Electronic Supplementary Information for Dalton Transactions

1 P n m a R = 0.04 : Jun 30 17:31:49 2004

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S u p p o r t i n g i n f o r m a t i o n
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B E L O N G I N G TO T H E P A P E R

The [2,5,12-$C_3B_8H_{15}$]$^-$ anion, the first representative of the eleven-vertex *hypho* family of tricarbaboranes

b y

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X-Ray crystallography:

Crystal data for **1** : $C_3H_{15}B_8$. $C_4H_{12}N$, M = 211.78, orthorhombic, *Pnma* (No 62), a = 13.8290(2) Å, b = 14.6120(2)Å, c = 13.8060(2)Å, V = 2789.77(7)Å^3, Z = 8, D_x = 1.008 Mg m^{-3}. An colourless crystal of dimensions 0.6x0.5x0.5mm was mounted on glass capillary with epoxy glue and measured at Nonius KappaCCD diffractometer by monochromatized MoKα radiation (λ = 0.71073 Å) at 150(2)K. A absorption was neglected (μ = 0.049 mm^{-1}); a total of 47791 measured reflections in the range h = -17 to 17, k = –18 to 18, l = –17 to 17 (θ_{max}= 27.5˚), from which 3307 were unique (R_{int}=0.042) , 2919 observed according to the $I > 2\sigma(I)$ criterion. The structure was solved by direct methods (SIR92) and refined by full-matrix least squares based on F^2 (SHELXL97). The hydrogen atoms of cluster were found on difference Fourier map and refined isotropically, those of methyl moieties of cation were fixed into idealised positions (riding model) and assigned temperature factors $H_{iso}(H) = 1.5\ U_{eq}$(pivot atom) . The refinement converged (Δ/σ_{max}=0.000) to R = 0.041 for observed reflections and $wR2$ = 0.121, GOF = 1.100 for 228 parameters and all 3307 reflections. The final difference map displayed no peaks of chemical significance ($\Delta\rho_{max}$ = 0.223, $\Delta\rho_{min}$ -0.141 e.Å^{-3}).

SIR92 Altomare, A.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.; Burla, M.C.; Polidori, G. ; Camalli, M. . *J. Appl. Cryst.* **1994**, *27*, 435.

Sheldrick, G. M. (1997). SHELXL97. University of Gőttingen, Germany.

Electronic Supplementary Information for Dalton Transactions

C o n t e n t s
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Table S1 - Crystal Data and Details of the Structure Determination
for: 1 P n m a R = 0.04

Formula			C3 H15 B8, C4 H12 N
Formula Weight			211.78
Crystal System			Orthorhombic
Space group		Pnma	(No. 62)
a, b, c [Angstrom]	13.8290(2)	14.6120(2)	13.8060(2)
V [Ang**3]			2789.77(7)
Z			8
D(calc) [g/cm**3]			1.008
Mu(MoKa) [/mm]			0.049
F(000)			928
Crystal Size [mm]		0.50 x 0.50 x	0.60

Data Collection

Temperature (K)			150
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			2.0, 27.5
Dataset		-17: 17 ; -18: 18 ; -17: 17	
Tot., Uniq. Data, R(int)		47791, 3307,	0.042
Observed data [I > 2.0 sigma(I)]			2919

Refinement

Nref, Npar	3307, 228
R, wR2, S	0.0412, 0.1206, 1.10
w = 1/[\s^2^(Fo^2^)+(0.0574P)^2^+0.7536P] where P=(Fo^2^+2Fc^2^)/3	
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.14, 0.22

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
for: 1 P n m a R = 0.04

Atom	x	y	z	U(eq) [Ang^2]
C2	-0.00603(7)	0.13522(7)	-0.03404(7)	0.0215(3)
C12	0.15688(11)	1/4	-0.03758(11)	0.0259(4)
B3	-0.10509(8)	0.18562(8)	0.01542(8)	0.0223(3)
B8	0.00172(8)	0.15427(8)	0.08492(8)	0.0201(3)
B9	-0.06779(12)	1/4	0.11893(11)	0.0212(4)
B13	0.10810(8)	0.16515(8)	0.01685(8)	0.0214(3)
B14	0.06298(12)	1/4	0.12210(11)	0.0205(4)
C2'	-0.06062(7)	0.13460(7)	0.53277(7)	0.0226(3)
C12'	-0.07313(11)	1/4	0.69477(10)	0.0244(4)
B3'	-0.00648(8)	0.18603(8)	0.43601(9)	0.0219(3)
B8'	0.05782(8)	0.15428(7)	0.54567(8)	0.0211(3)
B9'	0.09498(11)	1/4	0.47780(12)	0.0206(4)
B13'	-0.01535(8)	0.16508(8)	0.64919(9)	0.0230(3)
B14'	0.09166(11)	1/4	0.60917(12)	0.0217(4)
N1	0.25106(5)	0.00531(5)	0.25237(5)	0.0190(2)
C3	0.20674(8)	-0.05942(7)	0.18115(8)	0.0278(3)
C4	0.17398(8)	0.06416(7)	0.29541(8)	0.0293(3)
C5	0.29964(8)	-0.04781(8)	0.33086(8)	0.0317(3)
C6	0.32410(8)	0.06358(7)	0.20200(8)	0.0272(3)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: 1 P n m a R = 0.04

Atom	x	y	z	U(iso) [Ang^2]
H2A	-0.0148(8)	0.0715(9)	-0.0489(9)	0.027(3)
H2B	0.0047(8)	0.1737(10)	-0.0928(10)	0.034(4)
H3	-0.1721(9)	0.1472(8)	0.0210(8)	0.026(3)
H8	-0.0035(7)	0.0888(9)	0.1251(9)	0.025(3)
H9	-0.1125(14)	1/4	0.1885(14)	0.037(5)
H12A	0.2262(16)	1/4	-0.0207(15)	0.050(6)
H12B	0.1510(15)	1/4	-0.1126(15)	0.044(5)
H13	0.1525(9)	0.1038(8)	0.0343(8)	0.025(3)
H14	0.1002(13)	1/4	0.1961(13)	0.032(5)
H33	-0.1233(14)	1/4	-0.0461(13)	0.035(5)
H2A'	-0.0745(9)	0.0703(9)	0.5222(9)	0.030(3)
H2B'	-0.1200(9)	0.1718(9)	0.5420(9)	0.031(3)
H3'	0.0013(8)	0.1468(10)	0.3674(11)	0.040(4)
H8'	0.0985(8)	0.0903(8)	0.5415(8)	0.024(3)
H9'	0.1640(13)	1/4	0.4369(13)	0.033(5)
H12C	-0.0626(14)	1/4	0.7695(15)	0.042(5)
H12D	-0.1501(14)	1/4	0.6795(13)	0.036(5)
H13'	0.0019(8)	0.1045(10)	0.6945(10)	0.034(4)
H14'	0.1623(12)	1/4	0.6499(12)	0.025(4)
H33'	-0.0670(13)	1/4	0.4192(13)	0.031(5)
H3A	0.25620	-0.09790	0.15420	0.0420
H3B	0.17620	-0.02530	0.13020	0.0420
H3C	0.15940	-0.09670	0.21330	0.0420
H4A	0.12680	0.02630	0.32700	0.0440

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: 1 P n m a R = 0.04

Atom	x	y	z	U(iso) [Ang^2]
H4B	0.14330	0.09900	0.24510	0.0440
H4C	0.20230	0.10510	0.34180	0.0440
H5A	0.32780	-0.00630	0.37680	0.0480
H5B	0.34940	-0.08550	0.30330	0.0480
H5C	0.25300	-0.08580	0.36290	0.0480
H6A	0.35210	0.10560	0.24750	0.0410
H6B	0.29320	0.09720	0.15090	0.0410
H6C	0.37390	0.02540	0.17520	0.0410

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for: 1 P n m a R = 0.04

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C2	0.0258(5)	0.0178(5)	0.0208(5)	-0.0028(4)	-0.0010(4)	0.0002(4)
C12	0.0220(7)	0.0252(7)	0.0306(8)	0	0.0055(6)	0
B3	0.0215(5)	0.0191(5)	0.0263(5)	-0.0002(4)	-0.0010(4)	-0.0018(4)
B8	0.0243(5)	0.0164(5)	0.0195(5)	0.0003(4)	0.0005(4)	0.0004(4)
B9	0.0254(8)	0.0176(7)	0.0207(7)	0	0.0040(6)	0
B13	0.0216(5)	0.0203(5)	0.0223(5)	-0.0014(4)	-0.0005(4)	0.0031(4)
B14	0.0249(8)	0.0186(7)	0.0181(7)	0	-0.0021(6)	0
C2'	0.0209(5)	0.0194(5)	0.0275(5)	-0.0013(4)	-0.0005(4)	-0.0038(4)
C12'	0.0290(8)	0.0230(7)	0.0211(7)	0	0.0003(6)	0
B3'	0.0204(5)	0.0217(5)	0.0236(5)	-0.0025(4)	-0.0007(4)	0.0000(4)
B8'	0.0196(5)	0.0175(5)	0.0262(5)	0.0001(4)	-0.0020(4)	0.0009(4)
B9'	0.0176(7)	0.0191(7)	0.0251(7)	0	-0.0001(6)	0
B13'	0.0260(5)	0.0195(5)	0.0235(5)	0.0031(4)	-0.0022(4)	-0.0017(4)
B14'	0.0210(7)	0.0191(7)	0.0250(8)	0	-0.0039(6)	0
N1	0.0201(4)	0.0174(4)	0.0194(4)	0.0013(3)	-0.0005(3)	0.0005(3)
C3	0.0300(5)	0.0237(5)	0.0296(5)	-0.0047(4)	-0.0004(4)	-0.0069(4)
C4	0.0300(6)	0.0271(5)	0.0308(6)	-0.0022(4)	0.0039(4)	0.0088(4)
C5	0.0302(6)	0.0332(6)	0.0316(6)	0.0119(5)	-0.0052(4)	0.0042(5)
C6	0.0279(5)	0.0261(5)	0.0276(5)	0.0020(4)	0.0012(4)	-0.0091(4)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: 1 P n m a R = 0.04

N1	-C3	1.4957(13)	C5	-H5B	0.9600
N1	-C4	1.4929(13)	C5	-H5A	0.9601
N1	-C5	1.4927(13)	C5	-H5C	0.9591
N1	-C6	1.4929(13)	C6	-H6C	0.9604
C2	-B13	1.7821(15)	C6	-H6B	0.9600
C2	-B3	1.6986(15)	C6	-H6A	0.9600
C2	-B8	1.6692(15)	B3	-B9	1.7870(17)
C12	-B13_a	1.5990(15)	B3	-B3_a	1.8814(17)
C12	-B13	1.5990(15)	B3	-B8	1.8200(16)
C2	-H2A	0.961(13)	B8	-B14	1.7140(15)
C2	-H2B	0.998(14)	B8	-B13	1.7529(16)
C12	-H12A	0.99(2)	B8	-B9	1.7610(15)
C12	-H12B	1.04(2)	B9	-B14	1.809(2)
C2'	-B8'	1.6725(15)	B13	-B14	2.0095(17)
C2'	-B3'	1.7058(16)	B3	-H33	1.292(12)
C2'	-B13'	1.7815(16)	B3	-H3	1.086(12)
C12'	-B13'_b	1.6044(15)	B8	-H8	1.108(13)
C12'	-B13'	1.6044(15)	B9	-H9	1.142(19)
C2'	-H2B'	0.993(13)	B13	-H13	1.113(12)
C2'	-H2A'	0.970(13)	B14	-H14	1.144(18)
C12'	-H12C	1.04(2)	B3'	-B8'	1.8160(16)
C12'	-H12D	1.085(19)	B3'	-B9'	1.7819(17)
C3	-H3A	0.9604	B3'	-B3'_b	1.8695(17)
C3	-H3B	0.9601	B8'	-B14'	1.7158(14)
C3	-H3C	0.9604	B8'	-B9'	1.7602(14)
C4	-H4A	0.9602	B8'	-B13'	1.7582(16)
C4	-H4C	0.9599	B9'	-B14'	1.814(2)
C4	-H4B	0.9600	B13'	-B14'	2.0087(17)

Table S5 - Bond Distances (Angstrom) (continued)
for: 1 P n m a R = 0.04

B3'	-H33'	1.276(12)	B9'	-H9'	1.109(18)
B3'	-H3'	1.112(15)	B13'	-H13'	1.110(14)
B8'	-H8'	1.093(12)	B14'	-H14'	1.127(17)

Table S6 - Bond Angles (Degrees)
for: 1 P n m a R = 0.04

C3	-N1	-C5	109.44(8)	B3'	-C2'	-H2A'	113.3(7)
C3	-N1	-C6	109.37(7)	B3'	-C2'	-H2B'	102.8(7)
C4	-N1	-C5	109.39(7)	B8'	-C2'	-H2A'	112.1(7)
C4	-N1	-C6	109.88(7)	B13'	-C2'	-H2B'	92.2(7)
C5	-N1	-C6	109.28(7)	B13'	-C2'	-H2A'	116.6(7)
C3	-N1	-C4	109.47(7)	B13'	-C12'	-H12D	114.4(5)
B3	-C2	-B8	65.41(6)	B13'_b	-C12'	-H12C	108.6(6)
B3	-C2	-B13	116.70(8)	B13'_b	-C12'	-H12D	114.4(5)
B8	-C2	-B13	60.94(6)	B13'	-C12'	-H12C	108.6(6)
B13	-C12	-B13_a	101.68(10)	H12C	-C12'	-H12D	109.2(14)
H2A	-C2	-H2B	113.0(11)	H3A	-C3	-H3C	109.42
B13	-C2	-H2B	92.9(7)	N1	-C3	-H3A	109.45
B3	-C2	-H2B	101.7(7)	H3A	-C3	-H3B	109.48
B8	-C2	-H2A	112.3(8)	N1	-C3	-H3B	109.48
B13	-C2	-H2A	115.7(7)	H3B	-C3	-H3C	109.47
B8	-C2	-H2B	134.1(8)	N1	-C3	-H3C	109.52
B3	-C2	-H2A	113.8(7)	N1	-C4	-H4A	109.52
B13_a	-C12	-H12A	107.4(7)	H4A	-C4	-H4C	109.47
B13	-C12	-H12B	115.8(6)	H4A	-C4	-H4B	109.50
H12A	-C12	-H12B	108.2(17)	N1	-C4	-H4C	109.46
B13_a	-C12	-H12B	115.8(6)	N1	-C4	-H4B	109.45
B13	-C12	-H12A	107.4(7)	H4B	-C4	-H4C	109.42
B8'	-C2'	-B13'	61.10(6)	N1	-C5	-H5A	109.49
B3'	-C2'	-B8'	65.03(6)	H5A	-C5	-H5C	109.50
B3'	-C2'	-B13'	116.24(8)	H5B	-C5	-H5C	109.44
B13'	-C12'	-B13'_b	101.32(10)	N1	-C5	-H5C	109.46
H2A'	-C2'	-H2B'	112.7(11)	H5A	-C5	-H5B	109.48
B8'	-C2'	-H2B'	134.6(7)	N1	-C5	-H5B	109.46

Table S6 - Bond Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

N1	-C6	-H6A	109.44	B3_a	-B9	-B8_a	61.72(6)
N1	-C6	-H6B	109.45	B3	-B9	-B8	61.72(6)
H6A	-C6	-H6C	109.54	B8	-B9	-B14	57.37(6)
H6B	-C6	-H6C	109.47	B3	-B9	-B8_a	111.25(9)
N1	-C6	-H6C	109.47	C2	-B13	-B8	56.35(6)
H6A	-C6	-H6B	109.46	C2	-B13	-B14	99.29(8)
C2	-B3	-B8	56.52(6)	C2	-B13	-C12	112.25(9)
B3_a	-B3	-B8	104.58(7)	C12	-B13	-B8	132.56(9)
B8	-B3	-B9	58.44(6)	B8	-B13	-B14	53.68(6)
C2	-B3	-B9	108.48(8)	C12	-B13	-B14	89.57(7)
B3_a	-B3	-B9	58.24(6)	B8	-B14	-B8_a	109.39(10)
C2	-B3	-B3_a	115.69(8)	B8_a	-B14	-B13_a	55.49(6)
C2	-B8	-B13	62.71(6)	B8_a	-B14	-B13	116.13(9)
C2	-B8	-B14	117.55(9)	B8	-B14	-B13	55.49(6)
C2	-B8	-B3	58.07(6)	B13	-B14	-B13_a	76.19(7)
C2	-B8	-B9	111.09(9)	B9	-B14	-B13_a	107.03(8)
B9	-B8	-B13	121.94(9)	B8	-B14	-B9	59.91(6)
B3	-B8	-B9	59.84(7)	B8	-B14	-B13_a	116.13(9)
B13	-B8	-B14	70.84(8)	B8_a	-B14	-B9	59.91(6)
B3	-B8	-B14	110.71(8)	B9	-B14	-B13	107.03(8)
B9	-B8	-B14	62.72(8)	B8	-B3	-H3	121.7(6)
B3	-B8	-B13	112.07(8)	B3_a	-B3	-H33	43.3(6)
B3	-B9	-B14	107.93(9)	C2	-B3	-H33	102.0(8)
B8_a	-B9	-B14	57.37(6)	B8	-B3	-H33	133.5(8)
B8	-B9	-B8_a	105.18(10)	H3	-B3	-H33	104.9(10)
B3	-B9	-B3_a	63.53(7)	B3_a	-B3	-H3	121.1(6)
B3_a	-B9	-B14	107.93(9)	C2	-B3	-H3	119.5(6)
B3_a	-B9	-B8	111.25(9)	B9	-B3	-H3	117.5(6)

Table S6 - Bond Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

B9	-B3	-H33	101.5(6)	C2'	-B8'	-B14'	117.50(9)
B14	-B8	-H8	125.9(6)	B3'	-B8'	-B9'	59.75(7)
B13	-B8	-H8	113.7(5)	C2'	-B8'	-B3'	58.37(6)
C2	-B8	-H8	110.1(7)	C2'	-B8'	-B9'	111.46(8)
B3	-B8	-H8	115.4(5)	B9'	-B8'	-B14'	62.91(8)
B9	-B8	-H8	121.1(6)	B13'	-B8'	-B14'	70.64(8)
B3	-B9	-H9	121.1(8)	B3'	-B8'	-B14'	110.57(8)
B8	-B9	-H9	121.3(4)	B9'	-B8'	-B13'	121.97(8)
B8_a	-B9	-H9	121.3(4)	B3'	-B9'	-B3'_b	63.28(7)
B3_a	-B9	-H9	121.1(8)	B8'_b	-B9'	-B14'	57.35(6)
B14	-B9	-H9	121.4(10)	B3'_b	-B9'	-B8'_b	61.68(6)
C2	-B13	-H13	112.1(6)	B8'	-B9'	-B8'_b	105.24(10)
B14	-B13	-H13	120.8(6)	B3'_b	-B9'	-B14'	107.68(9)
B8	-B13	-H13	105.9(6)	B3'	-B9'	-B8'	61.68(6)
C12	-B13	-H13	119.6(6)	B3'	-B9'	-B14'	107.68(9)
B8_a	-B14	-H14	119.3(3)	B8'	-B9'	-B14'	57.35(6)
B13_a	-B14	-H14	120.4(6)	B3'_b	-B9'	-B8'	111.06(9)
B13	-B14	-H14	120.4(6)	B3'	-B9'	-B8'_b	111.06(9)
B8	-B14	-H14	119.3(3)	C2'	-B13'	-C12'	111.85(9)
B9	-B14	-H14	118.1(9)	C2'	-B13'	-B14'	99.51(8)
C2'	-B3'	-B8'	56.60(6)	C12'	-B13'	-B14'	89.83(7)
C2'	-B3'	-B9'	108.85(9)	B8'	-B13'	-B14'	53.69(6)
C2'	-B3'	-B3'_b	116.14(8)	C12'	-B13'	-B8'	132.44(9)
B8'	-B3'	-B9'	58.57(6)	C2'	-B13'	-B8'	56.39(6)
B3'_b	-B3'	-B8'	104.80(8)	B8'	-B14'	-B8'_b	109.21(10)
B3'_b	-B3'	-B9'	58.36(6)	B13'	-B14'	-B13'_b	76.30(7)
C2'	-B8'	-B13'	62.51(6)	B8'_b	-B14'	-B13'_b	55.67(6)
B3'	-B8'	-B13'	111.90(8)	B9'	-B14'	-B13'_b	107.08(8)

Table S6 - Bond Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

B8'_b	-B14'	-B13'	116.31(9)	B3'	-B8'	-H8'	115.3(6)
B8'	-B14'	-B9'	59.74(6)	B13'	-B8'	-H8'	114.6(6)
B8'	-B14'	-B13'	55.67(6)	B14'	-B8'	-H8'	125.7(6)
B8'_b	-B14'	-B9'	59.74(6)	B8'_b	-B9'	-H9'	121.5(3)
B8'	-B14'	-B13'_b	116.31(9)	B3'	-B9'	-H9'	120.9(7)
B9'	-B14'	-B13'	107.08(8)	B8'	-B9'	-H9'	121.5(3)
B8'	-B3'	-H33'	131.3(8)	B14'	-B9'	-H9'	122.1(9)
C2'	-B3'	-H3'	118.8(7)	B3'_b	-B9'	-H9'	120.9(7)
C2'	-B3'	-H33'	100.2(8)	B8'	-B13'	-H13'	105.2(7)
B8'	-B3'	-H3'	122.1(7)	C2'	-B13'	-H13'	112.6(7)
H3'	-B3'	-H33'	106.6(10)	C12'	-B13'	-H13'	120.2(7)
B9'	-B3'	-H3'	118.0(6)	B14'	-B13'	-H13'	119.3(6)
B9'	-B3'	-H33'	101.0(6)	B13'_b	-B14'	-H14'	120.1(6)
B3'_b	-B3'	-H3'	121.0(8)	B8'	-B14'	-H14'	119.4(3)
B3'_b	-B3'	-H33'	42.9(6)	B9'	-B14'	-H14'	118.5(8)
B9'	-B8'	-H8'	120.1(6)	B13'	-B14'	-H14'	120.1(6)
C2'	-B8'	-H8'	110.6(6)	B8'_b	-B14'	-H14'	119.4(3)

Table S7 - Torsion Angles (Degrees)
for: 1 P n m a R = 0.04

B3	-C2	-B8	-B9	-28.99(8)
B3	-C2	-B8	-B13	-145.04(8)
B3	-C2	-B8	-B14	-98.33(10)
B13	-C2	-B8	-B3	145.04(8)
B13	-C2	-B8	-B9	116.04(9)
B13	-C2	-B8	-B14	46.71(9)
B3	-C2	-B13	-C12	-91.58(10)
B3	-C2	-B13	-B8	35.68(8)
B3	-C2	-B13	-B14	1.78(10)
B8	-C2	-B13	-C12	-127.27(10)
B8	-C2	-B3	-B9	28.03(7)
B8	-C2	-B3	-B3_a	90.95(9)
B13	-C2	-B3	-B8	-34.10(8)
B13	-C2	-B3	-B9	-6.08(11)
B13	-C2	-B3	-B3_a	56.85(11)
B8	-C2	-B13	-B14	-33.90(6)
B13	-C12	-B13_a	-B14	14.60(10)
B13_a	-C12	-B13	-B14	-14.60(10)
B13_a	-C12	-B13	-C2	85.27(11)
B13_a	-C12	-B13	-B8	21.20(16)
B8'	-C2'	-B13'	-B14'	33.67(6)
B8'	-C2'	-B13'	-C12'	127.34(10)
B13'	-C2'	-B3'	-B8'	34.52(8)
B8'	-C2'	-B3'	-B9'	-27.73(7)
B13'	-C2'	-B8'	-B14'	-46.20(9)
B13'	-C2'	-B8'	-B9'	-115.89(9)
B3'	-C2'	-B13'	-B14'	-2.26(10)
B3'	-C2'	-B13'	-B8'	-35.93(8)

Table S7 - Torsion Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

B8'	-C2'	-B3'	-B3'_b	-90.99(9)
B3'	-C2'	-B8'	-B14'	98.31(10)
B13'	-C2'	-B8'	-B3'	-144.51(8)
B3'	-C2'	-B8'	-B9'	28.62(8)
B13'	-C2'	-B3'	-B9'	6.80(11)
B13'	-C2'	-B3'	-B3'_b	-56.47(11)
B3'	-C2'	-B13'	-C12'	91.41(10)
B3'	-C2'	-B8'	-B13'	144.51(8)
B13'_b	-C12'	-B13'	-B8'	-22.51(16)
B13'	-C12'	-B13'_b	-B14'	-13.87(10)
B13'_b	-C12'	-B13'	-C2'	-86.31(10)
B13'_b	-C12'	-B13'	-B14'	13.87(10)
B8	-B3	-B3_a	-B9	-37.15(8)
B9	-B3	-B8	-B14	-38.16(9)
B3_a	-B3	-B8	-C2	-111.41(8)
B3_a	-B3	-B8	-B9	37.05(7)
B8	-B3	-B3_a	-C2_a	59.50(10)
C2	-B3	-B9	-B3_a	109.32(9)
C2	-B3	-B9	-B8_a	68.92(10)
C2	-B3	-B3_a	-B8_a	-59.50(10)
B8	-B3	-B9	-B14	35.14(6)
B8	-B3	-B9	-B3_a	136.70(9)
B8	-B3	-B9	-B8_a	96.31(10)
B3_a	-B3	-B9	-B8	-136.70(9)
B8	-B3	-B3_a	-B8_a	0.00(9)
C2	-B3	-B9	-B14	7.76(9)
C2	-B3	-B9	-B8	-27.38(7)
B9	-B3	-B8	-C2	-148.46(9)

Table S7 - Torsion Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

B9	-B3	-B8	-B13	-115.13(10)
C2	-B3	-B8	-B14	110.30(10)
C2	-B3	-B3_a	-B9	-96.65(10)
B3_a	-B3	-B8	-B13	-78.08(9)
B3_a	-B3	-B8	-B14	-1.11(11)
C2	-B3	-B8	-B13	33.33(8)
C2	-B3	-B3_a	-C2_a	0.00(11)
C2	-B3	-B8	-B9	148.46(9)
B3_a	-B3	-B9	-B14	-101.56(8)
B14	-B8	-B13	-C2	-136.91(8)
B14	-B8	-B13	-C12	-46.55(13)
B3	-B8	-B14	-B8_a	1.86(13)
B9	-B8	-B13	-C2	-98.94(11)
B3	-B8	-B13	-C12	58.71(15)
B9	-B8	-B13	-C12	-8.58(17)
B9	-B8	-B13	-B14	37.96(10)
B3	-B8	-B14	-B13	-107.08(9)
B14	-B8	-B9	-B3	139.44(9)
B14	-B8	-B9	-B3_a	98.24(10)
B3	-B8	-B14	-B13_a	-58.38(12)
B9	-B8	-B14	-B13	-144.03(9)
C2	-B8	-B9	-B3	28.41(8)
B3	-B8	-B13	-B14	105.25(9)
B3	-B8	-B14	-B9	36.95(9)
B9	-B8	-B14	-B8_a	-35.09(9)
B9	-B8	-B14	-B13_a	-95.33(10)
C2	-B8	-B14	-B9	100.81(10)
C2	-B8	-B14	-B13	-43.22(8)

Table S7 - Torsion Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

C2	-B8	-B14	-B8_a	65.72(13)
C2	-B8	-B14	-B13_a	5.48(13)
B3	-B8	-B13	-C2	-31.65(7)
B13	-B8	-B9	-B8_a	-7.68(14)
B13	-B8	-B9	-B3_a	57.41(13)
B13	-B8	-B9	-B14	-40.83(10)
B14	-B8	-B9	-B8_a	33.15(9)
C2	-B8	-B13	-C12	90.36(13)
C2	-B8	-B13	-B14	136.91(8)
B3	-B8	-B9	-B3_a	-41.20(8)
B13	-B8	-B14	-B9	144.03(9)
B13	-B8	-B14	-B8_a	108.94(10)
C2	-B8	-B9	-B14	-111.03(10)
C2	-B8	-B9	-B3_a	-12.79(12)
C2	-B8	-B9	-B8_a	-77.88(11)
B3	-B8	-B9	-B14	-139.44(9)
B13	-B8	-B14	-B13_a	48.70(9)
B13	-B8	-B9	-B3	98.61(10)
B3	-B8	-B9	-B8_a	-106.29(10)
B8_a	-B9	-B14	-B13	-110.79(9)
B8_a	-B9	-B14	-B8	-141.20(10)
B3	-B9	-B14	-B13_a	73.78(7)
B8	-B9	-B14	-B13	30.41(7)
B3_a	-B9	-B14	-B13	-73.78(7)
B8	-B9	-B14	-B13_a	110.79(9)
B3_a	-B9	-B14	-B8	-104.19(9)
B8	-B9	-B14	-B8_a	141.20(10)
B3	-B9	-B14	-B8_a	104.19(9)

Table S7 - Torsion Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

B3	-B9	-B14	-B13	-6.59(8)
B3	-B9	-B14	-B8	-37.00(7)
C2	-B13	-B14	-B13_a	-100.82(7)
C12	-B13	-B14	-B8	147.67(10)
C12	-B13	-B14	-B9	115.57(8)
B8	-B13	-B14	-B13_a	-136.01(9)
C2	-B13	-B14	-B8	35.19(7)
C2	-B13	-B14	-B9	3.08(8)
C2	-B13	-B14	-B8_a	-61.21(11)
B8	-B13	-B14	-B9	-32.11(7)
C12	-B13	-B14	-B8_a	51.27(11)
B8	-B13	-B14	-B8_a	-96.40(11)
C12	-B13	-B14	-B13_a	11.67(8)
B9'	-B3'	-B8'	-B13'	115.22(9)
B9'	-B3'	-B8'	-C2'	148.94(9)
B3'_b	-B3'	-B8'	-C2'	111.81(8)
B3'_b	-B3'	-B8'	-B9'	-37.12(7)
B3'_b	-B3'	-B8'	-B13'	78.10(9)
B3'_b	-B3'	-B8'	-B14'	1.44(11)
B3'_b	-B3'	-B9'	-B14'	101.33(8)
C2'	-B3'	-B3'_b	-B9'	96.92(10)
B9'	-B3'	-B8'	-B14'	38.57(9)
C2'	-B3'	-B9'	-B8'_b	-69.38(10)
B8'	-B3'	-B9'	-B14'	-35.41(6)
B8'	-B3'	-B9'	-B3'_b	-136.74(9)
B8'	-B3'	-B9'	-B8'_b	-96.45(10)
B3'_b	-B3'	-B9'	-B8'	136.74(9)
C2'	-B3'	-B8'	-B9'	-148.94(9)

Table S7 - Torsion Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

C2'	-B3'	-B8'	-B13'	-33.72(8)
C2'	-B3'	-B8'	-B14'	-110.37(10)
B8'	-B3'	-B3'_b	-B8'_b	0.00(10)
C2'	-B3'	-B3'_b	-C2'_b	0.00(12)
C2'	-B3'	-B3'_b	-B8'_b	59.70(10)
B8'	-B3'	-B3'_b	-B9'	37.22(8)
C2'	-B3'	-B9'	-B8'	27.08(7)
C2'	-B3'	-B9'	-B14'	-8.33(9)
C2'	-B3'	-B9'	-B3'_b	-109.66(9)
B8'	-B3'	-B3'_b	-C2'_b	-59.70(10)
B3'	-B8'	-B13'	-C12'	-57.68(15)
B3'	-B8'	-B13'	-B14'	-105.07(9)
B9'	-B8'	-B13'	-C2'	99.29(11)
B9'	-B8'	-B13'	-C12'	9.42(18)
B9'	-B8'	-B13'	-B14'	-37.98(10)
B14'	-B8'	-B13'	-C2'	137.27(8)
B13'	-B8'	-B9'	-B3'_b	-57.34(13)
C2'	-B8'	-B14'	-B9'	-101.36(10)
B13'	-B8'	-B9'	-B8'_b	7.70(14)
B14'	-B8'	-B9'	-B3'	-139.03(9)
B14'	-B8'	-B9'	-B3'_b	-98.04(10)
B14'	-B8'	-B9'	-B8'_b	-33.00(9)
C2'	-B8'	-B13'	-C12'	-89.87(13)
B14'	-B8'	-B13'	-C12'	47.40(13)
B3'	-B8'	-B13'	-C2'	32.20(7)
B9'	-B8'	-B14'	-B8'_b	34.81(9)
B9'	-B8'	-B14'	-B13'_b	95.21(10)
B13'	-B8'	-B14'	-B9'	-144.10(9)

Table S7 - Torsion Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

B13'	-B8'	-B14'	-B8'_b	-109.29(10)
B13'	-B8'	-B14'	-B13'_b	-48.89(9)
B3'	-B8'	-B9'	-B8'_b	106.04(10)
B13'	-B8'	-B9'	-B3'	-98.33(10)
B13'	-B8'	-B9'	-B14'	40.70(10)
C2'	-B8'	-B9'	-B3'	-28.17(8)
C2'	-B8'	-B14'	-B13'	42.74(8)
C2'	-B8'	-B14'	-B8'_b	-66.55(12)
C2'	-B8'	-B14'	-B13'_b	-6.16(13)
B3'	-B8'	-B14'	-B9'	-37.22(9)
C2'	-B8'	-B13'	-B14'	-137.27(8)
B9'	-B8'	-B14'	-B13'	144.10(9)
B3'	-B8'	-B14'	-B13'	106.88(9)
C2'	-B8'	-B9'	-B14'	110.86(10)
C2'	-B8'	-B9'	-B3'_b	12.82(12)
C2'	-B8'	-B9'	-B8'_b	77.87(11)
B3'	-B8'	-B9'	-B14'	139.03(9)
B3'	-B8'	-B9'	-B3'_b	40.99(8)
B3'	-B8'	-B14'	-B13'_b	57.99(12)
B3'	-B8'	-B14'	-B8'_b	-2.41(13)
B8'	-B9'	-B14'	-B13'	-30.44(7)
B3'	-B9'	-B14'	-B8'	37.29(7)
B8'	-B9'	-B14'	-B13'_b	-110.95(9)
B3'_b	-B9'	-B14'	-B8'	104.10(9)
B3'_b	-B9'	-B14'	-B13'	73.66(7)
B8'_b	-B9'	-B14'	-B8'	141.39(10)
B3'	-B9'	-B14'	-B13'	6.85(8)
B3'	-B9'	-B14'	-B8'_b	-104.10(9)

Table S7 - Torsion Angles (Degrees) (continued)
for: 1 P n m a R = 0.04

B8'	-B9'	-B14'	-B8'_b	-141.39(10)
B3'	-B9'	-B14'	-B13'_b	-73.66(7)
B8'_b	-B9'	-B14'	-B13'	110.95(9)
C2'	-B13'	-B14'	-B13'_b	101.00(8)
C12'	-B13'	-B14'	-B9'	-115.10(8)
C12'	-B13'	-B14'	-B8'_b	-50.96(11)
C12'	-B13'	-B14'	-B8'	-147.10(10)
B8'	-B13'	-B14'	-B9'	32.00(7)
C2'	-B13'	-B14'	-B8'_b	61.18(11)
B8'	-B13'	-B14'	-B13'_b	135.96(9)
C12'	-B13'	-B14'	-B13'_b	-11.14(8)
B8'	-B13'	-B14'	-B8'_b	96.14(11)
C2'	-B13'	-B14'	-B9'	-2.96(8)
C2'	-B13'	-B14'	-B8'	-34.96(7)

Table S8 - Contact Distances(Angstrom)
for: 1 P n m a R = 0.04

C5	.B13_w	3.3408(16)	H2B'	.H12A_r	2.43(2)
C5	.C12_x	3.5198(14)	H2A	.H2A_h	2.521(18)
C5	.C12_w	3.5198(14)	H2A	.H8_h	2.580(18)
C6	.B3'_m	3.5101(16)	H2A	.H3B_i	2.5879
C12	.C5_d	3.5198(14)	H2B	.H12B	2.33(2)
C12	.C5_c	3.5198(14)	H2B	.C2_a	2.911(15)
C2	.H2B_a	2.911(15)	H2B	.H12C_k	2.39(2)
C2'	.H2B'_b	2.948(13)	H2B	.H12C_j	2.39(2)
C4	.H3'	2.855(12)	H2B	.H2B_a	2.23(2)
C5	.H13_w	2.999(11)	H3'	.H4A	2.5344
C6	.H3'_m	2.899(12)	H3'	.C4	2.855(12)
C12	.H5C_c	3.0328	H3'	.H6C_f	2.5684
C12	.H5C_d	3.0328	H3'	.C6_f	2.899(12)
C12'	.H3C_n	2.8376	H3A	.H14'_z	2.4926
C12'	.H3C_o	2.8376	H3A	.H6C	2.4453
B3'	.C6_f	3.5101(16)	H3A	.H8'_y	2.5438
B13	.C5_c	3.3408(16)	H3A	.H5B	2.4354
B9	.H6A_f	3.0133	H3A	.H14'_y	2.4926
B9	.H6A_e	3.0133	H3B	.H4B	2.4540
B13'	.H3C_o	2.9276	H3B	.H6B	2.4297
B14	.H4B_g	2.9976	H3B	.H13	2.3279
B14	.H4B	2.9976	H3B	.H2A_h	2.5879
H2A'	.H8'_p	2.528(17)	H3C	.H13'_p	2.5708
H2B'	.H5C_o	2.5857	H3C	.H5C	2.4427
H2B'	.H2B'_b	2.285(19)	H3C	.B13'_p	2.9276
H2B'	.H12A_q	2.43(2)	H3C	.H4A	2.4285
H2B'	.H12D	2.25(2)	H3C	.C12'_p	2.8376
H2B'	.C2'_b	2.948(13)	H4A	.H3'	2.5344

Table S8 - Contact Distances(Angstrom) (continued)
for: 1 P n m a R = 0.04

H4A	.H5C	2.4443	H6C	.H13'_y	2.5737
H4A	.H3C	2.4285	H6C	.H3A	2.4453
H4B	.B14	2.9976	H6C	.H5B	2.4225
H4B	.H14	2.3835	H6C	.H8'_y	2.5320
H4B	.H6B	2.4473	H8	.H2A_h	2.580(18)
H4B	.H3B	2.4540	H8'	.H6C_s	2.5320
H4B	.H14	2.3835	H8'	.H2A'_p	2.528(17)
H4B	.B14	2.9976	H8'	.H3A_s	2.5438
H4C	.H6A	2.4467	H9	.H6A_e	2.3393
H4C	.H5A	2.4280	H9	.H6A_f	2.3393
H4C	.H9'	2.5470	H9'	.H4C	2.5470
H4C	.H9'	2.5470	H9'	.H4C_g	2.5470
H5A	.H4C	2.4280	H12A	.H2B'_m	2.43(2)
H5A	.H6A	2.4440	H12A	.H2B'_l	2.43(2)
H5B	.H6C	2.4225	H12B	.H2B_a	2.33(2)
H5B	.H3A	2.4354	H12B	.H2B	2.33(2)
H5B	.H13'_y	2.5616	H12C	.H2B_t	2.39(2)
H5C	.H4A	2.4443	H12C	.H2B_u	2.39(2)
H5C	.C12_x	3.0328	H12D	.H2B'_b	2.25(2)
H5C	.H3C	2.4427	H12D	.H2B'	2.25(2)
H5C	.C12_w	3.0328	H13	.H3B	2.3279
H5C	.H2B'_p	2.5857	H13	.H6B	2.5272
H6A	.H4C	2.4467	H13	.C5_c	2.999(11)
H6A	.H5A	2.4440	H13'	.H3C_o	2.5708
H6B	.H13	2.5272	H13'	.H5B_s	2.5616
H6B	.H3B	2.4297	H13'	.H6C_s	2.5737
H6B	.H4B	2.4473	H14	.H4B_g	2.3835
H6C	.H3'_m	2.5684	H14	.H4B	2.3835

Table S8 - Contact Distances(Angstrom) (continued)
for: 1 P n m a R = 0.04

H14'	.H3A_s	2.4926	H14'	.H3A_v	2.4926

Translation of Symmetry Code to Equiv.Pos

```
a =[  8555.00 ]  = x,1/2-y,z
b =[  8555.00 ]  = x,1/2-y,z
c =[  2554.00 ]  = 1/2-x,-y,-1/2+z
d =[  7554.00 ]  = 1/2-x,1/2+y,-1/2+z
e =[  3455.00 ]  = -1/2+x,1/2-y,1/2-z
f =[  6455.00 ]  = -1/2+x,y,1/2-z
g =[  8555.00 ]  = x,1/2-y,z
h =[  5555.00 ]  = -x,-y,-z
i =[  5555.00 ]  = -x,-y,-z
j =[  1554.00 ]  = x,y,-1+z
k =[  8554.00 ]  = x,1/2-y,-1+z
l =[  3555.00 ]  = 1/2+x,1/2-y,1/2-z
m =[  6555.00 ]  = 1/2+x,y,1/2-z
n =[  4556.00 ]  = -x,1/2+y,1-z
o =[  5556.00 ]  = -x,-y,1-z
p =[  5556.00 ]  = -x,-y,1-z
q =[  3455.00 ]  = -1/2+x,1/2-y,1/2-z
r =[  6455.00 ]  = -1/2+x,y,1/2-z
s =[  2555.00 ]  = 1/2-x,-y,1/2+z
t =[  1556.00 ]  = x,y,1+z
u =[  8556.00 ]  = x,1/2-y,1+z
v =[  7555.00 ]  = 1/2-x,1/2+y,1/2+z
w =[  2555.00 ]  = 1/2-x,-y,1/2+z
x =[  7545.00 ]  = 1/2-x,-1/2+y,1/2+z
y =[  2554.00 ]  = 1/2-x,-y,-1/2+z
z =[  7544.00 ]  = 1/2-x,-1/2+y,-1/2+z
* =[  4546.00 ]  = -x,-1/2+y,1-z
* =[  3555.00 ]  = 1/2+x,1/2-y,1/2-z
* =[  6555.00 ]  = 1/2+x,y,1/2-z
```

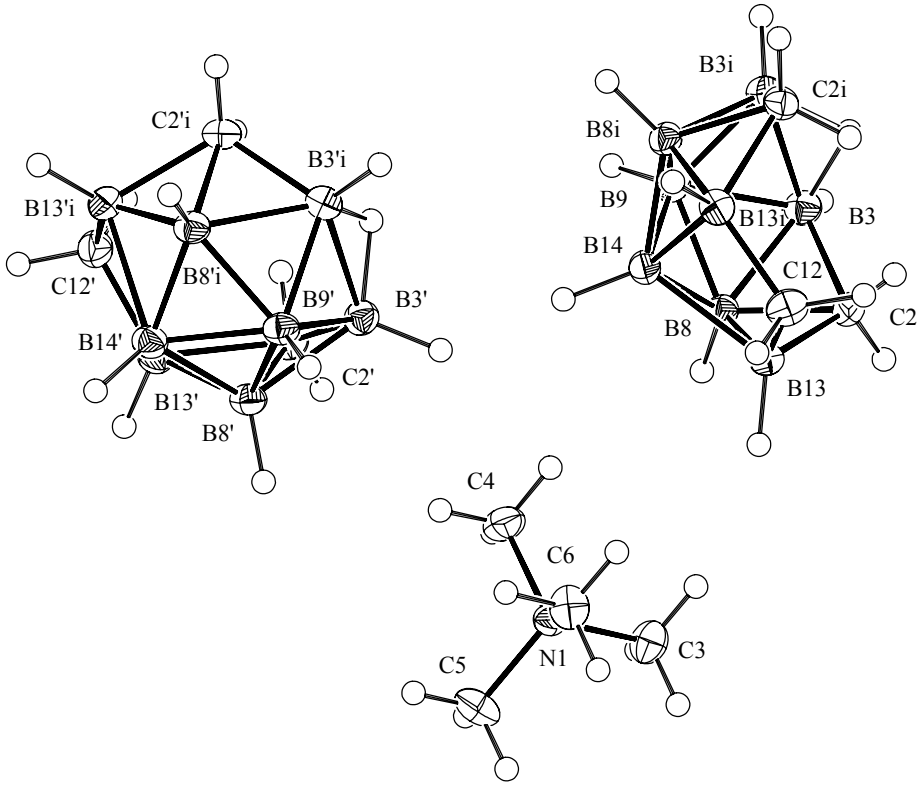

Fig s1. View on the asymmetric unit of **1** with atom numbering schema for symmetrically independent parts. Both carbaborane cages are situated on mirror plane going through atoms B9,C12, B14 and B9', C12' and B14' for cage 1 and 2 respectively. Displacement ellipsoids are drawn on 50% probability level.

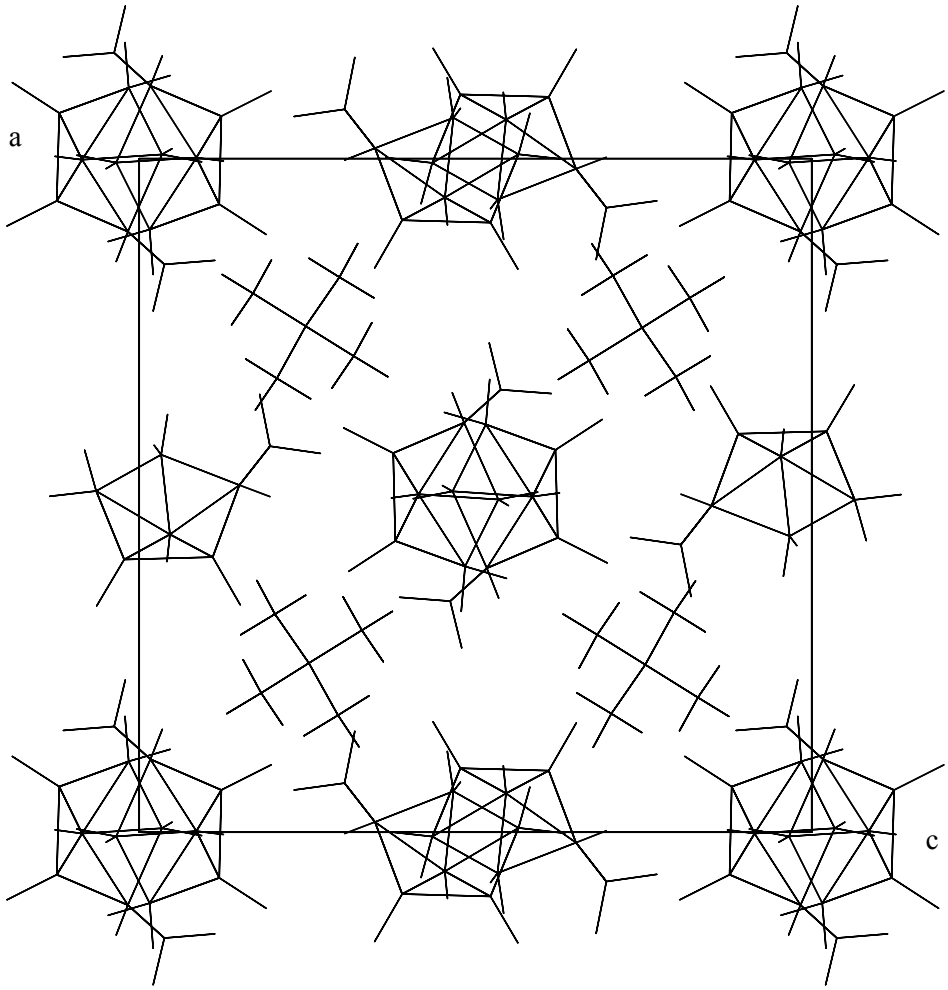

Fig s2. View on the unit cell of 1 along axis b.