9 Kristallstrukturdaten

Identification code	**1**	**2**	**5**
Empirical formula	$C_{12}H_{20}B_4N_8$	$C_{15}H_{25}B_5N_{10}$	$C_{20}H_{36}B_4N_8$
Formula weight	319.60	399.50	431.81
Temperature	173(2)	173(2)	173(2)
Crystal system	Monoclinic	Orthorhombic	Monoclinic
Space group	P2(1)/c	Pnma	P2(1)/c
Unit cell dimensions			
a [Å]	9.3506(2)	9.7400(6)	12.5847(2)
b [Å]	12.3406(2)	20.6899(12)	17.7859(3)
c [Å]	7.8260(2)	10.9517(6)	11.4299(2)
β [°]	100.4030(10)	90	106.3090(10)
Volume [$Å^3$]	888.21(3)	2207.0(2)	2455.41(7)
Z	2	4	4
Density (calculated) [g/cm^3]	1.195	1.202	1.168
Absorption coefficient [mm^{-1}]	0.075	0.076	0.071
F(000)	336	840	928
Crystal size [mm^3]	0.45 x 0.34 x 0.29	0.46 x 0.37 x 0.28	0.40 x 0.29 x 0.25
Theta range [°]	2.21 to 28.28°.	1.97 to 28.30°.	1.69 to 28.27°.
Index ranges	-12/12, 0/16, 0/10	0/13, 0/26, 0/14	-16/16, 0/23, 0/15
Reflections collected	8811	15034	22573
Independent reflections	2168 [R(int) = 0.022]	2757 [R(int) = 0.0331]	5999 [R(int) = 0.032]
Max. and min. transmission	0.771 and 0.914	1.0000 and 0.8967	0.901 and 0.768
parameters	149	192	433
Final R indices [I>2sigma(I)]	R1 = 0.0372	R1 = 0.0378	R1 = 0.0416
R indices (all data)	wR2 = 0.1069	wR2 = 0.1063	wR2 = 0.1254
Largest diff. peak and hole [e/ $Å^3$]	0.221 and -0.133	0.260 and -0.159	0.302 and -0.179

Identification code	**10**	**14**	**16**
Empirical formula	$C_8H_{18}B_2N_4Si$	$C_{31}H_{62}B_3N_5$	$C_{19}H_{38}B_2N_4$
Formula weight	219.97	537.29	344.15
Temperature [K]	190	173	173
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	C2/c	P2(1)/n	Pbcn
Unit cell dimensions			
a [Å]	16.3703(18)	23.000(8)	11.0322(6)
b [Å]	6.3079(5)	11.363(6)	13.3381(8)
c [Å]	14.2036(12)	26.976(11)	14.5648(8)
β [°]	117.210(2)	97.83(3)	90
Volume [Å^3]	1304.4(2)	6984(5)	2143.2(2)
Z	4	8	4
Density (calculated) [g/cm^3]	1.120	1.022	1.067
Absorption coefficient [mm^{-1}]	0.155	0.059	0.062
F(000)	472	2384	760
Crystal size [mm^3]	0.33 × 0.31 × 0.12	0.40 × 0.37 × 0.35	0.55 × 0.46 × 0.26
Theta range [°]	2.80 to 32.46	1.09 to 27.10	2.40 to 27.87
Index ranges	–24/21, 0/9, 0/21	–29/29, 0/14, 0/34	0/14, 0/17, 0/18
Reflections collected	13086	58271	13498
Independent reflections	2209 [R(int) = 0.0302]	15391 [R(int) = 0.0397]	2462 [R(int) = 0.0254]
Max. and min. transmission	1.0000 and 0.8733	1.0000 and 0.8058	1.0000 and 0.8827
parameters	105	1196	190
Final R indices [I>2sigma(I)]	R1 = 0.0367	R1 = 0.0543	R1 = 0.0367
R indices (all data)	wR2 = 0.1073	wR2 = 0.1632	wR2 = 0.1031
Largest diff. peak and hole [e/ Å^3]	0.428 and – 0.191	0.760 and –0.313	0.314 and –0.172

Identification code	**18**	**21**	**22**
Empirical formula	$C_{11}H_{22}B_2N_4$	$C_{21.50}H_{31}B_2ClN_4$ Ti	$C_{21}H_{30}B_2N_4Zr$
Formula weight	231.95	450.47	451.33
Temperature [K]	293	190	190
Crystal system	Monoclinic	Triclinic	Orthorhombic
Space group	P2(1)/c	P-1	Pna2(1)
Unit cell dimensions			
a [Å]	8.4793(9)	10.7849(12)	15.4843(8)
b [Å]	15.0945(16)	14.6931(16)	11.7675(6)
c [Å]	11.3155(12)	14.7532(16)	11.6797(6)
β [°]	107.601(2)	104.260(3)	90
Volume [$Å^3$]	1380.5(3)	2260.4(4)	2128.18(19)
Z	4	4	4
Density (calculated) [g/cm^3]	1.116	1.324	1.409
Absorption coefficient [mm^{-1}]	0.067	0.513	0.530
F(000)	504	948	936
Crystal size [mm^3]	0.42 × 0.30 × 0.28	0.30 × 0.23 × 0.04	0.60 × 0.44 × 0.38
Theta range [°]	2.32 to 32.40	1.95 to 25.00	2.17 to 32.16
Index ranges	–12/12, 0/21, 0/16	–12/12, –17/17, 0/17	0/23, 0/17, –6/16
Reflections collected	15064	25227	27203
Independent reflections	4572 [R(int) = 0.0244]	7947 [R(int) = 0.0912]	6995 [R(int) = 0.0209]
Max. and min. transmission	1.0000 and 0.7496	0.980 and 0.850	1.0000 and 0.8213
parameters	242	767	373
Final R indices [I>2sigma(I)]	R1 = 0.0450	R1 = 0.0754	R1 = 0.0205
R indices (all data)	wR2 = 0.1315	wR2 = 0.2396	wR2 = 0.0569
Largest diff. peak and hole [e/ Å3]	0.426 and –0.186	1.210 and –1.363	0.372 and –0.301

Identification code	**26**
Empirical formula	$C_{57}H_{56}B_2Cl_2N_4$
Formula weight	889.58
Temperature [K]	190(2)
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	
a [Å]	a = 25.757(2)
b [Å]	b = 8.9382(9)
c [Å]	c = 23.314(2)
β [°]	114.830(2)
Volume [$Å^3$]	4871.3(8)
Z	4
Density (calculated) [g/cm^3]	1.213
Absorption coefficient [mm^{-1}]	0.176
F(000)	1880
Crystal size [mm^3]	0.15 x 0.23 x 0.25
Theta range [°]	1.98 to 25.01°.
Index ranges	-30/27, 0/10, 0/27
Reflections collected	14615
Independent reflections	4291 [R(int) = 0.0679]
Max. and min. transmission	1.0000 and 0.6747
parameters	303
Final R indices [I>2sigma(I)]	R1 = 0.0659
R indices (all data)	wR2 = 0.2147
Largest diff. peak and hole [e/ Å3]	0.499 and -0.509