JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1996, 118(13), 3313-3314, DOI:10.1021/ja9541443

2/20/96 Revised

J3314-1

Table 1. Crystal data for $[Me_2PhNH][B_{11}CMe_{12}]\cdot MeOH$.

Identification code	bc51
Empirical formula	C22 H52 B11 N O
Formula mass	465.56
Crystal size	0.13 x 0.26 x 0.27 mm
Crystal color, habit	colorless block
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	
a = 13.1241(10) Å	$\alpha = 90°$
b = 13.2373(10) Å	$\beta = 90°$
c = 17.0648(13) Å	$\gamma = 90°$
Volume	2964.6(4) $Å^3$
Z	4
Density (calculated)	1.043 $Mg\cdot m^{-3}$
Absorption coefficient	0.055 mm^{-1}
F(000)	1016
Absorption correction	None

J3314-2

Table 2. Data collection for [Me_2PhNH][$B_{11}CMe_{12}$]·MeOH.

Diffractometer	Siemens CCD
Temperature	123(2) K
Radiation source	sealed tube (1.75 kW)
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
Cell measurement	
Reflections used	3796
θ range	$1.94° \leq \theta \leq 23.28°$
θ range, data coll'n	1.95° to 23.28°
Scan type	0.3° ω scans
Index ranges	$-14 \leq h \leq 14$, $-13 \leq k \leq 14$, $-14 \leq l \leq 19$
Reflections collected	11821
Independent reflections	4264 (R_{int} = 0.0691)

J3314-3

Table 3. Solution and refinement of $[Me_2PhNH][B_{11}CMe_{12}]\cdot MeOH$.

System for solution	Siemens SHELXTL[1,2]
Structure solution	direct
System for refinement	Siemens SHELXTL[1,2]
Hydrogen atoms	riding, with riding isotropic U
Data/ restraints/ parameters	4264 / 1 / 343
Final R indices[3] [I>2σ(I)]	R1 = 0.0690, wR2 = 0.1398
Reflections observed	3032
R indices (all data)	R1 = 0.1093, wR2 = 0.1660
Goodness-of-fit [4] on F^2	1.114
Absolute structure parameter	-2(4)
Largest diff. peak and hole	0.185 and -0.223 e·Å^{-3}

---

1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5 beta, 1995, Siemens Anayltical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co.Boston, 1991.

3) $$R1 = \frac{\sum ||Fo| - |Fc||}{\sum |Fo|} \quad ; \quad wR2 = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2 \right]}{\sum \left[w\left(Fo^2\right)^2 \right]}}$$

4) $$Goodness - of - Fit = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2 \right]}{(M - N)}}$$

where M is the number of reflections and N is the number of parameters refined.

J3314-4

Notes on the structure determination for $[Me_2PhNH][B_{11}CMe_{12}]\cdot MeOH$.

A suitable crystal was selected and mounted with silicone grease in the 123 K N_2 cold stream of a Siemens SMART 3-circle goniometer. Indexing was determined after collection of three sets of twenty 0.3°(ω) scans. Least-squares refinement of final cell dimensions was performed using all reflections harvested during data collection. A hemisphere of data was collected. Equivalent reflections were merged and all data were corrected for Lorentz and polarization effects. No merging was performed on Friedel opposites. Structure solution by direct methods in the non-centrosymmetric space group $P2_12_12_1$ revealed the complete non-hydrogen structure. In addition to the cation and anion, a methanol is present in the asymmetric unit. Attempts to determine the absolute structure were inconclusive.

Ammonium hydrogen H(1N) was located by difference map and refined with a riding model in subsequent cycles. All other hydrogens were placed at calculated positions, then refined using a riding model. Hydrogen thermal motion was modeled as isotropic; thermal parameters for hydrogen were calculated as 1.2 times the U_{eq} for the parent atom.

No disorder was observed in either the cation or the anion. The methanol is disordered across two sites, modeled at occupancies of 0.901 and 0.099 respectively.

The shortest intermolecular hydrogen-oxygen distance is 1.865(7) Å between H(1N) of the cation and the MeOH oxygen. The N-H(1N)···O angle is 172.14(19)°. No notable hydrogen bonds were observed for methanol hydrogen H(1O). There do not appear to be any hydrogen bonds involving the minor component of the methanol.

Closest contact between cation and anion is 2.42 Å between methyl hydrogens H(8B) and H(13B). The centroid of phenyl ring C(16) to C(21) is 2.97 Å to H(7A). Some additional cage dimensions are tabulated below.

The structure determination was performed using equipment acquired under National Science Foundation grant CHE-9505926. This equipment includes a Siemens SMART CCD diffractometer system, LT-2A low-temperature apparatus and Silicon Graphics Indigo2 XL workstation.

Cage diameter (Å)		Methyl diameter (Å)	
C1-B12	3.269(6)	C1M-C12M	6.390(6)
B2-B9	3.390(6)	C2M-C9M	6.555(6)
B3-B10	3.407(7)	C3M-C10M	6.554(6)
B4-B11	3.391(7)	C4M-C11M	6.575(6)
B5-B7	3.372(7)	C5M-C7M	6.558(6)
B6-B8	3.375(6)	C6M-C8M	6.572(6)

J3314-5

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for [Me_2PhNH][$B_{11}CMe_{12}$]·MeOH.

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

	x	y	z	U_{eq}
C(1)	5372(3)	3766(3)	3854(2)	29(1)
B(2)	6317(4)	4133(4)	3207(3)	29(1)
B(3)	5273(4)	4956(4)	3429(3)	32(1)
B(4)	4921(4)	4738(4)	4422(3)	28(1)
B(5)	5758(4)	3801(4)	4812(3)	32(1)
B(6)	6613(4)	3427(4)	4075(3)	30(1)
B(7)	6528(4)	5432(4)	3415(3)	30(1)
B(8)	5673(4)	5797(4)	4173(3)	33(1)
B(9)	5977(4)	5087(3)	5032(3)	25(1)
B(10)	7028(4)	4276(4)	4802(3)	28(1)
B(11)	7361(4)	4491(4)	3798(3)	30(1)
B(12)	6972(4)	5523(4)	4401(3)	26(1)
C(1M)	4635(4)	2949(3)	3589(3)	42(1)
C(2M)	6409(4)	3640(4)	2367(3)	54(2)
C(3M)	4426(4)	5190(4)	2796(3)	48(1)
C(4M)	3753(3)	4785(4)	4677(3)	45(1)
C(5M)	5342(4)	3000(4)	5433(3)	51(1)
C(6M)	6986(4)	2287(3)	4003(3)	55(2)
C(7M)	6897(4)	6181(4)	2741(3)	58(2)
C(8M)	5200(4)	6916(3)	4224(3)	49(1)
C(9M)	5800(3)	5508(4)	5894(2)	41(1)
C(10M)	7829(4)	3953(4)	5437(3)	46(1)
C(11M)	8493(3)	4341(4)	3478(3)	46(1)
C(12M)	7738(3)	6401(3)	4666(3)	35(1)
N	919(3)	6136(3)	3478(2)	38(1)
C(13)	1785(4)	6736(4)	3797(4)	74(2)
C(14)	132(4)	6811(3)	3115(3)	51(1)
C(15)	1272(3)	5305(3)	2973(2)	30(1)
C(16)	1335(3)	4355(3)	3283(3)	34(1)
C(17)	1704(3)	3585(4)	2817(3)	43(1)
C(18)	1999(4)	3791(5)	2057(3)	54(2)
C(19)	1925(4)	4752(5)	1770(3)	58(2)
C(20)	1558(3)	5522(4)	2217(3)	48(1)
O	99(4)	5343(5)	4834(3)	83(2)
C(21)	555(6)	5228(5)	5561(4)	65(2)
O'	251(51)	5103(44)	5132(38)	83(2)
C(21')	721(54)	5998(36)	4926(34)	65(2)

J3314-6

Table 5. Bond lengths [Å] for [Me_2PhNH][$B_{11}CMe_{12}$]·MeOH.

C(1)-C(1M)	1.520(5)	C(1)-B(5)	1.712(6)
C(1)-B(4)	1.716(6)	C(1)-B(2)	1.730(6)
C(1)-B(6)	1.731(6)	C(1)-B(3)	1.739(6)
B(2)-C(2M)	1.578(6)	B(2)-B(11)	1.766(7)
B(2)-B(7)	1.778(6)	B(2)-B(3)	1.791(7)
B(2)-B(6)	1.794(7)	B(3)-C(3M)	1.581(6)
B(3)-B(7)	1.764(7)	B(3)-B(8)	1.769(7)
B(3)-B(4)	1.780(7)	B(4)-C(4M)	1.594(7)
B(4)-B(8)	1.767(7)	B(4)-B(5)	1.786(7)
B(4)-B(9)	1.793(7)	B(5)-C(5M)	1.596(7)
B(5)-B(6)	1.758(7)	B(5)-B(9)	1.766(7)
B(5)-B(10)	1.781(7)	B(6)-C(6M)	1.591(6)
B(6)-B(10)	1.761(7)	B(6)-B(11)	1.780(7)
B(7)-C(7M)	1.594(7)	B(7)-B(8)	1.779(7)
B(7)-B(11)	1.782(7)	B(7)-B(12)	1.785(7)
B(8)-C(8M)	1.610(6)	B(8)-B(9)	1.785(7)
B(8)-B(12)	1.786(7)	B(9)-C(9M)	1.590(6)
B(9)-B(12)	1.788(7)	B(9)-B(10)	1.792(7)
B(10)-C(10M)	1.569(6)	B(10)-B(12)	1.788(7)
B(10)-B(11)	1.792(7)	B(11)-C(11M)	1.595(7)
B(11)-B(12)	1.785(7)	B(12)-C(12M)	1.601(6)
N-C(15)	1.472(5)	N-C(13)	1.490(6)
N-C(14)	1.499(5)	C(15)-C(16)	1.367(6)
C(15)-C(20)	1.373(6)	C(16)-C(17)	1.381(6)
C(17)-C(18)	1.381(7)	C(18)-C(19)	1.367(7)
C(19)-C(20)	1.361(7)	O-C(21)	1.386(8)
O'-C(21')	1.38(3)		

J 3314-7

Table 6. Bond angles [_] for [Me_2PhNH][$B_{11}CMe_{12}$]·MeOH.

C(1M)-C(1)-B(5)	119.5(3)	C(1M)-C(1)-B(4)	118.8(3)
B(5)-C(1)-B(4)	62.8(3)	C(1M)-C(1)-B(2)	117.8(3)
B(5)-C(1)-B(2)	113.0(3)	B(4)-C(1)-B(2)	113.4(3)
C(1M)-C(1)-B(6)	118.7(3)	B(5)-C(1)-B(6)	61.4(3)
B(4)-C(1)-B(6)	113.4(3)	B(2)-C(1)-B(6)	62.5(3)
C(1M)-C(1)-B(3)	118.2(3)	B(5)-C(1)-B(3)	113.3(3)
B(4)-C(1)-B(3)	62.0(3)	B(2)-C(1)-B(3)	62.1(3)
B(6)-C(1)-B(3)	113.3(3)	C(2M)-B(2)-C(1)	121.2(4)
C(2M)-B(2)-B(11)	124.7(4)	C(1)-B(2)-B(11)	105.4(3)
C(2M)-B(2)-B(7)	124.7(4)	C(1)-B(2)-B(7)	104.8(3)
B(11)-B(2)-B(7)	60.4(3)	C(2M)-B(2)-B(3)	120.1(4)
C(1)-B(2)-B(3)	59.2(3)	B(11)-B(2)-B(3)	108.1(3)
B(7)-B(2)-B(3)	59.3(3)	C(2M)-B(2)-B(6)	121.1(4)
C(1)-B(2)-B(6)	58.8(3)	B(11)-B(2)-B(6)	60.0(3)
B(7)-B(2)-B(6)	107.8(3)	B(3)-B(2)-B(6)	107.9(3)
C(3M)-B(3)-C(1)	121.1(4)	C(3M)-B(3)-B(7)	125.2(4)
C(1)-B(3)-B(7)	105.0(3)	C(3M)-B(3)-B(8)	125.2(4)
C(1)-B(3)-B(8)	104.3(3)	B(7)-B(3)-B(8)	60.5(3)
C(3M)-B(3)-B(4)	120.0(4)	C(1)-B(3)-B(4)	58.4(3)
B(7)-B(3)-B(4)	108.3(3)	B(8)-B(3)-B(4)	59.7(3)
C(3M)-B(3)-B(2)	120.8(4)	C(1)-B(3)-B(2)	58.7(3)
B(7)-B(3)-B(2)	60.0(3)	B(8)-B(3)-B(2)	107.9(3)
B(4)-B(3)-B(2)	107.6(3)	C(4M)-B(4)-C(1)	121.0(4)
C(4M)-B(4)-B(8)	124.9(4)	C(1)-B(4)-B(8)	105.4(3)
C(4M)-B(4)-B(3)	120.2(4)	C(1)-B(4)-B(3)	59.6(3)
B(8)-B(4)-B(3)	59.8(3)	C(4M)-B(4)-B(5)	121.2(4)
C(1)-B(4)-B(5)	58.5(3)	B(8)-B(4)-B(5)	107.2(3)
B(3)-B(4)-B(5)	107.9(3)	C(4M)-B(4)-B(9)	125.1(4)
C(1)-B(4)-B(9)	104.7(3)	B(8)-B(4)-B(9)	60.2(3)
B(3)-B(4)-B(9)	108.0(3)	B(5)-B(4)-B(9)	59.1(3)
C(5M)-B(5)-C(1)	120.9(4)	C(5M)-B(5)-B(6)	120.4(4)
C(1)-B(5)-B(6)	59.8(3)	C(5M)-B(5)-B(9)	123.8(4)
C(1)-B(5)-B(9)	106.1(3)	B(6)-B(5)-B(9)	108.7(3)
C(5M)-B(5)-B(10)	124.2(4)	C(1)-B(5)-B(10)	106.1(3)
B(6)-B(5)-B(10)	59.7(3)	B(9)-B(5)-B(10)	60.7(3)
C(5M)-B(5)-B(4)	119.9(4)	C(1)-B(5)-B(4)	58.7(3)
B(6)-B(5)-B(4)	108.8(3)	B(9)-B(5)-B(4)	60.6(3)
B(10)-B(5)-B(4)	109.1(3)	C(6M)-B(6)-C(1)	121.2(4)
C(6M)-B(6)-B(5)	121.3(4)	C(1)-B(6)-B(5)	58.8(3)
C(6M)-B(6)-B(10)	124.4(4)	C(1)-B(6)-B(10)	106.2(3)
B(5)-B(6)-B(10)	60.8(3)	C(6M)-B(6)-B(11)	124.0(4)
C(1)-B(6)-B(11)	104.8(3)	B(5)-B(6)-B(11)	108.6(3)

J3314-8

B(10)-B(6)-B(11)	60.8(3)	C(6M)-B(6)-B(2)	119.8(4)
C(1)-B(6)-B(2)	58.8(3)	B(5)-B(6)-B(2)	107.8(3)
B(10)-B(6)-B(2)	108.4(3)	B(11)-B(6)-B(2)	59.2(3)
C(7M)-B(7)-B(3)	121.1(4)	C(7M)-B(7)-B(2)	120.3(4)
B(3)-B(7)-B(2)	60.7(3)	C(7M)-B(7)-B(8)	123.2(4)
B(3)-B(7)-B(8)	59.9(3)	B(2)-B(7)-B(8)	108.0(3)
C(7M)-B(7)-B(11)	120.9(4)	B(3)-B(7)-B(11)	108.5(3)
B(2)-B(7)-B(11)	59.5(3)	B(8)-B(7)-B(11)	108.0(3)
C(7M)-B(7)-B(12)	122.6(4)	B(3)-B(7)-B(12)	108.5(3)
B(2)-B(7)-B(12)	107.7(3)	B(8)-B(7)-B(12)	60.1(3)
B(11)-B(7)-B(12)	60.1(3)	C(8M)-B(8)-B(4)	120.1(4)
C(8M)-B(8)-B(3)	120.2(4)	B(4)-B(8)-B(3)	60.5(3)
C(8M)-B(8)-B(7)	122.1(4)	B(4)-B(8)-B(7)	108.2(3)
B(3)-B(8)-B(7)	59.6(3)	C(8M)-B(8)-B(9)	121.8(4)
B(4)-B(8)-B(9)	60.7(3)	B(3)-B(8)-B(9)	108.9(3)
B(7)-B(8)-B(9)	108.3(3)	C(8M)-B(8)-B(12)	123.0(4)
B(4)-B(8)-B(12)	108.7(3)	B(3)-B(8)-B(12)	108.2(3)
B(7)-B(8)-B(12)	60.1(3)	B(9)-B(8)-B(12)	60.1(3)
C(9M)-B(9)-B(5)	120.7(4)	C(9M)-B(9)-B(8)	122.8(4)
B(5)-B(9)-B(8)	107.3(3)	C(9M)-B(9)-B(12)	123.4(4)
B(5)-B(9)-B(12)	107.6(3)	B(8)-B(9)-B(12)	60.0(3)
C(9M)-B(9)-B(10)	121.6(4)	B(5)-B(9)-B(10)	60.1(3)
B(8)-B(9)-B(10)	107.9(3)	B(12)-B(9)-B(10)	59.9(3)
C(9M)-B(9)-B(4)	121.0(4)	B(5)-B(9)-B(4)	60.2(3)
B(8)-B(9)-B(4)	59.2(3)	B(12)-B(9)-B(4)	107.4(3)
B(10)-B(9)-B(4)	108.3(3)	C(10M)-B(10)-B(6)	121.3(4)
C(10M)-B(10)-B(5)	121.6(4)	B(6)-B(10)-B(5)	59.5(3)
C(10M)-B(10)-B(12)	122.9(4)	B(6)-B(10)-B(12)	107.8(3)
B(5)-B(10)-B(12)	106.9(3)	C(10M)-B(10)-B(9)	121.9(4)
B(6)-B(10)-B(9)	107.3(3)	B(5)-B(10)-B(9)	59.3(3)
B(12)-B(10)-B(9)	59.9(3)	C(10M)-B(10)-B(11)	122.7(4)
B(6)-B(10)-B(11)	60.1(3)	B(5)-B(10)-B(11)	107.1(3)
B(12)-B(10)-B(11)	59.8(3)	B(9)-B(10)-B(11)	107.6(3)
C(11M)-B(11)-B(2)	119.6(4)	C(11M)-B(11)-B(6)	120.4(4)
B(2)-B(11)-B(6)	60.8(3)	C(11M)-B(11)-B(7)	122.2(4)
B(2)-B(11)-B(7)	60.1(3)	B(6)-B(11)-B(7)	108.2(3)
C(11M)-B(11)-B(12)	124.0(4)	B(2)-B(11)-B(12)	108.2(3)
B(6)-B(11)-B(12)	107.1(3)	B(7)-B(11)-B(12)	60.0(3)
C(11M)-B(11)-B(10)	122.3(4)	B(2)-B(11)-B(10)	108.3(3)
B(6)-B(11)-B(10)	59.1(3)	B(7)-B(11)-B(10)	108.2(3)
B(12)-B(11)-B(10)	60.0(3)	C(12M)-B(12)-B(7)	121.3(4)
C(12M)-B(12)-B(11)	122.6(4)	B(7)-B(12)-B(11)	59.9(3)
C(12M)-B(12)-B(8)	120.9(4)	B(7)-B(12)-B(8)	59.8(3)
B(11)-B(12)-B(8)	107.6(3)	C(12M)-B(12)-B(10)	122.4(4)
B(7)-B(12)-B(10)	108.2(3)	B(11)-B(12)-B(10)	60.2(3)

J3314-9

B(8)-B(12)-B(10)	108.0(3)	C(12M)-B(12)-B(9)	121.5(3)
B(7)-B(12)-B(9)	107.9(3)	B(11)-B(12)-B(9)	108.0(3)
B(8)-B(12)-B(9)	59.9(3)	B(10)-B(12)-B(9)	60.1(3)
C(15)-N-C(13)	111.8(4)	C(15)-N-C(14)	114.9(4)
C(13)-N-C(14)	111.1(3)	C(16)-C(15)-C(20)	122.6(4)
C(16)-C(15)-N	118.7(4)	C(20)-C(15)-N	118.7(4)
C(15)-C(16)-C(17)	118.6(4)	C(16)-C(17)-C(18)	119.5(5)
C(19)-C(18)-C(17)	120.0(5)	C(20)-C(19)-C(18)	121.4(5)
C(19)-C(20)-C(15)	117.9(5)		

J3314-10

Table 7. Anisotropic displacement parameters [Å² x 10³] for [Me₂PhNH][B₁₁CMe₁₂]·MeOH.

The anisotropic displacement factor exponent takes the form:
$-2(\pi)^2[(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	27(2)	27(2)	31(2)	0(2)	2(2)	-8(2)
B(2)	27(3)	32(3)	30(3)	-10(2)	4(2)	-5(2)
B(3)	35(3)	32(3)	28(3)	1(2)	-6(2)	0(2)
B(4)	28(3)	30(3)	24(3)	-2(2)	-6(2)	-1(2)
B(5)	32(3)	33(3)	31(3)	8(2)	-4(2)	-2(3)
B(6)	33(3)	23(3)	36(3)	-5(2)	-1(2)	2(2)
B(7)	34(3)	29(3)	26(3)	4(2)	-3(2)	-7(2)
B(8)	37(3)	26(3)	34(3)	3(2)	-6(3)	1(2)
B(9)	25(3)	23(3)	28(3)	0(2)	-2(2)	6(2)
B(10)	28(3)	26(3)	31(3)	1(2)	1(2)	2(2)
B(11)	30(3)	29(3)	29(3)	1(2)	3(2)	-1(2)
B(12)	28(3)	28(3)	23(3)	-2(2)	3(2)	3(2)
C(1M)	43(3)	40(3)	44(3)	-6(2)	3(2)	-14(2)
C(2M)	45(3)	73(4)	43(3)	-21(3)	7(3)	-14(3)
C(3M)	46(3)	57(3)	40(3)	6(3)	-14(2)	5(3)
C(4M)	34(3)	60(3)	40(3)	-14(3)	-1(2)	-4(3)
C(5M)	59(4)	47(3)	47(3)	11(3)	1(3)	-13(3)
C(6M)	47(3)	28(3)	90(4)	-13(3)	0(3)	9(2)
C(7M)	72(4)	61(3)	41(3)	13(3)	2(3)	-17(3)
C(8M)	52(3)	29(3)	66(4)	1(3)	-6(3)	8(2)
C(9M)	35(3)	54(3)	34(3)	-10(2)	3(2)	-5(2)
C(10M)	42(3)	52(3)	43(3)	5(2)	-9(2)	7(3)
C(11M)	38(3)	54(3)	47(3)	-14(3)	5(2)	-6(3)
C(12M)	31(3)	41(3)	32(3)	-6(2)	2(2)	-11(2)
N	32(2)	28(2)	53(3)	4(2)	-7(2)	-1(2)
C(13)	45(3)	48(3)	129(6)	-17(4)	-20(4)	-3(3)
C(14)	42(3)	38(3)	73(4)	15(3)	0(3)	6(2)
C(15)	23(2)	34(3)	34(3)	1(2)	-2(2)	-7(2)
C(16)	30(2)	34(3)	37(3)	0(2)	5(2)	0(2)
C(17)	43(3)	34(3)	51(3)	-3(2)	5(3)	0(2)
C(18)	32(3)	83(4)	47(3)	-28(3)	0(3)	3(3)
C(19)	45(3)	99(5)	31(3)	9(3)	1(3)	4(3)
C(20)	37(3)	62(3)	46(3)	19(3)	2(3)	4(3)
O	61(3)	159(6)	29(3)	17(3)	3(3)	23(4)
C(21)	110(6)	44(3)	40(4)	5(3)	-31(4)	4(4)
O'	61(3)	159(6)	29(3)	17(3)	3(3)	23(4)
C(21')	110(6)	44(3)	40(4)	5(3)	-31(4)	4(4)

J3314-11

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Me_2PhNH][B_{11}CMe_{12}]$·MeOH.

	x	y	z	U_{eq}
H(1M1)	4629(15)	2917(14)	3016(3)	51
H(1M2)	3949(5)	3108(11)	3780(13)	51
H(1M3)	4852(12)	2295(5)	3801(13)	51
H(2M1)	7001(14)	3923(16)	2095(7)	65
H(2M2)	5791(10)	3784(19)	2065(6)	65
H(2M3)	6492(22)	2908(5)	2421(3)	65
H(3M1)	4703(7)	5072(19)	2270(3)	57
H(3M2)	4212(15)	5897(7)	2842(10)	57
H(3M3)	3839(9)	4747(14)	2882(10)	57
H(4M1)	3613(6)	5438(9)	4925(14)	53
H(4M2)	3609(6)	4239(13)	5049(12)	53
H(4M3)	3320(3)	4707(20)	4213(3)	53
H(5M1)	5308(21)	3314(7)	5953(4)	61
H(5M2)	5802(12)	2417(10)	5451(12)	61
H(5M3)	4660(10)	2776(16)	5277(9)	61
H(6M1)	6791(20)	1915(6)	4476(8)	66
H(6M2)	7729(5)	2272(3)	3945(17)	66
H(6M3)	6669(18)	1973(7)	3544(10)	66
H(7M1)	7642(5)	6167(17)	2708(11)	70
H(7M2)	6670(19)	6869(5)	2862(9)	70
H(7M3)	6606(18)	5968(13)	2239(4)	70
H(8M1)	5666(11)	7397(4)	3975(15)	59
H(8M2)	5102(20)	7103(9)	4774(3)	59
H(8M3)	4542(11)	6931(6)	3952(15)	59
H(9M1)	5236(13)	5994(14)	5890(4)	49
H(9M2)	6421(7)	5844(17)	6077(6)	49
H(9M3)	5633(18)	4947(4)	6245(4)	49
H(10A)	8013(15)	4540(6)	5758(10)	55
H(10B)	8440(9)	3690(19)	5178(3)	55
H(10C)	7535(8)	3428(15)	5773(10)	55
H(11A)	8848(7)	3841(15)	3803(10)	56
H(11B)	8858(7)	4986(6)	3501(15)	56
H(11C)	8469(3)	4103(19)	2935(6)	56
H(12A)	7917(14)	6310(11)	5219(5)	42
H(12B)	7408(7)	7059(3)	4595(13)	42
H(12C)	8357(8)	6370(12)	4346(10)	42
H(1N)	601(3)	5861(3)	3893(2)	27(12)
H(13A)	2259(14)	6284(6)	4070(18)	89
H(13B)	1525(5)	7242(18)	4165(16)	89
H(13C)	2141(16)	7075(21)	3366(5)	89

J3314-12

H(14A)	-421(11)	6399(4)	2898(15)	61
H(14B)	445(6)	7208(16)	2694(11)	61
H(14C)	-143(15)	7267(15)	3515(5)	61
H(16A)	1130(3)	4228(3)	3807(3)	40
H(17A)	1754(3)	2917(4)	3018(3)	51
H(18A)	2254(4)	3265(5)	1733(3)	65
H(19A)	2133(4)	4886(5)	1247(3)	70
H(20A)	1503(3)	6187(4)	2013(3)	58
H(1O)	247(57)	5913(27)	4650(24)	99
H(21A)	1296(6)	5276(25)	5504(5)	78
H(21B)	375(22)	4566(12)	5778(10)	78
H(21C)	315(20)	5761(16)	5914(7)	78
H(1O')	0(534)	5158(209)	5583(187)	99
H(21D)	283(127)	6374(123)	4563(159)	78
H(21E)	1374(131)	5852(36)	4671(171)	78
H(21F)	841(229)	6405(111)	5397(43)	78