Energetic high-nitrogen compounds: preparation and characterization of 5-(fluorodinitromethyl)-2H-tetrazole and –tetrazolates

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Supplementary Information

Crystal Structure Report for sodium dinitrocyanomethide, $C_2H_2N_3NaO_5$

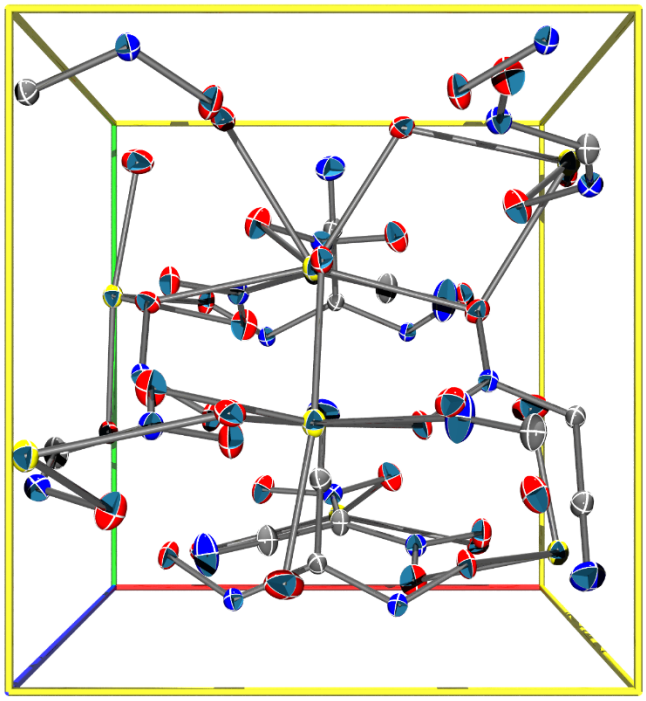

Figure S1. Packing diagram for the crystal structure of $C_2H_2N_3NaO_5$. View along the 001 direction.

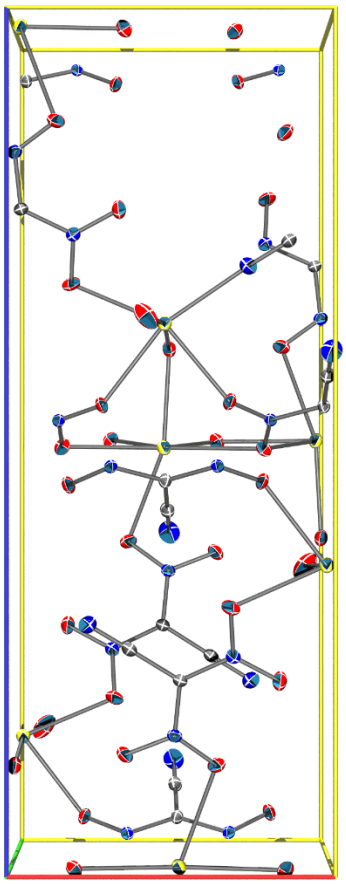

Figure S2. Packing diagram for the crystal structure of $C_2H_2N_3NaO_5$. View along the 010 direction.

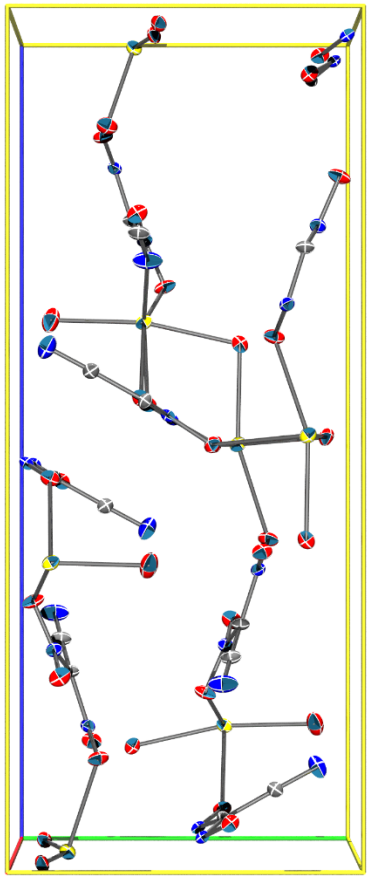

Figure S3. Packing diagram for the crystal structure of $C_2H_2N_3NaO_5$. View along the 100 direction.

Table S1. Sample and crystal data for $C_2H_2N_3NaO_5$

Identification code	NO22CCNNa	
Chemical formula	$C_2H_2N_3NaO_5$	
Formula weight	171.06 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.148 x 0.185 x 0.700 mm	
Crystal habit	clear yellow prism	
Crystal system	orthorhombic	
Space group	P 2_1 2_1 2_1	
Unit cell dimensions	a = 7.5138(6) Å	α = 90°
	b = 8.1663(6) Å	β = 90°
	c = 19.9151(14) Å	γ = 90°
Volume	1221.99(16) Å^3	
Z	8	
Density (calculated)	1.860 g/cm^3	
Absorption coefficient	0.237 mm^{-1}	
F(000)	688	

Table S2. Data collection and structure refinement for $C_2H_2N_3NaO_5$.

Diffractometer	Bruker APEX DUO
Radiation source	fine-focus tube, MoKα
Theta range for data collection	2.04 to 30.50°
Index ranges	-10<=h<=10, -11<=k<=11, -28<=l<=27
Reflections collected	30172
Independent reflections	3734 [R(int) = 0.0355]
Absorption correction	multi-scan
Max. and min. transmission	0.9660 and 0.8520
Structure solution technique	direct methods
Structure solution program	SHELXTL XT 2014/4 (Bruker AXS, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXTL XL 2014/6 (Bruker AXS, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	3734 / 0 / 201
Goodness-of-fit on F^2	1.060
Final R indices	3551 data; I>2σ(I) R1 = 0.0253, wR2 = 0.0651
	all data R1 = 0.0274, wR2 = 0.0661
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0372P)^2+0.2231P]$ where $P=(F_o^2+2F_c^2)/3$
Absolute structure parameter	0.1(1)
Largest diff. peak and hole	0.360 and -0.306 eÅ^{-3}
R.M.S. deviation from mean	0.051 eÅ^{-3}

Table S3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for $C_2H_2N_3NaO_5$.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
C1	0.98170(19)	0.38640(17)	0.54451(7)	0.0111(2)
C2	0.9879(2)	0.23515(18)	0.57913(7)	0.0142(3)
C3	0.0280(2)	0.33654(19)	0.77799(7)	0.0135(3)
C4	0.8714(2)	0.3679(2)	0.74112(8)	0.0169(3)
N1	0.81561(17)	0.45014(16)	0.52825(6)	0.0104(2)
N2	0.14153(17)	0.46024(16)	0.52758(6)	0.0106(2)
N3	0.9936(2)	0.11141(19)	0.60633(8)	0.0254(3)
N4	0.19101(18)	0.37860(17)	0.74918(6)	0.0133(2)
N5	0.01080(18)	0.28539(15)	0.84422(6)	0.0122(2)
N6	0.7435(2)	0.3917(3)	0.71184(8)	0.0289(4)
Na1	0.47850(9)	0.37895(8)	0.64290(3)	0.01413(13)
Na2	0.47560(8)	0.65522(7)	0.49546(3)	0.01415(13)
O1	0.68419(14)	0.37207(15)	0.54956(6)	0.0152(2)
O2	0.79752(15)	0.57655(14)	0.49395(6)	0.0147(2)
O3	0.28019(14)	0.38769(15)	0.54531(6)	0.0150(2)
O4	0.14895(16)	0.59222(14)	0.49632(6)	0.0150(2)
O5	0.33501(15)	0.35773(17)	0.77811(6)	0.0197(2)
O6	0.18246(17)	0.43980(17)	0.69138(6)	0.0203(3)
O7	0.14091(17)	0.25245(17)	0.87974(6)	0.0186(2)
O8	0.85611(16)	0.27725(16)	0.86673(6)	0.0183(2)
O1S	0.49294(15)	0.66061(13)	0.61653(5)	0.0151(2)
O2S	0.4228(2)	0.10316(17)	0.64656(8)	0.0302(3)

Table S4. Bond lengths (Å) for $C_2H_2N_3NaO_5$.

C1-N2	1.3855(19)	C1-N1	1.3904(19)
C1-C2	1.415(2)	C2-N3	1.147(2)
C3-N5	1.3896(18)	C3-N4	1.395(2)
C3-C4	1.411(2)	C4-N6	1.141(2)
N1-O2	1.2452(17)	N1-O1	1.2497(17)
N2-O4	1.2459(17)	N2-O3	1.2496(17)
N2-Na2	3.0406(15)	N3-Na2	2.9780(18)
N4-O5	1.2377(18)	N4-O6	1.2565(17)
N4-Na1	3.0243(14)	N5-O7	1.2362(18)
N5-O8	1.2476(18)	N5-Na2	3.0524(13)
N6-Na1	2.4207(17)	Na1-O2S	2.2920(15)
Na1-O1S	2.3618(13)	Na1-O1	2.4180(13)
Na1-N6	2.4207(17)	Na1-O3	2.4499(13)
Na1-O6	2.4754(14)	Na1-O5	2.9059(14)
Na1-H2S	2.6369	Na2-O1S	2.4150(13)
Na2-O4	2.4448(13)	Na2-O2	2.5029(13)
Na2-O4	2.5078(13)	Na2-O2	2.5755(13)
Na2-O7	2.5780(14)	Na2-O3	2.8133(14)
Na2-O8	2.9113(14)	Na2-N3	2.9779(18)
Na2-O1	2.9940(14)	Na2-N2	3.0407(15)
Na2-N5	3.0524(14)	O2-Na2	2.5754(13)
O3-Na1	2.4499(13)	O3-Na2	2.8134(14)
O4-Na2	2.4448(13)	O4-Na2	2.5078(13)
O7-Na2	2.5780(14)	O8-Na2	2.9112(13)
O1S-H1S	0.8866	O1S-H2S	0.7672
O2S-H3S	0.878	O2S-H4S	0.8777

Table S5. Bond angles (°) for $C_2H_2N_3NaO_5$.

N2-C1-N1	123.94(12)	N2-C1-C2	118.02(13)
N1-C1-C2	118.02(13)	N3-C2-C1	178.99(17)
N5-C3-N4	123.10(13)	N5-C3-C4	118.09(14)
N4-C3-C4	118.26(13)	N6-C4-C3	179.0(2)
O2-N1-O1	121.53(13)	O2-N1-C1	122.42(13)
O1-N1-C1	116.05(12)	O4-N2-O3	120.94(13)
O4-N2-C1	122.48(13)	O3-N2-C1	116.59(13)
O4-N2-Na2	53.48(7)	O3-N2-Na2	67.63(8)
C1-N2-Na2	174.10(10)	C2-N3-Na2	108.72(12)
O5-N4-O6	121.73(13)	O5-N4-C3	122.81(13)
O6-N4-C3	115.45(13)	O5-N4-Na1	72.64(8)
O6-N4-Na1	52.77(8)	C3-N4-Na1	156.19(10)
O7-N5-O8	121.30(13)	O7-N5-C3	122.33(13)
O8-N5-C3	116.36(13)	O7-N5-Na2	56.19(7)
O8-N5-Na2	71.64(8)	C3-N5-Na2	152.34(10)
C4-N6-Na1	167.30(18)	O2S-Na1-O1S	166.52(5)
O2S-Na1-O1	96.80(6)	O1S-Na1-O1	79.77(4)
O2S-Na1-N6	100.04(7)	O1S-Na1-N6	92.67(6)
O1-Na1-N6	84.91(5)	O2S-Na1-O3	86.72(5)
O1S-Na1-O3	79.82(4)	O1-Na1-O3	77.27(4)

N6-Na1-O3	161.61(6)	O2S-Na1-O6	91.19(6)
O1S-Na1-O6	86.13(5)	O1-Na1-O6	151.51(5)
N6-Na1-O6	120.61(6)	O3-Na1-O6	75.94(4)
O2S-Na1-O5	81.03(5)	O1S-Na1-O5	106.33(4)
O1-Na1-O5	161.47(5)	N6-Na1-O5	77.41(5)
O3-Na1-O5	120.74(4)	O6-Na1-O5	46.93(4)
O2S-Na1-N4	81.16(5)	O1S-Na1-N4	100.91(4)
O1-Na1-N4	174.00(5)	N6-Na1-N4	100.98(5)
O3-Na1-N4	96.94(4)	O6-Na1-N4	23.84(4)
O5-Na1-N4	23.99(3)	O2S-Na1-H2S	157.7
O1S-Na1-H2S	16.5	O1-Na1-H2S	95.3
N6-Na1-H2S	99.7	O3-Na1-H2S	77.7
O6-Na1-H2S	69.7	O5-Na1-H2S	93.2
N4-Na1-H2S	84.9	O1S-Na2-O4	83.63(4)
O1S-Na2-O2	87.97(4)	O4-Na2-O2	72.69(4)
O1S-Na2-O4	92.85(4)	O4-Na2-O4	133.95(4)
O2-Na2-O4	153.29(4)	O1S-Na2-O2	86.03(4)
O4-Na2-O2	63.50(4)	O2-Na2-O2	136.17(4)
O4-Na2-O2	70.45(4)	O1S-Na2-O7	154.89(5)
O4-Na2-O7	89.66(5)	O2-Na2-O7	113.11(4)
O4-Na2-O7	74.56(4)	O2-Na2-O7	69.39(4)
O1S-Na2-O3	71.94(4)	O4-Na2-O3	155.45(5)
O2-Na2-O3	108.01(4)	O4-Na2-O3	47.74(4)
O2-Na2-O3	111.13(4)	O7-Na2-O3	111.43(4)
O1S-Na2-O8	148.46(4)	O4-Na2-O8	70.60(4)
O2-Na2-O8	67.56(4)	O4-Na2-O8	118.03(4)
O2-Na2-O8	97.86(4)	O7-Na2-O8	45.96(4)
O3-Na2-O8	133.20(4)	O1S-Na2-N3	133.67(5)
O4-Na2-N3	129.66(5)	O2-Na2-N3	76.14(4)
O4-Na2-N3	84.20(5)	O2-Na2-N3	134.52(5)
O7-Na2-N3	67.71(4)	O3-Na2-N3	72.30(4)
O8-Na2-N3	61.28(4)	O1S-Na2-O1	68.07(4)
O4-Na2-O1	110.40(4)	O2-Na2-O1	45.59(4)
O4-Na2-O1	110.57(4)	O2-Na2-O1	154.07(4)
O7-Na2-O1	136.50(4)	O3-Na2-O1	63.03(3)
O8-Na2-O1	103.64(4)	N3-Na2-O1	69.91(4)
O1S-Na2-N2	81.03(4)	O4-Na2-N2	150.17(5)
O2-Na2-N2	131.75(4)	O4-Na2-N2	23.53(4)
O2-Na2-N2	89.96(4)	O7-Na2-N2	93.49(4)
O3-Na2-N2	24.25(3)	O8-Na2-N2	130.02(4)
N3-Na2-N2	78.33(4)	O1-Na2-N2	87.25(4)
O1S-Na2-N5	168.65(4)	O4-Na2-N5	85.08(4)
O2-Na2-N5	89.81(4)	O4-Na2-N5	94.13(4)
O2-Na2-N5	87.88(4)	O7-Na2-N5	23.48(4)
O3-Na2-N5	119.28(4)	O8-Na2-N5	24.00(3)
N3-Na2-N5	56.15(4)	O1-Na2-N5	117.41(4)
N2-Na2-N5	108.57(4)	N1-O1-Na1	138.96(10)
N1-O1-Na2	84.11(9)	Na1-O1-Na2	85.65(4)
N1-O2-Na2	108.16(9)	N1-O2-Na2	127.11(9)

Na2-O2-Na2	106.43(4)	N2-O3-Na1	138.17(10)
N2-O3-Na2	88.12(9)	Na1-O3-Na2	89.15(4)
N2-O4-Na2	132.26(10)	N2-O4-Na2	102.99(9)
Na2-O4-Na2	110.41(4)	N4-O5-Na1	83.38(9)
N4-O6-Na1	103.39(10)	N5-O7-Na2	100.33(9)
N5-O8-Na2	84.36(8)	Na1-O1S-Na2	101.64(4)
Na1-O1S-H1S	108.7	Na2-O1S-H1S	120.5
Na1-O1S-H2S	102.5	Na2-O1S-H2S	112.1
H1S-O1S-H2S	109.4	Na1-O2S-H3S	109.9
Na1-O2S-H4S	109.8	H3S-O2S-H4S	109.0

Table S6. Anisotropic atomic displacement parameters (Å²) for $C_2H_2N_3NaO_5$.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0093(6)	0.0115(5)	0.0125(6)	0.0016(5)	-0.0005(5)	0.0005(5)
C2	0.0117(7)	0.0160(6)	0.0148(6)	0.0010(5)	0.0013(5)	0.0015(6)
C3	0.0118(6)	0.0192(7)	0.0094(6)	0.0001(5)	0.0009(5)	-0.0002(6)
C4	0.0135(7)	0.0257(8)	0.0115(6)	-0.0017(6)	0.0024(5)	0.0012(6)
N1	0.0095(5)	0.0119(5)	0.0098(5)	-0.0026(5)	-0.0007(4)	0.0002(4)
N2	0.0095(5)	0.0124(6)	0.0098(5)	-0.0031(5)	0.0005(4)	-0.0010(5)
N3	0.0264(8)	0.0196(6)	0.0302(7)	0.0085(6)	0.0033(6)	0.0025(6)
N4	0.0127(6)	0.0149(6)	0.0122(5)	0.0009(5)	0.0011(4)	0.0000(5)
N5	0.0130(6)	0.0128(5)	0.0106(5)	-0.0016(4)	0.0011(5)	-0.0010(5)
N6	0.0184(7)	0.0506(11)	0.0177(7)	-0.0008(7)	-0.0023(5)	0.0048(7)
Na1	0.0122(3)	0.0166(3)	0.0135(3)	0.0025(2)	0.0001(2)	-0.0002(2)
Na2	0.0119(3)	0.0159(3)	0.0146(3)	0.0020(2)	-0.0014(2)	-0.0002(2)
O1	0.0099(5)	0.0187(5)	0.0169(5)	-0.0030(5)	0.0033(4)	-0.0035(4)
O2	0.0149(5)	0.0140(5)	0.0154(5)	0.0021(4)	-0.0032(4)	0.0027(4)
O3	0.0094(5)	0.0206(5)	0.0150(5)	-0.0024(4)	-0.0031(4)	0.0026(4)
O4	0.0157(5)	0.0116(5)	0.0179(5)	0.0026(4)	0.0033(4)	-0.0019(4)
O5	0.0115(5)	0.0262(6)	0.0214(5)	0.0046(5)	-0.0011(4)	-0.0003(5)
O6	0.0197(6)	0.0287(6)	0.0124(5)	0.0075(5)	0.0039(4)	0.0005(5)
O7	0.0180(6)	0.0253(6)	0.0125(5)	0.0030(5)	-0.0023(4)	0.0049(5)
O8	0.0148(5)	0.0246(6)	0.0155(5)	-0.0018(5)	0.0049(4)	-0.0043(5)
O1S	0.0108(5)	0.0164(5)	0.0180(5)	-0.0027(4)	-0.0011(4)	-0.0005(4)
O2S	0.0333(7)	0.0190(6)	0.0384(8)	0.0060(6)	-0.0170(6)	-0.0028(5)

Table S7. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²) for $C_2H_2N_3NaO_5$.

	x/a	y/b	z/c	U(eq)
H1S	0.5868	0.7036	0.6369	0.023
H2S	0.4076	0.6942	0.6326	0.023
H3S	0.3084	0.0859	0.6521	0.045
H4S	0.4809	0.0589	0.6802	0.045

Crystal Structure Report for ammonium dinitrocyanomethide, $C_2H_4N_4O_4$

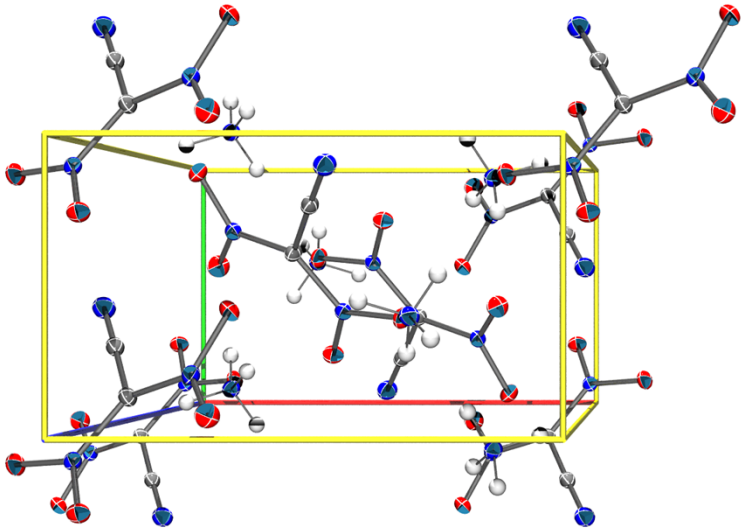

Figure S4. Packing diagram for the crystal structure of $C_2H_4N_4O_4$. View along the 001 direction.

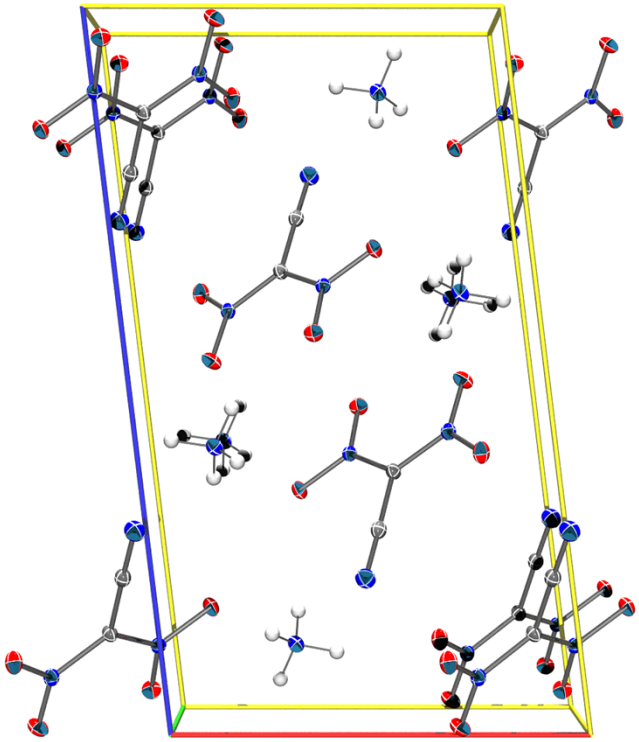

Figure S5. Packing diagram for the crystal structure of $C_2H_4N_4O_4$. View along the 010 direction.

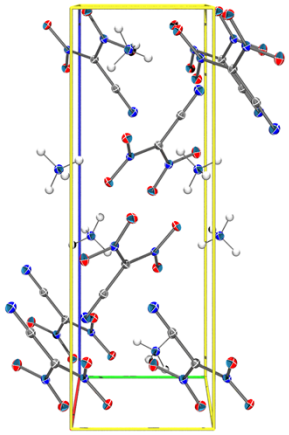

Figure S6. Packing diagram for the crystal structure of $C_2H_4N_4O_4$. View along the 100 direction.

Table S8. Sample and crystal data for $C_2H_4N_4O_4$.

Identification code	azole	
Chemical formula	$C_2H_4N_4O_4$	
Formula weight	148.09 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.120 x 0.212 x 0.431 mm	
Crystal habit	clear yellow prism	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 8.1144(12) Å	α = 90°
	b = 4.8009(8) Å	β = 96.914(3)°
	c = 14.218(2) Å	γ = 90°
Volume	549.85(15) $Å^3$	
Z	4	
Density (calculated)	1.789 g/cm^3	
Absorption coefficient	0.170 mm^{-1}	
F(000)	304	

Table S9. Data collection and structure refinement for $C_2H_4N_4O_4$.

Diffractometer	Bruker APEX DUO
Radiation source	fine-focus tube, MoKα
Theta range for data collection	2.76 to 30.54°
Index ranges	-11<=h<=11, -6<=k<=6, -19<=l<=20
Reflections collected	12950
Independent reflections	1681 [R(int) = 0.0265]
Coverage of independent reflections	99.9%
Absorption correction	multi-scan
Structure solution technique	direct methods
Structure solution program	SHELXTL XT 2013/1 (Bruker AXS, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXTL XL 2014/7 (Bruker AXS, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	1681 / 6 / 103
Goodness-of-fit on F^2	1.053
Final R indices	1485 data; I>2σ(I) R1 = 0.0292, wR2 = 0.0795
	all data R1 = 0.0335, wR2 = 0.0826
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0436P)^2+0.1928P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.376 and -0.329 $eÅ^{-3}$
R.M.S. deviation from mean	0.057 $eÅ^{-3}$

Table S10. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for $C_2H_4N_4O_4$.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
C1	0.60973(10)	0.37721(18)	0.35721(6)	0.01053(17)
C2	0.55559(11)	0.21066(19)	0.27753(6)	0.01149(17)
N1	0.50771(9)	0.59185(15)	0.38012(5)	0.00978(16)
N2	0.75523(9)	0.29671(16)	0.41397(5)	0.01067(16)
N3	0.50901(10)	0.07614(17)	0.21269(6)	0.01582(17)
N4	0.18470(10)	0.10068(16)	0.39417(6)	0.01173(16)
O1	0.54474(8)	0.75345(14)	0.44740(5)	0.01330(15)
O2	0.37096(8)	0.61373(14)	0.32749(5)	0.01306(15)
O3	0.80942(8)	0.42378(15)	0.48650(5)	0.01543(16)
O4	0.82365(8)	0.08223(14)	0.38679(5)	0.01473(15)

Table S11. Bond lengths (Å) for $C_2H_4N_4O_4$.

C1-N1	1.3850(11)	C1-N2	1.4019(11)
C1-C2	1.4127(12)	C2-N3	1.1515(12)
N1-O1	1.2401(10)	N1-O2	1.2658(10)
N2-O3	1.2328(10)	N2-O4	1.2528(10)
N4-H1	0.875(11)	N4-H2	0.868(11)
N4-H3	0.885(11)	N4-H4	0.877(10)

Table S12. Bond angles (°) for $C_2H_4N_4O_4$.

N1-C1-N2	123.74(8)	N1-C1-C2	118.21(8)
N2-C1-C2	117.69(8)	N3-C2-C1	178.96(9)
O1-N1-O2	121.19(7)	O1-N1-C1	123.41(7)
O2-N1-C1	115.40(7)	O3-N2-O4	122.55(7)
O3-N2-C1	122.42(8)	O4-N2-C1	115.01(7)
H1-N4-H2	110.7(12)	H1-N4-H3	110.1(12)
H2-N4-H3	112.0(12)	H1-N4-H4	105.2(12)
H2-N4-H4	109.3(12)	H3-N4-H4	109.2(11)

Table S13. Anisotropic atomic displacement parameters (Å²) for $C_2H_4N_4O_4$.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0096(4)	0.0106(4)	0.0111(4)	-0.0007(3)	0.0001(3)	0.0013(3)
C2	0.0104(4)	0.0109(4)	0.0133(4)	0.0014(3)	0.0021(3)	0.0013(3)
N1	0.0097(3)	0.0094(3)	0.0104(3)	0.0010(2)	0.0018(2)	-0.0005(2)
N2	0.0095(3)	0.0104(3)	0.0122(3)	0.0012(3)	0.0015(3)	-0.0005(3)
N3	0.0162(4)	0.0150(4)	0.0160(4)	-0.0019(3)	0.0005(3)	0.0006(3)
N4	0.0116(3)	0.0111(4)	0.0121(3)	0.0000(3)	-0.0003(3)	0.0006(3)
O1	0.0150(3)	0.0111(3)	0.0136(3)	-0.0038(2)	0.0012(2)	-0.0006(2)
O2	0.0098(3)	0.0144(3)	0.0142(3)	0.0003(2)	-0.0016(2)	0.0019(2)
O3	0.0157(3)	0.0165(3)	0.0129(3)	-0.0023(2)	-0.0034(2)	-0.0002(2)
O4	0.0118(3)	0.0121(3)	0.0203(3)	-0.0014(2)	0.0021(2)	0.0031(2)

Table S14. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²) for $C_2H_4N_4O_4$.

	x/a	y/b	z/c	U(eq)
H1	0.1704(16)	0.228(3)	0.3499(8)	0.014
H2	0.2380(16)	-0.041(2)	0.3752(9)	0.014
H3	0.2355(15)	0.173(3)	0.4471(8)	0.014
H4	0.0844(14)	0.049(3)	0.4036(9)	0.014

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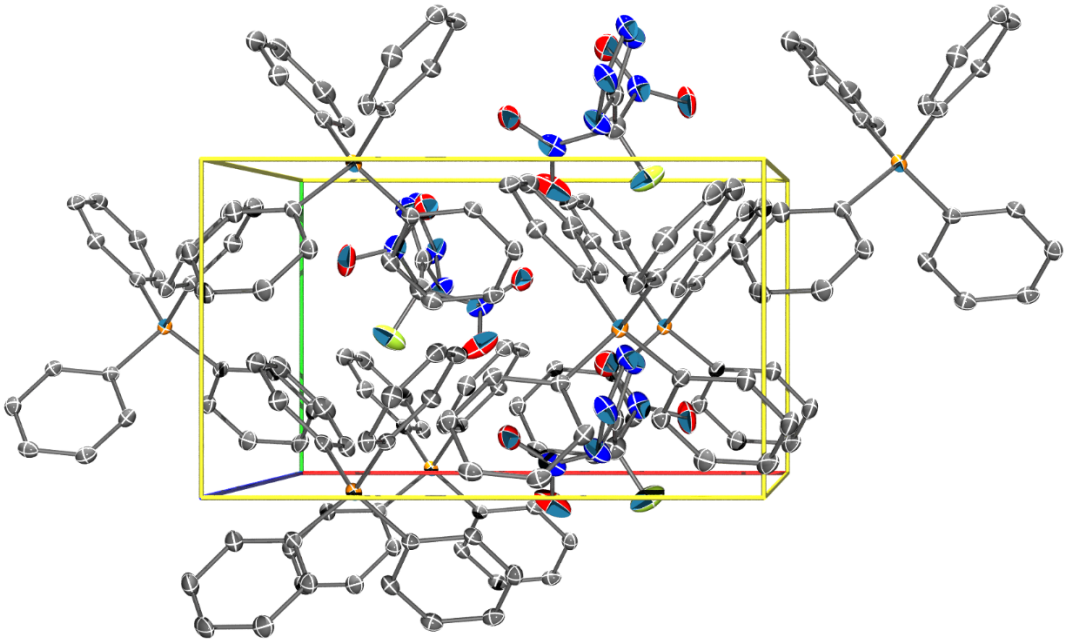

Figure S7. Packing diagram for the crystal structure of $C_{26}H_{20}N_3O_4P$. View along the 001 direction.

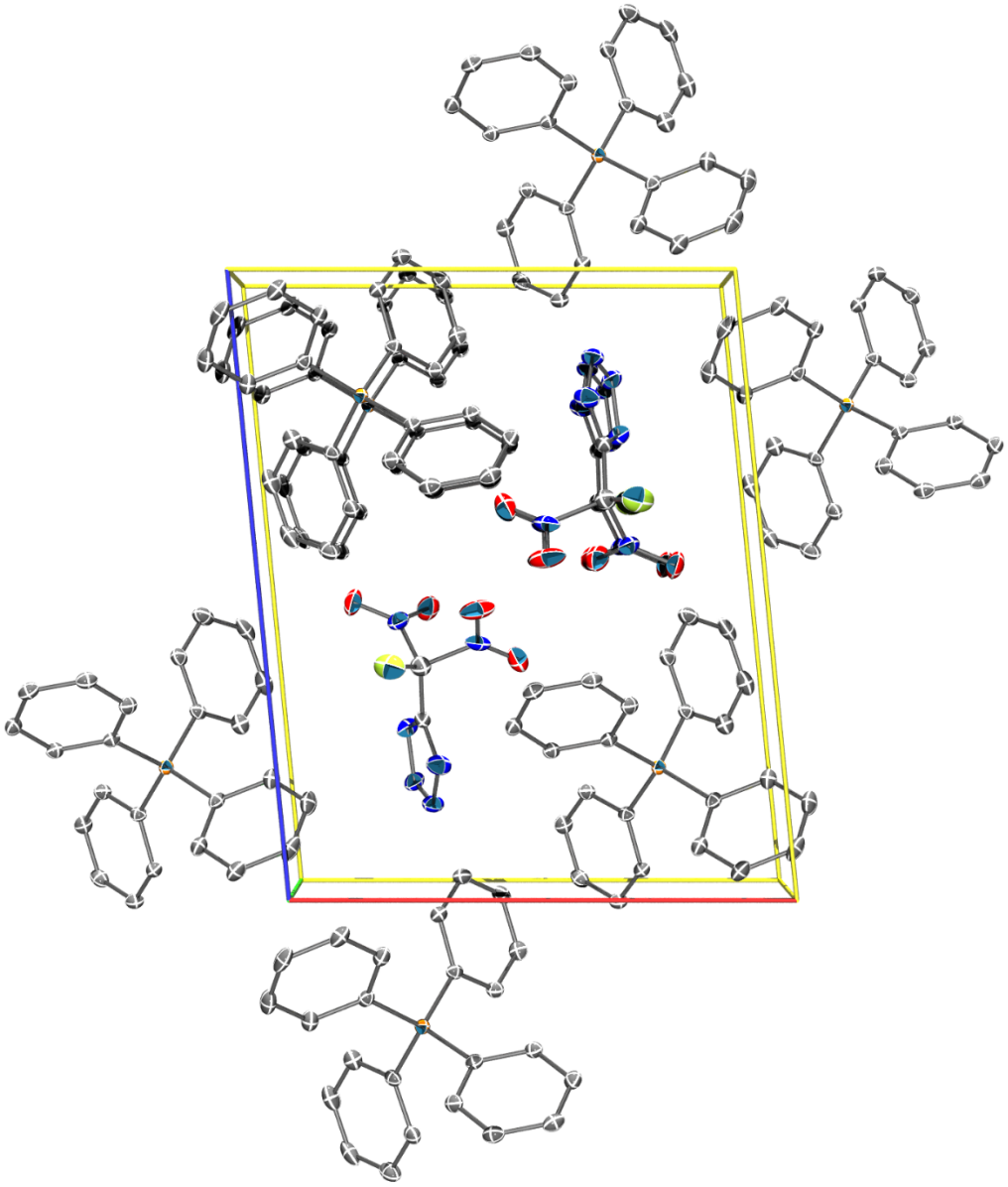

Figure S8. Packing diagram for the crystal structure of $C_{26}H_{20}N_3O_4P$. View along the 010 direction.

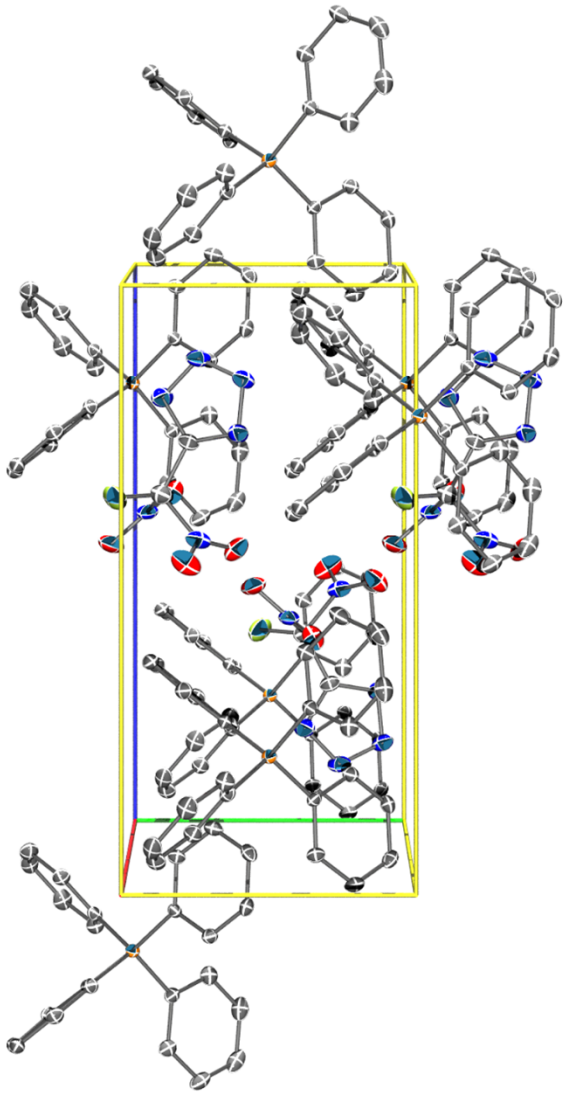

Figure S9. Packing diagram for the crystal structure of $C_{26}H_{20}N_3O_4P$. View along the 100 direction.

Table S15. Sample and crystal data for $C_{26}H_{20}N_3O_4P$.

Identification code	TPPNO22CCN	
Chemical formula	$C_{26}H_{20}N_3O_4P$	
Formula weight	469.42 g/mol	
Temperature	104(2) K	
Wavelength	0.71073 Å	
Crystal size	0.142 x 0.227 x 0.335 mm	
Crystal habit	clear yellow prism	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 11.6601(8) Å	α = 90°
	b = 14.2600(9) Å	β = 90.0990(10)°
	c = 13.4402(9) Å	γ = 90°
Volume	2234.7(3) $Å^3$	
Z	4	
Density (calculated)	1.395 g/cm^3	
Absorption coefficient	0.163 mm^{-1}	
F(000)	976	

Table S16. Data collection and structure refinement for $C_{26}H_{20}N_3O_4P$.

Diffractometer	Bruker APEX DUO
Radiation source	fine-focus tube, MoKα
Theta range for data collection	2.08 to 30.56°
Index ranges	-16<=h<=16, -20<=k<=20, -19<=l<=19
Reflections collected	55116
Independent reflections	6814 [R(int) = 0.0385]
Coverage of independent reflections	99.3%
Absorption correction	multi-scan
Max. and min. transmission	0.9770 and 0.9470
Structure solution technique	direct methods
Structure solution program	SHELXTL XT 2014/4 (Bruker AXS, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXTL XL 2014/6 (Bruker AXS, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	6814 / 0 / 307
Goodness-of-fit on F^2	1.035
Δ/σ_{max}	0.002
Final R indices	5611 data; I>2σ(I) R1 = 0.0359, wR2 = 0.0922
	all data R1 = 0.0476, wR2 = 0.0988
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0456P)^2+1.0542P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.398 and -0.257 $eÅ^{-3}$
R.M.S. deviation from mean	0.052 $eÅ^{-3}$

Table S17. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $C_{26}H_{20}N_3O_4P$.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
C1	0.57515(10)	0.24267(8)	0.13252(9)	0.0185(2)
C2	0.50448(11)	0.32182(9)	0.14897(9)	0.0212(2)

	x/a	y/b	z/c	U(eq)
C3	0.59960(9)	0.32770(8)	0.52773(8)	0.0150(2)
C4	0.56677(10)	0.38204(8)	0.60961(9)	0.0191(2)
C5	0.59821(11)	0.47605(9)	0.61419(9)	0.0213(2)
C6	0.66156(11)	0.51598(8)	0.53771(9)	0.0211(2)
C7	0.69228(11)	0.46280(9)	0.45572(9)	0.0226(2)
C8	0.66167(11)	0.36856(9)	0.45002(9)	0.0202(2)
C9	0.56301(10)	0.14923(8)	0.63784(8)	0.0158(2)
C10	0.48592(10)	0.17620(9)	0.71296(9)	0.0184(2)
C11	0.49076(11)	0.13231(9)	0.80531(9)	0.0229(2)
C12	0.56992(12)	0.06095(9)	0.82315(9)	0.0247(3)
C13	0.64447(11)	0.03337(9)	0.74845(10)	0.0237(2)
C14	0.64200(10)	0.07723(8)	0.65588(9)	0.0193(2)
C15	0.65965(10)	0.14884(8)	0.43770(8)	0.0156(2)
C16	0.77744(10)	0.15898(9)	0.45652(9)	0.0215(2)
C17	0.85578(11)	0.10880(10)	0.39975(10)	0.0247(3)
C18	0.81795(11)	0.04993(9)	0.32415(10)	0.0232(2)
C19	0.70127(11)	0.04131(8)	0.30431(9)	0.0207(2)
C20	0.62148(10)	0.09018(8)	0.36088(8)	0.0165(2)
C21	0.41860(9)	0.19620(8)	0.46439(8)	0.0144(2)
C22	0.33667(10)	0.13492(8)	0.50303(8)	0.0169(2)
C23	0.23005(10)	0.12686(9)	0.45640(9)	0.0206(2)
C24	0.20647(11)	0.17880(9)	0.37136(10)	0.0237(3)
C25	0.28844(11)	0.23953(9)	0.33219(10)	0.0239(2)
C26	0.39447(11)	0.24886(8)	0.37875(9)	0.0193(2)
N1	0.68924(9)	0.24737(7)	0.16393(7)	0.0192(2)
N2	0.52890(10)	0.16578(8)	0.08170(8)	0.0225(2)
N3	0.44779(11)	0.38689(9)	0.16124(9)	0.0303(3)
O1	0.71317(8)	0.31758(7)	0.21657(7)	0.0269(2)
O2	0.76089(8)	0.18777(6)	0.13965(7)	0.02471(19)
O3	0.42567(9)	0.17283(8)	0.05708(9)	0.0353(2)
O4	0.58609(9)	0.09499(7)	0.06506(8)	0.0293(2)
P1	0.55941(2)	0.20618(2)	0.51843(2)	0.01325(7)

Table S18. Bond lengths (Å) for $C_{26}H_{20}N_3O_4P$.

C1-N1	1.3966(15)	C1-N2	1.3994(16)
C1-C2	1.4150(17)	C2-N3	1.1513(17)
C3-C8	1.3989(16)	C3-C4	1.3998(16)
C3-P1	1.7994(11)	C4-C5	1.3911(17)
C4-H4	0.95	C5-C6	1.3890(18)
C5-H5	0.95	C6-C7	1.3853(18)
C6-H6	0.95	C7-C8	1.3925(17)
C7-H7	0.95	C8-H8	0.95
C9-C14	1.4002(16)	C9-C10	1.4065(16)
C9-P1	1.7991(11)	C10-C11	1.3912(16)
C10-H10	0.95	C11-C12	1.3943(19)
C11-H11	0.95	C12-C13	1.386(2)
C12-H12	0.95	C13-C14	1.3928(17)
C13-H13	0.95	C14-H14	0.95
C15-C20	1.4008(15)	C15-C16	1.4035(16)
C15-P1	1.7934(11)	C16-C17	1.3896(18)
C16-H16	0.95	C17-C18	1.3894(19)
C17-H17	0.95	C18-C19	1.3913(18)
C18-H18	0.95	C19-C20	1.3899(16)
C19-H19	0.95	C20-H20	0.95
C21-C22	1.3956(16)	C21-C26	1.4025(16)
C21-P1	1.7998(11)	C22-C23	1.3960(16)
C22-H22	0.95	C23-C24	1.3890(18)
C23-H23	0.95	C24-C25	1.3937(19)
C24-H24	0.95	C25-C26	1.3911(17)
C25-H25	0.95	C26-H26	0.95
N1-O2	1.2360(14)	N1-O1	1.2571(14)
N2-O4	1.2305(14)	N2-O3	1.2518(15)

Table S19. Bond angles (°) for $C_{26}H_{20}N_3O_4P$.

N1-C1-N2	123.45(11)	N1-C1-C2	117.98(11)
N2-C1-C2	118.50(11)	N3-C2-C1	179.00(15)
C8-C3-C4	119.93(10)	C8-C3-P1	118.96(9)
C4-C3-P1	121.08(9)	C5-C4-C3	119.73(11)
C5-C4-H4	120.1	C3-C4-H4	120.1
C6-C5-C4	120.18(11)	C6-C5-H5	119.9
C4-C5-H5	119.9	C7-C6-C5	120.19(11)
C7-C6-H6	119.9	C5-C6-H6	119.9
C6-C7-C8	120.36(11)	C6-C7-H7	119.8
C8-C7-H7	119.8	C7-C8-C3	119.59(11)
C7-C8-H8	120.2	C3-C8-H8	120.2
C14-C9-C10	119.81(10)	C14-C9-P1	119.99(9)
C10-C9-P1	120.20(9)	C11-C10-C9	119.50(11)
C11-C10-H10	120.2	C9-C10-H10	120.2
C10-C11-C12	120.50(12)	C10-C11-H11	119.7
C12-C11-H11	119.7	C13-C12-C11	119.89(11)
C13-C12-H12	120.1	C11-C12-H12	120.1
C12-C13-C14	120.50(12)	C12-C13-H13	119.7
C14-C13-H13	119.7	C13-C14-C9	119.78(12)

C13-C14-H14	120.1	C9-C14-H14	120.1
C20-C15-C16	120.26(11)	C20-C15-P1	120.77(9)
C16-C15-P1	118.85(9)	C17-C16-C15	119.47(11)
C17-C16-H16	120.3	C15-C16-H16	120.3
C18-C17-C16	120.30(12)	C18-C17-H17	119.9
C16-C17-H17	119.9	C17-C18-C19	120.18(11)
C17-C18-H18	119.9	C19-C18-H18	119.9
C20-C19-C18	120.40(11)	C20-C19-H19	119.8
C18-C19-H19	119.8	C19-C20-C15	119.37(11)
C19-C20-H20	120.3	C15-C20-H20	120.3
C22-C21-C26	120.28(10)	C22-C21-P1	121.59(8)
C26-C21-P1	118.06(9)	C21-C22-C23	119.61(11)
C21-C22-H22	120.2	C23-C22-H22	120.2
C24-C23-C22	120.03(11)	C24-C23-H23	120.0
C22-C23-H23	120.0	C23-C24-C25	120.48(11)
C23-C24-H24	119.8	C25-C24-H24	119.8
C26-C25-C24	119.94(11)	C26-C25-H25	120.0
C24-C25-H25	120.0	C25-C26-C21	119.66(11)
C25-C26-H26	120.2	C21-C26-H26	120.2
O2-N1-O1	123.15(10)	O2-N1-C1	122.08(10)
O1-N1-C1	114.75(10)	O4-N2-O3	122.62(11)
O4-N2-C1	121.53(11)	O3-N2-C1	115.82(11)
C15-P1-C9	108.64(5)	C15-P1-C3	108.13(5)
C9-P1-C3	111.53(5)	C15-P1-C21	108.35(5)
C9-P1-C21	110.13(5)	C3-P1-C21	109.97(5)

Table S20. Torsion angles (°) for $C_{26}H_{20}N_3O_4P$.

C8-C3-C4-C5	-1.36(18)	P1-C3-C4-C5	-179.37(9)
C3-C4-C5-C6	0.24(18)	C4-C5-C6-C7	0.99(19)
C5-C6-C7-C8	-1.09(19)	C6-C7-C8-C3	-0.04(19)
C4-C3-C8-C7	1.26(18)	P1-C3-C8-C7	179.31(10)
C14-C9-C10-C11	1.43(17)	P1-C9-C10-C11	-179.18(9)
C9-C10-C11-C12	-1.12(18)	C10-C11-C12-C13	0.00(19)
C11-C12-C13-C14	0.82(19)	C12-C13-C14-C9	-0.50(18)
C10-C9-C14-C13	-0.62(17)	P1-C9-C14-C13	179.98(9)
C20-C15-C16-C17	-1.40(18)	P1-C15-C16-C17	174.70(10)
C15-C16-C17-C18	0.8(2)	C16-C17-C18-C19	0.4(2)
C17-C18-C19-C20	-1.08(19)	C18-C19-C20-C15	0.47(18)
C16-C15-C20-C19	0.77(17)	P1-C15-C20-C19	-175.26(9)
C26-C21-C22-C23	-0.51(17)	P1-C21-C22-C23	-177.55(9)
C21-C22-C23-C24	0.76(18)	C22-C23-C24-C25	-0.30(19)
C23-C24-C25-C26	-0.4(2)	C24-C25-C26-C21	0.67(19)
C22-C21-C26-C25	-0.20(18)	P1-C21-C26-C25	176.94(10)
N2-C1-N1-O2	7.87(18)	C2-C1-N1-O2	-169.02(11)
N2-C1-N1-O1	-173.58(11)	C2-C1-N1-O1	9.53(16)
N1-C1-N2-O4	3.06(18)	C2-C1-N2-O4	179.94(12)
N1-C1-N2-O3	-178.84(11)	C2-C1-N2-O3	-1.97(17)
C20-C15-P1-C9	106.51(10)	C16-C15-P1-C9	-69.57(11)
C20-C15-P1-C3	-132.29(9)	C16-C15-P1-C3	51.63(11)
C20-C15-P1-C21	-13.13(11)	C16-C15-P1-C21	170.79(9)

C14-C9-P1-C15	4.16(11)	C10-C9-P1-C15	-175.23(9)
C14-C9-P1-C3	-114.93(10)	C10-C9-P1-C3	65.68(10)
C14-C9-P1-C21	122.69(9)	C10-C9-P1-C21	-56.70(10)
C8-C3-P1-C15	25.41(11)	C4-C3-P1-C15	-156.56(9)
C8-C3-P1-C9	144.80(9)	C4-C3-P1-C9	-37.17(11)
C8-C3-P1-C21	-92.72(10)	C4-C3-P1-C21	85.31(10)
C22-C21-P1-C15	105.94(10)	C26-C21-P1-C15	-71.16(10)
C22-C21-P1-C9	-12.76(11)	C26-C21-P1-C9	170.13(9)
C22-C21-P1-C3	-136.07(9)	C26-C21-P1-C3	46.83(10)

Table S21. Anisotropic atomic displacement parameters (Å^2) for $C_{26}H_{20}N_3O_4P$.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0179(5)	0.0194(5)	0.0183(5)	-0.0005(4)	-0.0001(4)	-0.0006(4)
C2	0.0202(5)	0.0232(6)	0.0203(5)	-0.0022(4)	0.0007(4)	-0.0024(4)
C3	0.0157(5)	0.0142(5)	0.0153(5)	-0.0014(4)	-0.0027(4)	-0.0010(4)
C4	0.0215(6)	0.0190(5)	0.0167(5)	-0.0021(4)	0.0011(4)	-0.0008(4)
C5	0.0244(6)	0.0187(5)	0.0207(5)	-0.0065(4)	-0.0011(4)	-0.0001(4)
C6	0.0215(6)	0.0160(5)	0.0257(6)	-0.0015(4)	-0.0047(5)	-0.0028(4)
C7	0.0253(6)	0.0198(5)	0.0228(6)	0.0009(5)	0.0021(5)	-0.0053(5)
C8	0.0243(6)	0.0184(5)	0.0179(5)	-0.0023(4)	0.0030(4)	-0.0026(4)
C9	0.0163(5)	0.0164(5)	0.0146(5)	0.0012(4)	-0.0039(4)	-0.0032(4)
C10	0.0154(5)	0.0214(5)	0.0185(5)	0.0011(4)	-0.0013(4)	-0.0030(4)
C11	0.0225(6)	0.0287(6)	0.0175(5)	0.0012(5)	-0.0009(4)	-0.0083(5)
C12	0.0283(6)	0.0268(6)	0.0191(5)	0.0059(5)	-0.0082(5)	-0.0100(5)
C13	0.0261(6)	0.0206(6)	0.0243(6)	0.0040(5)	-0.0103(5)	-0.0012(5)
C14	0.0200(5)	0.0183(5)	0.0195(5)	-0.0006(4)	-0.0051(4)	0.0001(4)
C15	0.0162(5)	0.0146(5)	0.0159(5)	-0.0004(4)	0.0002(4)	0.0007(4)
C16	0.0178(5)	0.0237(6)	0.0229(6)	-0.0039(5)	-0.0023(4)	-0.0003(4)
C17	0.0166(5)	0.0292(6)	0.0284(6)	0.0005(5)	0.0013(5)	0.0017(5)
C18	0.0249(6)	0.0212(6)	0.0234(6)	0.0008(5)	0.0081(5)	0.0041(5)
C19	0.0267(6)	0.0171(5)	0.0183(5)	-0.0015(4)	0.0040(4)	-0.0027(4)
C20	0.0183(5)	0.0150(5)	0.0161(5)	0.0007(4)	0.0004(4)	-0.0028(4)
C21	0.0144(5)	0.0140(5)	0.0150(5)	-0.0022(4)	-0.0020(4)	0.0019(4)
C22	0.0175(5)	0.0167(5)	0.0165(5)	-0.0005(4)	-0.0013(4)	0.0002(4)
C23	0.0162(5)	0.0214(5)	0.0241(6)	-0.0022(5)	-0.0013(4)	-0.0020(4)
C24	0.0180(5)	0.0262(6)	0.0270(6)	-0.0018(5)	-0.0084(5)	0.0025(5)
C25	0.0258(6)	0.0231(6)	0.0228(6)	0.0040(5)	-0.0084(5)	0.0026(5)
C26	0.0207(5)	0.0172(5)	0.0200(5)	0.0026(4)	-0.0033(4)	-0.0002(4)
N1	0.0190(5)	0.0213(5)	0.0172(4)	0.0021(4)	0.0015(4)	-0.0028(4)
N2	0.0234(5)	0.0211(5)	0.0231(5)	-0.0006(4)	-0.0040(4)	0.0000(4)
N3	0.0275(6)	0.0303(6)	0.0329(6)	-0.0078(5)	-0.0005(5)	0.0022(5)
O1	0.0240(5)	0.0313(5)	0.0253(4)	-0.0082(4)	-0.0007(4)	-0.0060(4)
O2	0.0188(4)	0.0208(4)	0.0345(5)	0.0035(4)	0.0013(4)	0.0023(3)
O3	0.0268(5)	0.0306(5)	0.0483(6)	-0.0066(5)	-0.0170(5)	0.0023(4)
O4	0.0318(5)	0.0198(4)	0.0363(5)	-0.0067(4)	-0.0046(4)	0.0037(4)
P1	0.01348(13)	0.01327(13)	0.01298(12)	-0.00092(10)	-0.00158(9)	-0.00022(10)

Table S22. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for $C_{26}H_{20}N_3O_4P$.

	x/a	y/b	z/c	U(eq)
H4	0.5232	0.3548	0.6618	0.023
H5	0.5763	0.5130	0.6698	0.026
H6	0.6839	0.5799	0.5416	0.025
H7	0.7345	0.4908	0.4031	0.027
H8	0.6828	0.3322	0.3937	0.024
H10	0.4310	0.2240	0.7007	0.022
H11	0.4397	0.1511	0.8566	0.027
H12	0.5728	0.0313	0.8864	0.03
H13	0.6977	-0.0158	0.7605	0.028
H14	0.6937	0.0584	0.6052	0.023
H16	0.8034	0.1998	0.5076	0.026
H17	0.9356	0.1148	0.4127	0.03

Crystal Structure Report for hydrazinium dinitromethide, $CH_6N_4O_4$

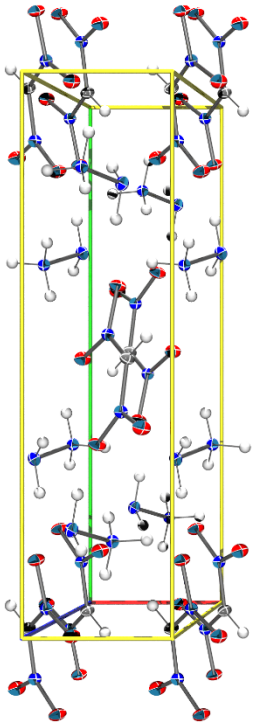

Figure S10. Packing diagram for the crystal structure of $CH_6N_4O_4$. View along the 001 direction.

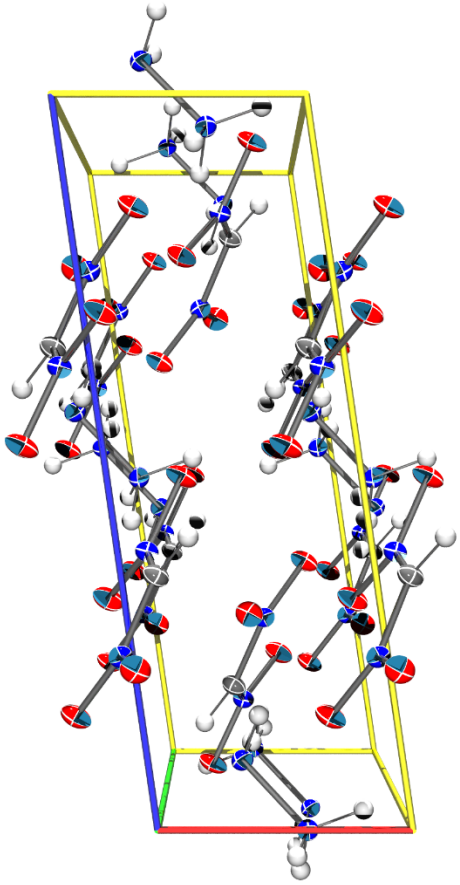

Figure S11. Packing diagram for the crystal structure of $CH_6N_4O_4$. View along the 010 direction.

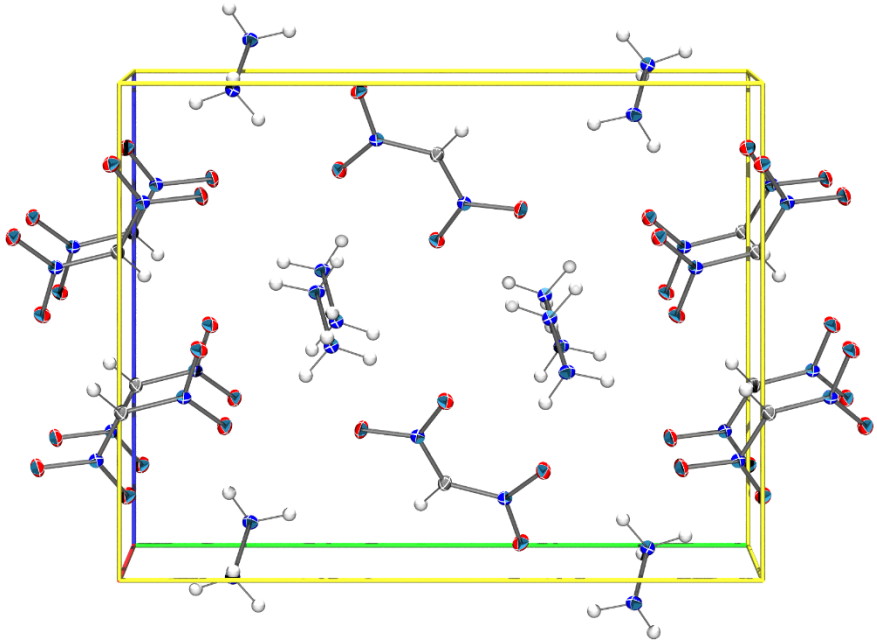

Figure S12. Packing diagram for the crystal structure of $CH_6N_4O_4$. View along the 100 direction.

Table S23. Sample and crystal data for $CH_6N_4O_4$.

Identification code	NO22C_N2H5	
Chemical formula	$CH_6N_4O_4$	
Formula weight	138.10 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.098 x 0.272 x 1.019 mm	
Crystal habit	clear yellow plate	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 3.6434(4) Å	α = 90°
	b = 13.7827(13) Å	β = 98.230(2)°
	c = 10.6457(10) Å	γ = 90°
Volume	529.08(9) $Å^3$	
Z	4	
Density (calculated)	1.734 g/cm^3	
Absorption coefficient	0.169 mm^{-1}	
F(000)	288	

Table S24. Data collection and structure refinement for $CH_6N_4O_4$.

Diffractometer	Bruker APEX DUO
Radiation source	fine-focus tube, MoKα
Theta range for data collection	2.43 to 30.61°
Index ranges	-5<=h<=5, -19<=k<=19, -15<=l<=14
Reflections collected	12436
Independent reflections	1614 [R(int) = 0.0231]
Absorption correction	multi-scan
Max. and min. transmission	0.9840 and 0.8470
Structure solution technique	direct methods
Structure solution program	SHELXTL XT 2014/4 (Bruker AXS, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXTL XL 2014/6 (Bruker AXS, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	1614 / 0 / 100
Goodness-of-fit on F^2	1.087
Δ/σ_{max}	0.001
Final R indices	1465 data; I>2σ(I) R1 = 0.0255, wR2 = 0.0746
	all data R1 = 0.0285, wR2 = 0.0769
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0442P)^2+0.1095P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.308 and -0.271 eÅ^{-3}
R.M.S. deviation from mean	0.048 eÅ^{-3}

Table S25. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for $CH_6N_4O_4$.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
C1	0.3641(2)	0.50613(5)	0.15481(7)	0.01206(15)
N1	0.39509(17)	0.60208(5)	0.12520(6)	0.01096(14)
N2	0.54237(17)	0.46290(5)	0.26182(6)	0.01089(14)
N3	0.86465(18)	0.30543(5)	0.57358(6)	0.01195(14)
N4	0.09230(18)	0.33019(5)	0.47678(6)	0.01092(14)
O1	0.58787(16)	0.66234(4)	0.19448(5)	0.01541(14)
O2	0.21327(17)	0.62862(4)	0.02069(5)	0.01605(14)
O3	0.75790(16)	0.50676(4)	0.34655(5)	0.01505(14)
O4	0.47962(17)	0.37323(4)	0.27230(6)	0.01509(14)

Table S26. Bond lengths (Å) for $CH_6N_4O_4$.

C1-N2	1.3647(9)	C1-N1	1.3680(10)
C1-H1	0.910(12)	N1-O1	1.2565(8)
N1-O2	1.2647(8)	N2-O3	1.2621(8)
N2-O4	1.2648(8)	N3-N4	1.4529(9)
N3-H2	0.904(12)	N3-H3	0.869(12)
N4-H4	0.890(12)	N4-H5	0.866(12)
N4-H6	0.890(12)		

Table S27. Bond angles (°) for $CH_6N_4O_4$.

N2-C1-N1	124.70(7)	N2-C1-H1	116.5(8)
N1-C1-H1	118.8(8)	O1-N1-O2	120.24(6)
O1-N1-C1	124.15(6)	O2-N1-C1	115.61(6)
O3-N2-O4	120.45(6)	O3-N2-C1	124.09(6)
O4-N2-C1	115.46(6)	N4-N3-H2	106.2(7)
N4-N3-H3	105.2(8)	H2-N3-H3	105.2(11)
N3-N4-H4	112.0(7)	N3-N4-H5	108.1(8)
H4-N4-H5	108.8(11)	N3-N4-H6	109.0(7)
H4-N4-H6	111.5(11)	H5-N4-H6	107.4(10)

Table S28. Torsion angles (°) for $CH_6N_4O_4$.

N2-C1-N1-O1	-1.20(12)	N2-C1-N1-O2	178.87(7)
N1-C1-N2-O3	0.05(12)	N1-C1-N2-O4	-179.77(7)

Table S29. Anisotropic atomic displacement parameters (Å^2) for $CH_6N_4O_4$.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0139(3)	0.0103(3)	0.0112(3)	0.0006(2)	-0.0010(2)	-0.0017(2)
N1	0.0119(3)	0.0111(3)	0.0096(3)	0.0001(2)	0.0006(2)	0.0001(2)
N2	0.0118(3)	0.0106(3)	0.0105(3)	-0.0001(2)	0.0022(2)	0.0000(2)
N3	0.0119(3)	0.0135(3)	0.0106(3)	0.0004(2)	0.0023(2)	-0.0013(2)
N4	0.0105(3)	0.0112(3)	0.0110(3)	0.0001(2)	0.0015(2)	0.0001(2)
O1	0.0195(3)	0.0112(3)	0.0136(3)	-0.00124(19)	-0.0040(2)	-0.0035(2)
O2	0.0201(3)	0.0140(3)	0.0119(3)	0.00288(19)	-0.0050(2)	-0.0009(2)
O3	0.0180(3)	0.0130(3)	0.0124(3)	-0.00141(19)	-0.0040(2)	-0.0009(2)
O4	0.0189(3)	0.0096(3)	0.0163(3)	0.00243(19)	0.0009(2)	-0.00215(19)

Table S30. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for $CH_6N_4O_4$.

	x/a	y/b	z/c	U(eq)
H1	0.213(3)	0.4675(9)	0.1007(11)	0.014
H2	-0.087(3)	0.2425(9)	0.5933(11)	0.014
H3	-0.041(3)	0.3378(9)	0.6405(11)	0.014
H4	0.333(3)	0.3256(9)	0.5055(11)	0.013
H5	0.039(3)	0.2903(9)	0.4140(11)	0.013
H6	0.032(3)	0.3895(9)	0.4477(11)	0.013

Crystal Structure Report for 5-(Fluorodinitromethyl)-2H-tetrazole $C_2HFN_6O_4$

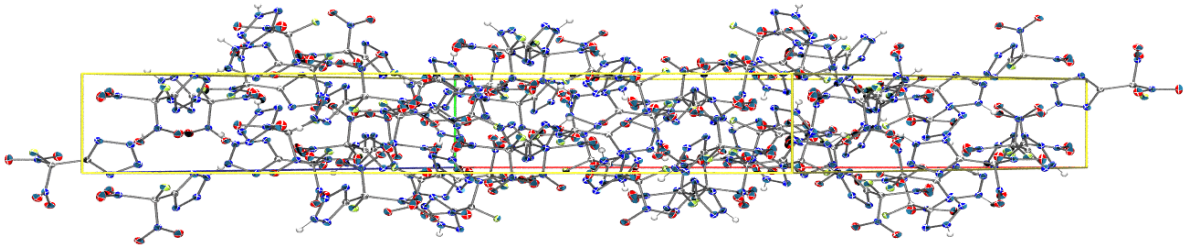

Figure S13. Packing diagram for the crystal structure of $C_2HFN_6O_4$. View along the 001 direction.

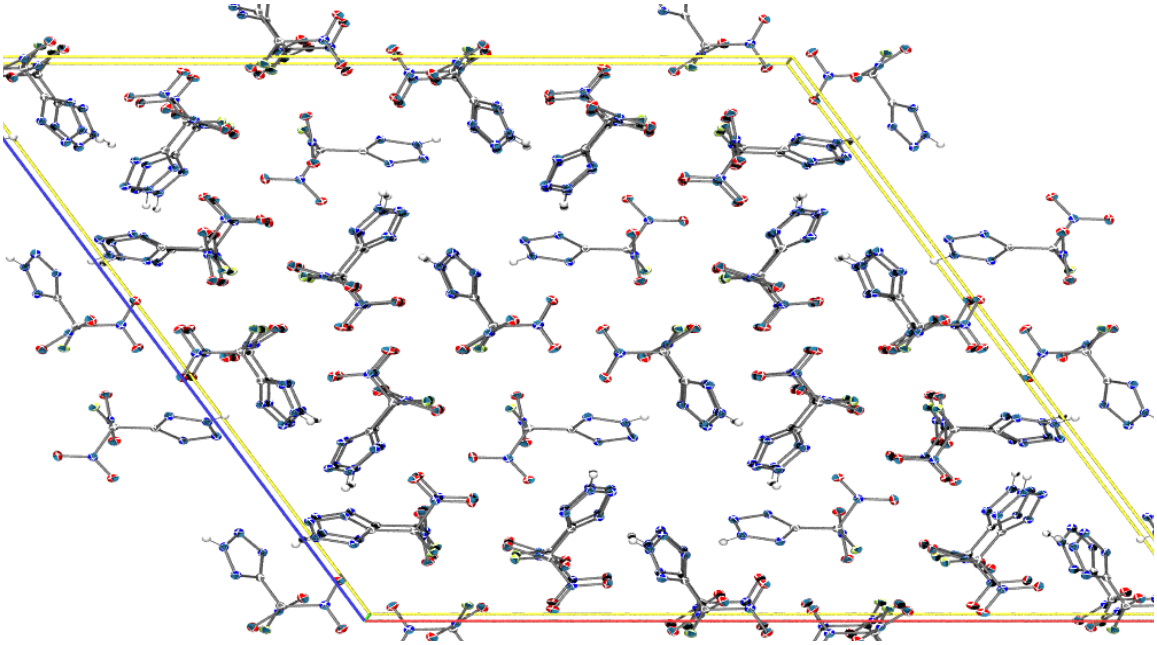

Figure S14. Packing diagram for the crystal structure of $C_2HFN_6O_4$. View along the 010 direction.

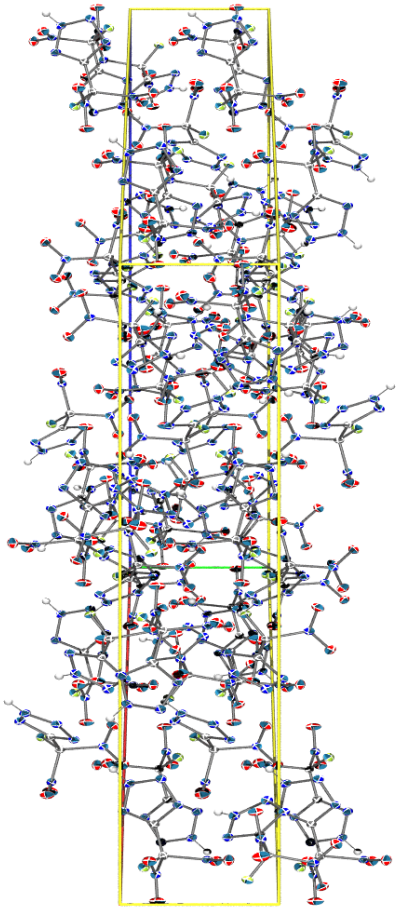

Figure S15. Packing diagram for the crystal structure of $C_2HFN_6O_4$. View along the 100 direction.

Table S31. Sample and crystal data for $C_2HFN_6O_4$.

Identification code	HFDNTz	
Chemical formula	$C_2HFN_6O_4$	
Formula weight	192.09 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.022 x 0.059 x 0.435 mm	
Crystal habit	clear colourless needle	
Crystal system	monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 28.8030(7) Å	α = 90°
	b = 5.37030(10) Å	β = 119.723(2)°
	c = 28.8969(10) Å	γ = 90°
Volume	3881.71(19) $Å^3$	
Z	24	
Density (calculated)	1.972 g/cm^3	
Absorption coefficient	0.200 mm^{-1}	
F(000)	2304	

Table S32. Data collection and structure refinement for $C_2HFN_6O_4$.

Diffractometer	Bruker APEX DUO
Radiation source	fine-focus tube, MoKα
Theta range for data collection	1.62 to 30.56°
Index ranges	-40<=h<=40, -7<=k<=7, -41<=l<=41
Reflections collected	46406
Independent reflections	5932 [R(int) = 0.0774]
Coverage of independent reflections	99.8%
Absorption correction	multi-scan
Max. and min. transmission	0.9960 and 0.9180
Structure solution technique	direct methods
Structure solution program	SHELXTL XT 2014/4 (Bruker AXS, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXTL XL 2014/6 (Bruker AXS, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	5932 / 0 / 361
Goodness-of-fit on F^2	1.035
Δ/σ_{max}	0.001
Final R indices	4146 data; I>2σ(I) R1 = 0.0414, wR2 = 0.0830
	all data R1 = 0.0760, wR2 = 0.0940
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0348P)^2+4.5858P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.456 and -0.324 $eÅ^{-3}$
R.M.S. deviation from mean	0.069 $eÅ^{-3}$

Table S33. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $C_2HFN_6O_4$.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

x/a	y/b	z/c	U(eq)

	x/a	y/b	z/c	U(eq)
C1	0.41234(6)	0.2864(3)	0.57465(7)	0.0121(3)
C2	0.41056(6)	0.2305(3)	0.52329(7)	0.0127(3)
C3	0.41128(6)	0.3749(3)	0.33780(6)	0.0122(3)
C4	0.36142(6)	0.4249(3)	0.33980(7)	0.0121(3)
C5	0.17640(6)	0.5410(3)	0.33778(7)	0.0127(3)
C6	0.22798(6)	0.5936(3)	0.38742(7)	0.0129(3)
F1	0.37321(4)	0.35649(19)	0.48278(4)	0.0170(2)
F2	0.35839(4)	0.29651(19)	0.37703(4)	0.0162(2)
F3	0.26858(4)	0.46927(19)	0.38982(4)	0.0159(2)
N1	0.38892(6)	0.4848(3)	0.58126(6)	0.0153(3)
N2	0.39901(6)	0.4479(3)	0.63070(6)	0.0146(3)
N3	0.42621(6)	0.2439(3)	0.65378(6)	0.0154(3)
N4	0.43524(5)	0.1361(3)	0.61775(6)	0.0134(3)
N5	0.39939(6)	0.9512(3)	0.51041(6)	0.0137(3)
N6	0.46433(6)	0.2767(3)	0.52542(6)	0.0147(3)
N7	0.44153(6)	0.1773(3)	0.36059(6)	0.0146(3)
N8	0.48099(6)	0.2183(3)	0.35030(6)	0.0145(3)
N9	0.47642(6)	0.4233(3)	0.32354(6)	0.0155(3)
N10	0.43111(5)	0.5276(3)	0.31476(6)	0.0136(3)
N11	0.31011(6)	0.3754(3)	0.28623(6)	0.0142(3)
N12	0.35918(5)	0.7041(3)	0.35128(6)	0.0138(3)
N13	0.16922(6)	0.3424(3)	0.30786(6)	0.0150(3)
N14	0.11986(6)	0.3833(3)	0.26850(6)	0.0150(3)
N15	0.09743(6)	0.5886(3)	0.27299(6)	0.0152(3)
N16	0.13361(5)	0.6936(3)	0.31795(6)	0.0138(3)
N17	0.24077(5)	0.8731(3)	0.38970(6)	0.0135(3)
N18	0.22574(6)	0.5375(3)	0.43854(6)	0.0138(3)
O1	0.35335(5)	0.8942(2)	0.48098(5)	0.0194(3)
O2	0.43838(5)	0.8143(2)	0.53273(5)	0.0187(3)
O3	0.46298(5)	0.2662(3)	0.48284(5)	0.0233(3)
O4	0.50279(5)	0.3148(2)	0.56923(5)	0.0193(3)
O5	0.31581(5)	0.3436(2)	0.24780(5)	0.0195(3)
O6	0.26907(5)	0.3743(3)	0.28804(5)	0.0232(3)
O7	0.34284(5)	0.8415(2)	0.31258(5)	0.0190(3)
O8	0.37553(5)	0.7585(2)	0.39735(5)	0.0193(3)
O9	0.26929(5)	0.9328(2)	0.37200(5)	0.0184(3)
O10	0.21908(5)	0.0077(2)	0.40771(5)	0.0185(3)
O11	0.18135(5)	0.5161(2)	0.43347(5)	0.0196(3)
O12	0.26855(5)	0.5227(3)	0.47907(5)	0.0224(3)

Table S34. Bond lengths (Å) for $C_2HFN_6O_4$.

C1-N1	1.325(2)	C1-N4	1.350(2)
C1-C2	1.490(2)	C2-F1	1.3180(19)
C2-N6	1.539(2)	C2-N5	1.540(2)
C3-N7	1.323(2)	C3-N10	1.349(2)
C3-C4	1.490(2)	C4-F2	1.3168(18)
C4-N12	1.543(2)	C4-N11	1.544(2)

C5-N13	1.323(2)	C5-N16	1.349(2)
C5-C6	1.494(2)	C6-F3	1.3182(18)
C6-N17	1.539(2)	C6-N18	1.540(2)
N1-N2	1.324(2)	N2-N3	1.319(2)
N2-H2	0.89(2)	N3-N4	1.325(2)
N5-O1	1.2071(18)	N5-O2	1.2245(18)
N6-O3	1.2129(18)	N6-O4	1.2170(19)
N7-N8	1.328(2)	N8-N9	1.314(2)
N8-H8	0.88(2)	N9-N10	1.3244(19)
N11-O6	1.2089(18)	N11-O5	1.2124(18)
N12-O8	1.2074(18)	N12-O7	1.2226(18)
N13-N14	1.326(2)	N14-N15	1.316(2)
N14-H14	0.91(2)	N15-N16	1.323(2)
N17-O9	1.2067(18)	N17-O10	1.2274(18)
N18-O12	1.2109(18)	N18-O11	1.2181(18)

Table S35. Bond angles (°) for $C_2HFN_6O_4$.

N1-C1-N4	113.51(15)	N1-C1-C2	122.49(15)
N4-C1-C2	123.92(15)	F1-C2-C1	113.02(13)
F1-C2-N6	108.34(13)	C1-C2-N6	113.00(13)
F1-C2-N5	107.74(13)	C1-C2-N5	109.68(13)
N6-C2-N5	104.60(12)	N7-C3-N10	113.46(14)
N7-C3-C4	122.34(15)	N10-C3-C4	124.15(15)
F2-C4-C3	113.12(14)	F2-C4-N12	107.84(13)
C3-C4-N12	109.11(13)	F2-C4-N11	108.10(13)
C3-C4-N11	113.08(13)	N12-C4-N11	105.18(12)
N13-C5-N16	113.48(15)	N13-C5-C6	122.60(15)
N16-C5-C6	123.87(15)	F3-C6-C5	112.88(14)
F3-C6-N17	107.73(12)	C5-C6-N17	109.19(14)
F3-C6-N18	107.95(13)	C5-C6-N18	112.91(13)
N17-C6-N18	105.83(13)	N2-N1-C1	100.36(14)
N3-N2-N1	115.32(14)	N3-N2-H2	122.7(14)
N1-N2-H2	122.0(14)	N2-N3-N4	105.32(13)
N3-N4-C1	105.48(14)	O1-N5-O2	128.25(15)
O1-N5-C2	116.23(14)	O2-N5-C2	115.48(13)
O3-N6-O4	128.16(15)	O3-N6-C2	115.24(14)
O4-N6-C2	116.59(13)	C3-N7-N8	100.41(13)
N9-N8-N7	115.09(14)	N9-N8-H8	121.8(13)
N7-N8-H8	123.1(13)	N8-N9-N10	105.59(13)
N9-N10-C3	105.45(14)	O6-N11-O5	128.20(15)
O6-N11-C4	115.33(14)	O5-N11-C4	116.47(13)
O8-N12-O7	128.69(15)	O8-N12-C4	115.92(14)
O7-N12-C4	115.33(13)	C5-N13-N14	100.41(14)
N15-N14-N13	115.09(14)	N15-N14-H14	121.1(13)
N13-N14-H14	123.8(13)	N14-N15-N16	105.51(13)
N15-N16-C5	105.51(14)	O9-N17-O10	128.31(15)
O9-N17-C6	116.08(13)	O10-N17-C6	115.56(13)
O12-N18-O11	127.95(15)	O12-N18-C6	115.71(13)

O11-N18-C6 116.33(14)

Table S36. Anisotropic atomic displacement parameters (Å²) for $C_2HFN_6O_4$.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0103(7)	0.0128(8)	0.0138(8)	-0.0012(6)	0.0064(6)	-0.0009(6)
C2	0.0118(7)	0.0121(8)	0.0133(8)	0.0012(6)	0.0057(6)	0.0013(6)
C3	0.0122(7)	0.0127(8)	0.0108(8)	-0.0012(6)	0.0051(6)	-0.0003(6)
C4	0.0135(7)	0.0121(8)	0.0106(8)	0.0000(6)	0.0059(6)	0.0004(6)
C5	0.0132(7)	0.0143(8)	0.0128(8)	0.0005(6)	0.0081(7)	-0.0010(6)
C6	0.0127(7)	0.0132(8)	0.0144(8)	-0.0005(6)	0.0080(7)	0.0003(6)
F1	0.0159(5)	0.0173(5)	0.0142(5)	0.0031(4)	0.0048(4)	0.0039(4)
F2	0.0196(5)	0.0168(5)	0.0149(5)	0.0026(4)	0.0105(4)	0.0003(4)
F3	0.0130(4)	0.0164(5)	0.0201(5)	-0.0005(4)	0.0096(4)	0.0026(4)
N1	0.0153(7)	0.0159(7)	0.0153(7)	-0.0005(6)	0.0081(6)	0.0019(5)
N2	0.0142(6)	0.0154(7)	0.0167(7)	-0.0019(6)	0.0094(6)	0.0017(5)
N3	0.0148(7)	0.0154(7)	0.0172(7)	-0.0005(6)	0.0088(6)	-0.0006(5)
N4	0.0132(6)	0.0139(7)	0.0140(7)	0.0005(6)	0.0074(6)	-0.0002(5)
N5	0.0142(6)	0.0147(7)	0.0143(7)	-0.0007(6)	0.0087(6)	-0.0011(5)
N6	0.0164(7)	0.0133(7)	0.0159(7)	-0.0006(6)	0.0092(6)	-0.0005(5)
N7	0.0138(6)	0.0151(7)	0.0148(7)	0.0008(6)	0.0072(6)	0.0022(5)
N8	0.0121(6)	0.0151(7)	0.0149(7)	0.0009(6)	0.0057(6)	0.0025(5)
N9	0.0125(6)	0.0171(7)	0.0152(7)	0.0007(6)	0.0057(6)	0.0008(5)
N10	0.0113(6)	0.0154(7)	0.0135(7)	-0.0007(6)	0.0057(6)	0.0004(5)
N11	0.0129(6)	0.0143(7)	0.0150(7)	-0.0008(6)	0.0067(6)	-0.0001(5)
N12	0.0120(6)	0.0149(7)	0.0161(7)	0.0001(6)	0.0083(6)	0.0008(5)
N13	0.0151(7)	0.0156(7)	0.0148(7)	-0.0033(6)	0.0077(6)	-0.0014(5)
N14	0.0161(7)	0.0163(7)	0.0128(7)	-0.0024(6)	0.0073(6)	-0.0022(6)
N15	0.0169(7)	0.0162(7)	0.0125(7)	-0.0004(6)	0.0074(6)	-0.0008(6)
N16	0.0136(6)	0.0156(7)	0.0117(7)	-0.0001(6)	0.0059(6)	-0.0009(5)
N17	0.0129(6)	0.0139(7)	0.0119(7)	-0.0010(5)	0.0047(6)	-0.0013(5)
N18	0.0156(7)	0.0126(7)	0.0134(7)	-0.0009(6)	0.0074(6)	-0.0006(5)
O1	0.0153(6)	0.0219(7)	0.0189(7)	-0.0043(5)	0.0069(5)	-0.0047(5)
O2	0.0173(6)	0.0147(6)	0.0229(7)	0.0011(5)	0.0091(5)	0.0033(5)
O3	0.0249(7)	0.0329(8)	0.0177(7)	-0.0025(6)	0.0148(6)	-0.0036(6)
O4	0.0141(6)	0.0253(7)	0.0156(6)	-0.0010(5)	0.0053(5)	-0.0024(5)
O5	0.0188(6)	0.0271(7)	0.0131(6)	-0.0018(5)	0.0083(5)	0.0008(5)
O6	0.0122(6)	0.0352(8)	0.0230(7)	-0.0030(6)	0.0093(6)	-0.0012(5)
O7	0.0214(6)	0.0164(6)	0.0184(6)	0.0041(5)	0.0091(5)	0.0030(5)
O8	0.0226(6)	0.0208(7)	0.0153(6)	-0.0042(5)	0.0100(5)	0.0005(5)
O9	0.0169(6)	0.0198(6)	0.0215(7)	0.0013(5)	0.0117(5)	-0.0031(5)
O10	0.0227(6)	0.0149(6)	0.0215(7)	-0.0033(5)	0.0137(6)	0.0004(5)
O11	0.0165(6)	0.0260(7)	0.0201(7)	-0.0017(5)	0.0120(5)	-0.0031(5)
O12	0.0173(6)	0.0313(8)	0.0131(6)	0.0015(5)	0.0034(5)	0.0001(5)

Table S37. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²) for $C_2HFN_6O_4$.

	x/a	y/b	z/c	U(eq)
H2	0.3874(8)	0.551(4)	0.6467(8)	0.018

	x/a	y/b	z/c	U(eq)
H8	0.5088(8)	0.118(4)	0.3612(8)	0.017
H14	0.1021(8)	0.280(4)	0.2400(8)	0.018

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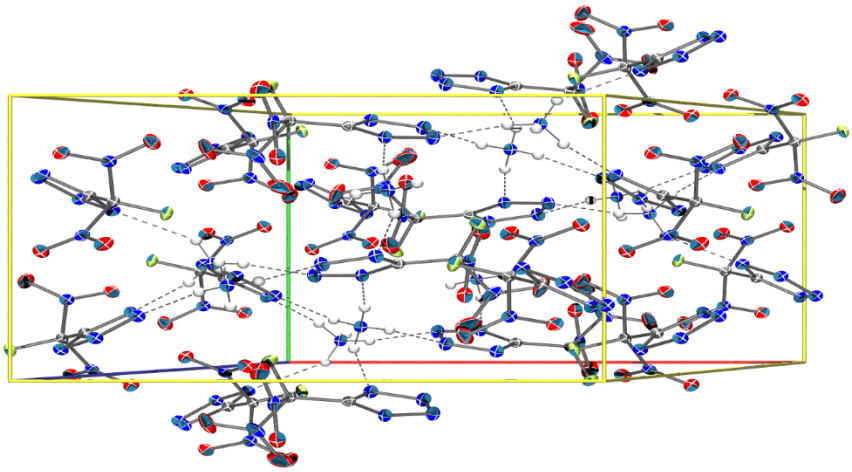

Figure S16. Packing diagram for the crystal structure of $C_2H_4FN_7O_4$. View along the 001 direction.

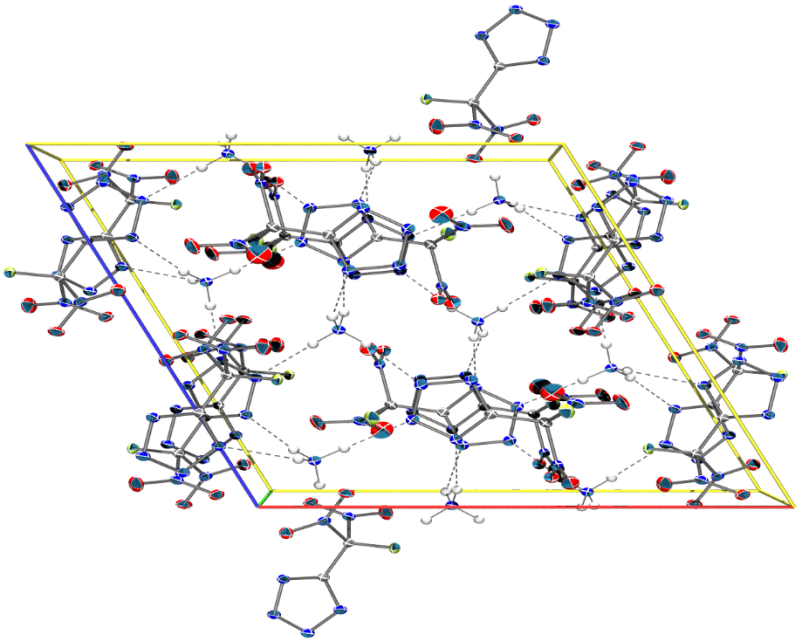

Figure S17. Packing diagram for the crystal structure of $C_2H_4FN_7O_4$. View along the 010 direction.

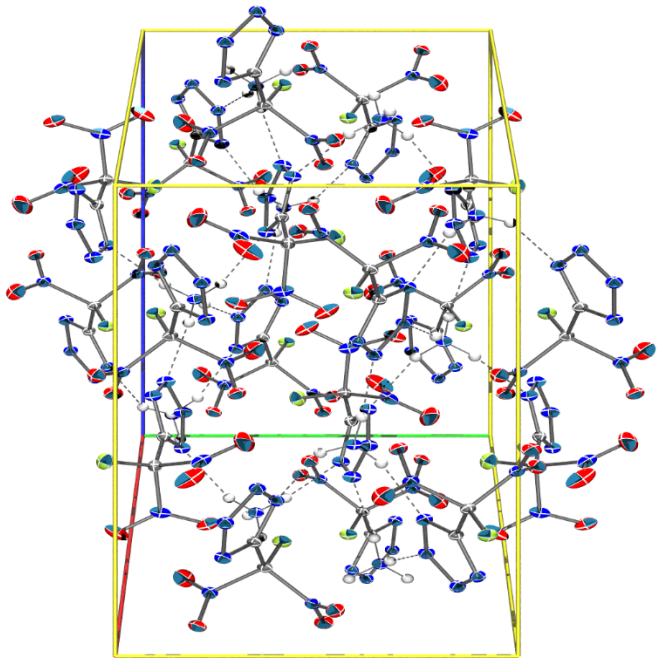

Figure S18. Packing diagram for the crystal structure of $C_2H_4FN_7O_4$. View along the 100 direction.

Table S38. Sample and crystal data for $C_2H_4FN_7O_4$.

Identification code	NH4FDNTz	
Chemical formula	$C_2H_4FN_7O_4$	
Formula weight	209.12 g/mol	
Temperature	101(2) K	
Wavelength	0.71073 Å	
Crystal size	0.120 x 0.420 x 0.440 mm	
Crystal habit	clear yellow prism	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 13.9642(7) Å	α = 90°
	b = 8.9672(5) Å	β = 115.47160(10)°
	c = 13.9957(7) Å	γ = 90°
Volume	1582.19(14) $Å^3$	
Z	8	
Density (calculated)	1.756 g/cm^3	
Absorption coefficient	0.174 mm^{-1}	
F(000)	848	

Table S39. Data collection and structure refinement for $C_2H_4FN_7O_4$.

Diffractometer	Bruker APEX DUO
Radiation source	fine-focus tube, MoKα
Theta range for data collection	1.62 to 30.49°
Index ranges	-19<=h<=19, -12<=k<=12, -19<=l<=19
Reflections collected	37464
Independent reflections	4778 [R(int) = 0.0384]
Absorption correction	multi-scan
Max. and min. transmission	0.9790 and 0.9270
Structure solution technique	direct methods
Structure solution program	SHELXTL XT 2014/4 (Bruker AXS, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXTL XL 2014/6 (Bruker AXS, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4778 / 0 / 277
Goodness-of-fit on F^2	1.026
Δ/σ_{max}	0.001
Final R indices	3941 data; $I>2\sigma(I)$ R1 = 0.0329, wR2 = 0.0786
	all data R1 = 0.0441, wR2 = 0.0845
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0393P)^2+0.5930P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.395 and -0.270 eÅ^{-3}
R.M.S. deviation from mean	0.053 eÅ^{-3}

Table S40. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for $C_2H_4FN_7O_4$.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
C1	0.01012(8)	0.84528(11)	0.26261(8)	0.01147(19)
C2	0.10443(8)	0.86925(12)	0.36478(8)	0.01166(19)
C3	0.45565(8)	0.59293(11)	0.24714(8)	0.01206(19)
C4	0.36164(8)	0.57596(12)	0.26877(8)	0.01285(19)
F1	0.18988(5)	0.91121(7)	0.35224(5)	0.01561(14)
F2	0.31081(5)	0.44813(8)	0.23409(6)	0.02102(15)
N1	0.92395(7)	0.77053(11)	0.25228(7)	0.01367(18)
N2	0.86068(7)	0.77843(11)	0.14802(7)	0.01404(18)
N3	0.90865(7)	0.85491(10)	0.10034(7)	0.01406(18)
N4	0.00440(7)	0.89930(10)	0.17137(7)	0.01342(18)
N5	0.08778(7)	0.98996(10)	0.43512(7)	0.01314(17)
N6	0.13297(7)	0.72909(10)	0.43491(7)	0.01364(17)
N7	0.45149(7)	0.56501(11)	0.15162(7)	0.01559(18)
N8	0.55055(8)	0.59330(11)	0.16450(8)	0.01730(19)
N9	0.60932(7)	0.63596(11)	0.26293(7)	0.01656(19)
N10	0.55073(7)	0.63701(11)	0.31809(7)	0.01405(18)
N11	0.39102(7)	0.58794(12)	0.38782(7)	0.01641(19)
N12	0.27951(8)	0.70063(12)	0.21906(8)	0.0199(2)
N13	0.35928(8)	0.16647(11)	0.48813(8)	0.01345(17)
N14	0.15787(8)	0.40633(11)	0.62437(8)	0.01328(17)
O1	0.00095(6)	0.04607(9)	0.40338(7)	0.01803(17)

	x/a	y/b	z/c	U(eq)
O2	0.16641(6)	0.01866(9)	0.51686(6)	0.01818(17)
O3	0.07301(6)	0.70054(9)	0.47503(6)	0.01679(16)
O4	0.21039(7)	0.65981(11)	0.44324(8)	0.0258(2)
O5	0.41499(7)	0.71214(10)	0.42587(7)	0.02151(18)
O6	0.38893(7)	0.47339(11)	0.43273(7)	0.0276(2)
O7	0.30835(9)	0.81132(12)	0.18964(9)	0.0373(3)
O8	0.19270(7)	0.67572(13)	0.21484(8)	0.0342(3)

Table S41. Bond lengths (Å) for $C_2H_4FN_7O_4$.

C1-N1	1.3298(13)	C1-N4	1.3357(13)
C1-C2	1.4850(14)	C2-F1	1.3328(11)
C2-N6	1.5381(14)	C2-N5	1.5466(14)
C3-N10	1.3309(13)	C3-N7	1.3366(14)
C3-C4	1.4764(14)	C4-F2	1.3256(12)
C4-N12	1.5372(14)	C4-N11	1.5389(14)
N1-N2	1.3438(12)	N2-N3	1.3224(13)
N3-N4	1.3383(12)	N5-O1	1.2072(12)
N5-O2	1.2248(12)	N6-O4	1.2083(12)
N6-O3	1.2191(12)	N7-N8	1.3401(13)
N8-N9	1.3211(13)	N9-N10	1.3449(13)
N11-O6	1.2110(13)	N11-O5	1.2177(13)
N12-O7	1.2081(15)	N12-O8	1.2088(14)
N13-H1	0.896(15)	N13-H2	0.873(15)
N13-H3	0.883(15)	N13-H4	0.898(15)
N14-H5	0.890(15)	N14-H6	0.865(16)
N14-H7	0.897(15)	N14-H8	0.916(15)

Table S42. Bond angles (°) for $C_2H_4FN_7O_4$.

N1-C1-N4	113.55(9)	N1-C1-C2	124.33(9)
N4-C1-C2	122.12(9)	F1-C2-C1	112.81(8)
F1-C2-N6	108.29(8)	C1-C2-N6	112.04(8)
F1-C2-N5	105.93(8)	C1-C2-N5	113.60(8)
N6-C2-N5	103.55(8)	N10-C3-N7	113.71(9)
N10-C3-C4	124.57(9)	N7-C3-C4	121.72(9)
F2-C4-C3	113.41(9)	F2-C4-N12	106.58(8)
C3-C4-N12	112.85(9)	F2-C4-N11	107.95(9)
C3-C4-N11	111.61(8)	N12-C4-N11	103.82(8)
C1-N1-N2	103.48(8)	N3-N2-N1	109.64(8)
N2-N3-N4	109.91(8)	C1-N4-N3	103.42(8)
O1-N5-O2	127.67(10)	O1-N5-C2	117.37(8)
O2-N5-C2	114.95(9)	O4-N6-O3	127.66(10)
O4-N6-C2	117.20(9)	O3-N6-C2	115.14(8)
C3-N7-N8	103.40(9)	N9-N8-N7	109.72(9)
N8-N9-N10	110.01(9)	C3-N10-N9	103.16(9)
O6-N11-O5	127.76(10)	O6-N11-C4	116.61(10)
O5-N11-C4	115.62(9)	O7-N12-O8	127.55(11)
O7-N12-C4	117.30(10)	O8-N12-C4	115.15(11)

H1-N13-H2	108.3(13)	H1-N13-H3	110.0(13)
H2-N13-H3	111.0(13)	H1-N13-H4	112.5(13)
H2-N13-H4	106.4(13)	H3-N13-H4	108.7(13)
H5-N14-H6	111.6(13)	H5-N14-H7	110.4(13)
H6-N14-H7	109.9(13)	H5-N14-H8	110.4(13)
H6-N14-H8	106.1(13)	H7-N14-H8	108.2(12)

Table S43. Anisotropic atomic displacement parameters (Å²) for $C_2H_4FN_7O_4$.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0111(4)	0.0126(4)	0.0101(4)	0.0001(3)	0.0040(4)	-0.0005(3)
C2	0.0112(4)	0.0132(5)	0.0107(4)	0.0004(3)	0.0049(4)	-0.0016(3)
C3	0.0118(4)	0.0117(4)	0.0118(5)	0.0003(4)	0.0043(4)	0.0004(3)
C4	0.0112(4)	0.0129(5)	0.0126(5)	-0.0005(4)	0.0032(4)	-0.0005(4)
F1	0.0116(3)	0.0209(3)	0.0158(3)	-0.0013(2)	0.0073(2)	-0.0042(2)
F2	0.0179(3)	0.0179(3)	0.0264(4)	-0.0052(3)	0.0086(3)	-0.0071(3)
N1	0.0124(4)	0.0160(4)	0.0114(4)	-0.0001(3)	0.0039(3)	-0.0025(3)
N2	0.0139(4)	0.0158(4)	0.0107(4)	0.0001(3)	0.0036(3)	-0.0009(3)
N3	0.0143(4)	0.0151(4)	0.0114(4)	0.0002(3)	0.0042(3)	-0.0009(3)
N4	0.0138(4)	0.0143(4)	0.0111(4)	0.0009(3)	0.0044(3)	-0.0011(3)
N5	0.0153(4)	0.0134(4)	0.0114(4)	0.0000(3)	0.0063(3)	-0.0025(3)
N6	0.0126(4)	0.0151(4)	0.0111(4)	0.0007(3)	0.0031(3)	-0.0003(3)
N7	0.0147(4)	0.0195(5)	0.0127(4)	-0.0021(3)	0.0061(3)	-0.0019(3)
N8	0.0157(4)	0.0222(5)	0.0148(4)	-0.0028(4)	0.0073(4)	-0.0031(4)
N9	0.0146(4)	0.0220(5)	0.0141(4)	-0.0010(4)	0.0071(4)	-0.0019(4)
N10	0.0121(4)	0.0174(4)	0.0126(4)	-0.0008(3)	0.0053(3)	-0.0009(3)
N11	0.0099(4)	0.0263(5)	0.0128(4)	0.0028(4)	0.0046(3)	0.0005(3)
N12	0.0179(5)	0.0242(5)	0.0128(4)	-0.0032(4)	0.0020(4)	0.0089(4)
N13	0.0122(4)	0.0162(4)	0.0110(4)	0.0007(3)	0.0041(3)	0.0004(3)
N14	0.0129(4)	0.0160(4)	0.0111(4)	-0.0003(3)	0.0053(3)	-0.0005(3)
O1	0.0163(4)	0.0187(4)	0.0190(4)	-0.0001(3)	0.0075(3)	0.0024(3)
O2	0.0178(4)	0.0214(4)	0.0113(4)	-0.0026(3)	0.0025(3)	-0.0049(3)
O3	0.0190(4)	0.0182(4)	0.0148(4)	0.0022(3)	0.0088(3)	-0.0016(3)
O4	0.0183(4)	0.0268(5)	0.0330(5)	0.0094(4)	0.0115(4)	0.0093(3)
O5	0.0167(4)	0.0305(5)	0.0173(4)	-0.0075(3)	0.0073(3)	-0.0028(3)
O6	0.0238(5)	0.0347(5)	0.0245(5)	0.0150(4)	0.0105(4)	0.0017(4)
O7	0.0472(6)	0.0250(5)	0.0417(6)	0.0151(4)	0.0210(5)	0.0168(5)
O8	0.0119(4)	0.0494(6)	0.0339(5)	-0.0176(5)	0.0029(4)	0.0069(4)

Table S44. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²) for $C_2H_4FN_7O_4$.

	x/a	y/b	z/c	U(eq)
H1	0.3941(11)	0.1516(16)	0.4481(11)	0.016
H2	0.3633(11)	0.0849(17)	0.5238(12)	0.016
H3	0.2925(12)	0.1902(16)	0.4478(11)	0.016
H4	0.3886(11)	0.2390(17)	0.5362(11)	0.016
H5	0.2283(12)	0.4053(16)	0.6585(11)	0.016
H6	0.1319(11)	0.4912(17)	0.6310(11)	0.016
H7	0.1369(11)	0.3855(16)	0.5556(12)	0.016
H8	0.1292(11)	0.3364(16)	0.6521(11)	0.016

Crystal Structure Report for $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$

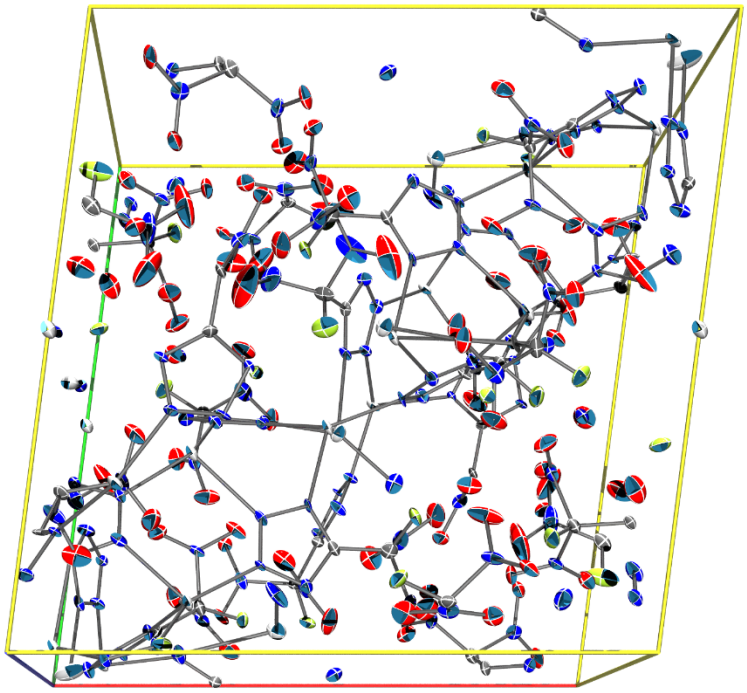

Figure S19. Packing diagram for the crystal structure of $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$. View along the 001 direction

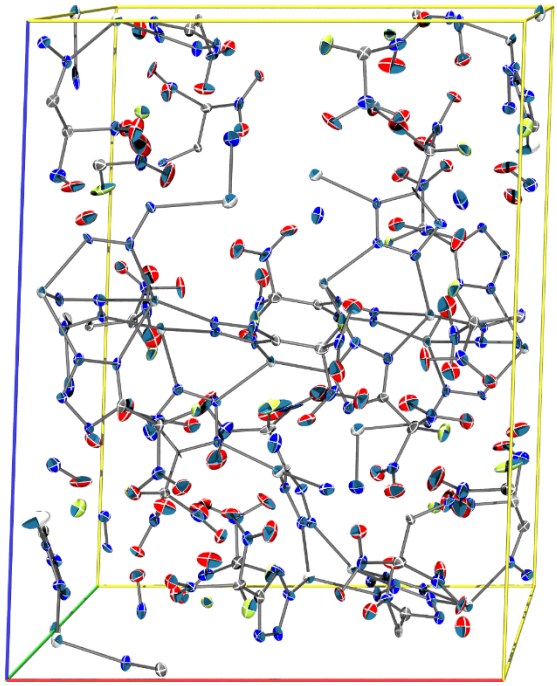

Figure S20. Packing diagram for the crystal structure of $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$. View along the 010 direction

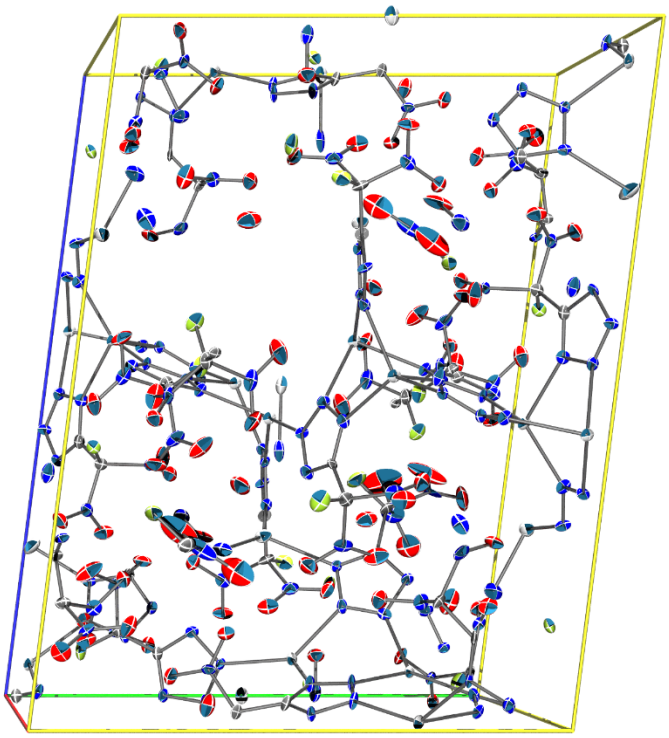

Figure S21. Packing diagram for the crystal structure of $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$. View along the 100 direction.

Table S45. Sample and crystal data for $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$.

Identification code	AgFDNTz	
Chemical formula	$C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$	
Formula weight	3689.60 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.020 x 0.030 x 0.100 mm	
Crystal habit	clear colourless rod	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 15.4270(10) Å	α = 82.7270(10)°
	b = 15.4526(10) Å	β = 88.1560(10)°
	c = 20.5225(13) Å	γ = 82.6690(10)°
Volume	4812.6(5) $Å^3$	
Z	2	
Density (calculated)	2.546 g/cm^3	
Absorption coefficient	2.540 mm^{-1}	
F(000)	3528	

Table S1. **Data collection and structure refinement for** $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$.

Diffractometer	Bruker APEX DUO
Radiation source	fine-focus tube, MoKα
Theta range for data collection	1.00 to 27.48°
Index ranges	-20<=h<=20, -20<=k<=20, -27<=l<=27
Reflections collected	22050
Independent reflections	22050 [R(int) = 0.0939]
Coverage of independent reflections	100.0%
Absorption correction	multi-scan
Max. and min. transmission	0.9510 and 0.7850
Structure solution technique	direct methods
Structure solution program	SHELXTL XT 2014/4 (Bruker AXS, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXTL XL 2014/6 (Bruker AXS, 2014)
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	22050 / 66 / 1576
Goodness-of-fit on F^2	0.992
Δ/σ_{max}	0.001
Final R indices	13724 data; I>2σ(I) R1 = 0.0584, wR2 = 0.0977
	all data R1 = 0.1174, wR2 = 0.1106
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0471P)^2]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	1.387 and -2.437 eÅ^{-3}
R.M.S. deviation from mean	0.211 eÅ^{-3}

Table S46. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å²) for $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
C1	0.7991(5)	0.9258(4)	0.5918(4)	0.0132(16)
C2	0.7293(5)	0.8806(5)	0.6252(4)	0.0166(17)
C3	0.1993(4)	0.9797(4)	0.7584(3)	0.0118(15)
C4	0.2211(5)	0.9528(5)	0.8280(4)	0.0167(17)
C5	0.9921(5)	0.2542(4)	0.5294(3)	0.0123(15)
C6	0.8979(5)	0.2498(4)	0.5206(4)	0.0172(17)
C7	0.2575(5)	0.4702(5)	0.2924(4)	0.0138(16)
C8	0.2281(5)	0.4883(5)	0.2237(4)	0.0196(18)
C9	0.4916(5)	0.2132(5)	0.4966(3)	0.0126(15)
C10	0.5866(5)	0.2111(5)	0.4842(4)	0.0202(18)
C11	0.6864(5)	0.5377(5)	0.3734(4)	0.0165(17)
C12	0.7500(5)	0.5639(5)	0.3222(4)	0.0187(17)
C13	0.4628(5)	0.6789(5)	0.2402(3)	0.0131(15)
C14	0.4192(5)	0.6938(5)	0.3044(4)	0.0204(18)
C15	0.4683(5)	0.2674(5)	0.0881(4)	0.0149(16)
C16	0.4359(5)	0.1861(5)	0.1188(4)	0.0151(16)
C17	0.7530(5)	0.4980(4)	0.0266(3)	0.0127(15)
C18	0.7485(5)	0.4070(4)	0.0134(3)	0.0120(15)

	x/a	y/b	z/c	U(eq)
C19	0.6914(5)	0.9931(5)	0.9852(4)	0.0170(17)
C20	0.6694(5)	0.0822(5)	0.9482(4)	0.0167(17)
C21	0.9797(4)	0.7732(5)	0.8046(4)	0.0151(16)
C22	0.0180(5)	0.7512(5)	0.7407(4)	0.0224(18)
C23	0.0161(5)	0.1999(4)	0.8712(4)	0.0144(16)
C24	0.0361(5)	0.2699(5)	0.8193(4)	0.0160(16)
N1	0.8569(4)	0.9631(4)	0.6214(3)	0.0138(13)
N2	0.9078(4)	0.9948(4)	0.5720(3)	0.0143(13)
N3	0.8817(4)	0.9746(4)	0.5155(3)	0.0131(13)
N4	0.8111(4)	0.9315(4)	0.5272(3)	0.0137(13)
N5	0.7474(4)	0.7799(4)	0.6285(3)	0.0170(14)
N6	0.7250(4)	0.8971(4)	0.6980(3)	0.0170(14)
N7	0.1223(4)	0.9763(4)	0.7320(3)	0.0138(13)
N8	0.1332(4)	0.0099(4)	0.6691(3)	0.0165(14)
N9	0.2134(4)	0.0315(4)	0.6596(3)	0.0148(14)
N10	0.2568(4)	0.0139(4)	0.7164(3)	0.0153(14)
N11	0.1464(4)	0.9069(4)	0.8639(3)	0.0188(14)
N12	0.3044(4)	0.8873(4)	0.8369(3)	0.0192(15)
N13	0.0446(4)	0.1909(4)	0.5617(3)	0.0147(13)
N14	0.1234(4)	0.2204(4)	0.5589(3)	0.0158(14)
N15	0.1143(4)	0.3004(4)	0.5259(3)	0.0136(13)
N16	0.0312(4)	0.3240(4)	0.5060(3)	0.0162(14)
N17	0.8803(4)	0.1885(4)	0.4708(3)	0.0205(15)
N18	0.8519(4)	0.3412(4)	0.4938(4)	0.0248(16)
N19	0.2023(4)	0.4629(4)	0.3435(3)	0.0146(13)
N20	0.2551(4)	0.4481(4)	0.3961(3)	0.0159(14)
N21	0.3382(4)	0.4467(4)	0.3759(3)	0.0131(13)
N22	0.3418(4)	0.4611(4)	0.3101(3)	0.0136(13)
N23	0.2208(4)	0.4055(4)	0.1909(3)	0.0210(15)
N24	0.2943(4)	0.5358(5)	0.1803(3)	0.0238(16)
N25	0.4384(4)	0.2875(4)	0.4850(3)	0.0129(13)
N26	0.3591(4)	0.2647(4)	0.5045(3)	0.0144(13)
N27	0.3681(4)	0.1804(4)	0.5262(3)	0.0113(13)
N28	0.4529(4)	0.1447(4)	0.5220(3)	0.0154(14)
N29	0.6082(5)	0.2363(5)	0.4108(4)	0.0289(17)
N30	0.6334(4)	0.1173(4)	0.5028(3)	0.0209(15)
N31	0.6165(4)	0.4997(4)	0.3608(3)	0.0187(14)
N32	0.5785(4)	0.4847(4)	0.4199(3)	0.0147(14)
N33	0.6239(4)	0.5137(4)	0.4650(3)	0.0154(14)
N34	0.6935(4)	0.5473(4)	0.4361(3)	0.0139(13)
N35	0.7816(5)	0.6509(5)	0.3304(3)	0.0251(16)
N36	0.7084(4)	0.5752(5)	0.2542(3)	0.0235(16)
N37	0.4726(4)	0.6000(4)	0.2191(3)	0.0138(13)
N38	0.5103(4)	0.6168(4)	0.1593(3)	0.0155(14)
N39	0.5194(4)	0.7007(4)	0.1481(3)	0.0148(13)
N40	0.4900(4)	0.7415(4)	0.1996(3)	0.0143(13)
N41	0.3202(5)	0.7210(6)	0.2985(5)	0.046(2)
N42	0.4564(6)	0.7705(6)	0.3314(4)	0.046(2)

	x/a	y/b	z/c	U(eq)
N43	0.4975(4)	0.3268(4)	0.1209(3)	0.0170(14)
N44	0.5149(4)	0.3903(4)	0.0731(3)	0.0169(14)
N45	0.4973(4)	0.3685(4)	0.0149(3)	0.0149(14)
N46	0.4680(4)	0.2901(4)	0.0234(3)	0.0165(14)
N47	0.3347(4)	0.1912(4)	0.1144(3)	0.0149(14)
N48	0.4529(4)	0.1700(5)	0.1931(3)	0.0217(16)
N49	0.6858(4)	0.5482(4)	0.0507(3)	0.0137(13)
N50	0.7148(4)	0.6248(4)	0.0531(3)	0.0148(14)
N51	0.7979(4)	0.6201(4)	0.0317(3)	0.0156(14)
N52	0.8226(4)	0.5402(4)	0.0142(3)	0.0123(13)
N53	0.7255(4)	0.3458(4)	0.0740(3)	0.0145(13)
N54	0.8369(4)	0.3671(4)	0.9884(3)	0.0188(15)
N55	0.6312(4)	0.9492(4)	0.0166(3)	0.0133(13)
N56	0.6734(4)	0.8690(4)	0.0338(3)	0.0116(13)
N57	0.7571(4)	0.8661(4)	0.0140(3)	0.0143(13)
N58	0.7703(4)	0.9446(4)	0.9822(3)	0.0155(14)
N59	0.6776(5)	0.0758(4)	0.8730(3)	0.0223(16)
N60	0.7310(5)	0.1500(4)	0.9591(3)	0.0231(16)
N61	0.9651(4)	0.7172(4)	0.8571(3)	0.0187(14)
N62	0.9317(4)	0.7679(4)	0.9026(3)	0.0161(14)
N63	0.9278(4)	0.8517(4)	0.8769(3)	0.0162(14)
N64	0.9571(4)	0.8568(4)	0.8150(3)	0.0135(13)
N65	0.1159(5)	0.7113(7)	0.7481(4)	0.050(2)
N66	0.9810(4)	0.6783(4)	0.7111(3)	0.0253(16)
N67	0.9652(4)	0.1388(4)	0.8616(3)	0.0196(15)
N68	0.9639(4)	0.0915(4)	0.9216(3)	0.0180(14)
N69	0.0100(4)	0.1231(4)	0.9632(3)	0.0144(13)
N70	0.0441(4)	0.1936(4)	0.9320(3)	0.0129(13)
N71	0.1310(4)	0.2874(5)	0.8222(3)	0.0225(16)
N72	0.0228(5)	0.2426(5)	0.7506(3)	0.0252(16)
N73	0.5918(4)	0.3561(4)	0.2465(3)	0.0265(16)
N74	0.8739(4)	0.1062(4)	0.7225(3)	0.0321(18)
N75	0.4020(4)	0.1055(5)	0.8162(3)	0.0313(18)
N76	0.4762(4)	0.9987(4)	0.6408(3)	0.0240(16)
N77	0.0119(5)	0.5125(4)	0.3946(3)	0.0276(16)
N78	0.9970(4)	0.4828(4)	0.1056(3)	0.0253(16)
O1	0.6829(4)	0.7403(3)	0.6419(3)	0.0266(13)
O2	0.8212(4)	0.7471(3)	0.6172(3)	0.0331(15)
O3	0.6678(4)	0.9518(4)	0.7134(3)	0.0310(14)
O4	0.7803(4)	0.8524(4)	0.7339(3)	0.0278(14)
O5	0.0941(3)	0.9528(4)	0.8935(3)	0.0312(15)
O6	0.1476(3)	0.8289(4)	0.8584(3)	0.0275(14)
O7	0.3469(3)	0.8907(3)	0.8852(3)	0.0224(13)
O8	0.3181(3)	0.8370(3)	0.7959(3)	0.0226(12)
O9	0.8057(4)	0.1693(4)	0.4704(3)	0.0361(16)
O10	0.9412(4)	0.1626(3)	0.4374(3)	0.0244(13)
O11	0.8302(4)	0.3905(4)	0.5339(3)	0.0443(17)
O12	0.8446(4)	0.3563(4)	0.4345(3)	0.0354(15)

	x/a	y/b	z/c	U(eq)
O13	0.1857(3)	0.4166(4)	0.1387(3)	0.0269(13)
O14	0.2532(4)	0.3353(4)	0.2212(3)	0.0379(16)
O15	0.2850(4)	0.6143(4)	0.1779(3)	0.0328(15)
O16	0.3521(4)	0.4885(4)	0.1546(3)	0.0331(15)
O17	0.6655(4)	0.2819(4)	0.3982(3)	0.0422(17)
O18	0.5618(4)	0.2087(4)	0.3724(3)	0.0334(15)
O19	0.6607(4)	0.1030(4)	0.5586(3)	0.0329(15)
O20	0.6368(4)	0.0668(4)	0.4617(3)	0.0325(15)
O21	0.8594(4)	0.6569(4)	0.3219(3)	0.0398(16)
O22	0.7260(4)	0.7084(4)	0.3466(3)	0.0388(16)
O23	0.7193(4)	0.5123(4)	0.2250(3)	0.0391(16)
O24	0.6677(4)	0.6478(4)	0.2369(3)	0.0391(16)
O25	0.2768(6)	0.6990(7)	0.3460(4)	0.100(4)
O26	0.2967(5)	0.7652(5)	0.2466(4)	0.056(2)
O27	0.5236(6)	0.7472(6)	0.3585(4)	0.076(3)
O28	0.4137(6)	0.8421(5)	0.3209(4)	0.070(2)
O29	0.3056(3)	0.1230(3)	0.1320(2)	0.0226(13)
O30	0.2952(3)	0.2616(3)	0.0936(3)	0.0229(13)
O31	0.5071(4)	0.1081(5)	0.2117(3)	0.0451(18)
O32	0.4097(4)	0.2192(4)	0.2255(3)	0.0302(14)
O33	0.6987(4)	0.2777(3)	0.0637(3)	0.0259(13)
O34	0.7359(4)	0.3692(4)	0.1272(3)	0.0306(14)
O35	0.8478(4)	0.3745(4)	0.9294(3)	0.0280(14)
O36	0.8893(4)	0.3353(4)	0.0303(3)	0.0311(14)
O37	0.6095(4)	0.0738(4)	0.8447(3)	0.0374(16)
O38	0.7520(4)	0.0677(3)	0.8517(3)	0.0253(13)
O39	0.7136(4)	0.2201(3)	0.9246(3)	0.0400(17)
O40	0.7861(4)	0.1299(3)	0.9993(3)	0.0220(13)
O41	0.1696(5)	0.7552(6)	0.7232(4)	0.076(3)
O42	0.1261(5)	0.6399(6)	0.7803(4)	0.067(2)
O43	0.0073(4)	0.6678(4)	0.6564(3)	0.0425(17)
O44	0.9290(5)	0.6399(5)	0.7429(3)	0.058(2)
O45	0.1432(4)	0.3639(4)	0.8202(3)	0.0310(14)
O46	0.1867(4)	0.2248(4)	0.8247(3)	0.0369(16)
O47	0.9687(4)	0.2887(4)	0.7161(3)	0.0414(17)
O48	0.0686(4)	0.1758(4)	0.7379(3)	0.0378(16)
F1	0.6512(3)	0.9041(3)	0.6003(2)	0.0196(10)
F2	0.2317(3)	0.0208(3)	0.8608(2)	0.0212(10)
F3	0.8568(3)	0.2226(3)	0.5760(2)	0.0259(11)
F4	0.1501(3)	0.5356(3)	0.2180(2)	0.0257(11)
F5	0.6236(3)	0.2654(3)	0.5173(2)	0.0257(11)
F6	0.8229(3)	0.5050(3)	0.3203(2)	0.0327(12)
F7	0.4288(4)	0.6244(3)	0.3492(2)	0.0412(14)
F8	0.4683(3)	0.1147(3)	0.0924(2)	0.0247(11)
F9	0.6891(3)	0.4025(3)	0.9685(2)	0.0179(9)
F10	0.5886(3)	0.1170(3)	0.9606(2)	0.0294(11)
F11	0.0150(4)	0.8197(3)	0.6958(2)	0.0431(14)
F12	0.9869(3)	0.3462(3)	0.8219(2)	0.0285(11)

	x/a	y/b	z/c	U(eq)
Ag1	0.03830(4)	0.03496(4)	0.58600(3)	0.01517(13)
Ag2	0.25363(3)	0.11380(4)	0.56713(3)	0.01490(13)
Ag3	0.41036(4)	0.05370(4)	0.72333(3)	0.02421(15)
Ag4	0.22602(4)	0.37803(4)	0.49944(3)	0.01564(13)
Ag5	0.45456(3)	0.43153(4)	0.44271(3)	0.01427(13)
Ag6	0.47699(4)	0.44687(4)	0.26441(3)	0.02209(14)
Ag7	0.53969(4)	0.52635(3)	0.08143(3)	0.01521(13)
Ag8	0.60913(4)	0.75007(3)	0.06546(3)	0.01413(13)
Ag9	0.86788(4)	0.73729(4)	0.00471(3)	0.01619(13)
Ag10	0.90825(4)	0.96458(3)	0.94478(3)	0.01610(13)
Ag11	0.95380(6)	0.98725(5)	0.75836(4)	0.0459(2)
Ag12	0.0	0.5	0.5	0.0247(2)
Ag13	0.0	0.5	0.0	0.0220(2)

Table S47. Bond lengths (Å) for $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$.

C1-N1	1.324(9)	C1-N4	1.325(8)
C1-C2	1.463(10)	C2-F1	1.313(8)
C2-N5	1.540(9)	C2-N6	1.545(9)
C3-N10	1.329(9)	C3-N7	1.331(9)
C3-C4	1.473(9)	C4-F2	1.348(8)
C4-N12	1.531(9)	C4-N11	1.547(9)
C5-N13	1.313(9)	C5-N16	1.332(8)
C5-C6	1.482(10)	C6-F3	1.331(8)
C6-N17	1.531(9)	C6-N18	1.541(9)
C7-N19	1.332(9)	C7-N22	1.347(9)
C7-C8	1.477(10)	C8-F4	1.327(8)
C8-N24	1.530(10)	C8-N23	1.536(10)
C9-N28	1.323(8)	C9-N25	1.323(9)
C9-C10	1.478(10)	C10-F5	1.336(9)
C10-N30	1.542(9)	C10-N29	1.542(10)
C11-N34	1.322(9)	C11-N31	1.339(9)
C11-C12	1.470(10)	C12-F6	1.357(9)
C12-N35	1.518(10)	C12-N36	1.535(10)
C13-N40	1.297(9)	C13-N37	1.335(9)
C13-C14	1.490(10)	C14-F7	1.318(8)
C14-N41	1.536(11)	C14-N42	1.550(11)
C15-N46	1.331(9)	C15-N43	1.333(9)
C15-C16	1.472(10)	C16-F8	1.325(8)
C16-N48	1.538(9)	C16-N47	1.557(9)
C17-N52	1.327(8)	C17-N49	1.334(9)
C17-C18	1.477(9)	C18-F9	1.335(8)
C18-N53	1.524(9)	C18-N54	1.524(9)
C19-N55	1.323(9)	C19-N58	1.349(9)
C19-C20	1.491(10)	C20-F10	1.323(8)
C20-N60	1.543(9)	C20-N59	1.558(9)
C21-N61	1.325(9)	C21-N64	1.336(9)
C21-C22	1.481(10)	C22-F11	1.309(8)

C22-N66	1.525(10)	C22-N65	1.561(12)
C23-N70	1.320(9)	C23-N67	1.339(9)
C23-C24	1.474(10)	C24-F12	1.325(8)
C24-N71	1.527(9)	C24-N72	1.548(10)
N1-N2	1.343(8)	N2-N3	1.327(8)
N2-Ag1	2.219(6)	N3-N4	1.348(7)
N3-Ag1	2.398(6)	N4-Ag2	2.425(6)
N5-O2	1.212(8)	N5-O1	1.239(7)
N6-O3	1.205(8)	N6-O4	1.228(8)
N7-N8	1.343(8)	N7-Ag11	2.626(6)
N8-N9	1.324(8)	N8-Ag1	2.247(6)
N9-N10	1.345(8)	N9-Ag2	2.262(6)
N10-Ag3	2.535(6)	N11-O5	1.207(8)
N11-O6	1.222(8)	N12-O8	1.212(8)
N12-O7	1.215(7)	N13-N14	1.348(8)
N13-Ag1	2.412(6)	N14-N15	1.326(8)
N14-Ag2	2.426(6)	N15-N16	1.349(8)
N15-Ag4	2.237(6)	N17-O10	1.202(8)
N17-O9	1.226(8)	N18-O11	1.202(8)
N18-O12	1.216(8)	N19-N20	1.352(8)
N20-N21	1.332(8)	N20-Ag4	2.314(6)
N21-N22	1.341(7)	N21-Ag5	2.265(6)
N22-Ag6	2.255(6)	N23-O13	1.200(7)
N23-O14	1.234(8)	N24-O15	1.199(8)
N24-O16	1.227(8)	N25-N26	1.351(7)
N25-Ag5	2.325(6)	N26-N27	1.314(7)
N26-Ag4	2.518(6)	N27-N28	1.357(8)
N27-Ag2	2.244(5)	N29-O17	1.201(8)
N29-O18	1.230(9)	N30-O20	1.214(8)
N30-O19	1.217(8)	N31-N32	1.337(8)
N32-N33	1.331(8)	N32-Ag5	2.190(5)
N33-N34	1.341(8)	N33-Ag5	2.401(6)
N34-Ag4	2.341(6)	N35-O21	1.220(8)
N35-O22	1.224(8)	N36-O23	1.196(8)
N36-O24	1.231(9)	N37-N38	1.351(8)
N37-Ag6	2.423(6)	N38-N39	1.312(8)
N38-Ag7	2.252(6)	N39-N40	1.335(8)
N39-Ag8	2.273(6)	N41-O25	1.202(10)
N41-O26	1.230(10)	N42-O27	1.185(11)
N42-O28	1.212(11)	N43-N44	1.344(8)
N44-N45	1.326(8)	N44-Ag7	2.212(6)
N45-N46	1.336(7)	N45-Ag7	2.428(6)
N46-Ag8	2.396(6)	N47-O29	1.208(7)
N47-O30	1.212(7)	N48-O32	1.196(8)
N48-O31	1.218(8)	N49-N50	1.325(7)
N49-Ag7	2.375(6)	N50-N51	1.337(8)
N50-Ag8	2.401(6)	N51-N52	1.334(8)
N51-Ag9	2.227(6)	N53-O34	1.215(7)
N53-O33	1.224(7)	N54-O35	1.209(8)

N54-O36	1.213(8)	N55-N56	1.335(8)
N56-N57	1.338(8)	N56-Ag8	2.214(5)
N57-N58	1.339(7)	N57-Ag9	2.475(6)
N58-Ag10	2.284(6)	N59-O38	1.213(8)
N59-O37	1.222(8)	N60-O40	1.188(8)
N60-O39	1.221(8)	N61-N62	1.344(8)
N62-N63	1.330(8)	N62-Ag9	2.306(6)
N63-N64	1.331(8)	N63-Ag10	2.351(6)
N64-Ag11	2.191(6)	N65-O41	1.198(10)
N65-O42	1.207(11)	N66-O44	1.189(8)
N66-O43	1.205(8)	N67-N68	1.351(8)
N68-N69	1.305(8)	N68-Ag10	2.231(6)
N69-N70	1.350(7)	N69-Ag10	2.463(6)
N70-Ag9	2.347(6)	N71-O46	1.206(8)
N71-O45	1.216(8)	N72-O47	1.211(8)
N72-O48	1.225(9)	N73-Ag6	2.167(6)
N73-H73A	0.91	N73-H73B	0.91
N73-H73C	0.91	N74-Ag11	2.139(6)
N74-H74A	0.91	N74-H74B	0.91
N74-H74C	0.91	N75-Ag3	2.153(6)
N75-H75A	0.91	N75-H75B	0.91
N75-H75C	0.91	N76-Ag3	2.158(6)
N76-H76A	0.91	N76-H76B	0.91
N76-H76C	0.91	N77-Ag12	2.152(6)
N77-H77A	0.91	N77-H77B	0.91
N77-H77C	0.91	N78-Ag13	2.150(6)
N78-H78A	0.91	N78-H78B	0.91
N78-H78C	0.91	Ag1-N3	2.398(6)
Ag2-N4	2.425(6)	Ag4-N34	2.341(6)
Ag5-N33	2.402(6)	Ag7-N45	2.428(6)
Ag8-N46	2.396(6)	Ag9-N70	2.347(6)
Ag10-N69	2.463(6)	Ag11-N7	2.626(6)
Ag12-N77	2.152(6)	Ag13-N78	2.151(6)

Table S48. Bond angles (°) for $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$.

N1-C1-N4	113.2(6)	N1-C1-C2	125.0(7)
N4-C1-C2	121.8(6)	F1-C2-C1	115.3(6)
F1-C2-N5	106.9(6)	C1-C2-N5	113.1(6)
F1-C2-N6	108.3(6)	C1-C2-N6	108.7(6)
N5-C2-N6	103.9(5)	N10-C3-N7	113.8(6)
N10-C3-C4	120.9(6)	N7-C3-C4	125.3(6)
F2-C4-C3	113.3(6)	F2-C4-N12	107.3(6)
C3-C4-N12	112.7(6)	F2-C4-N11	106.4(5)
C3-C4-N11	110.0(6)	N12-C4-N11	106.7(5)
N13-C5-N16	113.5(6)	N13-C5-C6	123.6(6)
N16-C5-C6	122.9(6)	F3-C6-C5	113.2(6)
F3-C6-N17	106.3(6)	C5-C6-N17	113.4(6)
F3-C6-N18	107.8(6)	C5-C6-N18	110.0(6)
N17-C6-N18	105.6(6)	N19-C7-N22	113.1(6)
N19-C7-C8	122.8(7)	N22-C7-C8	124.1(7)
F4-C8-C7	112.6(6)	F4-C8-N24	109.3(6)
C7-C8-N24	110.6(6)	F4-C8-N23	105.7(6)
C7-C8-N23	114.2(6)	N24-C8-N23	104.0(6)
N28-C9-N25	114.6(6)	N28-C9-C10	124.5(7)
N25-C9-C10	120.8(6)	F5-C10-C9	113.5(6)
F5-C10-N30	107.9(6)	C9-C10-N30	110.4(6)
F5-C10-N29	106.6(6)	C9-C10-N29	111.9(6)
N30-C10-N29	106.1(6)	N34-C11-N31	113.8(6)
N34-C11-C12	123.6(7)	N31-C11-C12	122.5(7)
F6-C12-C11	113.7(6)	F6-C12-N35	106.0(6)
C11-C12-N35	112.6(6)	F6-C12-N36	107.2(6)
C11-C12-N36	110.2(6)	N35-C12-N36	106.8(6)
N40-C13-N37	115.1(6)	N40-C13-C14	123.2(6)
N37-C13-C14	121.6(6)	F7-C14-C13	113.9(6)
F7-C14-N41	105.8(7)	C13-C14-N41	112.9(7)
F7-C14-N42	108.5(7)	C13-C14-N42	109.1(6)
N41-C14-N42	106.2(7)	N46-C15-N43	113.2(6)
N46-C15-C16	121.9(6)	N43-C15-C16	124.8(7)
F8-C16-C15	114.3(6)	F8-C16-N48	108.6(6)
C15-C16-N48	111.6(6)	F8-C16-N47	105.8(5)
C15-C16-N47	112.0(6)	N48-C16-N47	103.9(5)
N52-C17-N49	112.4(6)	N52-C17-C18	124.4(6)
N49-C17-C18	123.2(6)	F9-C18-C17	112.5(6)
F9-C18-N53	106.2(5)	C17-C18-N53	113.6(6)
F9-C18-N54	107.8(5)	C17-C18-N54	110.1(5)
N53-C18-N54	106.3(5)	N55-C19-N58	113.4(6)
N55-C19-C20	122.1(7)	N58-C19-C20	123.9(6)
F10-C20-C19	112.4(6)	F10-C20-N60	107.6(6)
C19-C20-N60	115.3(6)	F10-C20-N59	107.7(6)
C19-C20-N59	109.5(6)	N60-C20-N59	103.9(5)
N61-C21-N64	112.2(7)	N61-C21-C22	126.9(7)
N64-C21-C22	120.9(7)	F11-C22-C21	112.8(7)
F11-C22-N66	107.7(6)	C21-C22-N66	116.5(6)

F11-C22-N65	107.2(7)	C21-C22-N65	111.0(6)
N66-C22-N65	100.5(6)	N70-C23-N67	113.9(6)
N70-C23-C24	123.2(6)	N67-C23-C24	122.9(7)
F12-C24-C23	114.2(6)	F12-C24-N71	106.7(6)
C23-C24-N71	111.2(6)	F12-C24-N72	106.6(6)
C23-C24-N72	110.4(6)	N71-C24-N72	107.3(6)
C1-N1-N2	104.0(6)	N3-N2-N1	109.8(6)
N3-N2-Ag1	123.6(4)	N1-N2-Ag1	123.9(4)
N2-N3-N4	108.6(6)	N2-N3-Ag1	129.2(4)
N4-N3-Ag1	119.2(4)	C1-N4-N3	104.4(5)
C1-N4-Ag2	138.9(4)	N3-N4-Ag2	116.8(4)
O2-N5-O1	126.5(6)	O2-N5-C2	118.4(6)
O1-N5-C2	115.1(6)	O3-N6-O4	127.2(7)
O3-N6-C2	116.7(6)	O4-N6-C2	116.1(6)
C3-N7-N8	103.3(6)	C3-N7-Ag11	142.9(5)
N8-N7-Ag11	108.1(4)	N9-N8-N7	109.8(5)
N9-N8-Ag1	120.0(4)	N7-N8-Ag1	130.1(4)
N8-N9-N10	109.5(5)	N8-N9-Ag2	122.3(4)
N10-N9-Ag2	126.7(4)	C3-N10-N9	103.5(6)
C3-N10-Ag3	135.8(5)	N9-N10-Ag3	120.6(4)
O5-N11-O6	128.3(7)	O5-N11-C4	115.8(6)
O6-N11-C4	115.9(6)	O8-N12-O7	128.3(7)
O8-N12-C4	115.7(6)	O7-N12-C4	115.9(6)
C5-N13-N14	105.3(6)	C5-N13-Ag1	132.0(5)
N14-N13-Ag1	118.6(4)	N15-N14-N13	107.6(6)
N15-N14-Ag2	127.6(4)	N13-N14-Ag2	118.6(4)
N14-N15-N16	110.7(5)	N14-N15-Ag4	123.5(4)
N16-N15-Ag4	125.5(4)	C5-N16-N15	102.8(6)
O10-N17-O9	126.8(7)	O10-N17-C6	117.0(6)
O9-N17-C6	116.2(6)	O11-N18-O12	127.5(7)
O11-N18-C6	116.0(7)	O12-N18-C6	116.4(6)
C7-N19-N20	103.8(6)	N21-N20-N19	109.6(6)
N21-N20-Ag4	118.3(4)	N19-N20-Ag4	127.5(4)
N20-N21-N22	109.6(5)	N20-N21-Ag5	125.1(4)
N22-N21-Ag5	125.2(4)	N21-N22-C7	104.0(5)
N21-N22-Ag6	115.7(4)	C7-N22-Ag6	139.7(5)
O13-N23-O14	127.6(7)	O13-N23-C8	116.6(6)
O14-N23-C8	115.9(6)	O15-N24-O16	128.3(7)
O15-N24-C8	115.6(7)	O16-N24-C8	116.0(6)
C9-N25-N26	103.9(5)	C9-N25-Ag5	135.3(5)
N26-N25-Ag5	120.8(4)	N27-N26-N25	108.4(5)
N27-N26-Ag4	130.7(4)	N25-N26-Ag4	120.8(4)
N26-N27-N28	111.0(5)	N26-N27-Ag2	121.1(4)
N28-N27-Ag2	127.9(4)	C9-N28-N27	102.1(6)
O17-N29-O18	128.2(7)	O17-N29-C10	116.9(7)
O18-N29-C10	114.8(6)	O20-N30-O19	128.2(7)
O20-N30-C10	117.4(7)	O19-N30-C10	114.4(6)
N32-N31-C11	103.2(6)	N33-N32-N31	109.9(5)
N33-N32-Ag5	122.6(4)	N31-N32-Ag5	127.3(5)

N32-N33-N34	109.3(5)	N32-N33-Ag5	118.1(4)
N34-N33-Ag5	123.9(4)	C11-N34-N33	103.8(6)
C11-N34-Ag4	138.5(5)	N33-N34-Ag4	116.7(4)
O21-N35-O22	126.0(7)	O21-N35-C12	117.9(7)
O22-N35-C12	116.1(6)	O23-N36-O24	128.2(7)
O23-N36-C12	116.0(7)	O24-N36-C12	115.7(6)
C13-N37-N38	102.1(5)	C13-N37-Ag6	138.7(5)
N38-N37-Ag6	116.8(4)	N39-N38-N37	109.2(5)
N39-N38-Ag7	121.9(5)	N37-N38-Ag7	128.4(4)
N38-N39-N40	110.4(6)	N38-N39-Ag8	120.1(4)
N40-N39-Ag8	127.2(4)	C13-N40-N39	103.2(6)
O25-N41-O26	129.0(9)	O25-N41-C14	115.8(9)
O26-N41-C14	115.2(8)	O27-N42-O28	131.7(10)
O27-N42-C14	112.2(9)	O28-N42-C14	116.1(9)
C15-N43-N44	103.3(6)	N45-N44-N43	110.1(6)
N45-N44-Ag7	119.6(4)	N43-N44-Ag7	128.9(5)
N44-N45-N46	109.0(6)	N44-N45-Ag7	124.3(4)
N46-N45-Ag7	121.5(4)	C15-N46-N45	104.4(6)
C15-N46-Ag8	134.5(5)	N45-N46-Ag8	117.5(4)
O29-N47-O30	128.0(6)	O29-N47-C16	114.8(6)
O30-N47-C16	117.2(6)	O32-N48-O31	128.2(7)
O32-N48-C16	115.6(6)	O31-N48-C16	116.2(7)
N50-N49-C17	104.7(5)	N50-N49-Ag7	121.4(4)
C17-N49-Ag7	133.9(4)	N49-N50-N51	109.3(5)
N49-N50-Ag8	117.9(4)	N51-N50-Ag8	130.5(4)
N52-N51-N50	109.0(5)	N52-N51-Ag9	125.4(4)
N50-N51-Ag9	123.6(4)	C17-N52-N51	104.6(5)
O34-N53-O33	126.7(6)	O34-N53-C18	117.1(6)
O33-N53-C18	116.2(6)	O35-N54-O36	127.8(7)
O35-N54-C18	116.4(6)	O36-N54-C18	115.7(6)
C19-N55-N56	103.9(6)	N55-N56-N57	110.1(5)
N55-N56-Ag8	124.7(4)	N57-N56-Ag8	123.3(4)
N56-N57-N58	109.0(6)	N56-N57-Ag9	129.6(4)
N58-N57-Ag9	119.4(4)	N57-N58-C19	103.6(6)
N57-N58-Ag10	118.4(4)	C19-N58-Ag10	137.9(5)
O38-N59-O37	128.9(7)	O38-N59-C20	114.6(6)
O37-N59-C20	116.3(6)	O40-N60-O39	128.6(7)
O40-N60-C20	118.5(6)	O39-N60-C20	112.8(7)
C21-N61-N62	104.9(6)	N63-N62-N61	108.6(6)
N63-N62-Ag9	117.8(4)	N61-N62-Ag9	133.0(5)
N62-N63-N64	109.8(5)	N62-N63-Ag10	120.6(4)
N64-N63-Ag10	127.6(4)	N63-N64-C21	104.5(6)
N63-N64-Ag11	118.1(4)	C21-N64-Ag11	137.4(5)
O41-N65-O42	129.2(11)	O41-N65-C22	117.2(10)
O42-N65-C22	113.6(8)	O44-N66-O43	127.3(7)
O44-N66-C22	117.8(7)	O43-N66-C22	114.9(6)
C23-N67-N68	102.1(6)	N69-N68-N67	111.1(6)
N69-N68-Ag10	123.1(5)	N67-N68-Ag10	125.2(5)
N68-N69-N70	108.9(6)	N68-N69-Ag10	125.1(4)

N70-N69-Ag10	118.0(4)	C23-N70-N69	104.0(5)
C23-N70-Ag9	139.9(5)	N69-N70-Ag9	116.1(4)
O46-N71-O45	126.2(7)	O46-N71-C24	117.4(6)
O45-N71-C24	116.4(7)	O47-N72-O48	127.6(8)
O47-N72-C24	116.9(7)	O48-N72-C24	115.5(7)
Ag6-N73-H73A	109.5	Ag6-N73-H73B	109.5
H73A-N73-H73B	109.5	Ag6-N73-H73C	109.5
H73A-N73-H73C	109.5	H73B-N73-H73C	109.5
Ag11-N74-H74A	109.5	Ag11-N74-H74B	109.5
H74A-N74-H74B	109.5	Ag11-N74-H74C	109.5
H74A-N74-H74C	109.5	H74B-N74-H74C	109.5
Ag3-N75-H75A	109.5	Ag3-N75-H75B	109.5
H75A-N75-H75B	109.5	Ag3-N75-H75C	109.5
H75A-N75-H75C	109.5	H75B-N75-H75C	109.5
Ag3-N76-H76A	109.5	Ag3-N76-H76B	109.5
H76A-N76-H76B	109.5	Ag3-N76-H76C	109.5
H76A-N76-H76C	109.5	H76B-N76-H76C	109.5
Ag12-N77-H77A	109.5	Ag12-N77-H77B	109.5
H77A-N77-H77B	109.5	Ag12-N77-H77C	109.5
H77A-N77-H77C	109.5	H77B-N77-H77C	109.5
Ag13-N78-H78A	109.5	Ag13-N78-H78B	109.5
H78A-N78-H78B	109.5	Ag13-N78-H78C	109.5
H78A-N78-H78C	109.5	H78B-N78-H78C	109.5
N2-Ag1-N8	133.9(2)	N2-Ag1-N3	107.10(19)
N8-Ag1-N3	108.8(2)	N2-Ag1-N13	114.2(2)
N8-Ag1-N13	97.1(2)	N3-Ag1-N13	84.79(19)
N27-Ag2-N9	139.5(2)	N27-Ag2-N4	104.9(2)
N9-Ag2-N4	109.4(2)	N27-Ag2-N14	108.9(2)
N9-Ag2-N14	97.0(2)	N4-Ag2-N14	81.30(19)
N75-Ag3-N76	155.6(3)	N75-Ag3-N10	100.5(2)
N76-Ag3-N10	102.6(2)	N15-Ag4-N20	125.5(2)
N15-Ag4-N34	130.8(2)	N20-Ag4-N34	100.2(2)
N15-Ag4-N26	104.56(19)	N20-Ag4-N26	96.6(2)
N34-Ag4-N26	85.09(19)	N32-Ag5-N21	126.4(2)
N32-Ag5-N25	126.1(2)	N21-Ag5-N25	94.3(2)
N32-Ag5-N33	114.0(2)	N21-Ag5-N33	96.4(2)
N25-Ag5-N33	91.1(2)	N73-Ag6-N22	145.4(2)
N73-Ag6-N37	119.0(2)	N22-Ag6-N37	95.5(2)
N44-Ag7-N38	134.0(2)	N44-Ag7-N49	111.5(2)
N38-Ag7-N49	101.8(2)	N44-Ag7-N45	114.93(19)
N38-Ag7-N45	98.9(2)	N49-Ag7-N45	84.0(2)
N56-Ag8-N39	138.3(2)	N56-Ag8-N46	110.9(2)
N39-Ag8-N46	97.3(2)	N56-Ag8-N50	107.3(2)
N39-Ag8-N50	104.0(2)	N46-Ag8-N50	87.3(2)
N51-Ag9-N62	122.6(2)	N51-Ag9-N70	130.4(2)
N62-Ag9-N70	99.8(2)	N51-Ag9-N57	105.5(2)
N62-Ag9-N57	104.1(2)	N70-Ag9-N57	85.50(19)
N68-Ag10-N58	127.5(2)	N68-Ag10-N63	123.5(2)
N58-Ag10-N63	97.8(2)	N68-Ag10-N69	108.3(2)

N58-Ag10-N69	98.2(2)	N63-Ag10-N69	94.3(2)
N74-Ag11-N64	145.9(3)	N74-Ag11-N7	117.9(2)
N64-Ag11-N7	96.1(2)	N77-Ag12-N77	180.0
N78-Ag13-N78	180.0		

Table S49. Anisotropic atomic displacement parameters (Å^2) for $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.010(4)	0.009(4)	0.020(4)	-0.004(3)	0.003(3)	0.003(3)
C2	0.016(4)	0.023(4)	0.011(4)	0.001(3)	-0.004(3)	-0.007(3)
C3	0.010(4)	0.016(4)	0.010(4)	0.000(3)	0.000(3)	-0.006(3)
C4	0.017(4)	0.021(4)	0.012(4)	-0.002(3)	0.005(3)	-0.003(3)
C5	0.012(4)	0.015(4)	0.011(4)	-0.001(3)	0.001(3)	-0.008(3)
C6	0.021(4)	0.009(4)	0.022(4)	-0.001(3)	0.009(3)	-0.005(3)
C7	0.012(4)	0.014(4)	0.015(4)	0.002(3)	-0.001(3)	-0.005(3)
C8	0.014(4)	0.026(4)	0.018(4)	0.006(3)	-0.007(3)	-0.005(3)
C9	0.013(4)	0.017(4)	0.010(4)	0.000(3)	-0.003(3)	-0.009(3)
C10	0.020(4)	0.017(4)	0.022(5)	0.001(3)	0.004(4)	0.001(3)
C11	0.020(4)	0.011(4)	0.019(4)	0.001(3)	0.005(3)	-0.008(3)
C12	0.019(4)	0.022(4)	0.017(4)	-0.005(3)	0.009(3)	-0.008(3)
C13	0.012(4)	0.017(4)	0.009(4)	0.000(3)	0.000(3)	-0.002(3)
C14	0.026(5)	0.011(4)	0.022(5)	0.004(3)	0.006(4)	0.000(3)
C15	0.012(4)	0.012(4)	0.020(4)	-0.003(3)	0.007(3)	-0.002(3)
C16	0.016(4)	0.014(4)	0.016(4)	-0.004(3)	0.004(3)	-0.006(3)
C17	0.015(4)	0.004(3)	0.018(4)	0.003(3)	0.000(3)	-0.002(3)
C18	0.013(4)	0.014(4)	0.010(4)	-0.001(3)	0.000(3)	-0.006(3)
C19	0.016(4)	0.017(4)	0.019(4)	-0.001(3)	-0.004(3)	-0.004(3)
C20	0.015(4)	0.011(4)	0.024(5)	0.001(3)	0.005(3)	-0.005(3)
C21	0.008(4)	0.013(4)	0.023(4)	0.000(3)	0.004(3)	0.000(3)
C22	0.028(5)	0.021(4)	0.019(5)	0.005(3)	-0.003(4)	-0.010(4)
C23	0.016(4)	0.005(3)	0.021(4)	0.000(3)	0.003(3)	0.000(3)
C24	0.011(4)	0.015(4)	0.021(4)	0.002(3)	0.002(3)	-0.003(3)
N1	0.015(3)	0.017(3)	0.012(3)	-0.006(3)	0.002(3)	-0.008(3)
N2	0.012(3)	0.019(3)	0.013(3)	-0.006(3)	0.006(3)	-0.004(3)
N3	0.014(3)	0.012(3)	0.015(3)	-0.003(3)	0.001(3)	-0.005(3)
N4	0.007(3)	0.017(3)	0.018(4)	0.002(3)	0.001(3)	-0.006(3)
N5	0.024(4)	0.012(3)	0.016(4)	-0.001(3)	0.007(3)	-0.009(3)
N6	0.019(4)	0.020(4)	0.013(4)	0.002(3)	0.002(3)	-0.012(3)
N7	0.020(3)	0.015(3)	0.006(3)	-0.001(2)	0.005(3)	-0.004(3)
N8	0.017(3)	0.019(3)	0.015(4)	-0.003(3)	0.000(3)	-0.006(3)
N9	0.009(3)	0.021(3)	0.014(3)	0.004(3)	0.001(3)	-0.008(3)
N10	0.011(3)	0.024(3)	0.010(3)	0.003(3)	-0.003(3)	-0.004(3)
N11	0.019(4)	0.017(4)	0.018(4)	0.005(3)	-0.001(3)	-0.003(3)
N12	0.013(3)	0.024(4)	0.020(4)	0.002(3)	0.004(3)	-0.004(3)
N13	0.007(3)	0.022(3)	0.016(3)	0.000(3)	0.001(3)	-0.006(3)
N14	0.024(4)	0.011(3)	0.016(3)	-0.005(3)	0.006(3)	-0.012(3)
N15	0.010(3)	0.015(3)	0.018(4)	-0.007(3)	0.001(3)	-0.006(3)
N16	0.010(3)	0.016(3)	0.021(4)	0.003(3)	0.001(3)	-0.003(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N17	0.017(4)	0.018(3)	0.028(4)	-0.002(3)	-0.005(3)	-0.008(3)
N18	0.015(4)	0.017(4)	0.043(5)	-0.002(4)	0.001(3)	-0.006(3)
N19	0.011(3)	0.016(3)	0.016(4)	-0.001(3)	-0.005(3)	0.001(3)
N20	0.017(3)	0.017(3)	0.016(4)	-0.007(3)	-0.001(3)	-0.007(3)
N21	0.015(3)	0.012(3)	0.013(3)	0.002(3)	-0.001(3)	-0.007(3)
N22	0.014(3)	0.015(3)	0.013(3)	0.002(3)	-0.002(3)	-0.007(3)
N23	0.017(4)	0.030(4)	0.017(4)	-0.007(3)	0.001(3)	-0.005(3)
N24	0.023(4)	0.031(4)	0.020(4)	-0.002(3)	-0.004(3)	-0.011(3)
N25	0.006(3)	0.019(3)	0.014(3)	0.003(3)	0.000(2)	-0.006(3)
N26	0.010(3)	0.018(3)	0.017(3)	0.001(3)	0.004(3)	-0.011(3)
N27	0.011(3)	0.009(3)	0.013(3)	0.003(2)	0.002(2)	-0.006(2)
N28	0.011(3)	0.018(3)	0.017(4)	0.001(3)	0.000(3)	-0.005(3)
N29	0.019(4)	0.029(4)	0.032(5)	0.011(3)	0.012(3)	0.003(3)
N30	0.017(4)	0.017(4)	0.026(4)	0.006(3)	0.007(3)	-0.001(3)
N31	0.019(4)	0.026(4)	0.014(4)	-0.007(3)	0.000(3)	-0.010(3)
N32	0.011(3)	0.020(3)	0.014(3)	0.000(2)	0.001(2)	-0.011(2)
N33	0.015(3)	0.015(3)	0.018(4)	-0.002(3)	0.005(3)	-0.010(3)
N34	0.011(3)	0.015(3)	0.015(3)	-0.001(3)	0.001(3)	-0.001(3)
N35	0.027(3)	0.038(3)	0.013(3)	0.000(3)	0.003(3)	-0.015(3)
N36	0.024(4)	0.040(5)	0.011(4)	-0.006(3)	0.006(3)	-0.020(4)
N37	0.015(3)	0.016(3)	0.011(3)	-0.001(3)	0.000(3)	-0.008(3)
N38	0.015(3)	0.012(3)	0.020(4)	-0.003(3)	0.001(3)	-0.005(3)
N39	0.015(3)	0.018(3)	0.013(3)	-0.005(3)	0.000(3)	-0.004(3)
N40	0.013(3)	0.015(3)	0.016(3)	-0.005(3)	0.007(3)	-0.006(3)
N41	0.028(5)	0.056(6)	0.051(6)	-0.012(5)	0.016(4)	0.010(4)
N42	0.055(4)	0.052(4)	0.032(4)	-0.011(3)	0.016(3)	-0.013(4)
N43	0.019(3)	0.020(3)	0.014(3)	-0.002(3)	-0.002(3)	-0.010(3)
N44	0.019(3)	0.017(3)	0.015(3)	0.006(3)	-0.006(3)	-0.010(3)
N45	0.015(3)	0.011(3)	0.020(3)	0.002(2)	-0.001(2)	-0.009(2)
N46	0.020(3)	0.014(3)	0.018(4)	-0.001(3)	-0.006(3)	-0.009(3)
N47	0.017(3)	0.023(4)	0.006(3)	-0.003(3)	0.003(3)	-0.007(3)
N48	0.012(3)	0.029(4)	0.024(4)	0.012(3)	-0.004(3)	-0.015(3)
N49	0.010(3)	0.012(3)	0.021(4)	-0.005(3)	0.001(3)	-0.006(3)
N50	0.015(3)	0.010(3)	0.022(3)	-0.003(2)	0.001(2)	-0.010(2)
N51	0.012(3)	0.011(3)	0.024(4)	0.002(3)	-0.004(3)	-0.004(3)
N52	0.005(3)	0.008(3)	0.024(4)	-0.004(3)	-0.001(3)	-0.001(2)
N53	0.020(3)	0.011(3)	0.009(3)	0.005(3)	0.004(3)	0.002(3)
N54	0.015(3)	0.013(3)	0.029(4)	-0.003(3)	0.004(3)	-0.004(3)
N55	0.014(3)	0.012(3)	0.015(3)	-0.002(3)	0.002(3)	-0.005(3)
N56	0.007(3)	0.011(3)	0.018(4)	-0.003(3)	0.001(3)	-0.005(2)
N57	0.013(3)	0.014(3)	0.017(4)	0.000(3)	0.003(3)	-0.009(3)
N58	0.016(3)	0.011(3)	0.020(4)	0.001(3)	0.000(3)	-0.011(3)
N59	0.027(4)	0.012(3)	0.027(4)	0.003(3)	-0.002(3)	-0.004(3)
N60	0.037(4)	0.014(3)	0.019(4)	-0.001(3)	0.005(3)	-0.007(3)
N61	0.026(4)	0.014(3)	0.016(4)	0.000(3)	-0.002(3)	-0.005(3)
N62	0.015(3)	0.017(3)	0.016(4)	-0.005(3)	0.001(3)	-0.001(3)
N63	0.021(4)	0.014(3)	0.015(4)	-0.003(3)	0.000(3)	-0.007(3)
N64	0.013(3)	0.018(3)	0.011(3)	-0.003(3)	-0.004(3)	-0.007(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N65	0.030(5)	0.087(8)	0.044(6)	-0.038(5)	0.014(4)	-0.024(5)
N66	0.024(4)	0.032(4)	0.023(4)	-0.004(3)	0.000(3)	-0.013(3)
N67	0.023(4)	0.021(3)	0.015(4)	0.003(3)	0.005(3)	-0.011(3)
N68	0.016(3)	0.019(3)	0.020(4)	0.000(3)	-0.001(3)	-0.010(3)
N69	0.015(3)	0.012(3)	0.017(4)	0.000(3)	0.006(3)	-0.006(3)
N70	0.011(3)	0.008(3)	0.020(4)	0.000(3)	0.005(3)	-0.005(2)
N71	0.025(4)	0.037(4)	0.006(3)	-0.001(3)	0.006(3)	-0.012(4)
N72	0.032(3)	0.024(3)	0.022(3)	0.003(3)	0.004(3)	-0.018(3)
N73	0.031(4)	0.036(4)	0.012(4)	-0.003(3)	-0.002(3)	-0.003(3)
N74	0.027(4)	0.031(4)	0.039(5)	-0.010(3)	-0.010(3)	0.003(3)
N75	0.027(4)	0.041(4)	0.034(4)	-0.019(4)	0.010(3)	-0.023(3)
N76	0.020(4)	0.022(4)	0.028(4)	-0.001(3)	0.005(3)	0.000(3)
N77	0.032(4)	0.028(4)	0.023(4)	-0.007(3)	-0.001(3)	-0.002(3)
N78	0.028(4)	0.021(4)	0.027(4)	-0.002(3)	-0.008(3)	-0.004(3)
O1	0.034(3)	0.028(3)	0.024(3)	-0.007(2)	0.006(3)	-0.023(3)
O2	0.029(4)	0.018(3)	0.052(4)	-0.010(3)	0.017(3)	0.000(3)
O3	0.037(4)	0.029(3)	0.030(4)	-0.013(3)	0.012(3)	-0.011(3)
O4	0.028(3)	0.039(4)	0.018(3)	0.000(3)	-0.002(3)	-0.015(3)
O5	0.014(3)	0.045(4)	0.037(4)	-0.012(3)	0.016(3)	-0.008(3)
O6	0.016(3)	0.028(3)	0.038(4)	0.002(3)	-0.001(3)	-0.008(3)
O7	0.016(3)	0.032(3)	0.021(3)	0.001(2)	-0.006(2)	-0.011(2)
O8	0.026(3)	0.021(3)	0.020(3)	-0.005(2)	0.002(2)	0.002(2)
O9	0.018(3)	0.027(3)	0.063(5)	-0.003(3)	-0.010(3)	-0.006(3)
O10	0.027(3)	0.030(3)	0.019(3)	-0.005(2)	0.000(3)	-0.014(3)
O11	0.042(4)	0.034(4)	0.057(5)	-0.022(3)	0.000(3)	0.013(3)
O12	0.040(4)	0.026(3)	0.038(4)	0.007(3)	0.000(3)	-0.004(3)
O13	0.023(3)	0.043(4)	0.015(3)	-0.007(3)	-0.007(3)	-0.003(3)
O14	0.057(4)	0.024(3)	0.031(4)	0.001(3)	-0.016(3)	0.001(3)
O15	0.046(4)	0.020(3)	0.033(4)	0.004(3)	-0.012(3)	-0.010(3)
O16	0.024(3)	0.053(4)	0.022(4)	-0.001(3)	0.007(3)	-0.008(3)
O17	0.023(3)	0.045(4)	0.051(4)	0.025(3)	0.005(3)	-0.009(3)
O18	0.042(4)	0.042(4)	0.017(3)	-0.005(3)	0.007(3)	-0.011(3)
O19	0.040(4)	0.032(3)	0.022(3)	0.009(3)	0.001(3)	0.002(3)
O20	0.029(3)	0.023(3)	0.047(4)	-0.011(3)	-0.004(3)	-0.002(3)
O21	0.025(4)	0.062(4)	0.037(4)	-0.002(3)	0.001(3)	-0.028(3)
O22	0.052(4)	0.025(3)	0.042(4)	-0.002(3)	0.009(3)	-0.017(3)
O23	0.056(4)	0.037(4)	0.030(4)	-0.014(3)	0.006(3)	-0.021(3)
O24	0.030(4)	0.051(4)	0.034(4)	0.002(3)	-0.002(3)	-0.002(3)
O25	0.061(6)	0.161(10)	0.065(6)	-0.001(6)	0.042(5)	0.012(6)
O26	0.043(5)	0.065(5)	0.054(5)	-0.009(4)	0.005(4)	0.014(4)
O27	0.062(5)	0.123(6)	0.056(5)	-0.040(5)	0.007(4)	-0.037(5)
O28	0.112(6)	0.040(4)	0.059(5)	-0.016(4)	0.037(4)	-0.020(4)
O29	0.028(3)	0.025(3)	0.017(3)	0.002(2)	0.003(2)	-0.017(3)
O30	0.018(3)	0.020(3)	0.031(3)	-0.004(2)	0.001(2)	-0.002(2)
O31	0.022(3)	0.065(5)	0.037(4)	0.025(3)	0.002(3)	0.003(3)
O32	0.036(4)	0.042(4)	0.017(3)	-0.006(3)	0.002(3)	-0.018(3)
O33	0.027(3)	0.015(3)	0.035(4)	0.002(2)	0.001(3)	-0.006(2)
O34	0.054(4)	0.026(3)	0.013(3)	-0.001(2)	0.002(3)	-0.010(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O35	0.030(3)	0.035(3)	0.020(3)	-0.007(3)	0.008(3)	-0.008(3)
O36	0.023(3)	0.030(3)	0.037(4)	0.003(3)	-0.002(3)	0.003(3)
O37	0.041(4)	0.033(4)	0.039(4)	0.003(3)	-0.026(3)	-0.007(3)
O38	0.030(3)	0.028(3)	0.017(3)	0.000(2)	0.005(3)	-0.005(3)
O39	0.079(5)	0.014(3)	0.029(4)	0.005(3)	-0.006(3)	-0.020(3)
O40	0.026(3)	0.015(3)	0.029(3)	-0.005(2)	0.002(3)	-0.015(2)
O41	0.048(4)	0.114(6)	0.084(6)	-0.057(5)	0.028(4)	-0.036(4)
O42	0.049(5)	0.080(5)	0.069(5)	-0.019(4)	-0.011(4)	0.017(4)
O43	0.063(5)	0.043(4)	0.026(4)	-0.013(3)	0.015(3)	-0.016(3)
O44	0.076(5)	0.083(6)	0.031(4)	-0.026(4)	0.018(4)	-0.062(5)
O45	0.035(4)	0.027(3)	0.037(4)	-0.006(3)	0.004(3)	-0.023(3)
O46	0.021(3)	0.031(4)	0.055(5)	0.005(3)	0.008(3)	0.002(3)
O47	0.038(4)	0.054(4)	0.031(4)	0.007(3)	-0.011(3)	-0.012(3)
O48	0.061(5)	0.037(4)	0.017(3)	-0.007(3)	0.011(3)	-0.011(3)
F1	0.012(2)	0.029(2)	0.018(2)	-0.0045(19)	0.0023(18)	-0.0065(19)
F2	0.030(3)	0.018(2)	0.018(2)	-0.0056(19)	-0.001(2)	-0.009(2)
F3	0.018(2)	0.032(3)	0.027(3)	0.003(2)	0.008(2)	-0.009(2)
F4	0.019(2)	0.030(3)	0.026(3)	-0.004(2)	-0.008(2)	0.006(2)
F5	0.014(2)	0.023(2)	0.041(3)	-0.002(2)	0.000(2)	-0.011(2)
F6	0.018(3)	0.041(3)	0.036(3)	0.006(2)	0.006(2)	-0.003(2)
F7	0.059(4)	0.034(3)	0.025(3)	0.006(2)	0.016(3)	0.001(3)
F8	0.024(3)	0.014(2)	0.038(3)	-0.007(2)	0.009(2)	-0.0076(19)
F9	0.018(2)	0.018(2)	0.019(2)	-0.0035(18)	-0.0035(19)	-0.0027(18)
F10	0.017(2)	0.020(2)	0.047(3)	0.003(2)	0.009(2)	0.006(2)
F11	0.080(4)	0.031(3)	0.020(3)	-0.006(2)	0.018(3)	-0.017(3)
F12	0.028(3)	0.016(2)	0.040(3)	0.002(2)	0.005(2)	0.000(2)
Ag1	0.0125(3)	0.0197(3)	0.0149(3)	-0.0001(2)	-0.0002(2)	-0.0102(2)
Ag2	0.0107(3)	0.0176(3)	0.0166(3)	0.0029(2)	0.0000(2)	-0.0075(2)
Ag3	0.0267(4)	0.0242(3)	0.0229(4)	-0.0051(3)	0.0061(3)	-0.0069(3)
Ag4	0.0128(3)	0.0194(3)	0.0162(3)	-0.0006(2)	0.0011(2)	-0.0093(2)
Ag5	0.0112(3)	0.0184(3)	0.0145(3)	0.0004(2)	0.0000(2)	-0.0093(2)
Ag6	0.0202(3)	0.0263(3)	0.0182(3)	0.0003(3)	0.0028(3)	-0.0008(3)
Ag7	0.0180(3)	0.0133(3)	0.0162(3)	-0.0029(2)	0.0032(2)	-0.0093(2)
Ag8	0.0171(3)	0.0120(3)	0.0149(3)	-0.0018(2)	0.0038(2)	-0.0088(2)
Ag9	0.0168(3)	0.0137(3)	0.0197(3)	-0.0008(2)	0.0020(2)	-0.0096(2)
Ag10	0.0156(3)	0.0132(3)	0.0208(3)	-0.0008(2)	0.0035(2)	-0.0089(2)
Ag11	0.0720(6)	0.0264(4)	0.0302(4)	0.0107(3)	0.0129(4)	0.0114(4)
Ag12	0.0234(5)	0.0151(4)	0.0356(6)	-0.0011(4)	0.0013(4)	-0.0042(4)
Ag13	0.0167(4)	0.0211(4)	0.0298(5)	-0.0044(4)	0.0011(4)	-0.0073(4)

Table S50. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for $C_{24}H_{18}Ag_{12}F_{12}N_{78}O_{48}$.

	x/a	y/b	z/c	U(eq)
H73A	0.5892	0.3397	0.2056	0.04
H73B	0.5937	0.3077	0.2769	0.04
H73C	0.6406	0.3827	0.2494	0.04
H74A	0.8445	1.1293	-0.2433	0.048
H74B	0.8350	1.0944	-0.3066	0.048

	x/a	y/b	z/c	U(eq)
H74C	0.9083	1.1454	-0.2979	0.048
H75A	0.4445	0.1409	0.8179	0.047
H75B	0.4093	0.0603	0.8494	0.047
H75C	0.3487	0.1372	0.8206	0.047
H76A	0.4573	-0.0537	0.6368	0.036
H76B	0.5349	-0.0096	0.6473	0.036
H76C	0.4642	0.0363	0.6034	0.036
H77A	-0.0152	0.5659	0.3773	0.041
H77B	-0.0135	0.4692	0.3793	0.041
H77C	0.0694	0.5078	0.3826	0.041
H78A	0.0043	0.4244	0.1206	0.038
H78B	-0.0553	0.5079	0.1203	0.038
H78C	0.0409	0.5088	0.1207	0.038

Crystal Structure Report for $C_{26}H_{20}FN_6O_4P$

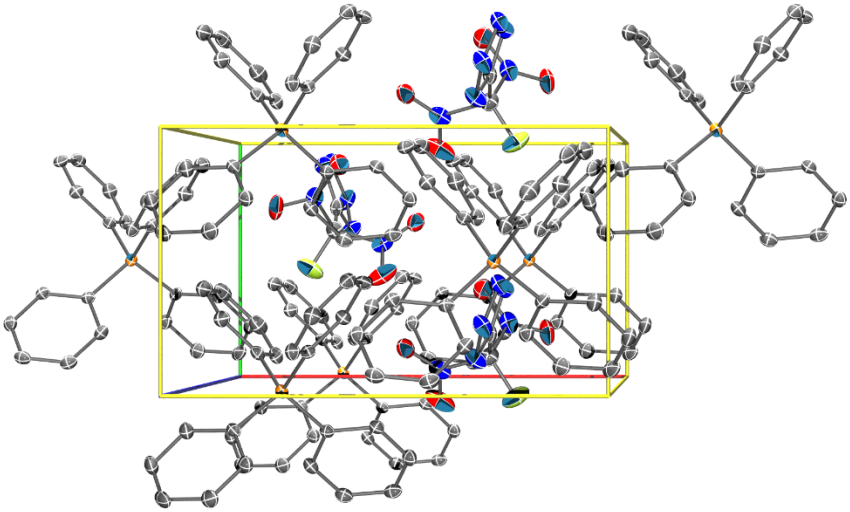

Figure S22. Packing diagram for the crystal structure of $C_{26}H_{20}FN_6O_4P$. View along the 001 direction

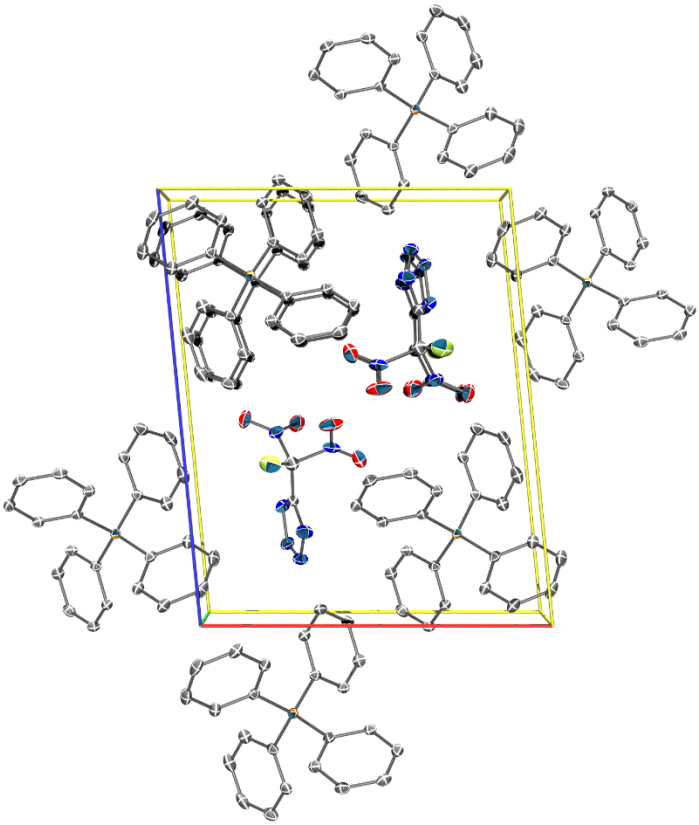

Figure S23. Packing diagram for the crystal structure of $C_{26}H_{20}FN_6O_4P$. View along the 010 direction

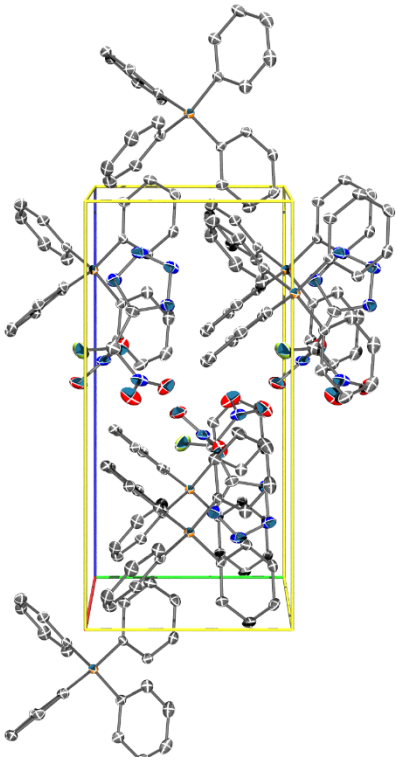

Figure S24. Packing diagram for the crystal structure of $C_{26}H_{20}FN_6O_4P$. View along the 100 direction

Table S51. Sample and crystal data for $C_{26}H_{20}FN_6O_4P$.

Identification code	TPPFDNTz	
Chemical formula	$C_{26}H_{20}FN_6O_4P$	
Formula weight	530.45 g/mol	
Temperature	101(2) K	
Wavelength	0.71073 Å	
Crystal size	0.060 x 0.170 x 0.490 mm	
Crystal habit	clear colourless rod	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 11.8077(14) Å	α = 90°
	b = 7.1276(8) Å	β = 95.585(2)°
	c = 14.7721(18) Å	γ = 90°
Volume	1237.3(3) $Å^3$	
Z	2	
Density (calculated)	1.424 g/cm^3	
Absorption coefficient	0.165 mm^{-1}	
F(000)	548	

Table S52. Data collection and structure refinement for $C_{26}H_{20}FN_6O_4P$.

Diffractometer	Bruker APEX DUO
Radiation source	fine-focus tube, MoKα
Theta range for data collection	1.73 to 30.54°
Index ranges	-16<=h<=16, -10<=k<=10, -20<=l<=20
Reflections collected	26729
Independent reflections	7495 [R(int) = 0.0451]
Absorption correction	multi-scan
Max. and min. transmission	0.9900 and 0.9240
Structure solution technique	direct methods
Structure solution program	SHELXTL XT 2014/4 (Bruker AXS, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXTL XL 2014/6 (Bruker AXS, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	7495 / 1 / 343
Goodness-of-fit on F^2	1.023
Final R indices	5985 data; I>2σ(I) R1 = 0.0435, wR2 = 0.0916
	all data R1 = 0.0660, wR2 = 0.1005
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0466P)^2+0.2111P]$ where $P=(F_o^2+2F_c^2)/3$
Absolute structure parameter	0.0(0)
Largest diff. peak and hole	0.488 and -0.292 eÅ^{-3}
R.M.S. deviation from mean	0.056 eÅ^{-3}

Table S53. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for $C_{26}H_{20}FN_6O_4P$.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
C1	0.2895(2)	0.7197(4)	0.27514(17)	0.0206(5)
C2	0.2976(3)	0.6241(4)	0.36416(19)	0.0270(6)
C3	0.6647(2)	0.3444(3)	0.24807(16)	0.0147(5)
C4	0.7107(2)	0.2030(4)	0.30569(17)	0.0187(5)
C5	0.6394(2)	0.0831(4)	0.34731(17)	0.0200(5)
C6	0.5218(2)	0.1014(4)	0.33023(17)	0.0201(5)
C7	0.4762(2)	0.2392(4)	0.27128(17)	0.0193(5)
C8	0.5468(2)	0.3625(4)	0.23034(16)	0.0162(5)
C9	0.8637(2)	0.3581(4)	0.14949(17)	0.0162(5)
C10	0.8234(2)	0.2380(4)	0.07869(17)	0.0197(5)
C11	0.8979(2)	0.1136(4)	0.04293(19)	0.0235(6)
C12	0.0110(2)	0.1061(4)	0.0785(2)	0.0260(6)
C13	0.0513(2)	0.2252(4)	0.1489(2)	0.0259(6)
C14	0.9781(2)	0.3526(4)	0.18422(18)	0.0214(6)
C15	0.8323(2)	0.6430(4)	0.28911(16)	0.0163(5)
C16	0.8047(2)	0.6279(4)	0.37887(17)	0.0194(5)
C17	0.8582(3)	0.7451(4)	0.44523(18)	0.0261(6)
C18	0.9381(2)	0.8756(4)	0.4229(2)	0.0277(6)
C19	0.9654(2)	0.8909(4)	0.3335(2)	0.0276(6)
C20	0.9118(2)	0.7763(4)	0.26629(19)	0.0228(6)
C21	0.6892(2)	0.6579(3)	0.11995(16)	0.0150(5)

	x/a	y/b	z/c	U(eq)
C22	0.7097(2)	0.6637(4)	0.02829(17)	0.0178(5)
C23	0.6567(2)	0.7992(4)	0.97178(17)	0.0208(6)
C24	0.5825(2)	0.9272(4)	0.00530(18)	0.0202(5)
C25	0.5596(2)	0.9192(4)	0.09604(17)	0.0194(5)
C26	0.6132(2)	0.7868(4)	0.15342(17)	0.0174(5)
F1	0.23655(19)	0.4658(3)	0.36487(13)	0.0455(6)
N1	0.3149(2)	0.6265(4)	0.20131(17)	0.0315(6)
N2	0.2939(2)	0.7541(4)	0.13452(15)	0.0290(6)
N3	0.2579(2)	0.9110(4)	0.16813(16)	0.0264(5)
N4	0.2544(2)	0.8930(4)	0.25860(16)	0.0264(5)
N5	0.4195(2)	0.5704(4)	0.40249(15)	0.0281(6)
N6	0.2590(2)	0.7542(4)	0.43795(16)	0.0299(6)
O1	0.49759(19)	0.6562(3)	0.37486(15)	0.0331(5)
O2	0.4252(2)	0.4430(4)	0.45776(15)	0.0465(7)
O3	0.32180(19)	0.8856(4)	0.45835(15)	0.0365(5)
O4	0.17022(19)	0.7144(4)	0.46911(16)	0.0399(6)
P1	0.76191(5)	0.50104(9)	0.20038(4)	0.01387(13)

Table S54. Bond lengths (Å) for $C_{26}H_{20}FN_6O_4P$.

C1-N4	1.319(4)	C1-N1	1.335(4)
C1-C2	1.476(4)	C2-F1	1.339(4)
C2-N6	1.534(4)	C2-N5	1.543(4)
C3-C4	1.395(3)	C3-C8	1.398(4)
C3-P1	1.793(3)	C4-C5	1.385(4)
C4-H4	0.95	C5-C6	1.394(4)
C5-H5	0.95	C6-C7	1.386(4)
C6-H6	0.95	C7-C8	1.390(3)
C7-H7	0.95	C8-H8	0.95
C9-C14	1.398(4)	C9-C10	1.399(4)
C9-P1	1.796(3)	C10-C11	1.389(4)
C10-H10	0.95	C11-C12	1.388(4)
C11-H11	0.95	C12-C13	1.390(4)
C12-H12	0.95	C13-C14	1.389(4)
C13-H13	0.95	C14-H14	0.95
C15-C16	1.400(3)	C15-C20	1.400(4)
C15-P1	1.794(3)	C16-C17	1.392(4)
C16-H16	0.95	C17-C18	1.387(5)
C17-H17	0.95	C18-C19	1.394(4)
C18-H18	0.95	C19-C20	1.390(4)
C19-H19	0.95	C20-H20	0.95
C21-C22	1.399(3)	C21-C26	1.407(3)
C21-P1	1.789(3)	C22-C23	1.385(4)
C22-H22	0.95	C23-C24	1.389(4)
C23-H23	0.95	C24-C25	1.394(4)
C24-H24	0.95	C25-C26	1.381(4)
C25-H25	0.95	C26-H26	0.95
N1-N2	1.347(4)	N2-N3	1.311(4)

N3-N4	1.347(3)	N5-O1	1.210(3)
N5-O2	1.218(3)	N6-O3	1.214(4)
N6-O4	1.219(3)		

Table S55. Bond angles (°) for $C_{26}H_{20}FN_6O_4P$.

N4-C1-N1	113.9(2)	N4-C1-C2	126.1(3)
N1-C1-C2	119.9(3)	F1-C2-C1	114.1(2)
F1-C2-N6	107.8(2)	C1-C2-N6	110.9(2)
F1-C2-N5	105.8(2)	C1-C2-N5	114.7(2)
N6-C2-N5	102.7(2)	C4-C3-C8	120.2(2)
C4-C3-P1	117.6(2)	C8-C3-P1	122.20(19)
C5-C4-C3	120.0(2)	C5-C4-H4	120.0
C3-C4-H4	120.0	C4-C5-C6	120.0(2)
C4-C5-H5	120.0	C6-C5-H5	120.0
C7-C6-C5	119.9(2)	C7-C6-H6	120.0
C5-C6-H6	120.0	C6-C7-C8	120.6(2)
C6-C7-H7	119.7	C8-C7-H7	119.7
C7-C8-C3	119.3(2)	C7-C8-H8	120.4
C3-C8-H8	120.4	C14-C9-C10	120.2(2)
C14-C9-P1	121.6(2)	C10-C9-P1	117.9(2)
C11-C10-C9	119.6(3)	C11-C10-H10	120.2
C9-C10-H10	120.2	C12-C11-C10	120.1(3)
C12-C11-H11	119.9	C10-C11-H11	119.9
C11-C12-C13	120.4(3)	C11-C12-H12	119.8
C13-C12-H12	119.8	C14-C13-C12	120.0(3)
C14-C13-H13	120.0	C12-C13-H13	120.0
C13-C14-C9	119.6(3)	C13-C14-H14	120.2
C9-C14-H14	120.2	C16-C15-C20	120.2(2)
C16-C15-P1	121.0(2)	C20-C15-P1	118.71(19)
C17-C16-C15	119.3(3)	C17-C16-H16	120.3
C15-C16-H16	120.3	C18-C17-C16	120.5(3)
C18-C17-H17	119.7	C16-C17-H17	119.7
C17-C18-C19	120.2(3)	C17-C18-H18	119.9
C19-C18-H18	119.9	C20-C19-C18	120.0(3)
C20-C19-H19	120.0	C18-C19-H19	120.0
C19-C20-C15	119.7(3)	C19-C20-H20	120.1
C15-C20-H20	120.1	C22-C21-C26	119.8(2)
C22-C21-P1	123.0(2)	C26-C21-P1	117.12(18)
C23-C22-C21	119.6(2)	C23-C22-H22	120.2
C21-C22-H22	120.2	C22-C23-C24	120.4(2)
C22-C23-H23	119.8	C24-C23-H23	119.8
C23-C24-C25	120.3(2)	C23-C24-H24	119.9
C25-C24-H24	119.9	C26-C25-C24	119.8(2)
C26-C25-H25	120.1	C24-C25-H25	120.1
C25-C26-C21	120.0(2)	C25-C26-H26	120.0
C21-C26-H26	120.0	C1-N1-N2	102.9(2)
N3-N2-N1	110.0(2)	N2-N3-N4	109.7(2)
C1-N4-N3	103.5(2)	O1-N5-O2	127.5(3)

O1-N5-C2	117.7(2)	O2-N5-C2	114.8(3)
O3-N6-O4	127.8(3)	O3-N6-C2	115.2(2)
O4-N6-C2	117.0(3)	C21-P1-C3	111.48(12)
C21-P1-C15	106.91(12)	C3-P1-C15	109.41(12)
C21-P1-C9	111.97(11)	C3-P1-C9	106.93(12)
C15-P1-C9	110.15(13)		

Table S56. Anisotropic atomic displacement parameters (Å^2) for $C_{26}H_{20}FN_6O_4P$.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0160(13)	0.0281(15)	0.0175(12)	0.0043(11)	0.0004(10)	0.0011(11)
C2	0.0270(15)	0.0297(16)	0.0242(14)	0.0023(12)	0.0021(11)	-0.0022(12)
C3	0.0174(12)	0.0139(12)	0.0131(11)	-0.0005(9)	0.0032(9)	0.0008(9)
C4	0.0183(13)	0.0199(14)	0.0180(12)	0.0007(10)	0.0023(10)	0.0052(10)
C5	0.0263(15)	0.0176(13)	0.0162(12)	0.0013(10)	0.0032(10)	0.0033(11)
C6	0.0269(14)	0.0165(14)	0.0179(12)	-0.0004(10)	0.0074(10)	-0.0026(11)
C7	0.0172(13)	0.0220(14)	0.0191(12)	-0.0020(11)	0.0046(10)	0.0008(10)
C8	0.0180(13)	0.0156(12)	0.0151(11)	0.0008(9)	0.0019(9)	0.0025(10)
C9	0.0165(12)	0.0162(12)	0.0164(11)	0.0033(10)	0.0047(9)	0.0032(10)
C10	0.0171(13)	0.0218(14)	0.0211(12)	0.0000(11)	0.0055(10)	0.0013(10)
C11	0.0240(14)	0.0243(15)	0.0240(13)	-0.0024(11)	0.0103(11)	0.0002(11)
C12	0.0238(15)	0.0218(15)	0.0351(15)	0.0017(12)	0.0169(12)	0.0057(11)
C13	0.0162(13)	0.0273(15)	0.0347(15)	0.0025(13)	0.0054(11)	0.0050(11)
C14	0.0168(13)	0.0230(14)	0.0245(13)	0.0002(11)	0.0031(10)	0.0015(11)
C15	0.0165(12)	0.0165(13)	0.0155(11)	-0.0009(10)	-0.0010(9)	0.0038(10)
C16	0.0160(13)	0.0226(14)	0.0193(12)	-0.0011(11)	-0.0008(9)	0.0037(11)
C17	0.0268(15)	0.0300(16)	0.0203(13)	-0.0077(12)	-0.0031(11)	0.0071(12)
C18	0.0208(14)	0.0261(16)	0.0334(15)	-0.0110(13)	-0.0111(12)	0.0071(12)
C19	0.0202(15)	0.0221(15)	0.0391(16)	-0.0022(13)	-0.0052(12)	-0.0003(12)
C20	0.0206(14)	0.0215(14)	0.0257(13)	0.0004(11)	-0.0001(11)	0.0001(11)
C21	0.0169(12)	0.0144(12)	0.0137(11)	0.0017(9)	0.0016(9)	-0.0012(9)
C22	0.0166(13)	0.0219(14)	0.0154(11)	0.0012(10)	0.0034(9)	0.0001(10)
C23	0.0214(14)	0.0261(14)	0.0148(11)	0.0028(10)	0.0019(10)	-0.0014(11)
C24	0.0210(14)	0.0184(13)	0.0201(12)	0.0050(10)	-0.0038(10)	-0.0017(10)
C25	0.0208(14)	0.0146(12)	0.0230(13)	-0.0027(10)	0.0022(10)	0.0023(10)
C26	0.0189(13)	0.0180(13)	0.0154(11)	-0.0006(10)	0.0014(10)	0.0013(10)
F1	0.0603(14)	0.0373(12)	0.0383(10)	0.0090(9)	0.0008(9)	-0.0216(10)
N1	0.0372(15)	0.0320(15)	0.0245(12)	0.0006(11)	-0.0011(10)	0.0127(12)
N2	0.0292(14)	0.0397(15)	0.0177(11)	0.0031(11)	0.0002(10)	0.0116(12)
N3	0.0257(13)	0.0322(14)	0.0221(11)	0.0067(11)	0.0068(9)	0.0073(11)
N4	0.0303(14)	0.0269(14)	0.0231(12)	0.0015(10)	0.0083(10)	0.0029(11)
N5	0.0395(16)	0.0301(14)	0.0137(11)	-0.0010(9)	-0.0024(10)	0.0085(12)
N6	0.0292(14)	0.0406(16)	0.0207(12)	0.0059(11)	0.0066(10)	0.0050(12)
O1	0.0255(11)	0.0323(13)	0.0399(12)	-0.0070(10)	-0.0056(9)	0.0035(10)
O2	0.076(2)	0.0425(15)	0.0228(11)	0.0110(10)	0.0135(11)	0.0283(13)
O3	0.0336(13)	0.0384(14)	0.0388(12)	-0.0149(11)	0.0103(10)	-0.0024(11)
O4	0.0209(11)	0.0566(16)	0.0438(13)	0.0164(12)	0.0117(10)	0.0073(11)
P1	0.0132(3)	0.0154(3)	0.0132(3)	0.0005(3)	0.0018(2)	0.0019(3)

Table S57. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for $C_{26}H_{20}FN_6O_4P$.

	x/a	y/b	z/c	U(eq)
H4	0.7909	0.1888	0.3164	0.022
H5	0.6707	-0.0116	0.3875	0.024
H6	0.4729	0.0194	0.3590	0.024
H7	0.3960	0.2494	0.2587	0.023
H8	0.5153	0.4581	0.1907	0.019
H10	0.7456	0.2414	0.0552	0.024
H11	0.8714	0.0335	-0.0060	0.028
H12	1.0612	0.0190	0.0546	0.031
H13	1.1288	0.2195	0.1729	0.031
H14	1.0057	0.4356	0.2317	0.026
H16	0.7500	0.5386	0.3943	0.023
H17	0.8399	0.7357	0.5063	0.031
H18	0.9744	0.9548	0.4687	0.033
H19	1.0206	0.9796	0.3185	0.033
H20	0.9291	0.7884	0.2051	0.027
H22	0.7596	0.5752	0.0050	0.021
H23	0.6712	0.8046	-0.0903	0.025
H24	0.5472	1.0205	-0.0338	0.024
H25	0.5072	1.0047	0.1183	0.023
H26	0.5988	0.7826	0.2155	0.021