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Supplementary Material

Acid form of Trofimenko's scorpionates, H(Tp$^{R,R'}$); comments on synthesis and solid-state structure of H(Tp^{tBu,Me})

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Acid Form of Trofimenko's Scorpionates, $H(Tp^{R,R'})$; Comments on Synthesis and Solid-State Structure of $H(Tp^{tBu,Me})$.

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STRUCTURE REPORT

XCL Code: TAK0502 **Date:** 20 May 2005

Updated: 13 September 2021

Compound: Hydrogen tris(3-*t*-butyl-5-methylpyrazolyl)borate

Formula: $C_{24}H_{41}BN_6$

Supervisor: J. Takats **Crystallographer:** R. McDonald

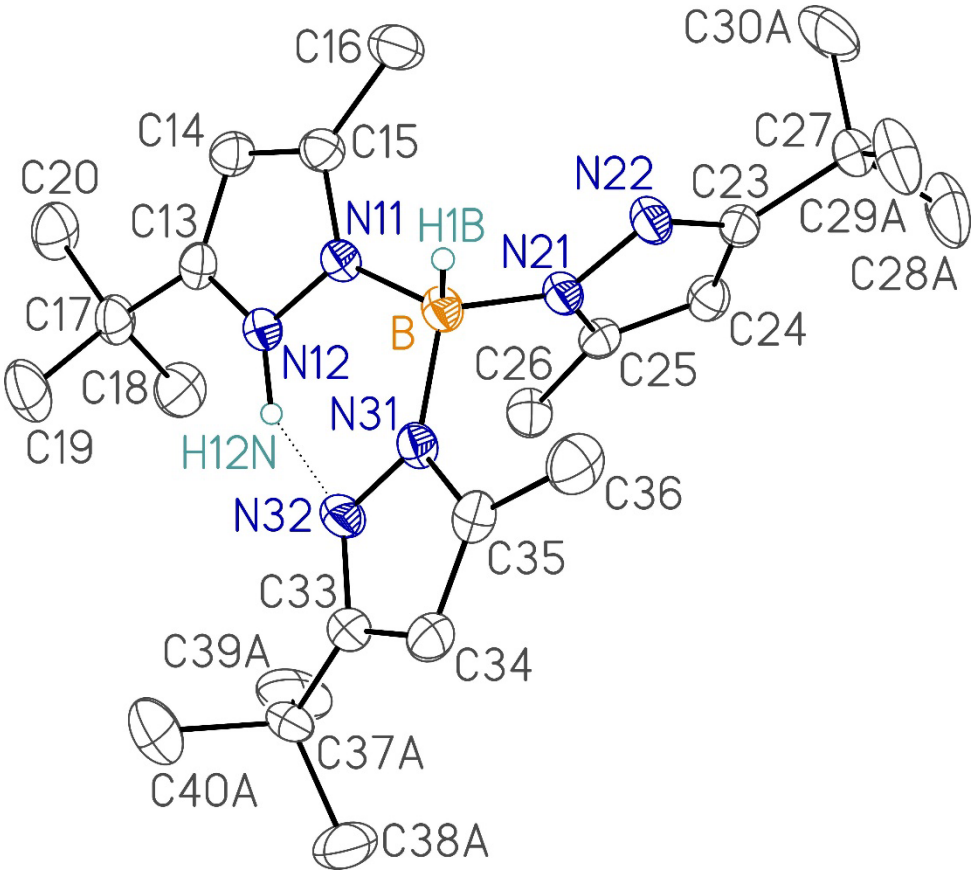
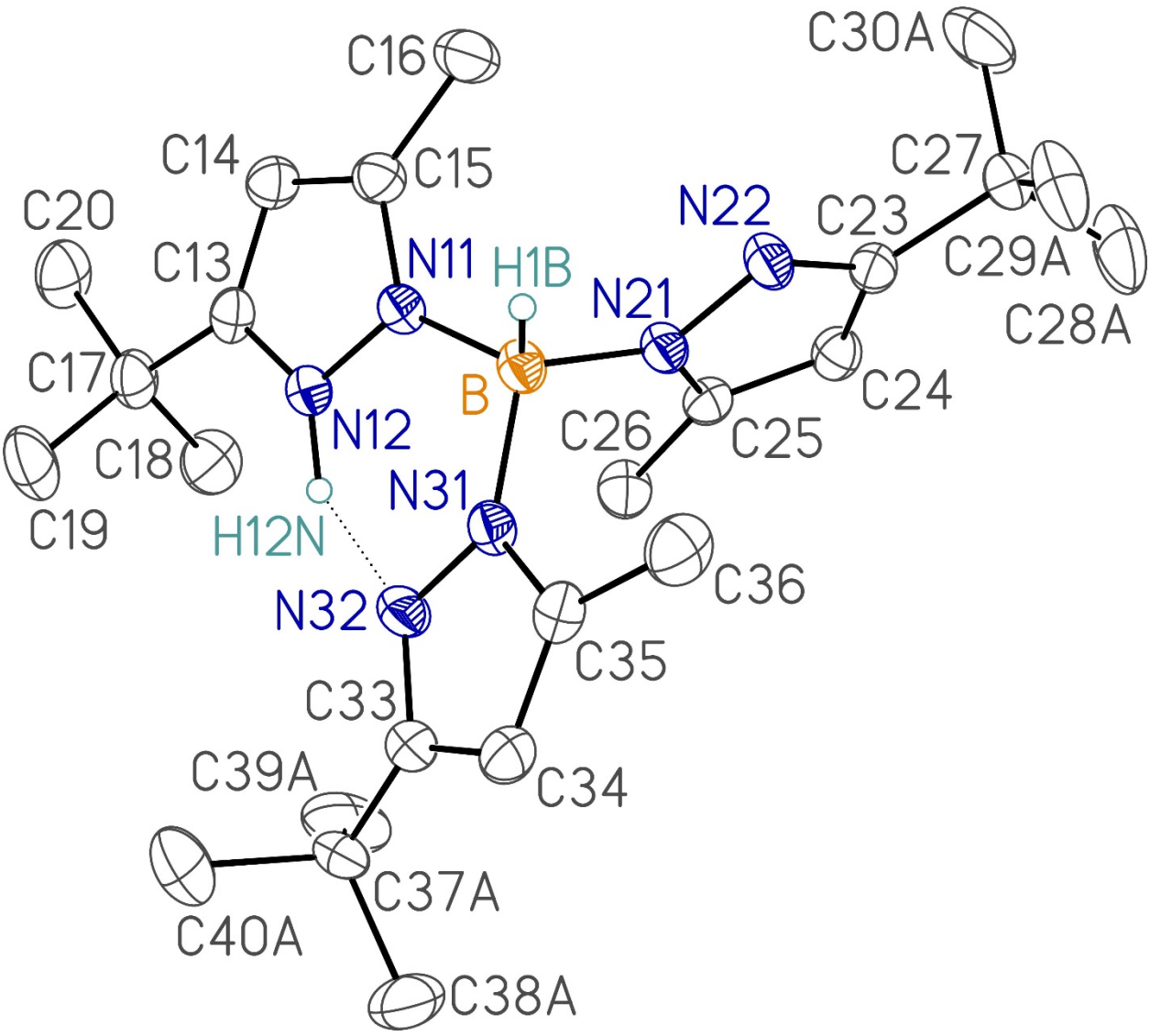
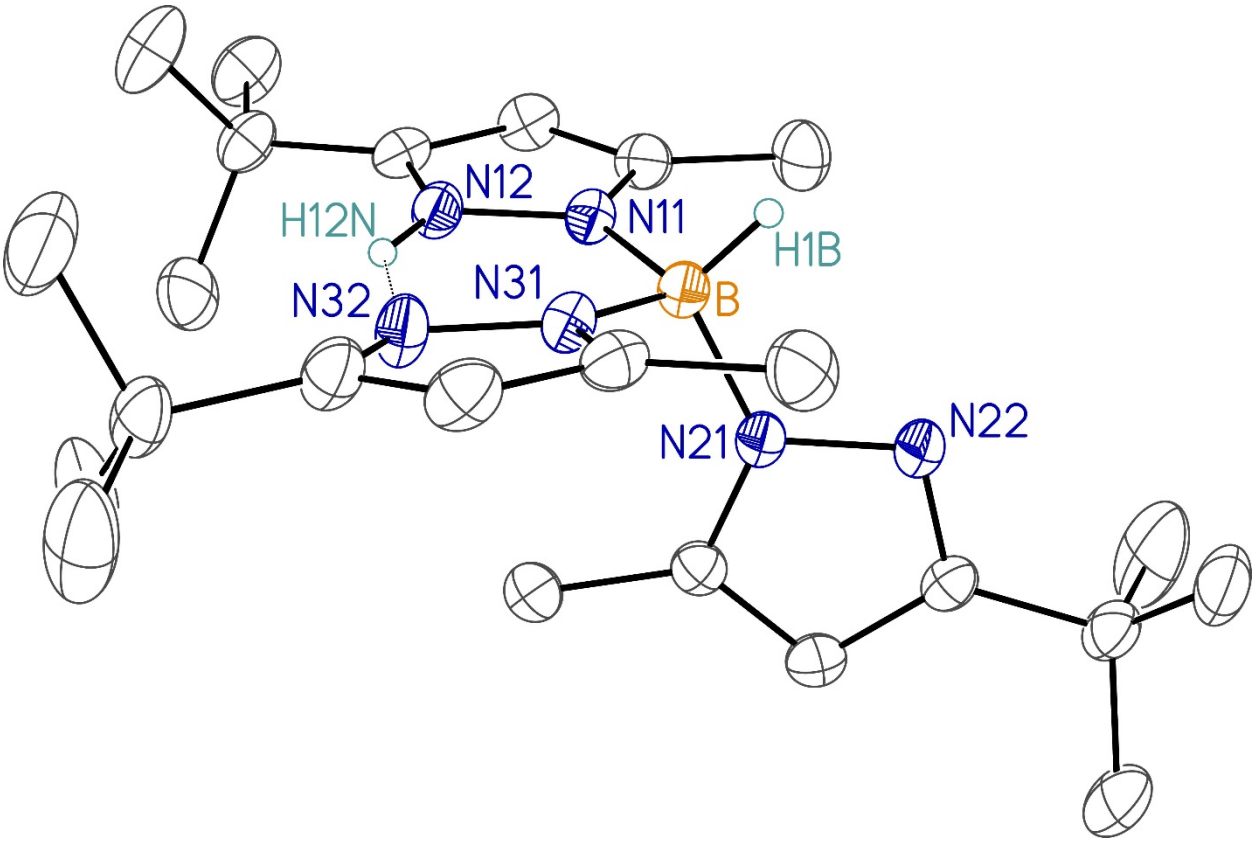


Figure Legends

Figure 1. Perspective view of the hydrogen tris(3-*t*-butyl-5-methylpyrazolyl)borate molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 20% probability level. The hydrogen atoms bound to N12 and B are shown with arbitrarily small thermal parameters; all other hydrogens are not shown.

Figure 2. Alternate view showing the near-parallel alignment of two of the pyrazolyl rings, as encouraged by the hydrogen-bonded interaction between N32 and H12N (dotted line); see Table 5 for distances and angles involving this interaction. The dihedral angle between these planes is 12.81(8)º; see Table 6 for least-squares planes calculations.


C16
C30A
C14
C15
C27
C20
N22
C23
C13
N11
H1B
N21
C29A
C28A
C17
B
C24
N12
C26
C25
C18
N31
C19
H12N
C36
N32
C35
C33
C39A
C34
C37A
C40A
C38A


N12
H12N
N11
H1B
N32
N31
B
N21
N22

List of Tables

Table 1. Crystallographic Experimental Details

A. Crystal Data	
formula	$C_{24}H_{41}BN_6$
formula weight	424.44
crystal dimensions (mm)	0.73 × 0.36 × 0.28
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	9.6716(17)
b (Å)	23.904(4)
c (Å)	11.451(2)
β (deg)	94.941(3)
V (Å^3)	2637.4(8)
Z	4
ρ_{calcd} (g cm^{-3})	1.069
μ (mm^{-1})	0.065
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.3°) (15 s exposures)
data collection 2θ limit (deg)	52.75
total data collected	20768 (-12 ≤ h ≤ 12, -29 ≤ k ≤ 29, -14 ≤ l ≤ 14)
independent reflections	5377 (R_{int} = 0.0327)
number of observed reflections (*NO*)	3992 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–97*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2014*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.9821–0.9544
data/restraints/parameters	5377 / 1[e] / 345
goodness-of-fit (*S*)[f] [all data]	1.031
final R indices[g]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0476
wR_2 [all data]	0.1354
largest difference peak and hole	0.203 and –0.189 e Å^{-3}

[a]Obtained from least-squares refinement of 4103 reflections with 4.56° < 2θ < 50.68°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1. Crystallographic Experimental Details (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[d]Sheldrick, G. M. *Acta Crystallogr.* **2015**, *C71*, 3–8.

[e]The C33–C37A and C33–C37B distances were constrained to be equal (within 0.01 Å) during refinement.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0635P)^2 + 0.5537P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[g]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters

Atom	*x*	*y*	*z*	U_{eq}, Å^2
N11	0.17582(12)	0.22085(5)	0.22742(10)	0.0402(3)*
N12	0.11218(13)	0.17209(5)	0.19405(11)	0.0415(3)*
N21	0.40930(12)	0.25800(5)	0.17694(10)	0.0387(3)*
N22	0.47306(13)	0.30781(5)	0.20820(11)	0.0445(3)*
N31	0.39741(12)	0.16715(5)	0.29242(10)	0.0403(3)*
N32	0.33878(13)	0.11849(5)	0.24869(12)	0.0488(3)*
C13	-0.02130(15)	0.18121(6)	0.15807(13)	0.0433(3)*
C14	-0.04414(16)	0.23774(7)	0.16970(14)	0.0488(4)*
C15	0.08072(16)	0.26158(6)	0.21252(13)	0.0459(4)*
C16	0.1158(2)	0.32128(7)	0.23811(17)	0.0611(5)*
C17	-0.11368(16)	0.13428(7)	0.11048(15)	0.0523(4)*
C18	-0.0582(2)	0.11322(9)	-0.00270(18)	0.0730(6)*
C19	-0.1141(2)	0.08743(9)	0.2009(2)	0.0784(6)*
C20	-0.26122(18)	0.15604(9)	0.08326(18)	0.0695(5)*
C23	0.52980(14)	0.32562(6)	0.11355(13)	0.0408(3)*
C24	0.50316(15)	0.28820(6)	0.02054(13)	0.0451(4)*
C25	0.42645(14)	0.24575(6)	0.06346(12)	0.0399(3)*
C26	0.36811(18)	0.19471(7)	0.00284(14)	0.0536(4)*
C27	0.60617(17)	0.38101(6)	0.11433(15)	0.0510(4)*
C28A[a]	0.7046(9)	0.3803(4)	0.0186(6)	0.093(3)*
C29A[a]	0.6951(6)	0.3853(2)	0.2339(4)	0.0773(13)*
C30A[a]	0.5067(9)	0.4252(3)	0.1013(8)	0.115(3)*
C28B[a]	0.7484(7)	0.3744(3)	0.0765(7)	0.087(2)*
C29B[a]	0.6077(6)	0.41141(19)	0.2300(4)	0.0787(14)*
C30B[a]	0.5267(10)	0.4212(3)	0.0209(7)	0.121(3)*
C33	0.42638(16)	0.07734(6)	0.28119(16)	0.0532(4)*
C34	0.54165(16)	0.09925(7)	0.34606(15)	0.0530(4)*
C35	0.52116(15)	0.15582(7)	0.35123(13)	0.0450(4)*
C36	0.61320(18)	0.20086(8)	0.40437(17)	0.0617(5)*
C37A[a,b]	0.392(2)	0.02026(18)	0.2267(8)	0.0569(19)*
C38A[a]	0.5231(9)	-0.0151(4)	0.2282(12)	0.123(5)*
C39A[a]	0.3239(7)	0.01960(18)	0.1038(5)	0.0995(17)*
C40A[a]	0.2946(8)	-0.0086(2)	0.3079(7)	0.1068(19)*
C37B[a,b]	0.398(2)	0.01499(18)	0.2649(8)	0.0569(19)*
C38B[a]	0.4990(13)	-0.0029(4)	0.1808(12)	0.146(6)*
C39B[a]	0.2490(6)	0.0093(2)	0.2111(8)	0.116(2)*
C40B[a]	0.4111(9)	-0.01843(17)	0.3740(5)	0.1085(19)*

Table 2. Atomic Coordinates and Displacement Parameters (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
B	0.33455(17)	0.22613(7)	0.26967(14)	0.0396(4)*
H12N	0.177(2)	0.1397(9)	0.2023(17)	0.078(6)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Refined with an occupancy factor of 0.5. [b]C37A and C37B were refined with common anisotropic displacement parameters.

Table 3. Selected Interatomic Distances (Å)

Atom1	Atom2	Distance	Atom1	Atom2	Distance
N11	N12	1.3575(16)	C23	C27	1.516(2)
N11	C15	1.3401(19)	C24	C25	1.373(2)
N11	B	1.574(2)	C25	C26	1.491(2)
N12	C13	1.3387(19)	C27	C28A	1.513(8)
N21	N22	1.3740(16)	C27	C29A	1.556(5)
N21	C25	1.3561(18)	C27	C30A	1.429(7)
N21	B	1.5371(19)	C27	C28B	1.486(7)
N22	C23	1.3265(18)	C27	C29B	1.509(5)
N31	N32	1.3698(16)	C27	C30B	1.586(7)
N31	C35	1.3493(19)	C33	C34	1.388(2)
N31	B	1.549(2)	C33	C37A	1.525(3)[a]
N32	C33	1.330(2)	C33	C37B	1.524(3)[a]
C13	C14	1.378(2)	C34	C35	1.369(2)
C13	C17	1.507(2)	C35	C36	1.493(2)
C14	C15	1.386(2)	C37A	C38A	1.52(2)
C15	C16	1.490(2)	C37A	C39A	1.503(11)
C17	C18	1.530(3)	C37A	C40A	1.544(15)
C17	C19	1.526(2)	C37B	C38B	1.49(2)
C17	C20	1.526(2)	C37B	C39B	1.521(18)
C23	C24	1.398(2)	C37B	C40B	1.479(10)

[a]Distances constrained to be equal (within 0.01 Å) during refinement.

Table 4. Selected Interatomic Angles (deg)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
N12	N11	C15	107.36(12)	C23	C27	C30A	108.8(3)
N12	N11	B	124.18(11)	C23	C27	C28B	111.6(3)
C15	N11	B	128.41(12)	C23	C27	C29B	113.17(19)
N11	N12	C13	110.41(12)	C23	C27	C30B	108.5(3)
N22	N21	C25	110.34(11)	C28A	C27	C29A	107.7(4)
N22	N21	B	118.47(11)	C28A	C27	C30A	113.1(5)
C25	N21	B	131.19(12)	C29A	C27	C30A	111.1(4)
N21	N22	C23	105.86(11)	C28B	C27	C29B	111.6(4)
N32	N31	C35	109.48(12)	C28B	C27	C30B	106.0(5)
N32	N31	B	124.58(12)	C29B	C27	C30B	105.5(4)
C35	N31	B	125.82(12)	N32	C33	C34	109.49(14)
N31	N32	C33	106.98(13)	N32	C33	C37A	115.9(6)
N12	C13	C14	106.76(13)	N32	C33	C37B	125.7(7)
N12	C13	C17	121.08(14)	C34	C33	C37A	133.8(7)
C14	C13	C17	132.09(14)	C34	C33	C37B	124.3(6)
C13	C14	C15	107.18(14)	C33	C34	C35	106.46(14)
N11	C15	C14	108.30(13)	N31	C35	C34	107.59(14)
N11	C15	C16	121.89(14)	N31	C35	C36	122.06(14)
C14	C15	C16	129.80(15)	C34	C35	C36	130.30(15)
C13	C17	C18	108.11(13)	C33	C37A	C38A	110.1(11)
C13	C17	C19	109.71(14)	C33	C37A	C39A	117.0(6)
C13	C17	C20	109.58(15)	C33	C37A	C40A	105.9(8)
C18	C17	C19	110.81(17)	C38A	C37A	C39A	107.7(9)
C18	C17	C20	109.23(15)	C38A	C37A	C40A	107.3(7)
C19	C17	C20	109.38(15)	C39A	C37A	C40A	108.4(10)
N22	C23	C24	110.80(13)	C33	C37B	C38B	103.6(9)
N22	C23	C27	120.75(13)	C33	C37B	C39B	107.0(9)
C24	C23	C27	128.41(14)	C33	C37B	C40B	115.0(5)
C23	C24	C25	105.67(13)	C38B	C37B	C39B	111.3(8)
N21	C25	C24	107.33(13)	C38B	C37B	C40B	112.1(11)
N21	C25	C26	123.39(13)	C39B	C37B	C40B	107.8(10)
C24	C25	C26	129.27(14)	N11	B	N21	109.37(11)
C23	C27	C28A	108.8(3)	N11	B	N31	109.69(11)
C23	C27	C29A	107.15(19)	N21	B	N31	111.48(12)

[a]Angle includes distances constrained to be equal (d(C33–C37A = d(C33–C37B) within 0.01 Å) during refinement.

Table 5. Hydrogen-Bonded Interactions

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠D–H···A (deg)
N12–H12N···N32	1.00(2)	1.68(2)	2.5690(18)	145.6(17)

Table 6. Torsional Angles (deg)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C15	N11	N12	C13	0.14(16)	N12	C13	C17	C19	56.6(2)
B	N11	N12	C13	-177.37(12)	N12	C13	C17	C20	176.73(14)
N12	N11	C15	C14	0.26(16)	C14	C13	C17	C18	112.25(19)
N12	N11	C15	C16	-178.54(14)	C14	C13	C17	C19	-126.81(19)
B	N11	C15	C14	177.62(13)	C14	C13	C17	C20	-6.7(2)
B	N11	C15	C16	-1.2(2)	C13	C14	C15	N11	-0.54(17)
N12	N11	B	N21	110.52(14)	C13	C14	C15	C16	178.13(16)
N12	N11	B	N31	-12.04(18)	N22	C23	C24	C25	-0.20(17)
C15	N11	B	N21	-66.44(18)	C27	C23	C24	C25	-177.73(14)
C15	N11	B	N31	171.00(13)	N22	C23	C27	C28A	158.0(3)
N11	N12	C13	C14	-0.47(16)	N22	C23	C27	C29A	41.8(3)
N11	N12	C13	C17	176.87(12)	N22	C23	C27	C30A	-78.4(4)
C25	N21	N22	C23	-0.39(15)	N22	C23	C27	C28B	126.4(4)
B	N21	N22	C23	179.26(12)	N22	C23	C27	C29B	-0.5(3)
N22	N21	C25	C24	0.27(16)	N22	C23	C27	C30B	-117.2(4)
N22	N21	C25	C26	-179.31(13)	C24	C23	C27	C28A	-24.7(4)
B	N21	C25	C24	-179.32(14)	C24	C23	C27	C29A	-140.9(3)
B	N21	C25	C26	1.1(2)	C24	C23	C27	C30A	98.9(4)
N22	N21	B	N11	118.47(13)	C24	C23	C27	C28B	-56.3(4)
N22	N21	B	N31	-120.05(13)	C24	C23	C27	C29B	176.9(3)
C25	N21	B	N11	-61.97(19)	C24	C23	C27	C30B	60.1(4)
C25	N21	B	N31	59.51(19)	C23	C24	C25	N21	-0.04(16)
N21	N22	C23	C24	0.36(16)	C23	C24	C25	C26	179.50(15)
N21	N22	C23	C27	178.11(13)	N32	C33	C34	C35	-0.38(19)
C35	N31	N32	C33	0.28(16)	C37A	C33	C34	C35	168.7(7)
B	N31	N32	C33	176.40(13)	C37B	C33	C34	C35	-172.8(7)
N32	N31	C35	C34	-0.52(17)	N32	C33	C37A	C38A	156.3(6)
N32	N31	C35	C36	177.10(14)	N32	C33	C37A	C39A	33.0(15)
B	N31	C35	C34	-176.58(13)	N32	C33	C37A	C40A	-88.0(7)
B	N31	C35	C36	1.0(2)	C34	C33	C37A	C38A	-12.2(11)
N32	N31	B	N11	18.86(18)	C34	C33	C37A	C39A	-135.6(9)
N32	N31	B	N21	-102.43(15)	C34	C33	C37A	C40A	103.4(11)
C35	N31	B	N11	-165.65(12)	N32	C33	C37B	C38B	114.8(10)
C35	N31	B	N21	73.06(17)	N32	C33	C37B	C39B	-2.9(11)
N31	N32	C33	C34	0.07(18)	N32	C33	C37B	C40B	-122.6(10)
N31	N32	C33	C37A	-171.2(6)	C34	C33	C37B	C38B	-74.0(8)
N31	N32	C33	C37B	172.4(6)	C34	C33	C37B	C39B	168.3(5)
N12	C13	C14	C15	0.61(17)	C34	C33	C37B	C40B	48.6(16)
C17	C13	C14	C15	-176.32(15)	C33	C34	C35	N31	0.54(18)
N12	C13	C17	C18	-64.32(19)	C33	C34	C35	C36	-176.82(17)

Table 7. Least-Squares Planes

Plane	Coefficients[a]			Defining Atoms with Deviations (Å)[b]			
1	-3.157(7)	-3.422(18)	10.981(3)	1.186(4)			
				N11	0.0004(8)	N12	0.0017(8)
				C13	-0.0031(9)	C14	0.0032(9)
				C15	-0.0023(9)		
2	7.31(4)	-11.798(15)	2.496(8)	0.642(6)			
				N21	0.0018(8)	N22	-0.0021(8)
				C23	0.0016(9)	C24	-0.0004(9)
				C25	-0.0008(9)		
3	-5.109(7)	-2.87(2)	10.110(5)	0.443(5)			
				N31	0.0022(8)	N32	-0.0006(9)
				C33	-0.0013(10)	C34	0.0026(10)
				C35	-0.0030(9)		

Dihedral angle between planes 1 and 2: 85.78(6)º

Dihedral angle between planes 1 and 3: 12.85(8)º

Dihedral angle between planes 2 and 3: 82.51(6)º

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.

Table 8. Anisotropic Displacement Parameters (U_{ij}, Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N11	0.0418(7)	0.0345(6)	0.0446(7)	0.0001(5)	0.0059(5)	-0.0040(5)
N12	0.0378(7)	0.0366(6)	0.0505(7)	-0.0005(5)	0.0054(5)	-0.0050(5)
N21	0.0411(6)	0.0346(6)	0.0406(6)	-0.0009(5)	0.0043(5)	-0.0054(5)
N22	0.0506(7)	0.0374(6)	0.0462(7)	-0.0018(5)	0.0085(6)	-0.0108(5)
N31	0.0392(6)	0.0373(6)	0.0443(7)	0.0013(5)	0.0036(5)	-0.0064(5)
N32	0.0440(7)	0.0329(6)	0.0689(9)	-0.0005(6)	0.0010(6)	-0.0048(5)
C13	0.0377(8)	0.0519(9)	0.0406(8)	0.0069(6)	0.0061(6)	-0.0037(6)
C14	0.0427(8)	0.0508(9)	0.0527(9)	0.0084(7)	0.0033(7)	0.0062(7)
C15	0.0496(9)	0.0422(8)	0.0464(8)	0.0041(7)	0.0069(7)	0.0041(7)
C16	0.0654(11)	0.0415(9)	0.0759(12)	-0.0008(8)	0.0031(9)	0.0051(8)
C17	0.0395(8)	0.0563(10)	0.0605(10)	0.0062(8)	0.0007(7)	-0.0103(7)
C18	0.0642(12)	0.0734(13)	0.0802(13)	-0.0217(11)	-0.0008(10)	-0.0149(10)
C19	0.0559(11)	0.0711(13)	0.1054(17)	0.0303(12)	-0.0082(11)	-0.0219(10)
C20	0.0452(10)	0.0831(14)	0.0784(13)	0.0112(10)	-0.0062(9)	-0.0088(9)
C23	0.0353(7)	0.0398(8)	0.0474(8)	0.0063(6)	0.0048(6)	0.0008(6)
C24	0.0449(8)	0.0501(9)	0.0409(8)	0.0034(6)	0.0077(6)	-0.0003(7)
C25	0.0364(7)	0.0420(8)	0.0413(8)	-0.0007(6)	0.0023(6)	0.0028(6)
C26	0.0574(10)	0.0560(10)	0.0482(9)	-0.0103(7)	0.0082(7)	-0.0081(8)
C27	0.0513(9)	0.0407(8)	0.0623(10)	0.0067(7)	0.0133(8)	-0.0066(7)
C28A	0.104(6)	0.091(4)	0.088(4)	-0.003(4)	0.041(4)	-0.051(4)
C29A	0.089(3)	0.074(3)	0.069(3)	-0.003(2)	0.009(3)	-0.046(3)
C30A	0.094(4)	0.035(2)	0.215(10)	0.026(5)	0.006(6)	0.000(2)
C28B	0.053(3)	0.053(3)	0.160(8)	-0.025(4)	0.044(4)	-0.017(2)
C29B	0.093(4)	0.053(3)	0.094(3)	-0.010(2)	0.032(3)	-0.031(2)
C30B	0.109(6)	0.077(4)	0.170(8)	0.073(5)	-0.032(6)	-0.015(4)
C33	0.0418(9)	0.0391(8)	0.0798(12)	0.0063(8)	0.0110(8)	0.0005(7)
C34	0.0391(8)	0.0545(10)	0.0658(10)	0.0110(8)	0.0065(7)	0.0051(7)
C35	0.0374(8)	0.0546(9)	0.0435(8)	0.0030(7)	0.0057(6)	-0.0031(7)
C36	0.0487(10)	0.0703(12)	0.0643(11)	-0.0130(9)	-0.0047(8)	-0.0042(8)
C37A[a]	0.0539(16)	0.0317(11)	0.085(6)	0.011(2)	0.008(5)	0.0029(18)
C38A	0.055(3)	0.050(3)	0.266(15)	-0.022(5)	0.025(5)	0.007(3)
C39A	0.121(4)	0.049(2)	0.124(4)	-0.031(3)	-0.016(4)	0.003(3)
C40A	0.109(5)	0.058(3)	0.159(6)	0.008(3)	0.040(4)	-0.026(3)
C37B[a]	0.0539(16)	0.0317(11)	0.085(6)	0.011(2)	0.008(5)	0.0029(18)
C38B	0.209(13)	0.068(6)	0.175(9)	-0.060(6)	0.104(9)	-0.031(6)
C39B	0.093(4)	0.044(3)	0.206(8)	-0.032(4)	-0.024(5)	-0.012(2)
C40B	0.173(6)	0.036(2)	0.118(4)	0.013(2)	0.022(4)	0.000(3)
B	0.0422(9)	0.0374(8)	0.0394(8)	-0.0019(7)	0.0045(7)	-0.0062(7)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

[a]C37A and C37B were refined with common anisotropic displacement parameters.

Table 9. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H14	-0.129488	0.256822	0.151728	0.059
H16A	0.137967	0.326096	0.322651	0.073
H16B	0.036428	0.344953	0.211909	0.073
H16C	0.196231	0.332060	0.196605	0.073
H18A	-0.116895	0.082607	-0.035216	0.088
H18B	-0.059180	0.143870	-0.059616	0.088
H18C	0.037109	0.099711	0.014242	0.088
H19A	-0.174294	0.056991	0.169690	0.094
H19B	-0.019446	0.073306	0.218285	0.094
H19C	-0.148874	0.101902	0.272954	0.094
H20A	-0.321161	0.125465	0.052326	0.083
H20B	-0.296093	0.170633	0.155129	0.083
H20C	-0.261180	0.186004	0.024853	0.083
H24	0.532103	0.291467	-0.056374	0.054
H26A[a]	0.407437	0.161321	0.042736	0.064
H26B[a]	0.391527	0.194771	-0.078744	0.064
H26C[a]	0.266988	0.194468	0.004659	0.064
H28A[a]	0.770108	0.349193	0.032092	0.111
H28B[a]	0.651599	0.375482	-0.057621	0.111
H28C[a]	0.755822	0.415655	0.019300	0.111
H29A[a]	0.762356	0.354555	0.240655	0.093
H29B[a]	0.744540	0.421115	0.238287	0.093
H29C[a]	0.634386	0.382905	0.297933	0.093
H30A[a]	0.446046	0.423628	0.165500	0.139
H30B[a]	0.554990	0.461318	0.103157	0.139
H30C[a]	0.450767	0.421145	0.026237	0.139
H28D[a]	0.743722	0.354528	0.001345	0.104
H28E[a]	0.790108	0.411326	0.067570	0.104
H28F[a]	0.805318	0.352865	0.135572	0.104
H29D[a]	0.512498	0.415058	0.252282	0.094
H29E[a]	0.663326	0.390218	0.290361	0.094
H29F[a]	0.648116	0.448679	0.222360	0.094
H30D[a]	0.431554	0.427047	0.041673	0.146
H30E[a]	0.574919	0.457210	0.020271	0.146
H30F[a]	0.524418	0.404079	-0.057057	0.146
H34	0.619436	0.078983	0.380144	0.064
H36A	0.638825	0.226328	0.342718	0.074
H36B	0.697231	0.184078	0.443599	0.074
H36C	0.563966	0.221754	0.461664	0.074
H38A[a]	0.570016	-0.015450	0.307536	0.148

Table 9. Derived Parameters for Hydrogen Atoms (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H38B[a]	0.498244	-0.053456	0.204385	0.148
H38C[a]	0.585264	0.000730	0.173637	0.148
H39A[a]	0.238991	0.042160	0.100230	0.119
H39B[a]	0.387492	0.035208	0.050154	0.119
H39C[a]	0.300472	-0.018978	0.080902	0.119
H40A[a]	0.337811	-0.008489	0.388567	0.128
H40B[a]	0.206328	0.011726	0.304771	0.128
H40C[a]	0.277705	-0.047226	0.282042	0.128
H38D[a]	0.486733	0.020237	0.109937	0.175
H38E[a]	0.593733	0.001713	0.217371	0.175
H38F[a]	0.483049	-0.042225	0.159877	0.175
H39D[a]	0.237172	0.031117	0.138436	0.140
H39E[a]	0.228744	-0.030146	0.193740	0.140
H39F[a]	0.185206	0.023288	0.266388	0.140
H40D[a]	0.343114	-0.005449	0.426629	0.130
H40E[a]	0.394267	-0.057962	0.355103	0.130
H40F[a]	0.504951	-0.014024	0.412598	0.130
H1B	0.344167	0.247818	0.344618	0.048

[a]Included with an occupancy factor of 0.5.