

## Bis(8-methyl-2,8-dicarba-closo-dodecaboran-2-yl) triselenide

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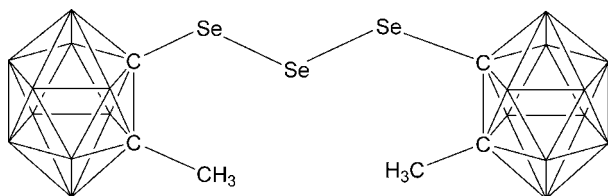
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Key indicators: single-crystal X-ray study;  $T = 297$  K; mean  $\sigma(\text{C}-\text{C}) = 0.010$  Å;  $R$  factor = 0.053;  $wR$  factor = 0.113; data-to-parameter ratio = 15.5.

In the title compound,  $\text{C}_6\text{H}_{26}\text{B}_{20}\text{Se}_3$ , the geometry around the central Se atom is V-shaped, with the Se—Se—Se angle being  $105.60(4)^\circ$ . The Se—Se bond lengths are consistent with single covalent bonds.

### Related literature

For general background to diorganotriseselenides, see: Atanassov *et al.* (2004); Hansen *et al.* (1989); Klapötke *et al.* (2006, 2007, 2008); Kulcsar *et al.* (2007); Kumar *et al.* (2004).



### Experimental

#### Crystal data

$\text{C}_6\text{H}_{26}\text{B}_{20}\text{Se}_3$   
 $M_r = 551.35$   
Orthorhombic,  $Pna2_1$   
 $a = 18.947(2)$  Å  
 $b = 11.2734(13)$  Å  
 $c = 10.8533(12)$  Å

$V = 2318.2(5)$  Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 4.75$  mm<sup>-1</sup>  
 $T = 297$  K  
 $0.40 \times 0.30 \times 0.20$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.252$ ,  $T_{\max} = 0.450$   
16082 measured reflections  
4083 independent reflections  
3398 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.069$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$   
 $wR(F^2) = 0.113$   
 $S = 1.05$   
4083 reflections  
264 parameters  
1 restraint  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.61$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.38$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983), 1920 Friedel pairs  
Flack parameter: 0.01 (2)

Data collection: SMART (Bruker, 2000); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2006); software used to prepare material for publication: enCIFer (Allen *et al.*, 2004) and publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2331).

### References

- Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.  
Atanassov, P. K., Linden, A. & Heimgartner, H. (2004). *Helv. Chim. Acta*, **87**, 1873–1887.  
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.  
Bruker (2000). *SMART* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Bruker (2001). *SAINTE-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
Hansen, F., Henriksen, L., Larsen, S. & Teuber, L. (1989). *Acta Chem. Scand.* **43**, 450–457.  
Klapötke, T. M., Krumm, B. & Polborn, K. (2008). *Z. Anorg. Allg. Chem.* **634**, 1287–1290.  
Klapötke, T. M., Krumm, B., Polborn, K. & Scherr, M. (2006). *Eur. J. Inorg. Chem.* pp. 2937–2941.  
Klapötke, T. M., Krumm, B. & Scherr, M. (2007). *Acta Cryst.* **E63**, o1965–o1966.  
Kulcsar, M., Silvestru, A. & Cziplé, F. (2007). *Acta Cryst.* **C63**, o701–o703.  
Kumar, S., Kandasamy, K., Singh, H. B., Wolmershauser, G. & Butcher, R. J. (2004). *Organometallics*, **23**, 4199–4208.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

**supplementary materials**

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## Bis(8-methyl-2,8-dicarba-*closo*-dodecaboran-2-yl) triselenide

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### Comment

Several diorganotriselenides of type R—Se—Se—Se—R have been reported:  $R = 2,6-(2,4,6\text{-Me}_3\text{C}_6\text{H}_2)_2\text{C}_6\text{H}_3$  and  $R = 2,6-(2,4,6\text{-}i\text{Pr}_3\text{C}_6\text{H}_2)_2\text{C}_6\text{H}_3$  (Klapötke *et al.*, 2007);  $R = 2-(\text{Me}_2\text{NCH}_2)\text{C}_6\text{H}_4-$  (Kulcsar *et al.*, 2007);  $R = (\text{Me}_2\text{PhSi})_2\text{ClC}$  (Klapötke *et al.*, 2007);  $R = (\text{Me}_2\text{PhSi})_3\text{C}$  (Klapötke *et al.*, 2006);  $R = 4\text{-}(\text{phenylamino})$  quinazolin-2-yl (Atanassov *et al.*, 2004);  $R = 2\text{-}(2\text{-phenyl-5,6-dihydro-4H-1,3-oxazinyl})$  (Kumar *et al.*, 2004). We report here the structure of the title compound, the first (to our knowledge), dicarboranetriselenide described so far.

The asymmetric unit of the title compound (Fig. 1) consists of a discrete molecule. The geometry around the central Se atom is V-shaped, with a Se—Se—Se angle of 105.60 (4)°. The Se—Se bond lengths are consistent with single covalent bonds. The values for the Se—Se bond distances of 2.3102 (12) Å and 2.3120 (13) Å, as well as for the torsion angles C1—Se1—Se2—Se3 -95.3 (2)° and C4—Se3—Se2—Se1 -84.8 (2)°, compare well with the corresponding values found in other triselenides (Kulcsar *et al.*, 2007; Klapötke *et al.*, 2007; Klapötke *et al.*, 2006; Hansen *et al.*, 1989).

### Experimental

A mixture of [2-(MeC<sub>2</sub>B<sub>10</sub>H<sub>10</sub>SeCH<sub>2</sub>)py] (0.184 g, 5.6 mmol) and [Cu(MeCN)<sub>4</sub>]PF<sub>6</sub> (0.208 g, 5.6 mmol) in CDCl<sub>3</sub> was stirred for 2 h. The resulting solution was filtered and allowed to stand at room temperature. After two weeks, yellow crystals of the title compound [(MeC<sub>2</sub>B<sub>10</sub>H<sub>10</sub>)<sub>2</sub>Se<sub>3</sub>] were obtained.

### Refinement

All hydrogen atoms were placed in calculated positions using a riding model, with C—H = 0.96 Å and B—H = 1.1 Å with  $U_{\text{iso}}=1.5\text{Ueq}$  (C) for methyl H and  $U_{\text{iso}}=1.2\text{Ueq}$  (B) for the rest of H. The methyl groups were allowed to rotate while retaining tetrahedral geometry.

### Figures

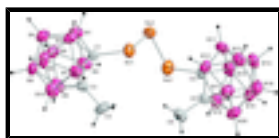


Fig. 1. Graphical representation of the molecular structure of [(MeC<sub>2</sub>B<sub>10</sub>H<sub>10</sub>)<sub>2</sub>Se<sub>3</sub>]. Displacement ellipsoids are drawn at the 50% probability level.

## Bis(8-methyl-2,8-dicarba-*closo*-dodecaboran-2-yl) triselenide

### Crystal data

C<sub>6</sub>H<sub>26</sub>B<sub>20</sub>Se<sub>3</sub>

$F(000) = 1056$

# supplementary materials

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|                                |   |
|--------------------------------|---|
| $M_r = 551.35$                 | $D_x = 1.580 \text{ Mg m}^{-3}$                         |
| Orthorhombic, $Pna2_1$         | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: P 2c -2n          | Cell parameters from 2078 reflections                   |
| $a = 18.947 (2) \text{ \AA}$   | $\theta = 2.6\text{--}18.5^\circ$                       |
| $b = 11.2734 (13) \text{ \AA}$ | $\mu = 4.75 \text{ mm}^{-1}$                            |
| $c = 10.8533 (12) \text{ \AA}$ | $T = 297 \text{ K}$                                     |
| $V = 2318.2 (5) \text{ \AA}^3$ | Block, yellow   |
| $Z = 4$                        | $0.40 \times 0.30 \times 0.20 \text{ mm}$               |

## Data collection

|  |  |
|--|--|
| Bruker SMART CCD area-detector diffractometer            | 4083 independent reflections   |
| Radiation source: fine-focus sealed tube graphite        | 3398 reflections with $I > 2\sigma(I)$                                 |
| $\varphi$ and $\omega$ scans                             | $R_{\text{int}} = 0.069$   |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | $\theta_{\text{max}} = 25.0^\circ$ , $\theta_{\text{min}} = 2.1^\circ$ |
| $T_{\text{min}} = 0.252$ , $T_{\text{max}} = 0.450$      | $h = -22 \rightarrow 22$   |
| 16082 measured reflections                               | $k = -13 \rightarrow 13$   |
|  | $l = -12 \rightarrow 12$   |

## Refinement

|  |  |
|--|--|
| Refinement on $F^2$  | Secondary atom site location: difference Fourier map     |
| Least-squares matrix: full                                     | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.053$                                | H-atom parameters constrained                            |
| $wR(F^2) = 0.113$  | $w = 1/[\sigma^2(F_o^2) + (0.0497P)^2]$                  |
| $S = 1.05$   | where $P = (F_o^2 + 2F_c^2)/3$                           |
| 4083 reflections   | $(\Delta/\sigma)_{\text{max}} = 0.001$                   |
| 264 parameters   | $\Delta\rho_{\text{max}} = 0.61 \text{ e \AA}^{-3}$      |
| 1 restraint  | $\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$     |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 1920 Friedel pairs     |
|  | Flack parameter: 0.01 (2)                                |

## Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

|     | <i>x</i>   | <i>y</i>    | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|-------------|--------------|----------------------------------|
| B1  | 0.8152 (5) | -0.3444 (9) | 0.1248 (8)   | 0.049 (2)                        |
| H1  | 0.8670     | -0.3770     | 0.0938       | 0.059*                           |
| B2  | 0.8058 (4) | -0.2509 (8) | 0.2541 (8)   | 0.042 (2)                        |
| H2  | 0.8520     | -0.2206     | 0.3068       | 0.051*                           |
| B3  | 0.7474 (5) | -0.3072 (7) | 0.0166 (9)   | 0.045 (2)                        |
| H3  | 0.7554     | -0.3158     | -0.0834      | 0.055*                           |
| B4  | 0.7359 (5) | -0.4328 (9) | 0.1164 (9)   | 0.056 (3)                        |
| H4  | 0.7359     | -0.5246     | 0.0820       | 0.067*                           |
| B5  | 0.7735 (6) | -0.3945 (7) | 0.2635 (9)   | 0.053 (2)                        |
| H5  | 0.7987     | -0.4607     | 0.3236       | 0.064*                           |
| B6  | 0.7228 (5) | -0.2797 (9) | 0.3243 (9)   | 0.051 (2)                        |
| H6  | 0.7145     | -0.2702     | 0.4241       | 0.061*                           |
| B7  | 0.6993 (4) | -0.1897 (8) | 0.0820 (9)   | 0.044 (2)                        |
| H7  | 0.6766     | -0.1191     | 0.0244       | 0.052*                           |
| B8  | 0.6658 (5) | -0.3341 (8) | 0.0858 (10)  | 0.051 (2)                        |
| H8  | 0.6203     | -0.3608     | 0.0295       | 0.061*                           |
| B9  | 0.6807 (5) | -0.3890 (8) | 0.2379 (9)   | 0.052 (2)                        |
| H9  | 0.6445     | -0.4526     | 0.2816       | 0.062*                           |
| B10 | 0.6567 (5) | -0.2416 (9) | 0.2160 (8)   | 0.050 (2)                        |
| H10 | 0.6050     | -0.2070     | 0.2448       | 0.060*                           |
| B11 | 1.0502 (5) | 0.1868 (9)  | 0.0637 (9)   | 0.052 (3)                        |
| H11 | 1.0780     | 0.1126      | 0.0193       | 0.063*                           |
| B12 | 0.9589 (4) | 0.2115 (7)  | 0.0395 (8)   | 0.040 (2)                        |
| H12 | 0.9263     | 0.1528      | -0.0181      | 0.048*                           |
| B13 | 1.0214 (5) | 0.3096 (9)  | -0.0207 (10) | 0.054 (3)                        |
| H13 | 1.0303     | 0.3162      | -0.1206      | 0.064*                           |
| B14 | 1.0909 (5) | 0.3232 (9)  | 0.0901 (10)  | 0.055 (2)                        |
| H14 | 1.1458     | 0.3398      | 0.0620       | 0.067*                           |
| B15 | 1.0710 (5) | 0.2338 (9)  | 0.2168 (9)   | 0.052 (3)                        |
| H15 | 1.1123     | 0.1906      | 0.2720       | 0.062*                           |
| B16 | 0.9918 (5) | 0.2851 (8)  | 0.2848 (9)   | 0.052 (3)                        |
| H16 | 0.9804     | 0.2735      | 0.3834       | 0.063*                           |
| B17 | 0.9455 (5) | 0.3657 (8)  | 0.0479 (9)   | 0.050 (2)                        |
| H17 | 0.9046     | 0.4099      | -0.0074      | 0.060*                           |
| B18 | 1.0262 (5) | 0.4347 (9)  | 0.0783 (10)  | 0.059 (3)                        |
| H18 | 1.0388     | 0.5237      | 0.0431       | 0.070*                           |
| B19 | 1.0556 (6) | 0.3843 (9)  | 0.2281 (10)  | 0.059 (3)                        |
| H19 | 1.0870     | 0.4404      | 0.2904       | 0.071*                           |
| B20 | 0.9641 (5) | 0.4120 (8)  | 0.2017 (10)  | 0.052 (2)                        |
| H20 | 0.9357     | 0.4852      | 0.2468       | 0.063*                           |
| C1  | 0.7868 (3) | -0.2037 (6) | 0.1094 (7)   | 0.0353 (16)                      |
| C2  | 0.7330 (4) | -0.1659 (7) | 0.2261 (6)   | 0.0407 (18)                      |
| C3  | 0.7363 (5) | -0.0404 (7) | 0.2731 (8)   | 0.060 (2)                        |
| H3A | 0.7809     | -0.0271     | 0.3125       | 0.091*                           |
| H3B | 0.6989     | -0.0276     | 0.3313       | 0.091*                           |

## supplementary materials

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|     |             |              |             |             |
|-----|-------------|--------------|-------------|-------------|
| H3C | 0.7311      | 0.0137       | 0.2053      | 0.091*      |
| C4  | 0.9916 (4)  | 0.1729 (6)   | 0.1812 (7)  | 0.0371 (17) |
| C5  | 0.9286 (4)  | 0.2786 (6)   | 0.1715 (7)  | 0.0382 (17) |
| C6  | 0.8535 (4)  | 0.2487 (8)   | 0.2121 (8)  | 0.059 (2)   |
| H6A | 0.8493      | 0.1646       | 0.2238      | 0.089*      |
| H6B | 0.8207      | 0.2741       | 0.1499      | 0.089*      |
| H6C | 0.8432      | 0.2887       | 0.2881      | 0.089*      |
| Se1 | 0.83965 (4) | -0.08061 (7) | 0.02743 (8) | 0.0485 (2)  |
| Se2 | 0.95387 (4) | -0.10616 (7) | 0.09702 (9) | 0.0543 (2)  |
| Se3 | 0.96638 (4) | 0.02322 (7)  | 0.26085 (7) | 0.0528 (2)  |

### Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|------------|------------|------------|-------------|-------------|-------------|
| B1  | 0.050 (6)  | 0.047 (5)  | 0.050 (6)  | 0.014 (4)   | 0.003 (4)   | 0.004 (4)   |
| B2  | 0.037 (5)  | 0.061 (6)  | 0.028 (4)  | 0.007 (4)   | -0.003 (4)  | 0.005 (5)   |
| B3  | 0.057 (6)  | 0.042 (5)  | 0.038 (5)  | 0.004 (4)   | -0.009 (5)  | -0.012 (4)  |
| B4  | 0.071 (7)  | 0.041 (5)  | 0.056 (6)  | 0.000 (5)   | 0.003 (5)   | -0.011 (5)  |
| B5  | 0.075 (7)  | 0.034 (5)  | 0.050 (5)  | 0.004 (4)   | 0.009 (5)   | 0.008 (5)   |
| B6  | 0.039 (5)  | 0.072 (7)  | 0.042 (5)  | 0.002 (5)   | 0.005 (4)   | 0.008 (5)   |
| B7  | 0.036 (5)  | 0.044 (5)  | 0.050 (5)  | 0.004 (4)   | -0.010 (4)  | 0.003 (4)   |
| B8  | 0.053 (6)  | 0.042 (5)  | 0.058 (5)  | -0.017 (4)  | -0.012 (5)  | 0.013 (5)   |
| B9  | 0.062 (6)  | 0.031 (5)  | 0.062 (6)  | -0.012 (4)  | 0.006 (5)   | 0.001 (4)   |
| B10 | 0.048 (6)  | 0.056 (6)  | 0.045 (5)  | 0.000 (5)   | -0.006 (4)  | 0.009 (5)   |
| B11 | 0.036 (5)  | 0.059 (6)  | 0.062 (7)  | 0.005 (5)   | 0.010 (4)   | -0.008 (5)  |
| B12 | 0.049 (6)  | 0.035 (5)  | 0.036 (5)  | -0.002 (4)  | -0.004 (4)  | 0.003 (4)   |
| B13 | 0.045 (6)  | 0.057 (7)  | 0.058 (6)  | -0.002 (5)  | 0.003 (5)   | -0.001 (5)  |
| B14 | 0.041 (5)  | 0.061 (6)  | 0.065 (6)  | -0.013 (4)  | 0.007 (5)   | 0.005 (6)   |
| B15 | 0.030 (5)  | 0.065 (7)  | 0.061 (7)  | -0.007 (5)  | -0.013 (4)  | -0.006 (5)  |
| B16 | 0.046 (6)  | 0.058 (6)  | 0.053 (7)  | -0.004 (5)  | -0.007 (5)  | 0.001 (5)   |
| B17 | 0.062 (6)  | 0.039 (5)  | 0.050 (6)  | 0.006 (5)   | 0.004 (5)   | 0.005 (4)   |
| B18 | 0.065 (7)  | 0.048 (6)  | 0.063 (6)  | -0.016 (5)  | 0.003 (5)   | 0.001 (5)   |
| B19 | 0.064 (7)  | 0.051 (6)  | 0.062 (7)  | -0.019 (5)  | -0.012 (5)  | -0.008 (5)  |
| B20 | 0.060 (7)  | 0.040 (6)  | 0.057 (6)  | 0.012 (4)   | -0.007 (5)  | -0.008 (5)  |
| C1  | 0.037 (4)  | 0.036 (4)  | 0.033 (4)  | 0.002 (3)   | -0.003 (3)  | -0.003 (3)  |
| C2  | 0.039 (4)  | 0.047 (5)  | 0.036 (4)  | 0.005 (3)   | 0.004 (3)   | -0.005 (3)  |
| C3  | 0.081 (6)  | 0.044 (5)  | 0.057 (5)  | 0.007 (4)   | -0.002 (5)  | -0.019 (4)  |
| C4  | 0.037 (4)  | 0.032 (4)  | 0.043 (4)  | 0.001 (3)   | -0.005 (3)  | 0.006 (3)   |
| C5  | 0.039 (4)  | 0.043 (4)  | 0.032 (4)  | 0.004 (4)   | 0.005 (3)   | 0.003 (3)   |
| C6  | 0.050 (5)  | 0.065 (6)  | 0.063 (6)  | 0.003 (4)   | 0.014 (4)   | 0.011 (5)   |
| Se1 | 0.0563 (5) | 0.0459 (4) | 0.0434 (4) | -0.0062 (4) | 0.0029 (4)  | 0.0088 (4)  |
| Se2 | 0.0457 (5) | 0.0423 (4) | 0.0749 (6) | 0.0014 (4)  | 0.0136 (5)  | -0.0047 (5) |
| Se3 | 0.0621 (5) | 0.0472 (5) | 0.0491 (4) | -0.0042 (4) | -0.0055 (5) | 0.0111 (4)  |

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

|       |            |         |            |
|-------|------------|---------|------------|
| B1—C1 | 1.683 (11) | B12—C5  | 1.719 (11) |
| B1—B2 | 1.763 (13) | B12—B13 | 1.746 (13) |
| B1—B3 | 1.790 (12) | B12—B17 | 1.759 (12) |

|          |            |             |             |
|----------|------------|-------------|-------------|
| B1—B5    | 1.791 (13) | B12—H12     | 1.1000      |
| B1—B4    | 1.806 (14) | B13—B17     | 1.738 (13)  |
| B1—H1    | 1.1000     | B13—B18     | 1.776 (14)  |
| B2—C1    | 1.696 (11) | B13—B14     | 1.790 (14)  |
| B2—C2    | 1.708 (11) | B13—H13     | 1.1000      |
| B2—B5    | 1.734 (12) | B14—B15     | 1.746 (14)  |
| B2—B6    | 1.778 (12) | B14—B18     | 1.761 (15)  |
| B2—H2    | 1.1000     | B14—B19     | 1.779 (15)  |
| B3—C1    | 1.713 (10) | B14—H14     | 1.1000      |
| B3—B8    | 1.745 (13) | B15—C4      | 1.699 (11)  |
| B3—B7    | 1.758 (12) | B15—B19     | 1.725 (14)  |
| B3—B4    | 1.796 (13) | B15—B16     | 1.768 (13)  |
| B3—H3    | 1.1000     | B15—H15     | 1.1000      |
| B4—B9    | 1.754 (14) | B16—C4      | 1.693 (12)  |
| B4—B8    | 1.764 (14) | B16—C5      | 1.719 (12)  |
| B4—B5    | 1.801 (14) | B16—B19     | 1.758 (14)  |
| B4—H4    | 1.1000     | B16—B20     | 1.771 (13)  |
| B5—B6    | 1.741 (13) | B16—H16     | 1.1000      |
| B5—B9    | 1.781 (14) | B17—C5      | 1.693 (11)  |
| B5—H5    | 1.1000     | B17—B18     | 1.746 (13)  |
| B6—C2    | 1.678 (12) | B17—B20     | 1.783 (14)  |
| B6—B9    | 1.741 (13) | B17—H17     | 1.1000      |
| B6—B10   | 1.770 (13) | B18—B20     | 1.800 (15)  |
| B6—H6    | 1.1000     | B18—B19     | 1.811 (15)  |
| B7—C1    | 1.693 (10) | B18—H18     | 1.1000      |
| B7—C2    | 1.710 (11) | B19—B20     | 1.786 (14)  |
| B7—B8    | 1.747 (12) | B19—H19     | 1.1000      |
| B7—B10   | 1.762 (13) | B20—C5      | 1.680 (12)  |
| B7—H7    | 1.1000     | B20—H20     | 1.1000      |
| B8—B10   | 1.764 (14) | C1—C2       | 1.682 (9)   |
| B8—B9    | 1.785 (14) | C1—Se1      | 1.928 (7)   |
| B8—H8    | 1.1000     | C2—C3       | 1.506 (11)  |
| B9—B10   | 1.739 (13) | C3—H3A      | 0.9600      |
| B9—H9    | 1.1000     | C3—H3B      | 0.9600      |
| B10—C2   | 1.681 (12) | C3—H3C      | 0.9600      |
| B10—H10  | 1.1000     | C4—C5       | 1.690 (10)  |
| B11—C4   | 1.699 (12) | C4—Se3      | 1.955 (7)   |
| B11—B14  | 1.743 (13) | C5—C6       | 1.527 (10)  |
| B11—B13  | 1.747 (14) | C6—H6A      | 0.9600      |
| B11—B12  | 1.772 (12) | C6—H6B      | 0.9600      |
| B11—B15  | 1.789 (14) | C6—H6C      | 0.9600      |
| B11—H11  | 1.1000     | Se1—Se2     | 2.3102 (12) |
| B12—C4   | 1.715 (11) | Se2—Se3     | 2.3120 (13) |
| C1—B1—B2 | 58.9 (5)   | B11—B13—B14 | 59.1 (5)    |
| C1—B1—B3 | 59.0 (5)   | B18—B13—B14 | 59.2 (6)    |
| B2—B1—B3 | 108.0 (6)  | B17—B13—H13 | 121.6       |
| C1—B1—B5 | 103.9 (6)  | B12—B13—H13 | 121.1       |
| B2—B1—B5 | 58.4 (5)   | B11—B13—H13 | 121.5       |
| B3—B1—B5 | 108.0 (7)  | B18—B13—H13 | 122.3       |

## supplementary materials

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|          |           |             |           |
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| C1—B1—B4 | 104.5 (6) | B14—B13—H13 | 122.9     |
| B2—B1—B4 | 106.7 (6) | B11—B14—B15 | 61.7 (5)  |
| B3—B1—B4 | 59.9 (5)  | B11—B14—B18 | 108.1 (6) |
| B5—B1—B4 | 60.1 (5)  | B15—B14—B18 | 108.6 (7) |
| C1—B1—H1 | 124.7     | B11—B14—B19 | 108.3 (7) |
| B2—B1—H1 | 122.3     | B15—B14—B19 | 58.6 (6)  |
| B3—B1—H1 | 121.1     | B18—B14—B19 | 61.5 (6)  |
| B5—B1—H1 | 123.0     | B11—B14—B13 | 59.2 (5)  |
| B4—B1—H1 | 122.7     | B15—B14—B13 | 108.7 (6) |
| C1—B2—C2 | 59.2 (4)  | B18—B14—B13 | 60.0 (5)  |
| C1—B2—B5 | 105.8 (6) | B19—B14—B13 | 108.9 (7) |
| C2—B2—B5 | 104.4 (6) | B11—B14—H14 | 121.5     |
| C1—B2—B1 | 58.2 (5)  | B15—B14—H14 | 121.4     |
| C2—B2—B1 | 106.0 (6) | B18—B14—H14 | 121.1     |
| B5—B2—B1 | 61.6 (5)  | B19—B14—H14 | 121.5     |
| C1—B2—B6 | 105.4 (6) | B13—B14—H14 | 121.6     |
| C2—B2—B6 | 57.5 (5)  | C4—B15—B19  | 105.4 (7) |
| B5—B2—B6 | 59.4 (5)  | C4—B15—B14  | 104.2 (6) |
| B1—B2—B6 | 108.7 (7) | B19—B15—B14 | 61.6 (6)  |
| C1—B2—H2 | 123.6     | C4—B15—B16  | 58.4 (5)  |
| C2—B2—H2 | 124.2     | B19—B15—B16 | 60.4 (6)  |
| B5—B2—H2 | 122.7     | B14—B15—B16 | 108.8 (7) |
| B1—B2—H2 | 121.3     | C4—B15—B11  | 58.2 (5)  |
| B6—B2—H2 | 122.5     | B19—B15—B11 | 108.7 (7) |
| C1—B3—B8 | 104.6 (6) | B14—B15—B11 | 59.1 (6)  |
| C1—B3—B7 | 58.4 (4)  | B16—B15—B11 | 107.3 (6) |
| B8—B3—B7 | 59.8 (5)  | C4—B15—H15  | 125.1     |
| C1—B3—B1 | 57.4 (5)  | B19—B15—H15 | 121.1     |
| B8—B3—B1 | 108.2 (7) | B14—B15—H15 | 122.1     |
| B7—B3—B1 | 106.5 (6) | B16—B15—H15 | 121.5     |
| C1—B3—B4 | 103.6 (6) | B11—B15—H15 | 122.1     |
| B8—B3—B4 | 59.7 (5)  | C4—B16—C5   | 59.4 (4)  |
| B7—B3—B4 | 106.7 (6) | C4—B16—B19  | 104.2 (7) |
| B1—B3—B4 | 60.5 (5)  | C5—B16—B19  | 104.9 (7) |
| C1—B3—H3 | 125.5     | C4—B16—B15  | 58.7 (5)  |
| B8—B3—H3 | 122.1     | C5—B16—B15  | 106.2 (6) |
| B7—B3—H3 | 122.4     | B19—B16—B15 | 58.6 (5)  |
| B1—B3—H3 | 121.9     | C4—B16—B20  | 105.3 (6) |
| B4—B3—H3 | 122.8     | C5—B16—B20  | 57.5 (5)  |
| B9—B4—B8 | 61.0 (6)  | B19—B16—B20 | 60.8 (6)  |
| B9—B4—B3 | 107.7 (6) | B15—B16—B20 | 107.7 (7) |
| B8—B4—B3 | 58.7 (5)  | C4—B16—H16  | 123.8     |
| B9—B4—B5 | 60.1 (6)  | C5—B16—H16  | 123.6     |
| B8—B4—B5 | 108.2 (7) | B19—B16—H16 | 123.5     |
| B3—B4—B5 | 107.3 (6) | B15—B16—H16 | 122.3     |
| B9—B4—B1 | 107.6 (7) | B20—B16—H16 | 122.2     |
| B8—B4—B1 | 106.7 (7) | C5—B17—B13  | 106.6 (7) |
| B3—B4—B1 | 59.6 (5)  | C5—B17—B18  | 106.0 (7) |
| B5—B4—B1 | 59.5 (5)  | B13—B17—B18 | 61.3 (6)  |



|           |           |             |           |
|-----------|-----------|-------------|-----------|
| B9—B4—H4  | 121.3     | C5—B17—B12  | 59.7 (5)  |
| B8—B4—H4  | 122.0     | B13—B17—B12 | 59.9 (5)  |
| B3—B4—H4  | 122.5     | B18—B17—B12 | 108.9 (7) |
| B5—B4—H4  | 121.8     | C5—B17—B20  | 57.7 (5)  |
| B1—B4—H4  | 122.5     | B13—B17—B20 | 110.2 (7) |
| B2—B5—B6  | 61.5 (5)  | B18—B17—B20 | 61.3 (6)  |
| B2—B5—B9  | 107.9 (6) | B12—B17—B20 | 108.1 (7) |
| B6—B5—B9  | 59.2 (5)  | C5—B17—H17  | 124.2     |
| B2—B5—B1  | 60.0 (5)  | B13—B17—H17 | 120.9     |
| B6—B5—B1  | 109.1 (6) | B18—B17—H17 | 121.1     |
| B9—B5—B1  | 107.1 (7) | B12—B17—H17 | 121.4     |
| B2—B5—B4  | 108.2 (7) | B20—B17—H17 | 121.1     |
| B6—B5—B4  | 107.2 (7) | B17—B18—B14 | 107.7 (7) |
| B9—B5—B4  | 58.7 (6)  | B17—B18—B13 | 59.1 (5)  |
| B1—B5—B4  | 60.4 (6)  | B14—B18—B13 | 60.8 (6)  |
| B2—B5—H5  | 121.0     | B17—B18—B20 | 60.4 (6)  |
| B6—B5—H5  | 121.2     | B14—B18—B20 | 107.4 (7) |
| B9—B5—H5  | 122.9     | B13—B18—B20 | 107.7 (7) |
| B1—B5—H5  | 121.4     | B17—B18—B19 | 107.4 (7) |
| B4—B5—H5  | 122.3     | B14—B18—B19 | 59.7 (6)  |
| C2—B6—B9  | 104.6 (7) | B13—B18—B19 | 108.0 (7) |
| C2—B6—B5  | 105.3 (6) | B20—B18—B19 | 59.3 (6)  |
| B9—B6—B5  | 61.5 (6)  | B17—B18—H18 | 122.1     |
| C2—B6—B10 | 58.3 (5)  | B14—B18—H18 | 121.7     |
| B9—B6—B10 | 59.4 (6)  | B13—B18—H18 | 121.7     |
| B5—B6—B10 | 108.6 (7) | B20—B18—H18 | 122.0     |
| C2—B6—B2  | 59.1 (5)  | B19—B18—H18 | 122.1     |
| B9—B6—B2  | 107.7 (7) | B15—B19—B16 | 61.0 (6)  |
| B5—B6—B2  | 59.0 (5)  | B15—B19—B14 | 59.8 (6)  |
| B10—B6—B2 | 107.3 (6) | B16—B19—B14 | 107.9 (7) |
| C2—B6—H6  | 124.6     | B15—B19—B20 | 108.9 (7) |
| B9—B6—H6  | 122.2     | B16—B19—B20 | 60.0 (5)  |
| B5—B6—H6  | 121.6     | B14—B19—B20 | 107.3 (7) |
| B10—B6—H6 | 121.9     | B15—B19—B18 | 107.3 (7) |
| B2—B6—H6  | 122.1     | B16—B19—B18 | 107.6 (7) |
| C1—B7—C2  | 59.2 (4)  | B14—B19—B18 | 58.7 (6)  |
| C1—B7—B8  | 105.3 (6) | B20—B19—B18 | 60.1 (6)  |
| C2—B7—B8  | 105.1 (6) | B15—B19—H19 | 121.2     |
| C1—B7—B3  | 59.5 (4)  | B16—B19—H19 | 121.5     |
| C2—B7—B3  | 107.1 (6) | B14—B19—H19 | 122.5     |
| B8—B7—B3  | 59.7 (5)  | B20—B19—H19 | 121.5     |
| C1—B7—B10 | 105.8 (6) | B18—B19—H19 | 122.5     |
| C2—B7—B10 | 57.9 (5)  | C5—B20—B16  | 59.7 (5)  |
| B8—B7—B10 | 60.4 (6)  | C5—B20—B17  | 58.4 (5)  |
| B3—B7—B10 | 108.7 (7) | B16—B20—B17 | 107.4 (6) |
| C1—B7—H7  | 123.3     | C5—B20—B19  | 105.3 (6) |
| C2—B7—H7  | 123.5     | B16—B20—B19 | 59.2 (5)  |
| B8—B7—H7  | 123.1     | B17—B20—B19 | 106.9 (7) |
| B3—B7—H7  | 121.2     | C5—B20—B18  | 104.1 (6) |

## supplementary materials

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|             |           |             |           |
|-------------|-----------|-------------|-----------|
| B10—B7—H7   | 122.1     | B16—B20—B18 | 107.5 (7) |
| B3—B8—B7    | 60.5 (5)  | B17—B20—B18 | 58.3 (6)  |
| B3—B8—B4    | 61.6 (5)  | B19—B20—B18 | 60.7 (6)  |
| B7—B8—B4    | 108.6 (6) | C5—B20—H20  | 124.2     |
| B3—B8—B10   | 109.2 (6) | B16—B20—H20 | 121.6     |
| B7—B8—B10   | 60.3 (5)  | B17—B20—H20 | 122.7     |
| B4—B8—B10   | 107.2 (7) | B19—B20—H20 | 122.3     |
| B3—B8—B9    | 108.5 (7) | B18—B20—H20 | 122.9     |
| B7—B8—B9    | 106.7 (7) | C2—C1—B1    | 111.0 (6) |
| B4—B8—B9    | 59.2 (5)  | C2—C1—B7    | 60.9 (5)  |
| B10—B8—B9   | 58.7 (5)  | B1—C1—B7    | 114.7 (6) |
| B3—B8—H8    | 120.2     | C2—C1—B2    | 60.7 (4)  |
| B7—B8—H8    | 121.8     | B1—C1—B2    | 62.9 (5)  |
| B4—B8—H8    | 121.5     | B7—C1—B2    | 113.5 (6) |
| B10—B8—H8   | 122.0     | C2—C1—B3    | 110.5 (5) |
| B9—B8—H8    | 122.9     | B1—C1—B3    | 63.6 (5)  |
| B10—B9—B6   | 61.1 (5)  | B7—C1—B3    | 62.1 (5)  |
| B10—B9—B4   | 108.8 (7) | B2—C1—B3    | 115.0 (6) |
| B6—B9—B4    | 109.3 (7) | C2—C1—Se1   | 118.7 (5) |
| B10—B9—B5   | 108.2 (6) | B1—C1—Se1   | 123.9 (5) |
| B6—B9—B5    | 59.3 (5)  | B7—C1—Se1   | 111.1 (5) |
| B4—B9—B5    | 61.3 (6)  | B2—C1—Se1   | 122.9 (5) |
| B10—B9—B8   | 60.1 (5)  | B3—C1—Se1   | 116.4 (5) |
| B6—B9—B8    | 109.0 (6) | C3—C2—B6    | 120.6 (7) |
| B4—B9—B8    | 59.8 (6)  | C3—C2—B10   | 122.3 (6) |
| B5—B9—B8    | 108.2 (7) | B6—C2—B10   | 63.6 (5)  |
| B10—B9—H9   | 121.2     | C3—C2—C1    | 117.9 (6) |
| B6—B9—H9    | 121.0     | B6—C2—C1    | 110.7 (6) |
| B4—B9—H9    | 120.8     | B10—C2—C1   | 110.1 (6) |
| B5—B9—H9    | 121.8     | C3—C2—B2    | 115.7 (6) |
| B8—B9—H9    | 121.7     | B6—C2—B2    | 63.3 (5)  |
| C2—B10—B9   | 104.5 (7) | B10—C2—B2   | 114.9 (6) |
| C2—B10—B7   | 59.5 (5)  | C1—C2—B2    | 60.1 (4)  |
| B9—B10—B7   | 108.1 (7) | C3—C2—B7    | 118.2 (6) |
| C2—B10—B8   | 105.6 (6) | B6—C2—B7    | 114.7 (6) |
| B9—B10—B8   | 61.3 (5)  | B10—C2—B7   | 62.6 (5)  |
| B7—B10—B8   | 59.4 (5)  | C1—C2—B7    | 59.9 (4)  |
| C2—B10—B6   | 58.1 (5)  | B2—C2—B7    | 112.1 (6) |
| B9—B10—B6   | 59.5 (6)  | C2—C3—H3A   | 109.5     |
| B7—B10—B6   | 107.7 (6) | C2—C3—H3B   | 109.5     |
| B8—B10—B6   | 108.6 (7) | H3A—C3—H3B  | 109.5     |
| C2—B10—H10  | 124.5     | C2—C3—H3C   | 109.5     |
| B9—B10—H10  | 122.2     | H3A—C3—H3C  | 109.5     |
| B7—B10—H10  | 121.6     | H3B—C3—H3C  | 109.5     |
| B8—B10—H10  | 121.6     | C5—C4—B16   | 61.1 (5)  |
| B6—B10—H10  | 121.9     | C5—C4—B15   | 110.8 (6) |
| C4—B11—B14  | 104.3 (7) | B16—C4—B15  | 62.8 (5)  |
| C4—B11—B13  | 105.2 (6) | C5—C4—B11   | 110.5 (6) |
| B14—B11—B13 | 61.7 (6)  | B16—C4—B11  | 115.3 (6) |

|             |            |                 |            |
|-------------|------------|-----------------|------------|
| C4—B11—B12  | 59.2 (5)   | B15—C4—B11      | 63.5 (5)   |
| B14—B11—B12 | 108.5 (7)  | C5—C4—B12       | 60.6 (4)   |
| B13—B11—B12 | 59.5 (5)   | B16—C4—B12      | 114.0 (6)  |
| C4—B11—B15  | 58.2 (5)   | B15—C4—B12      | 114.9 (6)  |
| B14—B11—B15 | 59.2 (6)   | B11—C4—B12      | 62.5 (5)   |
| B13—B11—B15 | 108.8 (7)  | C5—C4—Se3       | 117.6 (4)  |
| B12—B11—B15 | 107.8 (6)  | B16—C4—Se3      | 110.6 (5)  |
| C4—B11—H11  | 124.9      | B15—C4—Se3      | 117.7 (5)  |
| B14—B11—H11 | 122.1      | B11—C4—Se3      | 124.9 (5)  |
| B13—B11—H11 | 121.5      | B12—C4—Se3      | 121.9 (5)  |
| B12—B11—H11 | 121.5      | C6—C5—B20       | 120.9 (6)  |
| B15—B11—H11 | 121.8      | C6—C5—C4        | 119.0 (6)  |
| C4—B12—C5   | 59.0 (4)   | B20—C5—C4       | 109.6 (6)  |
| C4—B12—B13  | 104.6 (6)  | C6—C5—B17       | 122.2 (7)  |
| C5—B12—B13  | 105.1 (6)  | B20—C5—B17      | 63.8 (5)   |
| C4—B12—B17  | 104.8 (6)  | C4—C5—B17       | 108.9 (5)  |
| C5—B12—B17  | 58.2 (5)   | C6—C5—B16       | 116.9 (6)  |
| B13—B12—B17 | 59.4 (5)   | B20—C5—B16      | 62.8 (5)   |
| C4—B12—B11  | 58.3 (5)   | C4—C5—B16       | 59.5 (4)   |
| C5—B12—B11  | 105.8 (6)  | B17—C5—B16      | 114.1 (6)  |
| B13—B12—B11 | 59.5 (5)   | C6—C5—B12       | 117.1 (6)  |
| B17—B12—B11 | 106.7 (6)  | B20—C5—B12      | 115.0 (6)  |
| C4—B12—H12  | 124.0      | C4—C5—B12       | 60.4 (4)   |
| C5—B12—H12  | 123.4      | B17—C5—B12      | 62.1 (5)   |
| B13—B12—H12 | 123.3      | B16—C5—B12      | 112.5 (6)  |
| B17—B12—H12 | 123.0      | C5—C6—H6A       | 109.5      |
| B11—B12—H12 | 122.5      | C5—C6—H6B       | 109.5      |
| B17—B13—B12 | 60.6 (5)   | H6A—C6—H6B      | 109.5      |
| B17—B13—B11 | 108.8 (7)  | C5—C6—H6C       | 109.5      |
| B12—B13—B11 | 61.0 (5)   | H6A—C6—H6C      | 109.5      |
| B17—B13—B18 | 59.6 (6)   | H6B—C6—H6C      | 109.5      |
| B12—B13—B18 | 108.1 (7)  | C1—Se1—Se2      | 104.2 (2)  |
| B11—B13—B18 | 107.2 (7)  | Se1—Se2—Se3     | 105.60 (4) |
| B17—B13—B14 | 106.8 (7)  | C4—Se3—Se2      | 103.3 (2)  |
| B12—B13—B14 | 107.6 (7)  |                 |            |
| B3—B1—B2—C1 | -34.0 (5)  | B11—B13—B18—B14 | 35.7 (6)   |
| B5—B1—B2—C1 | -134.4 (6) | B17—B13—B18—B20 | 37.3 (7)   |
| B4—B1—B2—C1 | -97.1 (6)  | B12—B13—B18—B20 | -0.4 (9)   |
| C1—B1—B2—C2 | 36.4 (5)   | B11—B13—B18—B20 | -64.7 (8)  |
| B3—B1—B2—C2 | 2.4 (8)    | B14—B13—B18—B20 | -100.5 (8) |
| B5—B1—B2—C2 | -98.0 (7)  | B17—B13—B18—B19 | 99.9 (7)   |
| B4—B1—B2—C2 | -60.7 (7)  | B12—B13—B18—B19 | 62.2 (8)   |
| C1—B1—B2—B5 | 134.4 (6)  | B11—B13—B18—B19 | -2.1 (9)   |
| B3—B1—B2—B5 | 100.4 (7)  | B14—B13—B18—B19 | -37.9 (7)  |
| B4—B1—B2—B5 | 37.3 (6)   | C4—B15—B19—B16  | 38.7 (6)   |
| C1—B1—B2—B6 | 96.9 (6)   | B14—B15—B19—B16 | 136.8 (7)  |
| B3—B1—B2—B6 | 62.9 (8)   | B11—B15—B19—B16 | 99.8 (7)   |
| B5—B1—B2—B6 | -37.5 (6)  | C4—B15—B19—B14  | -98.1 (7)  |
| B4—B1—B2—B6 | -0.2 (8)   | B16—B15—B19—B14 | -136.8 (7) |

## supplementary materials

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|             |            |                 |            |
|-------------|------------|-----------------|------------|
| B2—B1—B3—C1 | 34.0 (5)   | B11—B15—B19—B14 | -37.0 (6)  |
| B5—B1—B3—C1 | 95.7 (7)   | C4—B15—B19—B20  | 1.3 (9)    |
| B4—B1—B3—C1 | 133.2 (6)  | B14—B15—B19—B20 | 99.4 (8)   |
| C1—B1—B3—B8 | -96.0 (7)  | B16—B15—B19—B20 | -37.4 (7)  |
| B2—B1—B3—B8 | -62.0 (8)  | B11—B15—B19—B20 | 62.4 (9)   |
| B5—B1—B3—B8 | -0.3 (8)   | C4—B15—B19—B18  | -62.2 (8)  |
| B4—B1—B3—B8 | 37.2 (6)   | B14—B15—B19—B18 | 35.9 (6)   |
| C1—B1—B3—B7 | -33.0 (6)  | B16—B15—B19—B18 | -100.9 (7) |
| B2—B1—B3—B7 | 1.0 (8)    | B11—B15—B19—B18 | -1.1 (9)   |
| B5—B1—B3—B7 | 62.7 (8)   | C4—B16—B19—B15  | -38.6 (6)  |
| B4—B1—B3—B7 | 100.2 (7)  | C5—B16—B19—B15  | -100.1 (7) |
| C1—B1—B3—B4 | -133.2 (6) | B20—B16—B19—B15 | -138.5 (7) |
| B2—B1—B3—B4 | -99.2 (7)  | C4—B16—B19—B14  | -0.1 (9)   |
| B5—B1—B3—B4 | -37.5 (6)  | C5—B16—B19—B14  | -61.7 (8)  |
| C1—B3—B4—B9 | 61.2 (8)   | B15—B16—B19—B14 | 38.4 (6)   |
| B8—B3—B4—B9 | -37.9 (7)  | B20—B16—B19—B14 | -100.0 (8) |
| B7—B3—B4—B9 | 0.6 (8)    | C4—B16—B19—B20  | 99.9 (7)   |
| B1—B3—B4—B9 | 100.4 (8)  | C5—B16—B19—B20  | 38.3 (6)   |
| C1—B3—B4—B8 | 99.1 (7)   | B15—B16—B19—B20 | 138.5 (7)  |
| B7—B3—B4—B8 | 38.5 (6)   | C4—B16—B19—B18  | 61.8 (8)   |
| B1—B3—B4—B8 | 138.3 (7)  | C5—B16—B19—B18  | 0.3 (9)    |
| C1—B3—B4—B5 | -2.1 (8)   | B15—B16—B19—B18 | 100.4 (8)  |
| B8—B3—B4—B5 | -101.2 (7) | B20—B16—B19—B18 | -38.0 (7)  |
| B7—B3—B4—B5 | -62.7 (8)  | B11—B14—B19—B15 | 38.0 (6)   |
| B1—B3—B4—B5 | 37.1 (6)   | B18—B14—B19—B15 | 139.1 (7)  |
| C1—B3—B4—B1 | -39.2 (5)  | B13—B14—B19—B15 | 100.9 (7)  |
| B8—B3—B4—B1 | -138.3 (7) | B11—B14—B19—B16 | -1.0 (9)   |
| B7—B3—B4—B1 | -99.8 (7)  | B15—B14—B19—B16 | -39.0 (6)  |
| C1—B1—B4—B9 | -60.4 (8)  | B18—B14—B19—B16 | 100.1 (7)  |
| B2—B1—B4—B9 | 1.0 (9)    | B13—B14—B19—B16 | 61.9 (9)   |
| B3—B1—B4—B9 | -100.6 (7) | B11—B14—B19—B20 | -64.2 (9)  |
| B5—B1—B4—B9 | 37.5 (6)   | B15—B14—B19—B20 | -102.2 (7) |
| C1—B1—B4—B8 | 3.8 (8)    | B18—B14—B19—B20 | 36.9 (6)   |
| B2—B1—B4—B8 | 65.1 (8)   | B13—B14—B19—B20 | -1.3 (9)   |
| B3—B1—B4—B8 | -36.4 (6)  | B11—B14—B19—B18 | -101.1 (7) |
| B5—B1—B4—B8 | 101.7 (7)  | B15—B14—B19—B18 | -139.1 (7) |
| C1—B1—B4—B3 | 40.2 (6)   | B13—B14—B19—B18 | -38.2 (6)  |
| B2—B1—B4—B3 | 101.5 (7)  | B17—B18—B19—B15 | 64.4 (9)   |
| B5—B1—B4—B3 | 138.1 (7)  | B14—B18—B19—B15 | -36.3 (6)  |
| C1—B1—B4—B5 | -97.9 (7)  | B13—B18—B19—B15 | 2.0 (9)    |
| B2—B1—B4—B5 | -36.6 (6)  | B20—B18—B19—B15 | 102.3 (7)  |
| B3—B1—B4—B5 | -138.1 (7) | B17—B18—B19—B16 | 0.1 (9)    |
| C1—B2—B5—B6 | -98.9 (6)  | B14—B18—B19—B16 | -100.6 (7) |
| C2—B2—B5—B6 | -37.3 (6)  | B13—B18—B19—B16 | -62.3 (9)  |
| B1—B2—B5—B6 | -138.0 (7) | B20—B18—B19—B16 | 38.0 (6)   |
| C1—B2—B5—B9 | -60.7 (8)  | B17—B18—B19—B14 | 100.7 (7)  |
| C2—B2—B5—B9 | 0.8 (8)    | B13—B18—B19—B14 | 38.3 (6)   |
| B1—B2—B5—B9 | -99.8 (7)  | B20—B18—B19—B14 | 138.6 (7)  |
| B6—B2—B5—B9 | 38.2 (6)   | B17—B18—B19—B20 | -37.9 (6)  |

|              |            |                 |            |
|--------------|------------|-----------------|------------|
| C1—B2—B5—B1  | 39.1 (6)   | B14—B18—B19—B20 | -138.6 (7) |
| C2—B2—B5—B1  | 100.6 (6)  | B13—B18—B19—B20 | -100.2 (7) |
| B6—B2—B5—B1  | 138.0 (7)  | C4—B16—B20—C5   | 36.8 (5)   |
| C1—B2—B5—B4  | 1.3 (8)    | B19—B16—B20—C5  | 134.7 (7)  |
| C2—B2—B5—B4  | 62.8 (8)   | B15—B16—B20—C5  | 98.3 (7)   |
| B1—B2—B5—B4  | -37.8 (6)  | C4—B16—B20—B17  | 1.8 (9)    |
| B6—B2—B5—B4  | 100.2 (8)  | C5—B16—B20—B17  | -35.1 (6)  |
| C1—B1—B5—B2  | -39.0 (6)  | B19—B16—B20—B17 | 99.7 (7)   |
| B3—B1—B5—B2  | -100.5 (7) | B15—B16—B20—B17 | 63.2 (8)   |
| B4—B1—B5—B2  | -137.9 (7) | C4—B16—B20—B19  | -97.9 (7)  |
| C1—B1—B5—B6  | -0.5 (9)   | C5—B16—B20—B19  | -134.7 (7) |
| B2—B1—B5—B6  | 38.5 (6)   | B15—B16—B20—B19 | -36.4 (6)  |
| B3—B1—B5—B6  | -62.0 (8)  | C4—B16—B20—B18  | -59.7 (8)  |
| B4—B1—B5—B6  | -99.4 (8)  | C5—B16—B20—B18  | -96.5 (7)  |
| C1—B1—B5—B9  | 62.1 (8)   | B19—B16—B20—B18 | 38.3 (7)   |
| B2—B1—B5—B9  | 101.2 (7)  | B15—B16—B20—B18 | 1.8 (9)    |
| B3—B1—B5—B9  | 0.6 (8)    | B13—B17—B20—C5  | -97.4 (7)  |
| B4—B1—B5—B9  | -36.8 (6)  | B18—B17—B20—C5  | -135.7 (7) |
| C1—B1—B5—B4  | 98.9 (7)   | B12—B17—B20—C5  | -33.6 (6)  |
| B2—B1—B5—B4  | 137.9 (7)  | C5—B17—B20—B16  | 35.6 (6)   |
| B3—B1—B5—B4  | 37.4 (6)   | B13—B17—B20—B16 | -61.8 (9)  |
| B9—B4—B5—B2  | -100.3 (7) | B18—B17—B20—B16 | -100.1 (7) |
| B8—B4—B5—B2  | -61.4 (9)  | B12—B17—B20—B16 | 2.0 (9)    |
| B3—B4—B5—B2  | 0.5 (9)    | C5—B17—B20—B19  | 97.9 (7)   |
| B1—B4—B5—B2  | 37.7 (6)   | B13—B17—B20—B19 | 0.5 (9)    |
| B9—B4—B5—B6  | -35.3 (6)  | B18—B17—B20—B19 | -37.9 (7)  |
| B8—B4—B5—B6  | 3.5 (9)    | B12—B17—B20—B19 | 64.3 (8)   |
| B3—B4—B5—B6  | 65.5 (8)   | C5—B17—B20—B18  | 135.7 (7)  |
| B1—B4—B5—B6  | 102.6 (7)  | B13—B17—B20—B18 | 38.4 (7)   |
| B8—B4—B5—B9  | 38.9 (6)   | B12—B17—B20—B18 | 102.2 (7)  |
| B3—B4—B5—B9  | 100.8 (7)  | B15—B19—B20—C5  | -1.6 (10)  |
| B1—B4—B5—B9  | 137.9 (7)  | B16—B19—B20—C5  | -39.5 (6)  |
| B9—B4—B5—B1  | -137.9 (7) | B14—B19—B20—C5  | 61.6 (8)   |
| B8—B4—B5—B1  | -99.1 (7)  | B18—B19—B20—C5  | 97.9 (7)   |
| B3—B4—B5—B1  | -37.1 (6)  | B15—B19—B20—B16 | 37.8 (7)   |
| B2—B5—B6—C2  | 38.3 (6)   | B14—B19—B20—B16 | 101.0 (8)  |
| B9—B5—B6—C2  | -98.5 (7)  | B18—B19—B20—B16 | 137.3 (7)  |
| B1—B5—B6—C2  | 0.4 (9)    | B15—B19—B20—B17 | -62.7 (9)  |
| B4—B5—B6—C2  | -63.4 (8)  | B16—B19—B20—B17 | -100.5 (7) |
| B2—B5—B6—B9  | 136.8 (7)  | B14—B19—B20—B17 | 0.5 (9)    |
| B1—B5—B6—B9  | 98.9 (8)   | B18—B19—B20—B17 | 36.8 (6)   |
| B4—B5—B6—B9  | 35.1 (6)   | B15—B19—B20—B18 | -99.5 (8)  |
| B2—B5—B6—B10 | 99.4 (7)   | B16—B19—B20—B18 | -137.3 (7) |
| B9—B5—B6—B10 | -37.4 (6)  | B14—B19—B20—B18 | -36.3 (6)  |
| B1—B5—B6—B10 | 61.5 (9)   | B17—B18—B20—C5  | 37.8 (6)   |
| B4—B5—B6—B10 | -2.3 (9)   | B14—B18—B20—C5  | -63.1 (8)  |
| B9—B5—B6—B2  | -136.8 (7) | B13—B18—B20—C5  | 1.0 (9)    |
| B1—B5—B6—B2  | -37.9 (6)  | B19—B18—B20—C5  | -99.8 (7)  |
| B4—B5—B6—B2  | -101.7 (7) | B17—B18—B20—B16 | 100.0 (7)  |

## supplementary materials

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|              |            |                 |            |
|--------------|------------|-----------------|------------|
| C1—B2—B6—C2  | -36.4 (5)  | B14—B18—B20—B16 | -0.9 (9)   |
| B5—B2—B6—C2  | -135.9 (7) | B13—B18—B20—B16 | 63.2 (9)   |
| B1—B2—B6—C2  | -97.4 (6)  | B19—B18—B20—B16 | -37.6 (6)  |
| C1—B2—B6—B9  | 60.3 (8)   | B14—B18—B20—B17 | -100.9 (7) |
| C2—B2—B6—B9  | 96.7 (7)   | B13—B18—B20—B17 | -36.8 (7)  |
| B5—B2—B6—B9  | -39.2 (7)  | B19—B18—B20—B17 | -137.6 (7) |
| B1—B2—B6—B9  | -0.7 (8)   | B17—B18—B20—B19 | 137.6 (7)  |
| C1—B2—B6—B5  | 99.5 (7)   | B14—B18—B20—B19 | 36.8 (7)   |
| C2—B2—B6—B5  | 135.9 (7)  | B13—B18—B20—B19 | 100.9 (7)  |
| B1—B2—B6—B5  | 38.5 (6)   | B2—B1—C1—C2     | -38.4 (6)  |
| C1—B2—B6—B10 | -2.2 (8)   | B3—B1—C1—C2     | 103.2 (6)  |
| C2—B2—B6—B10 | 34.2 (6)   | B5—B1—C1—C2     | 0.4 (8)    |
| B5—B2—B6—B10 | -101.7 (8) | B4—B1—C1—C2     | 62.6 (7)   |
| B1—B2—B6—B10 | -63.3 (8)  | B2—B1—C1—B7     | -105.0 (7) |
| B8—B3—B7—C1  | 134.4 (7)  | B3—B1—C1—B7     | 36.6 (7)   |
| B1—B3—B7—C1  | 32.6 (6)   | B5—B1—C1—B7     | -66.2 (8)  |
| B4—B3—B7—C1  | 96.0 (7)   | B4—B1—C1—B7     | -4.0 (9)   |
| C1—B3—B7—C2  | -36.6 (5)  | B3—B1—C1—B2     | 141.6 (6)  |
| B8—B3—B7—C2  | 97.8 (7)   | B5—B1—C1—B2     | 38.8 (6)   |
| B1—B3—B7—C2  | -4.0 (8)   | B4—B1—C1—B2     | 101.0 (6)  |
| B4—B3—B7—C2  | 59.3 (7)   | B2—B1—C1—B3     | -141.6 (6) |
| C1—B3—B7—B8  | -134.4 (7) | B5—B1—C1—B3     | -102.8 (7) |
| B1—B3—B7—B8  | -101.8 (7) | B4—B1—C1—B3     | -40.6 (6)  |
| B4—B3—B7—B8  | -38.4 (6)  | B2—B1—C1—Se1    | 113.0 (6)  |
| C1—B3—B7—B10 | -97.7 (7)  | B3—B1—C1—Se1    | -105.4 (6) |
| B8—B3—B7—B10 | 36.7 (6)   | B5—B1—C1—Se1    | 151.8 (5)  |
| B1—B3—B7—B10 | -65.2 (7)  | B4—B1—C1—Se1    | -146.0 (5) |
| B4—B3—B7—B10 | -1.8 (8)   | B8—B7—C1—C2     | -98.7 (7)  |
| C1—B3—B8—B7  | 38.9 (6)   | B3—B7—C1—C2     | -138.4 (6) |
| B1—B3—B8—B7  | 98.9 (7)   | B10—B7—C1—C2    | -35.7 (6)  |
| B4—B3—B8—B7  | 136.4 (7)  | C2—B7—C1—B1     | 101.2 (7)  |
| C1—B3—B8—B4  | -97.5 (6)  | B8—B7—C1—B1     | 2.6 (9)    |
| B7—B3—B8—B4  | -136.4 (7) | B3—B7—C1—B1     | -37.2 (7)  |
| B1—B3—B8—B4  | -37.6 (6)  | B10—B7—C1—B1    | 65.5 (8)   |
| C1—B3—B8—B10 | 2.2 (8)    | C2—B7—C1—B2     | 31.5 (6)   |
| B7—B3—B8—B10 | -36.7 (6)  | B8—B7—C1—B2     | -67.2 (8)  |
| B1—B3—B8—B10 | 62.1 (8)   | B3—B7—C1—B2     | -107.0 (6) |
| B4—B3—B8—B10 | 99.7 (7)   | B10—B7—C1—B2    | -4.3 (8)   |
| C1—B3—B8—B9  | -60.2 (7)  | C2—B7—C1—B3     | 138.4 (6)  |
| B7—B3—B8—B9  | -99.1 (7)  | B8—B7—C1—B3     | 39.8 (6)   |
| B1—B3—B8—B9  | -0.2 (8)   | B10—B7—C1—B3    | 102.7 (7)  |
| B4—B3—B8—B9  | 37.3 (6)   | C2—B7—C1—Se1    | -112.0 (5) |
| C1—B7—B8—B3  | -39.7 (6)  | B8—B7—C1—Se1    | 149.4 (5)  |
| C2—B7—B8—B3  | -101.3 (6) | B3—B7—C1—Se1    | 109.6 (6)  |
| B10—B7—B8—B3 | -139.4 (7) | B10—B7—C1—Se1   | -147.7 (5) |
| C1—B7—B8—B4  | 0.1 (9)    | B5—B2—C1—C2     | 97.6 (6)   |
| C2—B7—B8—B4  | -61.5 (8)  | B1—B2—C1—C2     | 138.3 (6)  |
| B3—B7—B8—B4  | 39.8 (6)   | B6—B2—C1—C2     | 35.6 (5)   |
| B10—B7—B8—B4 | -99.6 (7)  | C2—B2—C1—B1     | -138.3 (6) |

|              |            |              |            |
|--------------|------------|--------------|------------|
| C1—B7—B8—B10 | 99.7 (7)   | B5—B2—C1—B1  | -40.7 (6)  |
| C2—B7—B8—B10 | 38.1 (6)   | B6—B2—C1—B1  | -102.7 (7) |
| B3—B7—B8—B10 | 139.4 (7)  | C2—B2—C1—B7  | -31.5 (6)  |
| C1—B7—B8—B9  | 62.6 (8)   | B5—B2—C1—B7  | 66.1 (8)   |
| C2—B7—B8—B9  | 1.0 (8)    | B1—B2—C1—B7  | 106.8 (7)  |
| B3—B7—B8—B9  | 102.2 (7)  | B6—B2—C1—B7  | 4.1 (8)    |
| B10—B7—B8—B9 | -37.2 (6)  | C2—B2—C1—B3  | -100.5 (6) |
| B9—B4—B8—B3  | 138.0 (7)  | B5—B2—C1—B3  | -2.9 (8)   |
| B5—B4—B8—B3  | 99.5 (7)   | B1—B2—C1—B3  | 37.9 (6)   |
| B1—B4—B8—B3  | 36.8 (6)   | B6—B2—C1—B3  | -64.8 (7)  |
| B9—B4—B8—B7  | 98.8 (7)   | C2—B2—C1—Se1 | 107.1 (6)  |
| B3—B4—B8—B7  | -39.3 (6)  | B5—B2—C1—Se1 | -155.3 (5) |
| B5—B4—B8—B7  | 60.3 (9)   | B1—B2—C1—Se1 | -114.6 (6) |
| B1—B4—B8—B7  | -2.4 (9)   | B6—B2—C1—Se1 | 142.7 (5)  |
| B9—B4—B8—B10 | 35.1 (6)   | B8—B3—C1—C2  | -1.4 (8)   |
| B3—B4—B8—B10 | -102.9 (7) | B7—B3—C1—C2  | 38.3 (6)   |
| B5—B4—B8—B10 | -3.4 (9)   | B1—B3—C1—C2  | -103.9 (6) |
| B1—B4—B8—B10 | -66.1 (8)  | B4—B3—C1—C2  | -63.2 (7)  |
| B3—B4—B8—B9  | -138.0 (7) | B8—B3—C1—B1  | 102.5 (7)  |
| B5—B4—B8—B9  | -38.5 (6)  | B7—B3—C1—B1  | 142.2 (7)  |
| B1—B4—B8—B9  | -101.2 (7) | B4—B3—C1—B1  | 40.7 (6)   |
| C2—B6—B9—B10 | -38.3 (6)  | B8—B3—C1—B7  | -39.6 (6)  |
| B5—B6—B9—B10 | -138.0 (7) | B1—B3—C1—B7  | -142.2 (7) |
| B2—B6—B9—B10 | -100.0 (7) | B4—B3—C1—B7  | -101.4 (7) |
| C2—B6—B9—B4  | 63.1 (8)   | B8—B3—C1—B2  | 64.9 (7)   |
| B5—B6—B9—B4  | -36.7 (7)  | B7—B3—C1—B2  | 104.6 (6)  |
| B10—B6—B9—B4 | 101.3 (7)  | B1—B3—C1—B2  | -37.6 (6)  |
| B2—B6—B9—B4  | 1.3 (9)    | B4—B3—C1—B2  | 3.1 (8)    |
| C2—B6—B9—B5  | 99.8 (6)   | B8—B3—C1—Se1 | -140.8 (5) |
| B10—B6—B9—B5 | 138.0 (7)  | B7—B3—C1—Se1 | -101.1 (6) |
| B2—B6—B9—B5  | 38.0 (6)   | B1—B3—C1—Se1 | 116.7 (6)  |
| C2—B6—B9—B8  | -0.6 (8)   | B4—B3—C1—Se1 | 157.4 (5)  |
| B5—B6—B9—B8  | -100.4 (7) | B9—B6—C2—C3  | 152.4 (7)  |
| B10—B6—B9—B8 | 37.7 (6)   | B5—B6—C2—C3  | -143.7 (7) |
| B2—B6—B9—B8  | -62.3 (8)  | B10—B6—C2—C3 | 113.6 (8)  |
| B8—B4—B9—B10 | -36.1 (6)  | B2—B6—C2—C3  | -105.5 (7) |
| B3—B4—B9—B10 | 0.8 (9)    | B9—B6—C2—B10 | 38.8 (6)   |
| B5—B4—B9—B10 | 101.0 (7)  | B5—B6—C2—B10 | 102.7 (7)  |
| B1—B4—B9—B10 | 63.7 (8)   | B2—B6—C2—B10 | 140.9 (7)  |
| B8—B4—B9—B6  | -101.2 (7) | B9—B6—C2—C1  | -64.1 (7)  |
| B3—B4—B9—B6  | -64.3 (9)  | B5—B6—C2—C1  | -0.2 (8)   |
| B5—B4—B9—B6  | 35.8 (6)   | B10—B6—C2—C1 | -102.9 (6) |
| B1—B4—B9—B6  | -1.4 (9)   | B2—B6—C2—C1  | 38.1 (6)   |
| B8—B4—B9—B5  | -137.0 (6) | B9—B6—C2—B2  | -102.1 (7) |
| B3—B4—B9—B5  | -100.2 (7) | B5—B6—C2—B2  | -38.2 (6)  |
| B1—B4—B9—B5  | -37.3 (6)  | B10—B6—C2—B2 | -140.9 (7) |
| B3—B4—B9—B8  | 36.9 (6)   | B9—B6—C2—B7  | 1.3 (8)    |
| B5—B4—B9—B8  | 137.0 (6)  | B5—B6—C2—B7  | 65.2 (8)   |
| B1—B4—B9—B8  | 99.7 (7)   | B10—B6—C2—B7 | -37.5 (6)  |

## supplementary materials

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| B2—B5—B9—B10 | -1.1 (9)   | B2—B6—C2—B7   | 103.4 (6)  |
| B6—B5—B9—B10 | 38.1 (6)   | B9—B10—C2—C3  | -149.8 (7) |
| B1—B5—B9—B10 | -64.4 (8)  | B7—B10—C2—C3  | 107.6 (8)  |
| B4—B5—B9—B10 | -101.9 (7) | B8—B10—C2—C3  | 146.5 (7)  |
| B2—B5—B9—B6  | -39.2 (6)  | B6—B10—C2—C3  | -111.0 (8) |
| B1—B5—B9—B6  | -102.5 (7) | B9—B10—C2—B6  | -38.8 (6)  |
| B4—B5—B9—B6  | -140.0 (7) | B7—B10—C2—B6  | -141.5 (7) |
| B2—B5—B9—B4  | 100.8 (7)  | B8—B10—C2—B6  | -102.5 (7) |
| B6—B5—B9—B4  | 140.0 (7)  | B9—B10—C2—C1  | 65.0 (7)   |
| B1—B5—B9—B4  | 37.5 (6)   | B7—B10—C2—C1  | -37.7 (6)  |
| B2—B5—B9—B8  | 62.5 (8)   | B8—B10—C2—C1  | 1.3 (8)    |
| B6—B5—B9—B8  | 101.7 (7)  | B6—B10—C2—C1  | 103.8 (6)  |
| B1—B5—B9—B8  | -0.8 (8)   | B9—B10—C2—B2  | -0.4 (8)   |
| B4—B5—B9—B8  | -38.3 (6)  | B7—B10—C2—B2  | -103.1 (7) |
| B3—B8—B9—B10 | 101.6 (7)  | B8—B10—C2—B2  | -64.1 (7)  |
| B7—B8—B9—B10 | 37.9 (6)   | B6—B10—C2—B2  | 38.4 (6)   |
| B4—B8—B9—B10 | 140.0 (7)  | B9—B10—C2—B7  | 102.7 (7)  |
| B3—B8—B9—B6  | 63.5 (8)   | B8—B10—C2—B7  | 39.0 (6)   |
| B7—B8—B9—B6  | -0.2 (9)   | B6—B10—C2—B7  | 141.5 (7)  |
| B4—B8—B9—B6  | 101.8 (8)  | B1—C1—C2—C3   | 144.5 (7)  |
| B10—B8—B9—B6 | -38.1 (6)  | B7—C1—C2—C3   | -108.1 (7) |
| B3—B8—B9—B4  | -38.3 (6)  | B2—C1—C2—C3   | 105.1 (7)  |
| B7—B8—B9—B4  | -102.1 (7) | B3—C1—C2—C3   | -146.9 (6) |
| B10—B8—B9—B4 | -140.0 (7) | Se1—C1—C2—C3  | -8.6 (9)   |
| B3—B8—B9—B5  | 0.6 (8)    | B1—C1—C2—B6   | -0.2 (8)   |
| B7—B8—B9—B5  | -63.1 (8)  | B7—C1—C2—B6   | 107.3 (7)  |
| B4—B8—B9—B5  | 39.0 (6)   | B2—C1—C2—B6   | -39.5 (6)  |
| B10—B8—B9—B5 | -101.0 (7) | B3—C1—C2—B6   | 68.5 (7)   |
| B6—B9—B10—C2 | 38.2 (6)   | Se1—C1—C2—B6  | -153.2 (5) |
| B4—B9—B10—C2 | -64.1 (8)  | B1—C1—C2—B10  | -68.6 (7)  |
| B5—B9—B10—C2 | 0.9 (9)    | B7—C1—C2—B10  | 38.8 (6)   |
| B8—B9—B10—C2 | -100.0 (7) | B2—C1—C2—B10  | -107.9 (6) |
| B6—B9—B10—B7 | 100.3 (7)  | B3—C1—C2—B10  | 0.1 (8)    |
| B4—B9—B10—B7 | -1.9 (9)   | Se1—C1—C2—B10 | 138.4 (5)  |
| B5—B9—B10—B7 | 63.1 (8)   | B1—C1—C2—B2   | 39.3 (6)   |
| B8—B9—B10—B7 | -37.8 (6)  | B7—C1—C2—B2   | 146.7 (6)  |
| B6—B9—B10—B8 | 138.2 (7)  | B3—C1—C2—B2   | 107.9 (6)  |
| B4—B9—B10—B8 | 35.9 (6)   | Se1—C1—C2—B2  | -113.7 (5) |
| B5—B9—B10—B8 | 100.9 (7)  | B1—C1—C2—B7   | -107.4 (6) |
| B4—B9—B10—B6 | -102.2 (8) | B2—C1—C2—B7   | -146.7 (6) |
| B5—B9—B10—B6 | -37.2 (6)  | B3—C1—C2—B7   | -38.8 (6)  |
| B8—B9—B10—B6 | -138.2 (7) | Se1—C1—C2—B7  | 99.5 (6)   |
| C1—B7—B10—C2 | 36.3 (6)   | C1—B2—C2—C3   | -108.8 (7) |
| B8—B7—B10—C2 | 135.2 (6)  | B5—B2—C2—C3   | 151.2 (7)  |
| B3—B7—B10—C2 | 98.9 (6)   | B1—B2—C2—C3   | -144.8 (7) |
| C1—B7—B10—B9 | -60.2 (8)  | B6—B2—C2—C3   | 112.9 (8)  |
| C2—B7—B10—B9 | -96.6 (7)  | C1—B2—C2—B6   | 138.3 (6)  |
| B8—B7—B10—B9 | 38.7 (6)   | B5—B2—C2—B6   | 38.2 (6)   |
| B3—B7—B10—B9 | 2.3 (8)    | B1—B2—C2—B6   | 102.3 (7)  |



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| C1—B7—B10—B8    | -98.9 (6)  | C1—B2—C2—B10   | 99.8 (6)   |
| C2—B7—B10—B8    | -135.2 (6) | B5—B2—C2—B10   | -0.3 (8)   |
| B3—B7—B10—B8    | -36.4 (6)  | B1—B2—C2—B10   | 63.8 (7)   |
| C1—B7—B10—B6    | 2.6 (9)    | B6—B2—C2—B10   | -38.5 (6)  |
| C2—B7—B10—B6    | -33.7 (6)  | B5—B2—C2—C1    | -100.0 (7) |
| B8—B7—B10—B6    | 101.5 (7)  | B1—B2—C2—C1    | -36.0 (5)  |
| B3—B7—B10—B6    | 65.1 (8)   | B6—B2—C2—C1    | -138.3 (6) |
| B3—B8—B10—C2    | -2.2 (8)   | C1—B2—C2—B7    | 30.8 (5)   |
| B7—B8—B10—C2    | -39.0 (5)  | B5—B2—C2—B7    | -69.2 (8)  |
| B4—B8—B10—C2    | 63.0 (8)   | B1—B2—C2—B7    | -5.2 (8)   |
| B9—B8—B10—C2    | 98.3 (7)   | B6—B2—C2—B7    | -107.5 (7) |
| B3—B8—B10—B9    | -100.5 (7) | C1—B7—C2—C3    | 107.6 (7)  |
| B7—B8—B10—B9    | -137.3 (7) | B8—B7—C2—C3    | -153.3 (7) |
| B4—B8—B10—B9    | -35.3 (6)  | B3—B7—C2—C3    | 144.3 (7)  |
| B3—B8—B10—B7    | 36.8 (6)   | B10—B7—C2—C3   | -113.9 (8) |
| B4—B8—B10—B7    | 102.0 (7)  | C1—B7—C2—B6    | -100.6 (6) |
| B9—B8—B10—B7    | 137.3 (7)  | B8—B7—C2—B6    | -1.5 (8)   |
| B3—B8—B10—B6    | -63.2 (8)  | B3—B7—C2—B6    | -63.8 (7)  |
| B7—B8—B10—B6    | -100.0 (7) | B10—B7—C2—B6   | 37.9 (6)   |
| B4—B8—B10—B6    | 2.0 (8)    | C1—B7—C2—B10   | -138.4 (6) |
| B9—B8—B10—B6    | 37.3 (6)   | B8—B7—C2—B10   | -39.3 (6)  |
| B9—B6—B10—C2    | -135.2 (7) | B3—B7—C2—B10   | -101.7 (7) |
| B5—B6—B10—C2    | -96.9 (7)  | B8—B7—C2—C1    | 99.1 (6)   |
| B2—B6—B10—C2    | -34.5 (6)  | B3—B7—C2—C1    | 36.7 (5)   |
| C2—B6—B10—B9    | 135.2 (7)  | B10—B7—C2—C1   | 138.4 (6)  |
| B5—B6—B10—B9    | 38.3 (6)   | C1—B7—C2—B2    | -30.9 (6)  |
| B2—B6—B10—B9    | 100.7 (7)  | B8—B7—C2—B2    | 68.3 (7)   |
| C2—B6—B10—B7    | 34.3 (6)   | B3—B7—C2—B2    | 5.9 (8)    |
| B9—B6—B10—B7    | -100.9 (8) | B10—B7—C2—B2   | 107.6 (7)  |
| B5—B6—B10—B7    | -62.6 (8)  | B19—B16—C4—C5  | -99.1 (7)  |
| B2—B6—B10—B7    | -0.2 (9)   | B15—B16—C4—C5  | -137.6 (6) |
| C2—B6—B10—B8    | 97.1 (7)   | B20—B16—C4—C5  | -36.0 (6)  |
| B9—B6—B10—B8    | -38.1 (6)  | C5—B16—C4—B15  | 137.6 (6)  |
| B5—B6—B10—B8    | 0.2 (9)    | B19—B16—C4—B15 | 38.5 (6)   |
| B2—B6—B10—B8    | 62.6 (8)   | B20—B16—C4—B15 | 101.6 (7)  |
| B14—B11—B12—C4  | -96.0 (7)  | C5—B16—C4—B11  | 100.4 (7)  |
| B13—B11—B12—C4  | -134.9 (7) | B19—B16—C4—B11 | 1.3 (8)    |
| B15—B11—B12—C4  | -33.3 (6)  | B15—B16—C4—B11 | -37.2 (7)  |
| C4—B11—B12—C5   | 36.5 (5)   | B20—B16—C4—B11 | 64.4 (8)   |
| B14—B11—B12—C5  | -59.5 (8)  | C5—B16—C4—B12  | 30.8 (6)   |
| B13—B11—B12—C5  | -98.5 (6)  | B19—B16—C4—B12 | -68.3 (8)  |
| B15—B11—B12—C5  | 3.2 (8)    | B15—B16—C4—B12 | -106.8 (7) |
| C4—B11—B12—B13  | 134.9 (7)  | B20—B16—C4—B12 | -5.2 (8)   |
| B14—B11—B12—B13 | 39.0 (7)   | C5—B16—C4—Se3  | -111.0 (5) |
| B15—B11—B12—B13 | 101.7 (7)  | B19—B16—C4—Se3 | 149.9 (5)  |
| C4—B11—B12—B17  | 97.4 (7)   | B15—B16—C4—Se3 | 111.4 (6)  |
| B14—B11—B12—B17 | 1.4 (9)    | B20—B16—C4—Se3 | -147.0 (5) |
| B13—B11—B12—B17 | -37.6 (6)  | B19—B15—C4—C5  | -0.5 (8)   |
| B15—B11—B12—B17 | 64.1 (8)   | B14—B15—C4—C5  | -64.5 (8)  |

## supplementary materials

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| C4—B12—B13—B17  | -98.8 (7)  | B16—B15—C4—C5  | 39.1 (6)   |
| C5—B12—B13—B17  | -37.6 (6)  | B11—B15—C4—C5  | -103.2 (6) |
| B11—B12—B13—B17 | -137.3 (7) | B19—B15—C4—B16 | -39.6 (6)  |
| C4—B12—B13—B11  | 38.5 (6)   | B14—B15—C4—B16 | -103.6 (7) |
| C5—B12—B13—B11  | 99.7 (6)   | B11—B15—C4—B16 | -142.4 (7) |
| B17—B12—B13—B11 | 137.3 (7)  | B19—B15—C4—B11 | 102.7 (8)  |
| C4—B12—B13—B18  | -61.6 (8)  | B14—B15—C4—B11 | 38.8 (6)   |
| C5—B12—B13—B18  | -0.4 (8)   | B16—B15—C4—B11 | 142.4 (7)  |
| B17—B12—B13—B18 | 37.3 (7)   | B19—B15—C4—B12 | 65.8 (8)   |
| B11—B12—B13—B18 | -100.0 (7) | B14—B15—C4—B12 | 1.8 (9)    |
| C4—B12—B13—B14  | 0.9 (8)    | B16—B15—C4—B12 | 105.4 (7)  |
| C5—B12—B13—B14  | 62.1 (8)   | B11—B15—C4—B12 | -36.9 (7)  |
| B17—B12—B13—B14 | 99.8 (8)   | B19—B15—C4—Se3 | -139.9 (6) |
| B11—B12—B13—B14 | -37.6 (7)  | B14—B15—C4—Se3 | 156.1 (6)  |
| C4—B11—B13—B17  | -0.4 (9)   | B16—B15—C4—Se3 | -100.2 (6) |
| B14—B11—B13—B17 | -98.7 (8)  | B11—B15—C4—Se3 | 117.4 (6)  |
| B12—B11—B13—B17 | 38.6 (6)   | B14—B11—C4—C5  | 64.9 (7)   |
| B15—B11—B13—B17 | -61.5 (8)  | B13—B11—C4—C5  | 0.8 (8)    |
| C4—B11—B13—B12  | -39.0 (6)  | B12—B11—C4—C5  | -38.4 (6)  |
| B14—B11—B13—B12 | -137.3 (7) | B15—B11—C4—C5  | 103.7 (7)  |
| B15—B11—B13—B12 | -100.1 (7) | B14—B11—C4—B16 | -1.9 (9)   |
| C4—B11—B13—B18  | 62.5 (8)   | B13—B11—C4—B16 | -66.0 (8)  |
| B14—B11—B13—B18 | -35.8 (6)  | B12—B11—C4—B16 | -105.2 (7) |
| B12—B11—B13—B18 | 101.6 (7)  | B15—B11—C4—B16 | 36.9 (7)   |
| B15—B11—B13—B18 | 1.5 (9)    | B14—B11—C4—B15 | -38.8 (6)  |
| C4—B11—B13—B14  | 98.3 (7)   | B13—B11—C4—B15 | -102.9 (7) |
| B12—B11—B13—B14 | 137.3 (7)  | B12—B11—C4—B15 | -142.1 (7) |
| B15—B11—B13—B14 | 37.2 (6)   | B14—B11—C4—B12 | 103.3 (7)  |
| C4—B11—B14—B15  | 38.4 (6)   | B13—B11—C4—B12 | 39.2 (6)   |
| B13—B11—B14—B15 | 138.2 (7)  | B15—B11—C4—B12 | 142.1 (7)  |
| B12—B11—B14—B15 | 100.2 (7)  | B14—B11—C4—Se3 | -145.5 (6) |
| C4—B11—B14—B18  | -63.5 (8)  | B13—B11—C4—Se3 | 150.5 (5)  |
| B13—B11—B14—B18 | 36.3 (7)   | B12—B11—C4—Se3 | 111.3 (7)  |
| B12—B11—B14—B18 | -1.7 (9)   | B15—B11—C4—Se3 | -106.6 (7) |
| B15—B11—B14—B18 | -101.8 (7) | B13—B12—C4—C5  | 99.0 (6)   |
| C4—B11—B14—B19  | 1.7 (9)    | B17—B12—C4—C5  | 37.4 (5)   |
| B13—B11—B14—B19 | 101.5 (7)  | B11—B12—C4—C5  | 138.1 (6)  |
| B12—B11—B14—B19 | 63.5 (9)   | C5—B12—C4—B16  | -30.9 (6)  |
| B15—B11—B14—B19 | -36.7 (6)  | B13—B12—C4—B16 | 68.1 (8)   |
| C4—B11—B14—B13  | -99.8 (7)  | B17—B12—C4—B16 | 6.5 (8)    |
| B12—B11—B14—B13 | -38.0 (7)  | B11—B12—C4—B16 | 107.2 (7)  |
| B15—B11—B14—B13 | -138.2 (7) | C5—B12—C4—B15  | -100.8 (7) |
| B17—B13—B14—B11 | 102.2 (7)  | B13—B12—C4—B15 | -1.8 (8)   |
| B12—B13—B14—B11 | 38.4 (6)   | B17—B12—C4—B15 | -63.4 (8)  |
| B18—B13—B14—B11 | 139.4 (7)  | B11—B12—C4—B15 | 37.3 (7)   |
| B17—B13—B14—B15 | 63.9 (9)   | C5—B12—C4—B11  | -138.1 (6) |
| B12—B13—B14—B15 | 0.1 (10)   | B13—B12—C4—B11 | -39.1 (6)  |
| B11—B13—B14—B15 | -38.3 (7)  | B17—B12—C4—B11 | -100.8 (6) |
| B18—B13—B14—B15 | 101.1 (8)  | C5—B12—C4—Se3  | 106.1 (6)  |

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|-----------------|------------|----------------|------------|
| B17—B13—B14—B18 | -37.2 (7)  | B13—B12—C4—Se3 | -154.9 (5) |
| B12—B13—B14—B18 | -101.0 (7) | B17—B12—C4—Se3 | 143.4 (5)  |
| B11—B13—B14—B18 | -139.4 (7) | B11—B12—C4—Se3 | -115.8 (6) |
| B17—B13—B14—B19 | 1.7 (9)    | B16—B20—C5—C6  | 106.6 (8)  |
| B12—B13—B14—B19 | -62.1 (8)  | B17—B20—C5—C6  | -113.5 (8) |
| B11—B13—B14—B19 | -100.5 (7) | B19—B20—C5—C6  | 145.8 (7)  |
| B18—B13—B14—B19 | 38.9 (7)   | B18—B20—C5—C6  | -151.2 (7) |
| B11—B14—B15—C4  | -38.3 (6)  | B16—B20—C5—C4  | -37.9 (6)  |
| B18—B14—B15—C4  | 62.6 (8)   | B17—B20—C5—C4  | 102.0 (6)  |
| B19—B14—B15—C4  | 100.0 (7)  | B19—B20—C5—C4  | 1.3 (8)    |
| B13—B14—B15—C4  | -1.1 (9)   | B18—B20—C5—C4  | 64.3 (7)   |
| B11—B14—B15—B19 | -138.4 (7) | B16—B20—C5—B17 | -139.9 (7) |
| B18—B14—B15—B19 | -37.4 (7)  | B19—B20—C5—B17 | -100.7 (7) |
| B13—B14—B15—B19 | -101.1 (8) | B18—B20—C5—B17 | -37.8 (6)  |
| B11—B14—B15—B16 | -99.4 (7)  | B17—B20—C5—B16 | 139.9 (7)  |
| B18—B14—B15—B16 | 1.6 (9)    | B19—B20—C5—B16 | 39.2 (6)   |
| B19—B14—B15—B16 | 39.0 (6)   | B18—B20—C5—B16 | 102.2 (7)  |
| B13—B14—B15—B16 | -62.1 (9)  | B16—B20—C5—B12 | -103.6 (7) |
| B18—B14—B15—B11 | 101.0 (7)  | B17—B20—C5—B12 | 36.4 (6)   |
| B19—B14—B15—B11 | 138.4 (7)  | B19—B20—C5—B12 | -64.3 (8)  |
| B13—B14—B15—B11 | 37.2 (7)   | B18—B20—C5—B12 | -1.4 (8)   |
| B14—B11—B15—C4  | 135.0 (7)  | B16—C4—C5—C6   | -105.9 (7) |
| B13—B11—B15—C4  | 96.7 (7)   | B15—C4—C5—C6   | -145.8 (7) |
| B12—B11—B15—C4  | 33.6 (6)   | B11—C4—C5—C6   | 145.7 (7)  |
| C4—B11—B15—B19  | -96.9 (7)  | B12—C4—C5—C6   | 106.5 (7)  |
| B14—B11—B15—B19 | 38.1 (7)   | Se3—C4—C5—C6   | -6.4 (8)   |
| B13—B11—B15—B19 | -0.2 (9)   | B16—C4—C5—B20  | 39.3 (6)   |
| B12—B11—B15—B19 | -63.2 (8)  | B15—C4—C5—B20  | -0.6 (8)   |
| C4—B11—B15—B14  | -135.0 (7) | B11—C4—C5—B20  | -69.0 (7)  |
| B13—B11—B15—B14 | -38.3 (6)  | B12—C4—C5—B20  | -108.2 (6) |
| B12—B11—B15—B14 | -101.3 (7) | Se3—C4—C5—B20  | 138.9 (6)  |
| C4—B11—B15—B16  | -33.0 (6)  | B16—C4—C5—B17  | 107.5 (6)  |
| B14—B11—B15—B16 | 102.0 (7)  | B15—C4—C5—B17  | 67.6 (7)   |
| B13—B11—B15—B16 | 63.6 (8)   | B11—C4—C5—B17  | -0.9 (8)   |
| B12—B11—B15—B16 | 0.6 (9)    | B12—C4—C5—B17  | -40.1 (6)  |
| B19—B15—B16—C4  | 135.0 (7)  | Se3—C4—C5—B17  | -153.0 (5) |
| B14—B15—B16—C4  | 95.4 (7)   | B15—C4—C5—B16  | -39.9 (6)  |
| B11—B15—B16—C4  | 32.9 (6)   | B11—C4—C5—B16  | -108.4 (7) |
| C4—B15—B16—C5   | -37.2 (5)  | B12—C4—C5—B16  | -147.6 (6) |
| B19—B15—B16—C5  | 97.8 (7)   | Se3—C4—C5—B16  | 99.5 (6)   |
| B14—B15—B16—C5  | 58.3 (8)   | B16—C4—C5—B12  | 147.6 (6)  |
| B11—B15—B16—C5  | -4.2 (8)   | B15—C4—C5—B12  | 107.7 (7)  |
| C4—B15—B16—B19  | -135.0 (7) | B11—C4—C5—B12  | 39.2 (6)   |
| B14—B15—B16—B19 | -39.6 (7)  | Se3—C4—C5—B12  | -112.9 (6) |
| B11—B15—B16—B19 | -102.0 (8) | B13—B17—C5—C6  | -144.7 (7) |
| C4—B15—B16—B20  | -97.6 (7)  | B18—B17—C5—C6  | 151.1 (7)  |
| B19—B15—B16—B20 | 37.4 (7)   | B12—B17—C5—C6  | -105.9 (8) |
| B14—B15—B16—B20 | -2.1 (9)   | B20—B17—C5—C6  | 111.6 (8)  |
| B11—B15—B16—B20 | -64.6 (8)  | B13—B17—C5—B20 | 103.7 (7)  |

## supplementary materials

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|                 |            |                |            |
|-----------------|------------|----------------|------------|
| B12—B13—B17—C5  | 38.7 (6)   | B18—B17—C5—B20 | 39.6 (6)   |
| B11—B13—B17—C5  | -0.1 (9)   | B12—B17—C5—B20 | 142.5 (7)  |
| B18—B13—B17—C5  | -99.5 (7)  | B13—B17—C5—C4  | 0.6 (8)    |
| B14—B13—B17—C5  | -62.4 (8)  | B18—B17—C5—C4  | -63.6 (7)  |
| B12—B13—B17—B18 | 138.1 (7)  | B12—B17—C5—C4  | 39.4 (5)   |
| B11—B13—B17—B18 | 99.4 (7)   | B20—B17—C5—C4  | -103.1 (6) |
| B14—B13—B17—B18 | 37.1 (7)   | B13—B17—C5—B16 | 64.9 (8)   |
| B11—B13—B17—B12 | -38.8 (6)  | B18—B17—C5—B16 | 0.7 (8)    |
| B18—B13—B17—B12 | -138.1 (7) | B12—B17—C5—B16 | 103.7 (6)  |
| B14—B13—B17—B12 | -101.1 (8) | B20—B17—C5—B16 | -38.8 (6)  |
| B12—B13—B17—B20 | 99.7 (7)   | B13—B17—C5—B12 | -38.8 (6)  |
| B11—B13—B17—B20 | 61.0 (9)   | B18—B17—C5—B12 | -102.9 (7) |
| B18—B13—B17—B20 | -38.4 (7)  | B20—B17—C5—B12 | -142.5 (7) |
| B14—B13—B17—B20 | -1.3 (9)   | C4—B16—C5—C6   | 109.4 (7)  |
| C4—B12—B17—C5   | -37.7 (5)  | B19—B16—C5—C6  | -152.7 (7) |
| B13—B12—B17—C5  | -136.1 (7) | B15—B16—C5—C6  | 146.3 (7)  |
| B11—B12—B17—C5  | -98.5 (7)  | B20—B16—C5—C6  | -112.8 (8) |
| C4—B12—B17—B13  | 98.4 (7)   | C4—B16—C5—B20  | -137.8 (6) |
| C5—B12—B17—B13  | 136.1 (7)  | B19—B16—C5—B20 | -39.9 (6)  |
| B11—B12—B17—B13 | 37.6 (6)   | B15—B16—C5—B20 | -100.9 (7) |
| C4—B12—B17—B18  | 60.1 (8)   | B19—B16—C5—C4  | 97.9 (7)   |
| C5—B12—B17—B18  | 97.8 (7)   | B15—B16—C5—C4  | 36.9 (6)   |
| B13—B12—B17—B18 | -38.3 (7)  | B20—B16—C5—C4  | 137.8 (6)  |
| B11—B12—B17—B18 | -0.6 (9)   | C4—B16—C5—B17  | -98.5 (6)  |
| C4—B12—B17—B20  | -4.9 (8)   | B19—B16—C5—B17 | -0.6 (9)   |
| C5—B12—B17—B20  | 32.8 (6)   | B15—B16—C5—B17 | -61.7 (8)  |
| B13—B12—B17—B20 | -103.3 (8) | B20—B16—C5—B17 | 39.3 (7)   |
| B11—B12—B17—B20 | -65.7 (8)  | C4—B16—C5—B12  | -30.3 (6)  |
| C5—B17—B18—B14  | 62.5 (8)   | B19—B16—C5—B12 | 67.6 (8)   |
| B13—B17—B18—B14 | -38.0 (7)  | B15—B16—C5—B12 | 6.6 (8)    |
| B12—B17—B18—B14 | -0.4 (9)   | B20—B16—C5—B12 | 107.5 (7)  |
| B20—B17—B18—B14 | 100.3 (8)  | C4—B12—C5—C6   | -109.6 (7) |
| C5—B17—B18—B13  | 100.5 (7)  | B13—B12—C5—C6  | 152.2 (7)  |
| B12—B17—B18—B13 | 37.6 (7)   | B17—B12—C5—C6  | 114.0 (7)  |
| B20—B17—B18—B13 | 138.4 (7)  | B11—B12—C5—C6  | -145.8 (7) |
| C5—B17—B18—B20  | -37.9 (6)  | C4—B12—C5—B20  | 99.3 (6)   |
| B13—B17—B18—B20 | -138.4 (7) | B13—B12—C5—B20 | 1.1 (8)    |
| B12—B17—B18—B20 | -100.7 (7) | B17—B12—C5—B20 | -37.1 (6)  |
| C5—B17—B18—B19  | -0.5 (8)   | B11—B12—C5—B20 | 63.1 (8)   |
| B13—B17—B18—B19 | -101.0 (7) | B13—B12—C5—C4  | -98.2 (6)  |
| B12—B17—B18—B19 | -63.3 (8)  | B17—B12—C5—C4  | -136.4 (6) |
| B20—B17—B18—B19 | 37.4 (7)   | B11—B12—C5—C4  | -36.2 (5)  |
| B11—B14—B18—B17 | 1.3 (9)    | C4—B12—C5—B17  | 136.4 (6)  |
| B15—B14—B18—B17 | -64.1 (9)  | B13—B12—C5—B17 | 38.2 (6)   |
| B19—B14—B18—B17 | -100.2 (8) | B11—B12—C5—B17 | 100.2 (7)  |
| B13—B14—B18—B17 | 37.3 (6)   | C4—B12—C5—B16  | 30.0 (6)   |
| B11—B14—B18—B13 | -36.0 (7)  | B13—B12—C5—B16 | -68.2 (7)  |
| B15—B14—B18—B13 | -101.4 (7) | B17—B12—C5—B16 | -106.4 (7) |
| B19—B14—B18—B13 | -137.5 (7) | B11—B12—C5—B16 | -6.2 (8)   |

|                 |            |                |            |
|-----------------|------------|----------------|------------|
| B11—B14—B18—B20 | 64.9 (9)   | C2—C1—Se1—Se2  | 106.1 (5)  |
| B15—B14—B18—B20 | -0.5 (9)   | B1—C1—Se1—Se2  | -43.2 (6)  |
| B19—B14—B18—B20 | -36.6 (6)  | B7—C1—Se1—Se2  | 173.6 (4)  |
| B13—B14—B18—B20 | 100.9 (7)  | B2—C1—Se1—Se2  | 34.2 (6)   |
| B11—B14—B18—B19 | 101.5 (7)  | B3—C1—Se1—Se2  | -117.9 (4) |
| B15—B14—B18—B19 | 36.1 (6)   | C1—Se1—Se2—Se3 | -95.3 (2)  |
| B13—B14—B18—B19 | 137.5 (7)  | C5—C4—Se3—Se2  | 104.6 (5)  |
| B12—B13—B18—B17 | -37.7 (6)  | B16—C4—Se3—Se2 | 171.9 (4)  |
| B11—B13—B18—B17 | -102.1 (7) | B15—C4—Se3—Se2 | -118.8 (5) |
| B14—B13—B18—B17 | -137.8 (7) | B11—C4—Se3—Se2 | -43.1 (6)  |
| B17—B13—B18—B14 | 137.8 (7)  | B12—C4—Se3—Se2 | 33.7 (6)   |
| B12—B13—B18—B14 | 100.0 (7)  | Se1—Se2—Se3—C4 | -84.8 (2)  |

Fig. 1

