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CHARGE DISTRIBUTION WITHIN 1,2-DICARBA-*closo*-DODECABORANE: DIPOLE MOMENTS OF ITS PHENYL DERIVATIVES

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The dipole moment of 1,2-dicarba-*closo*-dodecaborane is oriented with the positive end towards the carbon atoms as follows from measurements on phenyl derivatives with variable substituents. Towards the phenyl group, the substituent 1,2-$C_2B_{10}H_{11}$ behaves as a weak electron acceptor.

Keywords: Dipole moments; Carboranes; Boranes; Electronic structure; Charge distribution; *Ab initio* calculations.

Hofmann and Lipscomb proposed in their pioneer work[1] the experimental availability of three positional isomers of icosahedral clusters $C_2B_{10}H_{12}$. On the basis of LCAO-MO calculations, they argued that the atomic charge on carbon atoms is positive, although simple atomic concepts such as electronegativity would have implied the opposite. The dipole moment of 1,2-$C_2B_{10}H_{12}$ (**1**) was determined[2] to be 4.53 D in agreement with our present measurement (4.50 D). It lies in the C_2 axis but the positions of the positive and negative ends are not evident. A comparison with the dipole moments of the bromo derivatives[3] 1,2-Br_2-1,2-$C_2B_{10}H_{10}$ and 9,12-Br_2-1,2-$C_2B_{10}H_{10}$ should confirm qualitatively the above proposal but there is an inherent weakness that the electron distribution can be affected by the immediately bonded substituents.

Our intention in this work was to gain more information about the electron distribution in the molecule of **1** by the method common in organic chemistry[4,5] – introducing, at a greater distance, non-interacting substituents with known partial dipole moments *viz.*, in the *para* position of the benzene ring. Our first task was thus confirming the direction of the vector

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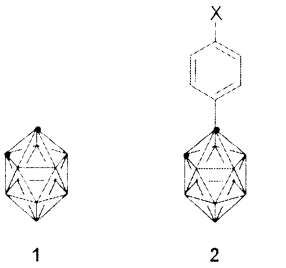
of **1**. Once the phenyl group was introduced, we could deal with the second problem, a possible interaction of the $C_2B_{10}H_{11}$ group with the benzene ring. For this purpose we prepared[6] 1-(4-substituted phenyl)-1,2-dicarba-*closo*-dodecaboranes **2a**–**2e** with variable *para* substituents (X = H, CH_3, Br, Cl, NO_2 for **2a**, **2b**, **2c**, **2d**, **2e**, respectively; see Fig. 1) and measured the



2	X
a	H
b	CH_3
c	Br
d	Cl
e	NO_2

corresponding dipole moments[7]. Their vector analysis is presented in Fig. 1. The dipole moment of a given derivative, *e.g.* the vector ***CIZ*** for **2d**, can be represented with a very good approximation[4] as a sum of the two vectors: the unknown dipole moment of **2a** (***HZ***) and the known moment of the

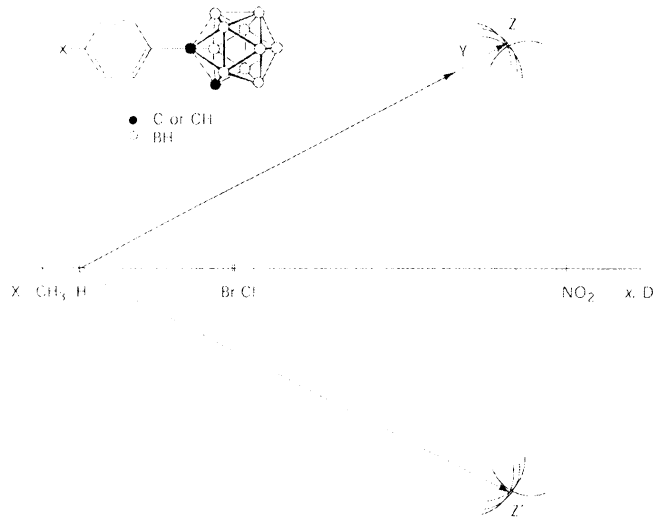


FIG. 1
Vector analysis of experimental dipole moments of **1**, ***HY***, **2a**, ***HZ*** and **2b**–**2e** (points CH_3, Cl, Br, NO_2). The moments are shown by the arrows from the positive towards the negative end

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substituent, vector ***CIH***. In geometrical terms, the task is to construct a triangle given its three sides. This procedure was repeated for the four substituted compounds **2b**–**2e** and good agreement was reached in graphical representation, similar to that in standard examples[9] (see the arcs in Fig. 1 intersecting with a good precision in one point). Note that in principle two equivalent solutions are possible, points Z and Z′, of which Z is considered with respect to the choice of the carbaborane orientation towards the benzene ring in the molecular diagram in Fig. 1. The dipole moment of **2a** (vector ***HZ*** as a mean value) was determined to be 5.0 D at an angle of 28° to the exohedral C–C_{ar} bond, *i.e.*, practically in the symmetry axis of the carbaborane moiety. (An electron diffraction study of **2a** (ref.[10]) yielded an angle of 31° between this axis and the C–C_{ar} bond.)

This result allows answering the two above questions. First, directions of the dipole moments of **1** (vector ***HY*** in the symmetry axis) and **2a** (vector ***HZ***), coincide within the experimental errors; also their absolute values are very close. There is no doubt that even the dipole moment of **1** as well as that of **2a**, is oriented with the positive end towards the carbon atoms and with the negative end inside the carbaborane skeleton, in agreement with the assumptions[1,2,+].

Second, a more detailed analysis is possible, comparing the dipole moment of **1** (vector ***HY***, Fig. 1) and that of **2a** (vector ***HZ***). Their difference in the absolute value is 0.5 D. Generally, this difference is called a mesomeric dipole moment[12] and interpreted as an electron shift from the benzene ring into the carbaborane skeleton. If the group $C_2B_{10}H_{11}$ is considered as an organic substituent, it is classified as a weak acceptor. This is in agreement with the substituent constants[13] σ_m and σ_p, 0.47 and 0.49, respectively; as expected $\sigma_p > \sigma_m$ but the difference is minute. For common simple organic substituents X, the mesomeric dipole moment was defined[14] as the vector difference between the dipole moments of compounds C_6H_5X and CH_3X. However, the mesomeric dipole moments of acceptors need not be inter-

+ The RMP2(fc)/6-31G* geometry optimisation of **1** with the C_{2v} symmetry restriction (NIMAG = 0 at RHF/6-31G*) using the Gaussian94 program package[11] provided the total Mulliken charge on C(1,2) of −0.51 (Note that μ of **1** was calculated to be 4.53 D at this correlated level and, according to Gaussian convention, it points away from the negatively charged part of **1**.) Because of the well-known drawbacks of the Mulliken approach[12a], we also employed the natural population analysis (NPA) of Weinhold, Reed and Weinstock[12] to get the charge distribution of **1** in a more sophisticated manner. However, these calculations yielded the total charge on carbons of −0.57, *i.e.*, a value very close to that provided by the Mulliken scheme.

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preted[15] on the basis of resonance or conjugation: the enhanced dipole moment can be also due to electron shifts within the benzene ring (polarisation) without giving a double bond character to the bond C–X. Indeed, the length of the C C_{Ar} exoskeletal linkage in **2a** was determined to be 150.0(8), 150.3(4) and 151.6 pm as followed from the electron diffraction, X-ray diffraction and RHF/6-31G* studies, respectively[10]. In any case, the acceptor character of the group $C_2B_{10}H_{11}$ is in agreement with the NMR (ref.[16]) and MCD (ref.[17]) studies. Note that most aromatic acceptor substituents possess dipole moments oriented out from the benzene ring but there is not a strict relationship[18].

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6. Compounds **2a**, **2b**, **2c** and **2d** were prepared by allowing to react 6,9-bis(ligand)decaborane(12), 6,9-$L_2B_{10}H_{12}$, where L was CH_3CN, with a substituted phenylacetylene, 4-X-C_6H_4CCH (X = H, CH_3, Br, Cl). See, *e.g.*, Heying T. L., Ager J. W., Jr., Clark S. L., Mangold D. J., Goldstein H. L., Hillman M., Polak R. J., Szymanski J. W.: *Inorg. Chem.* **1963**, *2*, 1089. Compound **2d** was obtained by nitration of **2a**: Hawthorne M. F., Berry F. T., Wegner A. P.: *J. Am. Chem. Soc.* **1965**, *87*, 4746. The purity of all compounds was checked by analytical TLC and the structures of the molecules were confirmed on the basis of $^1H\{^{11}B\}$ and $^{11}B\{^1H\}$ NMR spectra recorded on a Varian Unity-500 instrument in $CDCl_3$ solution. Example: NMR spectrum of **2a** (in ppm, see also ref.[10] for a comparison): B(3,6) –12.2, B(4,5) –11.7, B(7,11) –13.7, B(8,10) –9.9, B(9) –3.0, B(12) –5.0. The corresponding boron atoms in **2b**–**2d** resonated at about the same frequencies as in **2a**.
7. Dipole moments were measured at 25 °C in benzene (five solutions, weight fraction $1.8 \cdot 10^{-4}$ to $1.1 \cdot 10^{-3}$) by the method of Guggenheim and Smith[8]. Relative permittivities were measured at 6 MHz on a home-made DK-meter with direct frequency reading. Refractive indices were measured on an Aerograph refractive index detector (Varian). The following dipole moments were obtained: **1** 4.50, **2a** 4.94, **2b** 5.32, **2c** 3.66, **2d** 3.64 and **2e** 2.26 D; the estimated uncertainty was 0.05 D. For constructing Fig. 1, the following

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standard bond moments were used: H–C_{al} 0.3, H–C_{ar} 0, C_{ar}–Cl 1.6, C_{ar}–Br 1.57 and C_{ar}–NO_2 4.0 D.

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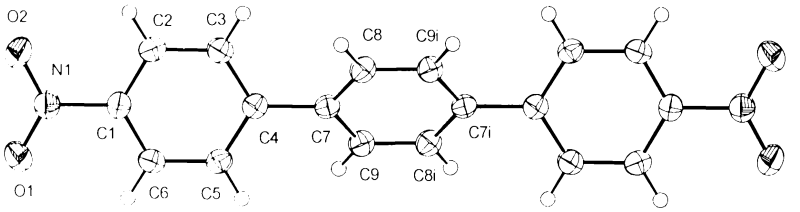
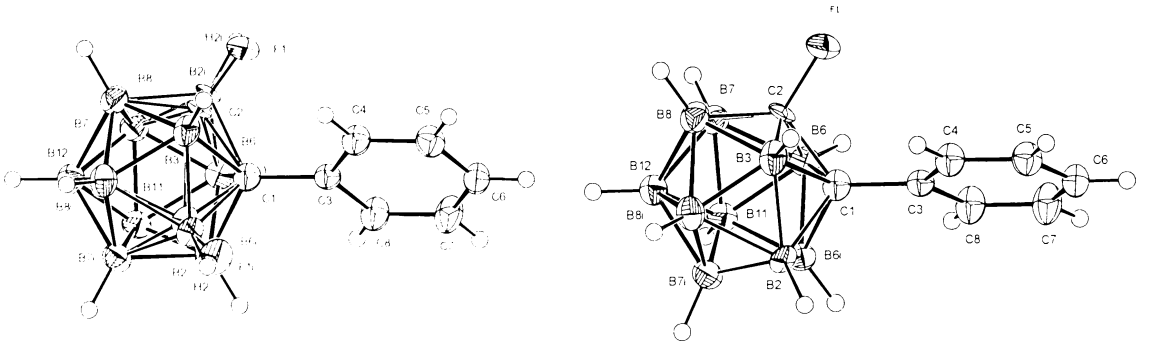
Pohledy na molekuly látek XXVIIa, XX, XXII, XXIII, XXXII a VIII s číslováním atomů. Teplotní elipsoidy jsou kresleny na hladině pravděpodobnosti 50%.

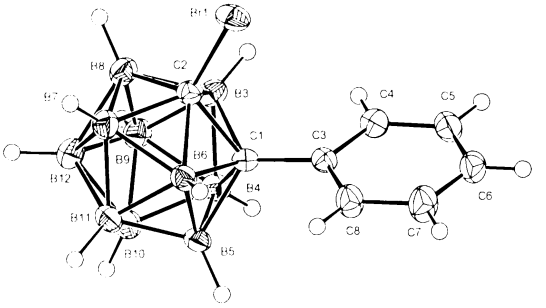
Příloha č. 2 RTG - XLVIIa (4,4''-dinitro-p-terfenyl)



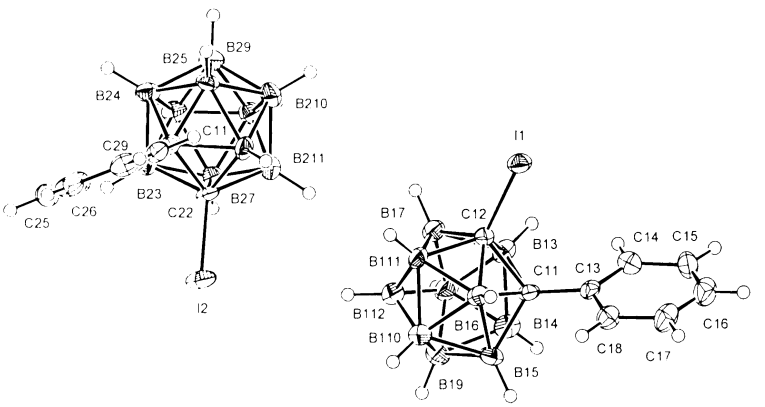
Příloha č. 3 RTG - XX (1-fenyl-2-fluor-1,2-dikarba-kloso-dodekaboran(12))



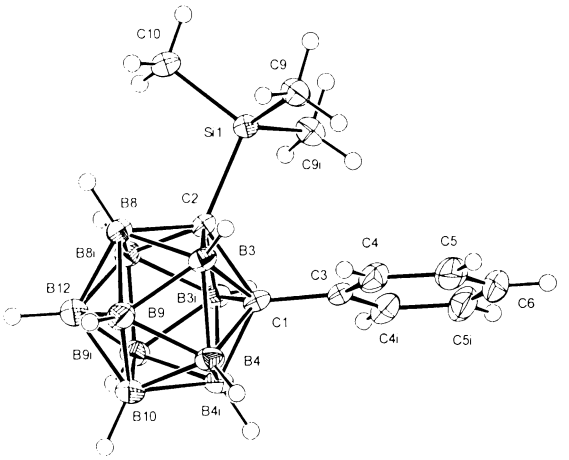
Příloha č. 4 RTG - XXII (1-fenyl-2-brom-1,2-dikarba-kloso-dodekaboran(12))



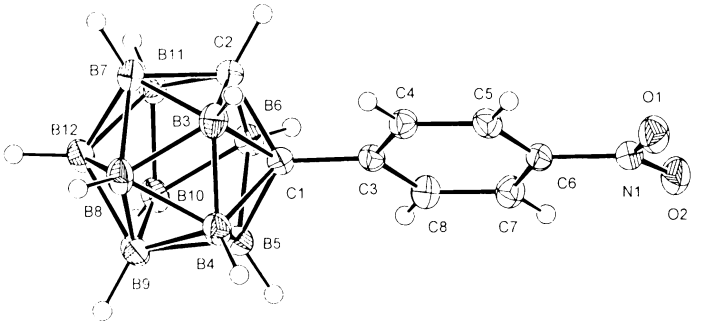
Příloha č. 5 RTG - XXIII (1-fenyl-2-jod-1,2-dikarba-kloso-dodekaboran(12))



Příloha č. 6 RTG - XXXII (1-fenyl-2-trimethylsilyl-1,2-dikarba-kloso-dodekaboran(12))



Příloha č. 7 RTG - VIII (1-(4-nitrofenyl)-1,2-dikarba-kloso-dodekaboran(12))



Příloha č. 2

RTG - XLVIIa (4,4''-dinitro-p-terfenyl)

Experimental

Crystal data

$C_{18}H_{12}N_2O_4$
M_r = 320.30
Triclinic
$P\bar{1}$
a = 3.8740 (2) Å
b = 9.8730 (4) Å
c = 12.0300 (5) Å
α = 100.732 (3)°
β = 95.755 (2)°
γ = 98.952 (3)°
V = 442.59 (3) Å^3
Z = 1
D_x = 1.202 Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 1982 reflections
θ = 1–27.5°
μ = 0.087 mm^{-1}
T = 150 (2) K
Bar
Yellow
0.5 × 0.12 × 0.025 mm
Crystal source: synthesized by the authors

Data collection

Nonius KappaCCD area detector diffractometer
φ and ω scans to fill the Ewald sphere
Absorption correction: none
10711 measured reflections
1998 independent reflections

1483 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.52°
h = −5 → 5
k = −12 → 12
l = −15 → 15

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.0582
$wR(F^2)$ = 0.1983
S = 1.111
1998 reflections
109 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1349P)^2 + 0.0000P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.000
$\Delta\rho_{max}$ = 0.300 e Å^{-3}
$\Delta\rho_{min}$ = −0.197 e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* ($Å^2$)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
C1	1.1901 (4)	0.72934 (15)	0.44866 (12)	0.0285 (4)
C2	1.0454 (4)	0.81626 (16)	0.38686 (13)	0.0314 (4)
C3	0.8810 (4)	0.75960 (16)	0.27684 (13)	0.0303 (4)
C4	0.8591 (4)	0.61843 (16)	0.22829 (13)	0.0268 (4)
C5	1.0092 (4)	0.53341 (16)	0.29398 (13)	0.0288 (4)
C6	1.1753 (4)	0.58896 (15)	0.40401 (13)	0.0296 (4)
C7	0.6771 (4)	0.55737 (15)	0.11103 (12)	0.0276 (4)
C8	0.6729 (4)	0.63731 (16)	0.02730 (13)	0.0304 (4)
C9	0.5017 (4)	0.41857 (16)	0.08186 (13)	0.0298 (4)
N1	1.3635 (4)	0.78772 (14)	0.56552 (12)	0.0348 (4)
O1	1.5241 (3)	0.71338 (13)	0.61544 (10)	0.0460 (4)
O2	1.3416 (4)	0.90834 (12)	0.60908 (11)	0.0524 (5)

Table 2. *Anisotropic displacement parameters* ($Å^2$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.0267 (8)	0.0315 (8)	0.0259 (8)	0.0032 (6)	0.0036 (6)	0.0036 (6)
C2	0.0339 (9)	0.0282 (8)	0.0329 (8)	0.0082 (6)	0.0065 (7)	0.0048 (6)
C3	0.0304 (8)	0.0317 (8)	0.0302 (8)	0.0077 (6)	0.0044 (6)	0.0081 (6)
C4	0.0249 (8)	0.0292 (8)	0.0272 (8)	0.0046 (6)	0.0070 (6)	0.0062 (6)
C5	0.0281 (8)	0.0284 (8)	0.0302 (8)	0.0069 (6)	0.0063 (6)	0.0041 (6)
C6	0.0298 (9)	0.0312 (8)	0.0308 (8)	0.0091 (6)	0.0059 (6)	0.0099 (6)
C7	0.0256 (8)	0.0310 (8)	0.0272 (8)	0.0089 (6)	0.0066 (6)	0.0035 (6)
C8	0.0321 (9)	0.0274 (8)	0.0307 (8)	0.0037 (6)	0.0050 (6)	0.0047 (6)
C9	0.0333 (9)	0.0297 (8)	0.0277 (8)	0.0061 (6)	0.0069 (6)	0.0075 (6)
N1	0.0393 (8)	0.0335 (8)	0.0303 (7)	0.0058 (6)	0.0016 (6)	0.0057 (6)
O1	0.0564 (8)	0.0427 (7)	0.0382 (7)	0.0126 (6)	−0.0079 (6)	0.0107 (6)
O2	0.0761 (10)	0.0352 (7)	0.0385 (7)	0.0133 (7)	−0.0103 (7)	−0.0043 (5)

Table 3. *Selected geometric parameters (Å, °)*

C1—C6	1.380 (2)	C5—H5	0.9300
C1—C2	1.381 (2)	C6—H6	0.9300
C1—N1	1.466 (2)	C7—C8	1.391 (2)
C2—C3	1.384 (2)	C7—C9	1.395 (2)
C2—H2	0.9300	C8—C9^{i}	1.387 (2)
C3—C4	1.396 (2)	C8—H8	0.9300
C3—H3	0.9300	C9—C8^{i}	1.387 (2)
C4—C5	1.402 (2)	C9—H9	0.9300
C4—C7	1.484 (2)	N1—O2	1.2281 (18)
C5—C6	1.384 (2)	N1—O1	1.2318 (17)
C6—C1—C2	122.07 (14)	C1—C6—C5	118.96 (14)
C6—C1—N1	118.90 (14)	C1—C6—H6	120.5
C2—C1—N1	119.03 (14)	C5—C6—H6	120.5
C1—C2—C3	118.41 (14)	C8—C7—C9	118.03 (14)
C1—C2—H2	120.8	C8—C7—C4	121.08 (14)
C3—C2—H2	120.8	C9—C7—C4	120.89 (14)
C2—C3—C4	121.49 (14)	C9^{i}—C8—C7	121.20 (14)
C2—C3—H3	119.3	C9^{i}—C8—H8	119.4
C4—C3—H3	119.3	C7—C8—H8	119.4
C3—C4—C5	118.29 (14)	C8^{i}—C9—C7	120.77 (14)
C3—C4—C7	121.27 (14)	C8^{i}—C9—H9	119.6
C5—C4—C7	120.44 (14)	C7—C9—H9	119.6
C6—C5—C4	120.78 (14)	O2—N1—O1	123.11 (13)
C6—C5—H5	119.6	O2—N1—C1	118.46 (13)
C4—C5—H5	119.6	O1—N1—C1	118.43 (13)
C6—C1—C2—C3	0.0 (2)	C5—C4—C7—C8	−149.54 (15)
N1—C1—C2—C3	−179.69 (13)	C3—C4—C7—C9	−147.82 (15)
C1—C2—C3—C4	0.1 (2)	C5—C4—C7—C9	31.1 (2)
C2—C3—C4—C5	−0.1 (2)	C9—C7—C8—C9^{i}	0.4 (2)
C2—C3—C4—C7	178.91 (13)	C4—C7—C8—C9^{i}	−178.97 (13)
C3—C4—C5—C6	−0.1 (2)	C8—C7—C9—C8^{i}	−0.4 (2)
C7—C4—C5—C6	−179.12 (12)	C4—C7—C9—C8^{i}	178.97 (13)
C2—C1—C6—C5	−0.2 (2)	C6—C1—N1—O2	−172.01 (14)
N1—C1—C6—C5	179.50 (12)	C2—C1—N1—O2	7.7 (2)
C4—C5—C6—C1	0.3 (2)	C6—C1—N1—O1	7.9 (2)
C3—C4—C7—C8	31.5 (2)	C2—C1—N1—O1	−172.36 (15)

Symmetry codes: (i) $1-x, 1-y, -z$.

Příloha č. 3

RTG - XX (1-fenyl-2-fluor-1,2-dikarba-kloso-dodekaboran(12))

Experimental

Crystal data

$C_8H_{15}B_{10}F$
M_r = 238.30
Monoclinic
$P2_1/m$
a = 8.6380 (3) Å
b = 7.5040 (3) Å
c = 10.5330 (4) Å
β = 106.145 (2)°
V = 655.82 (4) Å^3
Z = 2
D_x = 1.207 Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 1566 reflections
θ = 1–27.5°
μ = 0.067 mm^{-1}
T = 150 (2) K
Plate
Colourless
0.3 × 0.17 × 0.1 mm
Crystal source: synthesized by the authors

Data collection

Nonius KappaCCD area detector diffractometer
φ and ω scans to fill the Ewald sphere
Absorption correction: none
9428 measured reflections
1604 independent reflections

1357 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.45°
h = −11 → 11
k = −9 → 9
l = −13 → 13

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.0467
$wR(F^2)$ = 0.1385
S = 1.077
1604 reflections
109 parameters
H-atom parameters constrained

$w=1/[\sigma^2(F_o^2) + (0.0796P)^2 + 0.1410P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.000
$\Delta\rho_{max}$ = 0.319 e Å^{-3}
$\Delta\rho_{min}$ = −0.208 e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$

	Occupancy	x	y	z	U_{eq}
C1	1	0.22993 (18)	1/4	0.30067 (16)	0.0258 (4)
C2	0.50	0.3225 (16)	0.0868 (11)	0.2553 (12)	0.0221 (11)
F1	0.50	0.3269 (2)	−0.0565 (2)	0.33735 (17)	0.0373 (4)
B2	0.50	0.3236 (19)	0.0465 (13)	0.2707 (14)	0.0221 (11)
C3	1	0.15548 (18)	1/4	0.41369 (15)	0.0234 (3)
C4	1	0.24807 (19)	1/4	0.54482 (16)	0.0295 (4)
C5	1	0.1747 (2)	1/4	0.64633 (17)	0.0319 (4)
C6	1	0.0086 (2)	1/4	0.61832 (17)	0.0316 (4)
C7	1	−0.0835 (2)	1/4	0.48876 (19)	0.0398 (5)
C8	1	−0.01172 (19)	1/4	0.38652 (17)	0.0340 (4)
B3	1	0.4386 (2)	1/4	0.33296 (19)	0.0293 (4)
B6	1	0.13643 (15)	0.36815 (17)	0.15972 (12)	0.0260 (3)
B7	1	0.29304 (17)	0.05824 (18)	0.09291 (13)	0.0295 (3)
B8	1	0.48065 (16)	0.13160 (19)	0.20100 (13)	0.0308 (3)
B11	1	0.1773 (2)	1/4	0.02741 (18)	0.0274 (4)
B12	1	0.3903 (2)	1/4	0.05205 (19)	0.0291 (4)

Table 2. *Anisotropic displacement parameters* (Å²)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.0182 (7)	0.0339 (9)	0.0230 (8)	0.000	0.0020 (6)	0.000
C2	0.0279 (7)	0.017 (4)	0.022 (3)	0.004 (3)	0.0079 (14)	0.014 (2)
F1	0.0409 (8)	0.0279 (8)	0.0446 (9)	0.0094 (7)	0.0145 (7)	0.0141 (7)
B2	0.0279 (7)	0.017 (4)	0.022 (3)	0.004 (3)	0.0079 (14)	0.014 (2)
C3	0.0214 (8)	0.0236 (7)	0.0242 (8)	0.000	0.0046 (6)	0.000
C4	0.0218 (8)	0.0381 (9)	0.0267 (8)	0.000	0.0037 (6)	0.000
C5	0.0314 (9)	0.0389 (9)	0.0241 (8)	0.000	0.0056 (7)	0.000
C6	0.0314 (9)	0.0354 (9)	0.0309 (9)	0.000	0.0136 (7)	0.000
C7	0.0218 (8)	0.0616 (13)	0.0368 (10)	0.000	0.0093 (7)	0.000
C8	0.0209 (8)	0.0514 (11)	0.0277 (9)	0.000	0.0035 (7)	0.000
B3	0.0165 (8)	0.0438 (11)	0.0258 (9)	0.000	0.0032 (7)	0.000
B6	0.0245 (6)	0.0268 (6)	0.0243 (6)	0.0028 (5)	0.0027 (5)	0.0019 (5)
B7	0.0347 (7)	0.0258 (6)	0.0284 (7)	0.0012 (5)	0.0096 (5)	−0.0018 (5)
B8	0.0256 (6)	0.0365 (7)	0.0311 (7)	0.0061 (5)	0.0092 (5)	0.0021 (6)
B11	0.0288 (9)	0.0284 (9)	0.0228 (9)	0.000	0.0034 (7)	0.000
B12	0.0307 (10)	0.0304 (9)	0.0271 (9)	0.000	0.0097 (8)	0.000

Table 3. *Selected geometric parameters (Å, °)*

C1—C3	1.502 (2)	C7—H7	0.9300
C1—C2	1.606 (12)	C8—H8	0.9300
C1—C2^{i}	1.606 (12)	B3—C2^{i}	1.649 (12)
C1—B6	1.7250 (18)	B3—B8	1.770 (2)
C1—B6^{i}	1.7250 (18)	B3—B8^{i}	1.770 (2)
C1—B3	1.739 (2)	B3—B2^{i}	1.840 (13)
C1—B2	1.796 (13)	B3—H3	1.1000
C1—B2^{i}	1.796 (13)	B6—C2^{i}	1.677 (13)
C2—F1	1.373 (5)	B6—B11	1.768 (2)
C2—B3	1.649 (12)	B6—B6^{i}	1.773 (3)
C2—B8	1.656 (12)	B6—B7^{i}	1.7776 (18)
C2—B7	1.672 (13)	B6—B2^{i}	1.827 (14)
C2—B6^{i}	1.677 (13)	B6—H6A	1.1000
C2—H2	1.4417	B7—B6^{i}	1.7775 (18)
F1—H2	0.2424	B7—B11	1.7784 (18)
B2—B7	1.820 (14)	B7—B12	1.7785 (17)
B2—B6^{i}	1.827 (14)	B7—B8	1.789 (2)
B2—B8	1.828 (13)	B7—H7A	1.1000
B2—B3	1.840 (13)	B8—B8^{i}	1.777 (3)
B2—H2	1.1000	B8—B12	1.783 (2)
C3—C4	1.390 (2)	B8—H8A	1.1000
C3—C8	1.392 (2)	B11—B6^{i}	1.768 (2)
C4—C5	1.386 (2)	B11—B7^{i}	1.7784 (18)
C4—H4	0.9300	B11—B12	1.785 (3)
C5—C6	1.383 (2)	B11—H11	1.1000
C5—H5	0.9300	B12—B7^{i}	1.7785 (17)
C6—C7	1.375 (3)	B12—B8^{i}	1.783 (2)
C6—H6	0.9300	B12—H12	1.1000
C7—C8	1.384 (2)		
C3—C1—C2	126.4 (3)	B6—C1—B6^{i}	61.86 (10)
C3—C1—C2^{i}	126.4 (3)	C3—C1—B3	119.60 (13)
C2—C1—C2^{i}	99.4 (7)	C2—C1—B3	58.9 (5)
C3—C1—B6	118.74 (10)	C2^{i}—C1—B3	58.9 (5)
C2—C1—B6	106.8 (4)	B6—C1—B3	112.34 (10)
C2^{i}—C1—B6	60.3 (5)	B6^{i}—C1—B3	112.34 (10)
C3—C1—B6^{i}	118.75 (10)	C3—C1—B2	116.9 (4)
C2—C1—B6^{i}	60.3 (5)	C2—C1—B2	9.6 (6)
C2^{i}—C1—B6^{i}	106.8 (4)	C2^{i}—C1—B2	108.09 (15)

B6—C1—B2	114.3 (4)	B7—B2—B3	103.6 (4)
B6^{i}—C1—B2	62.5 (5)	B6^{i}—B2—B3	103.4 (5)
B3—C1—B2	62.7 (5)	B8—B2—B3	57.7 (4)
C3—C1—B2^{i}	116.9 (4)	C1—B2—H2	127.7
C2—C1—B2^{i}	108.08 (15)	B7—B2—H2	122.2
C2^{i}—C1—B2^{i}	9.6 (6)	B6^{i}—B2—H2	122.3
B6—C1—B2^{i}	62.5 (5)	B8—B2—H2	124.8
B6^{i}—C1—B2^{i}	114.3 (4)	B3—B2—H2	126.8
B3—C1—B2^{i}	62.7 (5)	C4—C3—C8	118.79 (15)
B2—C1—B2^{i}	116.4 (8)	C4—C3—C1	122.17 (14)
F1—C2—C1	109.8 (7)	C8—C3—C1	119.04 (14)
F1—C2—B3	111.3 (8)	C5—C4—C3	120.41 (15)
C1—C2—B3	64.6 (4)	C5—C4—H4	119.8
F1—C2—B8	119.7 (7)	C3—C4—H4	119.8
C1—C2—B8	118.3 (5)	C6—C5—C4	120.36 (16)
B3—C2—B8	64.8 (4)	C6—C5—H5	119.8
F1—C2—B7	120.9 (7)	C4—C5—H5	119.8
C1—C2—B7	117.1 (6)	C7—C6—C5	119.44 (15)
B3—C2—B7	120.1 (5)	C7—C6—H6	120.3
B8—C2—B7	65.0 (4)	C5—C6—H6	120.3
F1—C2—B6^{i}	113.0 (7)	C6—C7—C8	120.74 (16)
C1—C2—B6^{i}	63.4 (4)	C6—C7—H7	119.6
B3—C2—B6^{i}	119.8 (5)	C8—C7—H7	119.6
B8—C2—B6^{i}	119.8 (6)	C7—C8—C3	120.26 (16)
B7—C2—B6^{i}	64.1 (5)	C7—C8—H8	119.9
F1—C2—H2	9.5	C3—C8—H8	119.9
C1—C2—H2	118.3	C2—B3—C2^{i}	96.0 (7)
B3—C2—H2	117.9	C2—B3—C1	56.5 (4)
B8—C2—H2	115.1	C2^{i}—B3—C1	56.5 (4)
B7—C2—H2	111.6	C2—B3—B8	57.8 (4)
B6^{i}—C2—H2	112.0	C2^{i}—B3—B8	102.3 (4)
C2—F1—H2	101.7	C1—B3—B8	105.93 (11)
C1—B2—B7	101.3 (5)	C2—B3—B8^{i}	102.3 (4)
C1—B2—B6^{i}	56.8 (4)	C2^{i}—B3—B8^{i}	57.8 (4)
B7—B2—B6^{i}	58.3 (4)	C1—B3—B8^{i}	105.93 (11)
C1—B2—B8	101.2 (4)	B8—B3—B8^{i}	60.24 (11)
B7—B2—B8	58.7 (4)	C2—B3—B2^{i}	104.26 (15)
B6^{i}—B2—B8	104.1 (5)	C2^{i}—B3—B2^{i}	9.3 (6)
C1—B2—B3	57.1 (4)	C1—B3—B2^{i}	60.2 (5)

B8—B3—B2^{i}	110.2 (4)	C2—B7—B12	101.3 (3)
B8^{i}—B3—B2^{i}	60.8 (5)	B6^{i}—B7—B12	107.88 (10)
C2—B3—B2	9.3 (6)	B11—B7—B12	60.26 (9)
C2^{i}—B3—B2	104.26 (15)	C2—B7—B8	57.1 (4)
C1—B3—B2	60.2 (5)	B6^{i}—B7—B8	107.87 (9)
B8—B3—B2	60.8 (5)	B11—B7—B8	108.06 (10)
B8^{i}—B3—B2	110.2 (4)	B12—B7—B8	59.98 (9)
B2^{i}—B3—B2	112.2 (8)	C2—B7—B2	10.1 (6)
C2—B3—H3	128.6	B6^{i}—B7—B2	61.0 (5)
C2^{i}—B3—H3	128.6	B11—B7—B2	110.1 (4)
C1—B3—H3	124.2	B12—B7—B2	110.2 (4)
B8—B3—H3	121.6	B8—B7—B2	60.9 (5)
B8^{i}—B3—H3	121.6	C2—B7—H7A	128.1
B2^{i}—B3—H3	119.3	B6^{i}—B7—H7A	121.1
B2—B3—H3	119.3	B11—B7—H7A	122.4
C2^{i}—B6—C1	56.3 (4)	B12—B7—H7A	122.9
C2^{i}—B6—B11	101.9 (3)	B8—B7—H7A	121.8
C1—B6—B11	105.81 (9)	B2—B7—H7A	117.9
C2^{i}—B6—B6^{i}	101.6 (3)	C2—B8—B3	57.4 (4)
C1—B6—B6^{i}	59.07 (5)	C2—B8—B8^{i}	101.7 (3)
B11—B6—B6^{i}	59.90 (5)	B3—B8—B8^{i}	59.88 (5)
C2^{i}—B6—B7^{i}	57.8 (4)	C2—B8—B12	101.8 (4)
C1—B6—B7^{i}	105.95 (9)	B3—B8—B12	107.79 (9)
B11—B6—B7^{i}	60.21 (8)	B8^{i}—B8—B12	60.11 (6)
B6^{i}—B6—B7^{i}	108.10 (6)	C2—B8—B7	57.9 (5)
C2^{i}—B6—B2^{i}	10.1 (6)	B3—B8—B7	107.86 (10)
C1—B6—B2^{i}	60.7 (5)	B8^{i}—B8—B7	107.93 (6)
B11—B6—B2^{i}	110.2 (4)	B12—B8—B7	59.73 (8)
B6^{i}—B6—B2^{i}	110.5 (4)	C2—B8—B2	9.7 (6)
B7^{i}—B6—B2^{i}	60.6 (5)	B3—B8—B2	61.5 (5)
C2^{i}—B6—H6A	127.6	B8^{i}—B8—B2	110.4 (4)
C1—B6—H6A	124.0	B12—B8—B2	109.6 (4)
B11—B6—H6A	122.7	B7—B8—B2	60.4 (5)
B6^{i}—B6—H6A	123.1	C2—B8—H8A	127.6
B7^{i}—B6—H6A	120.9	B3—B8—H8A	122.7
B2^{i}—B6—H6A	117.5	B8^{i}—B8—H8A	123.5
C2—B7—B6^{i}	58.1 (4)	B12—B8—H8A	122.2
C2—B7—B11	101.7 (3)	B7—B8—H8A	120.2
B6^{i}—B7—B11	59.63 (8)	B2—B8—H8A	117.9

Příloha č. 4

RTG - XXII (1-fenyl-2-brom-1,2-dikarba-kloso-dodekaboran(12))

Experimental

Crystal data

$C_8H_{15}B_{10}Br$
$M_r = 299.21$
Orthorhombic
Pbca
$a = 10.2670\ (5)$ Å
$b = 11.4420\ (6)$ Å
$c = 24.0940\ (12)$ Å
$V = 2830.4\ (2)$ Å^3
$Z = 8$
$D_x = 1.404$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 4741 reflections
$\theta = 1–27.5°$
$\mu = 2.874$ mm^{-1}
$T = 150\ (2)$ K
Prism
Colourless
$0.45 \times 0.41 \times 0.4$ mm
Crystal source: synthesized by the authors

Data collection

Nonius KappaCCD area detector diffractometer
φ and ω scans to fill the Ewald sphere
Absorption correction: none
18502 measured reflections
3192 independent reflections

2326 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.0418$
$\theta_{\rm max} = 27.57°$
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 11$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0406$
$wR(F^2) = 0.0885$
$S = 1.053$
3192 reflections
172 parameters
H-atom parameters constrained

$w=1/[\sigma^2(F_o^2) + (0.0284P)^2 + 3.5196P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.402$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.622$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Br1	0.44304 (3)	0.36190 (2)	**0.119412** (13)	0.03378 (11)
C1	0.3989 (3)	0.0974 (2)	0.12552 (10)	0.0210 (6)
C2	0.5024 (3)	0.2098 (2)	0.13805 (11)	0.0241 (6)
B3	0.4258 (3)	0.1450 (3)	0.19325 (12)	0.0265 (7)
B4	0.4190 (3)	−0.0063 (3)	0.17595 (13)	0.0274 (7)
B5	0.4879 (3)	−0.0235 (3)	0.10856 (14)	0.0278 (7)
B6	0.5364 (3)	0.1167 (3)	0.08396 (13)	0.0253 (7)
B7	0.6603 (3)	0.1706 (3)	0.12857 (14)	0.0305 (8)
B8	0.5922 (3)	0.1882 (3)	0.19638 (13)	0.0293 (7)
B9	0.5436 (3)	0.0487 (3)	0.22083 (13)	0.0304 (8)
B10	0.5821 (3)	−0.0561 (3)	0.16840 (14)	0.0311 (8)
B11	0.6538 (3)	0.0205 (3)	0.11105 (14)	0.0309 (8)
B12	0.6891 (4)	0.0639 (3)	0.18046 (14)	0.0335 (8)
C3	0.2685 (3)	0.1190 (2)	0.09944 (11)	0.0222 (6)
C4	0.1599 (3)	0.1442 (2)	0.13194 (11)	0.0278 (6)
C5	0.0382 (3)	0.1572 (3)	0.10820 (13)	0.0324 (7)
C6	0.0225 (3)	0.1460 (3)	0.05164 (13)	0.0351 (7)
C7	0.1294 (3)	0.1206 (3)	0.01885 (13)	0.0397 (8)
C8	0.2511 (3)	0.1066 (3)	0.04238 (11)	0.0340 (7)

Table 2. *Anisotropic displacement parameters* (Å²)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br1	0.04084 (19)	0.01968 (16)	0.04082 (18)	0.00184 (14)	0.00791 (14)	0.00229 (13)
C1	0.0256 (14)	0.0185 (13)	0.0189 (13)	−0.0004 (12)	0.0010 (11)	−0.0002 (10)
C2	0.0255 (14)	0.0196 (14)	0.0270 (14)	−0.0020 (12)	0.0018 (12)	−0.0012 (11)
B3	0.0296 (18)	0.0289 (17)	0.0211 (14)	−0.0045 (15)	0.0011 (12)	−0.0023 (14)
B4	0.036 (2)	0.0222 (16)	0.0241 (15)	0.0029 (15)	−0.0032 (14)	0.0043 (13)
B5	0.0302 (18)	0.0222 (17)	0.0310 (18)	0.0072 (15)	−0.0057 (14)	−0.0048 (14)
B6	0.0248 (17)	0.0268 (17)	0.0244 (15)	0.0028 (14)	0.0020 (12)	−0.0019 (13)
B7	0.0235 (17)	0.0360 (19)	0.0320 (18)	−0.0006 (15)	0.0006 (13)	−0.0062 (14)
B8	0.0282 (18)	0.0335 (18)	0.0261 (16)	−0.0027 (16)	−0.0022 (13)	−0.0046 (15)
B9	0.0338 (19)	0.0332 (19)	0.0241 (15)	0.0011 (16)	−0.0075 (14)	−0.0001 (14)
B10	0.033 (2)	0.0274 (18)	0.0329 (17)	0.0052 (15)	−0.0098 (14)	0.0005 (14)
B11	0.0280 (18)	0.0328 (19)	0.0320 (19)	0.0092 (16)	−0.0022 (14)	−0.0071 (15)
B12	0.0314 (19)	0.037 (2)	0.0322 (18)	−0.0002 (16)	−0.0087 (15)	−0.0030 (16)
C3	0.0239 (15)	0.0189 (13)	0.0239 (12)	0.0003 (12)	0.0014 (11)	0.0031 (11)
C4	0.0278 (15)	0.0270 (15)	0.0286 (15)	−0.0023 (13)	0.0033 (11)	0.0024 (12)

C5	0.0252 (16)	0.0279 (16)	0.0442 (18)	0.0018 (13)	0.0031 (13)	0.0022 (13)
C6	0.0279 (16)	0.0288 (16)	0.0485 (18)	0.0019 (14)	−0.0092 (13)	0.0044 (15)
C7	0.0352 (18)	0.052 (2)	0.0322 (16)	0.0050 (16)	−0.0098 (13)	0.0009 (15)
C8	0.0295 (15)	0.0459 (18)	0.0268 (14)	0.0062 (15)	−0.0025 (13)	−0.0021 (14)

Table 3. *Selected geometric parameters (Å, °)*

Br1—C2	1.898 (3)	B7—B12	1.772 (5)
C1—C3	1.499 (4)	B7—B8	1.788 (5)
C1—C2	1.695 (4)	B7—H7	1.1000
C1—B5	1.707 (4)	B8—B9	1.773 (5)
C1—B4	1.711 (4)	B8—B12	1.777 (5)
C1—B3	1.743 (4)	B8—H8	1.1000
C1—B6	1.745 (4)	B9—B10	1.786 (5)
C2—B7	1.697 (4)	B9—B12	1.791 (5)
C2—B8	1.699 (4)	B9—H9	1.1000
C2—B3	1.714 (4)	B10—B12	1.782 (5)
C2—B6	1.719 (4)	B10—B11	1.794 (5)
B3—B9	1.766 (5)	B10—H10	1.1000
B3—B8	1.780 (5)	B11—B12	1.782 (5)
B3—B4	1.782 (5)	B11—H11	1.1000
B3—H3	1.1000	B12—H12	1.1000
B4—B10	1.778 (5)	C3—C4	1.392 (4)
B4—B5	1.782 (5)	C3—C8	1.394 (4)
B4—B9	1.789 (5)	C4—C5	1.382 (4)
B4—H4	1.1000	C4—H4A	0.9300
B5—B10	1.776 (5)	C5—C6	1.379 (4)
B5—B11	1.777 (5)	C5—H5A	0.9300
B5—B6	1.781 (5)	C6—C7	1.384 (5)
B5—H5	1.1000	C6—H6A	0.9300
B6—B11	1.758 (5)	C7—C8	1.382 (4)
B6—B7	1.776 (5)	C7—H7A	0.9300
B6—H6	1.1000	C8—H8A	0.9300
B7—B11	1.770 (5)		
C3—C1—C2	120.6 (2)	C2—C1—B3	59.78 (16)
C3—C1—B5	120.7 (2)	B5—C1—B3	113.1 (2)
C2—C1—B5	108.8 (2)	B4—C1—B3	62.12 (18)
C3—C1—B4	121.3 (2)	C3—C1—B6	117.5 (2)
C2—C1—B4	108.9 (2)	C2—C1—B6	59.95 (17)
B5—C1—B4	62.84 (18)	B5—C1—B6	62.11 (18)
C3—C1—B3	118.8 (2)	B4—C1—B6	113.4 (2)

B3—C1—B6	111.7 (2)	B5—B4—B9	107.8 (2)
C1—C2—B7	112.0 (2)	B3—B4—B9	59.29 (18)
C1—C2—B8	112.2 (2)	C1—B4—H4	123.8
B7—C2—B8	63.55 (19)	B10—B4—H4	122.5
C1—C2—B3	61.48 (16)	B5—B4—H4	121.8
B7—C2—B3	115.4 (2)	B3—B4—H4	121.7
B8—C2—B3	62.89 (18)	B9—B4—H4	122.3
C1—C2—B6	61.45 (16)	C1—B5—B10	105.5 (2)
B7—C2—B6	62.63 (18)	C1—B5—B11	106.0 (2)
B8—C2—B6	115.3 (2)	B10—B5—B11	60.64 (19)
B3—C2—B6	114.4 (2)	C1—B5—B6	59.97 (17)
C1—C2—Br1	116.89 (19)	B10—B5—B6	107.9 (2)
B7—C2—Br1	121.1 (2)	B11—B5—B6	59.21 (19)
B8—C2—Br1	120.23 (19)	C1—B5—B4	58.67 (17)
B3—C2—Br1	115.64 (19)	B10—B5—B4	59.97 (18)
B6—C2—Br1	117.00 (18)	B11—B5—B4	108.5 (2)
C2—B3—C1	58.73 (16)	B6—B5—B4	108.3 (2)
C2—B3—B9	104.3 (2)	C1—B5—H5	123.7
C1—B3—B9	105.4 (2)	B10—B5—H5	122.2
C2—B3—B8	58.15 (17)	B11—B5—H5	122.0
C1—B3—B8	106.2 (2)	B6—B5—H5	121.5
B9—B3—B8	59.99 (19)	B4—B5—H5	121.4
C2—B3—B4	104.8 (2)	C2—B6—C1	58.60 (16)
C1—B3—B4	58.06 (16)	C2—B6—B11	104.2 (2)
B9—B3—B4	60.55 (19)	C1—B6—B11	105.2 (2)
B8—B3—B4	108.5 (2)	C2—B6—B7	58.09 (18)
C2—B3—H3	124.5	C1—B6—B7	106.0 (2)
C1—B3—H3	123.6	B11—B6—B7	60.11 (19)
B9—B3—H3	122.9	C2—B6—B5	104.4 (2)
B8—B3—H3	121.8	C1—B6—B5	57.91 (17)
B4—B3—H3	122.1	B11—B6—B5	60.28 (19)
C1—B4—B10	105.3 (2)	B7—B6—B5	108.2 (2)
C1—B4—B5	58.48 (17)	C2—B6—H6	124.7
B10—B4—B5	59.86 (19)	C1—B6—H6	123.7
C1—B4—B3	59.82 (17)	B11—B6—H6	123.0
B10—B4—B3	107.4 (2)	B7—B6—H6	121.8
B5—B4—B3	107.8 (2)	B5—B6—H6	122.5
C1—B4—B9	105.8 (2)	C2—B7—B11	104.6 (2)
B10—B4—B9	60.08 (19)	C2—B7—B12	104.3 (2)

B11—B7—B12	60.4 (2)	B8—B9—H9	121.4
C2—B7—B6	59.29 (18)	B10—B9—H9	122.1
B11—B7—B6	59.44 (18)	B4—B9—H9	121.7
B12—B7—B6	107.9 (2)	B12—B9—H9	122.1
C2—B7—B8	58.27 (18)	B5—B10—B4	60.18 (18)
B11—B7—B8	108.2 (2)	B5—B10—B12	107.9 (2)
B12—B7—B8	59.88 (19)	B4—B10—B12	108.5 (2)
B6—B7—B8	108.2 (2)	B5—B10—B9	108.2 (2)
C2—B7—H7	124.9	B4—B10—B9	60.26 (19)
B11—B7—H7	122.3	B12—B10—B9	60.27 (19)
B12—B7—H7	122.4	B5—B10—B11	59.71 (19)
B6—B7—H7	121.4	B4—B10—B11	108.0 (2)
B8—B7—H7	121.5	B12—B10—B11	59.79 (19)
C2—B8—B9	104.7 (2)	B9—B10—B11	107.9 (2)
C2—B8—B12	104.0 (2)	B5—B10—H10	121.8
B9—B8—B12	60.6 (2)	B4—B10—H10	121.4
C2—B8—B3	58.96 (17)	B12—B10—H10	121.6
B9—B8—B3	59.62 (19)	B9—B10—H10	121.5
B12—B8—B3	107.8 (2)	B11—B10—H10	122.0
C2—B8—B7	58.18 (18)	B6—B11—B7	60.45 (19)
B9—B8—B7	108.2 (2)	B6—B11—B5	60.51 (18)
B12—B8—B7	59.60 (19)	B7—B11—B5	108.6 (2)
B3—B8—B7	107.8 (2)	B6—B11—B12	108.3 (2)
C2—B8—H8	125.1	B7—B11—B12	59.86 (19)
B9—B8—H8	122.1	B5—B11—B12	107.8 (2)
B12—B8—H8	122.5	B6—B11—B10	108.1 (2)
B3—B8—H8	121.6	B7—B11—B10	107.8 (2)
B7—B8—H8	121.7	B5—B11—B10	59.66 (19)
B3—B9—B8	60.40 (18)	B12—B11—B10	59.78 (19)
B3—B9—B10	107.7 (2)	B6—B11—H11	121.3
B8—B9—B10	107.9 (2)	B7—B11—H11	121.5
B3—B9—B4	60.16 (18)	B5—B11—H11	121.5
B8—B9—B4	108.5 (2)	B12—B11—H11	121.9
B10—B9—B4	59.66 (18)	B10—B11—H11	122.1
B3—B9—B12	107.8 (2)	B7—B12—B8	60.51 (19)
B8—B9—B12	59.82 (19)	B7—B12—B10	108.2 (2)
B10—B9—B12	59.75 (19)	B8—B12—B10	107.9 (3)
B4—B9—B12	107.6 (2)	B7—B12—B11	59.73 (19)
B3—B9—H9	121.6	B8—B12—B11	108.2 (2)

B10—B12—B11	60.4 (2)	C5—C4—H4A	119.6
B7—B12—B9	108.1 (2)	C3—C4—H4A	119.6
B8—B12—B9	59.6 (2)	C6—C5—C4	120.3 (3)
B10—B12—B9	60.0 (2)	C6—C5—H5A	119.8
B11—B12—B9	108.2 (2)	C4—C5—H5A	119.8
B7—B12—H12	121.6	C5—C6—C7	119.4 (3)
B8—B12—H12	121.7	C5—C6—H6A	120.3
B10—B12—H12	121.6	C7—C6—H6A	120.3
B11—B12—H12	121.6	C8—C7—C6	120.5 (3)
B9—B12—H12	121.8	C8—C7—H7A	119.7
C4—C3—C8	118.2 (3)	C6—C7—H7A	119.7
C4—C3—C1	120.9 (2)	C7—C8—C3	120.6 (3)
C8—C3—C1	120.7 (2)	C7—C8—H8A	119.7
C5—C4—C3	120.9 (3)	C3—C8—H8A	119.7
C3—C1—C2—B7	−144.4 (2)	B6—C2—B3—C1	−32.4 (2)
B5—C1—C2—B7	1.5 (3)	Br1—C2—B3—C1	108.1 (2)
B4—C1—C2—B7	68.3 (3)	C1—C2—B3—B9	99.5 (2)
B3—C1—C2—B7	107.9 (2)	B7—C2—B3—B9	−2.8 (3)
B6—C1—C2—B7	−38.4 (2)	B8—C2—B3—B9	−40.0 (2)
C3—C1—C2—B8	146.3 (2)	B6—C2—B3—B9	67.1 (3)
B5—C1—C2—B8	−67.8 (3)	Br1—C2—B3—B9	−152.40 (19)
B4—C1—C2—B8	−0.9 (3)	C1—C2—B3—B8	139.5 (2)
B3—C1—C2—B8	38.6 (2)	B7—C2—B3—B8	37.2 (2)
B6—C1—C2—B8	−107.6 (2)	B6—C2—B3—B8	107.1 (3)
C3—C1—C2—B3	107.7 (3)	Br1—C2—B3—B8	−112.4 (2)
B5—C1—C2—B3	−106.4 (2)	C1—C2—B3—B4	36.7 (2)
B4—C1—C2—B3	−39.5 (2)	B7—C2—B3—B4	−65.6 (3)
B6—C1—C2—B3	−146.3 (2)	B8—C2—B3—B4	−102.8 (2)
C3—C1—C2—B6	−106.1 (2)	B6—C2—B3—B4	4.3 (3)
B5—C1—C2—B6	39.9 (2)	Br1—C2—B3—B4	144.81 (19)
B4—C1—C2—B6	106.7 (2)	C3—C1—B3—C2	−110.6 (3)
B3—C1—C2—B6	146.3 (2)	B5—C1—B3—C2	99.0 (2)
C3—C1—C2—Br1	1.6 (3)	B4—C1—B3—C2	137.0 (2)
B5—C1—C2—Br1	147.55 (19)	B6—C1—B3—C2	31.2 (2)
B4—C1—C2—Br1	−145.61 (19)	C3—C1—B3—B9	151.7 (2)
B3—C1—C2—Br1	−106.1 (2)	C2—C1—B3—B9	−97.6 (2)
B6—C1—C2—Br1	107.7 (2)	B5—C1—B3—B9	1.4 (3)
B7—C2—B3—C1	−102.3 (2)	B4—C1—B3—B9	39.4 (2)
B8—C2—B3—C1	−139.5 (2)	B6—C1—B3—B9	−66.5 (3)

Příloha č. 5

RTG - XXIII (1-fenyl-2-jod-1,2-dikarba-kloso-dodekaboran(12))

Experimental

Crystal data

$C_8H_{15}B_{10}I$
$M_r = 346.20$
Monoclinic
$P2_1$
$a = 12.0590\ (4)$ Å
$b = 7.1940\ (2)$ Å
$c = 16.9420\ (6)$ Å
$\beta = 90.5190\ (16)°$
$V = 1469.70\ (8)$ Å^3
$Z = 4$
$D_x = 1.565$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 19985 reflections
$\theta = 1–27.5°$
$\mu = 2.149$ mm^{-1}
$T = 150\ (2)$ K
Plate
Colourless
0.15 × 0.12 × 0.075 mm
Crystal source: synthesized by the authors

Data collection

Nonius KappaCCD area detector diffractometer
φ and ω scans to fill the Ewald sphere
Absorption correction:
multiscans (SORTAV; Blessing 1997)
$T_{min} = 0.716$, $T_{max} = 0.852$
19130 measured reflections
6751 independent reflections

6047 reflections with
>2sigma(I)
$R_{int} = 0.0490$
$\theta_{max} = 27.61°$
$h = -15 \rightarrow 15$
$k = -9 \rightarrow 9$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0383$
$wR(F^2) = 0.0854$
$S = 1.059$
6751 reflections
345 parameters
H-atom parameters constrained
$w=1/[\sigma^2(F_o^2) + (0.0183P)^2 + 4.2171P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.084$ e Å^{-3}
$\Delta\rho_{min} = -0.867$ e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.0053 (3)
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute structure: Flack H D (1983), *Acta Cryst.* A39, 876-881
Flack parameter = −0.03 (3)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
I1	0.72200 (3)	0.52716 (7)	**0.475273** (19)	0.03114 (10)
C11	0.6983 (5)	0.9306 (7)	0.3898 (3)	0.0239 (12)
C12	0.6687 (5)	0.7008 (8)	0.3823 (3)	0.0238 (12)
B13	0.5638 (6)	0.8517 (10)	0.4016 (5)	0.0304 (15)
B14	0.5931 (6)	1.0537 (14)	0.3466 (4)	0.0335 (19)
B15	0.7219 (5)	1.0215 (18)	0.2970 (3)	0.0316 (12)
B16	0.7702 (7)	0.7923 (9)	0.3242 (4)	0.0291 (15)
B17	0.5455 (6)	0.6630 (10)	0.3357 (4)	0.0309 (15)
B18	0.4964 (7)	0.8883 (10)	0.3101 (5)	0.0358 (17)
B19	0.5937 (7)	0.9911 (11)	0.2447 (4)	0.039 (2)
B110	0.7048 (8)	0.8278 (10)	0.2303 (5)	0.0366 (18)
B111	0.6738 (6)	0.6243 (10)	0.2880 (4)	0.0307 (16)
B112	0.5657 (8)	0.7467 (10)	0.2386 (5)	0.0381 (19)
C13	0.7614 (5)	1.0050 (13)	0.4595 (3)	0.0252 (14)
C14	0.7085 (5)	1.0431 (17)	0.5294 (3)	0.0331 (15)
C15	0.7674 (7)	1.1268 (9)	0.5917 (4)	0.0382 (16)
C16	0.8775 (7)	1.1659 (10)	0.5840 (4)	0.0430 (18)
C17	0.9310 (6)	1.1266 (9)	0.5154 (4)	0.0391 (16)
C18	0.8734 (5)	1.0473 (13)	0.4522 (4)	0.0311 (14)
I2	0.24830 (3)	0.52491 (7)	0.04530 (2)	0.03855 (12)
C21	0.1873 (5)	0.1176 (8)	0.1163 (3)	0.0246 (12)
C22	0.1636 (5)	0.3489 (7)	0.1236 (4)	0.0251 (12)
B23	0.0620 (6)	0.2105 (9)	0.0830 (4)	0.0254 (14)
B24	0.0672 (5)	0.0015 (13)	0.1380 (4)	0.0290 (17)
B25	0.1782 (5)	0.0196 (17)	0.2071 (3)	0.0261 (12)
B26	0.2419 (6)	0.2401 (9)	0.1954 (4)	0.0285 (15)
B27	0.0314 (6)	0.3948 (10)	0.1500 (4)	0.0298 (15)
B28	−0.0323 (6)	0.1755 (10)	0.1608 (4)	0.0303 (15)
B29	0.0395 (6)	0.0565 (12)	0.2380 (4)	0.034 (2)
B210	0.1481 (7)	0.2029 (11)	0.2738 (4)	0.0342 (17)
B211	0.1416 (7)	0.4156 (10)	0.2184 (4)	0.0316 (16)
B212	0.0160 (7)	0.2998 (10)	0.2450 (4)	0.0304 (15)
C23	0.2689 (5)	0.0443 (14)	0.0569 (3)	0.0239 (13)
C24	0.2373 (5)	0.0117 (16)	−0.0214 (3)	0.0283 (13)
C25	0.3126 (7)	−0.0646 (9)	−0.0737 (4)	0.0389 (17)
C26	0.4165 (6)	−0.1140 (9)	−0.0485 (4)	0.0351 (16)

C27	0.4472 (6)	−0.0869 (9)	0.0295 (4)	0.0353 (15)
C28	0.3739 (5)	−0.0099 (7)	0.0821 (4)	0.0289 (15)

Table 2. *Anisotropic displacement parameters* (Å^2)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I1	0.03581 (19)	0.02275 (16)	0.03482 (18)	−0.0008 (4)	−0.00165 (15)	0.0066 (3)
C11	0.029 (3)	0.016 (3)	0.027 (3)	−0.002 (2)	0.004 (3)	0.004 (2)
C12	0.030 (3)	0.019 (3)	0.022 (3)	0.000 (2)	0.000 (2)	0.002 (2)
B13	0.027 (4)	0.024 (3)	0.040 (4)	0.000 (3)	−0.003 (3)	−0.001 (3)
B14	0.025 (3)	0.033 (5)	0.042 (4)	0.000 (3)	−0.004 (3)	0.006 (4)
B15	0.042 (3)	0.027 (3)	0.025 (3)	0.000 (7)	0.002 (2)	0.007 (5)
B16	0.033 (4)	0.023 (3)	0.032 (4)	−0.002 (3)	0.008 (3)	0.000 (3)
B17	0.032 (4)	0.026 (3)	0.034 (4)	−0.005 (3)	−0.003 (3)	0.001 (3)
B18	0.037 (4)	0.029 (4)	0.041 (4)	−0.006 (3)	−0.012 (4)	0.004 (3)
B19	0.048 (4)	0.035 (6)	0.035 (4)	−0.002 (3)	−0.013 (3)	0.008 (3)
B110	0.047 (5)	0.032 (4)	0.031 (4)	−0.010 (3)	−0.003 (3)	0.006 (3)
B111	0.036 (4)	0.029 (4)	0.028 (4)	−0.015 (3)	0.005 (3)	−0.006 (3)
B112	0.051 (5)	0.029 (4)	0.034 (4)	−0.008 (3)	−0.007 (4)	0.003 (3)
C13	0.033 (3)	0.014 (4)	0.029 (2)	0.002 (3)	−0.008 (2)	0.001 (3)
C14	0.035 (3)	0.034 (4)	0.030 (3)	0.001 (4)	0.001 (2)	0.003 (4)
C15	0.051 (5)	0.036 (4)	0.027 (3)	0.002 (3)	−0.007 (3)	−0.006 (3)
C16	0.050 (5)	0.035 (4)	0.044 (4)	0.002 (3)	−0.022 (4)	−0.002 (3)
C17	0.031 (4)	0.036 (4)	0.051 (4)	−0.004 (3)	−0.010 (3)	−0.006 (3)
C18	0.027 (3)	0.030 (4)	0.036 (3)	−0.001 (3)	−0.002 (2)	−0.001 (3)
I2	0.0459 (2)	0.02175 (17)	0.0482 (2)	−0.0007 (4)	0.01676 (19)	0.0079 (4)
C21	0.028 (3)	0.018 (3)	0.028 (3)	0.001 (2)	−0.004 (2)	0.000 (2)
C22	0.030 (3)	0.014 (2)	0.032 (3)	−0.004 (2)	0.005 (3)	0.005 (2)
B23	0.028 (4)	0.023 (3)	0.025 (3)	0.002 (3)	−0.001 (3)	−0.004 (3)
B24	0.025 (3)	0.029 (5)	0.033 (3)	−0.004 (3)	0.001 (2)	0.008 (3)
B25	0.029 (3)	0.025 (3)	0.024 (3)	−0.001 (5)	−0.003 (2)	0.010 (5)
B26	0.029 (4)	0.027 (3)	0.029 (4)	−0.005 (3)	−0.008 (3)	−0.004 (3)
B27	0.033 (4)	0.025 (3)	0.032 (4)	−0.002 (3)	0.003 (3)	0.001 (3)
B28	0.024 (4)	0.032 (4)	0.035 (4)	−0.001 (3)	0.007 (3)	0.002 (3)
B29	0.037 (4)	0.030 (6)	0.034 (3)	−0.002 (3)	0.004 (3)	0.006 (3)
B210	0.043 (5)	0.037 (4)	0.023 (4)	0.001 (3)	0.005 (3)	−0.004 (3)
B211	0.036 (4)	0.031 (4)	0.028 (4)	−0.001 (3)	0.000 (3)	−0.005 (3)
B212	0.033 (4)	0.031 (4)	0.027 (3)	0.000 (3)	0.008 (3)	−0.001 (3)
C23	0.030 (2)	0.014 (3)	0.028 (2)	0.002 (3)	−0.002 (2)	0.000 (3)
C24	0.033 (3)	0.026 (3)	0.026 (2)	0.003 (4)	0.002 (2)	0.000 (4)
C25	0.058 (5)	0.031 (3)	0.028 (3)	−0.003 (3)	0.007 (3)	−0.002 (3)
C26	0.038 (4)	0.025 (3)	0.043 (4)	−0.001 (3)	0.018 (3)	0.000 (3)

C27	0.028 (3)	0.029 (3)	0.050 (4)	0.000 (2)	0.004 (3)	0.003 (3)
C28	0.031 (3)	0.021 (4)	0.034 (3)	−0.004 (2)	0.002 (2)	−0.002 (2)

Table 3. *Selected geometric parameters (Å, °)*

I1—C12	2.107 (6)	B110—B112	1.782 (12)
C11—C13	1.497 (9)	B110—B111	1.801 (10)
C11—C12	1.696 (8)	B110—H110	1.1000
C11—B14	1.707 (10)	B111—B112	1.775 (12)
C11—B15	1.729 (8)	B111—H111	1.1000
C11—B16	1.730 (9)	B112—H112	1.1000
C11—B13	1.732 (9)	C13—C14	1.379 (8)
C12—B111	1.692 (9)	C13—C18	1.392 (8)
C12—B17	1.698 (10)	C14—C15	1.402 (10)
C12—B13	1.700 (9)	C14—H14A	0.9300
C12—B16	1.709 (9)	C15—C16	1.364 (11)
B13—B18	1.763 (11)	C15—H15A	0.9300
B13—B14	1.763 (11)	C16—C17	1.364 (10)
B13—B17	1.770 (10)	C16—H16A	0.9300
B13—H13	1.1000	C17—C18	1.392 (9)
B14—B18	1.773 (11)	C17—H17A	0.9300
B14—B19	1.785 (11)	C18—H18A	0.9300
B14—B15	1.789 (9)	I2—C22	2.105 (5)
B14—H14	1.1000	C21—C23	1.509 (8)
B15—B19	1.789 (10)	C21—C22	1.692 (8)
B15—B110	1.806 (13)	C21—B25	1.696 (9)
B15—B16	1.807 (14)	C21—B24	1.714 (9)
B15—H15	1.1000	C21—B26	1.728 (9)
B16—B111	1.781 (10)	C21—B23	1.741 (9)
B16—B110	1.788 (11)	C22—B27	1.692 (10)
B16—H16	1.1000	C22—B211	1.699 (9)
B17—B112	1.771 (11)	C22—B23	1.717 (9)
B17—B111	1.775 (11)	C22—B26	1.720 (9)
B17—B18	1.778 (11)	B23—B28	1.766 (10)
B17—H17	1.1000	B23—B24	1.769 (11)
B18—B19	1.782 (11)	B23—B27	1.786 (10)
B18—B112	1.795 (12)	B23—H23	1.1000
B18—H18	1.1000	B24—B29	1.775 (10)
B19—B112	1.793 (11)	B24—B25	1.775 (9)
B19—B110	1.800 (12)	B24—B28	1.779 (11)
B19—H19	1.1000	B24—H24	1.1000

B25—B26	1.774 (13)	B210—B211	1.796 (11)
B25—B210	1.776 (13)	B210—B212	1.802 (12)
B25—B29	1.778 (10)	B210—H210	1.1000
B25—H25	1.1000	B211—B212	1.790 (11)
B26—B210	1.773 (10)	B211—H211	1.1000
B26—B211	1.794 (10)	B212—H212	1.1000
B26—H26	1.1000	C23—C28	1.389 (9)
B27—B212	1.761 (10)	C23—C24	1.397 (8)
B27—B211	1.761 (11)	C24—C25	1.388 (9)
B27—B28	1.766 (10)	C24—H24A	0.9300
B27—H27	1.1000	C25—C26	1.367 (11)
B28—B212	1.778 (11)	C25—H25A	0.9300
B28—B29	1.781 (11)	C26—C27	1.383 (10)
B28—H28	1.1000	C26—H26A	0.9300
B29—B212	1.777 (12)	C27—C28	1.377 (9)
B29—B210	1.782 (11)	C27—H27A	0.9300
B29—H29	1.1000	C28—H28A	0.9300
C13—C11—C12	120.9 (5)	C11—C12—B16	61.1 (4)
C13—C11—B14	121.5 (6)	B17—C12—B16	115.0 (5)
C12—C11—B14	108.5 (5)	B13—C12—B16	113.8 (5)
C13—C11—B15	119.7 (5)	B111—C12—I1	120.0 (4)
C12—C11—B15	109.7 (5)	C11—C12—I1	117.3 (4)
B14—C11—B15	62.7 (4)	B17—C12—I1	120.8 (4)
C13—C11—B16	117.3 (5)	B13—C12—I1	117.2 (4)
C12—C11—B16	59.8 (4)	B16—C12—I1	116.3 (4)
B14—C11—B16	113.4 (5)	C12—B13—C11	59.2 (4)
B15—C11—B16	63.0 (5)	C12—B13—B18	105.3 (5)
C13—C11—B13	119.7 (5)	C11—B13—B18	105.9 (5)
C12—C11—B13	59.5 (4)	C12—B13—B14	105.8 (5)
B14—C11—B13	61.7 (4)	C11—B13—B14	58.5 (4)
B15—C11—B13	113.0 (5)	B18—B13—B14	60.4 (4)
B16—C11—B13	111.1 (5)	C12—B13—B17	58.5 (4)
B111—C12—C11	112.2 (4)	C11—B13—B17	106.9 (5)
B111—C12—B17	63.2 (4)	B18—B13—B17	60.4 (4)
C11—C12—B17	112.0 (5)	B14—B13—B17	108.9 (5)
B111—C12—B13	115.0 (5)	C12—B13—H13	123.8
C11—C12—B13	61.3 (4)	C11—B13—H13	123.1
B17—C12—B13	62.8 (4)	B18—B13—H13	122.6
B111—C12—B16	63.2 (4)	B14—B13—H13	121.9

B17—B13—H13	121.4	B111—B16—B15	108.9 (6)
C11—B14—B13	59.9 (4)	B110—B16—B15	60.3 (4)
C11—B14—B18	106.6 (6)	C12—B16—H16	124.3
B13—B14—B18	59.8 (5)	C11—B16—H16	123.3
C11—B14—B19	105.9 (5)	B111—B16—H16	121.6
B13—B14—B19	107.8 (6)	B110—B16—H16	122.7
B18—B14—B19	60.1 (5)	B15—B16—H16	121.9
C11—B14—B15	59.2 (4)	C12—B17—B13	58.7 (4)
B13—B14—B15	108.7 (7)	C12—B17—B112	104.4 (5)
B18—B14—B15	108.7 (6)	B13—B17—B112	107.9 (5)
B19—B14—B15	60.1 (4)	C12—B17—B111	58.3 (4)
C11—B14—H14	123.3	B13—B17—B111	107.6 (5)
B13—B14—H14	121.4	B112—B17—B111	60.1 (5)
B18—B14—H14	121.8	C12—B17—B18	104.8 (5)
B19—B14—H14	122.4	B13—B17—B18	59.6 (4)
B15—B14—H14	121.1	B112—B17—B18	60.8 (5)
C11—B15—B14	58.0 (4)	B111—B17—B18	108.7 (5)
C11—B15—B19	104.8 (5)	C12—B17—H17	125.1
B14—B15—B19	59.9 (4)	B13—B17—H17	121.8
C11—B15—B110	105.0 (7)	B112—B17—H17	122.2
B14—B15—B110	107.4 (6)	B111—B17—H17	121.4
B19—B15—B110	60.1 (5)	B18—B17—H17	121.9
C11—B15—B16	58.6 (4)	B13—B18—B14	59.8 (4)
B14—B15—B16	106.1 (6)	B13—B18—B17	60.0 (4)
B19—B15—B16	106.8 (7)	B14—B18—B17	108.1 (6)
B110—B15—B16	59.3 (5)	B13—B18—B19	107.9 (6)
C11—B15—H15	124.5	B14—B18—B19	60.3 (4)
B14—B15—H15	122.4	B17—B18—B19	108.1 (6)
B19—B15—H15	122.4	B13—B18—B112	107.1 (6)
B110—B15—H15	122.3	B14—B18—B112	107.9 (6)
B16—B15—H15	122.7	B17—B18—B112	59.4 (4)
C12—B16—C11	59.1 (3)	B19—B18—B112	60.2 (4)
C12—B16—B111	57.9 (4)	B13—B18—H18	122.1
C11—B16—B111	106.4 (5)	B14—B18—H18	121.6
C12—B16—B110	104.8 (5)	B17—B18—H18	121.8
C11—B16—B110	105.7 (6)	B19—B18—H18	121.4
B111—B16—B110	60.6 (4)	B112—B18—H18	122.2
C12—B16—B15	105.5 (5)	B18—B19—B14	59.6 (4)
C11—B16—B15	58.5 (3)	B18—B19—B15	108.3 (5)

Příloha č. 6

RTG - XXXII (1-fenyl-2-trimethylsilyl-1,2-dikarba-kloso-dodekaboran(12))

Experimental

Crystal data

$C_{11}H_{24}B_{10}Si$
$M_r = 292.49$
Monoclinic
$P2_1/m$
$a = 8.8810\ (3)$ Å
$b = 11.1650\ (5)$ Å
$c = 9.0490\ (4)$ Å
$\beta = 102.8400\ (16)°$
$V = 874.83\ (6)$ Å^3
$Z = 2$
$D_x = 1.110$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 2030 reflections
$\theta = 1–27.5°$
$\mu = 0.118$ mm^{-1}
$T = 150\ (2)$ K
Prism
Colourless
0.3 × 0.21 × 0.2 mm
Crystal source: synthesized by the authors

Data collection

Nonius KappaCCD area detector diffractometer
φ and ω scans to fill the Ewald sphere
Absorption correction: none
8693 measured reflections
2110 independent reflections

1524 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.0511$
$\theta_{\rm max} = 27.46°$
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0482$
$wR(F^2) = 0.1363$
$S = 1.051$
2110 reflections
113 parameters
H-atom parameters constrained

$w=1/[\sigma^2(F_o^2) + (0.0731P)^2 + 0.0781P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.000$
$\Delta\rho_{\rm max} = 0.290$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.328$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
C1	0.3551 (2)	3/4	0.0836 (3)	0.0202 (5)
C2	0.1599 (2)	3/4	0.0633 (3)	0.0196 (5)
B3	0.2516 (2)	0.62200 (19)	0.0218 (2)	0.0226 (4)
B4	0.4057 (2)	0.67048 (19)	−0.0606 (2)	0.0247 (5)
B8	0.0760 (2)	0.6710 (2)	−0.0956 (2)	0.0253 (5)
B9	0.2286 (2)	0.6206 (2)	−0.1780 (2)	0.0299 (5)
B10	0.3226 (3)	3/4	−0.2297 (3)	0.0308 (7)
B12	0.1194 (3)	3/4	−0.2509 (3)	0.0327 (8)
C3	0.4605 (2)	3/4	0.2393 (3)	0.0214 (5)
C4	0.51395 (18)	0.64291 (19)	0.3100 (2)	0.0316 (5)
C5	0.6149 (2)	0.6434 (2)	0.4515 (2)	0.0430 (6)
C6	0.6645 (3)	3/4	0.5221 (3)	0.0458 (9)
Si1	0.06162 (7)	3/4	0.23453 (7)	0.0216 (2)
C9	0.11846 (19)	0.61352 (18)	0.35038 (19)	0.0292 (4)
C10	−0.1492 (3)	3/4	0.1526 (3)	0.0339 (7)

Table 2. *Anisotropic displacement parameters* (A²)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.0146 (10)	0.0190 (13)	0.0280 (13)	0.000	0.0072 (9)	0.000
C2	0.0145 (10)	0.0211 (14)	0.0231 (12)	0.000	0.0037 (9)	0.000
B3	0.0197 (8)	0.0195 (11)	0.0298 (11)	−0.0019 (8)	0.0080 (7)	−0.0034 (9)
B4	0.0222 (9)	0.0259 (12)	0.0287 (11)	0.0003 (8)	0.0112 (7)	−0.0036 (9)
B8	0.0201 (9)	0.0313 (13)	0.0247 (10)	−0.0032 (9)	0.0058 (7)	−0.0036 (9)
B9	0.0247 (10)	0.0374 (14)	0.0287 (11)	−0.0035 (9)	0.0085 (8)	−0.0100 (10)
B10	0.0246 (14)	0.044 (2)	0.0266 (15)	0.000	0.0115 (11)	0.000
B12	0.0247 (14)	0.048 (2)	0.0263 (16)	0.000	0.0069 (11)	0.000
C3	0.0145 (10)	0.0262 (15)	0.0241 (12)	0.000	0.0056 (9)	0.000
C4	0.0217 (8)	0.0335 (12)	0.0382 (11)	0.0017 (8)	0.0034 (7)	0.0050 (9)
C5	0.0263 (9)	0.0598 (16)	0.0409 (12)	0.0072 (10)	0.0030 (8)	0.0188 (12)
C6	0.0220 (13)	0.081 (3)	0.0314 (16)	0.000	−0.0001 (11)	0.000
Si1	0.0190 (3)	0.0246 (4)	0.0217 (4)	0.000	0.0058 (2)	0.000
C9	0.0329 (9)	0.0301 (12)	0.0257 (9)	−0.0015 (8)	0.0090 (7)	−0.0004 (8)
C10	0.0199 (12)	0.052 (2)	0.0312 (14)	0.000	0.0093 (10)	0.000

Table 3. *Selected geometric parameters (Å, °)*

C1—C3	1.509 (3)	B9—H9	1.1000
C1—C2	1.702 (3)	B10—B12	1.772 (4)
C1—B4	1.719 (3)	B10—B4^{i}	1.781 (3)
C1—B4^{i}	1.719 (3)	B10—B9^{i}	1.782 (3)
C1—B3	1.724 (2)	B10—H10	1.1000
C1—B3^{i}	1.724 (2)	B12—B8^{i}	1.773 (3)
C2—B8	1.710 (3)	B12—B9^{i}	1.783 (3)
C2—B8^{i}	1.710 (3)	B12—H12	1.1000
C2—B3	1.727 (2)	C3—C4^{i}	1.389 (2)
C2—B3^{i}	1.727 (2)	C3—C4	1.389 (2)
C2—Si1	1.940 (2)	C4—C5	1.390 (3)
B3—B8	1.767 (2)	C4—H4A	0.9300
B3—B9	1.775 (3)	C5—C6	1.377 (3)
B3—B4	1.782 (2)	C5—H5	0.9300
B3—H3	1.1000	C6—C5^{i}	1.377 (3)
B4—B4^{i}	1.776 (4)	C6—H6	0.9300
B4—B9	1.780 (3)	Si1—C10	1.854 (2)
B4—B10	1.781 (3)	Si1—C9	1.8548 (19)
B4—H4	1.1000	Si1—C9^{i}	1.8549 (19)
B8—B8^{i}	1.765 (4)	C9—H9A	0.9600
B8—B12	1.773 (3)	C9—H9B	0.9600
B8—B9	1.777 (2)	C9—H9C	0.9600
B8—H8	1.1000	C10—H10A	0.9600
B9—B10	1.782 (3)	C10—H10C	0.9600
B9—B12	1.783 (3)		
C3—C1—C2	120.45 (17)	B4^{i}—C1—B3^{i}	62.36 (10)
C3—C1—B4	119.75 (14)	B3—C1—B3^{i}	112.02 (17)
C2—C1—B4	110.49 (14)	C1—C2—B8	109.50 (14)
C3—C1—B4^{i}	119.75 (14)	C1—C2—B8^{i}	109.50 (14)
C2—C1—B4^{i}	110.48 (14)	B8—C2—B8^{i}	62.11 (16)
B4—C1—B4^{i}	62.21 (16)	C1—C2—B3	60.36 (9)
C3—C1—B3	118.58 (11)	B8—C2—B3	61.88 (10)
C2—C1—B3	60.54 (9)	B8^{i}—C2—B3	112.49 (15)
B4—C1—B3	62.36 (10)	C1—C2—B3^{i}	60.36 (9)
B4^{i}—C1—B3	113.12 (15)	B8—C2—B3^{i}	112.49 (15)
C3—C1—B3^{i}	118.58 (11)	B8^{i}—C2—B3^{i}	61.88 (10)
C2—C1—B3^{i}	60.54 (9)	B3—C2—B3^{i}	111.71 (17)
B4—C1—B3^{i}	113.12 (15)	C1—C2—Si1	122.82 (15)

B8—C2—Si1	118.83 (11)	B3—B8—B12	108.23 (14)
B8^{i}—C2—Si1	118.83 (11)	C2—B8—B9	106.60 (13)
B3—C2—Si1	119.41 (10)	B8^{i}—B8—B9	108.44 (10)
B3^{i}—C2—Si1	119.41 (10)	B3—B8—B9	60.09 (11)
C1—B3—C2	59.10 (11)	B12—B8—B9	60.29 (12)
C1—B3—B8	105.90 (14)	C2—B8—H8	123.4
C2—B3—B8	58.60 (11)	B8^{i}—B8—H8	121.6
C1—B3—B9	105.66 (15)	B3—B8—H8	121.5
C2—B3—B9	105.99 (15)	B12—B8—H8	121.9
B8—B3—B9	60.23 (10)	B9—B8—H8	121.7
C1—B3—B4	58.68 (11)	B3—B9—B8	59.68 (10)
C2—B3—B4	106.41 (14)	B3—B9—B4	60.17 (10)
B8—B3—B4	108.13 (14)	B8—B9—B4	107.78 (14)
B9—B3—B4	60.07 (11)	B3—B9—B10	107.80 (16)
C1—B3—H3	123.5	B8—B9—B10	107.40 (16)
C2—B3—H3	123.2	B4—B9—B10	59.99 (13)
B8—B3—H3	122.1	B3—B9—B12	107.46 (16)
B9—B3—H3	122.5	B8—B9—B12	59.73 (13)
B4—B3—H3	121.9	B4—B9—B12	107.67 (16)
C1—B4—B4^{i}	58.90 (8)	B10—B9—B12	59.63 (13)
C1—B4—B9	105.62 (13)	B3—B9—H9	121.9
B4^{i}—B4—B9	108.21 (10)	B8—B9—H9	122.1
C1—B4—B10	105.45 (14)	B4—B9—H9	121.7
B4^{i}—B4—B10	60.10 (8)	B10—B9—H9	122.0
B9—B4—B10	60.04 (11)	B12—B9—H9	122.1
C1—B4—B3	58.96 (10)	B12—B10—B4^{i}	108.11 (16)
B4^{i}—B4—B3	107.68 (9)	B12—B10—B4	108.11 (16)
B9—B4—B3	59.76 (11)	B4^{i}—B10—B4	59.81 (16)
B10—B4—B3	107.51 (14)	B12—B10—B9	60.21 (11)
C1—B4—H4	124.0	B4^{i}—B10—B9	107.93 (17)
B4^{i}—B4—H4	121.5	B4—B10—B9	59.97 (11)
B9—B4—H4	122.1	B12—B10—B9^{i}	60.21 (11)
B10—B4—H4	122.3	B4^{i}—B10—B9^{i}	59.96 (11)
B3—B4—H4	121.9	B4—B10—B9^{i}	107.92 (17)
C2—B8—B8^{i}	58.95 (8)	B9—B10—B9^{i}	108.32 (19)
C2—B8—B3	59.51 (10)	B12—B10—H10	121.5
B8^{i}—B8—B3	108.02 (10)	B4^{i}—B10—H10	121.8
C2—B8—B12	106.21 (14)	B4—B10—H10	121.8
B8^{i}—B8—B12	60.15 (8)	B9—B10—H10	121.6

B9^{i}—B10—H10	121.6	C6—C5—C4	120.3 (2)
B10—B12—B8^{i}	108.01 (17)	C6—C5—H5	119.8
B10—B12—B8	108.01 (17)	C4—C5—H5	119.8
B8^{i}—B12—B8	59.70 (16)	C5—C6—C5^{i}	119.8 (3)
B10—B12—B9	60.15 (11)	C5—C6—H6	120.1
B8^{i}—B12—B9	107.82 (17)	C5^{i}—C6—H6	120.1
B8—B12—B9	59.97 (10)	C10—Si1—C9	110.48 (7)
B10—B12—B9^{i}	60.16 (11)	C10—Si1—C9^{i}	110.47 (7)
B8^{i}—B12—B9^{i}	59.97 (10)	C9—Si1—C9^{i}	110.48 (12)
B8—B12—B9^{i}	107.82 (17)	C10—Si1—C2	105.92 (10)
B9—B12—B9^{i}	108.2 (2)	C9—Si1—C2	109.70 (6)
B10—B12—H12	121.6	C9^{i}—Si1—C2	109.70 (6)
B8^{i}—B12—H12	121.9	Si1—C9—H9A	109.5
B8—B12—H12	121.9	Si1—C9—H9B	109.5
B9—B12—H12	121.6	H9A—C9—H9B	109.5
B9^{i}—B12—H12	121.6	Si1—C9—H9C	109.5
C4^{i}—C3—C4	118.8 (2)	H9A—C9—H9C	109.5
C4^{i}—C3—C1	120.52 (11)	H9B—C9—H9C	109.5
C4—C3—C1	120.52 (11)	Si1—C10—H10A	109.5
C3—C4—C5	120.4 (2)	Si1—C10—H10C	109.5
C3—C4—H4A	119.8	H10A—C10—H10C	109.5
C5—C4—H4A	119.8		
C3—C1—C2—B8	−146.82 (10)	B3—C1—C2—B3^{i}	−144.44 (19)
B4—C1—C2—B8	−0.29 (15)	C3—C1—C2—Si1	0.0
B4^{i}—C1—C2—B8	66.64 (12)	B4—C1—C2—Si1	146.53 (10)
B3—C1—C2—B8	−39.04 (12)	B4^{i}—C1—C2—Si1	−146.53 (10)
B3^{i}—C1—C2—B8	105.40 (15)	B3—C1—C2—Si1	107.78 (10)
C3—C1—C2—B8^{i}	146.82 (10)	B3^{i}—C1—C2—Si1	−107.78 (10)
B4—C1—C2—B8^{i}	−66.64 (12)	C3—C1—B3—C2	110.80 (19)
B4^{i}—C1—C2—B8^{i}	0.29 (15)	B4—C1—B3—C2	−138.55 (15)
B3—C1—C2—B8^{i}	−105.40 (15)	B4^{i}—C1—B3—C2	−101.30 (15)
B3^{i}—C1—C2—B8^{i}	39.05 (12)	B3^{i}—C1—B3—C2	−33.11 (17)
C3—C1—C2—B3	−107.78 (10)	C3—C1—B3—B8	147.50 (15)
B4—C1—C2—B3	38.75 (12)	C2—C1—B3—B8	36.69 (13)
B4^{i}—C1—C2—B3	105.69 (15)	B4—C1—B3—B8	−101.86 (14)
B3^{i}—C1—C2—B3	144.44 (19)	B4^{i}—C1—B3—B8	−64.60 (16)
C3—C1—C2—B3^{i}	107.78 (10)	B3^{i}—C1—B3—B8	3.6 (2)
B4—C1—C2—B3^{i}	−105.69 (15)	C3—C1—B3—B9	−149.66 (16)
B4^{i}—C1—C2—B3^{i}	−38.75 (12)	C2—C1—B3—B9	99.54 (15)

Příloha č. 7

RTG - VIII (1-(4-nitrofenyl)-1,2-dikarba-kloso-dodekaboran(12))

Experimental

Crystal data

$C_8H_{15}B_{10}NO_2$
$M_r = 265.31$
Monoclinic
$P2_1/n$
$a = 7.0750\ (2)$ Å
$b = 19.2040\ (6)$ Å
$c = 10.0160\ (3)$ Å
$\beta = 93.8670\ (16)°$
$V = 1357.76\ (7)$ Å^3
$Z = 4$
$D_x = 1.298$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 2890 reflections
$\theta = 1–27.5°$
$\mu = 0.074$ mm^{-1}
$T = 150\ (2)$ K
Bar
Colourless
$0.3 \times 0.1 \times 0.1$ mm
Crystal source: synthesized by the authors

Data collection

Nonius KappaCCD area detector diffractometer
φ and ω scans to fill the Ewald sphere
Absorption correction: none
12275 measured reflections
3107 independent reflections

2253 reflections with $I > 2\sigma$igma(I)
$R_{\rm int} = 0.047$
$\theta_{\rm max} = 27.48°$
$h = -9 \rightarrow 9$
$k = -24 \rightarrow 24$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0501$
$wR(F^2) = 0.1476$
$S = 1.032$
3107 reflections
190 parameters
H-atom parameters constrained

w=$1/[\sigma^2(F_o^2) + (0.0791P)^2 + 0.4445P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.000$
$\Delta\rho_{\rm max} = 0.262$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.302$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
C1	0.2383 (2)	0.12219 (8)	0.85206 (16)	0.0202 (3)
C2	0.0683 (2)	0.18072 (8)	0.86591 (17)	0.0236 (4)
B3	0.2931 (3)	0.21027 (10)	0.8452 (2)	0.0269 (4)
B4	0.4424 (3)	0.15002 (10)	0.9365 (2)	0.0266 (4)
B5	0.2962 (3)	0.08539 (10)	1.00462 (19)	0.0261 (4)
B6	0.0563 (3)	0.10466 (10)	0.95443 (19)	0.0237 (4)
B7	0.1449 (3)	0.25119 (10)	0.9571 (2)	0.0274 (4)
B8	0.3854 (3)	0.23172 (10)	1.0075 (2)	0.0276 (4)
B9	0.3869 (3)	0.15487 (11)	1.1068 (2)	0.0280 (4)
B10	0.1472 (3)	0.12682 (11)	1.1173 (2)	0.0274 (4)
B11	−0.0007 (3)	0.18652 (10)	1.0243 (2)	0.0268 (4)
B12	0.2034 (3)	0.21768 (11)	1.1196 (2)	0.0268 (4)
C3	0.2419 (2)	0.07942 (8)	0.72582 (16)	0.0211 (4)
C4	0.2882 (2)	0.10913 (9)	0.60543 (16)	0.0239 (4)
C5	0.2949 (2)	0.06865 (9)	0.49147 (17)	0.0245 (4)
C6	0.2539 (2)	−0.00158 (9)	0.50014 (16)	0.0234 (4)
C7	0.2087 (2)	−0.03267 (9)	0.61753 (17)	0.0264 (4)
C8	0.2036 (2)	0.00849 (9)	0.73070 (18)	0.0261 (4)
N1	0.2588 (2)	−0.04434 (7)	0.37811 (14)	0.0265 (3)
O1	0.32259 (19)	−0.01804 (7)	0.27914 (13)	0.0351 (3)
O2	0.19867 (19)	−0.10416 (6)	0.38282 (13)	0.0360 (3)

Table 2. *Anisotropic displacement parameters* (A^2)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.0194 (8)	0.0217 (8)	0.0198 (8)	−0.0008 (6)	0.0021 (6)	−0.0005 (6)
C2	0.0223 (8)	0.0248 (8)	0.0235 (9)	0.0026 (6)	−0.0008 (6)	−0.0025 (7)
B3	0.0311 (10)	0.0224 (9)	0.0276 (11)	−0.0050 (8)	0.0051 (8)	−0.0024 (8)
B4	0.0195 (9)	0.0327 (10)	0.0275 (10)	−0.0025 (8)	0.0005 (7)	−0.0064 (8)
B5	0.0271 (10)	0.0281 (9)	0.0226 (10)	0.0021 (8)	−0.0012 (7)	0.0007 (8)
B6	0.0208 (9)	0.0287 (10)	0.0221 (10)	−0.0039 (7)	0.0038 (7)	−0.0010 (8)
B7	0.0319 (10)	0.0238 (9)	0.0261 (11)	0.0014 (8)	0.0000 (8)	−0.0060 (8)
B8	0.0247 (9)	0.0294 (10)	0.0290 (11)	−0.0069 (8)	0.0036 (8)	−0.0094 (8)
B9	0.0248 (10)	0.0360 (11)	0.0226 (10)	0.0018 (8)	−0.0036 (7)	−0.0055 (9)
B10	0.0303 (10)	0.0327 (10)	0.0191 (10)	−0.0036 (8)	0.0018 (7)	−0.0025 (8)
B11	0.0209 (9)	0.0344 (10)	0.0251 (10)	−0.0005 (8)	0.0023 (7)	−0.0080 (8)
B12	0.0233 (9)	0.0336 (10)	0.0233 (10)	−0.0024 (8)	0.0008 (7)	−0.0071 (8)
C3	0.0178 (7)	0.0242 (8)	0.0210 (8)	0.0008 (6)	−0.0001 (6)	−0.0022 (7)

C4	0.0258 (8)	0.0233 (8)	0.0228 (9)	0.0005 (6)	0.0021 (7)	−0.0001 (7)
C5	0.0239 (8)	0.0295 (9)	0.0202 (9)	0.0007 (7)	0.0015 (6)	0.0003 (7)
C6	0.0192 (7)	0.0265 (8)	0.0240 (9)	0.0028 (6)	−0.0021 (6)	−0.0059 (7)
C7	0.0266 (9)	0.0238 (8)	0.0288 (10)	−0.0019 (7)	0.0023 (7)	−0.0028 (7)
C8	0.0271 (8)	0.0261 (8)	0.0256 (9)	−0.0023 (7)	0.0049 (7)	−0.0013 (7)
N1	0.0277 (7)	0.0266 (8)	0.0246 (8)	0.0047 (6)	−0.0031 (6)	−0.0047 (6)
O1	0.0450 (8)	0.0370 (7)	0.0236 (7)	0.0027 (6)	0.0044 (6)	−0.0036 (6)
O2	0.0458 (8)	0.0258 (7)	0.0357 (8)	−0.0020 (6)	−0.0020 (6)	−0.0075 (6)

Table 3. *Selected geometric parameters (Å, °)*

C1—C3	1.509 (2)	B7—B8	1.781 (3)
C1—C2	1.659 (2)	B7—H7	1.1000
C1—B5	1.708 (2)	B8—B9	1.780 (3)
C1—B4	1.709 (2)	B8—B12	1.785 (3)
C1—B6	1.732 (2)	B8—H8	1.1000
C1—B3	1.738 (2)	B9—B12	1.783 (3)
C2—B11	1.694 (3)	B9—B10	1.789 (3)
C2—B7	1.701 (2)	B9—H9	1.1000
C2—B6	1.714 (3)	B10—B11	1.774 (3)
C2—B3	1.715 (3)	B10—B12	1.789 (3)
C2—H2	1.1000	B10—H10	1.1000
B3—B8	1.759 (3)	B11—B12	1.780 (3)
B3—B7	1.769 (3)	B11—H11	1.1000
B3—B4	1.778 (3)	B12—H12	1.1000
B3—H3	1.1000	C3—C8	1.390 (2)
B4—B9	1.778 (3)	C3—C4	1.393 (2)
B4—B8	1.780 (3)	C4—C5	1.384 (2)
B4—B5	1.781 (3)	C4—H4A	0.9300
B4—H4	1.1000	C5—C6	1.383 (2)
B5—B9	1.775 (3)	C5—H5A	0.9300
B5—B6	1.776 (3)	C6—C7	1.376 (2)
B5—B10	1.783 (3)	C6—N1	1.475 (2)
B5—H5	1.1000	C7—C8	1.384 (2)
B6—B10	1.765 (3)	C7—H7A	0.9300
B6—B11	1.778 (3)	C8—H8A	0.9300
B6—H6	1.1000	N1—O1	1.2255 (19)
B7—B12	1.773 (3)	N1—O2	1.2269 (18)
B7—B11	1.775 (3)		
C3—C1—C2	119.48 (13)	C2—C1—B5	109.69 (13)
C3—C1—B5	120.51 (13)	C3—C1—B4	121.54 (13)

C2—C1—B4	109.87 (12)	B7—B3—H3	121.6
B5—C1—B4	62.81 (11)	B4—B3—H3	122.2
C3—C1—B6	116.46 (13)	C1—B4—B3	59.75 (10)
C2—C1—B6	60.66 (10)	C1—B4—B9	104.92 (13)
B5—C1—B6	62.16 (11)	B3—B4—B9	107.31 (14)
B4—C1—B6	113.87 (13)	C1—B4—B8	105.47 (13)
C3—C1—B3	118.68 (14)	B3—B4—B8	59.27 (11)
C2—C1—B3	60.58 (10)	B9—B4—B8	60.01 (11)
B5—C1—B3	113.42 (13)	C1—B4—B5	58.56 (10)
B4—C1—B3	62.10 (11)	B3—B4—B5	108.08 (13)
B6—C1—B3	112.91 (13)	B9—B4—B5	59.85 (11)
C1—C2—B11	112.27 (13)	B8—B4—B5	107.96 (14)
C1—C2—B7	112.16 (12)	C1—B4—H4	124.0
B11—C2—B7	63.03 (11)	B3—B4—H4	121.6
C1—C2—B6	61.78 (10)	B9—B4—H4	122.6
B11—C2—B6	62.89 (11)	B8—B4—H4	122.4
B7—C2—B6	115.18 (13)	B5—B4—H4	121.6
C1—C2—B3	61.99 (10)	C1—B5—B9	105.10 (13)
B11—C2—B3	114.80 (13)	C1—B5—B6	59.59 (10)
B7—C2—B3	62.40 (11)	B9—B5—B6	107.95 (14)
B6—C2—B3	115.05 (13)	C1—B5—B4	58.62 (10)
C1—C2—H2	120.1	B9—B5—B4	60.01 (11)
B11—C2—H2	118.0	B6—B5—B4	108.36 (13)
B7—C2—H2	118.1	C1—B5—B10	105.40 (13)
B6—C2—H2	117.2	B9—B5—B10	60.38 (11)
B3—C2—H2	117.5	B6—B5—B10	59.47 (11)
C2—B3—C1	57.44 (9)	B4—B5—B10	108.36 (14)
C2—B3—B8	104.79 (14)	C1—B5—H5	124.2
C1—B3—B8	105.14 (14)	B9—B5—H5	122.3
C2—B3—B7	58.42 (11)	B6—B5—H5	121.4
C1—B3—B7	105.31 (14)	B4—B5—H5	121.4
B8—B3—B7	60.64 (11)	B10—B5—H5	122.2
C2—B3—B4	104.24 (13)	C2—B6—C1	57.56 (10)
C1—B3—B4	58.16 (10)	C2—B6—B10	104.19 (13)
B8—B3—B4	60.42 (11)	C1—B6—B10	105.14 (13)
B7—B3—B4	108.66 (15)	C2—B6—B5	104.15 (13)
C2—B3—H3	124.9	C1—B6—B5	58.25 (10)
C1—B3—H3	124.4	B10—B6—B5	60.45 (11)
B8—B3—H3	122.5	C2—B6—B11	58.02 (11)

C1—B6—B11	104.97 (13)	B5—B9—B8	108.21 (14)
B10—B6—B11	60.08 (11)	B4—B9—B8	60.04 (11)
B5—B6—B11	108.09 (13)	B5—B9—B12	108.23 (13)
C2—B6—H6	125.1	B4—B9—B12	108.23 (14)
C1—B6—H6	124.2	B8—B9—B12	60.12 (11)
B10—B6—H6	122.8	B5—B9—B10	60.01 (11)
B5—B6—H6	122.3	B4—B9—B10	108.17 (13)
B11—B6—H6	122.1	B8—B9—B10	108.21 (13)
C2—B7—B3	59.18 (10)	B12—B9—B10	60.12 (11)
C2—B7—B12	104.49 (14)	B5—B9—H9	121.6
B3—B7—B12	107.98 (14)	B4—B9—H9	121.6
C2—B7—B11	58.30 (11)	B8—B9—H9	121.6
B3—B7—B11	108.25 (13)	B12—B9—H9	121.6
B12—B7—B11	60.22 (11)	B10—B9—H9	121.6
C2—B7—B8	104.42 (13)	B6—B10—B11	60.32 (11)
B3—B7—B8	59.41 (11)	B6—B10—B5	60.08 (11)
B12—B7—B8	60.28 (11)	B11—B10—B5	107.98 (14)
B11—B7—B8	108.25 (14)	B6—B10—B12	108.27 (14)
C2—B7—H7	125.0	B11—B10—B12	59.93 (11)
B3—B7—H7	121.4	B5—B10—B12	107.63 (14)
B12—B7—H7	122.3	B6—B10—B9	107.83 (14)
B11—B7—H7	121.3	B11—B10—B9	107.60 (14)
B8—B7—H7	122.5	B5—B10—B9	59.61 (11)
B3—B8—B9	108.08 (13)	B12—B10—B9	59.77 (11)
B3—B8—B4	60.30 (11)	B6—B10—H10	121.4
B9—B8—B4	59.95 (11)	B11—B10—H10	121.7
B3—B8—B7	59.95 (11)	B5—B10—H10	121.9
B9—B8—B7	107.60 (13)	B12—B10—H10	121.8
B4—B8—B7	108.03 (13)	B9—B10—H10	122.1
B3—B8—B12	107.89 (13)	C2—B11—B10	104.63 (13)
B9—B8—B12	60.04 (11)	C2—B11—B7	58.67 (11)
B4—B8—B12	108.08 (14)	B10—B11—B7	108.34 (14)
B7—B8—B12	59.62 (11)	C2—B11—B6	59.09 (10)
B3—B8—H8	121.6	B10—B11—B6	59.59 (11)
B9—B8—H8	121.8	B7—B11—B6	108.47 (14)
B4—B8—H8	121.5	C2—B11—B12	104.47 (13)
B7—B8—H8	122.0	B10—B11—B12	60.47 (11)
B12—B8—H8	121.8	B7—B11—B12	59.84 (11)
B5—B9—B4	60.14 (11)	B6—B11—B12	108.12 (13)

C2—B11—H11	124.9	C8—C3—C1	119.29 (15)
B10—B11—H11	122.3	C4—C3—C1	121.38 (14)
B7—B11—H11	121.3	C5—C4—C3	120.45 (15)
B6—B11—H11	121.3	C5—C4—H4A	119.8
B12—B11—H11	122.4	C3—C4—H4A	119.8
B7—B12—B11	59.94 (11)	C6—C5—C4	118.47 (16)
B7—B12—B9	107.82 (14)	C6—C5—H5A	120.8
B11—B12—B9	107.61 (14)	C4—C5—H5A	120.8
B7—B12—B8	60.10 (11)	C7—C6—C5	122.60 (15)
B11—B12—B8	107.89 (14)	C7—C6—N1	119.11 (15)
B9—B12—B8	59.84 (11)	C5—C6—N1	118.30 (15)
B7—B12—B10	107.73 (13)	C6—C7—C8	118.19 (16)
B11—B12—B10	59.60 (11)	C6—C7—H7A	120.9
B9—B12—B10	60.11 (11)	C8—C7—H7A	120.9
B8—B12—B10	107.97 (14)	C7—C8—C3	120.98 (16)
B7—B12—H12	121.8	C7—C8—H8A	119.5
B11—B12—H12	122.0	C3—C8—H8A	119.5
B9—B12—H12	121.9	O1—N1—O2	124.37 (15)
B8—B12—H12	121.7	O1—N1—C6	118.12 (14)
B10—B12—H12	121.8	O2—N1—C6	117.51 (15)
C8—C3—C4	119.31 (15)		
C3—C1—C2—B11	144.50 (14)	B11—C2—B3—C1	103.12 (14)
B5—C1—C2—B11	−0.75 (17)	B7—C2—B3—C1	139.49 (14)
B4—C1—C2—B11	−68.01 (16)	B6—C2—B3—C1	32.89 (13)
B6—C1—C2—B11	38.88 (13)	C1—C2—B3—B8	−98.73 (14)
B3—C1—C2—B11	−107.19 (14)	B11—C2—B3—B8	4.39 (18)
C3—C1—C2—B7	−146.74 (15)	B7—C2—B3—B8	40.75 (13)
B5—C1—C2—B7	68.00 (16)	B6—C2—B3—B8	−65.85 (17)
B4—C1—C2—B7	0.75 (18)	C1—C2—B3—B7	−139.49 (14)
B6—C1—C2—B7	107.63 (15)	B11—C2—B3—B7	−36.36 (14)
B3—C1—C2—B7	−38.43 (14)	B6—C2—B3—B7	−106.60 (15)
C3—C1—C2—B6	105.62 (16)	C1—C2—B3—B4	−36.10 (12)
B5—C1—C2—B6	−39.63 (12)	B11—C2—B3—B4	67.02 (17)
B4—C1—C2—B6	−106.89 (14)	B7—C2—B3—B4	103.38 (15)
B3—C1—C2—B6	−146.07 (14)	B6—C2—B3—B4	−3.22 (18)
C3—C1—C2—B3	−108.31 (16)	C3—C1—B3—C2	109.60 (15)
B5—C1—C2—B3	106.43 (14)	B5—C1—B3—C2	−100.21 (14)
B4—C1—C2—B3	39.18 (13)	B4—C1—B3—C2	−137.76 (14)
B6—C1—C2—B3	146.07 (14)	B6—C1—B3—C2	−31.89 (13)