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Caesium tetramethylammonium dodecahydrido-*closo*-dodecaborate monohydrate

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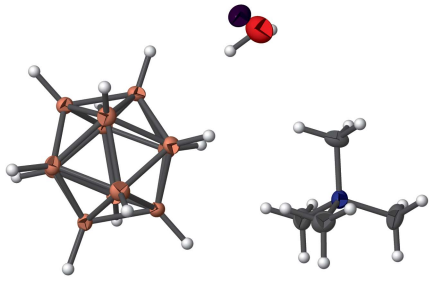
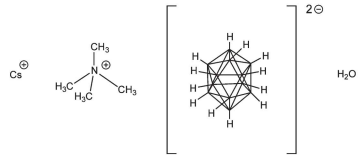
In the crystal structure of the hydrated double salt, $Cs^{+}\cdot[N(CH_3)_4]^{+}\cdot[B_{12}H_{12}]^{2-}\cdot H_2O$, the asymmetric unit contains one caesium and one tetramethylammonium cation, one dodecahydrido-*closo*-dodecaborate anion and one water molecule. The Cs^{+} cation is coordinated tetrahedrally by four $[B_{12}H_{12}]^{2-}$ clusters, with the water molecule completing the coordination sphere. The tetramethylammonium cation is surrounded distorted octahedrally by six $[B_{12}H_{12}]^{2-}$ anions. The crystal structure is stabilized by a three-dimensional network of O—H···H—B and C—H···H—B dihydrogen bonds.

3D view



Chemical scheme



Structure description

The crystal structures of dodecahydrido-*closo*-dodecaborates with heavier alkali metals $M_2[B_{12}H_{12}]$ (M = K, Rb, Cs) have been elucidated by single-crystal X-ray data [for the dicaesium salt, see: Tiritiris *et al.* (2000); for the dirubidium and dipotassium salts, see: Tiritiris & Schleid (2003)]. The crystal structures of the solvent-free and the acetonitrile-solvated bis(tetramethylammonium) salts have been also reported (Hofmann & Albert, 2001). In contrast, data for cationic mixed compounds with *closo*-borate anions are scarce. Until now, only two examples, namely $Cs[Na(NH_3)_6][B_{10}H_{10}]\cdot NH_3$ (Kraus & Albert, 2005) and the rare-earth-metal-containing compound $[La(H_2O)_9](H_3O)Cl_2[B_{12}H_{12}]\cdot H_2O$ (Tiritiris & Schleid, 2008), have been published. The title compound is the second in our series to have been structurally characterized (Fig. 1). The B—B bond lengths and the B—B—B angles are in typical ranges for a $[B_{12}H_{12}]^{2-}$ anion [1.771 (5)–1.795 (5) Å and 59.6 (2)–60.5 (2)°] and comparable with those of $Cs_2[B_{12}H_{12}]$ (Tiritiris *et al.*, 2000). Two anions are coordinating *via* triangular faces and another two *via* edges of H atoms to the caesium cation [Cs—H = 2.99 (4)–3.55 (3) Å]. The water molecule completes the coordination sphere of caesium, yielding a coordination number of 11

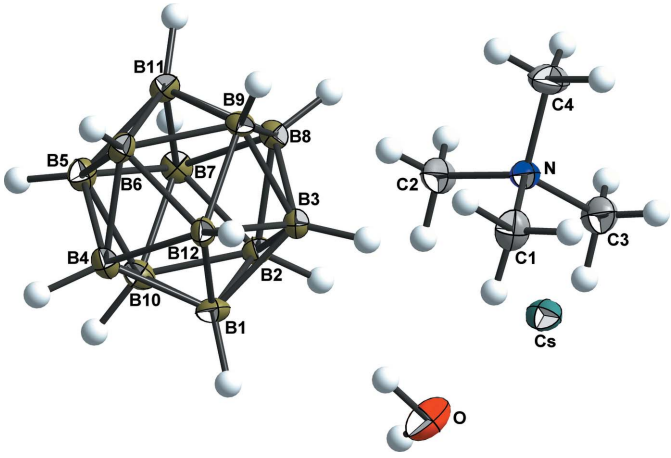


Figure 1
The molecular components of the title compound, with displacement ellipsoids drawn at the 50% probability level.

(Fig. 2). Every dodecahydrido-*closo*-dodecaborate anion is surrounded by four caesium and four tetramethylammonium cations, forming a slightly distorted cube.

The crystal structure is mainly stabilized by O—H···H—B dihydrogen bonds between the water molecules and the $[B_{12}H_{12}]^{2-}$ anions (Fig. 3 and Table 1). O—H···H—B dihydrogen-bonding interactions between the cluster anions and the water molecules were also observed in the crystal structure of $(NH_4)_2[B_{10}H_{10}]\cdot 1.5H_2O$ (Yisgedu *et al.*, 2010), there ranging from 2.12 (3) to 2.23 (3) Å. Taking additional C—H···H—B dihydrogen-bonding interactions between the anions and the tetramethylammonium cations into account, a three-dimensional network structure results (Fig. 4 and Table 1).

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O—H14···H7	0.91 (1)	2.11 (3)	2.86 (3)	135 (4)
O—H13···H1^{i}	0.91 (1)	2.45 (3)	3.24 (3)	146 (4)
O—H13···H2^{i}	0.91 (1)	2.47 (3)	3.07 (3)	124 (4)
O—H13···H3^{i}	0.91 (1)	2.39 (3)	3.11 (3)	136 (4)
C1—H1*A*···H3^{ii}	0.98	2.49	3.35 (5)	143
C2—H2*B*···H5	0.98	2.33	3.20 (5)	151
C2—H2*C*···H6^{iii}	0.98	2.49	3.29 (4)	138
C2—H2*B*···H9^{iii}	0.98	2.51	2.79 (4)	96
C3—H3*C*···H8^{iv}	0.98	2.51	3.18 (4)	126
C3—H3*C*···H11^{iv}	0.98	2.33	3.28 (4)	160
C4—H4*B*···H3^{ii}	0.98	2.30	3.21 (4)	152
C4—H4*C*···H1^{v}	0.98	2.52	2.82 (5)	98

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, -y, z-\frac{1}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (iv) $x-1, y, z$; (v) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.

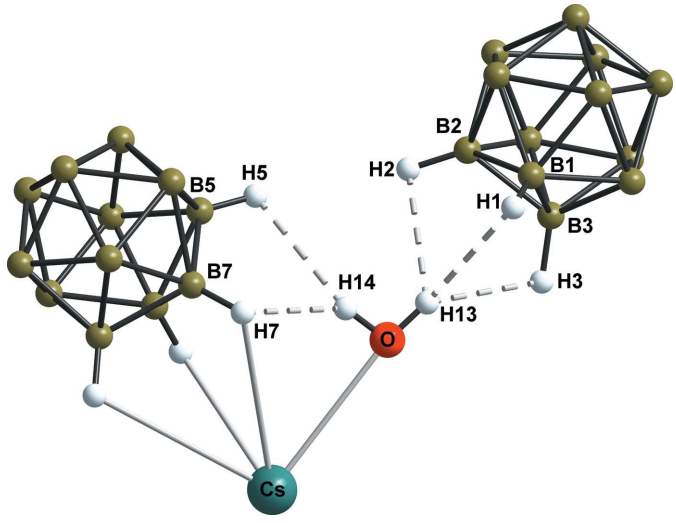


Figure 3
B—H···H—O dihydrogen bonds (depicted by grey dashed lines) between two $[B_{12}H_{12}]^{2-}$ anions and a water molecule.

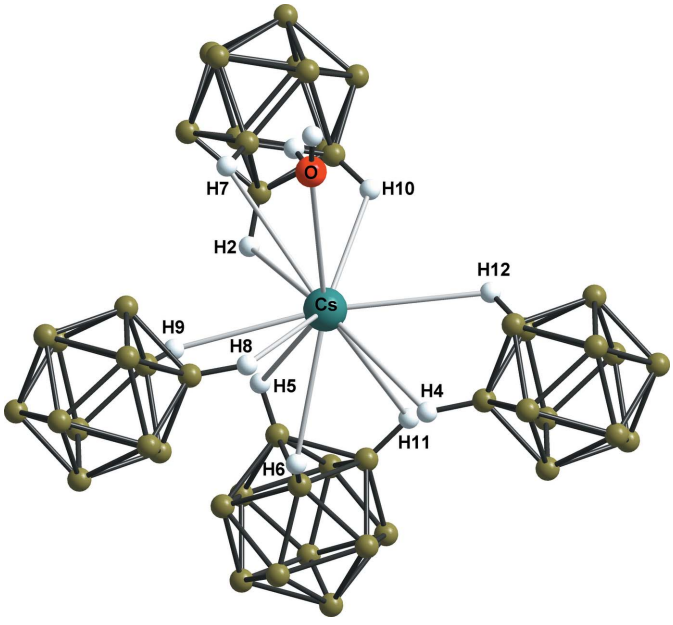


Figure 2
Tetrahedral coordination of caesium by four dodecahydrido-*closo*-dodecaborate anions with the water molecule completing the coordination sphere of the cation.

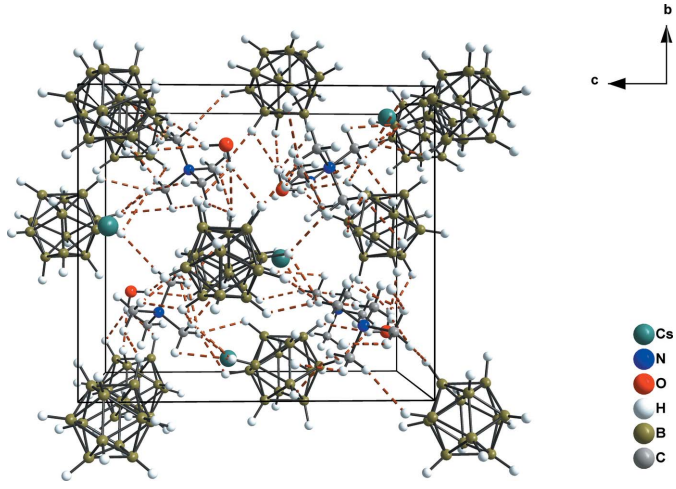


Figure 4
The molecular packing of the title compound (central projection with view along [100]). The O—H···H—B and C—H···H—B dihydrogen bonds are depicted by brown dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$Cs^+ \cdot C_4H_{12}N^+ \cdot B_{12}H_{12}^{2-} \cdot H_2O$
M_r	366.89
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	173
a, b, c (Å)	8.9771 (5), 12.8680 (8), 14.5449 (9)
V (Å^3)	1680.19 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.18
Crystal size (mm)	0.55 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker–Nonius KappaCCD
Absorption correction	Multi-scan (Blessing, 1995)
T_{min}, T_{max}	0.70, 0.80
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3552, 3279, 3143
R_{int}	0.017
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.703
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.063, 1.05
No. of reflections	3279
No. of parameters	231
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.59, −0.76
Absolute structure	Classical Flack method preferred over Parsons because s.u. lower
Absolute structure parameter	−0.02 (2)

Computer programs: *COLLECT* (Hooft, 2004), *DENZO-SMN* (Otwinowski & Minor, 1997), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg & Putz, 2005).

Synthesis and crystallization

The title compound was obtained by reaction of dicaesium dodecahydrido-*closo*-dodecaborate (Tiritiris *et al.*, 2000) with one equivalent of tetramethylammonium chloride in water. The crude product was recrystallized from an aqueous solution. After slow evaporation of the solvent at ambient temperature, colorless single crystals suitable for X-ray analysis emerged.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The residual electron-density peak of 1.585 e Å^{-3} is located 0.80 Å from the Cs atom.

Acknowledgements

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full crystallographic data

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Caesium tetramethylammonium dodecahydro-*closo*-dodecaborate monohydrate

Crystal data

$Cs^+ \cdot C_4H_{12}N^+ \cdot B_{12}H_{12}^{2-} \cdot H_2O$
M_r = 366.89
Orthorhombic, $P2_12_12_1$
a = 8.9771 (5) Å
b = 12.8680 (8) Å
c = 14.5449 (9) Å
V = 1680.19 (17) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.450 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3552 reflections
θ = 2.1–30.0°
μ = 2.18 mm^{-1}
T = 173 K
Needle, colorless
0.55 × 0.15 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ scans, and ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.70, T_{max} = 0.80
3552 measured reflections
3279 independent reflections
3143 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 30.0°, θ_{min} = 2.1°
h = −12→12
k = −18→18
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.063
S = 1.05
3279 reflections
231 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.3622P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}
Absolute structure: Classical Flack method preferred over Parsons because s.u. lower
Absolute structure parameter: −0.02 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cs	0.46732 (2)	−0.05439 (2)	0.08106 (2)	0.02735 (7)
N	0.0367 (4)	0.24156 (19)	0.20442 (17)	0.0211 (4)
C1	0.1556 (4)	0.2290 (3)	0.1332 (2)	0.0294 (7)
H1A	0.1203	0.1821	0.0848	0.044*
H1B	0.2451	0.1998	0.1617	0.044*
H1C	0.1792	0.2969	0.1064	0.044*
C2	0.0955 (5)	0.3074 (3)	0.2815 (2)	0.0311 (7)
H2A	0.1245	0.3757	0.2575	0.047*
H2B	0.1824	0.2735	0.3090	0.047*
H2C	0.0179	0.3162	0.3282	0.047*
C3	−0.0051 (4)	0.1366 (3)	0.2403 (3)	0.0321 (7)
H3A	0.0835	0.1023	0.2655	0.048*
H3B	−0.0460	0.0945	0.1902	0.048*
H3C	−0.0800	0.1442	0.2889	0.048*
C4	−0.0966 (5)	0.2926 (3)	0.1634 (3)	0.0366 (8)
H4A	−0.1771	0.2946	0.2088	0.055*
H4B	−0.1293	0.2531	0.1094	0.055*
H4C	−0.0710	0.3636	0.1448	0.055*
B1	0.3945 (4)	−0.0349 (2)	0.4200 (3)	0.0221 (6)
H1	0.319 (6)	−0.088 (4)	0.424 (3)	0.046 (14)*
B2	0.5537 (4)	−0.0493 (3)	0.3474 (2)	0.0212 (6)
H2	0.576 (5)	−0.116 (3)	0.307 (2)	0.014 (9)*
B3	0.5763 (4)	−0.0442 (3)	0.4691 (2)	0.0194 (6)
H3	0.612 (6)	−0.116 (3)	0.508 (3)	0.027 (11)*
B4	0.3427 (4)	0.0984 (3)	0.4197 (2)	0.0196 (5)
H4	0.223 (5)	0.121 (3)	0.427 (3)	0.026 (11)*
B5	0.4688 (5)	0.1664 (3)	0.3468 (2)	0.0216 (6)
H5	0.432 (6)	0.230 (4)	0.306 (3)	0.031 (12)*
B6	0.4908 (4)	0.1712 (2)	0.4688 (2)	0.0193 (6)
H6	0.469 (5)	0.243 (3)	0.511 (3)	0.017 (8)*
B7	0.5994 (4)	0.0747 (3)	0.3028 (2)	0.0204 (6)
H7	0.657 (4)	0.084 (3)	0.237 (2)	0.007 (7)*
B8	0.7029 (4)	0.0239 (3)	0.3968 (2)	0.0195 (6)
H8	0.823 (5)	0.002 (3)	0.390 (3)	0.019 (9)*
B9	0.6352 (4)	0.0829 (3)	0.4998 (2)	0.0174 (6)

H9	0.710 (5)	0.102 (3)	0.559 (3)	0.022 (10)*
B10	0.4091 (4)	0.0385 (3)	0.3175 (2)	0.0217 (6)
H10	0.341 (4)	0.019 (3)	0.260 (3)	0.016 (9)*
B11	0.6495 (4)	0.1574 (3)	0.3959 (2)	0.0194 (6)
H11	0.736 (5)	0.219 (3)	0.382 (3)	0.023 (10)*
B12	0.4455 (4)	0.0463 (3)	0.5141 (2)	0.0176 (5)
H12	0.386 (5)	0.037 (3)	0.588 (3)	0.028 (10)*
O	0.5166 (5)	0.1878 (2)	0.0878 (2)	0.0446 (8)
H13	0.521 (7)	0.2572 (11)	0.077 (3)	0.050*
H14	0.536 (8)	0.186 (3)	0.1489 (12)	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs	0.02633 (10)	0.02544 (9)	0.03026 (10)	0.00137 (8)	−0.00146 (9)	−0.00831 (7)
N	0.0214 (11)	0.0215 (10)	0.0204 (9)	0.0031 (11)	−0.0029 (12)	−0.0024 (9)
C1	0.0323 (16)	0.0317 (15)	0.0242 (14)	−0.0050 (15)	0.0087 (13)	−0.0039 (13)
C2	0.0313 (17)	0.0370 (17)	0.0250 (15)	0.0055 (16)	−0.0081 (14)	−0.0105 (12)
C3	0.0290 (17)	0.0291 (14)	0.0383 (16)	−0.0020 (12)	0.0050 (14)	0.0048 (14)
C4	0.0323 (18)	0.0396 (19)	0.0380 (19)	0.0146 (17)	−0.0126 (17)	−0.0078 (15)
B1	0.0217 (13)	0.0206 (13)	0.0239 (13)	−0.0072 (11)	−0.0002 (15)	0.0005 (13)
B2	0.0222 (15)	0.0185 (12)	0.0230 (13)	−0.0011 (14)	−0.0019 (12)	−0.0028 (11)
B3	0.0193 (13)	0.0167 (12)	0.0223 (13)	0.0014 (11)	−0.0026 (11)	0.0017 (11)
B4	0.0164 (12)	0.0252 (13)	0.0172 (12)	0.0035 (11)	0.0015 (13)	0.0025 (13)
B5	0.0221 (14)	0.0233 (13)	0.0193 (12)	0.0015 (16)	0.0020 (15)	0.0044 (11)
B6	0.0219 (16)	0.0166 (12)	0.0195 (12)	0.0017 (12)	0.0021 (11)	0.0007 (10)
B7	0.0201 (14)	0.0250 (15)	0.0159 (12)	0.0009 (13)	0.0027 (12)	−0.0018 (11)
B8	0.0178 (13)	0.0214 (13)	0.0193 (13)	0.0002 (11)	−0.0003 (11)	−0.0016 (11)
B9	0.0170 (13)	0.0189 (12)	0.0163 (12)	−0.0011 (11)	−0.0010 (11)	−0.0022 (11)
B10	0.0194 (14)	0.0281 (16)	0.0176 (12)	−0.0011 (14)	−0.0015 (12)	−0.0013 (12)
B11	0.0217 (14)	0.0166 (12)	0.0201 (13)	−0.0008 (12)	0.0035 (12)	0.0001 (11)
B12	0.0171 (13)	0.0174 (12)	0.0185 (11)	0.0020 (12)	−0.0010 (10)	0.0035 (11)
O	0.062 (2)	0.0283 (11)	0.0440 (14)	0.0055 (14)	0.0030 (19)	0.0019 (12)

Geometric parameters (Å, º)

Cs—O	3.149 (3)	B3—B9	1.776 (5)
Cs—B6^{i}	3.624 (3)	B3—B12	1.778 (5)
Cs—B10	3.678 (3)	B3—B8	1.780 (5)
Cs—B4^{ii}	3.684 (3)	B3—H3	1.13 (4)
Cs—B9^{iii}	3.777 (3)	B4—B6	1.776 (5)
Cs—B5^{i}	3.786 (3)	B4—B10	1.778 (5)
Cs—B7	3.816 (3)	B4—B5	1.782 (5)
Cs—B12^{ii}	3.833 (3)	B4—B12	1.785 (5)
Cs—B11^{i}	3.868 (3)	B4—Cs^{iv}	3.684 (3)
Cs—B2	3.951 (3)	B4—H4	1.12 (5)
Cs—H7	3.35 (3)	B5—B11	1.776 (6)
Cs—H10	2.99 (4)	B5—B7	1.783 (5)

Cs—H14	3.30 (4)	B5—B10	1.783 (5)
N—C4	1.490 (5)	B5—B6	1.786 (5)
N—C3	1.496 (4)	B5—Cs^{v}	3.786 (3)
N—C1	1.496 (4)	B5—H5	1.06 (5)
N—C2	1.501 (4)	B6—B9	1.782 (5)
C1—H1A	0.9800	B6—B11	1.785 (5)
C1—H1B	0.9800	B6—B12	1.785 (5)
C1—H1C	0.9800	B6—Cs^{v}	3.624 (3)
C2—H2A	0.9800	B6—H6	1.12 (4)
C2—H2B	0.9800	B7—B8	1.778 (5)
C2—H2C	0.9800	B7—B11	1.780 (5)
C3—H3A	0.9800	B7—B10	1.784 (6)
C3—H3B	0.9800	B7—H7	1.09 (3)
C3—H3C	0.9800	B8—B11	1.784 (5)
C4—H4A	0.9800	B8—B9	1.786 (5)
C4—H4B	0.9800	B8—H8	1.11 (4)
C4—H4C	0.9800	B9—B12	1.779 (5)
B1—B10	1.771 (5)	B9—B11	1.795 (5)
B1—B4	1.778 (5)	B9—Cs^{vi}	3.777 (3)
B1—B12	1.781 (5)	B9—H9	1.12 (4)
B1—B3	1.785 (5)	B10—H10	1.07 (4)
B1—B2	1.787 (5)	B11—Cs^{v}	3.868 (3)
B1—H1	0.97 (5)	B11—H11	1.13 (4)
B2—B7	1.771 (5)	B12—Cs^{iv}	3.833 (3)
B2—B10	1.775 (5)	B12—H12	1.21 (4)
B2—B3	1.784 (5)	O—H13	0.908 (11)
B2—B8	1.789 (5)	O—H14	0.906 (11)
B2—H2	1.05 (4)		

O—Cs—B6^{i}	162.90 (9)	B1—B4—Cs^{iv}	92.75 (17)
O—Cs—B10	70.69 (8)	B5—B4—Cs^{iv}	159.22 (19)
B6^{i}—Cs—B10	121.23 (8)	B12—B4—Cs^{iv}	80.98 (15)
O—Cs—B4^{ii}	106.14 (9)	B6—B4—H4	123 (2)
B6^{i}—Cs—B4^{ii}	78.53 (7)	B10—B4—H4	121 (2)
B10—Cs—B4^{ii}	122.55 (8)	B1—B4—H4	120 (2)
O—Cs—B9^{iii}	88.46 (9)	B5—B4—H4	123 (2)
B6^{i}—Cs—B9^{iii}	75.21 (7)	B12—B4—H4	121 (2)
B10—Cs—B9^{iii}	117.29 (8)	B11—B5—B4	108.0 (2)
B4^{ii}—Cs—B9^{iii}	119.97 (7)	B11—B5—B7	60.0 (2)
O—Cs—B5^{i}	155.38 (9)	B4—B5—B7	107.8 (2)
B6^{i}—Cs—B5^{i}	27.78 (7)	B11—B5—B10	108.1 (2)
B10—Cs—B5^{i}	94.07 (7)	B4—B5—B10	59.8 (2)
B4^{ii}—Cs—B5^{i}	98.34 (8)	B7—B5—B10	60.0 (2)
B9^{iii}—Cs—B5^{i}	81.46 (8)	B11—B5—B6	60.1 (2)
O—Cs—B7	59.96 (8)	B4—B5—B6	59.72 (19)
B6^{i}—Cs—B7	124.11 (7)	B7—B5—B6	107.9 (3)
B10—Cs—B7	27.46 (8)	B10—B5—B6	107.6 (2)
B4^{ii}—Cs—B7	147.12 (8)	B11—B5—Cs^{v}	79.17 (16)

B9^{iii}—Cs—B7	90.75 (7)	B4—B5—Cs^{v}	113.42 (17)
B5^{i}—Cs—B7	97.57 (7)	B7—B5—Cs^{v}	128.9 (2)
O—Cs—B12^{ii}	96.70 (9)	B10—B5—Cs^{v}	171.0 (2)
B6^{i}—Cs—B12^{ii}	94.36 (7)	B6—B5—Cs^{v}	71.04 (15)
B10—Cs—B12^{ii}	95.23 (7)	B11—B5—H5	124 (3)
B4^{ii}—Cs—B12^{ii}	27.38 (7)	B4—B5—H5	121 (3)
B9^{iii}—Cs—B12^{ii}	146.78 (7)	B7—B5—H5	121 (3)
B5^{i}—Cs—B12^{ii}	104.05 (8)	B10—B5—H5	119 (3)
B7—Cs—B12^{ii}	120.21 (7)	B6—B5—H5	124 (2)
O—Cs—B11^{i}	169.75 (8)	Cs^{v}—B5—H5	58 (2)
B6^{i}—Cs—B11^{i}	27.32 (7)	B4—B6—B9	108.0 (2)
B10—Cs—B11^{i}	101.07 (8)	B4—B6—B11	107.9 (2)
B4^{ii}—Cs—B11^{i}	72.72 (7)	B9—B6—B11	60.43 (19)
B9^{iii}—Cs—B11^{i}	100.97 (7)	B4—B6—B12	60.16 (18)
B5^{i}—Cs—B11^{i}	26.81 (8)	B9—B6—B12	59.81 (18)
B7—Cs—B11^{i}	115.35 (7)	B11—B6—B12	108.2 (2)
B12^{ii}—Cs—B11^{i}	77.64 (7)	B4—B6—B5	60.0 (2)
O—Cs—B2	85.74 (8)	B9—B6—B5	108.1 (2)
B6^{i}—Cs—B2	101.06 (7)	B11—B6—B5	59.7 (2)
B10—Cs—B2	26.60 (8)	B12—B6—B5	108.1 (2)
B4^{ii}—Cs—B2	140.83 (8)	B4—B6—Cs^{v}	120.77 (17)
B9^{iii}—Cs—B2	97.07 (7)	B9—B6—Cs^{v}	126.64 (19)
B5^{i}—Cs—B2	73.40 (7)	B11—B6—Cs^{v}	83.99 (15)
B7—Cs—B2	26.28 (7)	B12—B6—Cs^{v}	167.23 (18)
B12^{ii}—Cs—B2	116.00 (7)	B5—B6—Cs^{v}	81.17 (16)
B11^{i}—Cs—B2	89.09 (7)	B4—B6—H6	121 (2)
O—Cs—H7	51.8 (6)	B9—B6—H6	121 (2)
B6^{i}—Cs—H7	126.9 (6)	B11—B6—H6	123 (2)
B10—Cs—H7	42.7 (6)	B12—B6—H6	120 (2)
B4^{ii}—Cs—H7	153.8 (6)	B5—B6—H6	123 (2)
B9^{iii}—Cs—H7	77.6 (6)	Cs^{v}—B6—H6	48 (2)
B5^{i}—Cs—H7	103.8 (6)	B2—B7—B8	60.54 (19)
B7—Cs—H7	15.8 (6)	B2—B7—B11	108.6 (2)
B12^{ii}—Cs—H7	130.4 (6)	B8—B7—B11	60.17 (19)
B11^{i}—Cs—H7	126.0 (6)	B2—B7—B5	108.2 (2)
B2—Cs—H7	39.3 (6)	B8—B7—B5	108.1 (2)
O—Cs—H10	73.3 (7)	B11—B7—B5	59.8 (2)
B6^{i}—Cs—H10	121.4 (7)	B2—B7—B10	59.9 (2)
B10—Cs—H10	14.1 (8)	B8—B7—B10	108.2 (2)
B4^{ii}—Cs—H10	108.4 (8)	B11—B7—B10	107.9 (2)
B9^{iii}—Cs—H10	131.4 (8)	B5—B7—B10	60.0 (2)
B5^{i}—Cs—H10	96.7 (7)	B2—B7—Cs	81.10 (15)
B7—Cs—H10	41.0 (8)	B8—B7—Cs	130.72 (18)
B12^{ii}—Cs—H10	81.1 (8)	B11—B7—Cs	168.97 (19)
B11^{i}—Cs—H10	97.2 (7)	B5—B7—Cs	112.79 (19)
B2—Cs—H10	38.4 (7)	B10—B7—Cs	71.96 (15)
H7—Cs—H10	55.5 (9)	B2—B7—H7	121.9 (17)
O—Cs—H14	15.9 (3)	B8—B7—H7	117.7 (19)

B6^{i}—Cs—H14	162.2 (11)	B11—B7—H7	118.7 (18)
B10—Cs—H14	56.2 (6)	B5—B7—H7	123.5 (18)
B4^{ii}—Cs—H14	118.4 (8)	B10—B7—H7	125.9 (19)
B9^{iii}—Cs—H14	90.4 (12)	Cs—B7—H7	57.0 (18)
B5^{i}—Cs—H14	141.0 (5)	B7—B8—B3	107.6 (2)
B7—Cs—H14	44.1 (3)	B7—B8—B11	59.99 (19)
B12^{ii}—Cs—H14	103.4 (11)	B3—B8—B11	107.9 (2)
B11^{i}—Cs—H14	157.2 (6)	B7—B8—B9	108.1 (2)
B2—Cs—H14	69.8 (3)	B3—B8—B9	59.74 (19)
H7—Cs—H14	37.3 (8)	B11—B8—B9	60.37 (19)
H10—Cs—H14	61.0 (11)	B7—B8—B2	59.54 (19)
C4—N—C3	109.7 (3)	B3—B8—B2	59.99 (19)
C4—N—C1	110.1 (3)	B11—B8—B2	107.7 (2)
C3—N—C1	108.8 (3)	B9—B8—B2	107.8 (2)
C4—N—C2	109.4 (3)	B7—B8—H8	122 (2)
C3—N—C2	109.7 (3)	B3—B8—H8	123 (2)
C1—N—C2	109.1 (3)	B11—B8—H8	120 (2)
N—C1—H1A	109.5	B9—B8—H8	121 (2)
N—C1—H1B	109.5	B2—B8—H8	124 (2)
H1A—C1—H1B	109.5	B3—B9—B12	60.04 (18)
N—C1—H1C	109.5	B3—B9—B6	107.9 (2)
H1A—C1—H1C	109.5	B12—B9—B6	60.18 (18)
H1B—C1—H1C	109.5	B3—B9—B8	59.96 (18)
N—C2—H2A	109.5	B12—B9—B8	108.1 (2)
N—C2—H2B	109.5	B6—B9—B8	107.8 (2)
H2A—C2—H2B	109.5	B3—B9—B11	107.6 (2)
N—C2—H2C	109.5	B12—B9—B11	108.0 (2)
H2A—C2—H2C	109.5	B6—B9—B11	59.86 (19)
H2B—C2—H2C	109.5	B8—B9—B11	59.74 (18)
N—C3—H3A	109.5	B3—B9—Cs^{vi}	105.67 (17)
N—C3—H3B	109.5	B12—B9—Cs^{vi}	147.34 (16)
H3A—C3—H3B	109.5	B6—B9—Cs^{vi}	145.92 (18)
N—C3—H3C	109.5	B8—B9—Cs^{vi}	84.24 (16)
H3A—C3—H3C	109.5	B11—B9—Cs^{vi}	104.33 (17)
H3B—C3—H3C	109.5	B3—B9—H9	125 (2)
N—C4—H4A	109.5	B12—B9—H9	123 (2)
N—C4—H4B	109.5	B6—B9—H9	119 (2)
H4A—C4—H4B	109.5	B8—B9—H9	122 (2)
N—C4—H4C	109.5	B11—B9—H9	119 (2)
H4A—C4—H4C	109.5	B1—B10—B2	60.5 (2)
H4B—C4—H4C	109.5	B1—B10—B4	60.13 (19)
B10—B1—B4	60.1 (2)	B2—B10—B4	108.4 (2)
B10—B1—B12	108.4 (2)	B1—B10—B7	108.1 (2)
B4—B1—B12	60.21 (18)	B2—B10—B7	59.7 (2)
B10—B1—B3	107.8 (2)	B4—B10—B7	108.0 (2)
B4—B1—B3	107.8 (2)	B1—B10—B5	108.3 (2)
B12—B1—B3	59.82 (18)	B2—B10—B5	108.0 (3)
B10—B1—B2	59.9 (2)	B4—B10—B5	60.05 (19)

B4—B1—B2	107.9 (2)	B7—B10—B5	60.0 (2)
B12—B1—B2	108.0 (2)	B1—B10—Cs	128.64 (19)
B3—B1—B2	59.92 (19)	B2—B10—Cs	85.29 (16)
B10—B1—H1	119 (3)	B4—B10—Cs	166.1 (2)
B4—B1—H1	120 (3)	B7—B10—Cs	80.58 (15)
B12—B1—H1	123 (3)	B5—B10—Cs	118.74 (18)
B3—B1—H1	125 (3)	B1—B10—H10	120 (2)
B2—B1—H1	122 (3)	B2—B10—H10	117 (2)
B7—B2—B10	60.4 (2)	B4—B10—H10	125 (2)
B7—B2—B3	107.7 (2)	B7—B10—H10	121 (2)
B10—B2—B3	107.6 (2)	B5—B10—H10	125 (2)
B7—B2—B8	59.9 (2)	B5—B11—B7	60.2 (2)
B10—B2—B8	108.1 (2)	B5—B11—B8	108.1 (2)
B3—B2—B8	59.77 (19)	B7—B11—B8	59.84 (19)
B7—B2—B1	108.0 (2)	B5—B11—B6	60.19 (18)
B10—B2—B1	59.61 (19)	B7—B11—B6	108.0 (2)
B3—B2—B1	60.0 (2)	B8—B11—B6	107.8 (2)
B8—B2—B1	107.9 (2)	B5—B11—B9	107.9 (2)
B7—B2—Cs	72.62 (14)	B7—B11—B9	107.6 (2)
B10—B2—Cs	68.11 (14)	B8—B11—B9	59.88 (18)
B3—B2—Cs	175.1 (2)	B6—B11—B9	59.71 (18)
B8—B2—Cs	123.34 (18)	B5—B11—Cs^{v}	74.01 (15)
B1—B2—Cs	115.14 (18)	B7—B11—Cs^{v}	124.80 (18)
B7—B2—H2	119 (2)	B8—B11—Cs^{v}	174.59 (19)
B10—B2—H2	121 (2)	B6—B11—Cs^{v}	68.69 (14)
B3—B2—H2	124 (2)	B9—B11—Cs^{v}	114.82 (17)
B8—B2—H2	120 (2)	B5—B11—H11	121 (2)
B1—B2—H2	124 (2)	B7—B11—H11	117 (2)
Cs—B2—H2	59 (2)	B8—B11—H11	120 (2)
B9—B3—B12	60.05 (19)	B6—B11—H11	126 (2)
B9—B3—B8	60.31 (19)	B9—B11—H11	125 (2)
B12—B3—B8	108.4 (2)	Cs^{v}—B11—H11	62 (2)
B9—B3—B2	108.5 (2)	B3—B12—B9	59.91 (18)
B12—B3—B2	108.3 (2)	B3—B12—B1	60.21 (19)
B8—B3—B2	60.24 (19)	B9—B12—B1	108.2 (2)
B9—B3—B1	108.1 (2)	B3—B12—B4	107.8 (2)
B12—B3—B1	59.97 (19)	B9—B12—B4	107.8 (2)
B8—B3—B1	108.3 (2)	B1—B12—B4	59.80 (18)
B2—B3—B1	60.1 (2)	B3—B12—B6	107.7 (2)
B9—B3—H3	123 (2)	B9—B12—B6	60.01 (18)
B12—B3—H3	123 (2)	B1—B12—B6	107.6 (2)
B8—B3—H3	121 (2)	B4—B12—B6	59.67 (18)
B2—B3—H3	120 (2)	B3—B12—Cs^{iv}	138.56 (19)
B1—B3—H3	121 (2)	B9—B12—Cs^{iv}	161.41 (18)
B6—B4—B10	108.3 (2)	B1—B12—Cs^{iv}	87.86 (16)
B6—B4—B1	108.2 (2)	B4—B12—Cs^{iv}	71.64 (14)
B10—B4—B1	59.7 (2)	B6—B12—Cs^{iv}	106.82 (16)
B6—B4—B5	60.26 (19)	B3—B12—H12	124 (2)

B10—B4—B5	60.11 (19)	B9—B12—H12	124 (2)
B1—B4—B5	108.0 (2)	B1—B12—H12	121 (2)
B6—B4—B12	60.17 (19)	B4—B12—H12	120 (2)
B10—B4—B12	107.9 (2)	B6—B12—H12	121.6 (19)
B1—B4—B12	59.99 (19)	Cs^{iv}—B12—H12	49 (2)
B5—B4—B12	108.3 (2)	Cs—O—H13	168 (3)
B6—B4—Cs^{iv}	113.02 (18)	Cs—O—H14	92 (3)
B10—B4—Cs^{iv}	136.02 (19)	H13—O—H14	100.6 (16)
B10—B1—B2—B7	37.6 (2)	B2—B1—B10—B5	−100.8 (3)
B4—B1—B2—B7	0.1 (3)	B4—B1—B10—Cs	−166.9 (3)
B12—B1—B2—B7	−63.6 (3)	B12—B1—B10—Cs	155.69 (19)
B3—B1—B2—B7	−100.5 (3)	B3—B1—B10—Cs	92.4 (3)
B4—B1—B2—B10	−37.5 (2)	B2—B1—B10—Cs	55.1 (2)
B12—B1—B2—B10	−101.2 (2)	B7—B2—B10—B1	−138.1 (2)
B3—B1—B2—B10	−138.1 (3)	B3—B2—B10—B1	−37.4 (2)
B10—B1—B2—B3	138.1 (3)	B8—B2—B10—B1	−100.5 (2)
B4—B1—B2—B3	100.6 (3)	Cs—B2—B10—B1	140.03 (18)
B12—B1—B2—B3	36.9 (2)	B7—B2—B10—B4	−100.5 (3)
B10—B1—B2—B8	100.9 (3)	B3—B2—B10—B4	0.3 (3)
B4—B1—B2—B8	63.4 (3)	B8—B2—B10—B4	−62.8 (3)
B12—B1—B2—B8	−0.3 (3)	B1—B2—B10—B4	37.7 (2)
B3—B1—B2—B8	−37.2 (2)	Cs—B2—B10—B4	177.7 (2)
B10—B1—B2—Cs	−41.18 (18)	B3—B2—B10—B7	100.8 (3)
B4—B1—B2—Cs	−78.7 (2)	B8—B2—B10—B7	37.6 (2)
B12—B1—B2—Cs	−142.37 (18)	B1—B2—B10—B7	138.1 (2)
B3—B1—B2—Cs	−179.3 (2)	Cs—B2—B10—B7	−81.83 (15)
B7—B2—B3—B9	0.3 (3)	B7—B2—B10—B5	−36.9 (2)
B10—B2—B3—B9	−63.5 (3)	B3—B2—B10—B5	63.9 (3)
B8—B2—B3—B9	37.6 (2)	B8—B2—B10—B5	0.7 (3)
B1—B2—B3—B9	−100.7 (2)	B1—B2—B10—B5	101.2 (2)
B7—B2—B3—B12	63.9 (3)	Cs—B2—B10—B5	−118.7 (2)
B10—B2—B3—B12	0.2 (3)	B7—B2—B10—Cs	81.83 (15)
B8—B2—B3—B12	101.2 (3)	B3—B2—B10—Cs	−177.4 (2)
B1—B2—B3—B12	−37.0 (2)	B8—B2—B10—Cs	119.46 (19)
B7—B2—B3—B8	−37.3 (2)	B1—B2—B10—Cs	−140.03 (18)
B10—B2—B3—B8	−101.1 (3)	B6—B4—B10—B1	100.8 (2)
B1—B2—B3—B8	−138.3 (2)	B5—B4—B10—B1	138.5 (3)
B7—B2—B3—B1	100.9 (3)	B12—B4—B10—B1	37.2 (2)
B10—B2—B3—B1	37.2 (2)	Cs^{iv}—B4—B10—B1	−58.4 (3)
B8—B2—B3—B1	138.3 (2)	B6—B4—B10—B2	63.0 (3)
B10—B1—B3—B9	64.0 (3)	B1—B4—B10—B2	−37.8 (2)
B4—B1—B3—B9	0.5 (3)	B5—B4—B10—B2	100.6 (3)
B12—B1—B3—B9	−37.3 (2)	B12—B4—B10—B2	−0.6 (3)
B2—B1—B3—B9	101.3 (3)	Cs^{iv}—B4—B10—B2	−96.2 (3)
B10—B1—B3—B12	101.3 (2)	B6—B4—B10—B7	−0.2 (3)
B4—B1—B3—B12	37.8 (2)	B1—B4—B10—B7	−101.0 (3)
B2—B1—B3—B12	138.7 (3)	B5—B4—B10—B7	37.5 (2)

B10—B1—B3—B8	0.2 (3)	B12—B4—B10—B7	−63.8 (3)
B4—B1—B3—B8	−63.3 (3)	Cs^{iv}—B4—B10—B7	−159.4 (2)
B12—B1—B3—B8	−101.2 (2)	B6—B4—B10—B5	−37.6 (2)
B2—B1—B3—B8	37.5 (2)	B1—B4—B10—B5	−138.5 (3)
B10—B1—B3—B2	−37.3 (2)	B12—B4—B10—B5	−101.3 (3)
B4—B1—B3—B2	−100.8 (3)	Cs^{iv}—B4—B10—B5	163.2 (3)
B12—B1—B3—B2	−138.7 (3)	B6—B4—B10—Cs	−126.6 (8)
B10—B1—B4—B6	−101.0 (3)	B1—B4—B10—Cs	132.5 (9)
B12—B1—B4—B6	37.4 (2)	B5—B4—B10—Cs	−89.0 (9)
B3—B1—B4—B6	−0.3 (3)	B12—B4—B10—Cs	169.7 (7)
B2—B1—B4—B6	−63.5 (3)	Cs^{iv}—B4—B10—Cs	74.2 (9)
B12—B1—B4—B10	138.3 (3)	B2—B7—B10—B1	37.7 (2)
B3—B1—B4—B10	100.7 (3)	B8—B7—B10—B1	−0.2 (3)
B2—B1—B4—B10	37.4 (2)	B11—B7—B10—B1	−63.9 (3)
B10—B1—B4—B5	−37.2 (2)	B5—B7—B10—B1	−101.1 (2)
B12—B1—B4—B5	101.1 (3)	Cs—B7—B10—B1	127.7 (2)
B3—B1—B4—B5	63.5 (3)	B8—B7—B10—B2	−37.9 (2)
B2—B1—B4—B5	0.2 (3)	B11—B7—B10—B2	−101.6 (2)
B10—B1—B4—B12	−138.3 (3)	B5—B7—B10—B2	−138.8 (2)
B3—B1—B4—B12	−37.6 (2)	Cs—B7—B10—B2	90.04 (15)
B2—B1—B4—B12	−100.9 (3)	B2—B7—B10—B4	101.3 (2)
B10—B1—B4—Cs^{iv}	143.71 (19)	B8—B7—B10—B4	63.3 (3)
B12—B1—B4—Cs^{iv}	−77.94 (16)	B11—B7—B10—B4	−0.3 (3)
B3—B1—B4—Cs^{iv}	−115.6 (2)	B5—B7—B10—B4	−37.5 (2)
B2—B1—B4—Cs^{iv}	−178.88 (19)	Cs—B7—B10—B4	−168.7 (2)
B6—B4—B5—B11	37.3 (2)	B2—B7—B10—B5	138.8 (2)
B10—B4—B5—B11	−100.9 (3)	B8—B7—B10—B5	100.8 (2)
B1—B4—B5—B11	−63.8 (3)	B11—B7—B10—B5	37.2 (2)
B12—B4—B5—B11	−0.3 (3)	Cs—B7—B10—B5	−131.21 (17)
Cs^{iv}—B4—B5—B11	113.6 (5)	B2—B7—B10—Cs	−90.04 (15)
B6—B4—B5—B7	100.7 (3)	B8—B7—B10—Cs	−127.97 (19)
B10—B4—B5—B7	−37.4 (2)	B11—B7—B10—Cs	168.4 (2)
B1—B4—B5—B7	−0.4 (3)	B5—B7—B10—Cs	131.21 (17)
B12—B4—B5—B7	63.1 (3)	B11—B5—B10—B1	63.5 (3)
Cs^{iv}—B4—B5—B7	177.0 (5)	B4—B5—B10—B1	−37.3 (2)
B6—B4—B5—B10	138.1 (3)	B7—B5—B10—B1	100.8 (3)
B1—B4—B5—B10	37.0 (2)	B6—B5—B10—B1	−0.1 (4)
B12—B4—B5—B10	100.5 (2)	B11—B5—B10—B2	−0.6 (3)
Cs^{iv}—B4—B5—B10	−145.5 (6)	B4—B5—B10—B2	−101.3 (3)
B10—B4—B5—B6	−138.1 (3)	B7—B5—B10—B2	36.8 (2)
B1—B4—B5—B6	−101.1 (3)	B6—B5—B10—B2	−64.1 (3)
B12—B4—B5—B6	−37.6 (2)	B11—B5—B10—B4	100.7 (2)
Cs^{iv}—B4—B5—B6	76.3 (6)	B7—B5—B10—B4	138.1 (2)
B6—B4—B5—Cs^{v}	−48.48 (17)	B6—B5—B10—B4	37.2 (2)
B10—B4—B5—Cs^{v}	173.4 (2)	B11—B5—B10—B7	−37.4 (2)
B1—B4—B5—Cs^{v}	−149.57 (19)	B4—B5—B10—B7	−138.1 (2)
B12—B4—B5—Cs^{v}	−86.1 (2)	B6—B5—B10—B7	−100.9 (3)
Cs^{iv}—B4—B5—Cs^{v}	27.9 (7)	B11—B5—B10—Cs	−95.2 (2)

B10—B4—B6—B9	−63.3 (3)	B4—B5—B10—Cs	164.1 (2)
B1—B4—B6—B9	−0.1 (3)	B7—B5—B10—Cs	−57.8 (2)
B5—B4—B6—B9	−100.9 (3)	B6—B5—B10—Cs	−158.7 (2)
B12—B4—B6—B9	37.2 (2)	B4—B5—B11—B7	100.6 (3)
Cs^{iv}—B4—B6—B9	101.1 (2)	B10—B5—B11—B7	37.4 (2)
B10—B4—B6—B11	0.5 (3)	B6—B5—B11—B7	137.7 (2)
B1—B4—B6—B11	63.8 (3)	Cs^{v}—B5—B11—B7	−148.06 (17)
B5—B4—B6—B11	−37.0 (2)	B4—B5—B11—B8	63.5 (3)
B12—B4—B6—B11	101.1 (2)	B7—B5—B11—B8	−37.1 (2)
Cs^{iv}—B4—B6—B11	164.99 (17)	B10—B5—B11—B8	0.2 (3)
B10—B4—B6—B12	−100.6 (2)	B6—B5—B11—B8	100.6 (2)
B1—B4—B6—B12	−37.3 (2)	Cs^{v}—B5—B11—B8	174.8 (2)
B5—B4—B6—B12	−138.1 (2)	B4—B5—B11—B6	−37.1 (2)
Cs^{iv}—B4—B6—B12	63.90 (17)	B7—B5—B11—B6	−137.7 (2)
B10—B4—B6—B5	37.5 (2)	B10—B5—B11—B6	−100.3 (2)
B1—B4—B6—B5	100.8 (3)	Cs^{v}—B5—B11—B6	74.24 (15)
B12—B4—B6—B5	138.1 (2)	B4—B5—B11—B9	0.2 (3)
Cs^{iv}—B4—B6—B5	−158.0 (2)	B7—B5—B11—B9	−100.5 (2)
B10—B4—B6—Cs^{v}	94.2 (2)	B10—B5—B11—B9	−63.1 (3)
B1—B4—B6—Cs^{v}	157.45 (18)	B6—B5—B11—B9	37.2 (2)
B5—B4—B6—Cs^{v}	56.7 (2)	Cs^{v}—B5—B11—B9	111.49 (19)
B12—B4—B6—Cs^{v}	−165.2 (2)	B4—B5—B11—Cs^{v}	−111.3 (2)
Cs^{iv}—B4—B6—Cs^{v}	−101.34 (16)	B7—B5—B11—Cs^{v}	148.06 (17)
B11—B5—B6—B4	−138.4 (2)	B10—B5—B11—Cs^{v}	−174.6 (2)
B7—B5—B6—B4	−100.6 (3)	B6—B5—B11—Cs^{v}	−74.24 (15)
B10—B5—B6—B4	−37.3 (3)	B2—B7—B11—B5	−100.7 (3)
Cs^{v}—B5—B6—B4	133.41 (17)	B8—B7—B11—B5	−138.4 (2)
B11—B5—B6—B9	−37.6 (2)	B10—B7—B11—B5	−37.3 (2)
B4—B5—B6—B9	100.8 (2)	Cs—B7—B11—B5	50.0 (11)
B7—B5—B6—B9	0.2 (3)	B2—B7—B11—B8	37.7 (2)
B10—B5—B6—B9	63.5 (3)	B5—B7—B11—B8	138.4 (2)
Cs^{v}—B5—B6—B9	−125.8 (2)	B10—B7—B11—B8	101.2 (2)
B4—B5—B6—B11	138.4 (2)	Cs—B7—B11—B8	−171.6 (11)
B7—B5—B6—B11	37.8 (2)	B2—B7—B11—B6	−62.8 (3)
B10—B5—B6—B11	101.1 (3)	B8—B7—B11—B6	−100.5 (2)
Cs^{v}—B5—B6—B11	−88.18 (15)	B5—B7—B11—B6	37.9 (2)
B11—B5—B6—B12	−100.9 (2)	B10—B7—B11—B6	0.6 (3)
B4—B5—B6—B12	37.5 (2)	Cs—B7—B11—B6	87.9 (11)
B7—B5—B6—B12	−63.1 (3)	B2—B7—B11—B9	0.2 (3)
B10—B5—B6—B12	0.3 (4)	B8—B7—B11—B9	−37.5 (2)
Cs^{v}—B5—B6—B12	171.0 (2)	B5—B7—B11—B9	100.9 (3)
B11—B5—B6—Cs^{v}	88.18 (15)	B10—B7—B11—B9	63.7 (3)
B4—B5—B6—Cs^{v}	−133.41 (17)	Cs—B7—B11—B9	151.0 (10)
B7—B5—B6—Cs^{v}	126.0 (2)	B2—B7—B11—Cs^{v}	−139.0 (2)
B10—B5—B6—Cs^{v}	−170.7 (3)	B8—B7—B11—Cs^{v}	−176.7 (2)
B10—B2—B7—B8	137.9 (2)	B5—B7—B11—Cs^{v}	−38.3 (2)
B3—B2—B7—B8	37.3 (2)	B10—B7—B11—Cs^{v}	−75.5 (2)
B1—B2—B7—B8	100.6 (3)	Cs—B7—B11—Cs^{v}	11.7 (12)

Cs—B2—B7—B8	−147.87 (18)	B7—B8—B11—B5	37.3 (2)
B10—B2—B7—B11	100.3 (3)	B3—B8—B11—B5	−63.1 (3)
B3—B2—B7—B11	−0.3 (3)	B9—B8—B11—B5	−100.6 (2)
B8—B2—B7—B11	−37.6 (2)	B2—B8—B11—B5	0.2 (3)
B1—B2—B7—B11	63.1 (3)	B3—B8—B11—B7	−100.4 (3)
Cs—B2—B7—B11	174.6 (2)	B9—B8—B11—B7	−137.9 (3)
B10—B2—B7—B5	36.9 (2)	B2—B8—B11—B7	−37.0 (2)
B3—B2—B7—B5	−63.7 (3)	B7—B8—B11—B6	100.9 (3)
B8—B2—B7—B5	−100.9 (3)	B3—B8—B11—B6	0.5 (3)
B1—B2—B7—B5	−0.3 (3)	B9—B8—B11—B6	−37.0 (2)
Cs—B2—B7—B5	111.2 (2)	B2—B8—B11—B6	63.9 (3)
B3—B2—B7—B10	−100.6 (3)	B7—B8—B11—B9	137.9 (3)
B8—B2—B7—B10	−137.9 (2)	B3—B8—B11—B9	37.5 (2)
B1—B2—B7—B10	−37.2 (2)	B2—B8—B11—B9	100.8 (3)
Cs—B2—B7—B10	74.25 (15)	B4—B6—B11—B5	37.2 (2)
B10—B2—B7—Cs	−74.25 (15)	B9—B6—B11—B5	138.2 (2)
B3—B2—B7—Cs	−174.9 (2)	B12—B6—B11—B5	100.8 (2)
B8—B2—B7—Cs	147.87 (18)	Cs^{v}—B6—B11—B5	−83.27 (16)
B1—B2—B7—Cs	−111.5 (2)	B4—B6—B11—B7	−0.7 (3)
B11—B5—B7—B2	101.3 (2)	B9—B6—B11—B7	100.3 (2)
B4—B5—B7—B2	0.4 (3)	B12—B6—B11—B7	62.9 (3)
B10—B5—B7—B2	−36.9 (2)	B5—B6—B11—B7	−37.9 (2)
B6—B5—B7—B2	63.5 (3)	Cs^{v}—B6—B11—B7	−121.1 (2)
Cs^{v}—B5—B7—B2	143.25 (19)	B4—B6—B11—B8	−63.9 (3)
B11—B5—B7—B8	37.3 (2)	B9—B6—B11—B8	37.1 (2)
B4—B5—B7—B8	−63.6 (3)	B12—B6—B11—B8	−0.3 (3)
B10—B5—B7—B8	−101.0 (2)	B5—B6—B11—B8	−101.1 (3)
B6—B5—B7—B8	−0.5 (3)	Cs^{v}—B6—B11—B8	175.6 (2)
Cs^{v}—B5—B7—B8	79.2 (3)	B4—B6—B11—B9	−101.0 (2)
B4—B5—B7—B11	−100.9 (2)	B12—B6—B11—B9	−37.4 (2)
B10—B5—B7—B11	−138.3 (2)	B5—B6—B11—B9	−138.2 (2)
B6—B5—B7—B11	−37.8 (2)	Cs^{v}—B6—B11—B9	138.57 (17)
Cs^{v}—B5—B7—B11	41.9 (2)	B4—B6—B11—Cs^{v}	120.4 (2)
B11—B5—B7—B10	138.3 (2)	B9—B6—B11—Cs^{v}	−138.57 (17)
B4—B5—B7—B10	37.4 (2)	B12—B6—B11—Cs^{v}	−176.0 (2)
B6—B5—B7—B10	100.4 (3)	B5—B6—B11—Cs^{v}	83.27 (16)
Cs^{v}—B5—B7—B10	−179.8 (2)	B3—B9—B11—B5	63.5 (3)
B11—B5—B7—Cs	−170.8 (2)	B12—B9—B11—B5	0.1 (3)
B4—B5—B7—Cs	88.2 (2)	B6—B9—B11—B5	−37.5 (2)
B10—B5—B7—Cs	50.89 (17)	B8—B9—B11—B5	101.0 (2)
B6—B5—B7—Cs	151.3 (2)	Cs^{vi}—B9—B11—B5	175.38 (17)
Cs^{v}—B5—B7—Cs	−128.94 (16)	B3—B9—B11—B7	−0.1 (3)
B2—B7—B8—B3	−37.3 (2)	B12—B9—B11—B7	−63.5 (3)
B11—B7—B8—B3	100.9 (2)	B6—B9—B11—B7	−101.0 (3)
B5—B7—B8—B3	63.8 (3)	B8—B9—B11—B7	37.5 (2)
B10—B7—B8—B3	0.3 (3)	Cs^{vi}—B9—B11—B7	111.9 (2)
Cs—B7—B8—B3	−81.2 (3)	B3—B9—B11—B8	−37.5 (2)
B2—B7—B8—B11	−138.2 (2)	B12—B9—B11—B8	−100.9 (2)

B5—B7—B8—B11	−37.1 (2)	B6—B9—B11—B8	−138.4 (2)
B10—B7—B8—B11	−100.6 (2)	Cs^{vi}—B9—B11—B8	74.39 (17)
Cs—B7—B8—B11	177.9 (3)	B3—B9—B11—B6	100.9 (2)
B2—B7—B8—B9	−100.4 (3)	B12—B9—B11—B6	37.5 (2)
B11—B7—B8—B9	37.8 (2)	B8—B9—B11—B6	138.4 (2)
B5—B7—B8—B9	0.7 (3)	Cs^{vi}—B9—B11—B6	−147.16 (19)
B10—B7—B8—B9	−62.8 (3)	B3—B9—B11—Cs^{v}	143.70 (18)
Cs—B7—B8—B9	−144.3 (2)	B12—B9—B11—Cs^{v}	80.3 (2)
B11—B7—B8—B2	138.2 (2)	B6—B9—B11—Cs^{v}	42.79 (18)
B5—B7—B8—B2	101.1 (3)	B8—B9—B11—Cs^{v}	−178.8 (2)
B10—B7—B8—B2	37.7 (2)	Cs^{vi}—B9—B11—Cs^{v}	−104.37 (13)
Cs—B7—B8—B2	−43.9 (2)	B8—B3—B12—B9	−37.4 (2)
B9—B3—B8—B7	−101.1 (2)	B2—B3—B12—B9	−101.2 (3)
B12—B3—B8—B7	−63.9 (3)	B1—B3—B12—B9	−138.3 (2)
B2—B3—B8—B7	37.1 (2)	B9—B3—B12—B1	138.3 (2)
B1—B3—B8—B7	−0.3 (3)	B8—B3—B12—B1	100.9 (2)
B9—B3—B8—B11	−37.8 (2)	B2—B3—B12—B1	37.1 (2)
B12—B3—B8—B11	−0.5 (3)	B9—B3—B12—B4	100.7 (2)
B2—B3—B8—B11	100.4 (3)	B8—B3—B12—B4	63.3 (3)
B1—B3—B8—B11	63.0 (3)	B2—B3—B12—B4	−0.5 (3)
B12—B3—B8—B9	37.3 (2)	B1—B3—B12—B4	−37.6 (2)
B2—B3—B8—B9	138.2 (3)	B9—B3—B12—B6	37.7 (2)
B1—B3—B8—B9	100.8 (2)	B8—B3—B12—B6	0.3 (3)
B9—B3—B8—B2	−138.2 (3)	B2—B3—B12—B6	−63.5 (3)
B12—B3—B8—B2	−101.0 (3)	B1—B3—B12—B6	−100.6 (2)
B1—B3—B8—B2	−37.4 (2)	B9—B3—B12—Cs^{iv}	−177.2 (3)
B10—B2—B8—B7	−37.8 (2)	B8—B3—B12—Cs^{iv}	145.4 (2)
B3—B2—B8—B7	−138.1 (3)	B2—B3—B12—Cs^{iv}	81.6 (3)
B1—B2—B8—B7	−100.9 (3)	B1—B3—B12—Cs^{iv}	44.5 (3)
Cs—B2—B8—B7	37.4 (2)	B6—B9—B12—B3	137.7 (2)
B7—B2—B8—B3	138.1 (2)	B8—B9—B12—B3	37.2 (2)
B10—B2—B8—B3	100.3 (3)	B11—B9—B12—B3	100.3 (2)
B1—B2—B8—B3	37.3 (2)	Cs^{vi}—B9—B12—B3	−71.2 (3)
Cs—B2—B8—B3	175.5 (2)	B3—B9—B12—B1	−37.4 (2)
B7—B2—B8—B11	37.2 (2)	B6—B9—B12—B1	100.3 (2)
B10—B2—B8—B11	−0.6 (3)	B8—B9—B12—B1	−0.3 (3)
B3—B2—B8—B11	−100.9 (3)	B11—B9—B12—B1	62.9 (3)
B1—B2—B8—B11	−63.6 (3)	Cs^{vi}—B9—B12—B1	−108.7 (3)
Cs—B2—B8—B11	74.7 (3)	B3—B9—B12—B4	−100.6 (2)
B7—B2—B8—B9	101.0 (3)	B6—B9—B12—B4	37.1 (2)
B10—B2—B8—B9	63.1 (3)	B8—B9—B12—B4	−63.5 (3)
B3—B2—B8—B9	−37.2 (2)	B11—B9—B12—B4	−0.3 (3)
B1—B2—B8—B9	0.1 (3)	Cs^{vi}—B9—B12—B4	−171.9 (2)
Cs—B2—B8—B9	138.38 (19)	B3—B9—B12—B6	−137.7 (2)
B8—B3—B9—B12	138.5 (2)	B8—B9—B12—B6	−100.6 (2)
B2—B3—B9—B12	100.9 (2)	B11—B9—B12—B6	−37.4 (2)
B1—B3—B9—B12	37.3 (2)	Cs^{vi}—B9—B12—B6	151.0 (3)
B12—B3—B9—B6	−37.8 (2)	B3—B9—B12—Cs^{iv}	174.2 (5)

B8—B3—B9—B6	100.6 (2)	B6—B9—B12—Cs^{iv}	−48.1 (5)
B2—B3—B9—B6	63.1 (3)	B8—B9—B12—Cs^{iv}	−148.6 (4)
B1—B3—B9—B6	−0.6 (3)	B11—B9—B12—Cs^{iv}	−85.5 (5)
B12—B3—B9—B8	−138.5 (2)	Cs^{vi}—B9—B12—Cs^{iv}	103.0 (5)
B2—B3—B9—B8	−37.6 (2)	B10—B1—B12—B3	−100.3 (3)
B1—B3—B9—B8	−101.2 (2)	B4—B1—B12—B3	−137.7 (2)
B12—B3—B9—B11	−101.0 (2)	B2—B1—B12—B3	−37.0 (2)
B8—B3—B9—B11	37.4 (2)	B10—B1—B12—B9	−63.0 (3)
B2—B3—B9—B11	−0.1 (3)	B4—B1—B12—B9	−100.4 (2)
B1—B3—B9—B11	−63.7 (3)	B3—B1—B12—B9	37.3 (2)
B12—B3—B9—Cs^{vi}	147.95 (17)	B2—B1—B12—B9	0.3 (3)
B8—B3—B9—Cs^{vi}	−73.58 (17)	B10—B1—B12—B4	37.4 (2)
B2—B3—B9—Cs^{vi}	−111.1 (2)	B3—B1—B12—B4	137.7 (2)
B1—B3—B9—Cs^{vi}	−174.76 (17)	B2—B1—B12—B4	100.8 (3)
B4—B6—B9—B3	0.4 (3)	B10—B1—B12—B6	0.4 (3)
B11—B6—B9—B3	−100.3 (2)	B4—B1—B12—B6	−37.0 (2)
B12—B6—B9—B3	37.8 (2)	B3—B1—B12—B6	100.7 (2)
B5—B6—B9—B3	−63.1 (3)	B2—B1—B12—B6	63.7 (3)
Cs^{v}—B6—B9—B3	−155.45 (17)	B10—B1—B12—Cs^{iv}	107.3 (2)
B4—B6—B9—B12	−37.4 (2)	B4—B1—B12—Cs^{iv}	69.94 (15)
B11—B6—B9—B12	−138.1 (2)	B3—B1—B12—Cs^{iv}	−152.35 (17)
B5—B6—B9—B12	−100.9 (3)	B2—B1—B12—Cs^{iv}	170.7 (2)
Cs^{v}—B6—B9—B12	166.8 (2)	B6—B4—B12—B3	−100.5 (2)
B4—B6—B9—B8	63.7 (3)	B10—B4—B12—B3	0.7 (3)
B11—B6—B9—B8	−37.0 (2)	B1—B4—B12—B3	37.8 (2)
B12—B6—B9—B8	101.1 (2)	B5—B4—B12—B3	−62.9 (3)
B5—B6—B9—B8	0.3 (3)	Cs^{iv}—B4—B12—B3	136.3 (2)
Cs^{v}—B6—B9—B8	−92.1 (2)	B6—B4—B12—B9	−37.3 (2)
B4—B6—B9—B11	100.7 (2)	B10—B4—B12—B9	64.0 (3)
B12—B6—B9—B11	138.1 (2)	B1—B4—B12—B9	101.1 (2)
B5—B6—B9—B11	37.3 (2)	B5—B4—B12—B9	0.4 (3)
Cs^{v}—B6—B9—B11	−55.1 (2)	Cs^{iv}—B4—B12—B9	−160.45 (19)
B4—B6—B9—Cs^{vi}	170.4 (2)	B6—B4—B12—B1	−138.3 (2)
B11—B6—B9—Cs^{vi}	69.7 (3)	B10—B4—B12—B1	−37.1 (2)
B12—B6—B9—Cs^{vi}	−152.2 (3)	B5—B4—B12—B1	−100.7 (3)
B5—B6—B9—Cs^{vi}	106.9 (3)	Cs^{iv}—B4—B12—B1	98.49 (16)
Cs^{v}—B6—B9—Cs^{vi}	14.6 (4)	B10—B4—B12—B6	101.2 (3)
B7—B8—B9—B3	100.2 (3)	B1—B4—B12—B6	138.3 (2)
B11—B8—B9—B3	137.9 (2)	B5—B4—B12—B6	37.6 (2)
B2—B8—B9—B3	37.3 (2)	Cs^{iv}—B4—B12—B6	−123.19 (16)
B7—B8—B9—B12	63.0 (3)	B6—B4—B12—Cs^{iv}	123.19 (16)
B3—B8—B9—B12	−37.2 (2)	B10—B4—B12—Cs^{iv}	−135.6 (2)
B11—B8—B9—B12	100.7 (2)	B1—B4—B12—Cs^{iv}	−98.49 (16)
B2—B8—B9—B12	0.1 (3)	B5—B4—B12—Cs^{iv}	160.8 (2)
B7—B8—B9—B6	−0.6 (3)	B4—B6—B12—B3	100.6 (2)
B3—B8—B9—B6	−100.8 (2)	B9—B6—B12—B3	−37.7 (2)
B11—B8—B9—B6	37.1 (2)	B11—B6—B12—B3	0.0 (3)
B2—B8—B9—B6	−63.5 (3)	B5—B6—B12—B3	63.1 (3)

B7—B8—B9—B11	−37.7 (2)	Cs^{v}—B6—B12—B3	−161.5 (8)
B3—B8—B9—B11	−137.9 (2)	B4—B6—B12—B9	138.3 (2)
B2—B8—B9—B11	−100.6 (3)	B11—B6—B12—B9	37.7 (2)
B7—B8—B9—Cs^{vi}	−148.0 (2)	B5—B6—B12—B9	100.8 (3)
B3—B8—B9—Cs^{vi}	111.84 (16)	Cs^{v}—B6—B12—B9	−123.8 (9)
B11—B8—B9—Cs^{vi}	−110.30 (17)	B4—B6—B12—B1	37.1 (2)
B2—B8—B9—Cs^{vi}	149.1 (2)	B9—B6—B12—B1	−101.2 (2)
B4—B1—B10—B2	138.1 (2)	B11—B6—B12—B1	−63.5 (3)
B12—B1—B10—B2	100.6 (3)	B5—B6—B12—B1	−0.4 (3)
B3—B1—B10—B2	37.4 (2)	Cs^{v}—B6—B12—B1	135.0 (8)
B12—B1—B10—B4	−37.4 (2)	B9—B6—B12—B4	−138.3 (2)
B3—B1—B10—B4	−100.7 (2)	B11—B6—B12—B4	−100.6 (2)
B2—B1—B10—B4	−138.1 (2)	B5—B6—B12—B4	−37.5 (2)
B4—B1—B10—B7	100.8 (3)	Cs^{v}—B6—B12—B4	97.9 (9)
B12—B1—B10—B7	63.3 (3)	B4—B6—B12—Cs^{iv}	−56.07 (16)
B3—B1—B10—B7	0.1 (3)	B9—B6—B12—Cs^{iv}	165.66 (18)
B2—B1—B10—B7	−37.3 (2)	B11—B6—B12—Cs^{iv}	−156.68 (17)
B4—B1—B10—B5	37.2 (2)	B5—B6—B12—Cs^{iv}	−93.6 (2)
B12—B1—B10—B5	−0.2 (4)	Cs^{v}—B6—B12—Cs^{iv}	41.8 (9)
B3—B1—B10—B5	−63.4 (3)		

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1/2, −*y*, *z*−1/2; (iii) −*x*+3/2, −*y*, *z*−1/2; (iv) −*x*+1/2, −*y*, *z*+1/2; (v) −*x*+1, *y*+1/2, −*z*+1/2; (vi) −*x*+3/2, −*y*, *z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O—H14···H7	0.91 (1)	2.11 (3)	2.86 (3)	135 (4)
O—H13···H1^{v}	0.91 (1)	2.45 (3)	3.24 (3)	146 (4)
O—H13···H2^{v}	0.91 (1)	2.47 (3)	3.07 (3)	124 (4)
O—H13···H3^{v}	0.91 (1)	2.39 (3)	3.11 (3)	136 (4)
C1—H1*A*···H3^{ii}	0.98	2.49	3.35 (5)	143
C2—H2*B*···H5	0.98	2.33	3.20 (5)	151
C2—H2*C*···H6^{vii}	0.98	2.49	3.29 (4)	138
C2—H2*B*···H9^{vii}	0.98	2.51	2.79 (4)	96
C3—H3*C*···H8^{viii}	0.98	2.51	3.18 (4)	126
C3—H3*C*···H11^{viii}	0.98	2.33	3.28 (4)	160
C4—H4*B*···H3^{ii}	0.98	2.30	3.21 (4)	152
C4—H4*C*···H1^{ix}	0.98	2.52	2.82 (5)	98

Symmetry codes: (ii) −*x*+1/2, −*y*, *z*−1/2; (v) −*x*+1, *y*+1/2, −*z*+1/2; (vii) *x*−1/2, −*y*+1/2, −*z*+1; (viii) *x*−1, *y*, *z*; (ix) −*x*, *y*+1/2, −*z*+1/2.