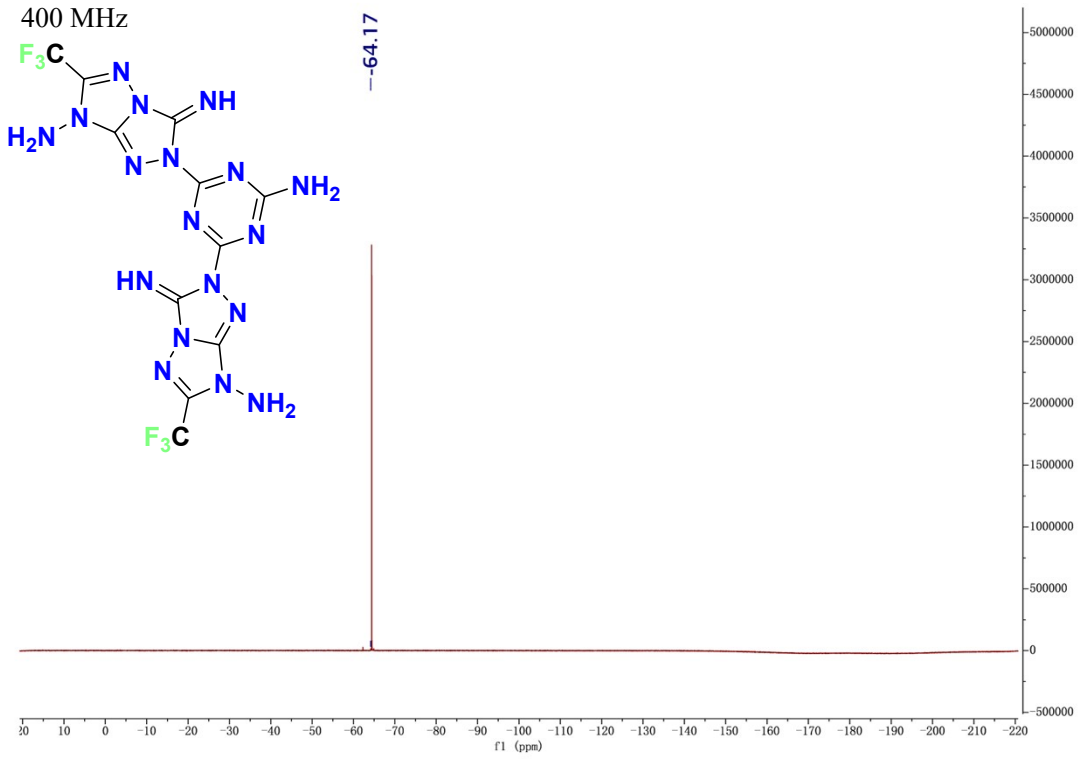


Figure S16. ^{19}F NMR of **6** in DMSO-d_6.

6. HRMS of **3** and **6**

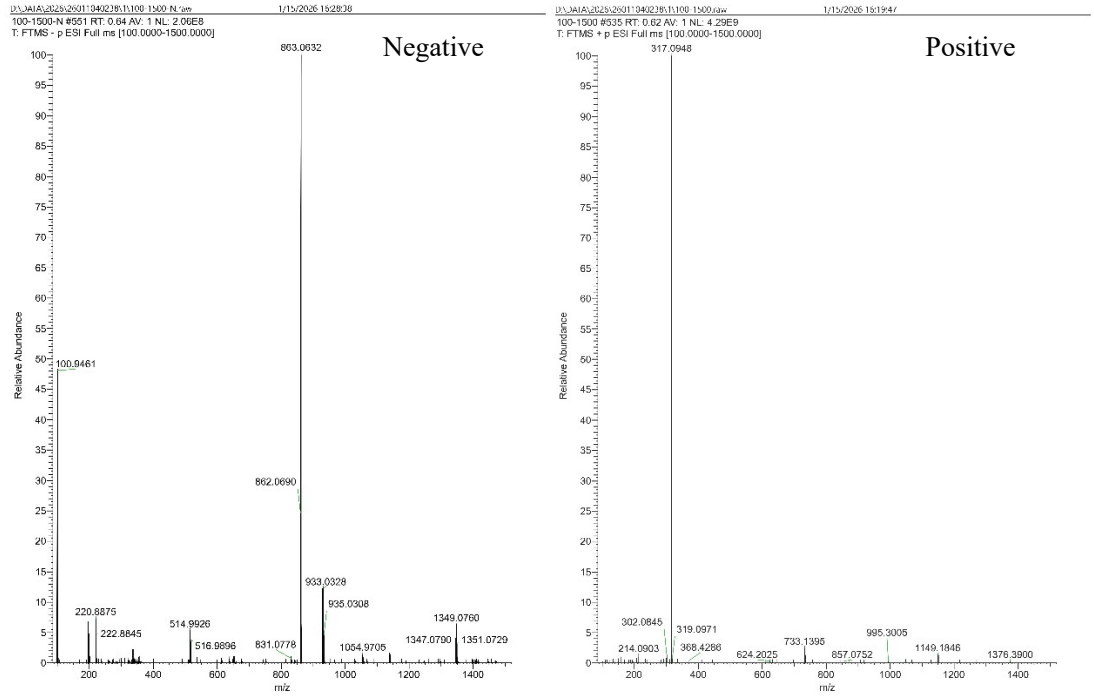


Figure S17. HRMS of **3**.

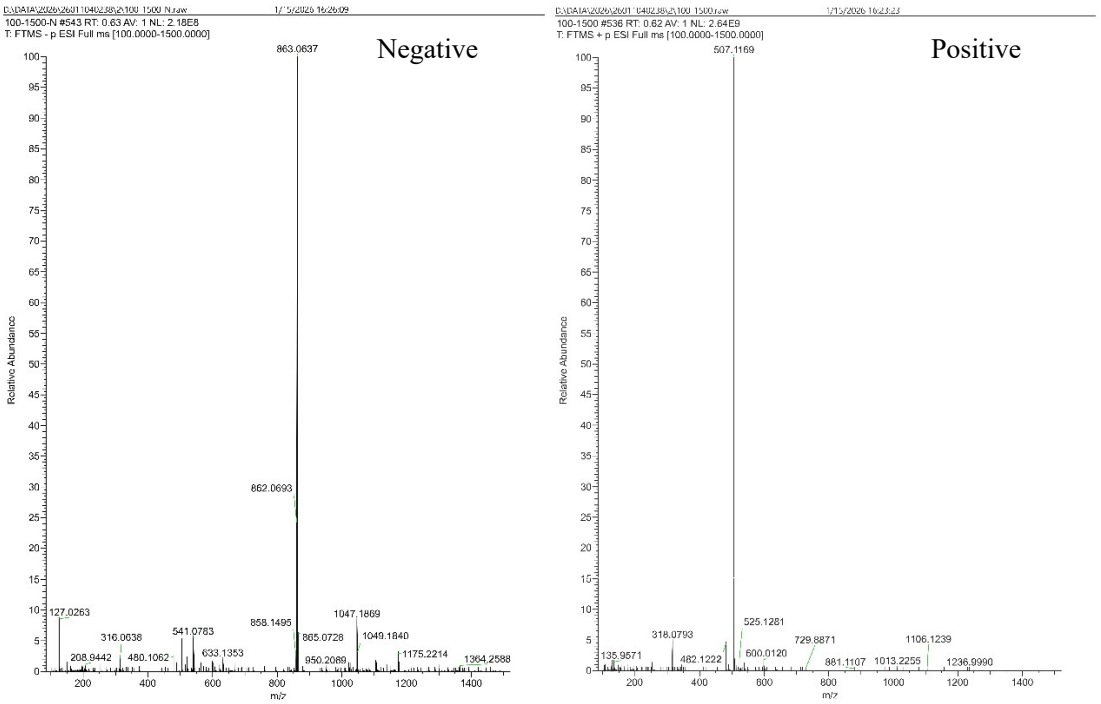


Figure S18. HRMS of **6**.

7. Ozawa curves of **3-6**

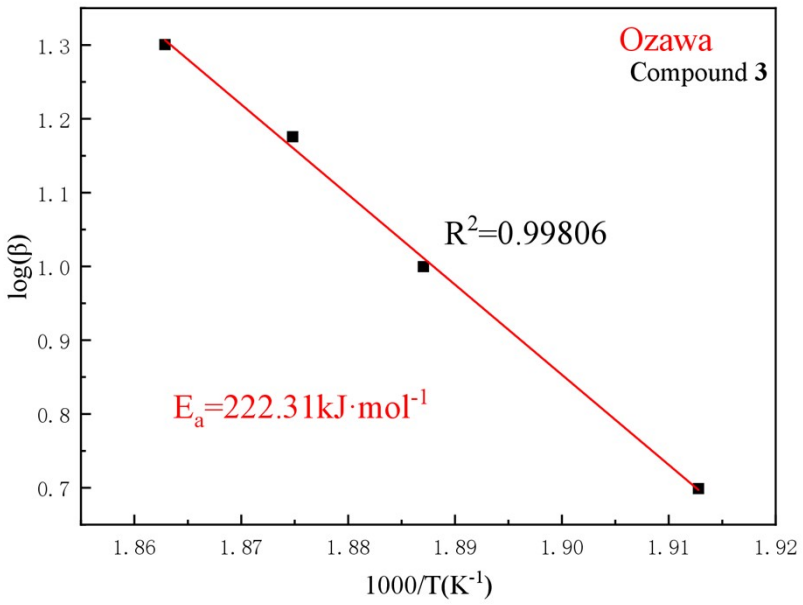


Figure S19. Ozawa curves of **3**.

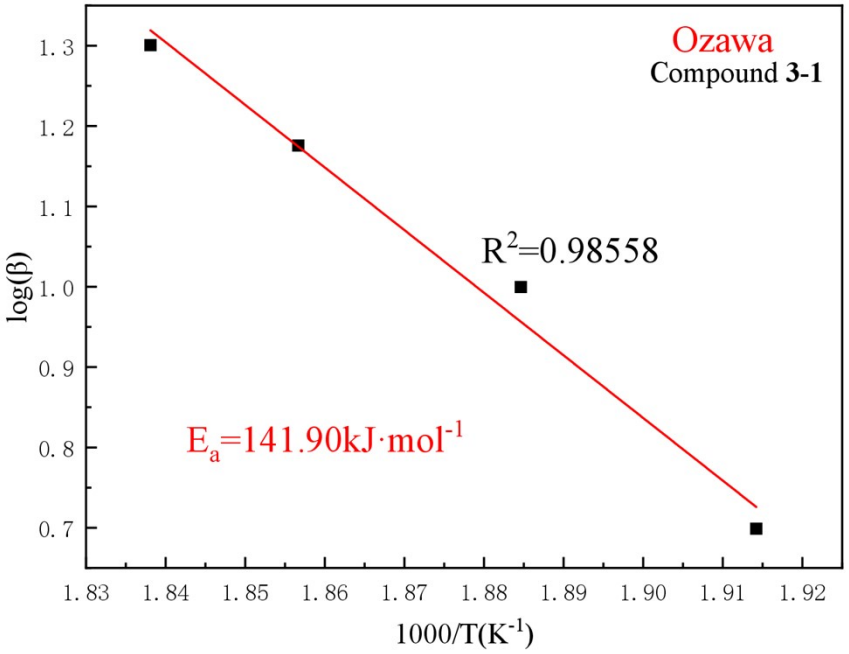


Figure S20. Ozawa curves of **4**.

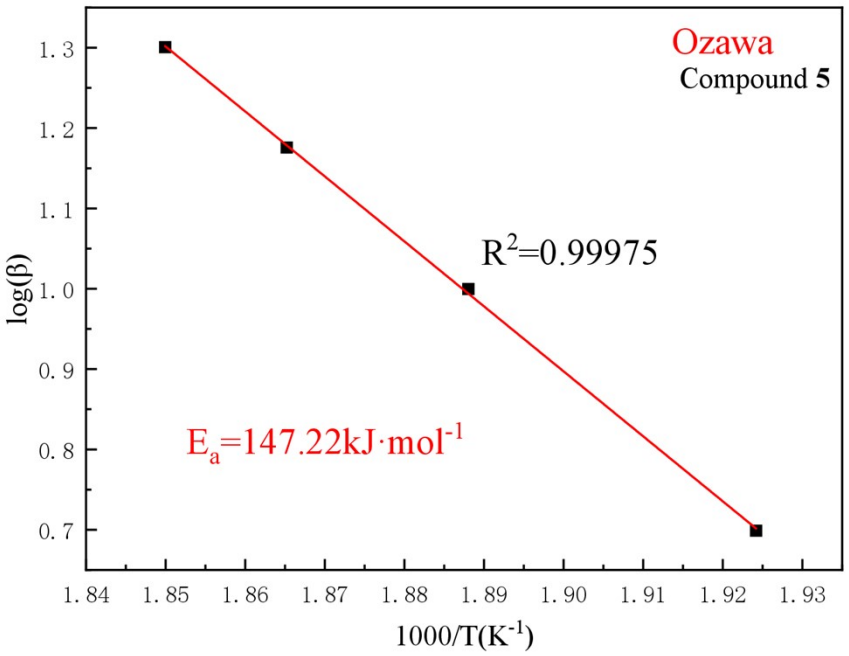


Figure S21. Ozawa curves of **5**.

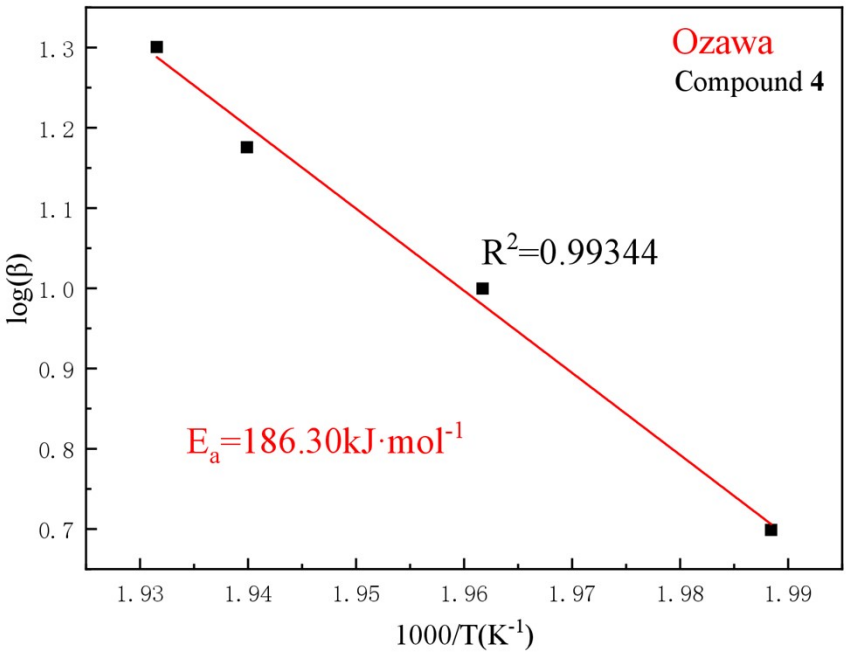


Figure S22. Ozawa curves of **6**.

References

[1] S. Kronister, D. Svatunek, C. Denk and H. Mikula, *Synlett,* 2018, 29, 1297–1302.
[2] A. D. Becke, *J. Chem Phys.***1993**, *98*, 5648-5652.
[3] a) A. Strömberg, O. Gropen, U. Wahlgren, *J. Comput. Chem.* **1983**, *4*, 181–186; b) M. N. Glukhovtsev, A. Pross,M. P. McGrath, L. Radom, *J. Chem. Phys.* **1995**, *103*, 1878–1885.
[4] H. D. B. Jenkins, D. Tudela and L. Glasser, *Inorg. Chem.*, 2002, **41**, 2364-2367.