Synthesis and Characterization of Energetic Bis(3,5-dinitro-1*H*-1,2,4-triazolyl)dihydro- and dichloroborates, Bis(5-nitro-2*H*-tetrazolyl)-, Bis(5-trinitromethyl-2*H*-tetrazolyl)-, and Bis(5-fluorodinitromethyl-2*H*-tetrazolyl)dihydroborate

Ralf Haiges, C. Bigler Jones(†), and Karl O. Christe**

Supporting Information

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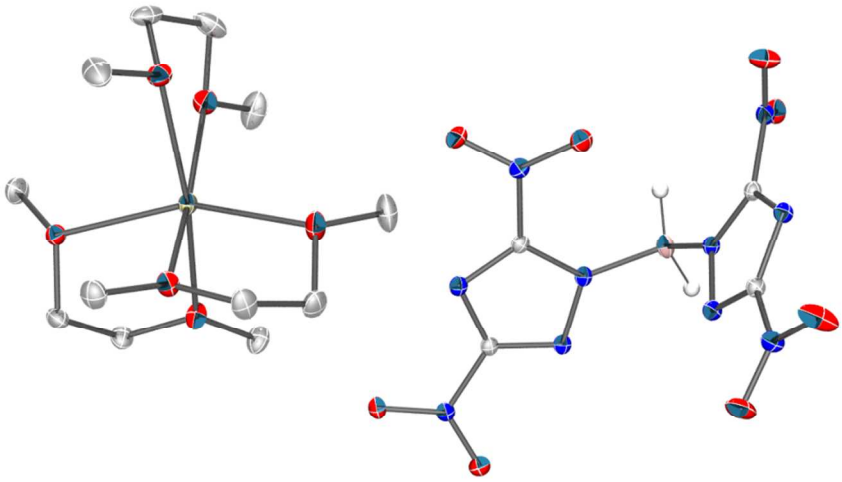

Figure S1: Asymmetric unit in the crystal structure of $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**.

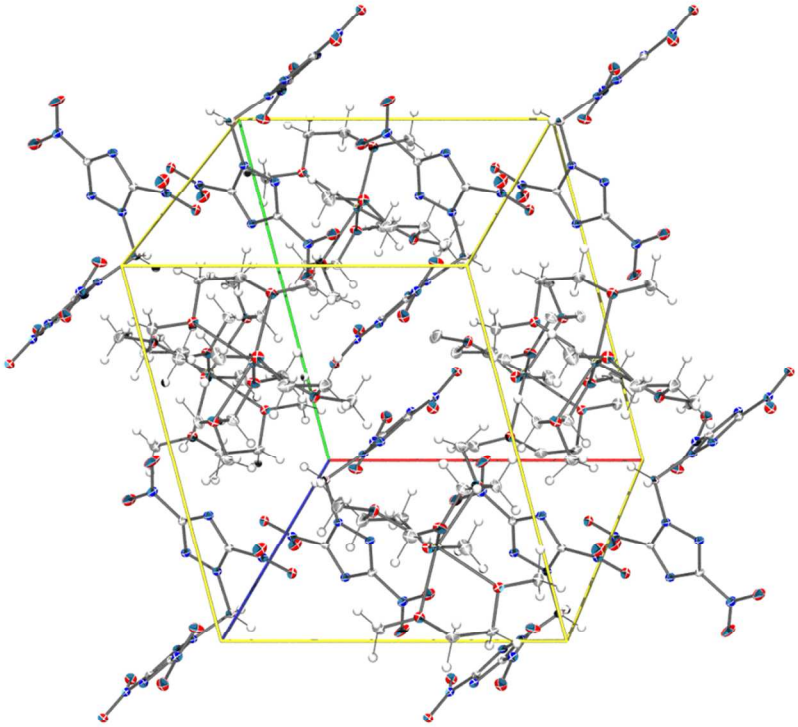

Figure S2: Unit cell of $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**. View normal to (001).

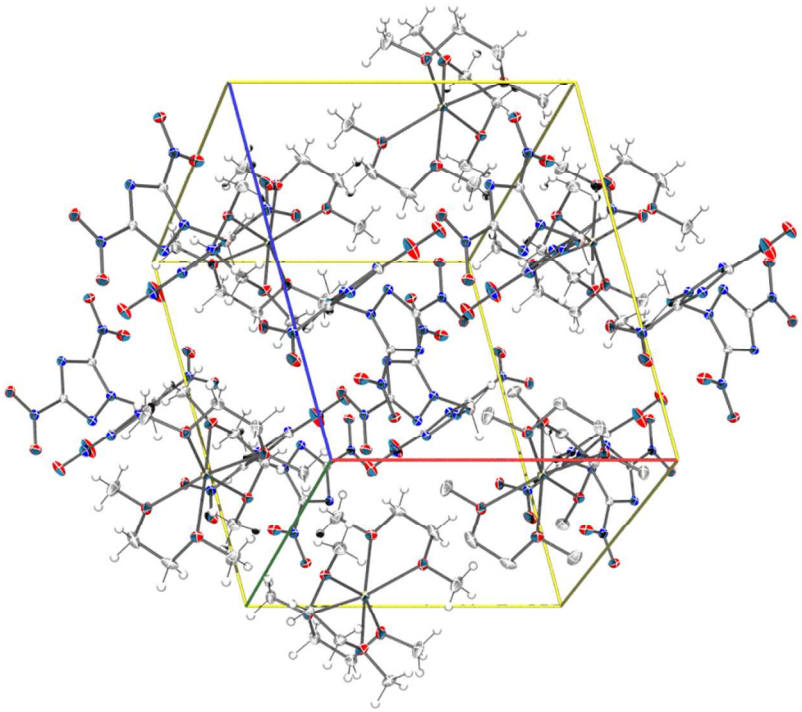

Figure S3: Unit cell of $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**. View normal to (010).

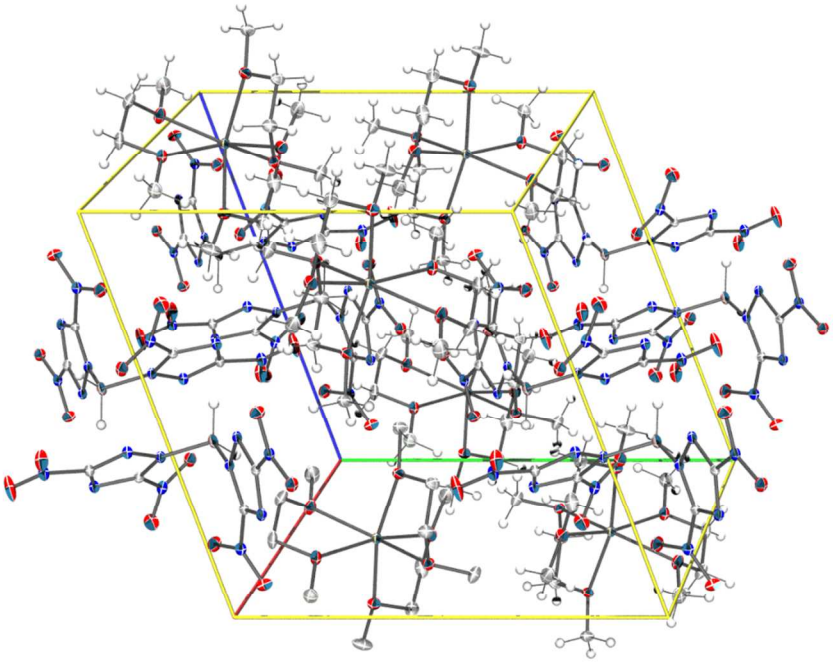

Figure S4: Unit cell of $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**. View normal to (100).

Table S1. Sample and crystal data for $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**.

Identification code	NaBH2DNT2	
Chemical formula	$C_{16}H_{32}BN_{10}NaO_{14}$	
Formula weight	622.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.270 x 0.450 x 0.570 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.1631(2) Å	α = 110.9310(10)°
	b = 12.6130(2) Å	β = 105.0920(10)°
	c = 12.6791(2) Å	γ = 104.7700(10)°
Volume	1485.24(4) $Å^3$	
Z	2	
Density (calculated)	1.392 g/cm^3	
Absorption coefficient	0.132 mm^{-1}	
F(000)	652	

Table S2. Data collection and structure refinement for $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**.

Diffractometer	Bruker APEX II CCD	
Radiation source	fine-focus tube, MoKα	
Theta range for data collection	1.87 to 30.03°	
Index ranges	-15<=h<=15, -17<=k<=17, -17<=l<=17	
Reflections collected	41074	
Independent reflections	8675 [R(int) = 0.0453]	
Absorption correction	multi-scan	
Max. and min. transmission	0.9650 and 0.9290	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL 2012-4 (Sheldrick, 2012)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	8675 / 30 / 414	
Goodness-of-fit on F^2	1.077	
Final R indices	7278 data; I>2σ(I)	R1 = 0.0324, wR2 = 0.0866
	all data	R1 = 0.0395, wR2 = 0.0902
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0460P)^2+0.1694P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.307 and -0.288 $eÅ^{-3}$	
R.M.S. deviation from mean	0.042 $eÅ^{-3}$	

Table S3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
B1	0.20284(10)	0.19117(9)	0.51104(10)	0.02175(19)
C1	0.37219(8)	0.27145(8)	0.41478(8)	0.01821(15)
C2	0.53050(8)	0.39609(7)	0.57176(8)	0.01784(15)
C3	0.09207(8)	0.94519(7)	0.38228(8)	0.01749(15)
C4	0.24737(8)	0.90677(8)	0.45921(8)	0.01854(15)
C5	0.5437(6)	0.1274(9)	0.1748(9)	0.0449(5)
O9	0.6489(2)	0.1331(2)	0.13072(19)	0.0311(4)
C6	0.7598(2)	0.1182(2)	0.2013(2)	0.0360(4)
C7	0.8459(3)	0.0939(2)	0.1285(3)	0.0339(6)
O10	0.8857(3)	0.1954(2)	0.1005(3)	0.0252(4)
C8	0.9830(5)	0.1882(5)	0.0466(3)	0.0329(7)
C5A	0.5328(15)	0.121(2)	0.168(2)	0.0449(5)
O9A	0.6648(6)	0.1646(5)	0.1713(5)	0.0311(4)
C6A	0.7165(5)	0.0724(5)	0.1510(6)	0.0360(4)
C7A	0.8583(8)	0.1243(7)	0.1635(7)	0.0339(6)
O10A	0.8632(7)	0.1693(6)	0.0788(7)	0.0252(4)
C8A	0.9938(12)	0.2024(14)	0.0744(11)	0.0329(7)
C9	0.48534(15)	0.40828(14)	0.09665(15)	0.0493(3)
C10	0.45790(11)	0.27319(11)	0.89891(12)	0.0416(3)
C11	0.53454(12)	0.23864(10)	0.82128(10)	0.0371(2)
C12	0.69554(12)	0.15117(12)	0.80283(11)	0.0434(3)
C13	0.79761(12)	0.47641(10)	0.39073(10)	0.0339(2)
C14	0.94452(10)	0.55557(9)	0.30901(9)	0.02842(19)
C15	0.99946(9)	0.51629(9)	0.21129(9)	0.02704(19)
C16	0.86628(11)	0.54317(11)	0.05129(11)	0.0364(2)
N1	0.33800(7)	0.26296(6)	0.50665(7)	0.01789(14)
N2	0.44452(7)	0.34673(6)	0.61231(7)	0.01852(14)
N3	0.49259(7)	0.35474(7)	0.45045(7)	0.01894(14)
N4	0.28564(8)	0.19459(7)	0.28633(7)	0.02165(15)
N5	0.66205(7)	0.49092(7)	0.65837(7)	0.01957(14)
N6	0.18943(7)	0.05341(6)	0.46841(7)	0.01779(14)
N7	0.29432(7)	0.02795(7)	0.51993(7)	0.01946(14)
N8	0.12260(7)	0.84858(6)	0.37170(7)	0.01924(14)
N9	0.96187(7)	0.93294(7)	0.30590(7)	0.02148(15)
N10	0.33003(8)	0.83966(7)	0.48491(7)	0.02335(15)
Na1	0.73200(3)	0.29550(3)	0.08548(3)	0.01950(8)
O1	0.19200(7)	0.10043(6)	0.25933(7)	0.03139(16)
O2	0.31196(7)	0.22849(7)	0.21306(6)	0.02914(15)
O3	0.69369(7)	0.51233(6)	0.76590(6)	0.02699(14)
O4	0.73249(6)	0.54252(6)	0.61738(6)	0.02393(13)
O5	0.91031(6)	0.00043(6)	0.35467(7)	0.02693(14)
O6	0.91357(8)	0.85565(7)	0.19900(7)	0.03588(17)
O7	0.44542(7)	0.89828(7)	0.55960(8)	0.03665(18)
O8	0.27817(8)	0.72809(7)	0.42903(9)	0.0486(2)
O11	0.55096(7)	0.35815(7)	0.02085(7)	0.02958(15)
O12	0.61689(7)	0.18468(6)	0.87101(6)	0.02760(14)
O13	0.84514(7)	0.44886(6)	0.29420(6)	0.02764(15)

	x/a	y/b	z/c	U(eq)
O14	0.89775(6)	0.45740(6)	0.09026(6)	0.02295(13)

Table S4. Bond lengths (Å) for $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**.

B1-N1	1.5756(12)	B1-N6	1.5773(12)
B1-H1B	1.092(10)	B1-H2B	1.106(10)
C1-N3	1.3186(11)	C1-N1	1.3467(10)
C1-N4	1.4494(11)	C2-N2	1.3244(10)
C2-N3	1.3388(11)	C2-N5	1.4557(11)
C3-N8	1.3182(10)	C3-N6	1.3406(11)
C3-N9	1.4559(11)	C4-N7	1.3208(11)
C4-N8	1.3424(11)	C4-N10	1.4535(11)
C5-O9	1.423(6)	C5-H5A	0.98
C5-H5B	0.98	C5-H5C	0.98
O9-C6	1.425(3)	O9-Na1	2.352(2)
C6-C7	1.510(3)	C6-H6A	0.99
C6-H6B	0.99	C7-O10	1.442(4)
C7-H7A	0.99	C7-H7B	0.99
O10-C8	1.432(5)	O10-Na1	2.383(4)
C8-H8A	0.98	C8-H8B	0.98
C8-H8C	0.98	C5A-O9A	1.417(13)
C5A-H5AA	0.98	C5A-H5AB	0.98
C5A-H5AC	0.98	O9A-C6A	1.399(7)
O9A-Na1	2.356(6)	C6A-C7A	1.492(9)
C6A-H6AA	0.99	C6A-H6AB	0.99
C7A-O10A	1.390(10)	C7A-H7AA	0.99
C7A-H7AB	0.99	O10A-C8A	1.431(11)
O10A-Na1	2.417(9)	C8A-H8AA	0.98
C8A-H8AB	0.98	C8A-H8AC	0.98
C9-O11	1.4243(13)	C9-H9A	0.98
C9-H9B	0.98	C9-H9C	0.98
C10-O11	1.4248(14)	C10-C11	1.4876(19)
C10-H10A	0.99	C10-H10B	0.99
C11-O12	1.4247(13)	C11-H11A	0.99
C11-H11B	0.99	C12-O12	1.4214(13)
C12-H12A	0.98	C12-H12B	0.98
C12-H12C	0.98	C13-O13	1.4243(12)
C13-H13A	0.98	C13-H13B	0.98
C13-H13C	0.98	C14-O13	1.4237(11)
C14-C15	1.5062(14)	C14-H14A	0.99
C14-H14B	0.99	C15-O14	1.4297(11)
C15-H15A	0.99	C15-H15B	0.99
C16-O14	1.4224(12)	C16-H16A	0.98
C16-H16B	0.98	C16-H16C	0.98
N1-N2	1.3578(10)	N4-O2	1.2223(10)
N4-O1	1.2290(10)	N5-O3	1.2223(10)
N5-O4	1.2271(9)	N6-N7	1.3579(10)
N9-O6	1.2188(11)	N9-O5	1.2238(10)
N10-O8	1.2149(11)	N10-O7	1.2173(10)
Na1-O14	2.3504(7)	Na1-O12	2.3555(8)
Na1-O13	2.3867(8)	Na1-O11	2.4073(7)

Table S5. Bond angles (°) for $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**.

N1-B1-N6	106.74(7)	N1-B1-H1B	107.9(6)
N6-B1-H1B	110.3(6)	N1-B1-H2B	106.5(6)
N6-B1-H2B	108.3(6)	H1B-B1-H2B	116.7(9)
N3-C1-N1	114.71(8)	N3-C1-N4	121.94(7)
N1-C1-N4	123.34(7)	N2-C2-N3	117.86(8)
N2-C2-N5	119.91(7)	N3-C2-N5	122.22(7)
N8-C3-N6	114.70(7)	N8-C3-N9	121.71(7)
N6-C3-N9	123.59(7)	N7-C4-N8	117.79(7)
N7-C4-N10	120.71(7)	N8-C4-N10	121.48(7)
O9-C5-H5A	109.5	O9-C5-H5B	109.5
H5A-C5-H5B	109.5	O9-C5-H5C	109.5
H5A-C5-H5C	109.5	H5B-C5-H5C	109.5
C5-O9-C6	113.8(4)	C5-O9-Na1	119.8(4)
C6-O9-Na1	108.71(14)	O9-C6-C7	108.3(2)
O9-C6-H6A	110.0	C7-C6-H6A	110.0
O9-C6-H6B	110.0	C7-C6-H6B	110.0
H6A-C6-H6B	108.4	O10-C7-C6	107.7(2)
O10-C7-H7A	110.2	C6-C7-H7A	110.2
O10-C7-H7B	110.2	C6-C7-H7B	110.2
H7A-C7-H7B	108.5	C8-O10-C7	111.1(4)
C8-O10-Na1	129.9(3)	C7-O10-Na1	115.0(2)
O10-C8-H8A	109.5	O10-C8-H8B	109.5
H8A-C8-H8B	109.5	O10-C8-H8C	109.5
H8A-C8-H8C	109.5	H8B-C8-H8C	109.5
O9A-C5A-H5AA	109.5	O9A-C5A-H5AB	109.5
H5AA-C5A-H5AB	109.5	O9A-C5A-H5AC	109.5
H5AA-C5A-H5AC	109.5	H5AB-C5A-H5AC	109.5
C6A-O9A-C5A	111.4(10)	C6A-O9A-Na1	113.5(3)
C5A-O9A-Na1	123.1(10)	O9A-C6A-C7A	109.3(5)
O9A-C6A-H6AA	109.8	C7A-C6A-H6AA	109.8
O9A-C6A-H6AB	109.8	C7A-C6A-H6AB	109.8
H6AA-C6A-H6AB	108.3	O10A-C7A-C6A	110.0(7)
O10A-C7A-H7AA	109.7	C6A-C7A-H7AA	109.7
O10A-C7A-H7AB	109.7	C6A-C7A-H7AB	109.7
H7AA-C7A-H7AB	108.2	C7A-O10A-C8A	111.9(9)
C7A-O10A-Na1	109.2(6)	C8A-O10A-Na1	124.2(8)
O10A-C8A-H8AA	109.5	O10A-C8A-H8AB	109.5
H8AA-C8A-H8AB	109.5	O10A-C8A-H8AC	109.5
H8AA-C8A-H8AC	109.5	H8AB-C8A-H8AC	109.5
O11-C9-H9A	109.5	O11-C9-H9B	109.5
H9A-C9-H9B	109.5	O11-C9-H9C	109.5
H9A-C9-H9C	109.5	H9B-C9-H9C	109.5
O11-C10-C11	108.68(8)	O11-C10-H10A	110.0
C11-C10-H10A	110.0	O11-C10-H10B	110.0
C11-C10-H10B	110.0	H10A-C10-H10B	108.3
O12-C11-C10	108.34(9)	O12-C11-H11A	110.0
C10-C11-H11A	110.0	O12-C11-H11B	110.0
C10-C11-H11B	110.0	H11A-C11-H11B	108.4
O12-C12-H12A	109.5	O12-C12-H12B	109.5

H12A-C12-H12B	109.5	O12-C12-H12C	109.5
H12A-C12-H12C	109.5	H12B-C12-H12C	109.5
O13-C13-H13A	109.5	O13-C13-H13B	109.5
H13A-C13-H13B	109.5	O13-C13-H13C	109.5
H13A-C13-H13C	109.5	H13B-C13-H13C	109.5
O13-C14-C15	108.13(8)	O13-C14-H14A	110.1
C15-C14-H14A	110.1	O13-C14-H14B	110.1
C15-C14-H14B	110.1	H14A-C14-H14B	108.4
O14-C15-C14	112.50(8)	O14-C15-H15A	109.1
C14-C15-H15A	109.1	O14-C15-H15B	109.1
C14-C15-H15B	109.1	H15A-C15-H15B	107.8
O14-C16-H16A	109.5	O14-C16-H16B	109.5
H16A-C16-H16B	109.5	O14-C16-H16C	109.5
H16A-C16-H16C	109.5	H16B-C16-H16C	109.5
C1-N1-N2	106.28(7)	C1-N1-B1	133.12(7)
N2-N1-B1	120.13(7)	C2-N2-N1	102.32(7)
C1-N3-C2	98.82(7)	O2-N4-O1	125.04(8)
O2-N4-C1	117.23(7)	O1-N4-C1	117.73(7)
O3-N5-O4	125.27(8)	O3-N5-C2	117.41(7)
O4-N5-C2	117.32(7)	C3-N6-N7	106.54(7)
C3-N6-B1	133.44(7)	N7-N6-B1	119.96(7)
C4-N7-N6	102.23(7)	C3-N8-C4	98.74(7)
O6-N9-O5	125.80(8)	O6-N9-C3	116.93(7)
O5-N9-C3	117.27(8)	O8-N10-O7	124.72(8)
O8-N10-C4	116.98(7)	O7-N10-C4	118.30(7)
O14-Na1-O9	156.03(6)	O14-Na1-O12	97.51(3)
O9-Na1-O12	96.99(6)	O14-Na1-O9A	149.98(13)
O12-Na1-O9A	108.09(12)	O14-Na1-O10	89.18(6)
O9-Na1-O10	70.32(8)	O12-Na1-O10	96.28(7)
O14-Na1-O13	73.32(2)	O9-Na1-O13	95.19(6)
O12-Na1-O13	166.17(3)	O9A-Na1-O13	83.79(12)
O10-Na1-O13	93.96(7)	O14-Na1-O11	94.95(3)
O9-Na1-O11	107.89(5)	O12-Na1-O11	70.28(3)
O9A-Na1-O11	108.07(14)	O10-Na1-O11	166.33(7)
O13-Na1-O11	99.71(3)	O14-Na1-O10A	94.46(16)
O12-Na1-O10A	90.06(18)	O9A-Na1-O10A	70.7(2)
O13-Na1-O10A	100.80(17)	O11-Na1-O10A	159.15(16)
C9-O11-C10	111.78(10)	C9-O11-Na1	124.23(7)
C10-O11-Na1	111.63(6)	C12-O12-C11	111.71(9)
C12-O12-Na1	116.19(6)	C11-O12-Na1	113.25(6)
C14-O13-C13	111.60(7)	C14-O13-Na1	112.36(5)
C13-O13-Na1	129.88(6)	C16-O14-C15	112.42(8)
C16-O14-Na1	122.22(6)	C15-O14-Na1	105.11(5)

Table S6. Anisotropic atomic displacement parameters ($Å^2$) for $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1].**

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}
B1	0.0237(4)	0.0144(4)	0.0306(5)	0.0102(4)	0.0145(4)	0.0084(3)
C1	0.0219(4)	0.0164(4)	0.0209(4)	0.0105(3)	0.0092(3)	0.0104(3)
C2	0.0196(4)	0.0159(4)	0.0224(4)	0.0108(3)	0.0091(3)	0.0096(3)
C3	0.0185(3)	0.0167(4)	0.0195(4)	0.0094(3)	0.0082(3)	0.0075(3)
C4	0.0196(4)	0.0160(4)	0.0209(4)	0.0087(3)	0.0076(3)	0.0080(3)
C5	0.0421(12)	0.0407(12)	0.0719(12)	0.0333(10)	0.0388(11)	0.0176(10)
O9	0.0301(6)	0.0337(11)	0.0476(12)	0.0284(9)	0.0232(9)	0.0170(8)
C6	0.0368(11)	0.0434(13)	0.0456(13)	0.0344(11)	0.0178(9)	0.0200(9)
C7	0.0343(9)	0.0285(14)	0.0542(19)	0.0275(12)	0.0201(12)	0.0198(10)
O10	0.0243(10)	0.0236(12)	0.0340(12)	0.0167(10)	0.0127(9)	0.0120(8)
C8	0.0284(9)	0.0365(16)	0.042(2)	0.0201(17)	0.0183(14)	0.0176(9)
C5A	0.0421(12)	0.0407(12)	0.0719(12)	0.0333(10)	0.0388(11)	0.0176(10)
O9A	0.0301(6)	0.0337(11)	0.0476(12)	0.0284(9)	0.0232(9)	0.0170(8)
C6A	0.0368(11)	0.0434(13)	0.0456(13)	0.0344(11)	0.0178(9)	0.0200(9)
C7A	0.0343(9)	0.0285(14)	0.0542(19)	0.0275(12)	0.0201(12)	0.0198(10)
O10A	0.0243(10)	0.0236(12)	0.0340(12)	0.0167(10)	0.0127(9)	0.0120(8)
C8A	0.0284(9)	0.0365(16)	0.042(2)	0.0201(17)	0.0183(14)	0.0176(9)
C9	0.0653(8)	0.0619(8)	0.0725(9)	0.0482(8)	0.0530(8)	0.0501(7)
C10	0.0230(5)	0.0322(6)	0.0557(7)	0.0169(5)	0.0006(5)	0.0091(4)
C11	0.0425(6)	0.0280(5)	0.0241(5)	0.0094(4)	-0.0032(4)	0.0085(4)
C12	0.0406(6)	0.0415(6)	0.0276(5)	-0.0003(5)	0.0166(5)	0.0048(5)
C13	0.0456(6)	0.0308(5)	0.0290(5)	0.0126(4)	0.0223(5)	0.0139(4)
C14	0.0302(5)	0.0216(4)	0.0239(4)	0.0057(4)	0.0095(4)	0.0032(4)
C15	0.0198(4)	0.0292(5)	0.0244(4)	0.0090(4)	0.0062(3)	0.0048(3)
C16	0.0365(5)	0.0347(6)	0.0439(6)	0.0278(5)	0.0135(5)	0.0105(4)
N1	0.0210(3)	0.0138(3)	0.0213(3)	0.0090(3)	0.0093(3)	0.0079(3)
N2	0.0215(3)	0.0140(3)	0.0215(3)	0.0087(3)	0.0087(3)	0.0077(3)
N3	0.0207(3)	0.0183(3)	0.0232(4)	0.0120(3)	0.0099(3)	0.0104(3)
N4	0.0240(3)	0.0213(4)	0.0224(4)	0.0108(3)	0.0093(3)	0.0113(3)
N5	0.0201(3)	0.0180(3)	0.0247(4)	0.0112(3)	0.0097(3)	0.0102(3)
N6	0.0198(3)	0.0154(3)	0.0207(3)	0.0093(3)	0.0093(3)	0.0076(3)
N7	0.0204(3)	0.0167(3)	0.0218(3)	0.0092(3)	0.0077(3)	0.0079(3)
N8	0.0199(3)	0.0156(3)	0.0211(3)	0.0079(3)	0.0069(3)	0.0068(3)
N9	0.0199(3)	0.0207(4)	0.0268(4)	0.0141(3)	0.0083(3)	0.0081(3)
N10	0.0220(3)	0.0183(3)	0.0269(4)	0.0093(3)	0.0054(3)	0.0092(3)
Na1	0.02166(16)	0.01706(16)	0.02190(17)	0.01008(14)	0.00931(13)	0.00801(13)
O1	0.0349(4)	0.0217(3)	0.0276(4)	0.0113(3)	0.0057(3)	0.0023(3)
O2	0.0302(3)	0.0377(4)	0.0238(3)	0.0174(3)	0.0128(3)	0.0122(3)
O3	0.0266(3)	0.0292(3)	0.0231(3)	0.0127(3)	0.0073(3)	0.0087(3)
O4	0.0221(3)	0.0226(3)	0.0317(3)	0.0148(3)	0.0139(3)	0.0084(2)
O5	0.0243(3)	0.0300(4)	0.0386(4)	0.0208(3)	0.0174(3)	0.0158(3)
O6	0.0328(4)	0.0324(4)	0.0275(4)	0.0066(3)	-0.0007(3)	0.0130(3)
O7	0.0239(3)	0.0255(4)	0.0454(5)	0.0141(3)	-0.0039(3)	0.0074(3)
O8	0.0339(4)	0.0164(3)	0.0660(6)	0.0049(4)	-0.0070(4)	0.0122(3)
O11	0.0286(3)	0.0352(4)	0.0352(4)	0.0189(3)	0.0166(3)	0.0192(3)
O12	0.0303(3)	0.0270(3)	0.0222(3)	0.0094(3)	0.0091(3)	0.0099(3)

O13	0.0385(4)	0.0191(3)	0.0250(3)	0.0078(3)	0.0178(3)	0.0082(3)
O14	0.0235(3)	0.0203(3)	0.0219(3)	0.0097(3)	0.0077(2)	0.0047(2)

Table S7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for $[Na(C_4H_{10}O_2)_3][BH_2(DNT)_2]$ **Na[1]**.

	x/a	y/b	z/c	U(eq)
H5A	0.4774	0.1503	0.1301	0.067
H5B	0.5812	0.1844	0.2625	0.067
H5C	0.5000	0.0434	0.1623	0.067
H6A	0.7270	0.0484	0.2190	0.043
H6B	0.8131	0.1936	0.2801	0.043
H7A	0.9263	0.0871	0.1769	0.041
H7B	0.7944	0.0159	0.0518	0.041
H8A	0.9476	0.1080	-0.0253	0.049
H8B	1.0661	0.1980	0.1066	0.049
H8C	1.0021	0.2537	0.0216	0.049
H5AA	0.4700	0.0659	0.0826	0.067
H5AB	0.5074	0.1914	0.2005	0.067
H5AC	0.5298	0.0770	0.2171	0.067
H6AA	0.6614	0.0036	0.0678	0.043
H6AB	0.7134	0.0401	0.2113	0.043
H7AA	0.9137	0.1916	0.2475	0.041
H7AB	0.8956	0.0596	0.1498	0.041
H8AA	1.0117	0.1280	0.0398	0.049
H8AB	1.0618	0.2574	0.1574	0.049
H8AC	0.9971	0.2445	0.0228	0.049
H9A	0.4386	0.4522	0.0630	0.074
H9B	0.5522	0.4656	0.1797	0.074
H9C	0.4201	0.3416	0.0994	0.074
H10A	0.3999	0.3112	-0.1336	0.05
H10B	0.3997	0.1990	-0.1017	0.05
H11A	0.4717	0.1793	-0.2640	0.045
H11B	0.5912	0.3125	-0.1797	0.045
H12A	0.6363	0.0957	-0.2832	0.065
H12B	0.7462	0.1095	-0.1639	0.065
H12C	0.7583	0.2253	-0.1914	0.065
H13A	0.7578	0.5374	0.3916	0.051
H13B	0.8728	0.5096	0.4693	0.051
H13C	0.7295	0.4012	0.3777	0.051
H14A	1.0177	0.5957	0.3913	0.034
H14B	0.9042	0.6151	0.3010	0.034
H15A	1.0698	0.5894	0.2212	0.032
H15B	1.0421	0.4590	0.2222	0.032
H16A	0.9482	0.6003	0.0563	0.055
H16B	0.8286	0.5894	0.1043	0.055
H16C	0.8003	0.4990	-0.0336	0.055
H1B	0.1203(11)	0.1964(11)	0.4470(10)	0.026(3)
H2B	0.2158(11)	0.2310(10)	0.6084(9)	0.025(3)

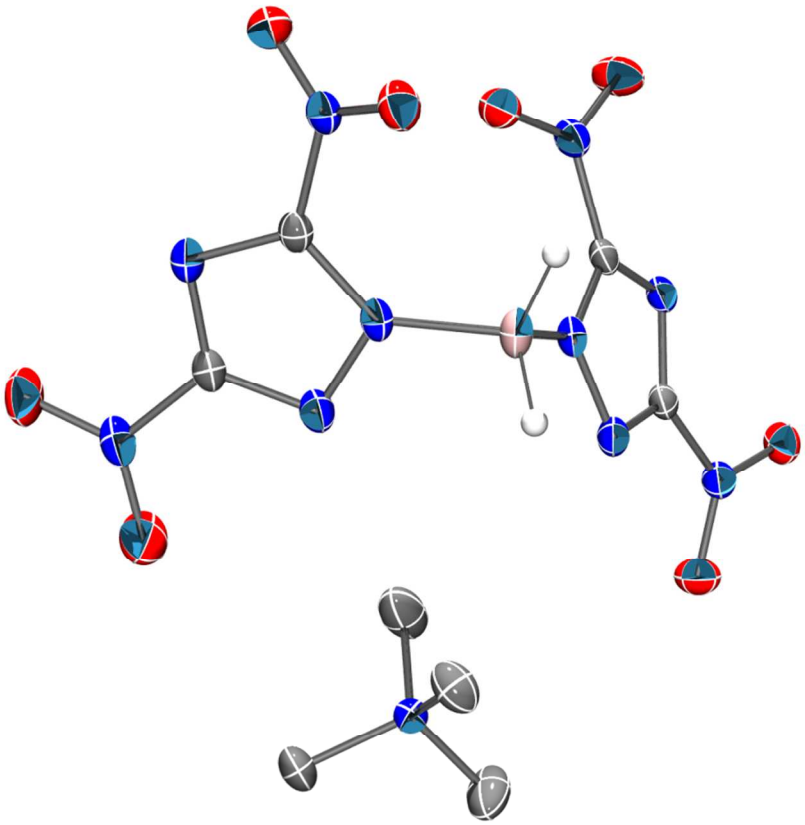

Figure S5: Asymmetric unit in the crystal structure of $NMe_4[BH_2(DNT)_2]$ **TMA[1]**.

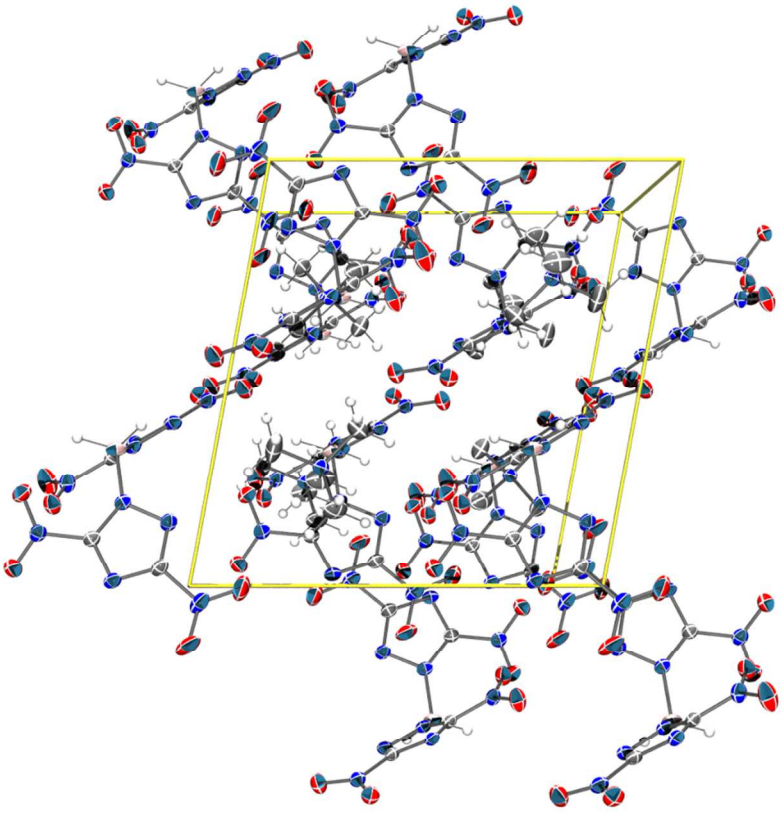

Figure S6: Unit cell of $NMe_4[BH_2(DNT)_2]$ **TMA[1]**. View normal to (001).

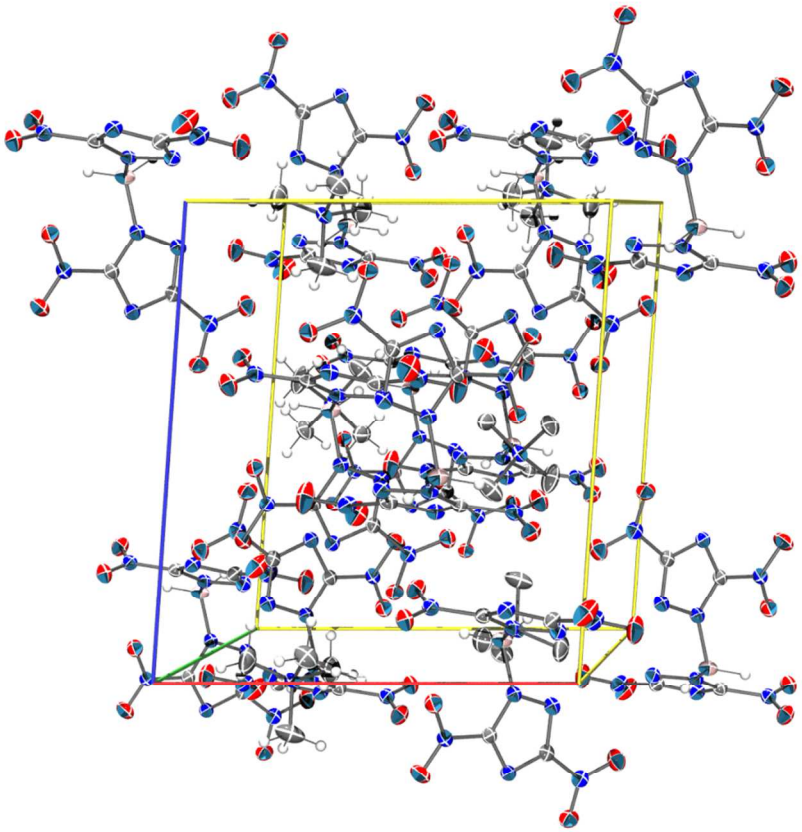

Figure S7: Unit cell of $NMe_4[BH_2(DNT)_2]$ **TMA[1]**. View normal to (010).

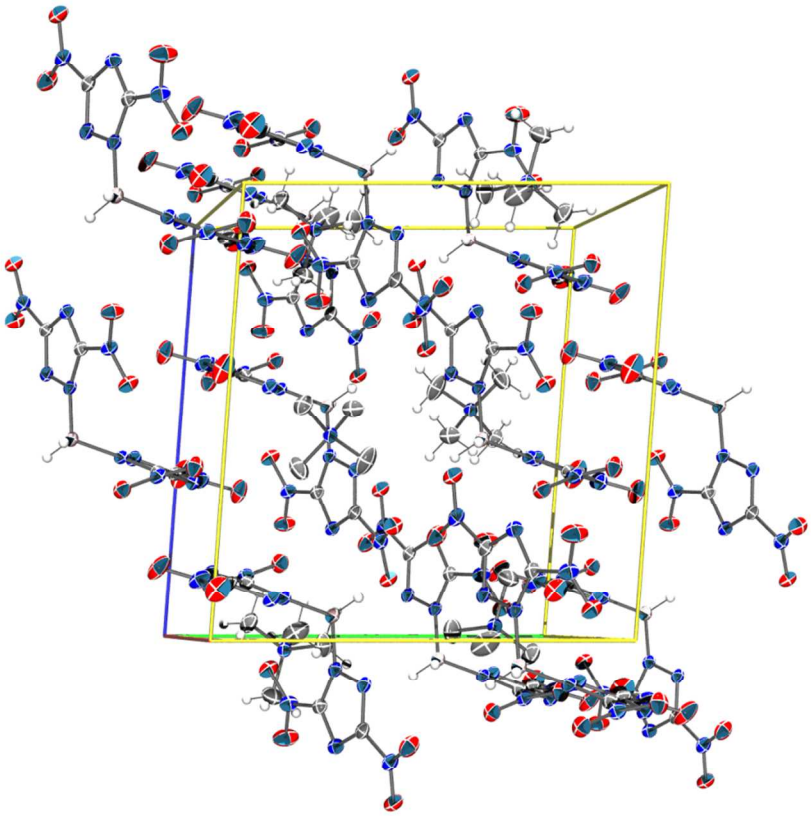

Figure S8: Unit cell of $NMe_4[BH_2(DNT)_2]$ **TMA[1]**. View normal to (100).

Table S8. Sample and crystal data for $NMe_4[BH_2(DNT)_2]$ **TMA[1]**.

Identification code	TMABH2DNT2	
Chemical formula	$C_8H_{14}BN_{11}O_8$	
Formula weight	403.11	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal size	0.090 x 0.250 x 0.300 mm	
Crystal habit	clear colourless blade	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.4579(5) Å	α = 85.815(2)°
	b = 12.0559(6) Å	β = 86.127(2)°
	c = 13.0552(6) Å	γ = 79.409(2)°
Volume	1765.24(14) $Å^3$	
Z	4	
Density (calculated)	1.517 g/cm^3	
Absorption coefficient	0.132 mm^{-1}	
F(000)	832	

Table S9. Data collection and structure refinement for $NMe_4[BH_2(DNT)_2]$ **TMA[1]**.

Diffractometer	Bruker APEX CCD	
Radiation source	fine-focus tube, MoKα	
Theta range for data collection	1.57 to 27.52°	
Index ranges	-14<=h<=14, -15<=k<=7, -16<=l<=16	
Reflections collected	10932	
Independent reflections	7604 [R(int) = 0.0208]	
Coverage of independent reflections	93.6%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9880 and 0.9610	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL 2012-4 (Sheldrick, 2012)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	7604 / 4 / 529	
Goodness-of-fit on F^2	1.039	
Δ/σ_{max}	0.011	
Final R indices	4953 data; I>2σ(I)	R1 = 0.0552, wR2 = 0.1407
	all data	R1 = 0.0854, wR2 = 0.1615
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0802P)^2+0.2997P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.461 and -0.231 $eÅ^{-3}$	
R.M.S. deviation from mean	0.054 $eÅ^{-3}$	

Table S10. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $NMe_4[BH_2(DNT)_2]$ **TMA[1]**.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
B1	0.3013(3)	0.3376(2)	0.54829(19)	0.0370(6)
B2	0.2372(3)	0.6809(2)	0.9476(2)	0.0386(6)
C1	0.40986(18)	0.41177(17)	0.29198(16)	0.0306(5)
C2	0.27529(17)	0.33268(17)	0.34486(15)	0.0301(5)
C3	0.4632(2)	0.06158(18)	0.61961(16)	0.0350(5)
C4	0.28692(19)	0.12456(17)	0.62097(15)	0.0311(5)
C5	0.0786(2)	0.95852(19)	0.87529(17)	0.0386(5)
C6	0.25285(19)	0.89161(18)	0.87249(16)	0.0326(5)
C7	0.12081(19)	0.60718(17)	0.20113(17)	0.0339(5)
C8	0.25108(18)	0.69277(17)	0.15128(16)	0.0325(5)
C9	0.8622(2)	0.1972(2)	0.5224(2)	0.0525(7)
C10	0.7248(3)	0.2179(2)	0.3859(2)	0.0730(10)
C11	0.6842(2)	0.3454(2)	0.5231(2)	0.0543(7)
C12	0.8480(3)	0.3593(3)	0.3993(3)	0.0747(10)
C13	0.8580(2)	0.6760(3)	0.9920(3)	0.0847(11)
C14	0.7269(3)	0.7436(3)	0.1402(2)	0.0792(10)
C15	0.6633(3)	0.6313(2)	0.0171(3)	0.0695(9)
C16	0.6842(3)	0.8224(2)	0.9664(2)	0.0649(8)
N1	0.33235(15)	0.34879(14)	0.42817(13)	0.0312(4)
N2	0.42322(16)	0.40187(14)	0.39232(13)	0.0335(4)
N3	0.32006(15)	0.37150(14)	0.25664(13)	0.0318(4)
N4	0.34288(16)	0.21024(14)	0.58672(13)	0.0324(4)
N5	0.46108(16)	0.16751(15)	0.58555(14)	0.0372(4)
N6	0.35896(17)	0.02827(15)	0.64264(13)	0.0357(4)
N7	0.17600(16)	0.27319(15)	0.34988(14)	0.0353(4)
N8	0.48988(16)	0.46845(15)	0.22385(14)	0.0362(4)
N9	0.57632(19)	0.98439(18)	0.63165(15)	0.0453(5)
N10	0.15807(17)	0.13575(16)	0.63511(14)	0.0374(4)
N11	0.19596(16)	0.80755(15)	0.90751(13)	0.0328(4)
N12	0.07807(16)	0.85319(16)	0.90964(14)	0.0387(5)
N13	0.18389(16)	0.98944(15)	0.85099(14)	0.0367(4)
N14	0.20145(15)	0.67010(14)	0.06656(13)	0.0317(4)
N15	0.11430(16)	0.61223(15)	0.10000(14)	0.0357(4)
N16	0.20432(16)	0.65445(15)	0.23868(14)	0.0357(4)
N17	0.96843(19)	0.03957(19)	0.86621(16)	0.0522(6)
N18	0.38228(16)	0.87858(16)	0.85639(14)	0.0374(4)
N19	0.04103(17)	0.54925(16)	0.26783(15)	0.0412(5)
N20	0.34846(17)	0.75409(17)	0.14850(15)	0.0415(5)
N21	0.78065(16)	0.27965(15)	0.45735(13)	0.0339(4)
N22	0.73500(16)	0.71968(15)	0.02937(14)	0.0359(4)
O1	0.15183(14)	0.22346(15)	0.43081(12)	0.0459(4)
O2	0.12219(15)	0.27719(16)	0.27142(12)	0.0539(5)
O3	0.45688(14)	0.50074(14)	0.13749(12)	0.0429(4)
O4	0.58328(15)	0.48056(15)	0.25723(13)	0.0504(4)
O5	0.66658(17)	0.02316(19)	0.6140(2)	0.0835(7)
O6	0.57204(17)	0.88673(15)	0.65693(16)	0.0654(6)

	x/a	y/b	z/c	U(eq)
O7	0.11565(15)	0.05381(15)	0.61657(14)	0.0523(5)
O8	0.10261(15)	0.22423(14)	0.66606(12)	0.0455(4)
O9	0.87540(17)	0.00647(19)	0.88846(18)	0.0736(6)
O10	0.97686(18)	0.13698(17)	0.84032(16)	0.0743(7)
O11	0.43594(15)	0.78898(14)	0.82653(13)	0.0494(4)
O12	0.42652(15)	0.95973(15)	0.87353(14)	0.0498(4)
O13	0.37215(15)	0.80667(15)	0.06845(13)	0.0493(4)
O14	0.40307(18)	0.7482(2)	0.22646(14)	0.0714(6)
O15	0.06460(16)	0.53009(14)	0.35866(12)	0.0496(4)
O16	0.95718(16)	0.52195(16)	0.22904(14)	0.0575(5)

Table S11. Bond lengths (Å) for $NMe_4[BH_2(DNT)_2]$ **TMA[1]**.

B1-N4	1.577(3)	B1-N1	1.586(3)
B1-H1	1.127(15)	B1-H2	1.103(15)
B2-N11	1.575(3)	B2-N14	1.582(3)
B2-H3	1.113(15)	B2-H4	1.099(15)
C1-N2	1.323(3)	C1-N3	1.337(3)
C1-N8	1.460(3)	C2-N3	1.318(3)
C2-N1	1.350(3)	C2-N7	1.448(3)
C3-N5	1.318(3)	C3-N6	1.337(3)
C3-N9	1.461(3)	C4-N6	1.319(3)
C4-N4	1.347(3)	C4-N10	1.458(3)
C5-N12	1.317(3)	C5-N13	1.338(3)
C5-N17	1.454(3)	C6-N13	1.317(3)
C6-N11	1.340(3)	C6-N18	1.465(3)
C7-N15	1.324(3)	C7-N16	1.336(3)
C7-N19	1.456(3)	C8-N16	1.317(3)
C8-N14	1.345(3)	C8-N20	1.444(3)
C9-N21	1.492(3)	C9-H9A	0.98
C9-H9B	0.98	C9-H9C	0.98
C10-N21	1.480(3)	C10-H10A	0.98
C10-H10B	0.98	C10-H10C	0.98
C11-N21	1.495(3)	C11-H11A	0.98
C11-H11B	0.98	C11-H11C	0.98
C12-N21	1.476(3)	C12-H12A	0.98
C12-H12B	0.98	C12-H12C	0.98
C13-N22	1.474(3)	C13-H13A	0.98
C13-H13B	0.98	C13-H13C	0.98
C14-N22	1.489(3)	C14-H14A	0.98
C14-H14B	0.98	C14-H14C	0.98
C15-N22	1.483(3)	C15-H15A	0.98
C15-H15B	0.98	C15-H15C	0.98
C16-N22	1.483(3)	C16-H16A	0.98
C16-H16B	0.98	C16-H16C	0.98
N1-N2	1.359(2)	N4-N5	1.357(2)
N7-O1	1.217(2)	N7-O2	1.224(2)
N8-O4	1.219(2)	N8-O3	1.227(2)
N9-O6	1.208(3)	N9-O5	1.213(3)
N10-O8	1.218(2)	N10-O7	1.224(2)
N11-N12	1.361(2)	N14-N15	1.352(3)
N17-O9	1.216(3)	N17-O10	1.217(3)
N18-O11	1.217(2)	N18-O12	1.222(2)
N19-O16	1.222(2)	N19-O15	1.230(2)
N20-O14	1.221(2)	N20-O13	1.223(2)

Table S12. Bond angles (°) for $NMe_4[BH_2(DNT)_2]$ **TMA[1]**.

N4-B1-N1	107.93(17)	N4-B1-H1	108.0(11)
N1-B1-H1	107.2(11)	N4-B1-H2	112.2(12)
N1-B1-H2	106.8(11)	H1-B1-H2	114.3(16)
N11-B2-N14	108.20(18)	N11-B2-H3	110.8(11)
N14-B2-H3	108.8(11)	N11-B2-H4	107.4(12)
N14-B2-H4	109.0(12)	H3-B2-H4	112.6(16)
N2-C1-N3	118.09(19)	N2-C1-N8	119.89(19)
N3-C1-N8	122.00(18)	N3-C2-N1	114.72(19)
N3-C2-N7	121.84(18)	N1-C2-N7	123.39(18)
N5-C3-N6	117.75(19)	N5-C3-N9	120.4(2)
N6-C3-N9	121.8(2)	N6-C4-N4	114.25(19)
N6-C4-N10	121.97(19)	N4-C4-N10	123.77(18)
N12-C5-N13	118.00(19)	N12-C5-N17	121.1(2)
N13-C5-N17	120.9(2)	N13-C6-N11	115.32(19)
N13-C6-N18	120.74(19)	N11-C6-N18	123.93(18)
N15-C7-N16	117.7(2)	N15-C7-N19	120.4(2)
N16-C7-N19	121.9(2)	N16-C8-N14	114.89(19)
N16-C8-N20	121.65(19)	N14-C8-N20	123.45(19)
N21-C9-H9A	109.5	N21-C9-H9B	109.5
H9A-C9-H9B	109.5	N21-C9-H9C	109.5
H9A-C9-H9C	109.5	H9B-C9-H9C	109.5
N21-C10-H10A	109.5	N21-C10-H10B	109.5
H10A-C10-H10B	109.5	N21-C10-H10C	109.5
H10A-C10-H10C	109.5	H10B-C10-H10C	109.5
N21-C11-H11A	109.5	N21-C11-H11B	109.5
H11A-C11-H11B	109.5	N21-C11-H11C	109.5
H11A-C11-H11C	109.5	H11B-C11-H11C	109.5
N21-C12-H12A	109.5	N21-C12-H12B	109.5
H12A-C12-H12B	109.5	N21-C12-H12C	109.5
H12A-C12-H12C	109.5	H12B-C12-H12C	109.5
N22-C13-H13A	109.5	N22-C13-H13B	109.5
H13A-C13-H13B	109.5	N22-C13-H13C	109.5
H13A-C13-H13C	109.5	H13B-C13-H13C	109.5
N22-C14-H14A	109.5	N22-C14-H14B	109.5
H14A-C14-H14B	109.5	N22-C14-H14C	109.5
H14A-C14-H14C	109.5	H14B-C14-H14C	109.5
N22-C15-H15A	109.5	N22-C15-H15B	109.5
H15A-C15-H15B	109.5	N22-C15-H15C	109.5
H15A-C15-H15C	109.5	H15B-C15-H15C	109.5
N22-C16-H16A	109.5	N22-C16-H16B	109.5
H16A-C16-H16B	109.5	N22-C16-H16C	109.5
H16A-C16-H16C	109.5	H16B-C16-H16C	109.5
C2-N1-N2	106.14(16)	C2-N1-B1	133.46(19)
N2-N1-B1	119.42(17)	C1-N2-N1	102.28(16)
C2-N3-C1	98.77(17)	C4-N4-N5	106.31(16)
C4-N4-B1	134.90(19)	N5-N4-B1	118.76(18)
C3-N5-N4	102.55(18)	C4-N6-C3	99.14(18)
O1-N7-O2	124.84(19)	O1-N7-C2	118.30(17)
O2-N7-C2	116.86(17)	O4-N8-O3	125.34(19)

O4-N8-C1	117.71(18)	O3-N8-C1	116.96(18)
O6-N9-O5	125.5(2)	O6-N9-C3	117.1(2)
O5-N9-C3	117.4(2)	O8-N10-O7	125.9(2)
O8-N10-C4	117.56(19)	O7-N10-C4	116.56(19)
C6-N11-N12	105.74(17)	C6-N11-B2	134.35(19)
N12-N11-B2	119.84(18)	C5-N12-N11	102.52(17)
C6-N13-C5	98.42(18)	C8-N14-N15	106.11(17)
C8-N14-B2	133.54(19)	N15-N14-B2	119.55(18)
C7-N15-N14	102.59(17)	C8-N16-C7	98.73(18)
O9-N17-O10	124.9(2)	O9-N17-C5	118.0(2)
O10-N17-C5	117.0(2)	O11-N18-O12	125.9(2)
O11-N18-C6	117.55(19)	O12-N18-C6	116.56(18)
O16-N19-O15	125.2(2)	O16-N19-C7	117.63(19)
O15-N19-C7	117.2(2)	O14-N20-O13	124.3(2)
O14-N20-C8	117.32(19)	O13-N20-C8	118.35(18)
C12-N21-C10	110.4(2)	C12-N21-C9	109.7(2)
C10-N21-C9	109.44(19)	C12-N21-C11	108.7(2)
C10-N21-C11	108.2(2)	C9-N21-C11	110.34(19)
C13-N22-C15	107.5(2)	C13-N22-C16	110.5(2)
C15-N22-C16	108.0(2)	C13-N22-C14	112.2(2)
C15-N22-C14	108.0(2)	C16-N22-C14	110.3(2)

Table S13. Anisotropic atomic displacement parameters ($Å^2$) for $NMe_4[BH_2(DNT)_2]$ **TMA[1]**.

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}
B1	0.0494(16)	0.0258(13)	0.0324(13)	0.0019(10)	-0.0025(11)	0.0004(12)
B2	0.0526(16)	0.0285(13)	0.0324(13)	0.0014(10)	-0.0055(12)	-0.0015(12)
C1	0.0276(10)	0.0269(11)	0.0350(11)	0.0039(9)	-0.0034(9)	-0.0001(9)
C2	0.0269(10)	0.0284(11)	0.0322(11)	0.0025(8)	-0.0056(9)	0.0022(9)
C3	0.0389(12)	0.0319(12)	0.0314(11)	0.0019(9)	-0.0042(9)	0.0006(10)
C4	0.0358(11)	0.0300(11)	0.0265(10)	0.0007(8)	-0.0047(9)	-0.0031(9)
C5	0.0344(12)	0.0399(13)	0.0356(12)	0.0072(10)	0.0009(10)	0.0044(10)
C6	0.0348(11)	0.0313(11)	0.0298(11)	0.0016(9)	-0.0023(9)	-0.0024(9)
C7	0.0336(11)	0.0260(11)	0.0389(12)	0.0060(9)	-0.0053(9)	0.0008(9)
C8	0.0297(11)	0.0299(11)	0.0351(12)	0.0020(9)	-0.0059(9)	0.0013(9)
C9	0.0460(14)	0.0500(15)	0.0586(16)	0.0098(12)	-0.0185(12)	-0.0005(12)
C10	0.085(2)	0.0547(18)	0.081(2)	-0.0214(15)	-0.0399(18)	0.0024(16)
C11	0.0434(14)	0.0663(18)	0.0468(15)	-0.0022(13)	-0.0010(12)	0.0057(13)
C12	0.0463(16)	0.0593(19)	0.112(3)	0.0292(18)	0.0129(17)	-0.0123(14)
C13	0.0349(15)	0.116(3)	0.092(2)	0.029(2)	-0.0020(15)	0.0014(17)
C14	0.118(3)	0.071(2)	0.0495(18)	-0.0126(15)	-0.0250(18)	-0.006(2)
C15	0.0652(19)	0.0552(18)	0.094(2)	-0.0064(16)	-0.0005(17)	-0.0264(16)
C16	0.080(2)	0.0456(16)	0.0653(19)	0.0162(13)	-0.0221(16)	-0.0030(15)
N1	0.0345(9)	0.0250(9)	0.0311(9)	0.0038(7)	-0.0038(7)	0.0008(8)
N2	0.0375(10)	0.0264(9)	0.0357(10)	0.0026(7)	-0.0059(8)	-0.0034(8)
N3	0.0287(9)	0.0304(9)	0.0334(10)	0.0032(7)	-0.0020(7)	0.0007(7)
N4	0.0389(10)	0.0292(9)	0.0271(9)	0.0024(7)	-0.0055(7)	-0.0010(8)
N5	0.0375(10)	0.0356(10)	0.0359(10)	0.0051(8)	-0.0049(8)	-0.0018(8)
N6	0.0425(11)	0.0274(9)	0.0353(10)	0.0021(7)	-0.0044(8)	-0.0017(8)
N7	0.0312(9)	0.0403(11)	0.0323(10)	0.0047(8)	-0.0027(8)	-0.0028(8)
N8	0.0358(10)	0.0331(10)	0.0379(10)	0.0014(8)	-0.0020(8)	-0.0034(8)
N9	0.0451(12)	0.0416(12)	0.0419(11)	0.0066(9)	-0.0009(9)	0.0068(10)
N10	0.0392(10)	0.0370(11)	0.0343(10)	0.0083(8)	-0.0084(8)	-0.0044(9)
N11	0.0344(10)	0.0310(10)	0.0310(9)	0.0022(7)	-0.0056(8)	-0.0014(8)
N12	0.0355(10)	0.0401(11)	0.0378(10)	0.0090(8)	-0.0042(8)	-0.0033(9)
N13	0.0378(10)	0.0312(10)	0.0362(10)	0.0058(8)	0.0013(8)	0.0018(8)
N14	0.0322(9)	0.0270(9)	0.0339(10)	0.0036(7)	-0.0064(8)	-0.0005(8)
N15	0.0381(10)	0.0274(9)	0.0408(11)	0.0049(8)	-0.0087(8)	-0.0039(8)
N16	0.0322(9)	0.0363(10)	0.0357(10)	0.0025(8)	-0.0058(8)	0.0007(8)
N17	0.0410(12)	0.0572(14)	0.0467(12)	0.0153(10)	0.0060(10)	0.0111(11)
N18	0.0365(10)	0.0384(11)	0.0350(10)	0.0041(8)	-0.0049(8)	-0.0020(9)
N19	0.0399(11)	0.0345(11)	0.0451(12)	0.0082(9)	-0.0027(9)	-0.0001(9)
N20	0.0354(10)	0.0521(13)	0.0373(11)	0.0007(9)	-0.0064(9)	-0.0089(9)
N21	0.0349(10)	0.0308(10)	0.0370(10)	0.0002(8)	-0.0077(8)	-0.0073(8)
N22	0.0376(10)	0.0336(10)	0.0374(10)	0.0005(8)	-0.0103(8)	-0.0067(8)
O1	0.0394(9)	0.0567(11)	0.0412(9)	0.0135(8)	-0.0042(7)	-0.0137(8)
O2	0.0469(10)	0.0802(13)	0.0390(10)	0.0043(9)	-0.0105(8)	-0.0235(10)
O3	0.0447(9)	0.0459(10)	0.0360(9)	0.0105(7)	-0.0026(7)	-0.0079(8)
O4	0.0434(10)	0.0618(12)	0.0498(10)	0.0051(8)	-0.0080(8)	-0.0209(9)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O5	0.0381(11)	0.0698(14)	0.133(2)	0.0293(14)	0.0026(12)	-0.0005(10)
O6	0.0598(12)	0.0369(10)	0.0889(15)	0.0122(10)	0.0006(10)	0.0111(9)
O7	0.0497(10)	0.0438(10)	0.0669(12)	0.0035(9)	-0.0174(9)	-0.0150(9)
O8	0.0428(9)	0.0424(10)	0.0461(10)	0.0032(8)	0.0024(8)	0.0020(8)
O9	0.0339(10)	0.0829(15)	0.0963(16)	0.0141(12)	-0.0021(10)	0.0014(10)
O10	0.0651(13)	0.0542(12)	0.0806(15)	0.0321(11)	0.0230(11)	0.0255(10)
O11	0.0423(9)	0.0411(10)	0.0584(11)	0.0000(8)	0.0067(8)	0.0046(8)
O12	0.0440(10)	0.0468(10)	0.0614(11)	-0.0030(8)	-0.0103(8)	-0.0131(8)
O13	0.0460(10)	0.0578(11)	0.0455(10)	0.0114(8)	-0.0065(8)	-0.0172(8)
O14	0.0678(13)	0.1132(18)	0.0448(11)	0.0047(11)	-0.0175(10)	-0.0455(13)
O15	0.0535(10)	0.0505(10)	0.0404(10)	0.0119(8)	-0.0020(8)	-0.0039(8)
O16	0.0516(11)	0.0608(12)	0.0637(12)	0.0163(9)	-0.0124(9)	-0.0239(9)

Table S14. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for $NMe_4[BH_2(DNT)_2]$ **TMA[1]**.

	x/a	y/b	z/c	U(eq)
H9A	0.9266	0.1567	0.4787	0.079
H9B	0.8177	0.1429	0.5591	0.079
H9C	0.8958	0.2377	0.5723	0.079
H10A	0.6660	0.2713	0.3475	0.109
H10B	0.6854	0.1615	0.4252	0.109
H10C	0.7860	0.1799	0.3378	0.109
H11A	0.7194	0.3870	0.5709	0.081
H11B	0.6388	0.2933	0.5621	0.081
H11C	0.6310	0.3988	0.4794	0.081
H12A	0.8851	0.3990	0.4475	0.112
H12B	0.7939	0.4143	0.3578	0.112
H12C	0.9098	0.3174	0.3540	0.112
H13A	0.8591	0.6614	-0.0810	0.127
H13B	0.8885	0.6056	0.0315	0.127
H13C	0.9081	0.7320	0.0005	0.127
H14A	0.7754	0.8005	0.1504	0.119
H14B	0.7561	0.6740	0.1813	0.119
H14C	0.6439	0.7722	0.1617	0.119
H15A	0.5796	0.6604	0.0357	0.104
H15B	0.6916	0.5645	0.0621	0.104
H15C	0.6714	0.6106	-0.0546	0.104
H16A	0.7344	0.8798	-0.0316	0.097
H16B	0.6038	0.8522	-0.0059	0.097
H16C	0.6807	0.8032	-0.1048	0.097
H1	0.3557(17)	0.3905(16)	0.5859(15)	0.036(6)
H2	0.2043(14)	0.3651(18)	0.5597(16)	0.039(6)
H3	0.3354(14)	0.6552(18)	-0.0638(16)	0.039(6)
H4	0.1884(18)	0.6288(17)	-0.0932(16)	0.041(6)

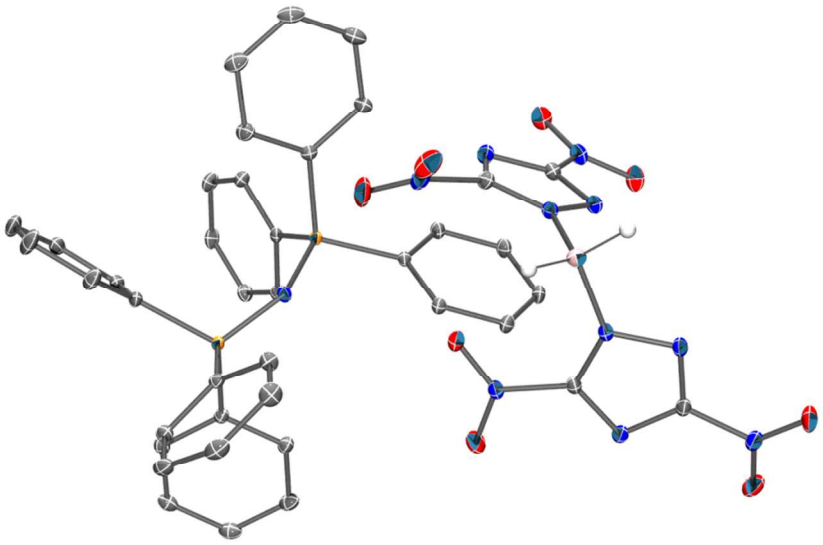

Figure S9: Asymmetric unit in the crystal structure of $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**.

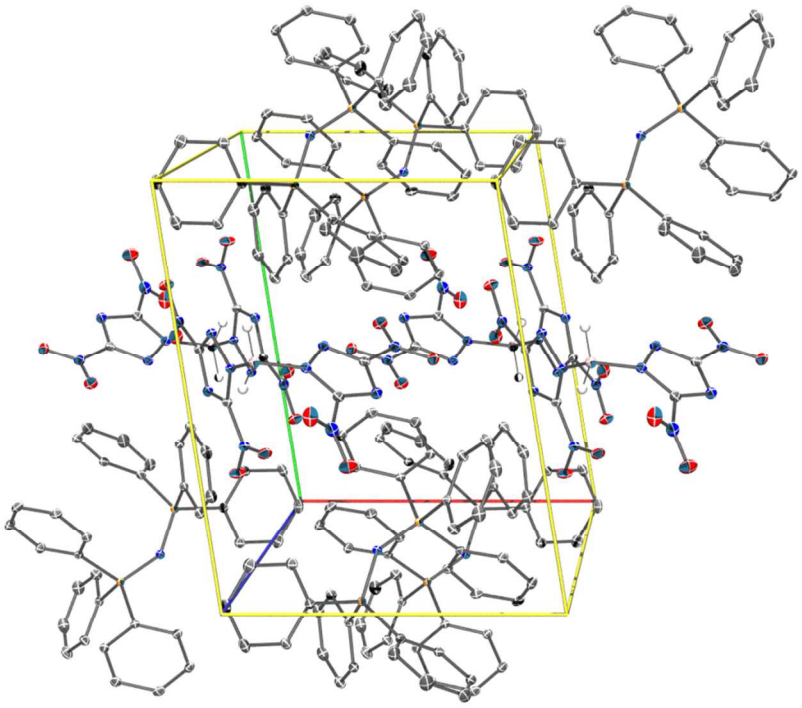

Figure S10: Unit cell of $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**. View normal to (001).

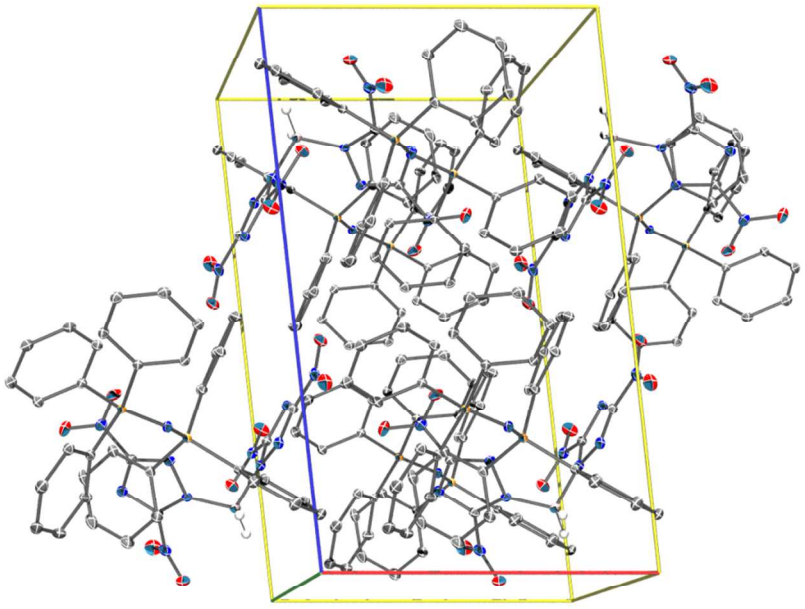

Figure S11: Unit cell of $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**. View normal to (010).

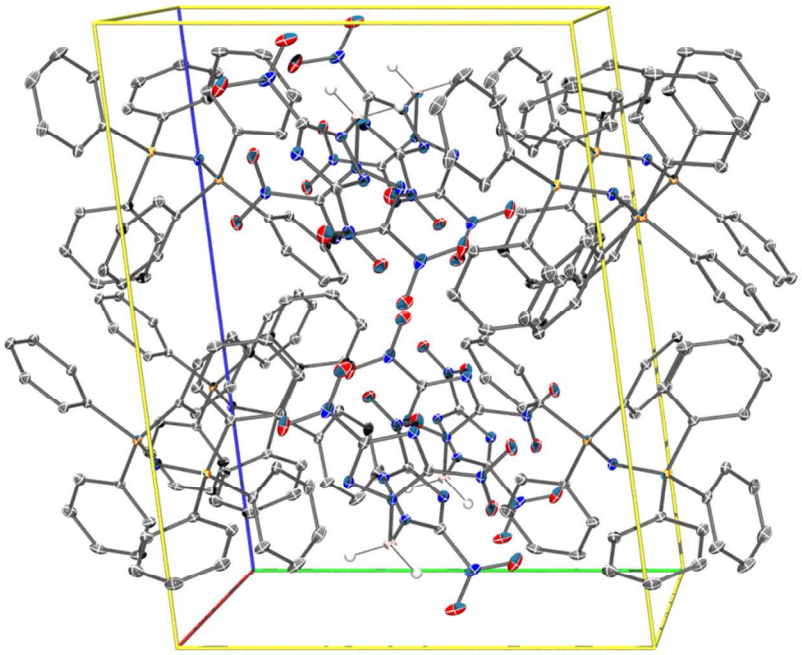

Figure S12: Unit cell of $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**. View normal to (100).

Table S15. Sample and crystal data for $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**.

Identification code	PNPBH2DNT2	
Chemical formula	$C_{40}H_{32}BN_{11}O_8P_2$	
Formula weight	867.52	
Temperature	104(2) K	
Wavelength	0.71073 Å	
Crystal size	0.280 x 0.320 x 0.500 mm	
Crystal habit	clear colourless prism	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.9418(5) Å	α = 97.5665(7)°
	b = 12.6744(6) Å	β = 96.2596(7)°
	c = 16.7980(8) Å	γ = 99.1580(7)°
Volume	2053.12(17) $Å^3$	
Z	2	
Density (calculated)	1.403 g/cm^3	
Absorption coefficient	0.174 mm^{-1}	
F(000)	896	

Table 3. Data collection and structure refinement for $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**.

Diffractometer	Bruker APEX II CCD	
Radiation source	fine-focus tube, MoKα	
Theta range for data collection	1.65 to 30.49°	
Index ranges	-13<=h<=14, -18<=k<=17, -23<=l<=23	
Reflections collected	39853	
Independent reflections	12196 [R(int) = 0.0253]	
Coverage of independent reflections	97.6%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9530 and 0.9182	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	12196 / 0 / 567	
Goodness-of-fit on F^2	1.024	
Δ/σ_{max}	0.001	
Final R indices	10230 data; I>2σ(I)	R1 = 0.0344, wR2 = 0.0875
	all data	R1 = 0.0436, wR2 = 0.0931
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0448P)^2+0.7093P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.421 and -0.308 $eÅ^{-3}$	
R.M.S. deviation from mean	0.049 $eÅ^{-3}$	

Table S16. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
B1	0.83068(13)	0.44943(10)	0.14520(7)	0.0191(2)
C1	0.52483(11)	0.46663(9)	0.23787(7)	0.0183(2)
C2	0.59572(12)	0.52826(9)	0.14249(7)	0.0195(2)
C3	0.04774(11)	0.45524(9)	0.33249(7)	0.0184(2)
C4	0.97195(11)	0.57284(8)	0.28105(6)	0.01610(19)
C5	0.79272(11)	0.03061(9)	0.18458(6)	0.01619(19)
C6	0.81843(12)	0.92911(9)	0.15460(7)	0.0212(2)
C7	0.93289(13)	0.92155(11)	0.11423(8)	0.0276(3)
C8	0.01908(13)	0.01444(12)	0.10358(7)	0.0277(3)
C9	0.99236(12)	0.11569(11)	0.13278(7)	0.0252(2)
C10	0.88028(11)	0.12454(9)	0.17418(7)	0.0201(2)
C11	0.72521(10)	0.12431(8)	0.33624(6)	0.01562(19)
C12	0.78266(11)	0.07333(9)	0.39752(7)	0.0195(2)
C13	0.85118(12)	0.13510(11)	0.46940(7)	0.0244(2)
C14	0.86227(12)	0.24710(10)	0.48050(7)	0.0248(2)
C15	0.80492(12)	0.29735(10)	0.41999(7)	0.0228(2)
C16	0.73653(11)	0.23688(9)	0.34755(7)	0.0189(2)
C17	0.53915(11)	0.11724(9)	0.18819(7)	0.0178(2)
C18	0.54555(13)	0.12537(11)	0.10651(8)	0.0272(3)
C19	0.45409(14)	0.17880(13)	0.06529(9)	0.0359(3)
C20	0.35610(13)	0.22232(12)	0.10489(9)	0.0330(3)
C21	0.34734(12)	0.21296(9)	0.18554(8)	0.0248(2)
C22	0.43918(11)	0.16111(9)	0.22779(7)	0.0192(2)
C23	0.34731(10)	0.94672(8)	0.32932(6)	0.01445(18)
C24	0.41051(11)	0.01137(9)	0.40203(6)	0.0175(2)
C25	0.34104(12)	0.08414(9)	0.44248(7)	0.0208(2)
C26	0.20844(13)	0.09239(9)	0.41083(7)	0.0231(2)
C27	0.14488(12)	0.02806(10)	0.33932(7)	0.0234(2)
C28	0.21384(11)	0.95488(9)	0.29824(7)	0.0189(2)
C29	0.33433(11)	0.78609(8)	0.18917(6)	0.01574(19)
C30	0.31217(12)	0.83604(10)	0.12048(7)	0.0220(2)
C31	0.21865(13)	0.78212(11)	0.05429(7)	0.0278(3)
C32	0.14876(13)	0.67871(11)	0.05626(7)	0.0287(3)
C33	0.17266(13)	0.62829(10)	0.12352(8)	0.0266(2)
C34	0.26484(11)	0.68169(9)	0.19041(7)	0.0203(2)
C35	0.49724(10)	0.77105(8)	0.34306(6)	0.01410(18)
C36	0.40505(11)	0.72668(9)	0.39206(7)	0.0179(2)
C37	0.44628(12)	0.65943(9)	0.44564(7)	0.0207(2)
C38	0.57946(12)	0.63740(9)	0.45115(7)	0.0203(2)
C39	0.67126(12)	0.68108(9)	0.40236(7)	0.0194(2)
C40	0.63065(11)	0.74771(8)	0.34786(6)	0.01654(19)
N1	0.68579(9)	0.46733(7)	0.16775(5)	0.01720(17)
N2	0.63887(10)	0.42644(7)	0.23252(6)	0.01822(18)
N3	0.49126(10)	0.53072(8)	0.18413(6)	0.02116(19)
N4	0.43955(11)	0.44186(8)	0.30028(6)	0.0225(2)
N5	0.61377(11)	0.59035(10)	0.07612(7)	0.0285(2)

	x/a	y/b	z/c	U(eq)
N6	0.92946(9)	0.48086(7)	0.22833(5)	0.01634(17)
N7	0.98058(10)	0.40212(7)	0.26276(6)	0.01906(18)
N8	0.04676(9)	0.56141(8)	0.34840(6)	0.01823(18)
N9	0.11607(10)	0.39872(9)	0.39048(7)	0.0244(2)
N10	0.93825(10)	0.67734(7)	0.26783(6)	0.01929(18)
N11	0.58204(9)	0.92438(7)	0.24976(6)	0.01645(17)
O1	0.48498(10)	0.39423(7)	0.35319(5)	0.0295(2)
O2	0.32760(10)	0.47143(8)	0.29554(6)	0.0309(2)
O3	0.65461(11)	0.54710(10)	0.01604(6)	0.0388(2)
O4	0.58675(12)	0.68188(9)	0.08672(7)	0.0430(3)
O5	0.12801(11)	0.30569(8)	0.36686(7)	0.0355(2)
O6	0.15454(10)	0.44804(8)	0.45902(6)	0.0329(2)
O7	0.86121(10)	0.68061(7)	0.20646(5)	0.02706(19)
O8	0.98807(11)	0.75495(7)	0.31948(6)	0.0321(2)
P1	0.65106(3)	0.04281(2)	0.240979(16)	0.01358(6)
P2	0.44719(3)	0.86140(2)	0.275726(15)	0.01272(6)

Table S17. Bond lengths (Å) for $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**.

B1-N1	1.5717(16)	B1-N6	1.5821(15)
B1-H1B	1.130(14)	B1-H2B	1.102(15)
C1-N2	1.3217(14)	C1-N3	1.3416(14)
C1-N4	1.4534(14)	C2-N3	1.3159(15)
C2-N1	1.3422(14)	C2-N5	1.4574(14)
C3-N7	1.3228(15)	C3-N8	1.3388(14)
C3-N9	1.4553(14)	C4-N8	1.3221(14)
C4-N6	1.3459(14)	C4-N10	1.4554(13)
C5-C6	1.3915(15)	C5-C10	1.4013(15)
C5-P1	1.7962(11)	C6-C7	1.3964(16)
C6-H6	0.95	C7-C8	1.3858(19)
C7-H7	0.95	C8-C9	1.3889(19)
C8-H8	0.95	C9-C10	1.3878(16)
C9-H9	0.95	C10-H10	0.95
C11-C16	1.3990(15)	C11-C12	1.4028(14)
C11-P1	1.7989(11)	C12-C13	1.3916(16)
C12-H12	0.95	C13-C14	1.3921(18)
C13-H13	0.95	C14-C15	1.3869(18)
C14-H14	0.95	C15-C16	1.3924(16)
C15-H15	0.95	C16-H16	0.95
C17-C18	1.3970(16)	C17-C22	1.4008(16)
C17-P1	1.8037(11)	C18-C19	1.3953(17)
C18-H18	0.95	C19-C20	1.383(2)
C19-H19	0.95	C20-C21	1.3863(19)
C20-H20	0.95	C21-C22	1.3935(15)
C21-H21	0.95	C22-H22	0.95
C23-C28	1.3968(14)	C23-C24	1.4012(14)
C23-P2	1.8017(10)	C24-C25	1.3891(15)
C24-H24	0.95	C25-C26	1.3919(17)
C25-H25	0.95	C26-C27	1.3855(17)
C26-H26	0.95	C27-C28	1.3940(16)
C27-H27	0.95	C28-H28	0.95
C29-C34	1.3958(15)	C29-C30	1.4008(15)
C29-P2	1.7949(11)	C30-C31	1.3928(16)
C30-H30	0.95	C31-C32	1.3886(19)
C31-H31	0.95	C32-C33	1.3862(19)
C32-H32	0.95	C33-C34	1.3922(16)
C33-H33	0.95	C34-H34	0.95
C35-C36	1.3988(14)	C35-C40	1.4004(14)
C35-P2	1.7994(10)	C36-C37	1.3918(15)
C36-H36	0.95	C37-C38	1.3918(16)
C37-H37	0.95	C38-C39	1.3902(16)
C38-H38	0.95	C39-C40	1.3950(14)
C39-H39	0.95	C40-H40	0.95
N1-N2	1.3609(12)	N4-O1	1.2243(13)
N4-O2	1.2275(13)	N5-O3	1.2241(15)
N5-O4	1.2268(16)	N6-N7	1.3558(12)
N9-O5	1.2220(14)	N9-O6	1.2251(14)
N10-O8	1.2216(13)	N10-O7	1.2248(13)

N11-P1	1.5806(9)	N11-P2	1.5822(9)

Table S18. Bond angles (°) for $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**.

N1-B1-N6	104.49(8)	N1-B1-H1B	109.4(7)
N6-B1-H1B	105.9(7)	N1-B1-H2B	110.3(8)
N6-B1-H2B	110.8(8)	H1B-B1-H2B	115.4(11)
N2-C1-N3	117.80(10)	N2-C1-N4	120.64(10)
N3-C1-N4	121.56(10)	N3-C2-N1	114.77(10)
N3-C2-N5	122.14(10)	N1-C2-N5	123.05(10)
N7-C3-N8	117.62(10)	N7-C3-N9	120.67(10)
N8-C3-N9	121.68(10)	N8-C4-N6	114.51(9)
N8-C4-N10	121.28(10)	N6-C4-N10	124.20(9)
C6-C5-C10	120.49(10)	C6-C5-P1	120.37(8)
C10-C5-P1	119.09(8)	C5-C6-C7	119.36(11)
C5-C6-H6	120.3	C7-C6-H6	120.3
C8-C7-C6	120.15(12)	C8-C7-H7	119.9
C6-C7-H7	119.9	C7-C8-C9	120.38(11)
C7-C8-H8	119.8	C9-C8-H8	119.8
C10-C9-C8	120.16(11)	C10-C9-H9	119.9
C8-C9-H9	119.9	C9-C10-C5	119.45(11)
C9-C10-H10	120.3	C5-C10-H10	120.3
C16-C11-C12	120.02(10)	C16-C11-P1	121.46(8)
C12-C11-P1	118.30(8)	C13-C12-C11	119.79(11)
C13-C12-H12	120.1	C11-C12-H12	120.1
C12-C13-C14	120.07(11)	C12-C13-H13	120.0
C14-C13-H13	120.0	C15-C14-C13	120.07(11)
C15-C14-H14	120.0	C13-C14-H14	120.0
C14-C15-C16	120.64(11)	C14-C15-H15	119.7
C16-C15-H15	119.7	C15-C16-C11	119.40(10)
C15-C16-H16	120.3	C11-C16-H16	120.3
C18-C17-C22	119.71(10)	C18-C17-P1	120.37(9)
C22-C17-P1	119.79(8)	C19-C18-C17	119.86(12)
C19-C18-H18	120.1	C17-C18-H18	120.1
C20-C19-C18	120.09(12)	C20-C19-H19	120.0
C18-C19-H19	120.0	C19-C20-C21	120.48(11)
C19-C20-H20	119.8	C21-C20-H20	119.8
C20-C21-C22	120.08(12)	C20-C21-H21	120.0
C22-C21-H21	120.0	C21-C22-C17	119.77(11)
C21-C22-H22	120.1	C17-C22-H22	120.1
C28-C23-C24	119.77(10)	C28-C23-P2	122.18(8)
C24-C23-P2	117.94(8)	C25-C24-C23	120.01(10)
C25-C24-H24	120.0	C23-C24-H24	120.0
C24-C25-C26	119.89(10)	C24-C25-H25	120.1
C26-C25-H25	120.1	C27-C26-C25	120.41(10)
C27-C26-H26	119.8	C25-C26-H26	119.8
C26-C27-C28	120.12(11)	C26-C27-H27	119.9
C28-C27-H27	119.9	C27-C28-C23	119.81(10)
C27-C28-H28	120.1	C23-C28-H28	120.1
C34-C29-C30	119.93(10)	C34-C29-P2	121.50(8)
C30-C29-P2	118.52(8)	C31-C30-C29	119.82(11)
C31-C30-H30	120.1	C29-C30-H30	120.1

C32-C31-C30	119.95(11)	C32-C31-H31	120.0
C30-C31-H31	120.0	C33-C32-C31	120.31(11)
C33-C32-H32	119.8	C31-C32-H32	119.8
C32-C33-C34	120.32(11)	C32-C33-H33	119.8
C34-C33-H33	119.8	C33-C34-C29	119.66(11)
C33-C34-H34	120.2	C29-C34-H34	120.2
C36-C35-C40	120.03(9)	C36-C35-P2	120.38(8)
C40-C35-P2	119.57(8)	C37-C36-C35	119.85(10)
C37-C36-H36	120.1	C35-C36-H36	120.1
C36-C37-C38	120.09(10)	C36-C37-H37	120.0
C38-C37-H37	120.0	C39-C38-C37	120.22(10)
C39-C38-H38	119.9	C37-C38-H38	119.9
C38-C39-C40	120.19(10)	C38-C39-H39	119.9
C40-C39-H39	119.9	C39-C40-C35	119.60(10)
C39-C40-H40	120.2	C35-C40-H40	120.2
C2-N1-N2	106.40(9)	C2-N1-B1	133.72(9)
N2-N1-B1	119.33(9)	C1-N2-N1	102.17(9)
C2-N3-C1	98.85(9)	O1-N4-O2	125.47(10)
O1-N4-C1	117.80(10)	O2-N4-C1	116.72(10)
O3-N5-O4	126.52(11)	O3-N5-C2	117.53(11)
O4-N5-C2	115.95(11)	C4-N6-N7	106.29(9)
C4-N6-B1	134.30(9)	N7-N6-B1	119.21(9)
C3-N7-N6	102.63(9)	C4-N8-C3	98.95(9)
O5-N9-O6	125.79(11)	O5-N9-C3	117.11(11)
O6-N9-C3	117.09(10)	O8-N10-O7	125.06(10)
O8-N10-C4	117.23(9)	O7-N10-C4	117.71(9)
P1-N11-P2	140.54(6)	N11-P1-C5	107.05(5)
N11-P1-C11	113.36(5)	C5-P1-C11	105.42(5)
N11-P1-C17	114.63(5)	C5-P1-C17	107.81(5)
C11-P1-C17	108.05(5)	N11-P2-C29	111.23(5)
N11-P2-C35	108.12(5)	C29-P2-C35	109.89(5)
N11-P2-C23	114.38(5)	C29-P2-C23	106.38(5)
C35-P2-C23	106.72(5)		

Table S19. Torsion angles (°) for $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**.

C10-C5-C6-C7	0.27(17)	P1-C5-C6-C7	-177.01(9)
C5-C6-C7-C8	-0.60(18)	C6-C7-C8-C9	-0.11(19)
C7-C8-C9-C10	1.14(18)	C8-C9-C10-C5	-1.46(17)
C6-C5-C10-C9	0.75(16)	P1-C5-C10-C9	178.07(9)
C16-C11-C12-C13	-0.17(16)	P1-C11-C12-C13	174.55(9)
C11-C12-C13-C14	0.19(17)	C12-C13-C14-C15	0.08(18)
C13-C14-C15-C16	-0.36(18)	C14-C15-C16-C11	0.38(17)
C12-C11-C16-C15	-0.11(16)	P1-C11-C16-C15	-174.66(8)
C22-C17-C18-C19	1.17(19)	P1-C17-C18-C19	176.98(11)
C17-C18-C19-C20	-0.9(2)	C18-C19-C20-C21	-0.3(2)
C19-C20-C21-C22	1.2(2)	C20-C21-C22-C17	-0.85(17)
C18-C17-C22-C21	-0.31(17)	P1-C17-C22-C21	-176.14(8)
C28-C23-C24-C25	-0.73(16)	P2-C23-C24-C25	175.37(8)
C23-C24-C25-C26	0.26(16)	C24-C25-C26-C27	0.29(17)
C25-C26-C27-C28	-0.37(18)	C26-C27-C28-C23	-0.11(17)
C24-C23-C28-C27	0.65(16)	P2-C23-C28-C27	-175.28(9)
C34-C29-C30-C31	1.33(17)	P2-C29-C30-C31	-176.03(9)
C29-C30-C31-C32	-0.64(19)	C30-C31-C32-C33	-0.69(19)
C31-C32-C33-C34	1.33(19)	C32-C33-C34-C29	-0.63(18)
C30-C29-C34-C33	-0.69(16)	P2-C29-C34-C33	176.59(9)
C40-C35-C36-C37	0.09(16)	P2-C35-C36-C37	-178.10(9)
C35-C36-C37-C38	0.76(17)	C36-C37-C38-C39	-0.96(17)
C37-C38-C39-C40	0.31(17)	C38-C39-C40-C35	0.53(16)
C36-C35-C40-C39	-0.73(16)	P2-C35-C40-C39	177.48(8)
N3-C2-N1-N2	-0.82(13)	N5-C2-N1-N2	177.02(10)
N3-C2-N1-B1	-171.99(11)	N5-C2-N1-B1	5.85(19)
N6-B1-N1-C2	122.52(12)	N6-B1-N1-N2	-47.75(12)
N3-C1-N2-N1	-0.60(13)	N4-C1-N2-N1	179.53(9)
C2-N1-N2-C1	0.78(11)	B1-N1-N2-C1	173.47(9)
N1-C2-N3-C1	0.44(13)	N5-C2-N3-C1	-177.43(11)
N2-C1-N3-C2	0.13(13)	N4-C1-N3-C2	180.00(10)
N2-C1-N4-O1	8.82(16)	N3-C1-N4-O1	-171.05(10)
N2-C1-N4-O2	-171.64(10)	N3-C1-N4-O2	8.49(16)
N3-C2-N5-O3	-140.39(12)	N1-C2-N5-O3	41.93(16)
N3-C2-N5-O4	39.99(17)	N1-C2-N5-O4	-137.69(12)
N8-C4-N6-N7	-0.48(12)	N10-C4-N6-N7	-179.36(9)
N8-C4-N6-B1	174.02(10)	N10-C4-N6-B1	-4.86(18)
N1-B1-N6-C4	-63.67(15)	N1-B1-N6-N7	110.28(10)
N8-C3-N7-N6	0.08(13)	N9-C3-N7-N6	178.13(9)
C4-N6-N7-C3	0.22(11)	B1-N6-N7-C3	-175.27(9)
N6-C4-N8-C3	0.49(12)	N10-C4-N8-C3	179.41(10)
N7-C3-N8-C4	-0.35(13)	N9-C3-N8-C4	-178.37(10)
N7-C3-N9-O5	11.73(16)	N8-C3-N9-O5	-170.31(11)
N7-C3-N9-O6	-167.13(11)	N8-C3-N9-O6	10.83(16)
N8-C4-N10-O8	3.86(15)	N6-C4-N10-O8	-177.33(11)
N8-C4-N10-O7	-175.37(10)	N6-C4-N10-O7	3.44(16)
P2-N11-P1-C5	-167.36(9)	P2-N11-P1-C11	76.83(11)
P2-N11-P1-C17	-47.86(11)	C6-C5-P1-N11	3.06(10)
C10-C5-P1-N11	-174.26(8)	C6-C5-P1-C11	124.04(9)

C10-C5-P1-C11	-53.28(9)	C6-C5-P1-C17	-120.74(9)
C10-C5-P1-C17	61.94(10)	C16-C11-P1-N11	-151.96(9)
C12-C11-P1-N11	33.40(10)	C16-C11-P1-C5	91.28(9)
C12-C11-P1-C5	-83.37(9)	C16-C11-P1-C17	-23.78(10)
C12-C11-P1-C17	161.58(8)	C18-C17-P1-N11	-99.50(10)
C22-C17-P1-N11	76.30(10)	C18-C17-P1-C5	19.57(11)
C22-C17-P1-C5	-164.62(9)	C18-C17-P1-C11	133.05(10)
C22-C17-P1-C11	-51.15(10)	P1-N11-P2-C29	105.99(10)
P1-N11-P2-C35	-133.27(9)	P1-N11-P2-C23	-14.55(12)
C34-C29-P2-N11	138.66(9)	C30-C29-P2-N11	-44.03(10)
C34-C29-P2-C35	18.97(10)	C30-C29-P2-C35	-163.72(9)
C34-C29-P2-C23	-96.19(9)	C30-C29-P2-C23	81.12(9)
C36-C35-P2-N11	162.98(9)	C40-C35-P2-N11	-15.22(10)
C36-C35-P2-C29	-75.45(10)	C40-C35-P2-C29	106.35(9)
C36-C35-P2-C23	39.49(10)	C40-C35-P2-C23	-138.71(8)
C28-C23-P2-N11	116.59(9)	C24-C23-P2-N11	-59.42(9)
C28-C23-P2-C29	-6.62(10)	C24-C23-P2-C29	177.38(8)
C28-C23-P2-C35	-123.90(9)	C24-C23-P2-C35	60.09(9)

Table S20. Anisotropic atomic displacement parameters ($Å^2$) for $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**.

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}
B1	0.0194(6)	0.0213(6)	0.0162(5)	0.0011(4)	0.0028(4)	0.0035(4)
C1	0.0203(5)	0.0158(5)	0.0191(5)	0.0033(4)	0.0043(4)	0.0026(4)
C2	0.0206(5)	0.0207(5)	0.0172(5)	0.0060(4)	0.0003(4)	0.0027(4)
C3	0.0160(5)	0.0184(5)	0.0227(5)	0.0082(4)	0.0033(4)	0.0042(4)
C4	0.0166(5)	0.0145(4)	0.0182(5)	0.0041(4)	0.0040(4)	0.0033(4)
C5	0.0147(4)	0.0198(5)	0.0144(4)	0.0054(4)	0.0012(4)	0.0024(4)
C6	0.0221(5)	0.0218(5)	0.0203(5)	0.0033(4)	0.0052(4)	0.0037(4)
C7	0.0277(6)	0.0320(6)	0.0253(6)	0.0016(5)	0.0093(5)	0.0098(5)
C8	0.0192(5)	0.0447(7)	0.0216(6)	0.0079(5)	0.0070(4)	0.0073(5)
C9	0.0175(5)	0.0342(6)	0.0241(6)	0.0119(5)	0.0032(4)	-0.0008(5)
C10	0.0169(5)	0.0214(5)	0.0223(5)	0.0075(4)	0.0022(4)	0.0008(4)
C11	0.0140(4)	0.0173(5)	0.0161(4)	0.0044(4)	0.0025(4)	0.0028(4)
C12	0.0186(5)	0.0215(5)	0.0188(5)	0.0065(4)	0.0007(4)	0.0035(4)
C13	0.0215(5)	0.0334(6)	0.0175(5)	0.0070(4)	-0.0004(4)	0.0016(5)
C14	0.0208(5)	0.0322(6)	0.0179(5)	-0.0017(4)	0.0037(4)	-0.0025(5)
C15	0.0212(5)	0.0202(5)	0.0254(5)	-0.0014(4)	0.0075(4)	-0.0001(4)
C16	0.0179(5)	0.0177(5)	0.0222(5)	0.0046(4)	0.0048(4)	0.0032(4)
C17	0.0153(5)	0.0171(5)	0.0213(5)	0.0084(4)	-0.0004(4)	0.0015(4)
C18	0.0225(6)	0.0385(7)	0.0251(6)	0.0172(5)	0.0037(4)	0.0086(5)
C19	0.0294(7)	0.0536(9)	0.0315(7)	0.0279(6)	0.0020(5)	0.0110(6)
C20	0.0218(6)	0.0379(7)	0.0429(8)	0.0243(6)	-0.0035(5)	0.0069(5)
C21	0.0165(5)	0.0198(5)	0.0388(7)	0.0096(5)	-0.0006(5)	0.0035(4)
C22	0.0168(5)	0.0155(5)	0.0251(5)	0.0060(4)	-0.0003(4)	0.0015(4)
C23	0.0159(4)	0.0131(4)	0.0159(4)	0.0051(3)	0.0031(4)	0.0039(4)
C24	0.0185(5)	0.0174(5)	0.0171(5)	0.0041(4)	0.0015(4)	0.0042(4)
C25	0.0277(6)	0.0167(5)	0.0183(5)	0.0018(4)	0.0035(4)	0.0056(4)
C26	0.0300(6)	0.0203(5)	0.0241(5)	0.0069(4)	0.0087(5)	0.0135(5)
C27	0.0212(5)	0.0269(6)	0.0256(6)	0.0073(5)	0.0031(4)	0.0123(4)
C28	0.0175(5)	0.0205(5)	0.0193(5)	0.0043(4)	0.0005(4)	0.0053(4)
C29	0.0143(4)	0.0176(5)	0.0153(4)	0.0008(4)	0.0026(4)	0.0037(4)
C30	0.0238(5)	0.0247(5)	0.0170(5)	0.0045(4)	0.0017(4)	0.0020(4)
C31	0.0273(6)	0.0403(7)	0.0146(5)	0.0031(5)	0.0005(4)	0.0045(5)
C32	0.0223(6)	0.0412(7)	0.0175(5)	-0.0073(5)	0.0018(4)	0.0003(5)
C33	0.0235(6)	0.0257(6)	0.0261(6)	-0.0046(5)	0.0056(5)	-0.0040(5)
C34	0.0188(5)	0.0195(5)	0.0215(5)	0.0011(4)	0.0036(4)	0.0012(4)
C35	0.0157(4)	0.0126(4)	0.0143(4)	0.0029(3)	0.0017(3)	0.0031(3)
C36	0.0173(5)	0.0174(5)	0.0210(5)	0.0064(4)	0.0051(4)	0.0045(4)
C37	0.0234(5)	0.0201(5)	0.0215(5)	0.0092(4)	0.0068(4)	0.0051(4)
C38	0.0256(5)	0.0184(5)	0.0195(5)	0.0079(4)	0.0026(4)	0.0075(4)
C39	0.0193(5)	0.0202(5)	0.0211(5)	0.0058(4)	0.0027(4)	0.0082(4)
C40	0.0169(5)	0.0172(5)	0.0170(5)	0.0044(4)	0.0036(4)	0.0048(4)
N1	0.0190(4)	0.0169(4)	0.0157(4)	0.0041(3)	0.0020(3)	0.0020(3)
N2	0.0206(4)	0.0173(4)	0.0180(4)	0.0052(3)	0.0052(3)	0.0031(3)
N3	0.0215(5)	0.0210(4)	0.0220(5)	0.0061(4)	0.0021(4)	0.0051(4)
N4	0.0255(5)	0.0184(4)	0.0255(5)	0.0044(4)	0.0096(4)	0.0044(4)
N5	0.0256(5)	0.0373(6)	0.0248(5)	0.0162(4)	0.0002(4)	0.0048(4)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N6	0.0175(4)	0.0140(4)	0.0185(4)	0.0037(3)	0.0040(3)	0.0039(3)
N7	0.0184(4)	0.0158(4)	0.0247(5)	0.0064(3)	0.0039(4)	0.0050(3)
N8	0.0174(4)	0.0188(4)	0.0193(4)	0.0049(3)	0.0023(3)	0.0037(3)
N9	0.0179(4)	0.0261(5)	0.0322(5)	0.0143(4)	0.0027(4)	0.0053(4)
N10	0.0207(4)	0.0156(4)	0.0225(4)	0.0047(3)	0.0039(4)	0.0037(3)
N11	0.0151(4)	0.0154(4)	0.0201(4)	0.0062(3)	0.0039(3)	0.0025(3)
O1	0.0397(5)	0.0286(5)	0.0259(4)	0.0120(4)	0.0136(4)	0.0110(4)
O2	0.0258(4)	0.0300(5)	0.0427(5)	0.0108(4)	0.0160(4)	0.0099(4)
O3	0.0360(5)	0.0631(7)	0.0219(4)	0.0168(5)	0.0062(4)	0.0124(5)
O4	0.0520(7)	0.0369(6)	0.0474(6)	0.0268(5)	0.0048(5)	0.0139(5)
O5	0.0369(5)	0.0244(5)	0.0500(6)	0.0171(4)	0.0033(5)	0.0120(4)
O6	0.0295(5)	0.0420(5)	0.0281(5)	0.0131(4)	-0.0041(4)	0.0079(4)
O7	0.0303(5)	0.0207(4)	0.0299(5)	0.0075(3)	-0.0047(4)	0.0068(3)
O8	0.0437(6)	0.0159(4)	0.0325(5)	-0.0019(3)	-0.0046(4)	0.0040(4)
P1	0.01313(12)	0.01381(12)	0.01466(12)	0.00556(9)	0.00163(9)	0.00226(9)
P2	0.01281(11)	0.01249(11)	0.01343(11)	0.00374(9)	0.00172(9)	0.00250(9)

Table S21. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for $[(Ph_3P)_2N][BH_2(DNT)_2]$ **PPN[1]**.

	x/a	y/b	z/c	U(eq)
H6	0.7587	0.8656	0.1615	0.025
H7	0.9517	0.8526	0.0940	0.033
H8	1.0969	1.0088	0.0761	0.033
H9	1.0509	1.1790	0.1244	0.03
H10	0.8631	1.1937	0.1953	0.024
H12	0.7748	0.9969	0.3900	0.023
H13	0.8904	1.1008	0.5109	0.029
H14	0.9092	1.2892	0.5296	0.03
H15	0.8124	1.3738	0.4281	0.027
H16	0.6979	1.2717	0.3062	0.023
H18	0.6120	1.0946	0.0791	0.033
H19	0.4591	1.1853	0.0100	0.043
H20	0.2943	1.2589	0.0766	0.04
H21	0.2786	1.2419	0.2120	0.03
H22	0.4340	1.1555	0.2833	0.023
H24	0.5009	1.0054	0.4237	0.021
H25	0.3840	1.1282	0.4917	0.025
H26	0.1612	1.1424	0.4384	0.028
H27	0.0542	1.0338	0.3182	0.028
H28	0.1702	0.9107	0.2493	0.023
H30	0.3608	0.9065	0.1190	0.026
H31	0.2027	0.8161	0.0078	0.033
H32	0.0843	0.6424	0.0113	0.034
H33	0.1259	0.5569	0.1240	0.032
H34	0.2804	0.6472	0.2367	0.024
H36	0.3145	0.7424	0.3888	0.021
H37	0.3834	0.6285	0.4785	0.025
H38	0.6077	0.5924	0.4884	0.024
H39	0.7619	0.6655	0.4062	0.023
H40	0.6931	0.7771	0.3142	0.02
H1B	0.8283(15)	0.3603(11)	0.1257(9)	0.021(3)
H2B	0.8639(15)	0.5024(12)	0.1014(9)	0.024(4)

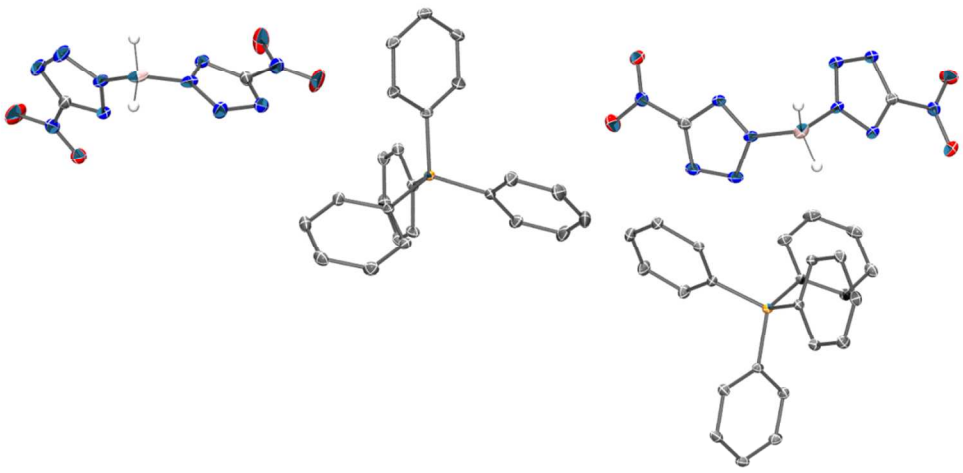

Figure S13: Asymmetric unit in the crystal structure of $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**.

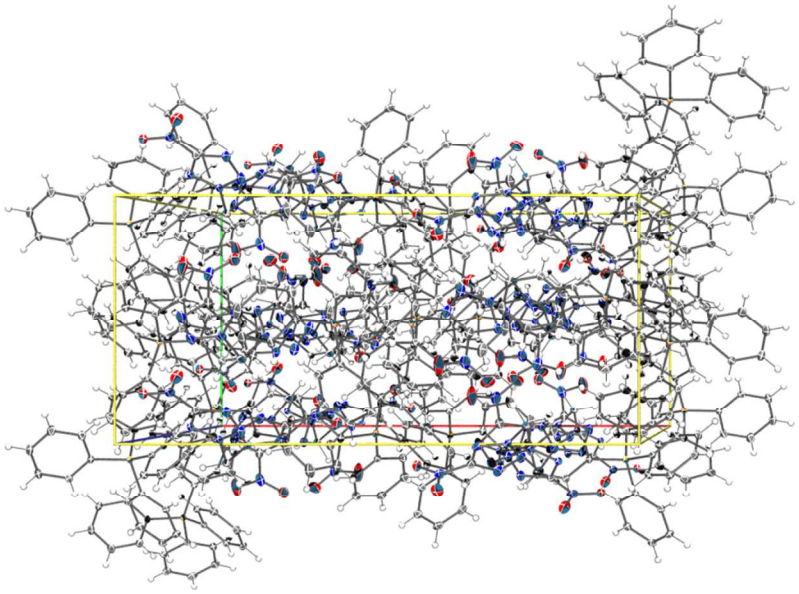

Figure S14: Unit cell of $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**. View normal to (001).

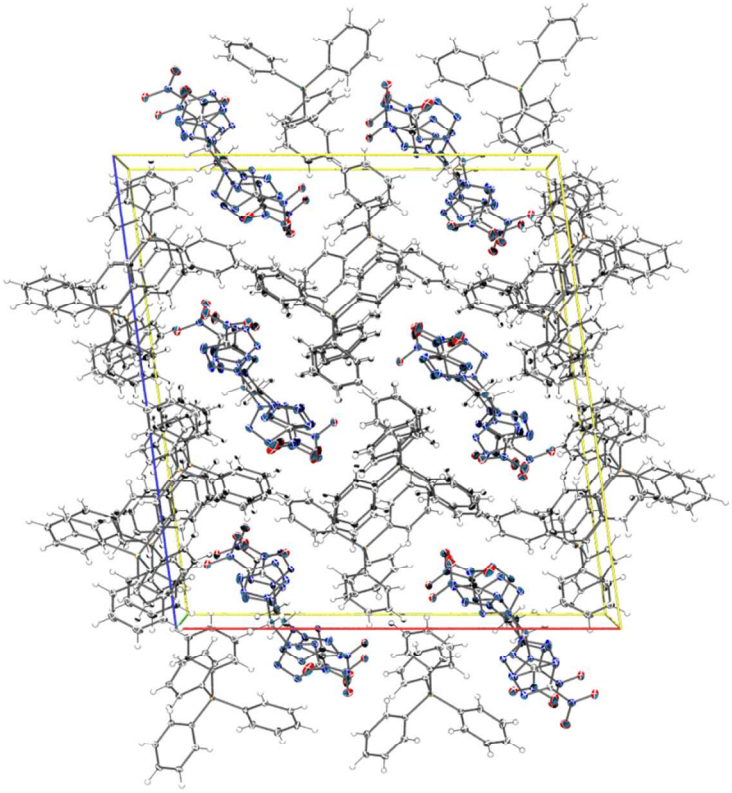

Figure S15: Unit cell of $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**. View normal to (010).

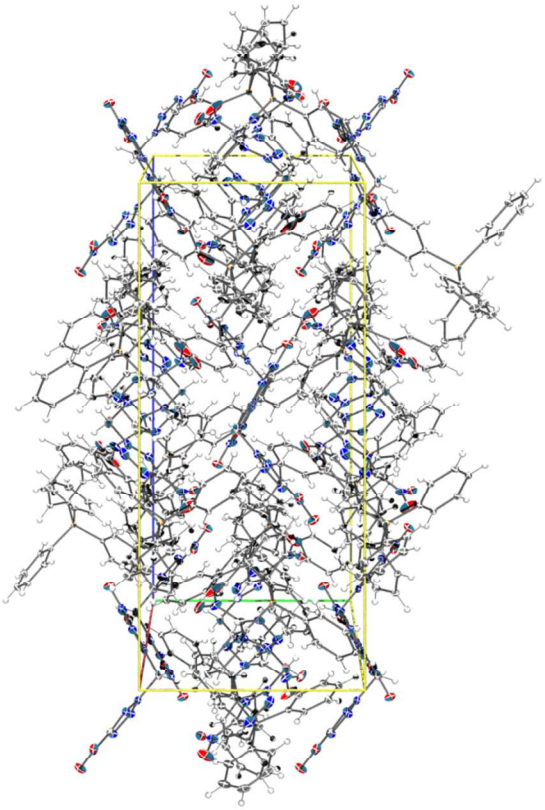

Figure S16: Unit cell of $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**. View normal to (100).

Table S22. Sample and crystal data for $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**.

Identification code	TPPBH2NTz2	
Chemical formula	$C_{26}H_{22}BN_{10}O_4P$	
Formula weight	580.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.240 x 0.250 x 0.490 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 22.1054(10) Å	α = 90°
	b = 10.5458(5) Å	β = 97.5540(10)°
	c = 23.8276(11) Å	γ = 90°
Volume	5506.5(4) $Å^3$	
Z	8	
Density (calculated)	1.400 g/cm^3	
Absorption coefficient	0.153 mm^{-1}	
F(000)	2400	

Table S23. Data collection and structure refinement for $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**.

Diffractometer	Bruker APEX II CCD	
Radiation source	fine-focus tube, MoKα	
Theta range for data collection	1.72 to 30.61°	
Index ranges	-31<=h<=31, -15<=k<=14, -34<=l<=33	
Reflections collected	129956	
Independent reflections	16662 [R(int) = 0.0535]	
Absorption correction	multi-scan	
Max. and min. transmission	0.9640 and 0.9290	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL 2012-4 (Sheldrick, 2012)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	16662 / 63 / 828	
Goodness-of-fit on F^2	1.018	
Δ/σ_{max}	0.001	
Final R indices	12310 data; I>2σ(I)	R1 = 0.0412, wR2 = 0.0973
	all data	R1 = 0.0658, wR2 = 0.1100
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0491P)^2+2.0302P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.428 and -0.409 $eÅ^{-3}$	
R.M.S. deviation from mean	0.051 $eÅ^{-3}$	

Table S24. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
B1	0.75818(9)	0.65718(17)	0.99716(9)	0.0365(4)
B2	0.21570(8)	0.57354(15)	0.51318(7)	0.0264(3)
C1	0.6860(5)	0.4474(10)	0.0783(6)	0.0305(18)
C2	0.80057(6)	0.42806(16)	0.89898(6)	0.0302(3)
C3	0.31000(6)	0.43037(13)	0.42029(6)	0.0231(3)
C4	0.18021(6)	0.35617(13)	0.61888(6)	0.0215(3)
C5	0.45197(6)	0.32764(12)	0.13119(5)	0.0204(2)
C6	0.50407(6)	0.25454(13)	0.14607(6)	0.0230(3)
C7	0.50871(7)	0.13631(14)	0.12166(6)	0.0282(3)
C8	0.46162(7)	0.09074(14)	0.08261(6)	0.0302(3)
C9	0.40955(7)	0.16284(15)	0.06780(6)	0.0299(3)
C10	0.40460(7)	0.28213(14)	0.09130(6)	0.0258(3)
C11	0.44005(6)	0.59430(12)	0.10121(5)	0.0192(2)
C12	0.48648(6)	0.59545(13)	0.06642(6)	0.0233(3)
C13	0.48327(7)	0.68104(14)	0.02197(6)	0.0277(3)
C14	0.43418(7)	0.76382(14)	0.01183(6)	0.0293(3)
C15	0.38779(7)	0.76101(14)	0.04556(6)	0.0290(3)
C16	0.39031(6)	0.67616(13)	0.09060(6)	0.0231(3)
C17	0.38112(6)	0.50049(14)	0.19669(5)	0.0221(3)
C18	0.37871(7)	0.60985(17)	0.22960(6)	0.0343(3)
C19	0.33005(8)	0.6281(2)	0.25995(7)	0.0454(4)
C20	0.28455(8)	0.5370(2)	0.25851(7)	0.0449(5)
C21	0.28685(7)	0.42928(18)	0.22604(7)	0.0394(4)
C22	0.33477(6)	0.41041(15)	0.19449(6)	0.0281(3)
C23	0.51202(6)	0.51588(12)	0.20885(5)	0.0197(2)
C24	0.52071(6)	0.44166(13)	0.25809(6)	0.0242(3)
C25	0.57218(7)	0.46009(15)	0.29726(6)	0.0283(3)
C26	0.61430(6)	0.55298(16)	0.28826(6)	0.0296(3)
C27	0.60524(6)	0.62721(15)	0.24009(6)	0.0289(3)
C28	0.55434(6)	0.60912(13)	0.19976(6)	0.0226(3)
C29	0.12204(6)	0.08879(12)	0.31013(5)	0.0189(2)
C30	0.13095(6)	0.98674(14)	0.27440(6)	0.0269(3)
C31	0.18784(7)	0.96617(16)	0.25761(7)	0.0322(3)
C32	0.23581(7)	0.04685(16)	0.27639(6)	0.0313(3)
C33	0.22728(6)	0.14870(15)	0.31131(6)	0.0262(3)
C34	0.17031(6)	0.17027(13)	0.32853(5)	0.0209(2)
C35	0.03305(5)	0.24053(12)	0.36929(5)	0.0168(2)
C36	0.07029(6)	0.28274(13)	0.41769(5)	0.0201(2)
C37	0.05511(6)	0.39253(13)	0.44476(6)	0.0234(3)
C38	0.00240(6)	0.45847(13)	0.42461(6)	0.0234(3)
C39	0.96443(6)	0.41473(13)	0.37757(6)	0.0235(3)
C40	0.97971(6)	0.30626(12)	0.34956(5)	0.0199(2)
C41	0.99241(5)	0.06883(12)	0.27705(5)	0.0172(2)
C42	0.99691(6)	0.14577(13)	0.22981(5)	0.0209(2)
C43	0.95212(6)	0.14000(13)	0.18336(6)	0.0239(3)
C44	0.90309(6)	0.05809(14)	0.18354(6)	0.0256(3)

	x/a	y/b	z/c	U(eq)
C45	0.89884(6)	0.98128(14)	0.23017(6)	0.0250(3)
C46	0.94323(6)	0.98604(12)	0.27747(5)	0.0203(2)
C47	0.05281(6)	0.97387(12)	0.39058(5)	0.0176(2)
C48	0.00126(6)	0.94900(13)	0.41700(5)	0.0223(3)
C49	0.00531(7)	0.86175(14)	0.46106(6)	0.0280(3)
C50	0.06061(7)	0.80370(14)	0.48006(6)	0.0323(3)
C51	0.11204(7)	0.83148(14)	0.45493(7)	0.0327(3)
C52	0.10854(6)	0.91538(13)	0.40980(6)	0.0243(3)
C1'	0.6912(3)	0.4134(8)	0.0783(4)	0.0279(11)
N1	0.73743(5)	0.46176(13)	0.05505(5)	0.0288(3)
N2	0.71882(6)	0.57203(13)	0.03182(6)	0.0309(3)
N3	0.6642(7)	0.6194(14)	0.0379(10)	0.0388(18)
N4	0.6427(3)	0.5348(10)	0.0733(3)	0.0347(14)
N5	0.6825(4)	0.3330(12)	0.1109(4)	0.044(2)
N6	0.75726(5)	0.47168(12)	0.92710(5)	0.0280(3)
N7	0.78635(5)	0.56624(12)	0.95600(6)	0.0289(3)
N8	0.84397(6)	0.57777(15)	0.94548(7)	0.0415(3)
N9	0.85336(6)	0.48923(16)	0.90848(7)	0.0439(4)
N10	0.79213(6)	0.31958(15)	0.86172(6)	0.0383(3)
N11	0.25626(6)	0.40585(13)	0.38973(5)	0.0298(3)
N12	0.21604(5)	0.45479(12)	0.41996(5)	0.0287(3)
N13	0.24707(5)	0.50551(10)	0.46649(5)	0.0216(2)
N14	0.30707(5)	0.49225(11)	0.46796(5)	0.0214(2)
N15	0.36758(6)	0.39210(12)	0.40269(5)	0.0272(3)
N16	0.16064(5)	0.42546(10)	0.57423(5)	0.0212(2)
N17	0.21276(5)	0.47740(11)	0.56316(5)	0.0210(2)
N18	0.26044(5)	0.44114(13)	0.59965(5)	0.0283(3)
N19	0.24020(5)	0.36177(13)	0.63603(5)	0.0283(3)
N20	0.13811(6)	0.28349(11)	0.64812(5)	0.0261(2)
N3'	0.6608(5)	0.5897(11)	0.0438(7)	0.0421(14)
N4'	0.6431(3)	0.4904(8)	0.0702(3)	0.0442(12)
N5'	0.6912(3)	0.2892(7)	0.1058(2)	0.0352(12)
O1	0.6361(2)	0.3228(16)	0.1338(6)	0.084(4)
O2	0.7251(5)	0.2580(9)	0.1153(4)	0.062(2)
O3	0.74305(5)	0.26536(12)	0.85633(5)	0.0401(3)
O4	0.83553(6)	0.29080(19)	0.83702(7)	0.0747(5)
O5	0.36571(6)	0.33415(13)	0.35796(5)	0.0438(3)
O6	0.41437(5)	0.42069(11)	0.43361(5)	0.0319(2)
O7	0.08385(5)	0.29032(10)	0.63054(5)	0.0306(2)
O8	0.15964(6)	0.22176(13)	0.68931(5)	0.0456(3)
O1'	0.6422(3)	0.2490(9)	0.11605(16)	0.0596(19)
O2'	0.7394(3)	0.2340(6)	0.1156(3)	0.0436(11)
P1	0.44571(2)	0.48430(3)	0.15889(2)	0.01760(7)
P2	0.04979(2)	0.09313(3)	0.33677(2)	0.01542(7)

Table S25. Bond lengths (Å) for $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**.

B1-N7	1.559(2)	B1-N2	1.560(2)
B1-H1B	1.113(14)	B1-H2B	1.115(14)
B2-N13	1.561(2)	B2-N17	1.572(2)
B2-H3B	1.103(12)	B2-H4B	1.102(13)
C1-N4	1.323(7)	C1-N1	1.338(8)
C1-N5	1.442(8)	C2-N6	1.3213(19)
C2-N9	1.327(2)	C2-N10	1.445(2)
C3-N14	1.3188(18)	C3-N11	1.3345(18)
C3-N15	1.4488(18)	C4-N16	1.3160(17)
C4-N19	1.3366(17)	C4-N20	1.4524(18)
C5-C6	1.3925(19)	C5-C10	1.4031(18)
C5-P1	1.7911(14)	C6-C7	1.385(2)
C6-H6	0.95	C7-C8	1.388(2)
C7-H7	0.95	C8-C9	1.386(2)
C8-H8	0.95	C9-C10	1.387(2)
C9-H9	0.95	C10-H10	0.95
C11-C16	1.3946(18)	C11-C12	1.4017(18)
C11-P1	1.7903(13)	C12-C13	1.3862(19)
C12-H12	0.95	C13-C14	1.389(2)
C13-H13	0.95	C14-C15	1.384(2)
C14-H14	0.95	C15-C16	1.3928(19)
C15-H15	0.95	C16-H16	0.95
C17-C22	1.3933(19)	C17-C18	1.400(2)
C17-P1	1.7936(13)	C18-C19	1.386(2)
C18-H18	0.95	C19-C20	1.388(3)
C19-H19	0.95	C20-C21	1.379(3)
C20-H20	0.95	C21-C22	1.391(2)
C21-H21	0.95	C22-H22	0.95
C23-C28	1.3936(18)	C23-C24	1.4026(19)
C23-P1	1.7937(13)	C24-C25	1.3871(19)
C24-H24	0.95	C25-C26	1.387(2)
C25-H25	0.95	C26-C27	1.382(2)
C26-H26	0.95	C27-C28	1.3933(19)
C27-H27	0.95	C28-H28	0.95
C29-C34	1.3949(18)	C29-C30	1.4021(18)
C29-P2	1.7951(12)	C30-C31	1.3861(19)
C30-H30	0.95	C31-C32	1.387(2)
C31-H31	0.95	C32-C33	1.387(2)
C32-H32	0.95	C33-C34	1.3936(18)
C33-H33	0.95	C34-H34	0.95
C35-C40	1.3949(17)	C35-C36	1.3988(17)
C35-P2	1.7969(13)	C36-C37	1.3877(18)
C36-H36	0.95	C37-C38	1.3873(19)
C37-H37	0.95	C38-C39	1.3879(19)
C38-H38	0.95	C39-C40	1.3883(18)
C39-H39	0.95	C40-H40	0.95
C41-C46	1.3954(17)	C41-C42	1.4018(17)
C41-P2	1.7957(12)	C42-C43	1.3859(18)
C42-H42	0.95	C43-C44	1.386(2)

C43-H43	0.95	C44-C45	1.388(2)
C44-H44	0.95	C45-C46	1.3947(18)
C45-H45	0.95	C46-H46	0.95
C47-C48	1.3971(18)	C47-C52	1.3999(18)
C47-P2	1.7910(13)	C48-C49	1.3902(19)
C48-H48	0.95	C49-C50	1.389(2)
C49-H49	0.95	C50-C51	1.384(2)
C50-H50	0.95	C51-C52	1.387(2)
C51-H51	0.95	C52-H52	0.95
C1'-N1	1.327(6)	C1'-N4'	1.331(5)
C1'-N5'	1.466(6)	N1-N2	1.3297(19)
N2-N3	1.331(15)	N2-N3'	1.362(10)
N3-N4	1.357(9)	N5-O2	1.224(7)
N5-O1	1.228(7)	N6-N7	1.3288(18)
N7-N8	1.3356(17)	N8-N9	1.319(2)
N10-O3	1.2183(18)	N10-O4	1.2277(18)
N11-N12	1.3207(18)	N12-N13	1.3363(16)
N13-N14	1.3297(15)	N15-O5	1.2246(16)
N15-O6	1.2260(16)	N16-N17	1.3330(15)
N17-N18	1.3314(16)	N18-N19	1.3243(18)
N20-O7	1.2193(15)	N20-O8	1.2209(16)
N3'-N4'	1.308(8)	N5'-O2'	1.210(5)
N5'-O1'	1.216(5)		

Table S26. Bond angles (°) for $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**.

N7-B1-N2	106.00(12)	N7-B1-H1B	107.1(10)
N2-B1-H1B	109.8(10)	N7-B1-H2B	110.0(10)
N2-B1-H2B	107.2(10)	H1B-B1-H2B	116.3(14)
N13-B2-N17	108.06(11)	N13-B2-H3B	109.8(9)
N17-B2-H3B	104.4(8)	N13-B2-H4B	110.0(9)
N17-B2-H4B	107.7(9)	H3B-B2-H4B	116.4(12)
N4-C1-N1	121.9(6)	N4-C1-N5	122.9(7)
N1-C1-N5	115.2(6)	N6-C2-N9	115.08(15)
N6-C2-N10	122.93(13)	N9-C2-N10	121.97(14)
N14-C3-N11	115.15(13)	N14-C3-N15	122.10(12)
N11-C3-N15	122.75(13)	N16-C4-N19	115.46(12)
N16-C4-N20	121.17(12)	N19-C4-N20	123.32(12)
C6-C5-C10	120.11(13)	C6-C5-P1	121.21(10)
C10-C5-P1	118.57(11)	C7-C6-C5	119.72(13)
C7-C6-H6	120.1	C5-C6-H6	120.1
C6-C7-C8	120.19(14)	C6-C7-H7	119.9
C8-C7-H7	119.9	C9-C8-C7	120.36(14)
C9-C8-H8	119.8	C7-C8-H8	119.8
C8-C9-C10	120.11(13)	C8-C9-H9	119.9
C10-C9-H9	119.9	C9-C10-C5	119.49(14)
C9-C10-H10	120.3	C5-C10-H10	120.3
C16-C11-C12	120.57(12)	C16-C11-P1	120.94(10)
C12-C11-P1	118.48(10)	C13-C12-C11	119.31(13)
C13-C12-H12	120.3	C11-C12-H12	120.3
C12-C13-C14	120.17(13)	C12-C13-H13	119.9
C14-C13-H13	119.9	C15-C14-C13	120.47(13)
C15-C14-H14	119.8	C13-C14-H14	119.8
C14-C15-C16	120.25(13)	C14-C15-H15	119.9
C16-C15-H15	119.9	C15-C16-C11	119.21(12)
C15-C16-H16	120.4	C11-C16-H16	120.4
C22-C17-C18	120.07(13)	C22-C17-P1	123.11(11)
C18-C17-P1	116.82(10)	C19-C18-C17	119.72(16)
C19-C18-H18	120.1	C17-C18-H18	120.1
C18-C19-C20	120.07(18)	C18-C19-H19	120.0
C20-C19-H19	120.0	C21-C20-C19	120.24(15)
C21-C20-H20	119.9	C19-C20-H20	119.9
C20-C21-C22	120.52(16)	C20-C21-H21	119.7
C22-C21-H21	119.7	C21-C22-C17	119.36(15)
C21-C22-H22	120.3	C17-C22-H22	120.3
C28-C23-C24	120.18(12)	C28-C23-P1	122.32(10)
C24-C23-P1	117.49(10)	C25-C24-C23	119.65(13)
C25-C24-H24	120.2	C23-C24-H24	120.2
C24-C25-C26	120.18(14)	C24-C25-H25	119.9
C26-C25-H25	119.9	C27-C26-C25	120.10(13)
C27-C26-H26	120.0	C25-C26-H26	120.0
C26-C27-C28	120.73(14)	C26-C27-H27	119.6
C28-C27-H27	119.6	C27-C28-C23	119.16(13)
C27-C28-H28	120.4	C23-C28-H28	120.4
C34-C29-C30	120.06(12)	C34-C29-P2	123.54(10)

C30-C29-P2	115.90(10)	C31-C30-C29	120.04(13)
C31-C30-H30	120.0	C29-C30-H30	120.0
C30-C31-C32	119.67(14)	C30-C31-H31	120.2
C32-C31-H31	120.2	C33-C32-C31	120.69(13)
C33-C32-H32	119.7	C31-C32-H32	119.7
C32-C33-C34	120.16(13)	C32-C33-H33	119.9
C34-C33-H33	119.9	C33-C34-C29	119.38(12)
C33-C34-H34	120.3	C29-C34-H34	120.3
C40-C35-C36	119.97(12)	C40-C35-P2	119.83(9)
C36-C35-P2	119.91(9)	C37-C36-C35	119.78(12)
C37-C36-H36	120.1	C35-C36-H36	120.1
C38-C37-C36	120.05(12)	C38-C37-H37	120.0
C36-C37-H37	120.0	C37-C38-C39	120.27(12)
C37-C38-H38	119.9	C39-C38-H38	119.9
C38-C39-C40	120.17(12)	C38-C39-H39	119.9
C40-C39-H39	119.9	C39-C40-C35	119.72(12)
C39-C40-H40	120.1	C35-C40-H40	120.1
C46-C41-C42	120.36(11)	C46-C41-P2	123.60(10)
C42-C41-P2	115.88(9)	C43-C42-C41	119.82(12)
C43-C42-H42	120.1	C41-C42-H42	120.1
C42-C43-C44	120.10(12)	C42-C43-H43	120.0
C44-C43-H43	120.0	C43-C44-C45	120.09(12)
C43-C44-H44	120.0	C45-C44-H44	120.0
C44-C45-C46	120.76(12)	C44-C45-H45	119.6
C46-C45-H45	119.6	C45-C46-C41	118.87(12)
C45-C46-H46	120.6	C41-C46-H46	120.6
C48-C47-C52	120.32(12)	C48-C47-P2	119.90(10)
C52-C47-P2	119.47(10)	C49-C48-C47	119.28(13)
C49-C48-H48	120.4	C47-C48-H48	120.4
C50-C49-C48	120.30(14)	C50-C49-H49	119.9
C48-C49-H49	119.9	C51-C50-C49	120.24(13)
C51-C50-H50	119.9	C49-C50-H50	119.9
C50-C51-C52	120.34(14)	C50-C51-H51	119.8
C52-C51-H51	119.8	C51-C52-C47	119.45(13)
C51-C52-H52	120.3	C47-C52-H52	120.3
N1-C1'-N4'	110.5(5)	N1-C1'-N5'	125.2(4)
N4'-C1'-N5'	124.2(5)	C1'-N1-N2	107.2(3)
N2-N1-C1	92.2(4)	N1-N2-N3	121.2(4)
N1-N2-N3'	106.3(4)	N1-N2-B1	124.06(12)
N3-N2-B1	114.7(4)	N3'-N2-B1	129.6(4)
N2-N3-N4	102.6(8)	C1-N4-N3	101.8(7)
O2-N5-O1	125.7(7)	O2-N5-C1	119.5(7)
O1-N5-C1	114.7(6)	C2-N6-N7	100.98(12)
N6-N7-N8	112.30(13)	N6-N7-B1	125.57(12)
N8-N7-B1	122.12(13)	N9-N8-N7	107.38(13)
N8-N9-C2	104.24(13)	O3-N10-O4	125.08(16)
O3-N10-C2	118.52(13)	O4-N10-C2	116.38(15)
N12-N11-C3	103.97(12)	N11-N12-N13	107.45(11)
N14-N13-N12	112.41(11)	N14-N13-B2	124.38(11)
N12-N13-B2	123.20(11)	C3-N14-N13	101.01(11)
O5-N15-O6	125.09(13)	O5-N15-C3	117.42(12)

O6-N15-C3	117.49(12)	C4-N16-N17	100.81(10)
N18-N17-N16	112.54(11)	N18-N17-B2	124.89(11)
N16-N17-B2	122.55(11)	N19-N18-N17	107.60(11)
N18-N19-C4	103.59(11)	O7-N20-O8	124.72(13)
O7-N20-C4	117.86(12)	O8-N20-C4	117.41(12)
N4'-N3'-N2	109.9(6)	N3'-N4'-C1'	105.9(5)
O2'-N5'-O1'	125.3(5)	O2'-N5'-C1'	117.7(5)
O1'-N5'-C1'	117.0(5)	C11-P1-C5	108.40(6)
C11-P1-C17	110.11(6)	C5-P1-C17	112.21(6)
C11-P1-C23	110.96(6)	C5-P1-C23	108.65(6)
C17-P1-C23	106.51(6)	C47-P2-C29	106.50(6)
C47-P2-C41	115.03(6)	C29-P2-C41	106.55(6)
C47-P2-C35	106.81(6)	C29-P2-C35	114.69(6)
C41-P2-C35	107.52(6)		

Table S27. Anisotropic atomic displacement parameters ($Å^2$) for $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**.

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}
B1	0.0299(9)	0.0253(8)	0.0506(11)	-0.0033(8)	-0.0091(8)	-0.0015(7)
B2	0.0243(7)	0.0183(7)	0.0369(9)	0.0031(6)	0.0048(6)	0.0025(6)
C1	0.030(3)	0.038(4)	0.024(3)	0.005(3)	0.007(2)	0.003(2)
C2	0.0214(7)	0.0401(9)	0.0292(7)	0.0096(6)	0.0039(5)	0.0013(6)
C3	0.0244(6)	0.0219(6)	0.0220(6)	0.0036(5)	-0.0006(5)	-0.0029(5)
C4	0.0203(6)	0.0225(6)	0.0217(6)	-0.0028(5)	0.0020(5)	0.0010(5)
C5	0.0232(6)	0.0204(6)	0.0174(6)	0.0001(5)	0.0019(5)	-0.0053(5)
C6	0.0230(6)	0.0244(7)	0.0216(6)	-0.0022(5)	0.0036(5)	-0.0038(5)
C7	0.0313(7)	0.0256(7)	0.0292(7)	-0.0029(6)	0.0092(6)	-0.0018(6)
C8	0.0405(8)	0.0249(7)	0.0274(7)	-0.0070(6)	0.0121(6)	-0.0108(6)
C9	0.0367(8)	0.0337(8)	0.0192(6)	-0.0055(6)	0.0030(6)	-0.0160(6)
C10	0.0272(7)	0.0290(7)	0.0199(6)	0.0002(5)	-0.0015(5)	-0.0076(6)
C11	0.0183(6)	0.0207(6)	0.0185(5)	0.0004(5)	0.0013(4)	-0.0024(5)
C12	0.0219(6)	0.0245(7)	0.0241(6)	0.0011(5)	0.0052(5)	0.0011(5)
C13	0.0324(7)	0.0289(7)	0.0233(6)	0.0014(5)	0.0101(6)	-0.0035(6)
C14	0.0373(8)	0.0276(7)	0.0224(6)	0.0063(5)	0.0011(6)	-0.0037(6)
C15	0.0264(7)	0.0284(7)	0.0309(7)	0.0066(6)	-0.0006(6)	0.0037(6)
C16	0.0181(6)	0.0264(7)	0.0247(6)	0.0020(5)	0.0023(5)	0.0002(5)
C17	0.0178(6)	0.0313(7)	0.0170(5)	0.0034(5)	0.0021(5)	-0.0014(5)
C18	0.0283(7)	0.0483(10)	0.0269(7)	-0.0111(7)	0.0063(6)	-0.0047(7)
C19	0.0370(9)	0.0718(13)	0.0287(8)	-0.0135(8)	0.0090(7)	0.0062(9)
C20	0.0298(8)	0.0782(14)	0.0294(8)	0.0133(9)	0.0133(7)	0.0100(8)
C21	0.0222(7)	0.0534(11)	0.0439(9)	0.0213(8)	0.0092(7)	-0.0010(7)
C22	0.0204(6)	0.0325(8)	0.0312(7)	0.0105(6)	0.0024(5)	-0.0014(6)
C23	0.0172(6)	0.0206(6)	0.0206(6)	-0.0041(5)	0.0000(5)	-0.0003(5)
C24	0.0259(7)	0.0235(6)	0.0222(6)	-0.0018(5)	-0.0001(5)	-0.0008(5)
C25	0.0308(7)	0.0328(8)	0.0197(6)	-0.0026(5)	-0.0025(5)	0.0071(6)
C26	0.0188(6)	0.0424(9)	0.0262(7)	-0.0110(6)	-0.0024(5)	0.0041(6)
C27	0.0190(6)	0.0357(8)	0.0318(7)	-0.0099(6)	0.0027(5)	-0.0060(6)
C28	0.0191(6)	0.0244(7)	0.0241(6)	-0.0035(5)	0.0027(5)	-0.0017(5)
C29	0.0157(5)	0.0218(6)	0.0194(6)	-0.0002(5)	0.0034(4)	0.0001(5)
C30	0.0226(7)	0.0290(7)	0.0299(7)	-0.0084(6)	0.0063(5)	-0.0027(5)
C31	0.0281(7)	0.0361(8)	0.0342(8)	-0.0112(6)	0.0103(6)	0.0016(6)
C32	0.0211(7)	0.0419(9)	0.0325(7)	-0.0031(6)	0.0098(6)	0.0007(6)
C33	0.0193(6)	0.0346(8)	0.0250(6)	-0.0004(6)	0.0040(5)	-0.0059(5)
C34	0.0205(6)	0.0232(6)	0.0191(6)	-0.0001(5)	0.0030(5)	-0.0023(5)
C35	0.0175(6)	0.0158(6)	0.0171(5)	0.0003(4)	0.0024(4)	-0.0008(4)
C36	0.0172(6)	0.0237(6)	0.0189(6)	-0.0016(5)	0.0002(4)	0.0001(5)
C37	0.0245(6)	0.0267(7)	0.0192(6)	-0.0042(5)	0.0033(5)	-0.0039(5)
C38	0.0305(7)	0.0189(6)	0.0217(6)	-0.0020(5)	0.0076(5)	0.0004(5)
C39	0.0253(6)	0.0209(6)	0.0239(6)	0.0012(5)	0.0020(5)	0.0064(5)
C40	0.0206(6)	0.0194(6)	0.0189(6)	-0.0003(5)	-0.0004(5)	0.0011(5)
C41	0.0164(5)	0.0172(6)	0.0172(5)	-0.0023(4)	-0.0004(4)	0.0004(4)
C42	0.0223(6)	0.0206(6)	0.0199(6)	0.0002(5)	0.0025(5)	-0.0027(5)
C43	0.0273(7)	0.0261(7)	0.0176(6)	0.0014(5)	0.0002(5)	0.0027(5)
C44	0.0223(6)	0.0319(7)	0.0207(6)	-0.0042(5)	-0.0043(5)	0.0027(5)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C45	0.0196(6)	0.0272(7)	0.0272(7)	-0.0045(5)	-0.0010(5)	-0.0052(5)
C46	0.0202(6)	0.0202(6)	0.0205(6)	-0.0004(5)	0.0022(5)	-0.0014(5)
C47	0.0186(6)	0.0159(6)	0.0177(5)	-0.0005(4)	-0.0003(4)	-0.0006(4)
C48	0.0223(6)	0.0242(6)	0.0202(6)	0.0010(5)	0.0026(5)	0.0007(5)
C49	0.0345(8)	0.0280(7)	0.0214(6)	0.0023(5)	0.0034(6)	-0.0076(6)
C50	0.0429(9)	0.0247(7)	0.0264(7)	0.0086(6)	-0.0060(6)	-0.0068(6)
C51	0.0293(7)	0.0231(7)	0.0422(9)	0.0103(6)	-0.0088(6)	-0.0002(6)
C52	0.0199(6)	0.0198(6)	0.0319(7)	0.0037(5)	-0.0012(5)	0.0010(5)
C1'	0.0139(16)	0.045(3)	0.0235(18)	-0.008(2)	-0.0014(12)	0.0033(16)
N1	0.0235(6)	0.0335(7)	0.0289(6)	-0.0046(5)	0.0016(5)	-0.0024(5)
N2	0.0220(6)	0.0348(7)	0.0337(7)	-0.0103(5)	-0.0046(5)	0.0057(5)
N3	0.029(2)	0.050(5)	0.039(3)	0.008(4)	0.009(2)	0.007(3)
N4	0.0263(19)	0.049(3)	0.029(2)	-0.005(2)	0.0062(15)	0.010(2)
N5	0.034(2)	0.056(4)	0.042(4)	0.021(4)	0.007(2)	-0.002(3)
N6	0.0211(6)	0.0333(7)	0.0291(6)	0.0019(5)	0.0010(5)	-0.0019(5)
N7	0.0214(6)	0.0259(6)	0.0374(7)	0.0093(5)	-0.0034(5)	-0.0041(5)
N8	0.0246(7)	0.0407(8)	0.0591(9)	0.0110(7)	0.0049(6)	-0.0102(6)
N9	0.0263(7)	0.0529(9)	0.0538(9)	0.0091(8)	0.0109(6)	-0.0050(6)
N10	0.0301(7)	0.0559(9)	0.0296(7)	-0.0012(6)	0.0061(5)	0.0104(6)
N11	0.0280(6)	0.0350(7)	0.0250(6)	0.0013(5)	-0.0022(5)	-0.0062(5)
N12	0.0246(6)	0.0321(7)	0.0272(6)	0.0031(5)	-0.0047(5)	-0.0054(5)
N13	0.0186(5)	0.0190(5)	0.0258(5)	0.0056(4)	-0.0029(4)	-0.0017(4)
N14	0.0192(5)	0.0200(5)	0.0237(5)	0.0033(4)	-0.0014(4)	-0.0008(4)
N15	0.0303(6)	0.0261(6)	0.0254(6)	0.0035(5)	0.0046(5)	-0.0009(5)
N16	0.0175(5)	0.0192(5)	0.0267(5)	-0.0016(4)	0.0025(4)	0.0006(4)
N17	0.0156(5)	0.0194(5)	0.0275(6)	-0.0025(4)	0.0009(4)	0.0012(4)
N18	0.0199(6)	0.0355(7)	0.0286(6)	0.0010(5)	-0.0006(5)	0.0013(5)
N19	0.0216(6)	0.0363(7)	0.0262(6)	0.0020(5)	0.0005(5)	0.0019(5)
N20	0.0290(6)	0.0244(6)	0.0251(6)	-0.0025(5)	0.0039(5)	-0.0022(5)
N3'	0.027(2)	0.057(4)	0.041(5)	-0.007(3)	-0.003(2)	0.019(3)
N4'	0.0281(16)	0.062(3)	0.0433(18)	-0.012(2)	0.0096(12)	0.012(2)
N5'	0.034(2)	0.052(3)	0.0189(13)	-0.0038(19)	0.0036(16)	-0.014(2)
O1	0.040(2)	0.126(8)	0.092(6)	0.069(6)	0.029(2)	0.007(3)
O2	0.073(4)	0.045(3)	0.077(4)	0.032(3)	0.038(4)	0.015(3)
O3	0.0371(6)	0.0467(7)	0.0373(6)	-0.0069(5)	0.0080(5)	0.0003(5)
O4	0.0368(8)	0.1131(15)	0.0776(11)	-0.0381(10)	0.0203(7)	0.0103(8)
O5	0.0479(7)	0.0537(8)	0.0306(6)	-0.0113(5)	0.0086(5)	0.0035(6)
O6	0.0239(5)	0.0363(6)	0.0353(6)	0.0018(5)	0.0034(4)	-0.0021(4)
O7	0.0225(5)	0.0288(5)	0.0414(6)	-0.0022(5)	0.0079(4)	-0.0011(4)
O8	0.0441(7)	0.0545(8)	0.0360(6)	0.0187(6)	-0.0032(5)	-0.0097(6)
O1'	0.0377(18)	0.104(4)	0.0364(16)	0.0211(19)	0.0020(11)	-0.028(2)
O2'	0.048(2)	0.035(2)	0.0497(18)	-0.0029(15)	0.0110(16)	-0.0009(15)
P1	0.01580(14)	0.01999(16)	0.01659(14)	0.00039(12)	0.00058(11)	-0.00310(12)
P2	0.01431(14)	0.01535(14)	0.01623(14)	-0.00018(11)	0.00059(11)	-0.00011(11)

Table S28. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for $[PPh_4][BH_2(NTz)_2]$ **TPP[2]**.

	x/a	y/b	z/c	U(eq)
H6	0.5363	0.2856	0.1729	0.028
H7	0.5442	0.0863	0.1317	0.034
H8	0.4651	0.0097	0.0659	0.036
H9	0.3772	0.1305	0.0415	0.036
H10	0.3694	0.3326	0.0805	0.031
H12	0.5198	0.5382	0.0732	0.028
H13	0.5147	0.6831	-0.0016	0.033
H14	0.4324	0.8228	-0.0185	0.035
H15	0.3541	0.8172	0.0380	0.035
H16	0.3585	0.6741	0.1138	0.028
H18	0.4103	0.6713	0.2311	0.041
H19	0.3278	0.7029	0.2818	0.055
H20	0.2517	0.5489	0.2800	0.054
H21	0.2555	0.3675	0.2252	0.047
H22	0.3359	0.3368	0.1717	0.034
H24	0.4915	0.3791	0.2646	0.029
H25	0.5786	0.4090	0.3303	0.034
H26	0.6494	0.5656	0.3152	0.036
H27	0.6340	0.6913	0.2344	0.035
H28	0.5486	0.6597	0.1665	0.027
H30	0.0980	-0.0683	0.2617	0.032
H31	0.1940	-0.1028	0.2334	0.039
H32	0.2749	0.0322	0.2652	0.038
H33	0.2604	0.2039	0.3235	0.031
H34	0.1644	0.2398	0.3526	0.025
H36	0.1058	0.2364	0.4320	0.024
H37	0.0808	0.4226	0.4771	0.028
H38	-0.0077	0.5339	0.4431	0.028
H39	-0.0721	0.4591	0.3645	0.028
H40	-0.0461	0.2769	0.3171	0.024
H42	0.0306	0.2017	0.2296	0.025
H43	-0.0450	0.1922	0.1513	0.029
H44	-0.1276	0.0545	0.1517	0.031
H45	-0.1347	-0.0752	0.2299	0.03
H46	-0.0600	-0.0662	0.3094	0.024
H48	-0.0362	-0.0087	0.4050	0.027
H49	-0.0299	-0.1583	0.4783	0.034
H50	0.0632	-0.2553	0.5104	0.039
H51	0.1499	-0.2071	0.4687	0.039
H52	0.1437	-0.0670	0.3921	0.029
H1B	0.7968(7)	0.6991(17)	0.0259(7)	0.044(5)
H2B	0.7266(8)	0.7256(17)	-0.0274(8)	0.046(5)
H3B	0.1675(6)	0.5931(15)	0.4972(7)	0.027(4)
H4B	0.2434(7)	0.6553(14)	0.5301(7)	0.031(4)

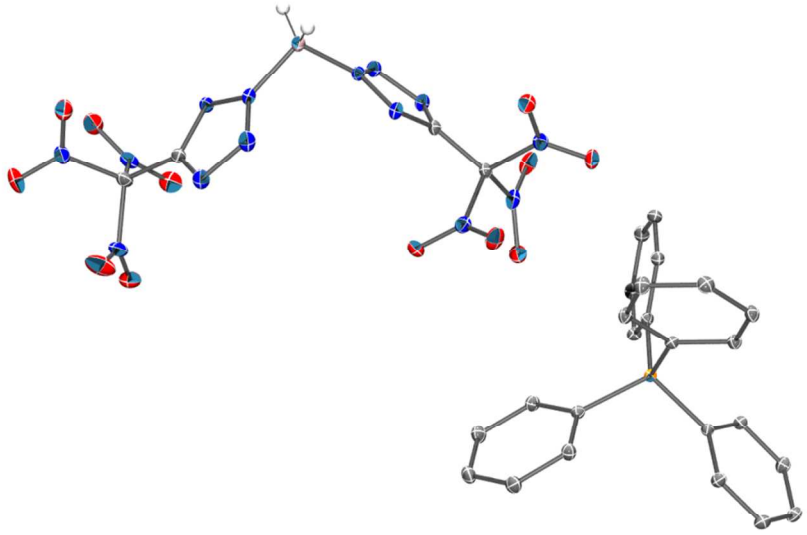

Figure S17: Asymmetric unit in the crystal structure of $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**.

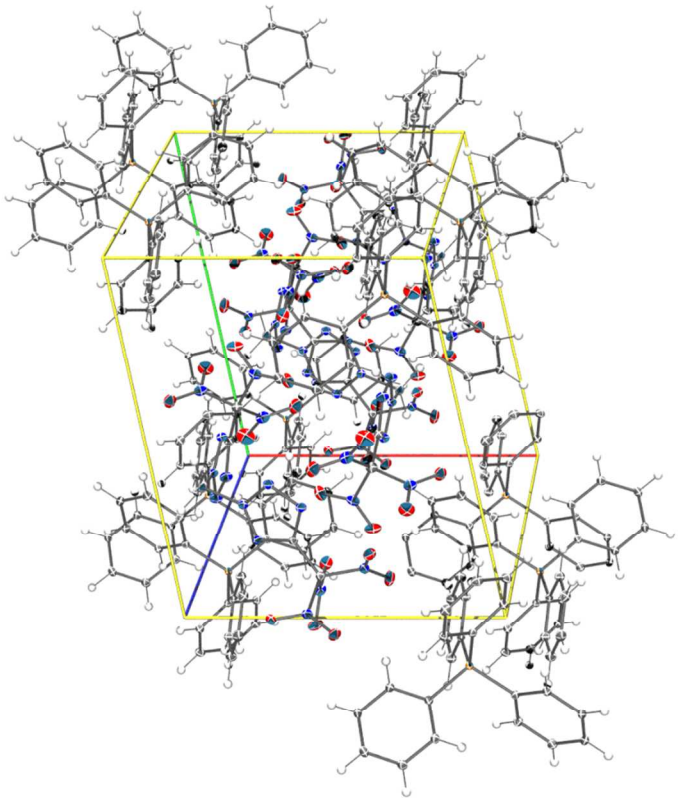

Figure S18: Unit cell of $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**. View normal to (001).

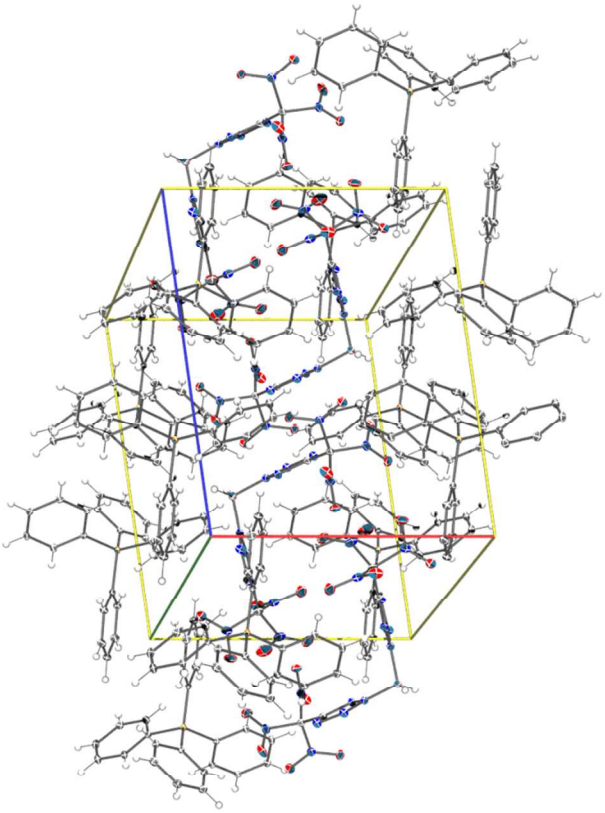

Figure S19: Unit cell of $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**. View normal to (010).

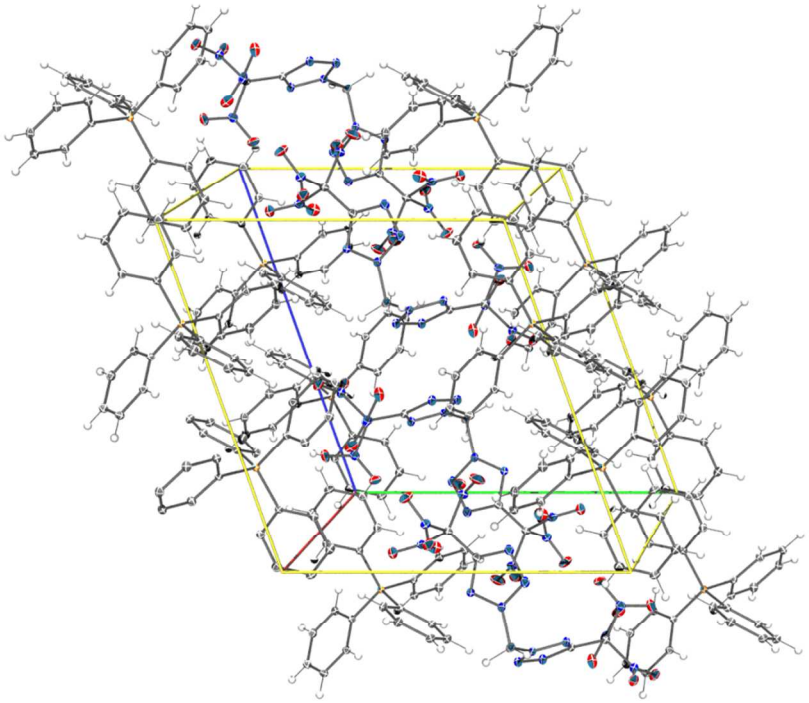

Figure S20: Unit cell of $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**. View normal to (100).

Table S29. Sample and crystal data for $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**.

Identification code	TPPBTNT	
Chemical formula	$C_{28}H_{22}BN_{14}O_{12}P$	
Formula weight	788.38	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.15 x 0.22 x 0.50 mm	
Crystal habit	clear colourless prism	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.0434(7) Å	α = 109.7350(10)°
	b = 12.7349(8) Å	β = 97.9540(10)°
	c = 13.7231(9) Å	γ = 102.8410(10)°
Volume	1722.62(19) $Å^3$	
Z	2	
Density (calculated)	1.520 Mg/cm^3	
Absorption coefficient	0.164 mm^{-1}	
F(000)	808	

Table S30. Data collection and structure refinement for $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**.

Diffractometer	Bruker APEX II CCD	
Radiation source	fine-focus tube, MoKα	
Theta range for data collection	1.62 to 30.46°	
Index ranges	-15<=h<=15, -18<=k<=18, -19<=l<=19	
Reflections collected	40440	
Independent reflections	10098 [R(int) = 0.0268]	
Coverage of independent reflections	96.2%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9757 and 0.9223	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	10098 / 0 / 513	
Goodness-of-fit on F^2	1.023	
Δ/σ_{max}	0.001	
Final R indices	8116 data; I>2σ(I)	R1 = 0.0414, wR2 = 0.1066
	all data	R1 = 0.0561, wR2 = 0.1154
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0579P)^2+0.9061P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.824 and -0.434 $eÅ^{-3}$	
R.M.S. deviation from mean	0.058 $eÅ^{-3}$	

Table S31. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
B1	0.24077(16)	0.48807(16)	0.27826(13)	0.0221(3)
C1	0.27196(13)	0.50121(12)	0.02479(11)	0.0193(3)
C2	0.29891(15)	0.56421(13)	0.95363(11)	0.0228(3)
C3	0.49730(13)	0.37557(11)	0.34574(10)	0.0164(2)
C4	0.55222(13)	0.27716(12)	0.33783(11)	0.0168(2)
C5	0.88461(12)	0.02013(12)	0.15276(10)	0.0158(2)
C6	0.92356(14)	0.12631(12)	0.14061(11)	0.0198(3)
C7	0.89705(15)	0.12971(14)	0.03972(12)	0.0240(3)
C8	0.83176(14)	0.02868(14)	0.95196(12)	0.0239(3)
C9	0.79208(14)	0.92307(13)	0.96376(12)	0.0235(3)
C10	0.81734(14)	0.91856(12)	0.06420(11)	0.0202(3)
C11	0.78162(12)	0.92594(11)	0.29951(10)	0.0152(2)
C12	0.66433(13)	0.94258(12)	0.26572(11)	0.0191(3)
C13	0.55442(13)	0.88236(13)	0.28424(12)	0.0212(3)
C14	0.56110(13)	0.80542(13)	0.33516(11)	0.0209(3)
C15	0.67719(13)	0.78874(12)	0.36840(11)	0.0198(3)
C16	0.78837(13)	0.84919(12)	0.35141(11)	0.0175(2)
C17	0.04145(12)	0.93068(11)	0.28054(10)	0.0149(2)
C18	0.01300(13)	0.81729(12)	0.20427(11)	0.0188(3)
C19	0.10166(14)	0.75515(12)	0.20268(11)	0.0209(3)
C20	0.21846(13)	0.80527(12)	0.27715(12)	0.0208(3)
C21	0.24598(13)	0.91685(12)	0.35360(12)	0.0206(3)
C22	0.15734(12)	0.97983(12)	0.35603(11)	0.0174(2)
C23	0.98180(12)	0.14872(11)	0.38498(10)	0.0151(2)
C24	0.09535(13)	0.22768(12)	0.38876(11)	0.0178(2)
C25	0.13960(14)	0.33670(12)	0.47103(11)	0.0210(3)
C26	0.07128(15)	0.36755(12)	0.54882(11)	0.0227(3)
C27	0.95914(14)	0.29014(12)	0.54562(11)	0.0211(3)
C28	0.91376(13)	0.18001(12)	0.46377(10)	0.0173(2)
N1	0.28481(12)	0.55831(10)	0.12825(9)	0.0193(2)
N2	0.24316(11)	0.47160(10)	0.15961(10)	0.0186(2)
N3	0.20808(13)	0.36787(11)	0.07973(10)	0.0264(3)
N4	0.22588(13)	0.38532(11)	0.99250(10)	0.0260(3)
N5	0.39736(14)	0.68266(12)	0.01742(10)	0.0269(3)
N6	0.17905(14)	0.58883(12)	0.90380(10)	0.0278(3)
N7	0.34233(16)	0.49367(13)	0.85713(11)	0.0318(3)
N8	0.37625(11)	0.35421(10)	0.29789(10)	0.0194(2)
N9	0.36470(11)	0.46134(10)	0.32245(9)	0.0175(2)
N10	0.47261(12)	0.54304(10)	0.38150(10)	0.0211(2)
N11	0.55912(12)	0.48952(10)	0.39731(10)	0.0209(2)
N12	0.69774(12)	0.31157(12)	0.36632(11)	0.0250(3)
N13	0.50893(12)	0.21217(11)	0.40889(10)	0.0222(2)
N14	0.50890(13)	0.18492(12)	0.22314(10)	0.0247(3)
O1	0.50363(12)	0.67845(12)	0.05084(11)	0.0393(3)
O2	0.35934(14)	0.76753(10)	0.03229(10)	0.0378(3)
O3	0.08829(12)	0.57646(12)	0.94353(10)	0.0352(3)

	x/a	y/b	z/c	U(eq)
O4	0.18765(14)	0.62046(13)	0.83026(10)	0.0414(3)
O5	0.45252(14)	0.52280(13)	0.85242(11)	0.0421(3)
O6	0.25444(17)	0.41165(13)	0.79285(11)	0.0539(4)
O7	0.74669(11)	0.39015(10)	0.45290(10)	0.0337(3)
O8	0.74889(12)	0.25508(13)	0.30280(11)	0.0374(3)
O9	0.58775(12)	0.17651(11)	0.44991(10)	0.0321(3)
O10	0.39800(10)	0.19951(10)	0.41441(9)	0.0268(2)
O11	0.46561(13)	0.08380(10)	0.21248(10)	0.0350(3)
O12	0.52449(12)	0.22456(12)	0.15495(9)	0.0324(3)
P1	0.92313(3)	0.00798(3)	0.27943(3)	0.01351(7)

Table S32. Bond lengths (Å) for $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**.

B1-N9	1.573(2)	B1-N2	1.575(2)
B1-H1	1.076(18)	B1-H2	1.059(19)
C1-N1	1.3288(18)	C1-N4	1.3400(19)
C1-C2	1.480(2)	C2-N5	1.530(2)
C2-N7	1.534(2)	C2-N6	1.548(2)
C3-N8	1.3292(17)	C3-N11	1.3436(17)
C3-C4	1.4881(19)	C4-N12	1.5247(18)
C4-N13	1.5371(18)	C4-N14	1.5425(18)
C5-C6	1.3981(19)	C5-C10	1.4012(18)
C5-P1	1.7981(14)	C6-C7	1.392(2)
C6-H6	0.95	C7-C8	1.388(2)
C7-H7	0.95	C8-C9	1.390(2)
C8-H8	0.95	C9-C10	1.391(2)
C9-H9	0.95	C10-H10	0.95
C11-C16	1.3985(18)	C11-C12	1.4000(18)
C11-P1	1.7881(13)	C12-C13	1.3890(19)
C12-H12	0.95	C13-C14	1.391(2)
C13-H13	0.95	C14-C15	1.386(2)
C14-H14	0.95	C15-C16	1.3910(19)
C15-H15	0.95	C16-H16	0.95
C17-C22	1.3937(18)	C17-C18	1.4021(18)
C17-P1	1.8036(13)	C18-C19	1.3870(19)
C18-H18	0.95	C19-C20	1.394(2)
C19-H19	0.95	C20-C21	1.388(2)
C20-H20	0.95	C21-C22	1.3937(19)
C21-H21	0.95	C22-H22	0.95
C23-C28	1.3998(18)	C23-C24	1.4045(18)
C23-P1	1.7891(13)	C24-C25	1.3886(19)
C24-H24	0.95	C25-C26	1.391(2)
C25-H25	0.95	C26-C27	1.386(2)
C26-H26	0.95	C27-C28	1.3955(19)
C27-H27	0.95	C28-H28	0.95
N1-N2	1.3289(16)	N2-N3	1.3319(17)
N3-N4	1.3215(19)	N5-O2	1.2094(19)
N5-O1	1.2190(19)	N6-O3	1.2107(19)
N6-O4	1.2139(18)	N7-O5	1.208(2)
N7-O6	1.225(2)	N8-N9	1.3304(16)
N9-N10	1.3310(16)	N10-N11	1.3252(17)
N12-O7	1.2183(18)	N12-O8	1.2206(19)
N13-O10	1.2160(16)	N13-O9	1.2221(16)
N14-O12	1.2186(17)	N14-O11	1.2198(18)

Table S33. Bond angles (°) for TPPBTNT.

N9-B1-N2	105.27(11)	N9-B1-H1	108.4(10)
N2-B1-H1	109.2(9)	N9-B1-H2	109.1(10)
N2-B1-H2	108.7(10)	H1-B1-H2	115.7(14)
N1-C1-N4	113.88(13)	N1-C1-C2	121.19(13)
N4-C1-C2	124.80(13)	C1-C2-N5	109.53(11)
C1-C2-N7	112.56(12)	N5-C2-N7	111.37(12)
C1-C2-N6	112.56(12)	N5-C2-N6	106.64(12)
N7-C2-N6	103.95(12)	N8-C3-N11	113.77(12)
N8-C3-C4	119.93(12)	N11-C3-C4	126.29(12)
C3-C4-N12	114.60(11)	C3-C4-N13	113.53(11)
N12-C4-N13	105.68(10)	C3-C4-N14	110.23(11)
N12-C4-N14	106.52(11)	N13-C4-N14	105.64(10)
C6-C5-C10	120.08(12)	C6-C5-P1	121.81(10)
C10-C5-P1	118.08(10)	C7-C6-C5	119.47(13)
C7-C6-H6	120.3	C5-C6-H6	120.3
C8-C7-C6	120.30(14)	C8-C7-H7	119.8
C6-C7-H7	119.8	C7-C8-C9	120.43(13)
C7-C8-H8	119.8	C9-C8-H8	119.8
C8-C9-C10	119.85(14)	C8-C9-H9	120.1
C10-C9-H9	120.1	C9-C10-C5	119.86(13)
C9-C10-H10	120.1	C5-C10-H10	120.1
C16-C11-C12	120.39(12)	C16-C11-P1	120.58(10)
C12-C11-P1	119.00(10)	C13-C12-C11	119.50(13)
C13-C12-H12	120.2	C11-C12-H12	120.2
C12-C13-C14	120.06(13)	C12-C13-H13	120.0
C14-C13-H13	120.0	C15-C14-C13	120.43(13)
C15-C14-H14	119.8	C13-C14-H14	119.8
C14-C15-C16	120.25(13)	C14-C15-H15	119.9
C16-C15-H15	119.9	C15-C16-C11	119.36(12)
C15-C16-H16	120.3	C11-C16-H16	120.3
C22-C17-C18	120.06(12)	C22-C17-P1	121.71(10)
C18-C17-P1	118.21(10)	C19-C18-C17	119.84(12)
C19-C18-H18	120.1	C17-C18-H18	120.1
C18-C19-C20	119.99(13)	C18-C19-H19	120.0
C20-C19-H19	120.0	C21-C20-C19	120.22(13)
C21-C20-H20	119.9	C19-C20-H20	119.9
C20-C21-C22	120.20(13)	C20-C21-H21	119.9
C22-C21-H21	119.9	C17-C22-C21	119.67(13)
C17-C22-H22	120.2	C21-C22-H22	120.2
C28-C23-C24	120.06(12)	C28-C23-P1	119.67(10)
C24-C23-P1	120.26(10)	C25-C24-C23	119.63(13)
C25-C24-H24	120.2	C23-C24-H24	120.2
C24-C25-C26	120.06(13)	C24-C25-H25	120.0
C26-C25-H25	120.0	C27-C26-C25	120.65(13)
C27-C26-H26	119.7	C25-C26-H26	119.7
C26-C27-C28	119.98(13)	C26-C27-H27	120.0
C28-C27-H27	120.0	C27-C28-C23	119.61(13)
C27-C28-H28	120.2	C23-C28-H28	120.2
C1-N1-N2	101.68(11)	N1-N2-N3	112.30(12)

N1-N2-B1	124.26(12)	N3-N2-B1	123.39(12)
N4-N3-N2	107.64(12)	N3-N4-C1	104.50(12)
O2-N5-O1	128.32(15)	O2-N5-C2	116.62(14)
O1-N5-C2	114.97(13)	O3-N6-O4	127.32(15)
O3-N6-C2	116.58(12)	O4-N6-C2	116.09(14)
O5-N7-O6	128.49(15)	O5-N7-C2	119.50(14)
O6-N7-C2	112.01(15)	C3-N8-N9	101.74(11)
N8-N9-N10	112.44(11)	N8-N9-B1	123.44(12)
N10-N9-B1	123.93(12)	N11-N10-N9	107.56(11)
N10-N11-C3	104.49(11)	O7-N12-O8	128.91(14)
O7-N12-C4	114.16(13)	O8-N12-C4	116.86(13)
O10-N13-O9	127.97(13)	O10-N13-C4	115.17(11)
O9-N13-C4	116.81(12)	O12-N14-O11	128.88(14)
O12-N14-C4	114.14(12)	O11-N14-C4	116.98(12)
C11-P1-C23	109.74(6)	C11-P1-C5	108.27(6)
C23-P1-C5	110.98(6)	C11-P1-C17	108.02(6)
C23-P1-C17	109.28(6)	C5-P1-C17	110.50(6)

Table S34. Anisotropic atomic displacement parameters ($Å^2$) for $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**.

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}
B1	0.0218(7)	0.0288(8)	0.0240(8)	0.0158(6)	0.0078(6)	0.0125(6)
C1	0.0209(6)	0.0182(6)	0.0174(6)	0.0052(5)	0.0027(5)	0.0065(5)
C2	0.0284(7)	0.0214(7)	0.0170(6)	0.0051(5)	0.0059(5)	0.0072(6)
C3	0.0164(6)	0.0167(6)	0.0175(6)	0.0087(5)	0.0031(5)	0.0042(5)
C4	0.0153(6)	0.0177(6)	0.0178(6)	0.0085(5)	0.0026(5)	0.0035(5)
C5	0.0136(5)	0.0180(6)	0.0174(6)	0.0075(5)	0.0046(4)	0.0057(5)
C6	0.0204(6)	0.0179(6)	0.0212(6)	0.0081(5)	0.0042(5)	0.0050(5)
C7	0.0251(7)	0.0254(7)	0.0257(7)	0.0148(6)	0.0066(6)	0.0067(6)
C8	0.0236(7)	0.0322(8)	0.0199(7)	0.0139(6)	0.0046(5)	0.0098(6)
C9	0.0228(7)	0.0257(7)	0.0189(6)	0.0066(5)	0.0004(5)	0.0067(6)
C10	0.0206(6)	0.0191(6)	0.0197(6)	0.0076(5)	0.0014(5)	0.0047(5)
C11	0.0132(5)	0.0145(6)	0.0168(6)	0.0053(4)	0.0032(4)	0.0032(4)
C12	0.0157(6)	0.0207(6)	0.0241(7)	0.0119(5)	0.0048(5)	0.0059(5)
C13	0.0131(6)	0.0256(7)	0.0273(7)	0.0129(6)	0.0046(5)	0.0056(5)
C14	0.0162(6)	0.0232(7)	0.0234(7)	0.0101(5)	0.0065(5)	0.0027(5)
C15	0.0195(6)	0.0222(6)	0.0206(6)	0.0119(5)	0.0056(5)	0.0055(5)
C16	0.0150(6)	0.0195(6)	0.0189(6)	0.0088(5)	0.0033(5)	0.0048(5)
C17	0.0138(5)	0.0162(6)	0.0160(6)	0.0072(5)	0.0047(4)	0.0048(4)
C18	0.0174(6)	0.0182(6)	0.0184(6)	0.0046(5)	0.0021(5)	0.0055(5)
C19	0.0215(7)	0.0177(6)	0.0233(7)	0.0060(5)	0.0067(5)	0.0071(5)
C20	0.0171(6)	0.0204(6)	0.0296(7)	0.0120(5)	0.0083(5)	0.0087(5)
C21	0.0136(6)	0.0217(7)	0.0260(7)	0.0096(5)	0.0019(5)	0.0051(5)
C22	0.0143(6)	0.0172(6)	0.0195(6)	0.0064(5)	0.0030(5)	0.0038(5)
C23	0.0139(5)	0.0153(6)	0.0159(6)	0.0058(4)	0.0023(4)	0.0047(4)
C24	0.0154(6)	0.0169(6)	0.0201(6)	0.0066(5)	0.0037(5)	0.0036(5)
C25	0.0197(6)	0.0173(6)	0.0224(7)	0.0071(5)	0.0010(5)	0.0016(5)
C26	0.0277(7)	0.0172(6)	0.0183(6)	0.0035(5)	0.0008(5)	0.0052(5)
C27	0.0256(7)	0.0219(7)	0.0163(6)	0.0056(5)	0.0055(5)	0.0101(5)
C28	0.0174(6)	0.0187(6)	0.0169(6)	0.0074(5)	0.0042(5)	0.0061(5)
N1	0.0233(6)	0.0172(5)	0.0185(5)	0.0076(4)	0.0050(4)	0.0068(4)
N2	0.0181(5)	0.0175(5)	0.0218(6)	0.0092(4)	0.0030(4)	0.0064(4)
N3	0.0314(7)	0.0183(6)	0.0241(6)	0.0069(5)	-0.0011(5)	0.0036(5)
N4	0.0314(7)	0.0189(6)	0.0223(6)	0.0051(5)	-0.0008(5)	0.0053(5)
N5	0.0339(7)	0.0236(6)	0.0207(6)	0.0078(5)	0.0087(5)	0.0029(5)
N6	0.0358(7)	0.0273(7)	0.0217(6)	0.0113(5)	0.0038(5)	0.0107(6)
N7	0.0481(9)	0.0301(7)	0.0217(6)	0.0089(5)	0.0152(6)	0.0171(6)
N8	0.0182(5)	0.0173(5)	0.0230(6)	0.0092(4)	0.0017(4)	0.0052(4)
N9	0.0188(5)	0.0169(5)	0.0186(5)	0.0086(4)	0.0047(4)	0.0054(4)
N10	0.0215(6)	0.0178(5)	0.0228(6)	0.0080(5)	0.0025(5)	0.0046(5)
N11	0.0201(6)	0.0174(5)	0.0241(6)	0.0086(5)	0.0020(4)	0.0040(4)
N12	0.0189(6)	0.0281(6)	0.0342(7)	0.0198(6)	0.0049(5)	0.0071(5)
N13	0.0237(6)	0.0208(6)	0.0240(6)	0.0110(5)	0.0057(5)	0.0061(5)
N14	0.0262(6)	0.0255(6)	0.0222(6)	0.0073(5)	0.0036(5)	0.0112(5)
O1	0.0287(6)	0.0415(7)	0.0393(7)	0.0108(6)	0.0068(5)	0.0024(5)
O2	0.0572(8)	0.0216(6)	0.0325(6)	0.0095(5)	0.0072(6)	0.0106(6)
O3	0.0346(6)	0.0457(7)	0.0360(7)	0.0232(6)	0.0104(5)	0.0188(6)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O4	0.0501(8)	0.0515(8)	0.0290(6)	0.0265(6)	0.0051(6)	0.0122(7)
O5	0.0495(8)	0.0525(8)	0.0379(7)	0.0199(6)	0.0248(6)	0.0279(7)
O6	0.0724(11)	0.0404(8)	0.0290(7)	-0.0053(6)	0.0143(7)	0.0058(7)
O7	0.0239(6)	0.0223(5)	0.0444(7)	0.0089(5)	-0.0096(5)	0.0032(4)
O8	0.0313(6)	0.0618(9)	0.0408(7)	0.0325(7)	0.0201(5)	0.0278(6)
O9	0.0341(6)	0.0412(7)	0.0363(6)	0.0267(6)	0.0113(5)	0.0197(5)
O10	0.0219(5)	0.0300(6)	0.0361(6)	0.0198(5)	0.0119(4)	0.0076(4)
O11	0.0430(7)	0.0190(5)	0.0346(6)	0.0044(5)	-0.0044(5)	0.0100(5)
O12	0.0391(7)	0.0456(7)	0.0223(5)	0.0177(5)	0.0120(5)	0.0203(6)
P1	0.01163(14)	0.01360(15)	0.01497(15)	0.00534(11)	0.00281(11)	0.00332(11)

Table S35. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for $[PPh_4][BH_2(TNTz)_2]$ **TPP[3]**.

	x/a	y/b	z/c	U(eq)
H6	0.9677	0.1956	0.2007	0.024
H7	0.9238	0.2015	0.0309	0.029
H8	0.8141	0.0317	-0.1166	0.029
H9	0.7478	-0.1459	-0.0966	0.028
H10	0.7891	-0.1532	0.0727	0.024
H12	0.6599	-0.0053	0.2304	0.023
H13	0.4746	-0.1063	0.2621	0.025
H14	0.4856	-0.2360	0.3473	0.025
H15	0.6808	-0.2642	0.4029	0.024
H16	0.8681	-0.1615	0.3748	0.021
H18	0.9332	-0.2169	0.1538	0.023
H19	1.0828	-0.3215	0.1509	0.025
H20	1.2794	-0.2371	0.2755	0.025
H21	1.3255	-0.0496	0.4044	0.025
H22	1.1758	0.0559	0.4089	0.021
H24	1.1416	0.2066	0.3353	0.021
H25	1.2166	0.3903	0.4742	0.025
H26	1.1018	0.4424	0.6047	0.027
H27	0.9132	0.3120	0.5991	0.025
H28	0.8371	0.1266	0.4615	0.021
H1	0.2479(17)	0.5776(15)	0.3231(14)	0.020(4)
H2	0.1595(18)	0.4256(16)	0.2783(15)	0.025(5)

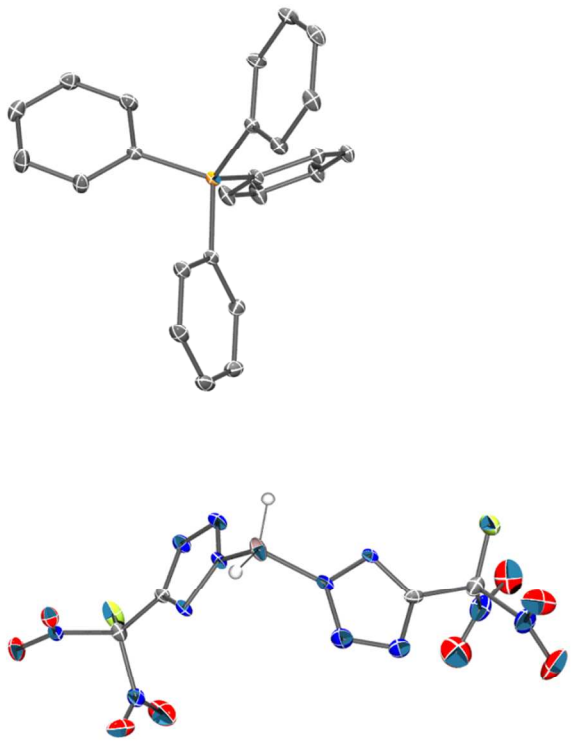

Figure S21: Asymmetric unit in the crystal structure of $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**.

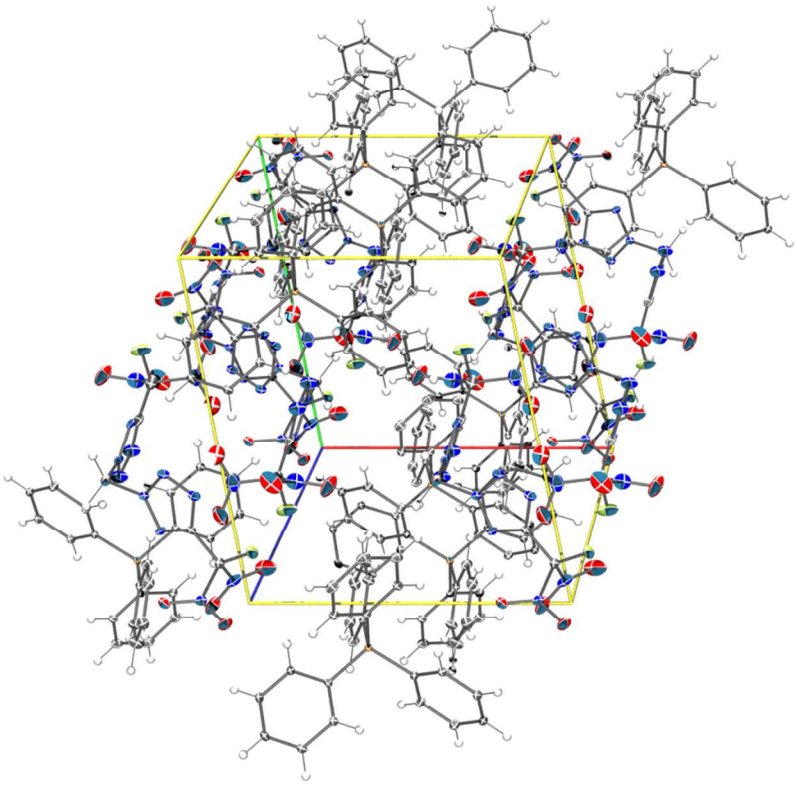

Figure S22: Unit cell of $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**. View normal to (001).

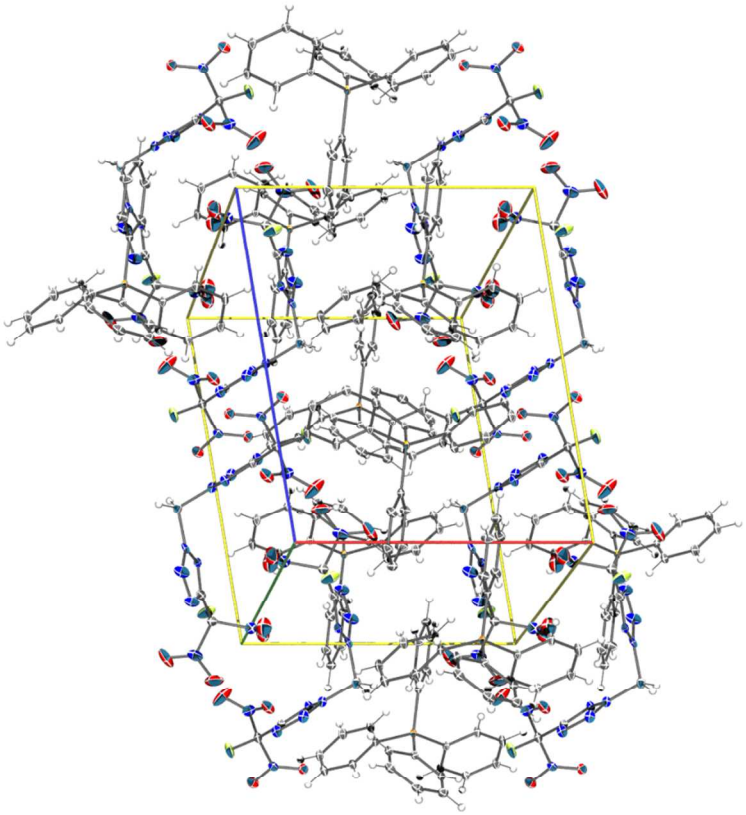

Figure S23: Unit cell of $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**. View normal to (010).

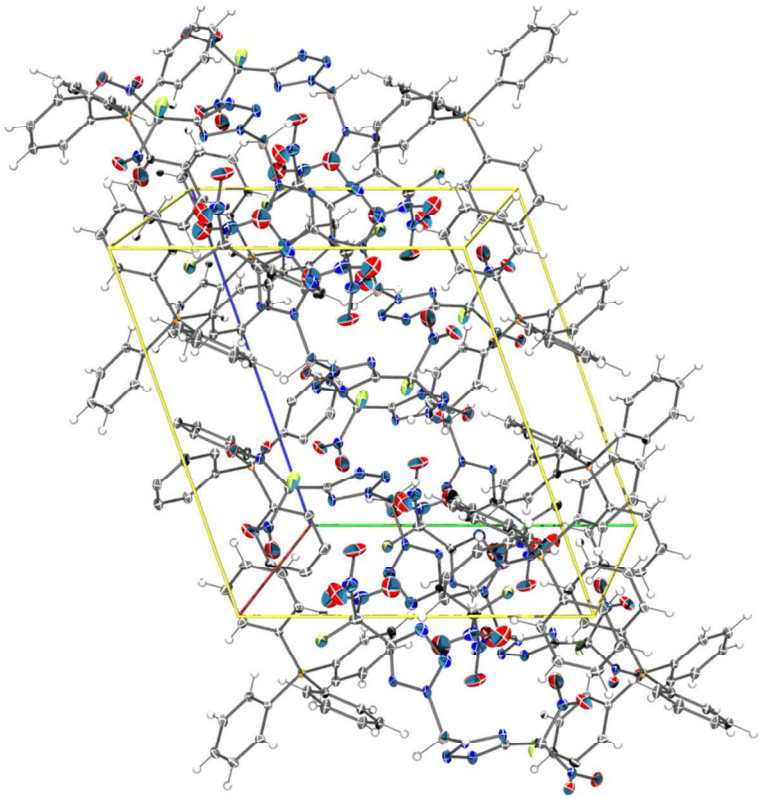

Figure S24: Unit cell of $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**. View normal to (100).

Table S36. Sample and crystal data for $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**.

Identification code	FDNTzBH2TPP	
Chemical formula	$C_{28}H_{22}BF_2N_{12}O_8P$	
Formula weight	734.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.120 x 0.520 x 0.630 mm	
Crystal habit	clear colourless prism	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.1504(6) Å	α = 109.3580(10)°
	b = 12.2645(6) Å	β = 99.4140(10)°
	c = 13.5087(7) Å	γ = 101.5770(10)°
Volume	1653.72(15) $Å^3$	
Z	2	
Density (calculated)	1.475 g/cm^3	
Absorption coefficient	0.163 mm^{-1}	
F(000)	752	

Table S37. Data collection and structure refinement for $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**.

Diffractometer	Bruker APEX II CCD	
Radiation source	fine-focus tube, MoKα	
Theta range for data collection	1.65 to 30.53°	
Index ranges	-15<=h<=15, -17<=k<=17, -18<=l<=19	
Reflections collected	40373	
Independent reflections	9869 [R(int) = 0.0216]	
Coverage of independent reflections	97.7%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9813 and 0.9047	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	9869 / 188 / 517	
Goodness-of-fit on F^2	1.042	
Δ/σ_{max}	0.001	
Final R indices	8258 data; I>2σ(I)	R1 = 0.0580, wR2 = 0.1561
	all data	R1 = 0.0690, wR2 = 0.1662
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0802P)^2+1.8199P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.178 and -0.958 $eÅ^{-3}$	
R.M.S. deviation from mean	0.075 $eÅ^{-3}$	

Table S38. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $[PPh_4][BH_2(FDNTz)_2]$ **TPP[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)
B1	0.2701(2)	0.5327(2)	0.7524(2)	0.0315(5)
C1	0.00399(15)	0.62441(15)	0.65244(14)	0.0200(3)
C2	0.93365(16)	0.70976(16)	0.63538(16)	0.0243(3)
C3	0.2238(5)	0.4644(3)	0.9875(4)	0.0256(7)
C4	0.1807(3)	0.3808(3)	0.0421(3)	0.0334(6)
C3A	0.2157(9)	0.4999(6)	0.9930(7)	0.0256(7)
C4A	0.1589(5)	0.4465(6)	0.0633(4)	0.0334(6)
C5	0.55392(14)	0.93850(14)	0.28580(13)	0.0172(3)
C6	0.66605(15)	0.99117(15)	0.36688(14)	0.0210(3)
C7	0.75771(16)	0.92880(16)	0.37014(16)	0.0252(3)
C8	0.73613(16)	0.81422(16)	0.29388(17)	0.0254(3)
C9	0.62351(18)	0.76062(16)	0.21344(16)	0.0264(4)
C10	0.53243(16)	0.82248(15)	0.20882(15)	0.0233(3)
C11	0.48071(14)	0.15952(14)	0.38222(13)	0.0170(3)
C12	0.59295(16)	0.24156(15)	0.38972(14)	0.0207(3)
C13	0.62957(18)	0.35653(16)	0.46949(16)	0.0269(4)
C14	0.5547(2)	0.38986(16)	0.54110(15)	0.0290(4)
C15	0.44436(19)	0.30903(18)	0.53446(15)	0.0283(4)
C16	0.40649(16)	0.19323(16)	0.45499(14)	0.0216(3)
C17	0.29266(14)	0.92169(14)	0.29248(14)	0.0181(3)
C18	0.30149(15)	0.83630(15)	0.33899(14)	0.0198(3)
C19	0.19187(16)	0.76476(16)	0.34622(15)	0.0234(3)
C20	0.07469(16)	0.77907(17)	0.30859(17)	0.0266(4)
C21	0.06586(16)	0.86497(18)	0.26340(18)	0.0292(4)
C22	0.17448(16)	0.93576(16)	0.25438(17)	0.0249(3)
C23	0.38932(14)	0.02275(14)	0.14741(13)	0.0170(3)
C24	0.31797(17)	0.91837(16)	0.05941(15)	0.0256(3)
C25	0.28466(18)	0.92227(17)	0.95719(15)	0.0282(4)
C26	0.32105(18)	0.02981(19)	0.94302(15)	0.0292(4)
C27	0.3930(2)	0.13310(19)	0.03014(17)	0.0333(4)
C28	0.42598(18)	0.13061(16)	0.13275(15)	0.0251(3)
F1	0.81259(11)	0.65551(13)	0.58568(14)	0.0454(4)
F2	0.1684(6)	0.2605(4)	0.9808(5)	0.0585(8)
F2A	0.0853(7)	0.5111(4)	0.1153(4)	0.0585(8)
N1	0.95559(15)	0.50515(14)	0.60109(14)	0.0282(3)
N2	0.04599(16)	0.45973(14)	0.63173(15)	0.0284(3)
N3	0.14307(14)	0.55064(13)	0.69898(13)	0.0226(3)
N4	0.12033(14)	0.65699(13)	0.71437(13)	0.0228(3)
N5	0.98754(15)	0.77895(13)	0.56838(12)	0.0234(3)
N6	0.9402(2)	0.80957(18)	0.74235(16)	0.0394(4)
N7	0.2092(4)	0.4291(4)	0.8821(5)	0.0195(7)
N8	0.2651(8)	0.5297(7)	0.8711(6)	0.0210(9)
N9	0.3122(10)	0.6203(6)	0.9661(5)	0.0425(12)
N10	0.2858(6)	0.5800(4)	0.0418(4)	0.0413(9)
N11	0.0470(4)	0.3742(4)	0.0609(3)	0.0476(7)
N12	0.2705(12)	0.4224(12)	0.1548(12)	0.0500(19)

	x/a	y/b	z/c	U(eq)
N7A	0.1872(8)	0.4471(8)	0.8853(9)	0.0195(7)
N8A	0.2509(16)	0.5326(12)	0.8579(10)	0.0210(9)
N9A	0.3113(18)	0.6326(11)	0.9439(10)	0.0425(12)
N10A	0.2891(11)	0.6135(7)	0.0294(8)	0.0413(9)
N11A	0.0864(6)	0.3123(6)	0.0021(5)	0.0476(7)
N12A	0.258(2)	0.442(2)	0.155(2)	0.0500(19)
O1	0.91567(16)	0.82550(15)	0.52937(14)	0.0388(4)
O2	0.09531(13)	0.78296(13)	0.56179(12)	0.0287(3)
O3	0.03132(19)	0.89518(17)	0.77632(14)	0.0496(5)
O4	0.8501(3)	0.7925(2)	0.7807(2)	0.0865(9)
O5	0.0208(5)	0.4647(5)	0.0840(5)	0.0794(11)
O6	0.9831(4)	0.2763(4)	0.0477(4)	0.0736(11)
O7	0.3720(5)	0.4097(5)	0.1580(5)	0.0733(14)
O8	0.226(2)	0.457(3)	0.2386(15)	0.076(3)
O5A	0.9732(8)	0.3003(8)	0.9987(8)	0.0794(11)
O6A	0.1745(11)	0.2644(13)	0.9825(13)	0.0736(11)
O7A	0.3566(11)	0.4339(10)	0.1334(9)	0.0733(14)
O8A	0.221(3)	0.469(5)	0.230(3)	0.076(3)
P1	0.43081(4)	0.01240(3)	0.27763(3)	0.01520(10)

Table S39. Bond lengths (Å) for $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**.

B1-N8A	1.476(14)	B1-N3	1.572(3)
B1-N8	1.626(8)	B1-H1B	1.114(16)
B1-H2B	1.116(17)	C1-N4	1.326(2)
C1-N1	1.342(2)	C1-C2	1.481(2)
C2-F1	1.328(2)	C2-N6	1.533(3)
C2-N5	1.544(2)	C3-N7	1.315(8)
C3-N10	1.333(6)	C3-C4	1.499(5)
C4-F2	1.398(6)	C4-N12	1.538(12)
C4-N11	1.543(5)	C3A-N7A	1.334(14)
C3A-N10A	1.345(10)	C3A-C4A	1.475(9)
C4A-F2A	1.369(7)	C4A-N12A	1.54(2)
C4A-N11A	1.546(9)	C5-C6	1.393(2)
C5-C10	1.401(2)	C5-P1	1.7984(16)
C6-C7	1.397(2)	C6-H6	0.95
C7-C8	1.385(3)	C7-H7	0.95
C8-C9	1.392(3)	C8-H8	0.95
C9-C10	1.390(2)	C9-H9	0.95
C10-H10	0.95	C11-C16	1.399(2)
C11-C12	1.405(2)	C11-P1	1.7921(16)
C12-C13	1.391(2)	C12-H12	0.95
C13-C14	1.393(3)	C13-H13	0.95
C14-C15	1.386(3)	C14-H14	0.95
C15-C16	1.396(2)	C15-H15	0.95
C16-H16	0.95	C17-C18	1.400(2)
C17-C22	1.400(2)	C17-P1	1.7922(16)
C18-C19	1.392(2)	C18-H18	0.95
C19-C20	1.389(2)	C19-H19	0.95
C20-C21	1.393(3)	C20-H20	0.95
C21-C22	1.390(2)	C21-H21	0.95
C22-H22	0.95	C23-C28	1.393(2)
C23-C24	1.399(2)	C23-P1	1.7972(17)
C24-C25	1.389(3)	C24-H24	0.95
C25-C26	1.385(3)	C25-H25	0.95
C26-C27	1.389(3)	C26-H26	0.95
C27-C28	1.387(3)	C27-H27	0.95
C28-H28	0.95	N1-N2	1.319(2)
N2-N3	1.328(2)	N3-N4	1.3338(19)
N5-O2	1.212(2)	N5-O1	1.221(2)
N6-O3	1.202(3)	N6-O4	1.216(3)
N7-N8	1.333(7)	N8-N9	1.325(7)
N9-N10	1.324(6)	N11-O5	1.160(6)
N11-O6	1.206(6)	N12-O7	1.169(14)
N12-O8	1.29(2)	N7A-N8A	1.337(12)
N8A-N9A	1.332(12)	N9A-N10A	1.304(10)
N11A-O5A	1.233(9)	N11A-O6A	1.262(15)
N12A-O8A	1.12(4)	N12A-O7A	1.20(3)

Table S40. Bond angles (°) for $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**.

N8A-B1-N3	102.8(7)	N8A-B1-N8	6.7(10)
N3-B1-N8	109.5(4)	N8A-B1-H1B	109.0(16)
N3-B1-H1B	106.5(15)	N8-B1-H1B	106.0(15)
N8A-B1-H2B	109.1(16)	N3-B1-H2B	109.9(16)
N8-B1-H2B	106.2(16)	H1B-B1-H2B	118.(2)
N4-C1-N1	113.96(15)	N4-C1-C2	124.24(15)
N1-C1-C2	121.73(16)	F1-C2-C1	112.13(15)
F1-C2-N6	107.83(17)	C1-C2-N6	111.97(15)
F1-C2-N5	107.10(15)	C1-C2-N5	113.68(14)
N6-C2-N5	103.59(14)	N7-C3-N10	113.9(4)
N7-C3-C4	123.0(4)	N10-C3-C4	123.0(4)
F2-C4-C3	113.3(3)	F2-C4-N12	111.4(6)
C3-C4-N12	109.4(7)	F2-C4-N11	101.4(4)
C3-C4-N11	115.0(3)	N12-C4-N11	105.9(7)
N7A-C3A-N10A	112.4(8)	N7A-C3A-C4A	123.8(8)
N10A-C3A-C4A	123.3(8)	F2A-C4A-C3A	112.2(5)
F2A-C4A-N12A	104.7(11)	C3A-C4A-N12A	113.1(13)
F2A-C4A-N11A	111.7(5)	C3A-C4A-N11A	112.4(5)
N12A-C4A-N11A	102.1(10)	C6-C5-C10	119.97(15)
C6-C5-P1	122.30(12)	C10-C5-P1	117.70(12)
C5-C6-C7	119.81(16)	C5-C6-H6	120.1
C7-C6-H6	120.1	C8-C7-C6	120.02(16)
C8-C7-H7	120.0	C6-C7-H7	120.0
C7-C8-C9	120.36(16)	C7-C8-H8	119.8
C9-C8-H8	119.8	C10-C9-C8	120.02(17)
C10-C9-H9	120.0	C8-C9-H9	120.0
C9-C10-C5	119.80(16)	C9-C10-H10	120.1
C5-C10-H10	120.1	C16-C11-C12	120.12(15)
C16-C11-P1	119.87(12)	C12-C11-P1	120.00(12)
C13-C12-C11	119.70(16)	C13-C12-H12	120.1
C11-C12-H12	120.1	C12-C13-C14	119.89(17)
C12-C13-H13	120.1	C14-C13-H13	120.1
C15-C14-C13	120.61(16)	C15-C14-H14	119.7
C13-C14-H14	119.7	C14-C15-C16	120.17(17)
C14-C15-H15	119.9	C16-C15-H15	119.9
C15-C16-C11	119.50(16)	C15-C16-H16	120.2
C11-C16-H16	120.2	C18-C17-C22	120.19(14)
C18-C17-P1	121.06(12)	C22-C17-P1	118.74(12)
C19-C18-C17	119.55(15)	C19-C18-H18	120.2
C17-C18-H18	120.2	C20-C19-C18	120.17(16)
C20-C19-H19	119.9	C18-C19-H19	119.9
C19-C20-C21	120.35(16)	C19-C20-H20	119.8
C21-C20-H20	119.8	C22-C21-C20	120.01(16)
C22-C21-H21	120.0	C20-C21-H21	120.0
C21-C22-C17	119.74(16)	C21-C22-H22	120.1
C17-C22-H22	120.1	C28-C23-C24	120.06(16)
C28-C23-P1	121.88(13)	C24-C23-P1	118.06(13)
C25-C24-C23	119.90(17)	C25-C24-H24	120.1
C23-C24-H24	120.1	C26-C25-C24	119.85(17)

C26-C25-H25	120.1	C24-C25-H25	120.1
C25-C26-C27	120.23(18)	C25-C26-H26	119.9
C27-C26-H26	119.9	C28-C27-C26	120.46(18)
C28-C27-H27	119.8	C26-C27-H27	119.8
C27-C28-C23	119.47(17)	C27-C28-H28	120.3
C23-C28-H28	120.3	N2-N1-C1	104.49(15)
N1-N2-N3	107.73(14)	N2-N3-N4	112.35(15)
N2-N3-B1	122.97(15)	N4-N3-B1	124.68(16)
C1-N4-N3	101.47(14)	O2-N5-O1	127.48(17)
O2-N5-C2	117.38(14)	O1-N5-C2	115.12(16)
O3-N6-O4	128.4(2)	O3-N6-C2	116.51(19)
O4-N6-C2	115.1(2)	C3-N7-N8	102.3(5)
N9-N8-N7	111.6(6)	N9-N8-B1	127.2(6)
N7-N8-B1	121.2(6)	N10-N9-N8	107.8(6)
N9-N10-C3	104.5(5)	O5-N11-O6	128.7(5)
O5-N11-C4	115.0(4)	O6-N11-C4	116.3(4)
O7-N12-O8	124.2(14)	O7-N12-C4	117.1(13)
O8-N12-C4	118.4(13)	C3A-N7A-N8A	102.0(9)
N9A-N8A-N7A	112.1(11)	N9A-N8A-B1	116.2(10)
N7A-N8A-B1	131.6(10)	N10A-N9A-N8A	107.5(11)
N9A-N10A-C3A	106.0(9)	O5A-N11A-O6A	148.8(10)
O5A-N11A-C4A	108.9(7)	O6A-N11A-C4A	102.2(8)
O8A-N12A-O7A	137.(3)	O8A-N12A-C4A	107.(3)
O7A-N12A-C4A	114.(2)	C11-P1-C17	111.17(8)
C11-P1-C23	109.98(7)	C17-P1-C23	106.79(7)
C11-P1-C5	109.59(7)	C17-P1-C5	107.60(7)
C23-P1-C5	111.67(7)		

Table S41. Torsion angles (°) for $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**.

N4-C1-C2-F1	-169.09(17)	N1-C1-C2-F1	14.1(3)
N4-C1-C2-N6	-47.7(2)	N1-C1-C2-N6	135.44(18)
N4-C1-C2-N5	69.2(2)	N1-C1-C2-N5	-107.59(19)
N7-C3-C4-F2	22.6(6)	N10-C3-C4-F2	-154.1(5)
N7-C3-C4-N12	147.6(6)	N10-C3-C4-N12	-29.1(8)
N7-C3-C4-N11	-93.4(4)	N10-C3-C4-N11	89.9(5)
N7A-C3A-C4A-F2A	-114.1(8)	N10A-C3A-C4A-F2A	56.9(11)
N7A-C3A-C4A-N12A	127.8(12)	N10A-C3A-C4A-N12A	-61.2(14)
N7A-C3A-C4A-N11A	12.8(9)	N10A-C3A-C4A-N11A	-176.2(8)
C10-C5-C6-C7	1.0(3)	P1-C5-C6-C7	179.08(13)
C5-C6-C7-C8	-1.0(3)	C6-C7-C8-C9	0.2(3)
C7-C8-C9-C10	0.5(3)	C8-C9-C10-C5	-0.5(3)
C6-C5-C10-C9	-0.3(3)	P1-C5-C10-C9	-178.44(14)
C16-C11-C12-C13	-0.3(2)	P1-C11-C12-C13	178.49(13)
C11-C12-C13-C14	-0.3(3)	C12-C13-C14-C15	0.7(3)
C13-C14-C15-C16	-0.5(3)	C14-C15-C16-C11	0.0(3)
C12-C11-C16-C15	0.4(2)	P1-C11-C16-C15	-178.35(13)
C22-C17-C18-C19	0.6(3)	P1-C17-C18-C19	-178.01(13)
C17-C18-C19-C20	-0.7(3)	C18-C19-C20-C21	0.0(3)
C19-C20-C21-C22	0.9(3)	C20-C21-C22-C17	-1.1(3)
C18-C17-C22-C21	0.3(3)	P1-C17-C22-C21	178.93(16)
C28-C23-C24-C25	0.5(3)	P1-C23-C24-C25	-179.54(14)
C23-C24-C25-C26	-0.7(3)	C24-C25-C26-C27	1.4(3)
C25-C26-C27-C28	-1.9(3)	C26-C27-C28-C23	1.7(3)
C24-C23-C28-C27	-1.0(3)	P1-C23-C28-C27	179.04(16)
N4-C1-N1-N2	-0.2(2)	C2-C1-N1-N2	176.93(16)
C1-N1-N2-N3	0.2(2)	N1-N2-N3-N4	-0.1(2)
N1-N2-N3-B1	-179.48(17)	N8A-B1-N3-N2	-94.5(6)
N8-B1-N3-N2	-94.2(4)	N8A-B1-N3-N4	86.2(6)
N8-B1-N3-N4	86.5(3)	N1-C1-N4-N3	0.1(2)
C2-C1-N4-N3	-176.94(16)	N2-N3-N4-C1	0.0(2)
B1-N3-N4-C1	179.34(17)	F1-C2-N5-O2	-143.68(16)
C1-C2-N5-O2	-19.3(2)	N6-C2-N5-O2	102.49(18)
F1-C2-N5-O1	37.5(2)	C1-C2-N5-O1	161.97(16)
N6-C2-N5-O1	-76.28(19)	F1-C2-N6-O3	-151.28(18)
C1-C2-N6-O3	84.9(2)	N5-C2-N6-O3	-38.0(2)
F1-C2-N6-O4	27.2(3)	C1-C2-N6-O4	-96.6(2)
N5-C2-N6-O4	140.5(2)	N10-C3-N7-N8	-0.4(6)
C4-C3-N7-N8	-177.3(5)	C3-N7-N8-N9	0.7(9)
C3-N7-N8-B1	-179.1(6)	N8A-B1-N8-N9	-94.(7)
N3-B1-N8-N9	-96.6(10)	N8A-B1-N8-N7	86.(6)
N3-B1-N8-N7	83.2(8)	N7-N8-N9-N10	-0.8(11)
B1-N8-N9-N10	178.9(8)	N8-N9-N10-C3	0.5(10)
N7-C3-N10-N9	-0.1(8)	C4-C3-N10-N9	176.9(6)
F2-C4-N11-O5	-159.9(5)	C3-C4-N11-O5	-37.2(5)
N12-C4-N11-O5	83.7(7)	F2-C4-N11-O6	18.6(5)
C3-C4-N11-O6	141.3(4)	N12-C4-N11-O6	-97.7(7)
F2-C4-N12-O7	55.2(14)	C3-C4-N12-O7	-70.9(12)
N11-C4-N12-O7	164.5(10)	F2-C4-N12-O8	-118.1(19)

C3-C4-N12-O8	115.8(19)	N11-C4-N12-O8	-9.(2)
N10A-C3A-N7A-N8A	2.2(12)	C4A-C3A-N7A-N8A	174.1(10)
C3A-N7A-N8A-N9A	-1.7(17)	C3A-N7A-N8A-B1	174.8(15)
N3-B1-N8A-N9A	-103.9(15)	N8-B1-N8A-N9A	78.(6)
N3-B1-N8A-N7A	79.6(18)	N8-B1-N8A-N7A	-98.(7)
N7A-N8A-N9A-N10A	1.(2)	B1-N8A-N9A-N10A	-176.5(14)
N8A-N9A-N10A-C3A	0.8(19)	N7A-C3A-N10A-N9A	-2.0(15)
C4A-C3A-N10A-N9A	-173.9(12)	F2A-C4A-N11A-O5A	12.2(8)
C3A-C4A-N11A-O5A	-114.9(7)	N12A-C4A-N11A-O5A	123.6(13)
F2A-C4A-N11A-O6A	-165.2(9)	C3A-C4A-N11A-O6A	67.7(10)
N12A-C4A-N11A-O6A	-53.8(14)	F2A-C4A-N12A-O8A	16.(4)
C3A-C4A-N12A-O8A	138.(3)	N11A-C4A-N12A-O8A	-101.(3)
F2A-C4A-N12A-O7A	-151.7(17)	C3A-C4A-N12A-O7A	-29.(2)
N11A-C4A-N12A-O7A	91.8(19)	C16-C11-P1-C17	-5.96(16)
C12-C11-P1-C17	175.25(13)	C16-C11-P1-C23	112.10(14)
C12-C11-P1-C23	-66.68(15)	C16-C11-P1-C5	-124.78(13)
C12-C11-P1-C5	56.44(15)	C18-C17-P1-C11	-100.46(15)
C22-C17-P1-C11	80.94(16)	C18-C17-P1-C23	139.56(14)
C22-C17-P1-C23	-39.04(16)	C18-C17-P1-C5	19.54(16)
C22-C17-P1-C5	-159.06(14)	C28-C23-P1-C11	16.27(16)
C24-C23-P1-C11	-163.65(13)	C28-C23-P1-C17	137.02(14)
C24-C23-P1-C17	-42.91(15)	C28-C23-P1-C5	-105.62(15)
C24-C23-P1-C5	74.46(15)	C6-C5-P1-C11	2.90(16)
C10-C5-P1-C11	-179.00(13)	C6-C5-P1-C17	-118.10(14)
C10-C5-P1-C17	59.99(15)	C6-C5-P1-C23	125.02(14)
C10-C5-P1-C23	-56.88(15)		

Table S42. Anisotropic atomic displacement parameters ($Å^2$) for $[PPh_4][BH_2(FDNTz)_2]$ **TPP[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}
B1	0.0259(10)	0.0351(11)	0.0498(13)	0.0285(10)	0.0166(9)	0.0161(8)
C1	0.0178(7)	0.0176(7)	0.0250(8)	0.0092(6)	0.0058(6)	0.0033(5)
C2	0.0175(7)	0.0253(8)	0.0325(9)	0.0144(7)	0.0051(6)	0.0064(6)
C3	0.0257(12)	0.025(2)	0.0227(10)	0.0020(17)	0.0035(8)	0.0130(16)
C4	0.0322(13)	0.0466(17)	0.0272(12)	0.0157(13)	0.0096(10)	0.0184(12)
C3A	0.0257(12)	0.025(2)	0.0227(10)	0.0020(17)	0.0035(8)	0.0130(16)
C4A	0.0322(13)	0.0466(17)	0.0272(12)	0.0157(13)	0.0096(10)	0.0184(12)
C5	0.0135(6)	0.0171(6)	0.0237(7)	0.0097(6)	0.0059(5)	0.0053(5)
C6	0.0154(7)	0.0194(7)	0.0275(8)	0.0100(6)	0.0028(6)	0.0035(6)
C7	0.0150(7)	0.0258(8)	0.0364(9)	0.0158(7)	0.0022(6)	0.0051(6)
C8	0.0176(7)	0.0239(8)	0.0423(10)	0.0187(7)	0.0097(7)	0.0097(6)
C9	0.0238(8)	0.0210(7)	0.0358(9)	0.0095(7)	0.0081(7)	0.0106(6)
C10	0.0185(7)	0.0192(7)	0.0290(8)	0.0059(6)	0.0027(6)	0.0064(6)
C11	0.0151(6)	0.0152(6)	0.0201(7)	0.0065(5)	0.0031(5)	0.0043(5)
C12	0.0181(7)	0.0169(7)	0.0249(8)	0.0077(6)	0.0034(6)	0.0018(6)
C13	0.0252(8)	0.0171(7)	0.0301(9)	0.0067(6)	-0.0036(7)	0.0002(6)
C14	0.0371(10)	0.0193(7)	0.0230(8)	0.0020(6)	-0.0029(7)	0.0101(7)
C15	0.0346(9)	0.0287(9)	0.0218(8)	0.0057(7)	0.0070(7)	0.0156(7)
C16	0.0201(7)	0.0239(8)	0.0225(8)	0.0090(6)	0.0064(6)	0.0086(6)
C17	0.0136(6)	0.0153(6)	0.0261(8)	0.0088(6)	0.0056(5)	0.0028(5)
C18	0.0161(7)	0.0198(7)	0.0251(8)	0.0114(6)	0.0040(6)	0.0045(6)
C19	0.0205(8)	0.0214(7)	0.0321(9)	0.0155(7)	0.0068(6)	0.0041(6)
C20	0.0168(7)	0.0256(8)	0.0422(10)	0.0193(8)	0.0098(7)	0.0029(6)
C21	0.0136(7)	0.0311(9)	0.0518(12)	0.0259(9)	0.0093(7)	0.0070(6)
C22	0.0151(7)	0.0234(8)	0.0438(10)	0.0206(7)	0.0090(7)	0.0065(6)
C23	0.0131(6)	0.0167(6)	0.0211(7)	0.0068(5)	0.0044(5)	0.0044(5)
C24	0.0252(8)	0.0183(7)	0.0272(8)	0.0052(6)	-0.0007(6)	0.0047(6)
C25	0.0264(8)	0.0267(8)	0.0235(8)	0.0030(7)	-0.0008(7)	0.0070(7)
C26	0.0257(8)	0.0389(10)	0.0216(8)	0.0124(7)	0.0048(6)	0.0050(7)
C27	0.0357(10)	0.0317(10)	0.0289(9)	0.0172(8)	0.0024(8)	-0.0035(8)
C28	0.0262(8)	0.0204(7)	0.0249(8)	0.0101(6)	0.0026(6)	-0.0015(6)
F1	0.0164(5)	0.0462(8)	0.0776(10)	0.0379(7)	-0.0009(6)	0.0023(5)
F2	0.107(2)	0.0398(12)	0.0528(14)	0.0277(11)	0.0460(15)	0.0342(14)
F2A	0.107(2)	0.0398(12)	0.0528(14)	0.0277(11)	0.0460(15)	0.0342(14)
N1	0.0250(7)	0.0188(7)	0.0363(8)	0.0100(6)	0.0041(6)	-0.0003(6)
N2	0.0288(8)	0.0168(6)	0.0388(9)	0.0103(6)	0.0102(7)	0.0039(6)
N3	0.0228(7)	0.0169(6)	0.0326(8)	0.0128(6)	0.0097(6)	0.0068(5)
N4	0.0217(7)	0.0157(6)	0.0306(7)	0.0094(5)	0.0024(6)	0.0064(5)
N5	0.0248(7)	0.0197(6)	0.0241(7)	0.0092(5)	0.0014(5)	0.0044(5)
N6	0.0601(12)	0.0384(10)	0.0390(10)	0.0211(8)	0.0239(9)	0.0341(9)
N7	0.0186(18)	0.0175(16)	0.0246(8)	0.0069(11)	0.0058(12)	0.0111(9)
N8	0.015(2)	0.0158(7)	0.0283(18)	0.0068(10)	-0.0044(14)	0.0053(10)
N9	0.0522(13)	0.0242(17)	0.032(3)	0.0034(15)	-0.008(2)	-0.0021(14)
N10	0.0535(14)	0.029(2)	0.0279(15)	0.0034(14)	-0.0021(12)	0.004(2)
N11	0.0386(15)	0.067(2)	0.0412(16)	0.0255(15)	0.0120(12)	0.0137(14)
N12	0.056(3)	0.050(5)	0.0315(10)	0.013(2)	-0.0052(16)	0.005(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N7A	0.0186(18)	0.0175(16)	0.0246(8)	0.0069(11)	0.0058(12)	0.0111(9)
N8A	0.015(2)	0.0158(7)	0.0283(18)	0.0068(10)	-0.0044(14)	0.0053(10)
N9A	0.0522(13)	0.0242(17)	0.032(3)	0.0034(15)	-0.008(2)	-0.0021(14)
N10A	0.0535(14)	0.029(2)	0.0279(15)	0.0034(14)	-0.0021(12)	0.004(2)
N11A	0.0386(15)	0.067(2)	0.0412(16)	0.0255(15)	0.0120(12)	0.0137(14)
N12A	0.056(3)	0.050(5)	0.0315(10)	0.013(2)	-0.0052(16)	0.005(2)
O1	0.0413(8)	0.0447(9)	0.0441(9)	0.0289(7)	0.0085(7)	0.0221(7)
O2	0.0244(6)	0.0279(6)	0.0348(7)	0.0155(6)	0.0074(5)	0.0028(5)
O3	0.0508(10)	0.0477(10)	0.0358(9)	-0.0034(7)	-0.0057(7)	0.0288(9)
O4	0.136(2)	0.0628(14)	0.112(2)	0.0468(14)	0.102(2)	0.0549(15)
O5	0.066(2)	0.084(3)	0.096(3)	0.036(2)	0.026(2)	0.030(2)
O6	0.0408(16)	0.090(3)	0.094(3)	0.050(2)	0.0130(17)	0.0019(16)
O7	0.052(2)	0.066(3)	0.073(3)	-0.001(2)	-0.0238(18)	0.0335(16)
O8	0.083(2)	0.094(6)	0.032(3)	0.022(3)	0.006(2)	-0.006(2)
O5A	0.066(2)	0.084(3)	0.096(3)	0.036(2)	0.026(2)	0.030(2)
O6A	0.0408(16)	0.090(3)	0.094(3)	0.050(2)	0.0130(17)	0.0019(16)
O7A	0.052(2)	0.066(3)	0.073(3)	-0.001(2)	-0.0238(18)	0.0335(16)
O8A	0.083(2)	0.094(6)	0.032(3)	0.022(3)	0.006(2)	-0.006(2)
P1	0.01139(17)	0.01329(17)	0.02075(19)	0.00666(14)	0.00397(13)	0.00261(13)

Table S43. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for $[PPh_4][BH_2(FDNTz)_2]$ **TPP[4]**.

	x/a	y/b	z/c	U(eq)
H6	0.6802	0.0693	0.4198	0.025
H7	0.8349	-0.0350	0.4247	0.03
H8	0.7985	-0.2281	0.2965	0.03
H9	0.6089	-0.3183	0.1617	0.032
H10	0.4558	-0.2138	0.1537	0.028
H12	0.6436	0.2186	0.3405	0.025
H13	0.7055	0.4122	0.4751	0.032
H14	0.5795	0.4687	0.5950	0.035
H15	0.3944	0.3325	0.5841	0.034
H16	0.3309	0.1377	0.4504	0.026
H18	0.3817	-0.1728	0.3655	0.024
H19	0.1972	-0.2940	0.3769	0.028
H20	0.0002	-0.2700	0.3137	0.032
H21	-0.0144	-0.1248	0.2388	0.035
H22	0.1685	-0.0065	0.2225	0.03
H24	0.2924	-0.1551	0.0695	0.031
H25	0.2370	-0.1487	-0.1029	0.034
H26	0.2967	0.0329	-0.1265	0.035
H27	0.4197	0.2060	0.0194	0.04
H28	0.4732	0.2019	0.1926	0.03
H1B	0.274(3)	0.4414(17)	0.702(2)	0.038(7)
H2B	0.351(2)	0.611(2)	0.766(2)	0.045(8)

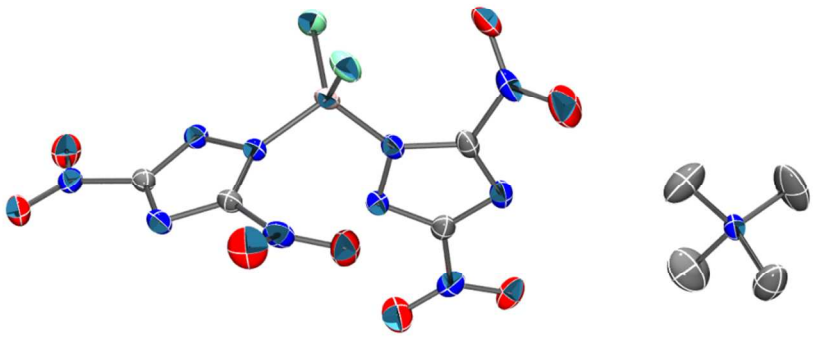

Figure S25: Asymmetric unit in the crystal structure of $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**.

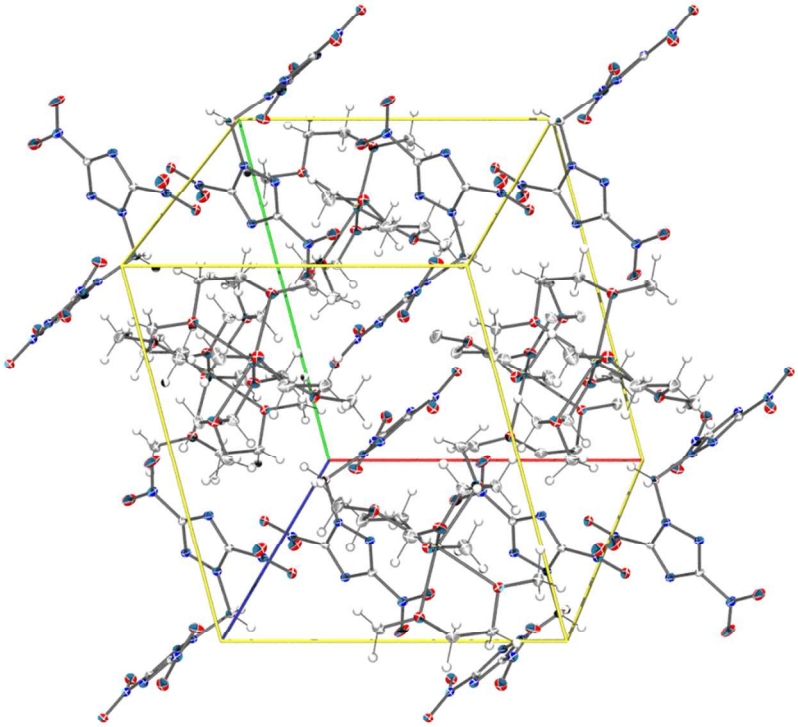

Figure S26: Unit cell of $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**. View normal to (001).

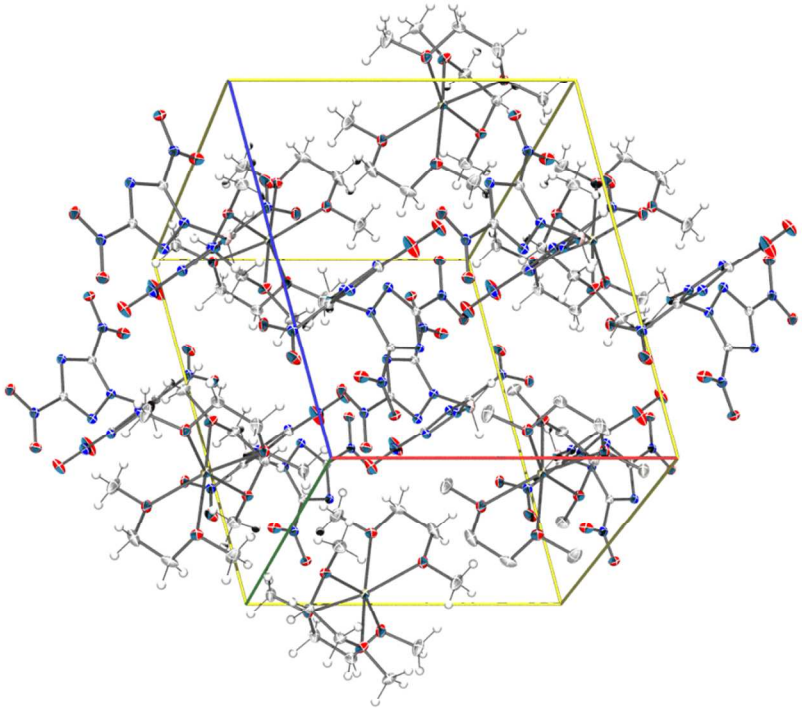

Figure S27: Unit cell of $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**. View normal to (010).

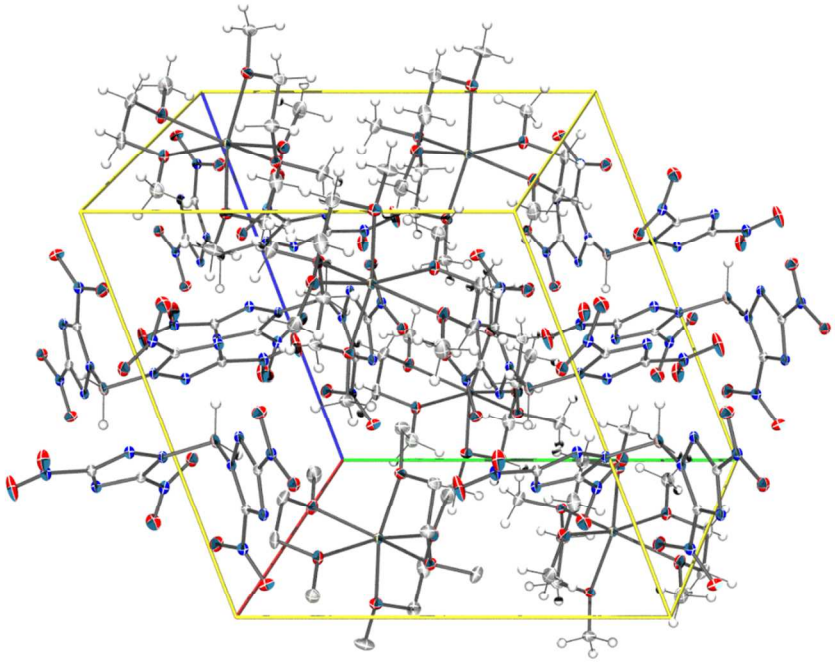

Figure S28: Unit cell of $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**. View normal to (100).

Table S45. Sample and crystal data for $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**.

Identification code	TMABCl2DNT2	
Chemical formula	$C_8H_{12}BCl_2N_{11}O_8$	
Formula weight	472.00	
Temperature	140(2) K	
Wavelength	0.71073 Å	
Crystal size	0.100 x 0.190 x 0.220 mm	
Crystal habit	clear colourless prism	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.4547(19) Å	α = 84.511(4)°
	b = 10.322(3) Å	β = 78.393(4)°
	c = 12.988(3) Å	γ = 77.534(4)°
Volume	954.5(4) $Å^3$	
Z	2	
Density (calculated)	1.642 g/cm^3	
Absorption coefficient	0.406 mm^{-1}	
F(000)	480	

Table S46. Data collection and structure refinement for $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**.

Diffractometer	Bruker APEX CCD	
Radiation source	fine-focus tube, MoKα	
Theta range for data collection	1.60 to 27.51°	
Index ranges	-6<=h<=9, -13<=k<=13, -16<=l<=16	
Reflections collected	5880	
Independent reflections	4103 [R(int) = 0.0170]	
Absorption correction	multi-scan	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2012 (Sheldrick, 2012)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	4103 / 6 / 292	
Goodness-of-fit on F^2	1.029	
Final R indices	3021 data; I>2σ(I)	R1 = 0.0580, wR2 = 0.1446
	all data	R1 = 0.0788, wR2 = 0.1619
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0765P)^2+0.7856P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.642 and -0.556 $eÅ^{-3}$	
R.M.S. deviation from mean	0.067 $eÅ^{-3}$	

Table S47. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $[NMe_4][BCl_2(DNT)_2]$ **TMA[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)
B1	0.7487(5)	0.8061(3)	0.7678(3)	0.0355(7)
C1	0.1058(4)	0.8581(3)	0.8993(2)	0.0337(6)
C2	0.9832(4)	0.9614(3)	0.7840(2)	0.0330(6)
C3	0.9989(4)	0.6793(3)	0.5230(2)	0.0368(7)
C4	0.7262(4)	0.7565(3)	0.5730(2)	0.0389(7)
C5	0.6115(12)	0.6937(8)	0.2959(5)	0.095(2)
C6	0.7074(11)	0.7480(6)	0.1152(5)	0.0751(17)
C7	0.5892(12)	0.5474(7)	0.1601(7)	0.107(3)
C8	0.8897(10)	0.5653(8)	0.2002(8)	0.105(3)
C5A	0.693(3)	0.5107(18)	0.2793(12)	0.095(2)
C6A	0.774(3)	0.7193(15)	0.2241(12)	0.0751(17)
C7A	0.512(3)	0.6717(17)	0.1696(18)	0.107(3)
C8A	0.835(3)	0.561(2)	0.1009(16)	0.105(3)
Cl1	0.56026(11)	0.95297(9)	0.77424(8)	0.0533(3)
Cl2	0.68112(14)	0.66742(9)	0.85279(7)	0.0547(3)
N1	0.9179(3)	0.8470(2)	0.80305(18)	0.0308(5)
N2	0.0015(3)	0.7785(2)	0.88094(18)	0.0341(5)
N3	0.0992(3)	0.9740(2)	0.8433(2)	0.0362(6)
N4	0.2157(4)	0.8229(3)	0.9823(2)	0.0444(6)
N5	0.9317(4)	0.0618(3)	0.7029(2)	0.0445(6)
N6	0.8141(3)	0.7607(2)	0.65354(19)	0.0342(5)
N7	0.9980(3)	0.7088(2)	0.61928(18)	0.0333(5)
N8	0.8366(4)	0.7062(3)	0.4891(2)	0.0411(6)
N9	0.1720(4)	0.6106(3)	0.4595(2)	0.0448(6)
N10	0.5233(4)	0.7962(3)	0.5799(3)	0.0542(8)
N11	0.6972(3)	0.6282(3)	0.19399(19)	0.0366(6)
O1	0.2799(3)	0.9104(3)	0.01021(19)	0.0560(6)
O2	0.2349(4)	0.7074(3)	0.0186(2)	0.0613(7)
O3	0.9104(5)	0.1765(2)	0.7251(3)	0.0732(9)
O4	0.9146(4)	0.0253(3)	0.6206(2)	0.0607(7)
O5	0.1586(4)	0.5618(2)	0.38031(17)	0.0515(6)
O6	0.3152(4)	0.6018(3)	0.4923(2)	0.0718(8)
O7	0.4712(4)	0.8564(4)	0.5032(3)	0.0850(10)
O8	0.4252(4)	0.7626(3)	0.6599(2)	0.0704(8)

Table S48. Bond lengths (Å) for $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**.

B1-N6	1.550(4)	B1-N1	1.574(4)
B1-Cl2	1.818(3)	B1-Cl1	1.827(4)
C1-N2	1.313(4)	C1-N3	1.336(4)
C1-N4	1.455(4)	C1-C2	2.010(4)
C2-N3	1.301(4)	C2-N1	1.355(3)
C2-N5	1.453(4)	C3-N7	1.314(4)
C3-N8	1.334(4)	C3-N9	1.462(4)
C3-C4	2.014(5)	C4-N8	1.302(4)
C4-N6	1.350(4)	C4-N10	1.466(4)
C5-N11	1.504(7)	C5-H5A	0.98
C5-H5B	0.98	C5-H5C	0.98
C6-N11	1.533(6)	C6-H6A	0.98
C6-H6B	0.98	C6-H6C	0.98
C7-N11	1.429(6)	C7-H7A	0.98
C7-H7B	0.98	C7-H7C	0.98
C8-N11	1.456(7)	C8-H8A	0.98
C8-H8B	0.98	C8-H8C	0.98
C5A-N11	1.563(15)	C5A-H5A1	0.98
C5A-H5A2	0.98	C5A-H5A3	0.98
C6A-N11	1.325(14)	C6A-H6A1	0.98
C6A-H6A2	0.98	C6A-H6A3	0.98
C7A-N11	1.445(16)	C7A-H7A1	0.98
C7A-H7A2	0.98	C7A-H7A3	0.98
C8A-N11	1.533(18)	C8A-H8A1	0.98
C8A-H8A2	0.98	C8A-H8A3	0.98
N1-N2	1.356(3)	N4-O1	1.222(4)
N4-O2	1.229(4)	N5-O4	1.206(4)
N5-O3	1.214(4)	N6-N7	1.359(3)
N9-O6	1.210(4)	N9-O5	1.218(3)
N10-O7	1.210(4)	N10-O8	1.212(4)

Table S49. Bond angles (°) for $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**.

N6-B1-N1	108.1(2)	N6-B1-Cl2	108.6(2)
N1-B1-Cl2	109.5(2)	N6-B1-Cl1	110.9(2)
N1-B1-Cl1	107.1(2)	Cl2-B1-Cl1	112.54(18)
N2-C1-N3	117.7(3)	N2-C1-N4	120.3(3)
N3-C1-N4	121.8(3)	N2-C1-C2	78.03(18)
N3-C1-C2	39.71(15)	N4-C1-C2	161.5(2)
N3-C2-N1	114.6(3)	N3-C2-N5	122.1(3)
N1-C2-N5	123.3(3)	N3-C2-C1	40.99(16)
N1-C2-C1	73.62(18)	N5-C2-C1	163.0(2)
N7-C3-N8	117.9(3)	N7-C3-N9	119.7(3)
N8-C3-N9	122.2(3)	N7-C3-C4	78.3(2)
N8-C3-C4	39.61(17)	N9-C3-C4	161.5(2)
N8-C4-N6	114.0(3)	N8-C4-N10	122.1(3)
N6-C4-N10	123.8(3)	N8-C4-C3	40.76(16)
N6-C4-C3	73.26(19)	N10-C4-C3	162.6(3)
N11-C5-H5A	109.5	N11-C5-H5B	109.5
H5A-C5-H5B	109.5	N11-C5-H5C	109.5
H5A-C5-H5C	109.5	H5B-C5-H5C	109.5
N11-C6-H6A	109.5	N11-C6-H6B	109.5
H6A-C6-H6B	109.5	N11-C6-H6C	109.5
H6A-C6-H6C	109.5	H6B-C6-H6C	109.5
N11-C7-H7A	109.5	N11-C7-H7B	109.5
H7A-C7-H7B	109.5	N11-C7-H7C	109.5
H7A-C7-H7C	109.5	H7B-C7-H7C	109.5
N11-C8-H8A	109.5	N11-C8-H8B	109.5
H8A-C8-H8B	109.5	N11-C8-H8C	109.5
H8A-C8-H8C	109.5	H8B-C8-H8C	109.5
N11-C5A-H5A1	109.5	N11-C5A-H5A2	109.5
H5A1-C5A-H5A2	109.5	N11-C5A-H5A3	109.5
H5A1-C5A-H5A3	109.5	H5A2-C5A-H5A3	109.5
N11-C6A-H6A1	109.5	N11-C6A-H6A2	109.5
H6A1-C6A-H6A2	109.5	N11-C6A-H6A3	109.5
H6A1-C6A-H6A3	109.5	H6A2-C6A-H6A3	109.5
N11-C7A-H7A1	109.5	N11-C7A-H7A2	109.5
H7A1-C7A-H7A2	109.5	N11-C7A-H7A3	109.5
H7A1-C7A-H7A3	109.5	H7A2-C7A-H7A3	109.5
N11-C8A-H8A1	109.5	N11-C8A-H8A2	109.5
H8A1-C8A-H8A2	109.5	N11-C8A-H8A3	109.5
H8A1-C8A-H8A3	109.5	H8A2-C8A-H8A3	109.5
C2-N1-N2	105.7(2)	C2-N1-B1	130.6(2)
N2-N1-B1	122.3(2)	C1-N2-N1	102.6(2)
C2-N3-C1	99.3(2)	O1-N4-O2	125.7(3)
O1-N4-C1	117.5(3)	O2-N4-C1	116.8(3)
O4-N5-O3	125.8(3)	O4-N5-C2	118.2(3)
O3-N5-C2	115.9(3)	C4-N6-N7	106.5(2)
C4-N6-B1	134.3(3)	N7-N6-B1	119.2(2)
C3-N7-N6	101.9(2)	C4-N8-C3	99.6(2)
O6-N9-O5	125.4(3)	O6-N9-C3	117.4(3)
O5-N9-C3	117.1(3)	O7-N10-O8	126.6(3)

O7-N10-C4	116.0(3)	O8-N10-C4	117.3(3)
C6A-N11-C7A	117.0(10)	C7-N11-C8	116.0(5)
C7-N11-C5	115.6(6)	C8-N11-C5	107.4(5)
C7-N11-C6	108.1(4)	C8-N11-C6	106.3(5)
C5-N11-C6	102.1(4)	C6A-N11-C8A	107.4(11)
C7A-N11-C8A	111.2(11)	C6A-N11-C5A	109.8(9)
C7A-N11-C5A	108.5(10)	C8A-N11-C5A	101.9(10)

Table S50. Torsion angles (°) for $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**.

N3-C2-N1-N2	-0.9(3)	N5-C2-N1-N2	178.1(3)
C1-C2-N1-N2	0.05(18)	N3-C2-N1-B1	165.5(3)
N5-C2-N1-B1	-15.5(5)	C1-C2-N1-B1	166.5(3)
N6-B1-N1-C2	81.5(4)	Cl2-B1-N1-C2	-160.4(2)
Cl1-B1-N1-C2	-38.1(4)	N6-B1-N1-N2	-114.0(3)
Cl2-B1-N1-N2	4.1(3)	Cl1-B1-N1-N2	126.4(2)
N3-C1-N2-N1	1.0(3)	N4-C1-N2-N1	177.7(2)
C2-C1-N2-N1	0.05(18)	C2-N1-N2-C1	-0.1(3)
B1-N1-N2-C1	-167.9(2)	N1-C2-N3-C1	1.4(3)
N5-C2-N3-C1	-177.6(3)	N2-C1-N3-C2	-1.5(3)
N4-C1-N3-C2	-178.1(3)	N2-C1-N4-O1	-165.7(3)
N3-C1-N4-O1	10.8(4)	C2-C1-N4-O1	6.9(8)
N2-C1-N4-O2	13.8(4)	N3-C1-N4-O2	-169.7(3)
C2-C1-N4-O2	-173.5(6)	N3-C2-N5-O4	140.9(3)
N1-C2-N5-O4	-37.9(4)	C1-C2-N5-O4	135.5(7)
N3-C2-N5-O3	-38.8(4)	N1-C2-N5-O3	142.3(3)
C1-C2-N5-O3	-44.3(9)	N8-C4-N6-N7	0.1(3)
N10-C4-N6-N7	176.2(3)	C3-C4-N6-N7	0.15(19)
N8-C4-N6-B1	-178.1(3)	N10-C4-N6-B1	-2.0(5)
C3-C4-N6-B1	-178.1(3)	N1-B1-N6-C4	-154.4(3)
Cl2-B1-N6-C4	86.9(4)	Cl1-B1-N6-C4	-37.3(4)
N1-B1-N6-N7	27.5(3)	Cl2-B1-N6-N7	-91.2(3)
Cl1-B1-N6-N7	144.7(2)	N8-C3-N7-N6	0.3(3)
N9-C3-N7-N6	-175.4(2)	C4-C3-N7-N6	0.15(19)
C4-N6-N7-C3	-0.2(3)	B1-N6-N7-C3	178.3(2)
N6-C4-N8-C3	0.0(3)	N10-C4-N8-C3	-176.2(3)
N7-C3-N8-C4	-0.2(3)	N9-C3-N8-C4	175.4(3)
N7-C3-N9-O6	-11.4(4)	N8-C3-N9-O6	173.1(3)
C4-C3-N9-O6	-177.6(6)	N7-C3-N9-O5	165.5(3)
N8-C3-N9-O5	-10.0(4)	C4-C3-N9-O5	-0.7(9)
N8-C4-N10-O7	-43.6(5)	N6-C4-N10-O7	140.6(3)
C3-C4-N10-O7	-52.0(10)	N8-C4-N10-O8	134.4(3)
N6-C4-N10-O8	-41.4(4)	C3-C4-N10-O8	126.0(8)

Table S51. Anisotropic atomic displacement parameters ($Å^2$) for $[NMe_4][BCl_2(DNT)_2]$ **TMA[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}
B1	0.0308(16)	0.0376(17)	0.0412(18)	-0.0025(14)	-0.0044(14)	-0.0156(14)
C1	0.0272(13)	0.0392(15)	0.0347(14)	-0.0077(12)	-0.0050(11)	-0.0048(11)
C2	0.0305(14)	0.0312(14)	0.0384(15)	-0.0025(12)	-0.0037(12)	-0.0109(11)
C3	0.0458(17)	0.0342(15)	0.0334(15)	0.0016(12)	-0.0078(13)	-0.0153(13)
C4	0.0405(16)	0.0376(16)	0.0456(17)	0.0010(13)	-0.0175(14)	-0.0157(13)
C5	0.122(6)	0.093(5)	0.052(3)	0.006(3)	-0.002(4)	0.002(4)
C6	0.112(5)	0.063(3)	0.057(3)	0.007(3)	-0.020(3)	-0.034(3)
C7	0.127(6)	0.078(4)	0.155(7)	0.022(5)	-0.085(6)	-0.065(5)
C8	0.076(4)	0.094(5)	0.137(7)	-0.009(5)	-0.034(5)	0.010(4)
C5A	0.122(6)	0.093(5)	0.052(3)	0.006(3)	-0.002(4)	0.002(4)
C6A	0.112(5)	0.063(3)	0.057(3)	0.007(3)	-0.020(3)	-0.034(3)
C7A	0.127(6)	0.078(4)	0.155(7)	0.022(5)	-0.085(6)	-0.065(5)
C8A	0.076(4)	0.094(5)	0.137(7)	-0.009(5)	-0.034(5)	0.010(4)
Cl1	0.0297(4)	0.0588(5)	0.0730(6)	-0.0219(4)	-0.0094(4)	-0.0046(3)
Cl2	0.0683(6)	0.0624(6)	0.0450(5)	0.0026(4)	-0.0065(4)	-0.0443(5)
N1	0.0305(12)	0.0320(12)	0.0316(12)	-0.0017(9)	-0.0050(10)	-0.0104(9)
N2	0.0346(13)	0.0345(13)	0.0329(12)	-0.0026(10)	-0.0048(10)	-0.0078(10)
N3	0.0296(12)	0.0389(13)	0.0425(14)	-0.0082(11)	-0.0051(10)	-0.0114(10)
N4	0.0345(14)	0.0633(19)	0.0351(13)	-0.0081(13)	-0.0056(11)	-0.0081(13)
N5	0.0433(15)	0.0382(15)	0.0542(17)	0.0112(12)	-0.0109(13)	-0.0169(12)
N6	0.0338(12)	0.0340(12)	0.0385(13)	-0.0006(10)	-0.0105(10)	-0.0117(10)
N7	0.0336(12)	0.0329(12)	0.0354(12)	-0.0034(10)	-0.0080(10)	-0.0091(10)
N8	0.0518(16)	0.0381(14)	0.0402(14)	0.0030(11)	-0.0188(12)	-0.0166(12)
N9	0.0565(17)	0.0383(14)	0.0383(14)	-0.0034(12)	-0.0018(13)	-0.0127(13)
N10	0.0426(16)	0.0600(19)	0.070(2)	-0.0130(16)	-0.0267(17)	-0.0127(14)
N11	0.0373(13)	0.0421(14)	0.0347(13)	-0.0007(11)	-0.0136(11)	-0.0116(11)
O1	0.0484(14)	0.0815(18)	0.0466(13)	-0.0171(12)	-0.0123(11)	-0.0221(13)
O2	0.0614(16)	0.0716(19)	0.0515(15)	0.0083(13)	-0.0230(13)	-0.0083(14)
O3	0.103(2)	0.0330(14)	0.090(2)	0.0113(13)	-0.0307(18)	-0.0212(14)
O4	0.0747(18)	0.0601(16)	0.0540(15)	0.0135(12)	-0.0290(14)	-0.0195(14)
O5	0.0827(18)	0.0352(12)	0.0359(12)	-0.0048(9)	-0.0092(12)	-0.0107(11)
O6	0.0437(15)	0.099(2)	0.0709(18)	-0.0373(16)	-0.0062(13)	-0.0010(14)
O7	0.0662(19)	0.095(2)	0.100(2)	0.0119(19)	-0.0491(19)	-0.0073(17)
O8	0.0430(14)	0.107(2)	0.0732(19)	-0.0237(17)	-0.0110(14)	-0.0333(16)

Table S52. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for $[NMe_4][BCl_2(DNT)_2]$ **TMA[5]**.

	x/a	y/b	z/c	U(eq)
H5A	0.4870	0.7463	0.2910	0.143
H5B	0.6908	0.7521	0.3096	0.143
H5C	0.6010	0.6255	0.3534	0.143
H6A	0.7704	0.7171	0.0455	0.113
H6B	0.7777	0.8063	0.1382	0.113
H6C	0.5806	0.7972	0.1114	0.113
H7A	0.6544	0.5117	0.0923	0.16
H7B	0.4667	0.6013	0.1523	0.16
H7C	0.5724	0.4740	0.2124	0.16
H8A	0.8918	0.4805	0.2413	0.157
H8B	0.9449	0.6236	0.2343	0.157
H8C	0.9618	0.5494	0.1290	0.157
H5A1	0.8036	0.4980	0.3121	0.143
H5A2	0.6937	0.4293	0.2461	0.143
H5A3	0.5799	0.5313	0.3331	0.143
H6A1	0.6780	0.7997	0.2406	0.113
H6A2	0.8729	0.7407	0.1672	0.113
H6A3	0.8269	0.6850	0.2868	0.113
H7A1	0.4187	0.6584	0.2323	0.16
H7A2	0.4992	0.6201	0.1129	0.16
H7A3	0.4931	0.7662	0.1469	0.16
H8A1	0.9064	0.6251	0.0612	0.157
H8A2	0.7659	0.5302	0.0547	0.157
H8A3	0.9210	0.4853	0.1271	0.157