Electronic Supplementary Information for Dalton Transactions


# Boron(8) substituted isonitrilium and ammonium derivatives new versatile cobalt bis(1,2-dicarbollide) building blocks for synthetic purposes.

**Vaclav Sicha[a], Jaromír Plešek[a], Magdalena Kvicalova[a], Ivana Císařová[b] and Bohumír Gruner[a]**

[a]Institute of Inorganic Chemistry, Academy of Sciences of the Czech, Republic, 250 68 Řež, Czech Republic, and [b]Dept. of Inorganic Chemistry, Faculty of Science, Charles University in Prague, Albertov 6, 128 40 Praha 2, Czech Republic
Correspondence e-mail: cisarova@mail.natur.cuni.cz

## Comment

## Experimental

### (2)

*Crystal data*

| | |
|---|---|
| $C_6H_{24}B_{18}CoN$ | $D_x$ = 1.335 Mg m$^{-3}$ |
| $M_r$ = 363.77 | Melting point: 568 K |
| Orthorhombic, $Pna2_1$ | Mo $K\alpha$ radiation<br>$\lambda$ = 0.71073 Å |
| Hall symbol: P 2c -2n | Cell parameters from 2415 reflections |
| $a$ = 22.05980 (10) Å | $\theta$ = 1–27.5° |
| $b$ = 7.0999 (2) Å | $\mu$ = 0.94 mm$^{-1}$ |
| $c$ = 11.5587 (3) Å | $T$ = 150 (2) K |
| $V$ = 1810.35 (7) Å$^3$ | Cell measurement pressure: 101.3 kPa |
| $Z$ = 4 | Plate, red |
| $F_{000}$ = 736 | 0.4 × 0.4 × 0.3 mm |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD area detector diffractometer | 3943 independent reflections |
| Radiation source: fine-focus sealed tube | 3795 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.045 |
| Detector resolution: 9.091 pixels mm$^{-1}$ | $\theta_{max}$ = 27.5° |
| $T$ = 150(2) K | $\theta_{min}$ = 3.0° |
| $P$ = 101.3 kPa | $h$ = −28→28 |
| φ and ω scans to fill the Ewald sphere | $k$ = −9→9 |
| Absorption correction: none | $l$ = −14→14 |
| 25157 measured reflections | |

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.065$

$S = 1.06$

3943 reflections

273 parameters

1 restraint

? constraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.5901P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.32$ e Å$^{-3}$

$\Delta\rho_{min} = -0.39$ e Å$^{-3}$

Extinction correction: none

Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881

Flack parameter: 0.00 (13)

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 $F^2 >$ 2sigma($F^2$) 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.

The crystal was refined as racemic twin, twin ration 0.54:0.46.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co3 | 0.422893 (8) | 0.24021 (2) | 0.91204 (4) | 0.01233 (7) |
| C1 | 0.36433 (8) | 0.3067 (3) | 1.04327 (15) | 0.0173 (3) |
| H1 | 0.3842 (9) | 0.381 (3) | 1.0979 (19) | 0.022 (5)* |
| C2 | 0.38405 (8) | 0.0868 (2) | 1.04180 (15) | 0.0179 (3) |
| H2 | 0.4144 (9) | 0.048 (3) | 1.093 (2) | 0.019 (5)* |
| B4 | 0.33920 (7) | 0.3831 (2) | 0.9126 (2) | 0.0157 (3) |
| H4 | 0.3429 (9) | 0.520 (3) | 0.8893 (19) | 0.024 (6)* |
| B5 | 0.28851 (9) | 0.3335 (3) | 1.02955 (18) | 0.0207 (4) |
| H5 | 0.2617 | 0.4466 | 1.0698 | 0.025* |
| B6 | 0.31850 (9) | 0.1484 (3) | 1.11407 (18) | 0.0211 (4) |
| H6 | 0.3117 | 0.1408 | 1.2082 | 0.025* |
| B7 | 0.37432 (8) | −0.0131 (2) | 0.9082 (2) | 0.0177 (3) |
| H7 | 0.3981 (10) | −0.132 (3) | 0.8766 (19) | 0.025 (6)* |
| B8 | 0.34197 (9) | 0.1749 (3) | 0.82487 (17) | 0.0163 (4) |

| | | | | |
|---|---|---|---|---|
| B9 | 0.27205 (9) | 0.2454 (3) | 0.88947 (18) | 0.0197 (5) |
| H9 | 0.2340 | 0.2997 | 0.8377 | 0.024* |
| B10 | 0.25982 (9) | 0.1005 (3) | 1.01361 (17) | 0.0220 (4) |
| H10 | 0.2139 | 0.0606 | 1.0416 | 0.026* |
| B11 | 0.32293 (9) | −0.0555 (3) | 1.02635 (19) | 0.0220 (4) |
| H11 | 0.3187 | −0.1968 | 1.0645 | 0.026* |
| B12 | 0.29371 (9) | 0.0014 (3) | 0.88742 (16) | 0.0212 (4) |
| H12 | 0.2696 | −0.1031 | 0.8343 | 0.025* |
| C1' | 0.50113 (8) | 0.3165 (2) | 0.99333 (15) | 0.0163 (3) |
| H1' | 0.4933 (9) | 0.321 (3) | 1.067 (2) | 0.013 (5)* |
| C2' | 0.47404 (6) | 0.47855 (19) | 0.90874 (18) | 0.0156 (3) |
| H2' | 0.4511 (8) | 0.578 (3) | 0.9436 (15) | 0.008 (4)* |
| B4' | 0.50714 (8) | 0.1044 (2) | 0.92436 (18) | 0.0163 (3) |
| H4' | 0.5058 (9) | −0.025 (3) | 0.9749 (19) | 0.019 (5)* |
| B5' | 0.57209 (9) | 0.2516 (3) | 0.9537 (2) | 0.0190 (5) |
| H5' | 0.6081 | 0.2066 | 1.0136 | 0.023* |
| B6' | 0.54933 (8) | 0.4900 (3) | 0.94656 (17) | 0.0187 (4) |
| H6' | 0.5698 | 0.5992 | 1.0016 | 0.022* |
| B7' | 0.45900 (8) | 0.3938 (3) | 0.77378 (16) | 0.0155 (3) |
| H7' | 0.4287 (9) | 0.467 (3) | 0.721 (2) | 0.027 (6)* |
| B8' | 0.48199 (8) | 0.1488 (3) | 0.77825 (16) | 0.0158 (4) |
| H8' | 0.4671 (8) | 0.042 (3) | 0.7193 (16) | 0.010 (4)* |
| B9' | 0.56150 (9) | 0.1489 (3) | 0.81503 (17) | 0.0192 (4) |
| H9' | 0.5915 | 0.0364 | 0.7834 | 0.023* |
| B10' | 0.58792 (9) | 0.3864 (3) | 0.82779 (18) | 0.0208 (4) |
| H10' | 0.6343 | 0.4273 | 0.8036 | 0.025* |
| B11' | 0.52443 (9) | 0.5374 (3) | 0.80468 (17) | 0.0192 (4) |
| H11' | 0.5294 | 0.6789 | 0.7670 | 0.023* |
| B12' | 0.53186 (9) | 0.3264 (3) | 0.72216 (16) | 0.0181 (4) |
| H12' | 0.5425 | 0.3302 | 0.6292 | 0.022* |
| N1 | 0.34117 (7) | 0.1754 (2) | 0.69449 (14) | 0.0189 (3) |
| C3 | 0.33764 (8) | 0.1731 (3) | 0.59612 (16) | 0.0188 (3) |
| C4 | 0.33273 (9) | 0.1684 (3) | 0.47097 (16) | 0.0240 (4) |
| H4A | 0.2994 | 0.0891 | 0.4491 | 0.036* |

| | | | | |
|---|---|---|---|---|
| H4B | 0.3696 | 0.1194 | 0.4386 | 0.036* |
| H4C | 0.3260 | 0.2936 | 0.4424 | 0.036* |

Atomic displacement parameters (Å$^2$)

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co3 | 0.01386 (10) | 0.01269 (10) | 0.01043 (10) | 0.00057 (6) | −0.00028 (10) | −0.00005 (10) |
| C1 | 0.0186 (8) | 0.0189 (8) | 0.0143 (8) | 0.0018 (6) | 0.0020 (7) | −0.0023 (7) |
| C2 | 0.0207 (8) | 0.0193 (8) | 0.0135 (7) | 0.0010 (6) | 0.0022 (7) | 0.0032 (6) |
| B4 | 0.0155 (7) | 0.0166 (7) | 0.0149 (8) | 0.0026 (6) | −0.0019 (9) | 0.0000 (9) |
| B5 | 0.0179 (9) | 0.0252 (10) | 0.0191 (9) | 0.0017 (8) | −0.0008 (8) | −0.0029 (8) |
| B6 | 0.0208 (9) | 0.0252 (10) | 0.0174 (10) | 0.0005 (8) | 0.0030 (7) | 0.0018 (8) |
| B7 | 0.0210 (8) | 0.0149 (7) | 0.0174 (8) | −0.0021 (6) | 0.0011 (9) | 0.0013 (10) |
| B8 | 0.0169 (9) | 0.0160 (9) | 0.0161 (9) | −0.0015 (7) | −0.0011 (7) | −0.0002 (7) |
| B9 | 0.0142 (9) | 0.0228 (9) | 0.0221 (15) | 0.0002 (6) | −0.0016 (7) | −0.0014 (7) |
| B10 | 0.0208 (9) | 0.0267 (10) | 0.0184 (10) | −0.0012 (8) | 0.0013 (7) | −0.0011 (8) |
| B11 | 0.0251 (10) | 0.0197 (9) | 0.0211 (10) | −0.0018 (7) | 0.0042 (7) | 0.0032 (8) |
| B12 | 0.0213 (9) | 0.0202 (8) | 0.0222 (11) | −0.0058 (7) | 0.0007 (7) | −0.0021 (7) |
| C1' | 0.0189 (8) | 0.0194 (8) | 0.0104 (7) | 0.0003 (6) | −0.0009 (6) | −0.0008 (6) |
| C2' | 0.0181 (7) | 0.0144 (6) | 0.0143 (6) | −0.0015 (5) | −0.0003 (8) | −0.0009 (8) |
| B4' | 0.0174 (8) | 0.0161 (7) | 0.0154 (9) | 0.0042 (6) | −0.0010 (7) | 0.0001 (8) |
| B5' | 0.0169 (11) | 0.0263 (12) | 0.0138 (9) | 0.0029 (7) | −0.0009 (7) | −0.0008 (7) |
| B6' | 0.0184 (9) | 0.0215 (9) | 0.0160 (9) | −0.0027 (7) | −0.0006 (7) | −0.0021 (7) |
| B7' | 0.0187 (8) | 0.0158 (8) | 0.0119 (8) | −0.0008 (7) | −0.0003 (7) | 0.0012 (6) |
| B8' | 0.0199 (9) | 0.0161 (9) | 0.0114 (9) | 0.0035 (6) | 0.0008 (7) | −0.0003 (7) |
| B9' | 0.0213 (9) | 0.0218 (10) | 0.0146 (9) | 0.0043 (7) | −0.0003 (7) | −0.0016 (7) |
| B10' | 0.0199 (9) | 0.0264 (10) | 0.0162 (9) | −0.0003 (8) | 0.0005 (7) | 0.0006 (8) |
| B11' | 0.0216 (9) | 0.0192 (9) | 0.0169 (9) | −0.0017 (7) | 0.0008 (7) | 0.0010 (7) |
| B12' | 0.0191 (9) | 0.0209 (9) | 0.0144 (9) | 0.0000 (7) | 0.0016 (7) | 0.0011 (7) |
| N1 | 0.0179 (7) | 0.0198 (8) | 0.0189 (8) | −0.0016 (6) | −0.0025 (6) | −0.0016 (6) |
| C3 | 0.0170 (7) | 0.0199 (8) | 0.0194 (9) | −0.0019 (6) | −0.0012 (6) | −0.0021 (7) |
| C4 | 0.0299 (10) | 0.0276 (10) | 0.0146 (9) | −0.0028 (7) | −0.0013 (7) | −0.0013 (7) |

**Table 1**
Geometric parameters (Å, °)

| | | | |
|---|---|---|---|
| Co3—C2' | 2.0342 (14) | B11—H11 | 1.1000 |
| Co3—C1' | 2.0384 (18) | B12—H12 | 1.1000 |
| Co3—C2 | 2.0421 (17) | C1'—C2' | 1.624 (2) |
| Co3—C1 | 2.0476 (18) | C1'—B5' | 1.695 (3) |
| Co3—B7' | 2.0922 (19) | C1'—B4' | 1.710 (2) |
| Co3—B7 | 2.0941 (16) | C1'—B6' | 1.714 (3) |
| Co3—B4' | 2.0987 (17) | C1'—H1' | 0.87 (2) |
| Co3—B8 | 2.1016 (19) | C2'—B11' | 1.690 (2) |
| Co3—B4 | 2.1066 (16) | C2'—B7' | 1.705 (3) |
| Co3—B8' | 2.1240 (18) | C2'—B6' | 1.719 (2) |
| C1—C2 | 1.621 (2) | C2'—H2' | 0.960 (18) |
| C1—B5 | 1.691 (3) | B4'—B9' | 1.771 (3) |
| C1—B4 | 1.698 (3) | B4'—B8' | 1.805 (3) |
| C1—B6 | 1.719 (3) | B4'—B5' | 1.806 (3) |
| C1—H1 | 0.93 (2) | B4'—H4' | 1.09 (2) |
| C2—B11 | 1.694 (3) | B5'—B6' | 1.767 (3) |
| C2—B7 | 1.713 (3) | B5'—B9' | 1.777 (3) |
| C2—B6 | 1.726 (3) | B5'—B10' | 1.777 (3) |
| C2—H2 | 0.93 (2) | B5'—H5' | 1.1000 |
| B4—B5 | 1.789 (3) | B6'—B11' | 1.762 (3) |
| B4—B8 | 1.793 (3) | B6'—B10' | 1.775 (3) |
| B4—B9 | 1.795 (3) | B6'—H6' | 1.1000 |
| B4—H4 | 1.01 (2) | B7'—B12' | 1.780 (3) |
| B5—B6 | 1.767 (3) | B7'—B11' | 1.803 (3) |
| B5—B9 | 1.773 (3) | B7'—B8' | 1.812 (3) |
| B5—B10 | 1.781 (3) | B7'—H7' | 1.05 (2) |
| B5—H5 | 1.1000 | B8'—B12' | 1.794 (3) |
| B6—B11 | 1.770 (3) | B8'—B9' | 1.805 (3) |
| B6—B10 | 1.772 (3) | B8'—H8' | 1.069 (19) |
| B6—H6 | 1.1000 | B9'—B12' | 1.780 (3) |
| B7—B8 | 1.794 (3) | B9'—B10' | 1.790 (3) |
| B7—B12 | 1.797 (3) | B9'—H9' | 1.1000 |

| | | | |
|---|---|---|---|
| B7—B11 | 1.800 (3) | B10'—B11' | 1.784 (3) |
| B7—H7 | 1.06 (2) | B10'—B12' | 1.789 (3) |
| B8—N1 | 1.507 (2) | B10'—H10' | 1.1000 |
| B8—B12 | 1.782 (3) | B11'—B12' | 1.784 (3) |
| B8—B9 | 1.785 (3) | B11'—H11' | 1.1000 |
| B9—B10 | 1.786 (3) | B12'—H12' | 1.1000 |
| B9—B12 | 1.798 (3) | N1—C3 | 1.140 (2) |
| B9—H9 | 1.1000 | C3—C4 | 1.451 (2) |
| B10—B12 | 1.784 (3) | C4—H4A | 0.9600 |
| B10—B11 | 1.785 (3) | C4—H4B | 0.9600 |
| B10—H10 | 1.1000 | C4—H4C | 0.9600 |
| B11—B12 | 1.777 (3) | | |

| | | | |
|---|---|---|---|
| C2'—Co3—C1' | 46.99 (7) | B12—B11—H11 | 122.6 |
| C2'—Co3—C2 | 133.64 (8) | B10—B11—H11 | 122.2 |
| C1'—Co3—C2 | 99.12 (7) | B7—B11—H11 | 120.7 |
| C2'—Co3—C1 | 99.90 (7) | B11—B12—B8 | 107.88 (14) |
| C1'—Co3—C1 | 97.55 (7) | B11—B12—B10 | 60.19 (11) |
| C2—Co3—C1 | 46.70 (7) | B8—B12—B10 | 108.01 (14) |
| C2'—Co3—B7' | 48.77 (8) | B11—B12—B7 | 60.49 (12) |
| C1'—Co3—B7' | 83.75 (7) | B8—B12—B7 | 60.17 (11) |
| C2—Co3—B7' | 177.12 (8) | B10—B12—B7 | 109.15 (14) |
| C1—Co3—B7' | 133.30 (7) | B11—B12—B9 | 107.67 (14) |
| C2'—Co3—B7 | 176.29 (8) | B8—B12—B9 | 59.83 (11) |
| C1'—Co3—B7 | 132.18 (8) | B10—B12—B9 | 59.83 (12) |
| C2—Co3—B7 | 48.92 (8) | B7—B12—B9 | 108.44 (13) |
| C1—Co3—B7 | 83.74 (8) | B11—B12—H12 | 121.8 |
| B7'—Co3—B7 | 128.77 (9) | B8—B12—H12 | 121.9 |
| C2'—Co3—B4' | 83.83 (6) | B10—B12—H12 | 121.4 |
| C1'—Co3—B4' | 48.79 (7) | B7—B12—H12 | 120.9 |
| C2—Co3—B4' | 94.39 (7) | B9—B12—H12 | 121.9 |
| C1—Co3—B4' | 127.91 (8) | C2'—C1'—B5' | 111.73 (14) |
| B7'—Co3—B4' | 87.38 (7) | C2'—C1'—B4' | 111.84 (14) |
| B7—Co3—B4' | 93.43 (7) | B5'—C1'—B4' | 64.06 (11) |
| C2'—Co3—B8 | 130.21 (7) | C2'—C1'—B6' | 61.94 (10) |

| | | | |
|---|---|---|---|
| C1'—Co3—B8 | 177.19 (7) | B5'—C1'—B6' | 62.45 (11) |
| C2—Co3—B8 | 83.00 (7) | B4'—C1'—B6' | 115.96 (14) |
| C1—Co3—B8 | 82.53 (8) | C2'—C1'—Co3 | 66.37 (8) |
| B7'—Co3—B8 | 94.14 (8) | B5'—C1'—Co3 | 125.81 (13) |
| B7—Co3—B8 | 50.64 (8) | B4'—C1'—Co3 | 67.45 (8) |
| B4'—Co3—B8 | 133.11 (8) | B6'—C1'—Co3 | 124.81 (11) |
| C2'—Co3—B4 | 94.91 (6) | C2'—C1'—H1' | 119.2 (14) |
| C1'—Co3—B4 | 127.77 (8) | B5'—C1'—H1' | 117.4 (13) |
| C2—Co3—B4 | 83.50 (8) | B4'—C1'—H1' | 120.4 (14) |
| C1—Co3—B4 | 48.22 (8) | B6'—C1'—H1' | 113.9 (13) |
| B7'—Co3—B4 | 94.88 (8) | Co3—C1'—H1' | 107.0 (13) |
| B7—Co3—B4 | 88.01 (6) | C1'—C2'—B11' | 111.20 (12) |
| B4'—Co3—B4 | 175.71 (10) | C1'—C2'—B7' | 111.88 (12) |
| B8—Co3—B4 | 50.45 (8) | B11'—C2'—B7' | 64.15 (12) |
| C2'—Co3—B8' | 84.26 (7) | C1'—C2'—B6' | 61.62 (11) |
| C1'—Co3—B8' | 84.10 (7) | B11'—C2'—B6' | 62.23 (11) |
| C2—Co3—B8' | 129.00 (7) | B7'—C2'—B6' | 115.94 (13) |
| C1—Co3—B8' | 175.54 (7) | C1'—C2'—Co3 | 66.64 (8) |
| B7'—Co3—B8' | 50.91 (7) | B11'—C2'—Co3 | 125.72 (12) |
| B7—Co3—B8' | 92.07 (8) | B7'—C2'—Co3 | 67.39 (8) |
| B4'—Co3—B8' | 50.62 (8) | B6'—C2'—Co3 | 124.76 (10) |
| B8—Co3—B8' | 96.02 (8) | C1'—C2'—H2' | 117.7 (11) |
| B4—Co3—B8' | 133.41 (9) | B11'—C2'—H2' | 117.5 (11) |
| C2—C1—B5 | 111.90 (14) | B7'—C2'—H2' | 122.8 (10) |
| C2—C1—B4 | 112.71 (13) | B6'—C2'—H2' | 111.6 (10) |
| B5—C1—B4 | 63.74 (11) | Co3—C2'—H2' | 108.4 (10) |
| C2—C1—B6 | 62.15 (12) | C1'—B4'—B9' | 103.17 (13) |
| B5—C1—B6 | 62.39 (12) | C1'—B4'—B8' | 104.96 (12) |
| B4—C1—B6 | 116.12 (14) | B9'—B4'—B8' | 60.62 (11) |
| C2—C1—Co3 | 66.47 (8) | C1'—B4'—B5' | 57.57 (10) |
| B5—C1—Co3 | 125.49 (12) | B9'—B4'—B5' | 59.56 (12) |
| B4—C1—Co3 | 67.71 (8) | B8'—B4'—B5' | 108.57 (14) |
| B6—C1—Co3 | 124.95 (12) | C1'—B4'—Co3 | 63.76 (8) |
| C2—C1—H1 | 115.1 (13) | B9'—B4'—Co3 | 117.98 (11) |

| | | | |
|---|---|---|---|
| B5—C1—H1 | 117.7 (12) | B8'—B4'—Co3 | 65.41 (8) |
| B4—C1—H1 | 125.2 (13) | B5'—B4'—Co3 | 116.70 (10) |
| B6—C1—H1 | 108.9 (13) | C1'—B4'—H4' | 119.3 (11) |
| Co3—C1—H1 | 109.6 (13) | B9'—B4'—H4' | 123.6 (11) |
| C1—C2—B11 | 111.23 (14) | B8'—B4'—H4' | 129.9 (11) |
| C1—C2—B7 | 112.01 (13) | B5'—B4'—H4' | 114.1 (11) |
| B11—C2—B7 | 63.79 (11) | Co3—B4'—H4' | 113.5 (11) |
| C1—C2—B6 | 61.73 (12) | C1'—B5'—B6' | 59.31 (11) |
| B11—C2—B6 | 62.32 (12) | C1'—B5'—B9' | 103.53 (14) |
| B7—C2—B6 | 115.86 (14) | B6'—B5'—B9' | 108.25 (15) |
| C1—C2—Co3 | 66.83 (8) | C1'—B5'—B10' | 104.84 (14) |
| B11—C2—Co3 | 125.07 (12) | B6'—B5'—B10' | 60.10 (11) |
| B7—C2—Co3 | 67.12 (8) | B9'—B5'—B10' | 60.49 (13) |
| B6—C2—Co3 | 124.89 (12) | C1'—B5'—B4' | 58.37 (10) |
| C1—C2—H2 | 118.0 (13) | B6'—B5'—B4' | 108.67 (13) |
| B11—C2—H2 | 117.6 (13) | B9'—B5'—B4' | 59.24 (12) |
| B7—C2—H2 | 122.4 (13) | B10'—B5'—B4' | 108.28 (16) |
| B6—C2—H2 | 111.8 (13) | C1'—B5'—H5' | 125.1 |
| Co3—C2—H2 | 108.5 (13) | B6'—B5'—H5' | 120.8 |
| C1—B4—B5 | 57.94 (11) | B9'—B5'—H5' | 122.9 |
| C1—B4—B8 | 103.22 (12) | B10'—B5'—H5' | 122.0 |
| B5—B4—B8 | 106.65 (13) | B4'—B5'—H5' | 121.5 |
| C1—B4—B9 | 103.19 (13) | C1'—B6'—C2' | 56.44 (10) |
| B5—B4—B9 | 59.32 (11) | C1'—B6'—B11' | 103.73 (13) |
| B8—B4—B9 | 59.67 (10) | C2'—B6'—B11' | 58.07 (11) |
| C1—B4—Co3 | 64.07 (8) | C1'—B6'—B5' | 58.24 (11) |
| B5—B4—Co3 | 117.09 (12) | C2'—B6'—B5' | 103.96 (13) |
| B8—B4—Co3 | 64.63 (8) | B11'—B6'—B5' | 108.38 (15) |
| B9—B4—Co3 | 117.43 (10) | C1'—B6'—B10' | 104.11 (14) |
| C1—B4—H4 | 121.1 (13) | C2'—B6'—B10' | 104.30 (13) |
| B5—B4—H4 | 116.2 (12) | B11'—B6'—B10' | 60.58 (11) |
| B8—B4—H4 | 129.6 (12) | B5'—B6'—B10' | 60.21 (13) |
| B9—B4—H4 | 123.4 (12) | C1'—B6'—H6' | 125.4 |
| Co3—B4—H4 | 113.0 (12) | C2'—B6'—H6' | 125.2 |

| | | | |
|---|---|---|---|
| C1—B5—B6 | 59.59 (11) | B11'—B6'—H6' | 122.1 |
| C1—B5—B9 | 104.38 (14) | B5'—B6'—H6' | 122.1 |
| B6—B5—B9 | 108.61 (14) | B10'—B6'—H6' | 122.8 |
| C1—B5—B10 | 104.87 (14) | C2'—B7'—B12' | 103.06 (13) |
| B6—B5—B10 | 59.93 (12) | C2'—B7'—B11' | 57.54 (10) |
| B9—B5—B10 | 60.33 (11) | B12'—B7'—B11' | 59.71 (11) |
| C1—B5—B4 | 58.32 (10) | C2'—B7'—B8' | 104.96 (12) |
| B6—B5—B4 | 109.28 (13) | B12'—B7'—B8' | 59.92 (11) |
| B9—B5—B4 | 60.50 (11) | B11'—B7'—B8' | 108.24 (13) |
| B10—B5—B4 | 109.06 (14) | C2'—B7'—Co3 | 63.84 (8) |
| C1—B5—H5 | 125.0 | B12'—B7'—Co3 | 117.36 (11) |
| B6—B5—H5 | 120.7 | B11'—B7'—Co3 | 116.63 (11) |
| B9—B5—H5 | 122.3 | B8'—B7'—Co3 | 65.45 (8) |
| B10—B5—H5 | 122.1 | C2'—B7'—H7' | 118.9 (12) |
| B4—B5—H5 | 120.8 | B12'—B7'—H7' | 121.0 (12) |
| C1—B6—C2 | 56.12 (10) | B11'—B7'—H7' | 110.2 (12) |
| C1—B6—B5 | 58.02 (11) | B8'—B7'—H7' | 132.4 (13) |
| C2—B6—B5 | 103.56 (14) | Co3—B7'—H7' | 117.7 (12) |
| C1—B6—B11 | 103.27 (14) | B12'—B8'—B9' | 59.27 (11) |
| C2—B6—B11 | 57.96 (11) | B12'—B8'—B4' | 105.81 (13) |
| B5—B6—B11 | 108.21 (15) | B9'—B8'—B4' | 58.74 (10) |
| C1—B6—B10 | 104.06 (14) | B12'—B8'—B7' | 59.15 (10) |
| C2—B6—B10 | 104.26 (14) | B9'—B8'—B7' | 106.16 (13) |
| B5—B6—B10 | 60.44 (12) | B4'—B8'—B7' | 106.29 (12) |
| B11—B6—B10 | 60.54 (12) | B12'—B8'—Co3 | 115.14 (11) |
| C1—B6—H6 | 125.6 | B9'—B8'—Co3 | 115.15 (11) |
| C2—B6—H6 | 125.5 | B4'—B8'—Co3 | 63.97 (8) |
| B5—B6—H6 | 122.2 | B7'—B8'—Co3 | 63.64 (8) |
| B11—B6—H6 | 122.3 | B12'—B8'—H8' | 117.0 (10) |
| B10—B6—H6 | 122.7 | B9'—B8'—H8' | 116.6 (9) |
| C2—B7—B8 | 103.03 (12) | B4'—B8'—H8' | 124.5 (10) |
| C2—B7—B12 | 102.74 (14) | B7'—B8'—H8' | 125.1 (10) |
| B8—B7—B12 | 59.48 (10) | Co3—B8'—H8' | 119.5 (10) |
| C2—B7—B11 | 57.59 (12) | B4'—B9'—B5' | 61.20 (11) |

| | | | |
|---|---|---|---|
| B8—B7—B11 | 106.32 (13) | B4'—B9'—B12' | 107.95 (13) |
| B12—B7—B11 | 59.19 (11) | B5'—B9'—B12' | 107.59 (14) |
| C2—B7—Co3 | 63.96 (8) | B4'—B9'—B10' | 109.27 (13) |
| B8—B7—Co3 | 64.90 (8) | B5'—B9'—B10' | 59.77 (11) |
| B12—B7—Co3 | 117.38 (10) | B12'—B9'—B10' | 60.17 (11) |
| B11—B7—Co3 | 116.72 (13) | B4'—B9'—B8' | 60.65 (11) |
| C2—B7—H7 | 125.4 (12) | B5'—B9'—B8' | 109.90 (14) |
| B8—B7—H7 | 127.2 (12) | B12'—B9'—B8' | 60.07 (11) |
| B12—B7—H7 | 119.4 (12) | B10'—B9'—B8' | 109.64 (14) |
| B11—B7—H7 | 116.2 (12) | B4'—B9'—H9' | 121.0 |
| Co3—B7—H7 | 116.0 (12) | B5'—B9'—H9' | 121.2 |
| N1—B8—B12 | 113.60 (14) | B12'—B9'—H9' | 122.3 |
| N1—B8—B9 | 114.05 (15) | B10'—B9'—H9' | 121.0 |
| B12—B8—B9 | 60.52 (11) | B8'—B9'—H9' | 120.4 |
| N1—B8—B4 | 124.28 (16) | B6'—B10'—B5' | 59.68 (11) |
| B12—B8—B4 | 108.67 (14) | B6'—B10'—B11' | 59.35 (11) |
| B9—B8—B4 | 60.20 (10) | B5'—B10'—B11' | 106.99 (14) |
| N1—B8—B7 | 122.88 (16) | B6'—B10'—B12' | 107.16 (14) |
| B12—B8—B7 | 60.34 (11) | B5'—B10'—B12' | 107.16 (15) |
| B9—B8—B7 | 109.14 (14) | B11'—B10'—B12' | 59.89 (11) |
| B4—B8—B7 | 108.87 (14) | B6'—B10'—B9' | 107.33 (14) |
| N1—B8—Co3 | 119.26 (13) | B5'—B10'—B9' | 59.75 (12) |
| B12—B8—Co3 | 117.74 (12) | B11'—B10'—B9' | 107.36 (15) |
| B9—B8—Co3 | 118.14 (12) | B12'—B10'—B9' | 59.64 (12) |
| B4—B8—Co3 | 64.92 (8) | B6'—B10'—H10' | 122.3 |
| B7—B8—Co3 | 64.47 (8) | B5'—B10'—H10' | 122.3 |
| B5—B9—B8 | 107.69 (14) | B11'—B10'—H10' | 122.2 |
| B5—B9—B10 | 60.04 (12) | B12'—B10'—H10' | 122.1 |
| B8—B9—B10 | 107.76 (14) | B9'—B10'—H10' | 122.0 |
| B5—B9—B4 | 60.19 (12) | C2'—B11'—B6' | 59.70 (10) |
| B8—B9—B4 | 60.13 (11) | C2'—B11'—B12' | 103.49 (13) |
| B10—B9—B4 | 108.58 (14) | B6'—B11'—B12' | 107.96 (14) |
| B5—B9—B12 | 107.32 (14) | C2'—B11'—B10' | 105.13 (13) |
| B8—B9—B12 | 59.65 (11) | B6'—B11'—B10' | 60.06 (11) |

| | | | |
|---|---|---|---|
| B10—B9—B12 | 59.70 (11) | B12'—B11'—B10' | 60.20 (11) |
| B4—B9—B12 | 107.92 (13) | C2'—B11'—B7' | 58.31 (10) |
| B5—B9—H9 | 122.0 | B6'—B11'—B7' | 109.02 (14) |
| B8—B9—H9 | 122.0 | B12'—B11'—B7' | 59.51 (11) |
| B10—B9—H9 | 121.6 | B10'—B11'—B7' | 108.56 (14) |
| B4—B9—H9 | 121.3 | C2'—B11'—H11' | 125.0 |
| B12—B9—H9 | 122.2 | B6'—B11'—H11' | 120.8 |
| B6—B10—B5 | 59.63 (12) | B12'—B11'—H11' | 123.1 |
| B6—B10—B12 | 107.78 (14) | B10'—B11'—H11' | 121.9 |
| B5—B10—B12 | 107.60 (14) | B7'—B11'—H11' | 121.2 |
| B6—B10—B11 | 59.68 (12) | B9'—B12'—B7' | 108.66 (14) |
| B5—B10—B11 | 106.90 (15) | B9'—B12'—B11' | 107.81 (13) |
| B12—B10—B11 | 59.72 (12) | B7'—B12'—B11' | 60.78 (11) |
| B6—B10—B9 | 107.80 (14) | B9'—B12'—B10' | 60.20 (12) |
| B5—B10—B9 | 59.62 (11) | B7'—B12'—B10' | 109.34 (14) |
| B12—B10—B9 | 60.47 (11) | B11'—B12'—B10' | 59.91 (11) |
| B11—B10—B9 | 107.81 (14) | B9'—B12'—B8' | 60.66 (11) |
| B6—B10—H10 | 121.9 | B7'—B12'—B8' | 60.93 (11) |
| B5—B10—H10 | 122.4 | B11'—B12'—B8' | 109.90 (13) |
| B12—B10—H10 | 121.7 | B10'—B12'—B8' | 110.14 (14) |
| B11—B10—H10 | 122.3 | B9'—B12'—H12' | 121.9 |
| B9—B10—H10 | 121.6 | B7'—B12'—H12' | 120.9 |
| C2—B11—B6 | 59.72 (11) | B11'—B12'—H12' | 121.4 |
| C2—B11—B12 | 104.39 (14) | B10'—B12'—H12' | 120.9 |
| B6—B11—B12 | 108.17 (15) | B8'—B12'—H12' | 120.1 |
| C2—B11—B10 | 105.02 (15) | C3—N1—B8 | 176.61 (18) |
| B6—B11—B10 | 59.79 (12) | N1—C3—C4 | 179.4 (2) |
| B12—B11—B10 | 60.10 (11) | C3—C4—H4A | 109.5 |
| C2—B11—B7 | 58.62 (10) | C3—C4—H4B | 109.5 |
| B6—B11—B7 | 109.44 (14) | H4A—C4—H4B | 109.5 |
| B12—B11—B7 | 60.32 (11) | C3—C4—H4C | 109.5 |
| B10—B11—B7 | 108.95 (14) | H4A—C4—H4C | 109.5 |
| C2—B11—H11 | 124.7 | H4B—C4—H4C | 109.5 |
| B6—B11—H11 | 120.8 | | |

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

**(6)**

*Crystal data*

| | |
|---|---|
| $C_{10}H_{35}B_{18}CoN_2$ | $D_x$ = 1.262 Mg m$^{-3}$ |
| $M_r$ = 436.91 | Melting point: 479 K |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation<br>λ = 0.71069 Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 8353 reflections |
| $a$ = 7.0734 (7) Å | θ = 1–26.5° |
| $b$ = 13.714 (2) Å | μ = 0.75 mm$^{-1}$ |
| $c$ = 23.709 (6) Å | $T$ = 150 (2) K |
| $V$ = 2299.9 (7) Å$^3$ | Cell measurement pressure: 101.3 kPa |
| $Z$ = 4 | Prism, red |
| $F_{000}$ = 904 | 0.40 × 0.24 × 0.12 mm |

*Data collection*

| | |
|---|---|
| KM4 CCD diffractometer | 4733 independent reflections |
| Radiation source: fine-focus sealed tube | 3491 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.043 |
| Detector resolution: 8.343 pixels mm$^{-1}$ | $\theta_{max}$ = 26.6° |
| $T$ = 150(2) K | $\theta_{min}$ = 3.0° |
| $P$ = 101.3 kPa | $h$ = −8→8 |
| φ and ω scans to fill the Ewald sphere | $k$ = −16→17 |
| Absorption correction: none | $l$ = −29→29 |
| 16379 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.035 | H-atom parameters constrained |
| $wR(F^2)$ = 0.087 | $w = 1/[\sigma^2(F_o^2) + (0.049P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 0.99 | $(\Delta/\sigma)_{max} < 0.001$ |
| 4733 reflections | $\Delta\rho_{max}$ = 0.66 e Å$^{-3}$ |
| 282 parameters | $\Delta\rho_{min}$ = −0.53 e Å$^{-3}$ |
| 1 restraint | Extinction correction: none |
| ? constraints | Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881 |
| Primary atom site location: structure-invariant direct | Flack parameter: 0.013 (17) |

methods

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co3 | 0.74668 (6) | 0.17305 (2) | 0.133189 (13) | 0.01749 (10) |
| C1 | 0.5023 (3) | 0.09275 (19) | 0.13161 (12) | 0.0185 (6) |
| H1A | 0.3980 | 0.1337 | 0.1150 | 0.022* |
| C2 | 0.6704 (4) | 0.0466 (2) | 0.09438 (13) | 0.0206 (7) |
| H2A | 0.6699 | 0.0566 | 0.0530 | 0.025* |
| B4 | 0.5746 (4) | 0.1181 (3) | 0.19802 (13) | 0.0200 (7) |
| H4 | 0.5192 | 0.1771 | 0.2248 | 0.024* |
| B5 | 0.4333 (5) | 0.0143 (2) | 0.18271 (14) | 0.0240 (8) |
| H5 | 0.2881 | 0.0082 | 0.1990 | 0.029* |
| B6 | 0.4896 (5) | −0.0293 (2) | 0.11521 (14) | 0.0237 (8) |
| H6 | 0.3838 | −0.0628 | 0.0873 | 0.028* |
| B7 | 0.8773 (4) | 0.0367 (2) | 0.13102 (15) | 0.0200 (7) |
| H7 | 1.0210 | 0.0412 | 0.1135 | 0.024* |
| B8 | 0.8165 (5) | 0.0791 (3) | 0.20084 (13) | 0.0208 (8) |
| B9 | 0.6308 (5) | 0.0027 (2) | 0.22693 (14) | 0.0215 (8) |
| H9 | 0.6156 | −0.0119 | 0.2723 | 0.026* |
| B10 | 0.5808 (5) | −0.0895 (3) | 0.17536 (15) | 0.0264 (8) |
| H10 | 0.5358 | −0.1635 | 0.1872 | 0.032* |
| B11 | 0.7283 (5) | −0.0668 (2) | 0.11640 (13) | 0.0226 (8) |
| H11 | 0.7776 | −0.1261 | 0.0888 | 0.027* |
| B12 | 0.8187 (5) | −0.0485 (3) | 0.18553 (14) | 0.0223 (8) |
| H12 | 0.9269 | −0.0967 | 0.2038 | 0.027* |
| C1' | 0.6825 (4) | 0.2703 (2) | 0.07088 (12) | 0.0214 (7) |
| H1A' | 0.5709 | 0.2527 | 0.0501 | 0.026* |
| C2' | 0.6376 (4) | 0.31032 (19) | 0.13362 (13) | 0.0230 (7) |
| H2A' | 0.5049 | 0.3090 | 0.1427 | 0.028* |
| B4' | 0.9041 (5) | 0.2260 (3) | 0.06503 (14) | 0.0219 (8) |

| | | | | |
|---|---|---|---|---|
| H4' | 0.9495 | 0.1668 | 0.0368 | 0.026* |
| B5' | 0.8394 (5) | 0.3420 (3) | 0.03680 (15) | 0.0270 (8) |
| H5' | 0.8416 | 0.3554 | −0.0089 | 0.032* |
| B6' | 0.6614 (6) | 0.3936 (3) | 0.07935 (15) | 0.0288 (9) |
| H6' | 0.5476 | 0.4393 | 0.0620 | 0.035* |
| B7' | 0.8272 (5) | 0.2987 (3) | 0.17714 (14) | 0.0234 (8) |
| H7' | 0.8224 | 0.2879 | 0.2231 | 0.028* |
| B8' | 1.0090 (4) | 0.2466 (2) | 0.13358 (14) | 0.0230 (7) |
| H8' | 1.1256 | 0.2023 | 0.1505 | 0.028* |
| B9' | 1.0474 (5) | 0.3309 (3) | 0.07689 (14) | 0.0264 (8) |
| H9' | 1.1877 | 0.3378 | 0.0573 | 0.032* |
| B10' | 0.8996 (5) | 0.4339 (3) | 0.08584 (15) | 0.0300 (9) |
| H10' | 0.9436 | 0.5075 | 0.0728 | 0.036* |
| B11' | 0.7600 (6) | 0.4127 (2) | 0.14684 (13) | 0.0299 (8) |
| H11' | 0.7090 | 0.4729 | 0.1735 | 0.036* |
| B12' | 1.0000 (5) | 0.3752 (3) | 0.14570 (14) | 0.0288 (9) |
| H12' | 1.1087 | 0.4115 | 0.1714 | 0.035* |
| N1 | 0.9710 (3) | 0.11126 (17) | 0.24122 (9) | 0.0229 (6) |
| H1 | 1.0990 | 0.0961 | 0.2332 | 0.028* |
| C4 | 1.1407 (4) | 0.1731 (2) | 0.32223 (12) | 0.0256 (7) |
| H4A | 1.1353 | 0.2401 | 0.3340 | 0.038* |
| H4B | 1.2456 | 0.1642 | 0.2971 | 0.038* |
| H4C | 1.1565 | 0.1321 | 0.3547 | 0.038* |
| N2 | 0.7994 (3) | 0.1596 (2) | 0.31860 (10) | 0.0343 (7) |
| H2 | 0.6938 | 0.1394 | 0.2947 | 0.041* |
| C3 | 0.9637 (4) | 0.1471 (2) | 0.29305 (12) | 0.0230 (7) |
| C5 | 0.7718 (5) | 0.1953 (2) | 0.37620 (11) | 0.0345 (8) |
| H5A | 0.7396 | 0.2641 | 0.3750 | 0.041* |
| H5B | 0.8890 | 0.1886 | 0.3971 | 0.041* |
| C6 | 0.6200 (6) | 0.1412 (3) | 0.40579 (15) | 0.0676 (14) |
| H6A | 0.6566 | 0.0733 | 0.4092 | 0.081* |
| H6B | 0.5053 | 0.1440 | 0.3834 | 0.081* |
| C7 | 0.5797 (6) | 0.1821 (3) | 0.46437 (15) | 0.0698 (13) |
| H7A | 0.6917 | 0.1750 | 0.4876 | 0.084* |

| | | | | |
|---|---|---|---|---|
| H7B | 0.5520 | 0.2512 | 0.4613 | 0.084* |
| C8 | 0.4150 (6) | 0.1313 (3) | 0.49291 (17) | 0.0782 (15) |
| H8A | 0.3047 | 0.1363 | 0.4695 | 0.117* |
| H8B | 0.3906 | 0.1615 | 0.5287 | 0.117* |
| H8C | 0.4455 | 0.0638 | 0.4986 | 0.117* |

Atomic displacement parameters (Å$^2$)

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co3 | 0.01460 (17) | 0.02230 (18) | 0.01557 (16) | 0.0002 (2) | 0.0006 (2) | −0.00209 (16) |
| C1 | 0.0128 (13) | 0.0226 (15) | 0.0201 (14) | 0.0028 (12) | 0.0002 (13) | −0.0004 (14) |
| C2 | 0.0158 (14) | 0.0274 (18) | 0.0186 (15) | 0.0018 (13) | 0.0011 (13) | −0.0046 (13) |
| B4 | 0.0164 (18) | 0.027 (2) | 0.0164 (17) | −0.0036 (16) | 0.0034 (14) | −0.0022 (14) |
| B5 | 0.0198 (18) | 0.0259 (19) | 0.0263 (19) | 0.0017 (16) | 0.0027 (15) | −0.0004 (15) |
| B6 | 0.0213 (18) | 0.0201 (18) | 0.030 (2) | −0.0041 (15) | −0.0029 (15) | −0.0020 (15) |
| B7 | 0.0186 (16) | 0.0237 (18) | 0.0176 (16) | 0.0040 (14) | −0.0074 (16) | −0.0044 (16) |
| B8 | 0.0166 (17) | 0.029 (2) | 0.0166 (17) | 0.0048 (14) | 0.0000 (14) | 0.0004 (15) |
| B9 | 0.0185 (18) | 0.026 (2) | 0.0205 (17) | 0.0036 (15) | 0.0006 (14) | 0.0010 (16) |
| B10 | 0.024 (2) | 0.028 (2) | 0.027 (2) | 0.0008 (17) | −0.0029 (17) | −0.0032 (16) |
| B11 | 0.023 (2) | 0.0198 (16) | 0.0254 (16) | 0.0038 (17) | −0.0020 (17) | −0.0022 (12) |
| B12 | 0.0209 (18) | 0.026 (2) | 0.0201 (18) | 0.0026 (14) | 0.0003 (14) | −0.0011 (15) |
| C1' | 0.0172 (16) | 0.0287 (18) | 0.0182 (15) | 0.0009 (13) | −0.0021 (12) | 0.0015 (13) |
| C2' | 0.0197 (15) | 0.0223 (17) | 0.0270 (16) | 0.0031 (12) | 0.0016 (14) | −0.0067 (15) |
| B4' | 0.0181 (18) | 0.027 (2) | 0.0205 (18) | −0.0037 (16) | 0.0025 (15) | −0.0020 (15) |
| B5' | 0.0271 (18) | 0.029 (2) | 0.0255 (18) | −0.0003 (17) | 0.0033 (16) | 0.0059 (16) |
| B6' | 0.033 (2) | 0.022 (2) | 0.031 (2) | −0.0006 (17) | 0.0049 (17) | 0.0007 (17) |
| B7' | 0.0223 (16) | 0.031 (2) | 0.0166 (17) | −0.0033 (15) | −0.0011 (15) | −0.0089 (15) |
| B8' | 0.0179 (16) | 0.0317 (19) | 0.0193 (16) | −0.0031 (15) | 0.0008 (17) | −0.0056 (17) |
| B9' | 0.0216 (17) | 0.030 (2) | 0.0273 (18) | −0.0090 (18) | 0.0044 (14) | −0.0024 (17) |
| B10' | 0.038 (2) | 0.027 (2) | 0.025 (2) | −0.0050 (18) | 0.0060 (18) | 0.0018 (17) |
| B11' | 0.0320 (19) | 0.0240 (17) | 0.0337 (19) | −0.002 (2) | 0.002 (2) | −0.0062 (13) |
| B12' | 0.029 (2) | 0.031 (2) | 0.026 (2) | −0.0040 (17) | −0.0007 (16) | −0.0056 (16) |
| N1 | 0.0179 (13) | 0.0300 (15) | 0.0209 (14) | 0.0018 (12) | 0.0006 (11) | 0.0007 (11) |
| C4 | 0.0233 (16) | 0.0261 (17) | 0.0275 (16) | −0.0013 (15) | −0.0046 (13) | −0.0041 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.0260 (16) | 0.0572 (19) | 0.0196 (12) | −0.0037 (13) | 0.0001 (10) | −0.0139 (12) |
| C3 | 0.0244 (17) | 0.0228 (17) | 0.0217 (16) | 0.0015 (13) | −0.0006 (14) | 0.0001 (13) |
| C5 | 0.0342 (19) | 0.049 (2) | 0.0204 (15) | 0.0016 (17) | 0.0019 (16) | −0.0085 (12) |
| C6 | 0.054 (2) | 0.115 (4) | 0.034 (2) | −0.045 (3) | 0.0024 (19) | −0.012 (2) |
| C7 | 0.081 (3) | 0.090 (4) | 0.039 (2) | −0.033 (3) | −0.008 (2) | 0.008 (2) |
| C8 | 0.079 (3) | 0.099 (4) | 0.057 (3) | 0.004 (3) | 0.008 (3) | −0.025 (3) |

**Table 2**
Geometric parameters (Å, °)

| | | | |
|---|---|---|---|
| Co3—C2' | 2.035 (3) | C2'—B7' | 1.700 (4) |
| Co3—C2 | 2.036 (3) | C2'—B6' | 1.729 (4) |
| Co3—C1' | 2.041 (3) | C2'—H2A' | 0.9631 |
| Co3—C1 | 2.050 (3) | B4'—B9' | 1.782 (5) |
| Co3—B7 | 2.086 (3) | B4'—B5' | 1.785 (5) |
| Co3—B4' | 2.093 (3) | B4'—B8' | 1.809 (5) |
| Co3—B7' | 2.093 (3) | B4'—H4' | 1.1000 |
| Co3—B4 | 2.100 (3) | B5'—B9' | 1.758 (5) |
| Co3—B8' | 2.113 (3) | B5'—B6' | 1.762 (5) |
| Co3—B8 | 2.116 (3) | B5'—B10' | 1.767 (5) |
| C1—C2 | 1.610 (4) | B5'—H5' | 1.1000 |
| C1—B4 | 1.692 (4) | B6'—B11' | 1.765 (5) |
| C1—B5 | 1.692 (4) | B6'—B10' | 1.780 (5) |
| C1—B6 | 1.720 (4) | B6'—H6' | 1.1000 |
| C1—H1A | 1.0078 | B7'—B12' | 1.775 (5) |
| C2—B11 | 1.691 (4) | B7'—B11' | 1.785 (5) |
| C2—B7 | 1.707 (4) | B7'—B8' | 1.798 (5) |
| C2—B6 | 1.721 (4) | B7'—H7' | 1.1000 |
| C2—H2A | 0.9904 | B8'—B12' | 1.788 (5) |
| B4—B9 | 1.770 (5) | B8'—B9' | 1.793 (5) |
| B4—B5 | 1.777 (5) | B8'—H8' | 1.1000 |
| B4—B8 | 1.794 (5) | B9'—B10' | 1.771 (5) |
| B4—H4 | 1.1000 | B9'—B12' | 1.773 (5) |
| B5—B9 | 1.754 (5) | B9'—H9' | 1.1000 |

| | | | |
|---|---|---|---|
| B5—B6 | 1.754 (5) | B10'—B11' | 1.775 (5) |
| B5—B10 | 1.774 (5) | B10'—B12' | 1.780 (5) |
| B5—H5 | 1.1000 | B10'—H10' | 1.1000 |
| B6—B11 | 1.766 (5) | B11'—B12' | 1.774 (5) |
| B6—B10 | 1.770 (5) | B11'—H11' | 1.1000 |
| B6—H6 | 1.1000 | B12'—H12' | 1.1000 |
| B7—B12 | 1.791 (5) | N1—C3 | 1.325 (3) |
| B7—B11 | 1.802 (4) | N1—H1 | 0.9479 |
| B7—B8 | 1.806 (5) | C4—C3 | 1.474 (4) |
| B7—H7 | 1.1000 | C4—H4A | 0.9600 |
| B8—N1 | 1.518 (4) | C4—H4B | 0.9600 |
| B8—B12 | 1.788 (5) | C4—H4C | 0.9600 |
| B8—B9 | 1.791 (5) | N2—C3 | 1.322 (3) |
| B9—B10 | 1.794 (5) | N2—C5 | 1.464 (3) |
| B9—B12 | 1.795 (5) | N2—H2 | 0.9767 |
| B9—H9 | 1.1000 | C5—C6 | 1.482 (4) |
| B10—B11 | 1.772 (5) | C5—H5A | 0.9700 |
| B10—B12 | 1.790 (5) | C5—H5B | 0.9700 |
| B10—H10 | 1.1000 | C6—C7 | 1.525 (5) |
| B11—B12 | 1.777 (4) | C6—H6A | 0.9700 |
| B11—H11 | 1.1000 | C6—H6B | 0.9700 |
| B12—H12 | 1.1000 | C7—C8 | 1.517 (3) |
| C1'—C2' | 1.617 (4) | C7—H7A | 0.9700 |
| C1'—B4' | 1.686 (5) | C7—H7B | 0.9700 |
| C1'—B5' | 1.689 (4) | C8—H8A | 0.9600 |
| C1'—B6' | 1.710 (5) | C8—H8B | 0.9600 |
| C1'—H1A' | 0.9612 | C8—H8C | 0.9600 |
| C2'—B11' | 1.679 (4) | | |

| | | | |
|---|---|---|---|
| C2'—Co3—C2 | 133.62 (11) | B10—B12—H12 | 121.2 |
| C2'—Co3—C1' | 46.75 (11) | B7—B12—H12 | 121.0 |
| C2—Co3—C1' | 99.81 (12) | B9—B12—H12 | 122.3 |
| C2'—Co3—C1 | 100.22 (11) | C2'—C1'—B4' | 112.4 (2) |
| C2—Co3—C1 | 46.42 (10) | C2'—C1'—B5' | 111.8 (2) |
| C1'—Co3—C1 | 98.63 (11) | B4'—C1'—B5' | 63.85 (19) |

| | | | |
|---|---|---|---|
| C2'—Co3—B7 | 175.84 (12) | C2'—C1'—B6' | 62.54 (19) |
| C2—Co3—B7 | 48.91 (12) | B4'—C1'—B6' | 116.5 (2) |
| C1'—Co3—B7 | 131.77 (13) | B5'—C1'—B6' | 62.4 (2) |
| C1—Co3—B7 | 83.76 (11) | C2'—C1'—Co3 | 66.41 (14) |
| C2'—Co3—B4' | 83.35 (13) | B4'—C1'—Co3 | 67.53 (15) |
| C2—Co3—B4' | 95.04 (13) | B5'—C1'—Co3 | 125.5 (2) |
| C1'—Co3—B4' | 48.13 (13) | B6'—C1'—Co3 | 125.5 (2) |
| C1—Co3—B4' | 128.40 (12) | C2'—C1'—H1A' | 113.3 |
| B7—Co3—B4' | 93.25 (14) | B4'—C1'—H1A' | 129.1 |
| C2'—Co3—B7' | 48.61 (12) | B5'—C1'—H1A' | 116.1 |
| C2—Co3—B7' | 176.87 (13) | B6'—C1'—H1A' | 103.7 |
| C1'—Co3—B7' | 83.28 (14) | Co3—C1'—H1A' | 112.9 |
| C1—Co3—B7' | 132.91 (12) | C1'—C2'—B11' | 110.8 (2) |
| B7—Co3—B7' | 129.04 (13) | C1'—C2'—B7' | 111.8 (2) |
| B4'—Co3—B7' | 87.35 (14) | B11'—C2'—B7' | 63.77 (19) |
| C2'—Co3—B4 | 96.23 (13) | C1'—C2'—B6' | 61.36 (19) |
| C2—Co3—B4 | 82.62 (12) | B11'—C2'—B6' | 62.37 (19) |
| C1'—Co3—B4 | 129.43 (13) | B7'—C2'—B6' | 115.9 (2) |
| C1—Co3—B4 | 48.09 (11) | C1'—C2'—Co3 | 66.83 (14) |
| B7—Co3—B4 | 87.31 (14) | B11'—C2'—Co3 | 125.4 (2) |
| B4'—Co3—B4 | 176.37 (13) | B7'—C2'—Co3 | 67.49 (15) |
| B7'—Co3—B4 | 95.09 (13) | B6'—C2'—Co3 | 124.79 (19) |
| C2'—Co3—B8' | 83.75 (12) | C1'—C2'—H2A' | 113.0 |
| C2—Co3—B8' | 129.92 (12) | B11'—C2'—H2A' | 118.5 |
| C1'—Co3—B8' | 83.49 (13) | B7'—C2'—H2A' | 129.1 |
| C1—Co3—B8' | 175.96 (12) | B6'—C2'—H2A' | 105.9 |
| B7—Co3—B8' | 92.25 (13) | Co3—C2'—H2A' | 110.7 |
| B4'—Co3—B8' | 50.96 (13) | C1'—B4'—B9' | 103.0 (2) |
| B7'—Co3—B8' | 50.61 (13) | C1'—B4'—B5' | 58.15 (18) |
| B4—Co3—B8' | 132.63 (13) | B9'—B4'—B5' | 59.06 (19) |
| C2'—Co3—B8 | 130.41 (13) | C1'—B4'—B8' | 104.6 (2) |
| C2—Co3—B8 | 83.44 (13) | B9'—B4'—B8' | 59.91 (18) |
| C1'—Co3—B8 | 176.73 (13) | B5'—B4'—B8' | 107.6 (2) |
| C1—Co3—B8 | 83.31 (12) | C1'—B4'—Co3 | 64.34 (15) |

| | | | |
|---|---|---|---|
| B7—Co3—B8 | 50.92 (13) | B9'—B4'—Co3 | 117.5 (2) |
| B4'—Co3—B8 | 132.28 (13) | B5'—B4'—Co3 | 117.6 (2) |
| B7'—Co3—B8 | 93.46 (14) | B8'—B4'—Co3 | 65.09 (15) |
| B4—Co3—B8 | 50.36 (13) | C1'—B4'—H4' | 126.0 |
| B8'—Co3—B8 | 94.73 (13) | B9'—B4'—H4' | 121.7 |
| C2—C1—B4 | 111.6 (2) | B5'—B4'—H4' | 120.3 |
| C2—C1—B5 | 110.8 (2) | B8'—B4'—H4' | 122.8 |
| B4—C1—B5 | 63.34 (18) | Co3—B4'—H4' | 111.6 |
| C2—C1—B6 | 62.12 (18) | C1'—B5'—B9' | 103.9 (2) |
| B4—C1—B6 | 115.2 (2) | C1'—B5'—B6' | 59.35 (19) |
| B5—C1—B6 | 61.86 (18) | B9'—B5'—B6' | 108.9 (3) |
| C2—C1—Co3 | 66.35 (13) | C1'—B5'—B10' | 105.0 (2) |
| B4—C1—Co3 | 67.52 (14) | B9'—B5'—B10' | 60.3 (2) |
| B5—C1—Co3 | 124.87 (19) | B6'—B5'—B10' | 60.6 (2) |
| B6—C1—Co3 | 124.82 (18) | C1'—B5'—B4' | 58.00 (18) |
| C2—C1—H1A | 123.1 | B9'—B5'—B4' | 60.4 (2) |
| B4—C1—H1A | 118.1 | B6'—B5'—B4' | 109.0 (2) |
| B5—C1—H1A | 115.0 | B10'—B5'—B4' | 109.1 (2) |
| B6—C1—H1A | 114.5 | C1'—B5'—H5' | 125.3 |
| Co3—C1—H1A | 109.0 | B9'—B5'—H5' | 122.4 |
| C1—C2—B11 | 111.8 (2) | B6'—B5'—H5' | 120.5 |
| C1—C2—B7 | 112.6 (2) | B10'—B5'—H5' | 121.7 |
| B11—C2—B7 | 64.05 (18) | B4'—B5'—H5' | 121.0 |
| C1—C2—B6 | 62.08 (17) | C1'—B6'—C2' | 56.11 (17) |
| B11—C2—B6 | 62.3 (2) | C1'—B6'—B5' | 58.21 (19) |
| B7—C2—B6 | 116.3 (2) | C2'—B6'—B5' | 103.3 (2) |
| C1—C2—Co3 | 67.23 (14) | C1'—B6'—B11' | 102.6 (3) |
| B11—C2—Co3 | 125.4 (2) | C2'—B6'—B11' | 57.44 (18) |
| B7—C2—Co3 | 67.07 (15) | B5'—B6'—B11' | 107.2 (3) |
| B6—C2—Co3 | 125.60 (19) | C1'—B6'—B10' | 103.6 (2) |
| C1—C2—H2A | 119.1 | C2'—B6'—B10' | 103.5 (3) |
| B11—C2—H2A | 115.7 | B5'—B6'—B10' | 59.86 (19) |
| B7—C2—H2A | 121.2 | B11'—B6'—B10' | 60.1 (2) |
| B6—C2—H2A | 111.4 | C1'—B6'—H6' | 125.7 |

| | | | |
|---|---|---|---|
| Co3—C2—H2A | 109.3 | C2'—B6'—H6' | 125.7 |
| C1—B4—B9 | 104.2 (2) | B5'—B6'—H6' | 122.5 |
| C1—B4—B5 | 58.34 (17) | B11'—B6'—H6' | 123.0 |
| B9—B4—B5 | 59.28 (18) | B10'—B6'—H6' | 123.2 |
| C1—B4—B8 | 105.2 (2) | C2'—B7'—B12' | 103.5 (2) |
| B9—B4—B8 | 60.32 (19) | C2'—B7'—B11' | 57.55 (18) |
| B5—B4—B8 | 107.8 (2) | B12'—B7'—B11' | 59.8 (2) |
| C1—B4—Co3 | 64.39 (13) | C2'—B7'—B8' | 104.7 (2) |
| B9—B4—Co3 | 118.3 (2) | B12'—B7'—B8' | 60.04 (19) |
| B5—B4—Co3 | 117.6 (2) | B11'—B7'—B8' | 107.9 (2) |
| B8—B4—Co3 | 65.27 (15) | C2'—B7'—Co3 | 63.91 (14) |
| C1—B4—H4 | 125.4 | B12'—B7'—Co3 | 117.7 (2) |
| B9—B4—H4 | 121.0 | B11'—B7'—Co3 | 116.6 (2) |
| B5—B4—H4 | 120.4 | B8'—B7'—Co3 | 65.26 (15) |
| B8—B4—H4 | 122.5 | C2'—B7'—H7' | 126.2 |
| Co3—B4—H4 | 111.4 | B12'—B7'—H7' | 121.1 |
| C1—B5—B9 | 104.8 (2) | B11'—B7'—H7' | 120.6 |
| C1—B5—B6 | 59.86 (17) | B8'—B7'—H7' | 122.5 |
| B9—B5—B6 | 109.5 (2) | Co3—B7'—H7' | 112.0 |
| C1—B5—B10 | 105.7 (2) | B12'—B8'—B9' | 59.35 (19) |
| B9—B5—B10 | 61.12 (19) | B12'—B8'—B7' | 59.36 (19) |
| B6—B5—B10 | 60.21 (19) | B9'—B8'—B7' | 106.4 (2) |
| C1—B5—B4 | 58.31 (17) | B12'—B8'—B4' | 106.5 (2) |
| B9—B5—B4 | 60.17 (18) | B9'—B8'—B4' | 59.29 (18) |
| B6—B5—B4 | 109.4 (2) | B7'—B8'—B4' | 106.5 (2) |
| B10—B5—B4 | 109.4 (2) | B12'—B8'—Co3 | 116.1 (2) |
| C1—B5—H5 | 124.7 | B9'—B8'—Co3 | 115.9 (2) |
| B9—B5—H5 | 121.8 | B7'—B8'—Co3 | 64.13 (14) |
| B6—B5—H5 | 120.4 | B4'—B8'—Co3 | 63.95 (14) |
| B10—B5—H5 | 121.5 | B12'—B8'—H8' | 120.9 |
| B4—B5—H5 | 121.0 | B9'—B8'—H8' | 121.1 |
| C1—B6—C2 | 55.80 (16) | B7'—B8'—H8' | 123.2 |
| C1—B6—B5 | 58.28 (18) | B4'—B8'—H8' | 123.2 |
| C2—B6—B5 | 103.0 (2) | Co3—B8'—H8' | 113.3 |

| | | | |
|---|---|---|---|
| C1—B6—B11 | 103.3 (2) | B5'—B9'—B10' | 60.1 (2) |
| C2—B6—B11 | 58.00 (18) | B5'—B9'—B12' | 108.1 (3) |
| B5—B6—B11 | 107.6 (2) | B10'—B9'—B12' | 60.3 (2) |
| C1—B6—B10 | 104.6 (2) | B5'—B9'—B4' | 60.57 (19) |
| C2—B6—B10 | 104.0 (2) | B10'—B9'—B4' | 109.1 (2) |
| B5—B6—B10 | 60.43 (19) | B12'—B9'—B4' | 108.3 (2) |
| B11—B6—B10 | 60.15 (19) | B5'—B9'—B8' | 109.6 (2) |
| C1—B6—H6 | 125.3 | B10'—B9'—B8' | 109.6 (2) |
| C2—B6—H6 | 125.8 | B12'—B9'—B8' | 60.18 (19) |
| B5—B6—H6 | 122.5 | B4'—B9'—B8' | 60.80 (18) |
| B11—B6—H6 | 122.6 | B5'—B9'—H9' | 121.3 |
| B10—B6—H6 | 122.6 | B10'—B9'—H9' | 121.0 |
| C2—B7—B12 | 102.7 (2) | B12'—B9'—H9' | 121.9 |
| C2—B7—B11 | 57.54 (18) | B4'—B9'—H9' | 121.1 |
| B12—B7—B11 | 59.28 (18) | B8'—B9'—H9' | 120.5 |
| C2—B7—B8 | 103.7 (2) | B5'—B10'—B9' | 59.6 (2) |
| B12—B7—B8 | 59.59 (19) | B5'—B10'—B11' | 106.6 (3) |
| B11—B7—B8 | 106.9 (2) | B9'—B10'—B11' | 107.2 (3) |
| C2—B7—Co3 | 64.02 (14) | B5'—B10'—B12' | 107.3 (3) |
| B12—B7—Co3 | 117.7 (2) | B9'—B10'—B12' | 59.92 (19) |
| B11—B7—Co3 | 116.9 (2) | B11'—B10'—B12' | 59.9 (2) |
| B8—B7—Co3 | 65.39 (15) | B5'—B10'—B6' | 59.56 (19) |
| C2—B7—H7 | 126.6 | B9'—B10'—B6' | 107.5 (2) |
| B12—B7—H7 | 121.5 | B11'—B10'—B6' | 59.5 (2) |
| B11—B7—H7 | 120.8 | B12'—B10'—B6' | 107.8 (3) |
| B8—B7—H7 | 123.2 | B5'—B10'—H10' | 122.5 |
| Co3—B7—H7 | 111.6 | B9'—B10'—H10' | 122.1 |
| N1—B8—B12 | 114.0 (2) | B11'—B10'—H10' | 122.5 |
| N1—B8—B9 | 118.7 (2) | B12'—B10'—H10' | 121.7 |
| B12—B8—B9 | 60.22 (19) | B6'—B10'—H10' | 121.9 |
| N1—B8—B4 | 128.6 (3) | C2'—B11'—B6' | 60.19 (19) |
| B12—B8—B4 | 107.0 (2) | C2'—B11'—B12' | 104.4 (2) |
| B9—B8—B4 | 59.19 (18) | B6'—B11'—B12' | 108.7 (2) |
| N1—B8—B7 | 120.0 (2) | C2'—B11'—B10' | 105.8 (2) |

| | | | |
|---|---|---|---|
| B12—B8—B7 | 59.78 (18) | B6'—B11'—B10' | 60.4 (2) |
| B9—B8—B7 | 107.6 (2) | B12'—B11'—B10' | 60.2 (2) |
| B4—B8—B7 | 106.8 (2) | C2'—B11'—B7' | 58.68 (17) |
| N1—B8—Co3 | 118.0 (2) | B6'—B11'—B7' | 109.9 (2) |
| B12—B8—Co3 | 116.37 (19) | B12'—B11'—B7' | 59.8 (2) |
| B9—B8—Co3 | 116.6 (2) | B10'—B11'—B7' | 108.9 (3) |
| B4—B8—Co3 | 64.37 (15) | C2'—B11'—H11' | 124.4 |
| B7—B8—Co3 | 63.69 (14) | B6'—B11'—H11' | 120.2 |
| B5—B9—B4 | 60.55 (18) | B12'—B11'—H11' | 122.7 |
| B5—B9—B8 | 108.9 (2) | B10'—B11'—H11' | 121.8 |
| B4—B9—B8 | 60.50 (18) | B7'—B11'—H11' | 120.9 |
| B5—B9—B10 | 59.98 (19) | B9'—B12'—B11' | 107.1 (2) |
| B4—B9—B10 | 108.8 (2) | B9'—B12'—B7' | 108.3 (2) |
| B8—B9—B10 | 108.8 (2) | B11'—B12'—B7' | 60.38 (19) |
| B5—B9—B12 | 107.4 (2) | B9'—B12'—B10' | 59.8 (2) |
| B4—B9—B12 | 107.7 (2) | B11'—B12'—B10' | 59.93 (19) |
| B8—B9—B12 | 59.81 (19) | B7'—B12'—B10' | 109.1 (3) |
| B10—B9—B12 | 59.84 (19) | B9'—B12'—B8' | 60.5 (2) |
| B5—B9—H9 | 121.6 | B11'—B12'—B8' | 108.8 (2) |
| B4—B9—H9 | 121.3 | B7'—B12'—B8' | 60.60 (19) |
| B8—B9—H9 | 121.1 | B10'—B12'—B8' | 109.4 (3) |
| B10—B9—H9 | 121.3 | B9'—B12'—H12' | 122.2 |
| B12—B9—H9 | 122.4 | B11'—B12'—H12' | 122.0 |
| B6—B10—B11 | 59.81 (19) | B7'—B12'—H12' | 121.1 |
| B6—B10—B5 | 59.35 (19) | B10'—B12'—H12' | 121.1 |
| B11—B10—B5 | 106.5 (3) | B8'—B12'—H12' | 120.7 |
| B6—B10—B12 | 107.8 (2) | C3—N1—B8 | 131.7 (2) |
| B11—B10—B12 | 59.87 (19) | C3—N1—H1 | 107.7 |
| B5—B10—B12 | 106.7 (2) | B8—N1—H1 | 119.9 |
| B6—B10—B9 | 107.0 (2) | C3—C4—H4A | 109.5 |
| B11—B10—B9 | 107.4 (2) | C3—C4—H4B | 109.5 |
| B5—B10—B9 | 58.90 (19) | H4A—C4—H4B | 109.5 |
| B12—B10—B9 | 60.12 (18) | C3—C4—H4C | 109.5 |
| B6—B10—H10 | 122.0 | H4A—C4—H4C | 109.5 |

| | | | |
|---|---|---|---|
| B11—B10—H10 | 122.2 | H4B—C4—H4C | 109.5 |
| B5—B10—H10 | 123.0 | C3—N2—C5 | 126.0 (2) |
| B12—B10—H10 | 121.8 | C3—N2—H2 | 111.7 |
| B9—B10—H10 | 122.2 | C5—N2—H2 | 122.2 |
| C2—B11—B6 | 59.68 (18) | N2—C3—N1 | 120.5 (3) |
| C2—B11—B10 | 105.2 (2) | N2—C3—C4 | 120.0 (2) |
| B6—B11—B10 | 60.04 (19) | N1—C3—C4 | 119.5 (3) |
| C2—B11—B12 | 104.0 (2) | N2—C5—C6 | 111.7 (3) |
| B6—B11—B12 | 108.5 (2) | N2—C5—H5A | 109.3 |
| B10—B11—B12 | 60.58 (19) | C6—C5—H5A | 109.3 |
| C2—B11—B7 | 58.41 (17) | N2—C5—H5B | 109.3 |
| B6—B11—B7 | 109.4 (2) | C6—C5—H5B | 109.3 |
| B10—B11—B7 | 109.3 (2) | H5A—C5—H5B | 107.9 |
| B12—B11—B7 | 60.06 (19) | C5—C6—C7 | 112.5 (3) |
| C2—B11—H11 | 125.0 | C5—C6—H6A | 109.1 |
| B6—B11—H11 | 120.6 | C7—C6—H6A | 109.1 |
| B10—B11—H11 | 121.7 | C5—C6—H6B | 109.1 |
| B12—B11—H11 | 122.6 | C7—C6—H6B | 109.1 |
| B7—B11—H11 | 120.8 | H6A—C6—H6B | 107.8 |
| B11—B12—B8 | 108.8 (2) | C8—C7—C6 | 112.4 (3) |
| B11—B12—B10 | 59.56 (19) | C8—C7—H7A | 109.1 |
| B8—B12—B10 | 109.1 (2) | C6—C7—H7A | 109.1 |
| B11—B12—B7 | 60.66 (18) | C8—C7—H7B | 109.1 |
| B8—B12—B7 | 60.63 (19) | C6—C7—H7B | 109.1 |
| B10—B12—B7 | 109.0 (2) | H7A—C7—H7B | 107.9 |
| B11—B12—B9 | 107.1 (2) | C7—C8—H8A | 109.5 |
| B8—B12—B9 | 59.97 (18) | C7—C8—H8B | 109.5 |
| B10—B12—B9 | 60.04 (18) | H8A—C8—H8B | 109.5 |
| B7—B12—B9 | 108.1 (2) | C7—C8—H8C | 109.5 |
| B11—B12—H12 | 121.9 | H8A—C8—H8C | 109.5 |
| B8—B12—H12 | 120.9 | H8B—C8—H8C | 109.5 |

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

**(7)**

*Crystal data*

| | |
|---|---|
| $C_{10}H_{35}B_{18}CoN_2$ | $D_x$ = 1.281 Mg m$^{-3}$ |
| $M_r$ = 436.91 | Melting point: 541 K |
| Orthorhombic, *Pbca* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 5708 reflections |
| *a* = 12.4127 (2) Å | θ = 1–27.5° |
| *b* = 12.1868 (2) Å | μ = 0.76 mm$^{-1}$ |
| *c* = 29.9491 (4) Å | *T* = 150 (2) K |
| *V* = 4530.43 (12) Å$^3$ | Cell measurement pressure: 101.3 kPa |
| *Z* = 8 | Prism, red |
| $F_{000}$ = 1808 | 0.55 × 0.5 × 0.2 mm |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD area detector diffractometer | 5178 independent reflections |
| Radiation source: fine-focus sealed tube | 4476 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.032 |
| Detector resolution: 9.091 pixels mm$^{-1}$ | $\theta_{max}$ = 27.5° |
| *T* = 150(2) K | $\theta_{min}$ = 2.1° |
| *P* = 101.3 kPa | *h* = −16→16 |
| φ and ω scans to fill the Ewald sphere | *k* = −15→15 |
| Absorption correction: none | *l* = −38→38 |
| 44317 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.035 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.091 | $w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 4.7024P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 1.03 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 5178 reflections | $\Delta\rho_{max}$ = 0.38 e Å$^{-3}$ |
| 287 parameters | $\Delta\rho_{min}$ = −0.29 e Å$^{-3}$ |
| ? constraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co3 | 0.490815 (17) | 0.202972 (18) | 0.158778 (7) | 0.01531 (8) |
| C1 | 0.48508 (14) | 0.33845 (15) | 0.19828 (6) | 0.0222 (4) |
| H1 | 0.4048 | 0.3751 | 0.1939 | 0.027* |
| C2 | 0.50162 (13) | 0.22665 (15) | 0.22601 (6) | 0.0215 (4) |
| H2 | 0.4329 | 0.1834 | 0.2411 | 0.026* |
| B4 | 0.57549 (16) | 0.35016 (17) | 0.15532 (7) | 0.0231 (4) |
| H4 | 0.5620 | 0.3920 | 0.1233 | 0.028* |
| B5 | 0.58761 (17) | 0.42658 (18) | 0.20683 (8) | 0.0281 (5) |
| H5 | 0.5797 | 0.5165 | 0.2073 | 0.034* |
| B6 | 0.53738 (18) | 0.34743 (19) | 0.25127 (8) | 0.0282 (5) |
| H6 | 0.4969 | 0.3845 | 0.2803 | 0.034* |
| B7 | 0.60475 (15) | 0.14967 (18) | 0.20583 (7) | 0.0217 (4) |
| H7 | 0.6104 | 0.0596 | 0.2068 | 0.026* |
| B8 | 0.66169 (15) | 0.22970 (18) | 0.16036 (7) | 0.0210 (4) |
| B9 | 0.70142 (17) | 0.35862 (19) | 0.18395 (7) | 0.0263 (4) |
| H9 | 0.7692 | 0.4048 | 0.1695 | 0.032* |
| B10 | 0.67831 (17) | 0.35615 (19) | 0.24250 (7) | 0.0281 (5) |
| H10 | 0.7322 | 0.3995 | 0.2657 | 0.034* |
| B11 | 0.61629 (17) | 0.22896 (19) | 0.25617 (7) | 0.0270 (5) |
| H11 | 0.6272 | 0.1893 | 0.2889 | 0.032* |
| B12 | 0.71870 (16) | 0.23400 (19) | 0.21528 (7) | 0.0249 (4) |
| H12 | 0.7983 | 0.1975 | 0.2216 | 0.030* |
| C1' | 0.39748 (14) | 0.06456 (15) | 0.16158 (6) | 0.0218 (4) |
| H1' | 0.4111 | 0.0270 | 0.1945 | 0.026* |
| C2' | 0.32835 (13) | 0.17501 (15) | 0.15632 (6) | 0.0210 (4) |
| H2' | 0.2934 | 0.2160 | 0.1857 | 0.025* |
| B4' | 0.49672 (16) | 0.05658 (17) | 0.12285 (7) | 0.0238 (4) |
| H4' | 0.5747 | 0.0151 | 0.1272 | 0.029* |
| B5' | 0.37580 (17) | −0.02191 (19) | 0.11853 (8) | 0.0290 (5) |
| H5' | 0.3772 | −0.1119 | 0.1210 | 0.035* |
| B6' | 0.26827 (16) | 0.05325 (18) | 0.14120 (7) | 0.0250 (4) |
| H6' | 0.2004 | 0.0135 | 0.1584 | 0.030* |

| | | | | |
|---|---|---|---|---|
| B7' | 0.37193 (16) | 0.25480 (18) | 0.11356 (7) | 0.0236 (4) |
| H7' | 0.3671 | 0.3448 | 0.1119 | 0.028* |
| B8' | 0.48077 (16) | 0.17890 (19) | 0.08906 (7) | 0.0242 (4) |
| H8' | 0.5471 | 0.2178 | 0.0706 | 0.029* |
| B9' | 0.42582 (17) | 0.0497 (2) | 0.07121 (8) | 0.0301 (5) |
| H9' | 0.4597 | 0.0062 | 0.0423 | 0.036* |
| B10' | 0.28507 (17) | 0.04861 (18) | 0.08240 (7) | 0.0258 (4) |
| H10' | 0.2281 | 0.0055 | 0.0604 | 0.031* |
| B11' | 0.25225 (16) | 0.17344 (18) | 0.10961 (7) | 0.0246 (4) |
| H11' | 0.1724 | 0.2117 | 0.1064 | 0.029* |
| B12' | 0.34778 (17) | 0.1729 (2) | 0.06572 (7) | 0.0285 (5) |
| H12' | 0.3301 | 0.2104 | 0.0331 | 0.034* |
| N1 | 0.72313 (12) | 0.17851 (14) | 0.12164 (5) | 0.0259 (3) |
| C3 | 0.82638 (14) | 0.17146 (16) | 0.11021 (6) | 0.0251 (4) |
| C4 | 0.91270 (15) | 0.22218 (18) | 0.13821 (7) | 0.0310 (4) |
| H4A | 0.8808 | 0.2725 | 0.1591 | 0.046* |
| H4B | 0.9623 | 0.2609 | 0.1194 | 0.046* |
| H4C | 0.9504 | 0.1658 | 0.1542 | 0.046* |
| N2 | 0.85516 (12) | 0.11870 (15) | 0.07307 (5) | 0.0299 (4) |
| C5 | 0.77663 (16) | 0.0715 (2) | 0.04176 (6) | 0.0348 (5) |
| H5A | 0.8067 | 0.0735 | 0.0119 | 0.042* |
| H5B | 0.7122 | 0.1165 | 0.0418 | 0.042* |
| C6 | 0.74567 (19) | −0.0461 (2) | 0.05292 (8) | 0.0458 (6) |
| H6A | 0.8089 | −0.0914 | 0.0526 | 0.069* |
| H6B | 0.6952 | −0.0726 | 0.0312 | 0.069* |
| H6C | 0.7134 | −0.0484 | 0.0820 | 0.069* |
| C7 | 0.96970 (15) | 0.0977 (2) | 0.06152 (7) | 0.0335 (5) |
| H7A | 0.9758 | 0.0255 | 0.0481 | 0.040* |
| H7B | 1.0124 | 0.0979 | 0.0887 | 0.040* |
| C8 | 1.01459 (18) | 0.1822 (2) | 0.02960 (8) | 0.0488 (7) |
| H8A | 0.9728 | 0.1823 | 0.0026 | 0.073* |
| H8B | 1.0881 | 0.1646 | 0.0227 | 0.073* |
| H8C | 1.0114 | 0.2535 | 0.0432 | 0.073* |
| H1A | 0.675 (2) | 0.139 (2) | 0.1030 (8) | 0.050 (7)* |

Atomic displacement parameters (Å$^2$)

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co3 | 0.01254 (12) | 0.01649 (12) | 0.01691 (13) | −0.00022 (8) | −0.00131 (8) | −0.00228 (8) |
| C1 | 0.0194 (8) | 0.0218 (9) | 0.0253 (9) | −0.0002 (7) | 0.0007 (7) | −0.0069 (7) |
| C2 | 0.0200 (8) | 0.0264 (9) | 0.0180 (8) | −0.0027 (7) | −0.0002 (6) | −0.0020 (7) |
| B4 | 0.0211 (9) | 0.0220 (10) | 0.0261 (10) | −0.0052 (8) | 0.0003 (8) | 0.0009 (8) |
| B5 | 0.0254 (10) | 0.0236 (10) | 0.0353 (12) | −0.0044 (8) | −0.0016 (9) | −0.0075 (9) |
| B6 | 0.0246 (10) | 0.0336 (11) | 0.0263 (10) | −0.0040 (9) | 0.0016 (8) | −0.0107 (9) |
| B7 | 0.0188 (9) | 0.0248 (10) | 0.0216 (10) | 0.0005 (8) | −0.0029 (7) | −0.0008 (8) |
| B8 | 0.0139 (8) | 0.0282 (10) | 0.0210 (9) | −0.0010 (7) | 0.0008 (7) | −0.0044 (8) |
| B9 | 0.0219 (10) | 0.0315 (11) | 0.0256 (11) | −0.0078 (8) | 0.0007 (8) | −0.0057 (9) |
| B10 | 0.0222 (10) | 0.0350 (12) | 0.0271 (11) | −0.0046 (9) | −0.0013 (8) | −0.0124 (9) |
| B11 | 0.0215 (10) | 0.0381 (12) | 0.0213 (10) | −0.0032 (9) | −0.0026 (8) | −0.0035 (9) |
| B12 | 0.0190 (9) | 0.0332 (12) | 0.0224 (10) | −0.0014 (8) | −0.0035 (8) | −0.0054 (9) |
| C1' | 0.0195 (8) | 0.0200 (8) | 0.0259 (9) | −0.0027 (7) | −0.0036 (7) | 0.0009 (7) |
| C2' | 0.0142 (8) | 0.0257 (9) | 0.0230 (9) | −0.0022 (6) | −0.0003 (6) | −0.0028 (7) |
| B4' | 0.0192 (9) | 0.0214 (10) | 0.0308 (11) | 0.0014 (7) | −0.0029 (8) | −0.0064 (8) |
| B5' | 0.0247 (10) | 0.0233 (10) | 0.0391 (13) | −0.0017 (8) | −0.0054 (9) | −0.0081 (9) |
| B6' | 0.0202 (10) | 0.0246 (10) | 0.0302 (11) | −0.0052 (8) | −0.0026 (8) | −0.0017 (9) |
| B7' | 0.0202 (9) | 0.0216 (10) | 0.0290 (11) | 0.0009 (8) | −0.0066 (8) | 0.0017 (8) |
| B8' | 0.0199 (9) | 0.0346 (11) | 0.0182 (9) | −0.0038 (8) | −0.0013 (7) | −0.0006 (8) |
| B9' | 0.0216 (10) | 0.0402 (13) | 0.0284 (11) | 0.0001 (9) | −0.0018 (8) | −0.0149 (10) |
| B10' | 0.0205 (9) | 0.0304 (11) | 0.0265 (11) | −0.0038 (8) | −0.0027 (8) | −0.0087 (9) |
| B11' | 0.0163 (9) | 0.0275 (11) | 0.0299 (11) | −0.0007 (8) | −0.0039 (8) | −0.0027 (9) |
| B12' | 0.0237 (10) | 0.0383 (12) | 0.0235 (11) | −0.0058 (9) | −0.0045 (8) | 0.0024 (9) |
| N1 | 0.0158 (7) | 0.0383 (9) | 0.0236 (8) | −0.0023 (6) | 0.0004 (6) | −0.0093 (7) |
| C3 | 0.0192 (8) | 0.0338 (10) | 0.0222 (9) | −0.0009 (7) | 0.0019 (7) | −0.0010 (8) |
| C4 | 0.0181 (9) | 0.0442 (12) | 0.0306 (10) | −0.0041 (8) | 0.0028 (7) | −0.0076 (9) |
| N2 | 0.0190 (7) | 0.0489 (11) | 0.0217 (8) | 0.0014 (7) | 0.0025 (6) | −0.0072 (7) |
| C5 | 0.0257 (10) | 0.0587 (14) | 0.0198 (9) | 0.0045 (9) | −0.0004 (7) | −0.0132 (9) |
| C6 | 0.0353 (12) | 0.0637 (16) | 0.0385 (12) | −0.0062 (11) | 0.0022 (10) | −0.0233 (12) |
| C7 | 0.0200 (9) | 0.0537 (13) | 0.0269 (10) | 0.0054 (9) | 0.0039 (7) | −0.0022 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0297 (11) | 0.0797 (19) | 0.0369 (13) | 0.0085 (11) | 0.0082 (9) | 0.0189 (13) |

**Table 3**
Geometric parameters (Å, °)

| | | | |
|---|---|---|---|
| Co3—C1 | 2.0324 (18) | C2'—B7' | 1.696 (3) |
| Co3—C2 | 2.0384 (18) | C2'—B6' | 1.721 (3) |
| Co3—C2' | 2.0465 (17) | C2'—H2' | 1.1000 |
| Co3—C1' | 2.0481 (17) | B4'—B9' | 1.781 (3) |
| Co3—B4 | 2.082 (2) | B4'—B5' | 1.784 (3) |
| Co3—B4' | 2.085 (2) | B4'—B8' | 1.813 (3) |
| Co3—B7 | 2.0995 (19) | B4'—H4' | 1.1000 |
| Co3—B7' | 2.100 (2) | B5'—B6' | 1.755 (3) |
| Co3—B8' | 2.112 (2) | B5'—B9' | 1.777 (3) |
| Co3—B8 | 2.1464 (19) | B5'—B10' | 1.783 (3) |
| C1—C2 | 1.609 (3) | B5'—H5' | 1.1000 |
| C1—B5 | 1.685 (3) | B6'—B11' | 1.755 (3) |
| C1—B4 | 1.713 (3) | B6'—B10' | 1.774 (3) |
| C1—B6 | 1.718 (3) | B6'—H6' | 1.1000 |
| C1—H1 | 1.1000 | B7'—B12' | 1.772 (3) |
| C2—B11 | 1.686 (3) | B7'—B11' | 1.790 (3) |
| C2—B7 | 1.698 (3) | B7'—B8' | 1.794 (3) |
| C2—B6 | 1.713 (3) | B7'—H7' | 1.1000 |
| C2—H2 | 1.1000 | B8'—B12' | 1.794 (3) |
| B4—B9 | 1.786 (3) | B8'—B9' | 1.797 (3) |
| B4—B5 | 1.808 (3) | B8'—H8' | 1.1000 |
| B4—B8 | 1.823 (3) | B9'—B10' | 1.779 (3) |
| B4—H4 | 1.1000 | B9'—B12' | 1.794 (3) |
| B5—B6 | 1.758 (3) | B9'—H9' | 1.1000 |
| B5—B10 | 1.774 (3) | B10'—B11' | 1.773 (3) |
| B5—B9 | 1.775 (3) | B10'—B12' | 1.775 (3) |
| B5—H5 | 1.1000 | B10'—H10' | 1.1000 |
| B6—B11 | 1.751 (3) | B11'—B12' | 1.770 (3) |
| B6—B10 | 1.772 (3) | B11'—H11' | 1.1000 |

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| B6—H6 | 1.1000 | B12'—H12' | 1.1000 |
| B7—B12 | 1.771 (3) | N1—C3 | 1.329 (2) |
| B7—B11 | 1.797 (3) | N1—H1A | 0.94 (3) |
| B7—B8 | 1.818 (3) | C3—N2 | 1.334 (2) |
| B7—H7 | 1.1000 | C3—C4 | 1.494 (3) |
| B8—N1 | 1.522 (2) | C4—H4A | 0.9600 |
| B8—B12 | 1.791 (3) | C4—H4B | 0.9600 |
| B8—B9 | 1.792 (3) | C4—H4C | 0.9600 |
| B9—B10 | 1.777 (3) | N2—C5 | 1.470 (2) |
| B9—B12 | 1.798 (3) | N2—C7 | 1.485 (2) |
| B9—H9 | 1.1000 | C5—C6 | 1.520 (3) |
| B10—B12 | 1.770 (3) | C5—H5A | 0.9700 |
| B10—B11 | 1.778 (3) | C5—H5B | 0.9700 |
| B10—H10 | 1.1000 | C6—H6A | 0.9600 |
| B11—B12 | 1.766 (3) | C6—H6B | 0.9600 |
| B11—H11 | 1.1000 | C6—H6C | 0.9600 |
| B12—H12 | 1.1000 | C7—C8 | 1.512 (3) |
| C1'—C2' | 1.604 (2) | C7—H7A | 0.9700 |
| C1'—B5' | 1.687 (3) | C7—H7B | 0.9700 |
| C1'—B4' | 1.695 (3) | C8—H8A | 0.9600 |
| C1'—B6' | 1.722 (3) | C8—H8B | 0.9600 |
| C1'—H1' | 1.1000 | C8—H8C | 0.9600 |
| C2'—B11' | 1.688 (3) | | |

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| C1—Co3—C2 | 46.55 (7) | B7—B12—H12 | 120.7 |
| C1—Co3—C2' | 96.99 (7) | B8—B12—H12 | 120.1 |
| C2—Co3—C2' | 97.12 (7) | B9—B12—H12 | 122.6 |
| C1—Co3—C1' | 128.71 (7) | C2'—C1'—B5' | 111.33 (14) |
| C2—Co3—C1' | 96.51 (7) | C2'—C1'—B4' | 111.70 (14) |
| C2'—Co3—C1' | 46.13 (7) | B5'—C1'—B4' | 63.70 (12) |
| C1—Co3—B4 | 49.20 (8) | C2'—C1'—B6' | 62.22 (11) |
| C2—Co3—B4 | 83.91 (8) | B5'—C1'—B6' | 61.99 (12) |
| C2'—Co3—B4 | 129.74 (8) | B4'—C1'—B6' | 115.46 (14) |
| C1'—Co3—B4 | 175.86 (8) | C2'—C1'—Co3 | 66.89 (9) |
| C1—Co3—B4' | 175.47 (8) | B5'—C1'—Co3 | 124.99 (13) |

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| C2—Co3—B4' | 128.95 (8) | B4'—C1'—Co3 | 66.93 (9) |
| C2'—Co3—B4' | 82.73 (8) | B6'—C1'—Co3 | 125.34 (12) |
| C1'—Co3—B4' | 48.41 (8) | C2'—C1'—H1' | 121.3 |
| B4—Co3—B4' | 133.95 (8) | B5'—C1'—H1' | 116.8 |
| C1—Co3—B7 | 83.35 (8) | B4'—C1'—H1' | 118.5 |
| C2—Co3—B7 | 48.43 (7) | B6'—C1'—H1' | 115.3 |
| C2'—Co3—B7 | 129.52 (8) | Co3—C1'—H1' | 107.0 |
| C1'—Co3—B7 | 95.66 (8) | C1'—C2'—B11' | 111.79 (14) |
| B4—Co3—B7 | 87.70 (8) | C1'—C2'—B7' | 112.62 (14) |
| B4'—Co3—B7 | 93.32 (8) | B11'—C2'—B7' | 63.86 (12) |
| C1—Co3—B7' | 96.11 (8) | C1'—C2'—B6' | 62.24 (11) |
| C2—Co3—B7' | 129.84 (8) | B11'—C2'—B6' | 61.95 (12) |
| C2'—Co3—B7' | 48.28 (8) | B7'—C2'—B6' | 115.70 (14) |
| C1'—Co3—B7' | 82.91 (8) | C1'—C2'—Co3 | 66.99 (9) |
| B4—Co3—B7' | 93.65 (8) | B11'—C2'—Co3 | 125.68 (12) |
| B4'—Co3—B7' | 87.09 (8) | B7'—C2'—Co3 | 67.51 (9) |
| B7—Co3—B7' | 177.70 (8) | B6'—C2'—Co3 | 125.44 (12) |
| C1—Co3—B8' | 133.33 (8) | C1'—C2'—H2' | 120.9 |
| C2—Co3—B8' | 179.58 (8) | B11'—C2'—H2' | 116.5 |
| C2'—Co3—B8' | 83.29 (7) | B7'—C2'—H2' | 118.0 |
| C1'—Co3—B8' | 83.84 (8) | B6'—C2'—H2' | 115.5 |
| B4—Co3—B8' | 95.76 (8) | Co3—C2'—H2' | 106.5 |
| B4'—Co3—B8' | 51.17 (9) | C1'—B4'—B9' | 103.76 (14) |
| B7—Co3—B8' | 131.32 (8) | C1'—B4'—B5' | 57.93 (11) |
| B7'—Co3—B8' | 50.42 (8) | B9'—B4'—B5' | 59.77 (13) |
| C1—Co3—B8 | 84.17 (7) | C1'—B4'—B8' | 104.80 (14) |
| C2—Co3—B8 | 83.78 (7) | B9'—B4'—B8' | 59.99 (13) |
| C2'—Co3—B8 | 178.83 (8) | B5'—B4'—B8' | 107.97 (15) |
| C1'—Co3—B8 | 133.08 (8) | C1'—B4'—Co3 | 64.67 (9) |
| B4—Co3—B8 | 51.05 (8) | B9'—B4'—Co3 | 118.08 (13) |
| B4'—Co3—B8 | 96.12 (8) | B5'—B4'—Co3 | 117.81 (13) |
| B7—Co3—B8 | 50.69 (8) | B8'—B4'—Co3 | 65.20 (10) |
| B7'—Co3—B8 | 131.53 (8) | C1'—B4'—H4' | 125.8 |
| B8'—Co3—B8 | 95.81 (8) | B9'—B4'—H4' | 121.1 |

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| C2—C1—B5 | 111.41 (14) | B5'—B4'—H4' | 120.2 |
| C2—C1—B4 | 112.00 (14) | B8'—B4'—H4' | 122.7 |
| B5—C1—B4 | 64.29 (12) | Co3—B4'—H4' | 111.3 |
| C2—C1—B6 | 61.90 (12) | C1'—B5'—B6' | 59.98 (12) |
| B5—C1—B6 | 62.20 (12) | C1'—B5'—B9' | 104.30 (15) |
| B4—C1—B6 | 116.15 (14) | B6'—B5'—B9' | 108.53 (16) |
| C2—C1—Co3 | 66.92 (9) | C1'—B5'—B10' | 105.29 (15) |
| B5—C1—Co3 | 125.44 (12) | B6'—B5'—B10' | 60.19 (12) |
| B4—C1—Co3 | 66.90 (9) | B9'—B5'—B10' | 59.98 (13) |
| B6—C1—Co3 | 125.18 (13) | C1'—B5'—B4' | 58.37 (11) |
| C2—C1—H1 | 121.4 | B6'—B5'—B4' | 109.38 (15) |
| B5—C1—H1 | 116.3 | B9'—B5'—B4' | 60.03 (12) |
| B4—C1—H1 | 118.0 | B10'—B5'—B4' | 108.48 (16) |
| B6—C1—H1 | 115.3 | C1'—B5'—H5' | 124.7 |
| Co3—C1—H1 | 107.0 | B6'—B5'—H5' | 120.4 |
| C1—C2—B11 | 111.73 (14) | B9'—B5'—H5' | 122.6 |
| C1—C2—B7 | 112.36 (14) | B10'—B5'—H5' | 122.2 |
| B11—C2—B7 | 64.12 (12) | B4'—B5'—H5' | 121.1 |
| C1—C2—B6 | 62.19 (12) | C2'—B6'—C1' | 55.54 (10) |
| B11—C2—B6 | 61.99 (13) | C2'—B6'—B11' | 58.09 (11) |
| B7—C2—B6 | 115.88 (14) | C1'—B6'—B11' | 103.29 (14) |
| C1—C2—Co3 | 66.53 (9) | C2'—B6'—B5' | 102.83 (14) |
| B11—C2—Co3 | 125.96 (12) | C1'—B6'—B5' | 58.03 (11) |
| B7—C2—Co3 | 67.66 (9) | B11'—B6'—B5' | 108.26 (16) |
| B6—C2—Co3 | 125.08 (13) | C2'—B6'—B10' | 103.75 (15) |
| C1—C2—H2 | 121.3 | C1'—B6'—B10' | 104.18 (14) |
| B11—C2—H2 | 116.2 | B11'—B6'—B10' | 60.33 (12) |
| B7—C2—H2 | 117.8 | B5'—B6'—B10' | 60.68 (13) |
| B6—C2—H2 | 115.5 | C2'—B6'—H6' | 126.0 |
| Co3—C2—H2 | 106.7 | C1'—B6'—H6' | 125.7 |
| C1—B4—B9 | 102.57 (14) | B11'—B6'—H6' | 122.2 |
| C1—B4—B5 | 57.09 (11) | B5'—B6'—H6' | 122.3 |
| B9—B4—B5 | 59.20 (12) | B10'—B6'—H6' | 122.7 |
| C1—B4—B8 | 104.79 (14) | C2'—B7'—B12' | 103.51 (15) |

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| B9—B4—B8 | 59.53 (12) | C2'—B7'—B11' | 57.84 (11) |
| B5—B4—B8 | 107.18 (14) | B12'—B7'—B11' | 59.61 (12) |
| C1—B4—Co3 | 63.90 (9) | C2'—B7'—B8' | 104.67 (14) |
| B9—B4—Co3 | 117.89 (13) | B12'—B7'—B8' | 60.41 (12) |
| B5—B4—Co3 | 116.32 (13) | B11'—B7'—B8' | 108.20 (15) |
| B8—B4—Co3 | 66.31 (9) | C2'—B7'—Co3 | 64.21 (9) |
| C1—B4—H4 | 126.5 | B12'—B7'—Co3 | 118.09 (13) |
| B9—B4—H4 | 121.7 | B11'—B7'—Co3 | 117.33 (13) |
| B5—B4—H4 | 121.2 | B8'—B7'—Co3 | 65.14 (9) |
| B8—B4—H4 | 122.3 | C2'—B7'—H7' | 126.1 |
| Co3—B4—H4 | 111.5 | B12'—B7'—H7' | 121.0 |
| C1—B5—B6 | 59.82 (12) | B11'—B7'—H7' | 120.3 |
| C1—B5—B10 | 105.22 (16) | B8'—B7'—H7' | 122.5 |
| B6—B5—B10 | 60.24 (13) | Co3—B7'—H7' | 111.6 |
| C1—B5—B9 | 104.18 (15) | B12'—B8'—B7' | 59.17 (12) |
| B6—B5—B9 | 108.57 (16) | B12'—B8'—B9' | 59.95 (12) |
| B10—B5—B9 | 60.10 (12) | B7'—B8'—B9' | 106.71 (14) |
| C1—B5—B4 | 58.61 (11) | B12'—B8'—B4' | 106.53 (15) |
| B6—B5—B4 | 109.49 (15) | B7'—B8'—B4' | 106.14 (14) |
| B10—B5—B4 | 108.51 (15) | B9'—B8'—B4' | 59.14 (12) |
| B9—B5—B4 | 59.77 (12) | B12'—B8'—Co3 | 116.43 (13) |
| C1—B5—H5 | 124.7 | B7'—B8'—Co3 | 64.44 (9) |
| B6—B5—H5 | 120.4 | B9'—B8'—Co3 | 115.99 (13) |
| B10—B5—H5 | 122.1 | B4'—B8'—Co3 | 63.63 (9) |
| B9—B5—H5 | 122.7 | B12'—B8'—H8' | 120.7 |
| B4—B5—H5 | 121.0 | B7'—B8'—H8' | 123.2 |
| C2—B6—C1 | 55.92 (11) | B9'—B8'—H8' | 120.8 |
| C2—B6—B11 | 58.24 (12) | B4'—B8'—H8' | 123.6 |
| C1—B6—B11 | 103.68 (14) | Co3—B8'—H8' | 113.2 |
| C2—B6—B5 | 103.24 (15) | B5'—B9'—B10' | 60.18 (13) |
| C1—B6—B5 | 57.98 (12) | B5'—B9'—B4' | 60.20 (12) |
| B11—B6—B5 | 108.52 (15) | B10'—B9'—B4' | 108.79 (15) |
| C2—B6—B10 | 104.00 (15) | B5'—B9'—B12' | 107.20 (15) |
| C1—B6—B10 | 103.89 (15) | B10'—B9'—B12' | 59.56 (12) |

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| B11—B6—B10 | 60.63 (13) | B4'—B9'—B12' | 107.89 (15) |
| B5—B6—B10 | 60.32 (13) | B5'—B9'—B8' | 109.02 (15) |
| C2—B6—H6 | 125.7 | B10'—B9'—B8' | 108.87 (15) |
| C1—B6—H6 | 125.6 | B4'—B9'—B8' | 60.87 (12) |
| B11—B6—H6 | 121.9 | B12'—B9'—B8' | 59.95 (12) |
| B5—B6—H6 | 122.3 | B5'—B9'—H9' | 121.7 |
| B10—B6—H6 | 122.9 | B10'—B9'—H9' | 121.3 |
| C2—B7—B12 | 102.98 (14) | B4'—B9'—H9' | 121.2 |
| C2—B7—B11 | 57.61 (11) | B12'—B9'—H9' | 122.5 |
| B12—B7—B11 | 59.34 (12) | B8'—B9'—H9' | 120.8 |
| C2—B7—B8 | 105.26 (14) | B11'—B10'—B6' | 59.30 (12) |
| B12—B7—B8 | 59.86 (11) | B11'—B10'—B12' | 59.87 (12) |
| B11—B7—B8 | 108.00 (15) | B6'—B10'—B12' | 107.68 (15) |
| C2—B7—Co3 | 63.90 (9) | B11'—B10'—B9' | 107.79 (15) |
| B12—B7—Co3 | 117.75 (13) | B6'—B10'—B9' | 107.58 (15) |
| B11—B7—Co3 | 116.78 (13) | B12'—B10'—B9' | 60.64 (13) |
| B8—B7—Co3 | 65.99 (9) | B11'—B10'—B5' | 106.24 (14) |
| C2—B7—H7 | 126.1 | B6'—B10'—B5' | 59.14 (12) |
| B12—B7—H7 | 121.6 | B12'—B10'—B5' | 107.77 (15) |
| B11—B7—H7 | 120.6 | B9'—B10'—B5' | 59.84 (13) |
| B8—B7—H7 | 122.0 | B11'—B10'—H10' | 122.5 |
| Co3—B7—H7 | 111.6 | B6'—B10'—H10' | 122.3 |
| N1—B8—B12 | 120.91 (15) | B12'—B10'—H10' | 121.4 |
| N1—B8—B9 | 121.47 (15) | B9'—B10'—H10' | 121.5 |
| B12—B8—B9 | 60.24 (12) | B5'—B10'—H10' | 122.6 |
| N1—B8—B7 | 123.07 (16) | C2'—B11'—B6' | 59.96 (12) |
| B12—B8—B7 | 58.77 (11) | C2'—B11'—B12' | 103.91 (14) |
| B9—B8—B7 | 106.39 (14) | B6'—B11'—B12' | 108.74 (16) |
| N1—B8—B4 | 124.14 (16) | C2'—B11'—B10' | 105.19 (15) |
| B12—B8—B4 | 106.52 (14) | B6'—B11'—B10' | 60.38 (12) |
| B9—B8—B4 | 59.21 (12) | B12'—B11'—B10' | 60.11 (13) |
| B7—B8—B4 | 105.42 (13) | C2'—B11'—B7' | 58.30 (11) |
| N1—B8—Co3 | 114.59 (12) | B6'—B11'—B7' | 109.43 (14) |
| B12—B8—Co3 | 114.53 (12) | B12'—B11'—B7' | 59.68 (12) |

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| B9—B8—Co3 | 114.44 (12) | B10'—B11'—B7' | 108.35 (15) |
| B7—B8—Co3 | 63.32 (9) | C2'—B11'—H11' | 124.9 |
| B4—B8—Co3 | 62.64 (9) | B6'—B11'—H11' | 120.2 |
| B5—B9—B10 | 59.91 (13) | B12'—B11'—H11' | 122.7 |
| B5—B9—B4 | 61.03 (12) | B10'—B11'—H11' | 122.1 |
| B10—B9—B4 | 109.36 (15) | B7'—B11'—H11' | 121.2 |
| B5—B9—B8 | 110.01 (14) | B11'—B12'—B7' | 60.71 (12) |
| B10—B9—B8 | 109.25 (15) | B11'—B12'—B10' | 60.02 (12) |
| B4—B9—B8 | 61.26 (11) | B7'—B12'—B10' | 109.11 (15) |
| B5—B9—B12 | 106.72 (15) | B11'—B12'—B9' | 107.26 (16) |
| B10—B9—B12 | 59.34 (12) | B7'—B12'—B9' | 107.81 (15) |
| B4—B9—B12 | 107.83 (14) | B10'—B12'—B9' | 59.80 (13) |
| B8—B9—B12 | 59.86 (12) | B11'—B12'—B8' | 109.07 (15) |
| B5—B9—H9 | 121.4 | B7'—B12'—B8' | 60.41 (12) |
| B10—B9—H9 | 121.3 | B10'—B12'—B8' | 109.19 (16) |
| B4—B9—H9 | 120.7 | B9'—B12'—B8' | 60.10 (12) |
| B8—B9—H9 | 120.3 | B11'—B12'—H12' | 121.6 |
| B12—B9—H9 | 123.0 | B7'—B12'—H12' | 121.2 |
| B12—B10—B6 | 107.30 (15) | B10'—B12'—H12' | 121.1 |
| B12—B10—B5 | 108.02 (15) | B9'—B12'—H12' | 122.5 |
| B6—B10—B5 | 59.44 (13) | B8'—B12'—H12' | 120.8 |
| B12—B10—B9 | 60.92 (12) | C3—N1—B8 | 134.90 (16) |
| B6—B10—B9 | 107.85 (15) | C3—N1—H1A | 114.8 (16) |
| B5—B10—B9 | 59.99 (13) | B8—N1—H1A | 110.1 (16) |
| B12—B10—B11 | 59.71 (12) | N1—C3—N2 | 120.28 (17) |
| B6—B10—B11 | 59.09 (13) | N1—C3—C4 | 121.33 (17) |
| B5—B10—B11 | 106.60 (15) | N2—C3—C4 | 118.39 (16) |
| B9—B10—B11 | 108.17 (15) | C3—C4—H4A | 109.5 |
| B12—B10—H10 | 121.5 | C3—C4—H4B | 109.5 |
| B6—B10—H10 | 122.4 | H4A—C4—H4B | 109.5 |
| B5—B10—H10 | 122.3 | C3—C4—H4C | 109.5 |
| B9—B10—H10 | 121.1 | H4A—C4—H4C | 109.5 |
| B11—B10—H10 | 122.5 | H4B—C4—H4C | 109.5 |
| C2—B11—B6 | 59.77 (12) | C3—N2—C5 | 122.90 (16) |

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| C2—B11—B12 | 103.68 (14) | C3—N2—C7 | 122.26 (16) |
| B6—B11—B12 | 108.40 (16) | C5—N2—C7 | 114.75 (15) |
| C2—B11—B10 | 104.87 (16) | N2—C5—C6 | 113.34 (18) |
| B6—B11—B10 | 60.27 (13) | N2—C5—H5A | 108.9 |
| B12—B11—B10 | 59.90 (12) | C6—C5—H5A | 108.9 |
| C2—B11—B7 | 58.26 (11) | N2—C5—H5B | 108.9 |
| B6—B11—B7 | 109.17 (15) | C6—C5—H5B | 108.9 |
| B12—B11—B7 | 59.61 (11) | H5A—C5—H5B | 107.7 |
| B10—B11—B7 | 108.07 (15) | C5—C6—H6A | 109.5 |
| C2—B11—H11 | 125.0 | C5—C6—H6B | 109.5 |
| B6—B11—H11 | 120.4 | H6A—C6—H6B | 109.5 |
| B12—B11—H11 | 122.9 | C5—C6—H6C | 109.5 |
| B10—B11—H11 | 122.3 | H6A—C6—H6C | 109.5 |
| B7—B11—H11 | 121.4 | H6B—C6—H6C | 109.5 |
| B11—B12—B10 | 60.39 (13) | N2—C7—C8 | 112.50 (18) |
| B11—B12—B7 | 61.04 (12) | N2—C7—H7A | 109.1 |
| B10—B12—B7 | 109.60 (14) | C8—C7—H7A | 109.1 |
| B11—B12—B8 | 110.57 (14) | N2—C7—H7B | 109.1 |
| B10—B12—B8 | 109.62 (15) | C8—C7—H7B | 109.1 |
| B7—B12—B8 | 61.37 (11) | H7A—C7—H7B | 107.8 |
| B11—B12—B9 | 107.78 (15) | C7—C8—H8A | 109.5 |
| B10—B12—B9 | 59.74 (13) | C7—C8—H8B | 109.5 |
| B7—B12—B9 | 108.15 (14) | H8A—C8—H8B | 109.5 |
| B8—B12—B9 | 59.90 (12) | C7—C8—H8C | 109.5 |
| B11—B12—H12 | 120.8 | H8A—C8—H8C | 109.5 |
| B10—B12—H12 | 121.0 | H8B—C8—H8C | 109.5 |

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

**(12)**

*Crystal data*

| | |
|---|---|
| $C_{18}H_{36}B_{18}CoN$ | $D_x$ = 1.285 Mg m$^{-3}$ |
| $M_r$ = 519.99 | Melting point: 556 K |
| Monoclinic, $P2_1$ | Mo $K\alpha$ radiation |

| | |
|---|---|
| | λ = 0.71073 Å |
| Hall symbol: P 2yb | Cell parameters from 5519 reflections |
| *a* = 13.6244 (2) Å | θ = 1–26.0° |
| *b* = 12.4912 (2) Å | μ = 0.65 mm$^{-1}$ |
| *c* = 16.4535 (3) Å | *T* = 150 (2) K |
| β = 106.3098 (10)° | Cell measurement pressure: 101.3 kPa |
| *V* = 2687.45 (8) Å$^3$ | Plate, red |
| *Z* = 4 | 0.4 × 0.4 × 0.25 mm |
| $F_{000}$ = 1072 | |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD area detector diffractometer | 10583 independent reflections |
| Radiation source: fine-focus sealed tube | 10184 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.044 |
| Detector resolution: 9.091 pixels mm$^{-1}$ | $\theta_{max}$ = 26.1° |
| *T* = 150(2) K | $\theta_{min}$ = 1.7° |
| *P* = 101.3 kPa | *h* = −16→16 |
| φ and ω scans to fill the Ewald sphere | *k* = −15→15 |
| Absorption correction: none | *l* = −10→20 |
| 38101 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.033 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.085 | $w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 2.0205P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 1.07 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 10583 reflections | $\Delta\rho_{max}$ = 0.48 e Å$^{-3}$ |
| 694 parameters | $\Delta\rho_{min}$ = −0.32 e Å$^{-3}$ |
| 1 restraint | Extinction correction: none |
| ? constraints | Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881 |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.010 (10) |

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co13 | −0.02134 (2) | −0.44298 (3) | −0.15698 (2) | 0.01691 (8) |
| C11 | −0.1069 (2) | −0.5796 (2) | −0.17573 (18) | 0.0219 (6) |
| H11 | −0.0996 | −0.6139 | −0.1127 | 0.026* |
| C12 | −0.0125 (2) | −0.5839 (2) | −0.21761 (17) | 0.0221 (6) |
| H12 | 0.0612 | −0.6211 | −0.1849 | 0.026* |
| B14 | −0.1803 (2) | −0.4672 (2) | −0.20403 (19) | 0.0215 (6) |
| H14 | −0.2227 | −0.4248 | −0.1659 | 0.026* |
| B15 | −0.2204 (2) | −0.5963 (3) | −0.2482 (2) | 0.0242 (6) |
| H15 | −0.2869 | −0.6362 | −0.2361 | 0.029* |
| B16 | −0.1134 (3) | −0.6712 (2) | −0.2544 (2) | 0.0239 (7) |
| H16 | −0.1096 | −0.7587 | −0.2463 | 0.029* |
| B17 | −0.0120 (3) | −0.4741 (2) | −0.27961 (19) | 0.0209 (6) |
| H17 | 0.0556 | −0.4361 | −0.2912 | 0.025* |
| B18 | −0.1233 (2) | −0.3993 (2) | −0.27549 (19) | 0.0193 (6) |
| B19 | −0.2334 (2) | −0.4842 (3) | −0.3156 (2) | 0.0248 (7) |
| H19 | −0.3087 | −0.4510 | −0.3490 | 0.030* |
| B110 | −0.1909 (3) | −0.6088 (3) | −0.3464 (2) | 0.0246 (6) |
| H110 | −0.2383 | −0.6554 | −0.3999 | 0.030* |
| B111 | −0.0550 (3) | −0.6035 (3) | −0.3233 (2) | 0.0264 (7) |
| H111 | −0.0130 | −0.6477 | −0.3608 | 0.032* |
| B112 | −0.1294 (3) | −0.4882 (3) | −0.3620 (2) | 0.0238 (7) |
| H112 | −0.1371 | −0.4571 | −0.4260 | 0.029* |
| C21 | 0.0763 (2) | −0.4834 (2) | −0.04202 (17) | 0.0214 (6) |
| H21 | 0.0763 | −0.5713 | −0.0379 | 0.026* |
| C22 | −0.0213 (2) | −0.4134 (2) | −0.03493 (16) | 0.0214 (6) |
| H22 | −0.0902 | −0.4514 | −0.0257 | 0.026* |
| B24 | 0.1379 (2) | −0.4258 (2) | −0.10783 (19) | 0.0218 (6) |
| H24 | 0.1795 | −0.4681 | −0.1466 | 0.026* |
| B25 | 0.1884 (2) | −0.4222 (3) | 0.0052 (2) | 0.0255 (7) |
| H25 | 0.2600 | −0.4637 | 0.0375 | 0.031* |
| B26 | 0.0856 (3) | −0.4171 (3) | 0.0515 (2) | 0.0266 (7) |
| H26 | 0.0897 | −0.4548 | 0.1128 | 0.032* |
| B27 | −0.0357 (2) | −0.3004 (2) | −0.09481 (19) | 0.0219 (6) |

| | | | | |
|---|---|---|---|---|
| H27 | −0.1086 | −0.2600 | −0.1250 | 0.026* |
| B28 | 0.0693 (2) | −0.3024 (2) | −0.1415 (2) | 0.0215 (6) |
| H28 | 0.0666 | −0.2623 | −0.2016 | 0.026* |
| B29 | 0.1852 (2) | −0.3033 (2) | −0.0559 (2) | 0.0238 (6) |
| H29 | 0.2554 | −0.2661 | −0.0630 | 0.029* |
| B210 | 0.1531 (3) | −0.2982 (3) | 0.0417 (2) | 0.0259 (7) |
| H210 | 0.2026 | −0.2569 | 0.0972 | 0.031* |
| B211 | 0.0169 (3) | −0.2975 (3) | 0.0177 (2) | 0.0265 (7) |
| H211 | −0.0234 | −0.2571 | 0.0584 | 0.032* |
| B212 | 0.0774 (2) | −0.2260 (3) | −0.0475 (2) | 0.0242 (6) |
| H212 | 0.0773 | −0.1380 | −0.0488 | 0.029* |
| N1 | −0.13460 (17) | −0.2742 (2) | −0.29684 (14) | 0.0219 (5) |
| C1A | −0.2460 (2) | −0.2393 (2) | −0.3196 (2) | 0.0292 (7) |
| H1A1 | −0.2812 | −0.2696 | −0.3743 | 0.035* |
| H1A2 | −0.2769 | −0.2694 | −0.2783 | 0.035* |
| C2A | −0.2639 (2) | −0.1204 (2) | −0.32337 (18) | 0.0250 (6) |
| C3A | −0.2590 (2) | −0.0622 (2) | −0.25019 (19) | 0.0299 (7) |
| H3A | −0.2444 | −0.0967 | −0.1981 | 0.036* |
| C4A | −0.2759 (2) | 0.0471 (3) | −0.2550 (2) | 0.0352 (7) |
| H4A | −0.2715 | 0.0859 | −0.2059 | 0.042* |
| C5A | −0.2992 (2) | 0.0991 (2) | −0.3323 (2) | 0.0359 (7) |
| H5A | −0.3112 | 0.1725 | −0.3353 | 0.043* |
| C6A | −0.3047 (2) | 0.0414 (3) | −0.4047 (2) | 0.0350 (7) |
| H6A | −0.3197 | 0.0762 | −0.4567 | 0.042* |
| C7A | −0.2879 (2) | −0.0682 (2) | −0.40073 (19) | 0.0301 (7) |
| H7A | −0.2927 | −0.1067 | −0.4501 | 0.036* |
| C1B | −0.0808 (2) | −0.2430 (2) | −0.36206 (19) | 0.0274 (6) |
| H1B1 | −0.1233 | −0.2652 | −0.4172 | 0.033* |
| H1B2 | −0.0176 | −0.2833 | −0.3506 | 0.033* |
| C2B | −0.0555 (2) | −0.1252 (2) | −0.36718 (19) | 0.0267 (6) |
| C3B | −0.0223 (2) | −0.0601 (2) | −0.2970 (2) | 0.0308 (7) |
| H3B | −0.0175 | −0.0874 | −0.2434 | 0.037* |
| C4B | 0.0040 (2) | 0.0461 (3) | −0.3060 (2) | 0.0393 (8) |
| H4B | 0.0252 | 0.0899 | −0.2586 | 0.047* |

| | | | | |
|---|---|---|---|---|
| C5B | −0.0014 (3) | 0.0865 (2) | −0.3854 (3) | 0.0431 (9) |
| H5B | 0.0154 | 0.1576 | −0.3916 | 0.052* |
| C6B | −0.0318 (3) | 0.0209 (3) | −0.4551 (3) | 0.0430 (9) |
| H6B | −0.0338 | 0.0475 | −0.5084 | 0.052* |
| C7B | −0.0593 (2) | −0.0840 (2) | −0.4466 (2) | 0.0320 (7) |
| H7B | −0.0805 | −0.1274 | −0.4943 | 0.038* |
| Co23 | 0.38502 (2) | 0.22591 (3) | −0.14808 (2) | 0.01743 (8) |
| C31 | 0.4421 (2) | 0.3633 (2) | −0.18378 (17) | 0.0216 (6) |
| H31 | 0.4942 | 0.3977 | −0.1261 | 0.026* |
| C32 | 0.3196 (2) | 0.3653 (2) | −0.20025 (18) | 0.0229 (6) |
| H32 | 0.2842 | 0.4017 | −0.1545 | 0.028* |
| B34 | 0.4830 (2) | 0.2522 (2) | −0.22498 (19) | 0.0219 (6) |
| H34 | 0.5569 | 0.2112 | −0.2003 | 0.026* |
| B35 | 0.4755 (3) | 0.3834 (3) | −0.2742 (2) | 0.0253 (7) |
| H35 | 0.5446 | 0.4257 | −0.2788 | 0.030* |
| B36 | 0.3722 (3) | 0.4541 (3) | −0.2551 (2) | 0.0260 (7) |
| H36 | 0.3740 | 0.5416 | −0.2467 | 0.031* |
| B37 | 0.2624 (3) | 0.2539 (2) | −0.2549 (2) | 0.0241 (7) |
| H37 | 0.1922 | 0.2143 | −0.2500 | 0.029* |
| B38 | 0.3672 (3) | 0.1816 (3) | −0.27615 (19) | 0.0221 (6) |
| B39 | 0.4254 (3) | 0.2688 (3) | −0.3366 (2) | 0.0265 (7) |
| H39 | 0.4618 | 0.2365 | −0.3832 | 0.032* |
| B310 | 0.3574 (3) | 0.3923 (3) | −0.3539 (2) | 0.0280 (7) |
| H310 | 0.3491 | 0.4394 | −0.4120 | 0.034* |
| B311 | 0.2581 (3) | 0.3845 (3) | −0.3036 (2) | 0.0282 (7) |
| H311 | 0.1852 | 0.4274 | −0.3277 | 0.034* |
| B312 | 0.2900 (3) | 0.2695 (3) | −0.3550 (2) | 0.0279 (7) |
| H312 | 0.2380 | 0.2376 | −0.4137 | 0.034* |
| C41 | 0.4045 (2) | 0.2674 (2) | −0.02411 (17) | 0.0247 (6) |
| H41 | 0.4095 | 0.3553 | −0.0208 | 0.030* |
| C42 | 0.4977 (2) | 0.1961 (2) | −0.03832 (17) | 0.0214 (6) |
| H42 | 0.5685 | 0.2329 | −0.0448 | 0.026* |
| B44 | 0.2884 (2) | 0.2118 (3) | −0.0693 (2) | 0.0257 (7) |
| H44 | 0.2162 | 0.2554 | −0.0950 | 0.031* |

| | | | | |
|---|---|---|---|---|
| B45 | 0.3475 (3) | 0.2081 (3) | 0.0422 (2) | 0.0288 (7) |
| H45 | 0.3140 | 0.2508 | 0.0865 | 0.035* |
| B46 | 0.4813 (3) | 0.2008 (3) | 0.0619 (2) | 0.0274 (7) |
| H46 | 0.5346 | 0.2381 | 0.1176 | 0.033* |
| B47 | 0.4535 (2) | 0.0829 (2) | −0.09480 (19) | 0.0216 (6) |
| H47 | 0.4906 | 0.0413 | −0.1372 | 0.026* |
| B48 | 0.3162 (2) | 0.0877 (2) | −0.1140 (2) | 0.0232 (6) |
| H48 | 0.2623 | 0.0482 | −0.1683 | 0.028* |
| B49 | 0.2922 (3) | 0.0909 (3) | −0.0125 (2) | 0.0282 (7) |
| H49 | 0.2221 | 0.0556 | −0.0033 | 0.034* |
| B410 | 0.4103 (3) | 0.0834 (3) | 0.0677 (2) | 0.0269 (7) |
| H410 | 0.4167 | 0.0426 | 0.1282 | 0.032* |
| B411 | 0.5098 (3) | 0.0798 (3) | 0.0174 (2) | 0.0241 (7) |
| H411 | 0.5824 | 0.0380 | 0.0454 | 0.029* |
| B412 | 0.3937 (3) | 0.0105 (3) | −0.0284 (2) | 0.0244 (7) |
| H412 | 0.3904 | −0.0775 | −0.0298 | 0.029* |
| N2 | 0.36208 (17) | 0.0571 (2) | −0.29825 (14) | 0.0219 (4) |
| C1C | 0.4409 (3) | 0.0270 (2) | −0.3441 (2) | 0.0325 (7) |
| H1C1 | 0.4211 | 0.0603 | −0.3996 | 0.039* |
| H1C2 | 0.5061 | 0.0576 | −0.3131 | 0.039* |
| C2C | 0.4564 (2) | −0.0906 (2) | −0.35572 (19) | 0.0266 (6) |
| C3C | 0.4438 (2) | −0.1306 (3) | −0.4369 (2) | 0.0356 (7) |
| H3C | 0.4234 | −0.0851 | −0.4834 | 0.043* |
| C4C | 0.4616 (3) | −0.2379 (3) | −0.4489 (2) | 0.0403 (8) |
| H4C | 0.4531 | −0.2639 | −0.5034 | 0.048* |
| C5C | 0.4916 (3) | −0.3065 (3) | −0.3806 (2) | 0.0407 (8) |
| H5C | 0.5023 | −0.3787 | −0.3889 | 0.049* |
| C6C | 0.5058 (2) | −0.2669 (3) | −0.2995 (2) | 0.0375 (7) |
| H6C | 0.5264 | −0.3126 | −0.2532 | 0.045* |
| C7C | 0.4894 (2) | −0.1600 (2) | −0.2871 (2) | 0.0328 (7) |
| H7C | 0.5006 | −0.1338 | −0.2324 | 0.039* |
| C1D | 0.2539 (2) | 0.0221 (2) | −0.34392 (19) | 0.0284 (6) |
| H1D1 | 0.2074 | 0.0544 | −0.3158 | 0.034* |
| H1D2 | 0.2364 | 0.0499 | −0.4013 | 0.034* |

| | | | | |
|---|---|---|---|---|
| C2D | 0.2365 (2) | −0.0974 (2) | −0.34803 (18) | 0.0247 (6) |
| C3D | 0.2056 (2) | −0.1462 (2) | −0.42599 (19) | 0.0299 (7) |
| H3D | 0.1954 | −0.1048 | −0.4746 | 0.036* |
| C4D | 0.1893 (2) | −0.2555 (2) | −0.4336 (2) | 0.0354 (7) |
| H4D | 0.1680 | −0.2875 | −0.4867 | 0.042* |
| C5D | 0.2051 (2) | −0.3162 (2) | −0.3609 (2) | 0.0347 (7) |
| H5D | 0.1966 | −0.3901 | −0.3652 | 0.042* |
| C6D | 0.2332 (2) | −0.2690 (3) | −0.2827 (2) | 0.0324 (6) |
| H6D | 0.2423 | −0.3107 | −0.2343 | 0.039* |
| C7D | 0.2479 (2) | −0.1596 (2) | −0.2753 (2) | 0.0311 (7) |
| H7D | 0.2654 | −0.1274 | −0.2222 | 0.037* |
| H1 | −0.103 (3) | −0.242 (3) | −0.250 (2) | 0.033 (9)* |
| H2 | 0.372 (3) | 0.020 (3) | −0.251 (2) | 0.038 (10)* |

Atomic displacement parameters (Å$^2$)

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co13 | 0.01697 (16) | 0.01564 (16) | 0.01764 (16) | −0.00007 (14) | 0.00408 (12) | −0.00062 (14) |
| C11 | 0.0226 (13) | 0.0185 (13) | 0.0239 (14) | −0.0037 (11) | 0.0052 (11) | 0.0001 (11) |
| C12 | 0.0233 (13) | 0.0174 (13) | 0.0254 (14) | 0.0000 (11) | 0.0066 (11) | −0.0006 (11) |
| B14 | 0.0207 (14) | 0.0199 (15) | 0.0215 (14) | −0.0021 (11) | 0.0022 (11) | 0.0009 (11) |
| B15 | 0.0231 (15) | 0.0222 (16) | 0.0250 (16) | −0.0041 (13) | 0.0029 (12) | 0.0026 (12) |
| B16 | 0.0262 (16) | 0.0161 (15) | 0.0275 (16) | −0.0049 (12) | 0.0045 (13) | −0.0008 (12) |
| B17 | 0.0268 (16) | 0.0176 (15) | 0.0189 (14) | −0.0009 (12) | 0.0077 (12) | −0.0017 (11) |
| B18 | 0.0230 (15) | 0.0143 (13) | 0.0189 (14) | −0.0014 (12) | 0.0029 (12) | −0.0002 (11) |
| B19 | 0.0220 (15) | 0.0219 (15) | 0.0255 (16) | −0.0040 (12) | −0.0016 (13) | 0.0020 (12) |
| B110 | 0.0264 (16) | 0.0207 (14) | 0.0248 (15) | −0.0066 (12) | 0.0039 (12) | 0.0010 (12) |
| B111 | 0.0346 (18) | 0.0188 (15) | 0.0278 (17) | −0.0046 (14) | 0.0119 (14) | −0.0041 (13) |
| B112 | 0.0311 (17) | 0.0189 (14) | 0.0217 (16) | −0.0073 (13) | 0.0080 (13) | −0.0014 (12) |
| C21 | 0.0196 (13) | 0.0217 (13) | 0.0205 (13) | 0.0031 (10) | 0.0021 (11) | −0.0002 (10) |
| C22 | 0.0210 (13) | 0.0252 (15) | 0.0186 (13) | 0.0019 (11) | 0.0067 (10) | 0.0005 (10) |
| B24 | 0.0188 (14) | 0.0223 (16) | 0.0226 (14) | 0.0030 (12) | 0.0034 (11) | −0.0021 (12) |
| B25 | 0.0237 (15) | 0.0234 (17) | 0.0274 (16) | 0.0039 (13) | 0.0037 (12) | 0.0000 (13) |
| B26 | 0.0251 (16) | 0.0316 (19) | 0.0206 (15) | −0.0007 (13) | 0.0023 (12) | −0.0032 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| B27 | 0.0210 (15) | 0.0214 (16) | 0.0219 (15) | −0.0001 (12) | 0.0033 (12) | −0.0024 (12) |
| B28 | 0.0200 (14) | 0.0191 (15) | 0.0251 (15) | −0.0017 (11) | 0.0058 (12) | −0.0015 (12) |
| B29 | 0.0212 (15) | 0.0235 (16) | 0.0248 (15) | −0.0001 (12) | 0.0036 (12) | −0.0026 (12) |
| B210 | 0.0291 (16) | 0.0238 (17) | 0.0223 (15) | 0.0007 (13) | 0.0028 (13) | −0.0061 (12) |
| B211 | 0.0241 (16) | 0.0321 (19) | 0.0238 (16) | 0.0012 (13) | 0.0078 (12) | −0.0085 (13) |
| B212 | 0.0245 (16) | 0.0202 (14) | 0.0256 (16) | 0.0007 (13) | 0.0036 (13) | −0.0045 (12) |
| N1 | 0.0246 (11) | 0.0185 (11) | 0.0213 (11) | −0.0006 (11) | 0.0046 (9) | 0.0003 (10) |
| C1A | 0.0233 (14) | 0.0250 (15) | 0.0352 (16) | 0.0001 (11) | 0.0014 (12) | 0.0046 (12) |
| C2A | 0.0209 (13) | 0.0211 (14) | 0.0303 (15) | 0.0003 (11) | 0.0029 (11) | 0.0013 (11) |
| C3A | 0.0283 (15) | 0.0310 (16) | 0.0276 (15) | 0.0034 (12) | 0.0033 (12) | 0.0019 (12) |
| C4A | 0.0286 (15) | 0.0326 (16) | 0.0372 (16) | 0.0014 (14) | −0.0024 (12) | −0.0115 (15) |
| C5A | 0.0289 (16) | 0.0210 (14) | 0.054 (2) | 0.0011 (12) | 0.0045 (14) | 0.0013 (14) |
| C6A | 0.0350 (16) | 0.0296 (17) | 0.0403 (17) | 0.0038 (14) | 0.0104 (13) | 0.0116 (14) |
| C7A | 0.0335 (16) | 0.0287 (15) | 0.0265 (15) | 0.0062 (13) | 0.0058 (12) | −0.0016 (12) |
| C1B | 0.0357 (16) | 0.0207 (14) | 0.0289 (15) | −0.0020 (11) | 0.0144 (13) | 0.0030 (11) |
| C2B | 0.0226 (13) | 0.0211 (14) | 0.0363 (16) | −0.0006 (11) | 0.0083 (12) | 0.0043 (12) |
| C3B | 0.0292 (16) | 0.0233 (15) | 0.0386 (17) | 0.0001 (12) | 0.0076 (13) | 0.0030 (12) |
| C4B | 0.0267 (15) | 0.0252 (16) | 0.064 (2) | −0.0037 (14) | 0.0084 (14) | −0.0069 (16) |
| C5B | 0.0306 (17) | 0.0179 (15) | 0.082 (3) | 0.0025 (12) | 0.0175 (17) | 0.0160 (16) |
| C6B | 0.0363 (18) | 0.0355 (18) | 0.061 (2) | 0.0068 (14) | 0.0206 (17) | 0.0240 (17) |
| C7B | 0.0299 (16) | 0.0277 (16) | 0.0395 (17) | 0.0001 (13) | 0.0116 (13) | 0.0068 (13) |
| Co23 | 0.01757 (16) | 0.01612 (17) | 0.01863 (16) | 0.00174 (14) | 0.00510 (13) | 0.00062 (14) |
| C31 | 0.0236 (14) | 0.0191 (13) | 0.0220 (14) | −0.0002 (11) | 0.0064 (11) | 0.0025 (11) |
| C32 | 0.0214 (14) | 0.0195 (13) | 0.0269 (14) | 0.0048 (11) | 0.0052 (11) | 0.0024 (11) |
| B34 | 0.0238 (15) | 0.0223 (16) | 0.0214 (15) | 0.0024 (12) | 0.0094 (12) | 0.0012 (11) |
| B35 | 0.0292 (16) | 0.0230 (16) | 0.0249 (16) | −0.0004 (13) | 0.0097 (13) | 0.0015 (13) |
| B36 | 0.0286 (17) | 0.0194 (15) | 0.0284 (17) | 0.0006 (13) | 0.0055 (13) | 0.0020 (13) |
| B37 | 0.0231 (15) | 0.0179 (16) | 0.0278 (17) | 0.0026 (12) | 0.0016 (13) | 0.0002 (12) |
| B38 | 0.0271 (16) | 0.0194 (15) | 0.0190 (15) | −0.0002 (12) | 0.0050 (12) | 0.0009 (12) |
| B39 | 0.0352 (18) | 0.0213 (15) | 0.0239 (16) | −0.0003 (13) | 0.0101 (14) | 0.0002 (12) |
| B310 | 0.0352 (18) | 0.0235 (16) | 0.0244 (17) | −0.0007 (15) | 0.0068 (14) | 0.0025 (13) |
| B311 | 0.0274 (17) | 0.0193 (15) | 0.0332 (19) | 0.0000 (14) | 0.0007 (14) | 0.0023 (14) |
| B312 | 0.0333 (18) | 0.0208 (15) | 0.0251 (17) | 0.0025 (14) | 0.0006 (14) | 0.0018 (13) |
| C41 | 0.0330 (16) | 0.0232 (13) | 0.0205 (14) | 0.0048 (12) | 0.0117 (12) | −0.0007 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C42 | 0.0214 (13) | 0.0214 (14) | 0.0205 (13) | 0.0027 (11) | 0.0048 (10) | 0.0009 (10) |
| B44 | 0.0254 (15) | 0.0261 (17) | 0.0281 (16) | 0.0021 (14) | 0.0117 (12) | 0.0040 (13) |
| B45 | 0.0339 (17) | 0.0274 (18) | 0.0294 (16) | 0.0052 (15) | 0.0159 (14) | 0.0039 (14) |
| B46 | 0.0337 (17) | 0.0287 (19) | 0.0197 (15) | 0.0017 (14) | 0.0074 (13) | 0.0003 (13) |
| B47 | 0.0243 (15) | 0.0168 (15) | 0.0234 (15) | 0.0017 (11) | 0.0061 (12) | 0.0040 (11) |
| B48 | 0.0208 (15) | 0.0225 (16) | 0.0279 (16) | −0.0013 (12) | 0.0096 (12) | 0.0020 (12) |
| B49 | 0.0250 (16) | 0.0311 (17) | 0.0318 (17) | 0.0014 (13) | 0.0134 (14) | 0.0046 (14) |
| B410 | 0.0335 (17) | 0.0262 (18) | 0.0255 (16) | 0.0037 (13) | 0.0158 (13) | 0.0056 (13) |
| B411 | 0.0281 (16) | 0.0226 (17) | 0.0217 (15) | 0.0035 (13) | 0.0072 (13) | 0.0060 (12) |
| B412 | 0.0284 (16) | 0.0217 (15) | 0.0250 (16) | −0.0008 (13) | 0.0106 (13) | 0.0025 (13) |
| N2 | 0.0254 (11) | 0.0177 (11) | 0.0215 (11) | 0.0007 (11) | 0.0051 (9) | −0.0008 (11) |
| C1C | 0.0353 (17) | 0.0263 (16) | 0.0395 (17) | −0.0015 (12) | 0.0167 (14) | −0.0013 (13) |
| C2C | 0.0247 (14) | 0.0242 (14) | 0.0349 (16) | −0.0009 (12) | 0.0151 (12) | −0.0050 (12) |
| C3C | 0.0330 (16) | 0.0439 (19) | 0.0313 (16) | 0.0028 (14) | 0.0113 (13) | −0.0038 (14) |
| C4C | 0.0402 (19) | 0.0414 (19) | 0.0420 (19) | −0.0068 (15) | 0.0160 (15) | −0.0188 (15) |
| C5C | 0.0316 (17) | 0.0276 (16) | 0.069 (2) | −0.0023 (13) | 0.0246 (17) | −0.0117 (16) |
| C6C | 0.0324 (16) | 0.0316 (16) | 0.0533 (19) | 0.0003 (15) | 0.0196 (14) | 0.0039 (16) |
| C7C | 0.0339 (17) | 0.0312 (16) | 0.0348 (17) | 0.0010 (13) | 0.0119 (14) | −0.0027 (13) |
| C1D | 0.0281 (15) | 0.0221 (14) | 0.0296 (15) | 0.0001 (11) | −0.0006 (12) | −0.0023 (11) |
| C2D | 0.0258 (14) | 0.0181 (13) | 0.0298 (15) | −0.0002 (11) | 0.0074 (11) | 0.0017 (11) |
| C3D | 0.0351 (16) | 0.0229 (15) | 0.0280 (15) | −0.0008 (12) | 0.0027 (13) | 0.0025 (12) |
| C4D | 0.0395 (17) | 0.0242 (16) | 0.0378 (17) | −0.0050 (13) | 0.0034 (14) | −0.0071 (13) |
| C5D | 0.0322 (17) | 0.0173 (13) | 0.056 (2) | −0.0023 (12) | 0.0142 (15) | 0.0027 (13) |
| C6D | 0.0342 (16) | 0.0261 (14) | 0.0426 (17) | 0.0034 (14) | 0.0199 (13) | 0.0113 (14) |
| C7D | 0.0347 (17) | 0.0310 (16) | 0.0292 (16) | 0.0037 (13) | 0.0114 (13) | 0.0014 (13) |

**Table 4**
Geometric parameters (Å, °)

| | | | |
|---|---|---|---|
| Co13—C11 | 2.041 (3) | Co23—C32 | 2.032 (3) |
| Co13—C22 | 2.042 (3) | Co23—C31 | 2.038 (3) |
| Co13—C12 | 2.043 (3) | Co23—C41 | 2.048 (3) |
| Co13—C21 | 2.047 (3) | Co23—C42 | 2.050 (3) |
| Co13—B27 | 2.090 (3) | Co23—B37 | 2.086 (3) |

| | | | |
|---|---|---|---|
| Co13—B17 | 2.093 (3) | Co23—B47 | 2.090 (3) |
| Co13—B24 | 2.103 (3) | Co23—B44 | 2.098 (3) |
| Co13—B14 | 2.107 (3) | Co23—B34 | 2.107 (3) |
| Co13—B28 | 2.121 (3) | Co23—B48 | 2.114 (3) |
| Co13—B18 | 2.123 (3) | Co23—B38 | 2.126 (3) |
| C11—C12 | 1.621 (4) | C31—C32 | 1.614 (4) |
| C11—B15 | 1.680 (4) | C31—B35 | 1.692 (4) |
| C11—B16 | 1.711 (4) | C31—B34 | 1.706 (4) |
| C11—B14 | 1.711 (4) | C31—B36 | 1.715 (4) |
| C11—H11 | 1.1000 | C31—H31 | 1.1000 |
| C12—B111 | 1.690 (4) | C32—B311 | 1.689 (4) |
| C12—B17 | 1.711 (4) | C32—B36 | 1.709 (4) |
| C12—B16 | 1.725 (4) | C32—B37 | 1.719 (4) |
| C12—H12 | 1.1000 | C32—H32 | 1.1000 |
| B14—B19 | 1.787 (4) | B34—B39 | 1.795 (4) |
| B14—B15 | 1.791 (4) | B34—B38 | 1.797 (4) |
| B14—B18 | 1.794 (4) | B34—B35 | 1.819 (4) |
| B14—H14 | 1.1000 | B34—H34 | 1.1000 |
| B15—B16 | 1.759 (5) | B35—B36 | 1.763 (5) |
| B15—B19 | 1.765 (4) | B35—B310 | 1.771 (5) |
| B15—B110 | 1.778 (5) | B35—B39 | 1.783 (5) |
| B15—H15 | 1.1000 | B35—H35 | 1.1000 |
| B16—B110 | 1.766 (5) | B36—B310 | 1.760 (5) |
| B16—B111 | 1.773 (5) | B36—B311 | 1.764 (5) |
| B16—H16 | 1.1000 | B36—H36 | 1.1000 |
| B17—B112 | 1.790 (4) | B37—B312 | 1.799 (5) |
| B17—B18 | 1.798 (4) | B37—B38 | 1.805 (5) |
| B17—B111 | 1.799 (4) | B37—B311 | 1.811 (4) |
| B17—H17 | 1.1000 | B37—H37 | 1.1000 |
| B18—N1 | 1.599 (4) | B38—N2 | 1.594 (4) |
| B18—B112 | 1.788 (4) | B38—B312 | 1.796 (4) |
| B18—B19 | 1.803 (4) | B38—B39 | 1.802 (4) |
| B19—B110 | 1.783 (5) | B39—B310 | 1.782 (5) |
| B19—B112 | 1.788 (5) | B39—B312 | 1.784 (5) |

| | | | |
|---|---|---|---|
| B19—H19 | 1.1000 | B39—H39 | 1.1000 |
| B110—B112 | 1.777 (5) | B310—B311 | 1.775 (5) |
| B110—B111 | 1.784 (5) | B310—B312 | 1.785 (5) |
| B110—H110 | 1.1000 | B310—H310 | 1.1000 |
| B111—B112 | 1.774 (5) | B311—B312 | 1.782 (5) |
| B111—H111 | 1.1000 | B311—H311 | 1.1000 |
| B112—H112 | 1.1000 | B312—H312 | 1.1000 |
| C21—C22 | 1.623 (4) | C41—C42 | 1.622 (4) |
| C21—B25 | 1.689 (4) | C41—B45 | 1.679 (4) |
| C21—B24 | 1.704 (4) | C41—B44 | 1.696 (4) |
| C21—B26 | 1.720 (4) | C41—B46 | 1.720 (4) |
| C21—H21 | 1.1000 | C41—H41 | 1.1000 |
| C22—B211 | 1.692 (4) | C42—B411 | 1.700 (4) |
| C22—B27 | 1.701 (4) | C42—B47 | 1.706 (4) |
| C22—B26 | 1.727 (4) | C42—B46 | 1.726 (4) |
| C22—H22 | 1.1000 | C42—H42 | 1.1000 |
| B24—B29 | 1.782 (4) | B44—B49 | 1.769 (5) |
| B24—B25 | 1.793 (4) | B44—B45 | 1.785 (5) |
| B24—B28 | 1.808 (4) | B44—B48 | 1.801 (5) |
| B24—H24 | 1.1000 | B44—H44 | 1.1000 |
| B25—B26 | 1.773 (5) | B45—B46 | 1.762 (5) |
| B25—B210 | 1.777 (4) | B45—B410 | 1.770 (5) |
| B25—B29 | 1.787 (4) | B45—B49 | 1.772 (5) |
| B25—H25 | 1.1000 | B45—H45 | 1.1000 |
| B26—B211 | 1.768 (5) | B46—B411 | 1.769 (5) |
| B26—B210 | 1.778 (5) | B46—B410 | 1.774 (5) |
| B26—H26 | 1.1000 | B46—H46 | 1.1000 |
| B27—B212 | 1.781 (4) | B47—B412 | 1.782 (4) |
| B27—B211 | 1.788 (4) | B47—B411 | 1.790 (4) |
| B27—B28 | 1.804 (4) | B47—B48 | 1.809 (4) |
| B27—H27 | 1.1000 | B47—H47 | 1.1000 |
| B28—B212 | 1.794 (4) | B48—B412 | 1.788 (4) |
| B28—B29 | 1.797 (4) | B48—B49 | 1.790 (5) |
| B28—H28 | 1.1000 | B48—H48 | 1.1000 |

| | | | |
|---|---|---|---|
| B29—B210 | 1.779 (4) | B49—B410 | 1.773 (5) |
| B29—B212 | 1.795 (4) | B49—B412 | 1.787 (5) |
| B29—H29 | 1.1000 | B49—H49 | 1.1000 |
| B210—B212 | 1.782 (4) | B410—B411 | 1.776 (5) |
| B210—B211 | 1.785 (5) | B410—B412 | 1.783 (4) |
| B210—H210 | 1.1000 | B410—H410 | 1.1000 |
| B211—B212 | 1.767 (5) | B411—B412 | 1.774 (5) |
| B211—H211 | 1.1000 | B411—H411 | 1.1000 |
| B212—H212 | 1.1000 | B412—H412 | 1.1000 |
| N1—C1B | 1.511 (3) | N2—C1D | 1.519 (4) |
| N1—C1A | 1.522 (4) | N2—C1C | 1.523 (4) |
| N1—H1 | 0.87 (4) | N2—H2 | 0.89 (4) |
| C1A—C2A | 1.503 (4) | C1C—C2C | 1.503 (4) |
| C1A—H1A1 | 0.9700 | C1C—H1C1 | 0.9700 |
| C1A—H1A2 | 0.9700 | C1C—H1C2 | 0.9700 |
| C2A—C7A | 1.385 (4) | C2C—C3C | 1.391 (4) |
| C2A—C3A | 1.392 (4) | C2C—C7C | 1.394 (4) |
| C3A—C4A | 1.382 (5) | C3C—C4C | 1.386 (5) |
| C3A—H3A | 0.9300 | C3C—H3C | 0.9300 |
| C4A—C5A | 1.383 (5) | C4C—C5C | 1.381 (5) |
| C4A—H4A | 0.9300 | C4C—H4C | 0.9300 |
| C5A—C6A | 1.377 (5) | C5C—C6C | 1.384 (5) |
| C5A—H5A | 0.9300 | C5C—H5C | 0.9300 |
| C6A—C7A | 1.387 (4) | C6C—C7C | 1.379 (5) |
| C6A—H6A | 0.9300 | C6C—H6C | 0.9300 |
| C7A—H7A | 0.9300 | C7C—H7C | 0.9300 |
| C1B—C2B | 1.519 (4) | C1D—C2D | 1.511 (4) |
| C1B—H1B1 | 0.9700 | C1D—H1D1 | 0.9700 |
| C1B—H1B2 | 0.9700 | C1D—H1D2 | 0.9700 |
| C2B—C3B | 1.380 (4) | C2D—C3D | 1.375 (4) |
| C2B—C7B | 1.392 (4) | C2D—C7D | 1.398 (4) |
| C3B—C4B | 1.393 (4) | C3D—C4D | 1.384 (4) |
| C3B—H3B | 0.9300 | C3D—H3D | 0.9300 |
| C4B—C5B | 1.382 (5) | C4D—C5D | 1.381 (5) |

| | | | |
|---|---|---|---|
| C4B—H4B | 0.9300 | C4D—H4D | 0.9300 |
| C5B—C6B | 1.375 (5) | C5D—C6D | 1.369 (5) |
| C5B—H5B | 0.9300 | C5D—H5D | 0.9300 |
| C6B—C7B | 1.382 (4) | C6D—C7D | 1.382 (5) |
| C6B—H6B | 0.9300 | C6D—H6D | 0.9300 |
| C7B—H7B | 0.9300 | C7D—H7D | 0.9300 |

| | | | |
|---|---|---|---|
| C11—Co13—C22 | 98.20 (11) | C32—Co23—C31 | 46.72 (11) |
| C11—Co13—C12 | 46.77 (11) | C32—Co23—C41 | 97.03 (11) |
| C22—Co13—C12 | 130.71 (11) | C31—Co23—C41 | 96.92 (11) |
| C11—Co13—C21 | 97.40 (11) | C32—Co23—C42 | 131.23 (11) |
| C22—Co13—C21 | 46.78 (11) | C31—Co23—C42 | 98.92 (11) |
| C12—Co13—C21 | 97.26 (11) | C41—Co23—C42 | 46.63 (11) |
| C11—Co13—B27 | 131.18 (12) | C32—Co23—B37 | 49.32 (11) |
| C22—Co13—B27 | 48.59 (11) | C31—Co23—B37 | 84.02 (12) |
| C12—Co13—B27 | 177.90 (12) | C41—Co23—B37 | 130.21 (13) |
| C21—Co13—B27 | 83.34 (11) | C42—Co23—B37 | 175.78 (13) |
| C11—Co13—B17 | 83.44 (12) | C32—Co23—B47 | 179.47 (13) |
| C22—Co13—B17 | 176.63 (12) | C31—Co23—B47 | 132.78 (12) |
| C12—Co13—B17 | 48.84 (11) | C41—Co23—B47 | 83.17 (12) |
| C21—Co13—B17 | 130.18 (12) | C42—Co23—B47 | 48.65 (11) |
| B27—Co13—B17 | 132.01 (12) | B37—Co23—B47 | 130.85 (12) |
| C11—Co13—B24 | 128.86 (12) | C32—Co23—B44 | 93.21 (12) |
| C22—Co13—B24 | 83.56 (11) | C31—Co23—B44 | 127.24 (12) |
| C12—Co13—B24 | 94.59 (11) | C41—Co23—B44 | 48.28 (12) |
| C21—Co13—B24 | 48.47 (11) | C42—Co23—B44 | 83.42 (12) |
| B27—Co13—B24 | 87.31 (12) | B37—Co23—B44 | 92.39 (13) |
| B17—Co13—B24 | 93.12 (12) | B47—Co23—B44 | 87.29 (13) |
| C11—Co13—B14 | 48.70 (11) | C32—Co23—B34 | 83.67 (12) |
| C22—Co13—B14 | 95.96 (11) | C31—Co23—B34 | 48.58 (11) |
| C12—Co13—B14 | 83.82 (11) | C41—Co23—B34 | 129.18 (12) |
| C21—Co13—B14 | 129.68 (12) | C42—Co23—B34 | 96.49 (12) |
| B27—Co13—B14 | 94.24 (12) | B37—Co23—B34 | 87.72 (13) |
| B17—Co13—B14 | 87.34 (13) | B47—Co23—B34 | 95.82 (12) |
| B24—Co13—B14 | 177.46 (12) | B44—Co23—B34 | 175.78 (13) |

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|---|---|---|---|
| C11—Co13—B28 | 177.90 (12) | C32—Co23—B48 | 129.55 (12) |
| C22—Co13—B28 | 83.83 (12) | C31—Co23—B48 | 176.27 (12) |
| C12—Co13—B28 | 131.31 (11) | C41—Co23—B48 | 83.45 (12) |
| C21—Co13—B28 | 83.57 (12) | C42—Co23—B48 | 84.05 (12) |
| B27—Co13—B28 | 50.72 (12) | B37—Co23—B48 | 92.90 (13) |
| B17—Co13—B28 | 94.51 (12) | B47—Co23—B48 | 50.95 (12) |
| B24—Co13—B28 | 50.68 (12) | B44—Co23—B48 | 50.63 (12) |
| B14—Co13—B28 | 131.79 (11) | B34—Co23—B48 | 133.58 (12) |
| C11—Co13—B18 | 82.96 (11) | C32—Co23—B38 | 83.68 (12) |
| C22—Co13—B18 | 132.54 (12) | C31—Co23—B38 | 83.12 (12) |
| C12—Co13—B18 | 83.46 (11) | C41—Co23—B38 | 179.07 (13) |
| C21—Co13—B18 | 179.26 (12) | C42—Co23—B38 | 132.44 (12) |
| B27—Co13—B18 | 95.93 (12) | B37—Co23—B38 | 50.73 (13) |
| B17—Co13—B18 | 50.48 (12) | B47—Co23—B38 | 96.11 (12) |
| B24—Co13—B18 | 131.70 (12) | B44—Co23—B38 | 132.35 (13) |
| B14—Co13—B18 | 50.17 (12) | B34—Co23—B38 | 50.24 (12) |
| B28—Co13—B18 | 96.09 (12) | B48—Co23—B38 | 96.57 (12) |
| C12—C11—B15 | 112.1 (2) | C32—C31—B35 | 111.8 (2) |
| C12—C11—B16 | 62.28 (18) | C32—C31—B34 | 112.5 (2) |
| B15—C11—B16 | 62.51 (18) | B35—C31—B34 | 64.73 (18) |
| C12—C11—B14 | 112.6 (2) | C32—C31—B36 | 61.70 (18) |
| B15—C11—B14 | 63.74 (18) | B35—C31—B36 | 62.32 (18) |
| B16—C11—B14 | 116.2 (2) | B34—C31—B36 | 116.6 (2) |
| C12—C11—Co13 | 66.69 (13) | C32—C31—Co23 | 66.46 (14) |
| B15—C11—Co13 | 125.73 (19) | B35—C31—Co23 | 126.66 (19) |
| B16—C11—Co13 | 125.41 (19) | B34—C31—Co23 | 67.82 (14) |
| B14—C11—Co13 | 67.66 (13) | B36—C31—Co23 | 124.79 (19) |
| C12—C11—H11 | 121.0 | C32—C31—H31 | 121.7 |
| B15—C11—H11 | 116.2 | B35—C31—H31 | 115.7 |
| B16—C11—H11 | 115.1 | B34—C31—H31 | 117.2 |
| B14—C11—H11 | 117.8 | B36—C31—H31 | 115.6 |
| Co13—C11—H11 | 106.7 | Co23—C31—H31 | 106.6 |
| C11—C12—B111 | 111.1 (2) | C31—C32—B311 | 111.6 (2) |
| C11—C12—B17 | 111.3 (2) | C31—C32—B36 | 62.07 (18) |

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| B111—C12—B17 | 63.89 (17) | B311—C32—B36 | 62.55 (19) |
| C11—C12—B16 | 61.40 (17) | C31—C32—B37 | 111.8 (2) |
| B111—C12—B16 | 62.54 (18) | B311—C32—B37 | 64.20 (18) |
| B17—C12—B16 | 115.7 (2) | B36—C32—B37 | 116.4 (2) |
| C11—C12—Co13 | 66.53 (13) | C31—C32—Co23 | 66.82 (13) |
| B111—C12—Co13 | 125.26 (18) | B311—C32—Co23 | 125.60 (19) |
| B17—C12—Co13 | 67.10 (13) | B36—C32—Co23 | 125.46 (19) |
| B16—C12—Co13 | 124.44 (19) | B37—C32—Co23 | 66.97 (14) |
| C11—C12—H12 | 122.0 | C31—C32—H32 | 121.5 |
| B111—C12—H12 | 116.3 | B311—C32—H32 | 116.2 |
| B17—C12—H12 | 118.3 | B36—C32—H32 | 114.9 |
| B16—C12—H12 | 115.6 | B37—C32—H32 | 118.1 |
| Co13—C12—H12 | 107.2 | Co23—C32—H32 | 106.9 |
| C11—B14—B19 | 102.6 (2) | C31—B34—B39 | 102.4 (2) |
| C11—B14—B15 | 57.27 (16) | C31—B34—B38 | 104.1 (2) |
| B19—B14—B15 | 59.10 (17) | B39—B34—B38 | 60.23 (18) |
| C11—B14—B18 | 103.8 (2) | C31—B34—B35 | 57.25 (16) |
| B19—B14—B18 | 60.47 (17) | B39—B34—B35 | 59.12 (17) |
| B15—B14—B18 | 107.4 (2) | B38—B34—B35 | 107.5 (2) |
| C11—B14—Co13 | 63.63 (13) | C31—B34—Co23 | 63.60 (13) |
| B19—B14—Co13 | 118.2 (2) | B39—B34—Co23 | 117.6 (2) |
| B15—B14—Co13 | 116.31 (19) | B38—B34—Co23 | 65.42 (14) |
| B18—B14—Co13 | 65.39 (14) | B35—B34—Co23 | 116.20 (18) |
| C11—B14—H14 | 126.9 | C31—B34—H34 | 126.8 |
| B19—B14—H14 | 121.1 | B39—B34—H34 | 121.5 |
| B15—B14—H14 | 121.1 | B38—B34—H34 | 122.5 |
| B18—B14—H14 | 122.6 | B35—B34—H34 | 121.0 |
| Co13—B14—H14 | 111.8 | Co23—B34—H34 | 112.0 |
| C11—B15—B16 | 59.61 (17) | C31—B35—B36 | 59.50 (17) |
| C11—B15—B19 | 104.9 (2) | C31—B35—B310 | 104.4 (2) |
| B16—B15—B19 | 108.9 (2) | B36—B35—B310 | 59.75 (19) |
| C11—B15—B110 | 105.0 (2) | C31—B35—B39 | 103.5 (2) |
| B16—B15—B110 | 59.91 (19) | B36—B35—B39 | 108.1 (2) |
| B19—B15—B110 | 60.43 (19) | B310—B35—B39 | 60.17 (19) |

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| C11—B15—B14 | 58.99 (16) | C31—B35—B34 | 58.01 (16) |
| B16—B15—B14 | 109.8 (2) | B36—B35—B34 | 108.7 (2) |
| B19—B15—B14 | 60.35 (17) | B310—B35—B34 | 108.2 (2) |
| B110—B15—B14 | 109.1 (2) | B39—B35—B34 | 59.77 (17) |
| C11—B15—H15 | 124.7 | C31—B35—H35 | 125.3 |
| B16—B15—H15 | 120.5 | B36—B35—H35 | 120.9 |
| B19—B15—H15 | 122.1 | B310—B35—H35 | 122.4 |
| B110—B15—H15 | 122.2 | B39—B35—H35 | 122.8 |
| B14—B15—H15 | 120.5 | B34—B35—H35 | 121.4 |
| C11—B16—C12 | 56.31 (16) | C32—B36—C31 | 56.24 (16) |
| C11—B16—B15 | 57.88 (17) | C32—B36—B310 | 104.2 (2) |
| C12—B16—B15 | 103.6 (2) | C31—B36—B310 | 103.8 (2) |
| C11—B16—B110 | 104.2 (2) | C32—B36—B35 | 104.0 (2) |
| C12—B16—B110 | 104.3 (2) | C31—B36—B35 | 58.18 (17) |
| B15—B16—B110 | 60.58 (19) | B310—B36—B35 | 60.36 (19) |
| C11—B16—B111 | 103.2 (2) | C32—B36—B311 | 58.16 (18) |
| C12—B16—B111 | 57.77 (17) | C31—B36—B311 | 103.5 (2) |
| B15—B16—B111 | 108.2 (2) | B310—B36—B311 | 60.5 (2) |
| B110—B16—B111 | 60.55 (19) | B35—B36—B311 | 108.5 (2) |
| C11—B16—H16 | 125.6 | C32—B36—H36 | 125.2 |
| C12—B16—H16 | 125.4 | C31—B36—H36 | 125.6 |
| B15—B16—H16 | 122.2 | B310—B36—H36 | 122.9 |
| B110—B16—H16 | 122.6 | B35—B36—H36 | 121.9 |
| B111—B16—H16 | 122.4 | B311—B36—H36 | 122.1 |
| C12—B17—B112 | 102.7 (2) | C32—B37—B312 | 102.2 (2) |
| C12—B17—B18 | 104.5 (2) | C32—B37—B38 | 103.9 (2) |
| B112—B17—B18 | 59.77 (18) | B312—B37—B38 | 59.79 (18) |
| C12—B17—B111 | 57.49 (16) | C32—B37—B311 | 57.10 (17) |
| B112—B17—B111 | 59.22 (18) | B312—B37—B311 | 59.14 (19) |
| B18—B17—B111 | 107.4 (2) | B38—B37—B311 | 107.1 (2) |
| C12—B17—Co13 | 64.06 (13) | C32—B37—Co23 | 63.71 (14) |
| B112—B17—Co13 | 117.7 (2) | B312—B37—Co23 | 117.7 (2) |
| B18—B17—Co13 | 65.63 (14) | B38—B37—Co23 | 65.77 (14) |
| B111—B17—Co13 | 116.83 (19) | B311—B37—Co23 | 116.29 (19) |

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| C12—B17—H17 | 126.4 | C32—B37—H37 | 127.0 |
| B112—B17—H17 | 121.6 | B312—B37—H37 | 121.6 |
| B18—B17—H17 | 122.6 | B38—B37—H37 | 122.7 |
| B111—B17—H17 | 120.8 | B311—B37—H37 | 121.1 |
| Co13—B17—H17 | 111.6 | Co23—B37—H37 | 111.7 |
| N1—B18—B112 | 116.8 (2) | N2—B38—B312 | 116.9 (2) |
| N1—B18—B14 | 125.0 (2) | N2—B38—B34 | 124.2 (2) |
| B112—B18—B14 | 107.2 (2) | B312—B38—B34 | 107.3 (2) |
| N1—B18—B17 | 122.0 (2) | N2—B38—B39 | 117.5 (2) |
| B112—B18—B17 | 59.90 (17) | B312—B38—B39 | 59.43 (19) |
| B14—B18—B17 | 107.7 (2) | B34—B38—B39 | 59.83 (18) |
| N1—B18—B19 | 118.4 (2) | N2—B38—B37 | 123.1 (2) |
| B112—B18—B19 | 59.73 (18) | B312—B38—B37 | 59.96 (19) |
| B14—B18—B19 | 59.58 (17) | B34—B38—B37 | 107.6 (2) |
| B17—B18—B19 | 107.7 (2) | B39—B38—B37 | 107.4 (2) |
| N1—B18—Co13 | 116.77 (18) | N2—B38—Co23 | 117.76 (19) |
| B112—B18—Co13 | 116.30 (19) | B312—B38—Co23 | 115.9 (2) |
| B14—B18—Co13 | 64.44 (13) | B34—B38—Co23 | 64.33 (14) |
| B17—B18—Co13 | 63.88 (14) | B39—B38—Co23 | 116.37 (19) |
| B19—B18—Co13 | 116.58 (18) | B37—B38—Co23 | 63.50 (14) |
| B15—B19—B110 | 60.17 (18) | B310—B39—B35 | 59.59 (18) |
| B15—B19—B14 | 60.55 (17) | B310—B39—B312 | 60.10 (19) |
| B110—B19—B14 | 109.0 (2) | B35—B39—B312 | 107.7 (2) |
| B15—B19—B112 | 107.1 (2) | B310—B39—B34 | 108.8 (2) |
| B110—B19—B112 | 59.69 (18) | B35—B39—B34 | 61.12 (18) |
| B14—B19—B112 | 107.5 (2) | B312—B39—B34 | 107.9 (2) |
| B15—B19—B18 | 108.1 (2) | B310—B39—B38 | 108.8 (2) |
| B110—B19—B18 | 108.3 (2) | B35—B39—B38 | 108.9 (2) |
| B14—B19—B18 | 59.94 (17) | B312—B39—B38 | 60.12 (18) |
| B112—B19—B18 | 59.72 (17) | B34—B39—B38 | 59.95 (17) |
| B15—B19—H19 | 121.8 | B310—B39—H39 | 121.4 |
| B110—B19—H19 | 121.2 | B35—B39—H39 | 121.4 |
| B14—B19—H19 | 121.3 | B312—B39—H39 | 122.0 |
| B112—B19—H19 | 122.5 | B34—B39—H39 | 121.2 |

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| B18—B19—H19 | 121.7 | B38—B39—H39 | 121.2 |
| B16—B110—B112 | 107.7 (2) | B36—B310—B35 | 59.89 (19) |
| B16—B110—B15 | 59.51 (19) | B36—B310—B311 | 59.87 (19) |
| B112—B110—B15 | 107.0 (2) | B35—B310—B311 | 107.7 (2) |
| B16—B110—B19 | 107.8 (2) | B36—B310—B39 | 108.2 (2) |
| B112—B110—B19 | 60.30 (19) | B35—B310—B39 | 60.24 (19) |
| B15—B110—B19 | 59.40 (19) | B311—B310—B39 | 108.0 (2) |
| B16—B110—B111 | 59.90 (19) | B36—B310—B312 | 108.1 (2) |
| B112—B110—B111 | 59.74 (19) | B35—B310—B312 | 108.1 (2) |
| B15—B110—B111 | 106.8 (2) | B311—B310—B312 | 60.05 (19) |
| B19—B110—B111 | 107.9 (2) | B39—B310—B312 | 60.01 (19) |
| B16—B110—H110 | 121.8 | B36—B310—H310 | 121.7 |
| B112—B110—H110 | 121.9 | B35—B310—H310 | 121.8 |
| B15—B110—H110 | 122.7 | B311—B310—H310 | 121.9 |
| B19—B110—H110 | 121.6 | B39—B310—H310 | 121.6 |
| B111—B110—H110 | 122.1 | B312—B310—H310 | 121.6 |
| C12—B111—B16 | 59.69 (17) | C32—B311—B36 | 59.29 (18) |
| C12—B111—B112 | 104.3 (2) | C32—B311—B310 | 104.5 (2) |
| B16—B111—B112 | 107.6 (2) | B36—B311—B310 | 59.65 (19) |
| C12—B111—B110 | 105.0 (2) | C32—B311—B312 | 104.1 (2) |
| B16—B111—B110 | 59.55 (19) | B36—B311—B312 | 108.1 (2) |
| B112—B111—B110 | 59.93 (19) | B310—B311—B312 | 60.3 (2) |
| C12—B111—B17 | 58.62 (17) | C32—B311—B37 | 58.71 (17) |
| B16—B111—B17 | 109.1 (2) | B36—B311—B37 | 109.2 (2) |
| B112—B111—B17 | 60.14 (18) | B310—B311—B37 | 108.7 (2) |
| B110—B111—B17 | 108.6 (2) | B312—B311—B37 | 60.10 (19) |
| C12—B111—H111 | 124.6 | C32—B311—H311 | 125.1 |
| B16—B111—H111 | 121.1 | B36—B311—H311 | 121.0 |
| B112—B111—H111 | 122.8 | B310—B311—H311 | 122.3 |
| B110—B111—H111 | 122.3 | B312—B311—H311 | 122.6 |
| B17—B111—H111 | 120.9 | B37—B311—H311 | 120.8 |
| B111—B112—B110 | 60.33 (19) | B311—B312—B39 | 107.6 (2) |
| B111—B112—B18 | 109.0 (2) | B311—B312—B310 | 59.7 (2) |
| B110—B112—B18 | 109.3 (2) | B39—B312—B310 | 59.89 (19) |

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| B111—B112—B19 | 108.1 (2) | B311—B312—B38 | 108.8 (2) |
| B110—B112—B19 | 60.01 (19) | B39—B312—B38 | 60.45 (18) |
| B18—B112—B19 | 60.55 (18) | B310—B312—B38 | 108.9 (2) |
| B111—B112—B17 | 60.64 (18) | B311—B312—B37 | 60.76 (19) |
| B110—B112—B17 | 109.4 (2) | B39—B312—B37 | 108.4 (2) |
| B18—B112—B17 | 60.34 (17) | B310—B312—B37 | 108.8 (2) |
| B19—B112—B17 | 108.7 (2) | B38—B312—B37 | 60.25 (18) |
| B111—B112—H112 | 121.4 | B311—B312—H312 | 121.7 |
| B110—B112—H112 | 121.0 | B39—B312—H312 | 121.9 |
| B18—B112—H112 | 120.9 | B310—B312—H312 | 121.5 |
| B19—B112—H112 | 121.7 | B38—B312—H312 | 121.0 |
| B17—B112—H112 | 121.0 | B37—B312—H312 | 121.1 |
| C22—C21—B25 | 112.1 (2) | C42—C41—B45 | 112.0 (2) |
| C22—C21—B24 | 112.2 (2) | C42—C41—B44 | 112.5 (2) |
| B25—C21—B24 | 63.79 (18) | B45—C41—B44 | 63.86 (19) |
| C22—C21—B26 | 62.12 (17) | C42—C41—B46 | 62.12 (18) |
| B25—C21—B26 | 62.66 (18) | B45—C41—B46 | 62.45 (19) |
| B24—C21—B26 | 116.0 (2) | B44—C41—B46 | 116.1 (2) |
| C22—C21—Co13 | 66.43 (13) | C42—C41—Co23 | 66.73 (14) |
| B25—C21—Co13 | 125.62 (19) | B45—C41—Co23 | 125.5 (2) |
| B24—C21—Co13 | 67.48 (13) | B44—C41—Co23 | 67.40 (14) |
| B26—C21—Co13 | 124.96 (18) | B46—C41—Co23 | 125.13 (19) |
| C22—C21—H21 | 121.3 | C42—C41—H41 | 121.0 |
| B25—C21—H21 | 116.0 | B45—C41—H41 | 116.2 |
| B24—C21—H21 | 118.0 | B44—C41—H41 | 117.9 |
| B26—C21—H21 | 115.2 | B46—C41—H41 | 115.3 |
| Co13—C21—H21 | 107.0 | Co23—C41—H41 | 106.9 |
| C21—C22—B211 | 111.0 (2) | C41—C42—B411 | 110.6 (2) |
| C21—C22—B27 | 111.7 (2) | C41—C42—B47 | 111.3 (2) |
| B211—C22—B27 | 63.61 (18) | B411—C42—B47 | 63.40 (17) |
| C21—C22—B26 | 61.70 (17) | C41—C42—B46 | 61.73 (18) |
| B211—C22—B26 | 62.28 (18) | B411—C42—B46 | 62.16 (18) |
| B27—C22—B26 | 115.7 (2) | B47—C42—B46 | 115.3 (2) |
| C21—C22—Co13 | 66.79 (13) | C41—C42—Co23 | 66.64 (14) |

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| B211—C22—Co13 | 124.99 (18) | B411—C42—Co23 | 124.43 (18) |
| B27—C22—Co13 | 67.19 (14) | B47—C42—Co23 | 66.92 (13) |
| B26—C22—Co13 | 124.91 (18) | B46—C42—Co23 | 124.69 (19) |
| C21—C22—H22 | 121.7 | C41—C42—H42 | 121.8 |
| B211—C22—H22 | 116.8 | B411—C42—H42 | 117.1 |
| B27—C22—H22 | 118.3 | B47—C42—H42 | 118.6 |
| B26—C22—H22 | 115.5 | B46—C42—H42 | 115.5 |
| Co13—C22—H22 | 107.0 | Co23—C42—H42 | 107.4 |
| C21—B24—B29 | 103.5 (2) | C41—B44—B49 | 103.4 (2) |
| C21—B24—B25 | 57.69 (17) | C41—B44—B45 | 57.60 (17) |
| B29—B24—B25 | 59.98 (17) | B49—B44—B45 | 59.79 (19) |
| C21—B24—B28 | 104.5 (2) | C41—B44—B48 | 104.7 (2) |
| B29—B24—B28 | 60.07 (17) | B49—B44—B48 | 60.19 (18) |
| B25—B24—B28 | 108.2 (2) | B45—B44—B48 | 108.2 (2) |
| C21—B24—Co13 | 64.05 (13) | C41—B44—Co23 | 64.33 (14) |
| B29—B24—Co13 | 117.83 (18) | B49—B44—Co23 | 117.9 (2) |
| B25—B24—Co13 | 117.09 (19) | B45—B44—Co23 | 117.19 (19) |
| B28—B24—Co13 | 65.16 (13) | B48—B44—Co23 | 65.14 (14) |
| C21—B24—H24 | 126.2 | C41—B44—H44 | 126.1 |
| B29—B24—H24 | 121.0 | B49—B44—H44 | 121.1 |
| B25—B24—H24 | 120.2 | B45—B44—H44 | 120.3 |
| B28—B24—H24 | 122.6 | B48—B44—H44 | 122.5 |
| Co13—B24—H24 | 111.8 | Co23—B44—H44 | 111.7 |
| C21—B25—B26 | 59.53 (17) | C41—B45—B46 | 59.91 (18) |
| C21—B25—B210 | 104.7 (2) | C41—B45—B410 | 105.1 (2) |
| B26—B25—B210 | 60.13 (18) | B46—B45—B410 | 60.28 (19) |
| C21—B25—B29 | 103.9 (2) | C41—B45—B49 | 104.0 (2) |
| B26—B25—B29 | 108.3 (2) | B46—B45—B49 | 108.7 (2) |
| B210—B25—B29 | 59.91 (18) | B410—B45—B49 | 60.10 (19) |
| C21—B25—B24 | 58.52 (17) | C41—B45—B44 | 58.54 (18) |
| B26—B25—B24 | 109.1 (2) | B46—B45—B44 | 109.6 (2) |
| B210—B25—B24 | 108.1 (2) | B410—B45—B44 | 108.3 (2) |
| B29—B25—B24 | 59.70 (17) | B49—B45—B44 | 59.65 (19) |
| C21—B25—H25 | 124.9 | C41—B45—H45 | 124.8 |

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| B26—B25—H25 | 120.6 | B46—B45—H45 | 120.2 |
| B210—B25—H25 | 122.4 | B410—B45—H45 | 122.2 |
| B29—B25—H25 | 122.8 | B49—B45—H45 | 122.7 |
| B24—B25—H25 | 121.3 | B44—B45—H45 | 121.1 |
| C21—B26—C22 | 56.18 (16) | C41—B46—C42 | 56.16 (16) |
| C21—B26—B211 | 103.1 (2) | C41—B46—B45 | 57.64 (18) |
| C22—B26—B211 | 57.88 (17) | C42—B46—B45 | 103.4 (2) |
| C21—B26—B25 | 57.81 (17) | C41—B46—B411 | 103.1 (2) |
| C22—B26—B25 | 103.5 (2) | C42—B46—B411 | 58.20 (17) |
| B211—B26—B25 | 107.9 (2) | B45—B46—B411 | 107.7 (2) |
| C21—B26—B210 | 103.4 (2) | C41—B46—B410 | 103.3 (2) |
| C22—B26—B210 | 103.9 (2) | C42—B46—B410 | 104.0 (2) |
| B211—B26—B210 | 60.45 (19) | B45—B46—B410 | 60.07 (19) |
| B25—B26—B210 | 60.03 (18) | B411—B46—B410 | 60.16 (18) |
| C21—B26—H26 | 125.9 | C41—B46—H46 | 126.0 |
| C22—B26—H26 | 125.5 | C42—B46—H46 | 125.3 |
| B211—B26—H26 | 122.4 | B45—B46—H46 | 122.5 |
| B25—B26—H26 | 122.4 | B411—B46—H46 | 122.4 |
| B210—B26—H26 | 123.1 | B410—B46—H46 | 123.2 |
| C22—B27—B212 | 103.6 (2) | C42—B47—B412 | 103.8 (2) |
| C22—B27—B211 | 57.96 (17) | C42—B47—B411 | 58.15 (16) |
| B212—B27—B211 | 59.37 (18) | B412—B47—B411 | 59.56 (18) |
| C22—B27—B28 | 105.0 (2) | C42—B47—B48 | 104.9 (2) |
| B212—B27—B28 | 60.07 (17) | B412—B47—B48 | 59.73 (17) |
| B211—B27—B28 | 107.8 (2) | B411—B47—B48 | 107.7 (2) |
| C22—B27—Co13 | 64.21 (13) | C42—B47—Co23 | 64.43 (13) |
| B212—B27—Co13 | 118.05 (19) | B412—B47—Co23 | 117.65 (19) |
| B211—B27—Co13 | 117.29 (19) | B411—B47—Co23 | 117.55 (18) |
| B28—B27—Co13 | 65.52 (13) | B48—B47—Co23 | 65.19 (14) |
| C22—B27—H27 | 125.8 | C42—B47—H47 | 125.6 |
| B212—B27—H27 | 121.2 | B412—B47—H47 | 121.3 |
| B211—B27—H27 | 120.5 | B411—B47—H47 | 120.3 |
| B28—B27—H27 | 122.4 | B48—B47—H47 | 122.8 |
| Co13—B27—H27 | 111.5 | Co23—B47—H47 | 111.6 |

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| B212—B28—B29 | 59.98 (17) | B412—B48—B49 | 59.92 (18) |
| B212—B28—B27 | 59.33 (17) | B412—B48—B44 | 106.7 (2) |
| B29—B28—B27 | 107.1 (2) | B49—B48—B44 | 59.02 (17) |
| B212—B28—B24 | 106.7 (2) | B412—B48—B47 | 59.40 (17) |
| B29—B28—B24 | 59.25 (16) | B49—B48—B47 | 106.8 (2) |
| B27—B28—B24 | 106.6 (2) | B44—B48—B47 | 106.4 (2) |
| B212—B28—Co13 | 115.89 (19) | B412—B48—Co23 | 116.20 (19) |
| B29—B28—Co13 | 116.25 (18) | B49—B48—Co23 | 116.10 (19) |
| B27—B28—Co13 | 63.76 (13) | B44—B48—Co23 | 64.24 (14) |
| B24—B28—Co13 | 64.16 (13) | B47—B48—Co23 | 63.86 (13) |
| B212—B28—H28 | 120.8 | B412—B48—H48 | 120.6 |
| B29—B28—H28 | 120.5 | B49—B48—H48 | 120.8 |
| B27—B28—H28 | 123.2 | B44—B48—H48 | 123.3 |
| B24—B28—H28 | 123.2 | B47—B48—H48 | 123.3 |
| Co13—B28—H28 | 113.4 | Co23—B48—H48 | 113.3 |
| B210—B29—B24 | 108.5 (2) | B44—B49—B45 | 60.56 (18) |
| B210—B29—B25 | 59.76 (18) | B44—B49—B410 | 108.9 (2) |
| B24—B29—B25 | 60.32 (17) | B45—B49—B410 | 59.90 (19) |
| B210—B29—B212 | 59.81 (18) | B44—B49—B412 | 108.2 (2) |
| B24—B29—B212 | 107.8 (2) | B45—B49—B412 | 107.6 (2) |
| B25—B29—B212 | 107.2 (2) | B410—B49—B412 | 60.09 (18) |
| B210—B29—B28 | 108.8 (2) | B44—B49—B48 | 60.79 (17) |
| B24—B29—B28 | 60.68 (16) | B45—B49—B48 | 109.2 (2) |
| B25—B29—B28 | 108.9 (2) | B410—B49—B48 | 109.1 (2) |
| B212—B29—B28 | 59.94 (17) | B412—B49—B48 | 59.98 (18) |
| B210—B29—H29 | 121.5 | B44—B49—H49 | 121.1 |
| B24—B29—H29 | 121.4 | B45—B49—H49 | 121.5 |
| B25—B29—H29 | 121.8 | B410—B49—H49 | 121.2 |
| B212—B29—H29 | 122.4 | B412—B49—H49 | 122.2 |
| B28—B29—H29 | 120.9 | B48—B49—H49 | 120.8 |
| B25—B210—B26 | 59.84 (18) | B45—B410—B49 | 60.00 (19) |
| B25—B210—B29 | 60.34 (18) | B45—B410—B46 | 59.65 (19) |
| B26—B210—B29 | 108.4 (2) | B49—B410—B46 | 108.1 (2) |
| B25—B210—B212 | 108.2 (2) | B45—B410—B411 | 107.1 (2) |

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| B26—B210—B212 | 107.6 (2) | B49—B410—B411 | 107.8 (2) |
| B29—B210—B212 | 60.53 (18) | B46—B410—B411 | 59.79 (18) |
| B25—B210—B211 | 107.0 (2) | B45—B410—B412 | 107.9 (2) |
| B26—B210—B211 | 59.50 (19) | B49—B410—B412 | 60.34 (19) |
| B29—B210—B211 | 107.7 (2) | B46—B410—B412 | 108.1 (2) |
| B212—B210—B211 | 59.39 (18) | B411—B410—B412 | 59.81 (18) |
| B25—B210—H210 | 121.9 | B45—B410—H410 | 122.2 |
| B26—B210—H210 | 121.8 | B49—B410—H410 | 121.5 |
| B29—B210—H210 | 121.2 | B46—B410—H410 | 121.7 |
| B212—B210—H210 | 121.7 | B411—B410—H410 | 122.2 |
| B211—B210—H210 | 122.6 | B412—B410—H410 | 121.6 |
| C22—B211—B212 | 104.5 (2) | C42—B411—B46 | 59.64 (17) |
| C22—B211—B26 | 59.84 (17) | C42—B411—B412 | 104.4 (2) |
| B212—B211—B26 | 108.8 (2) | B46—B411—B412 | 108.7 (2) |
| C22—B211—B210 | 105.1 (2) | C42—B411—B410 | 105.0 (2) |
| B212—B211—B210 | 60.22 (18) | B46—B411—B410 | 60.05 (18) |
| B26—B211—B210 | 60.05 (18) | B412—B411—B410 | 60.29 (18) |
| C22—B211—B27 | 58.44 (16) | C42—B411—B47 | 58.46 (16) |
| B212—B211—B27 | 60.12 (18) | B46—B411—B47 | 109.2 (2) |
| B26—B211—B27 | 109.4 (2) | B412—B411—B47 | 60.00 (17) |
| B210—B211—B27 | 108.6 (2) | B410—B411—B47 | 108.5 (2) |
| C22—B211—H211 | 124.7 | C42—B411—H411 | 124.8 |
| B212—B211—H211 | 122.3 | B46—B411—H411 | 120.6 |
| B26—B211—H211 | 120.5 | B412—B411—H411 | 122.4 |
| B210—B211—H211 | 122.2 | B410—B411—H411 | 122.1 |
| B27—B211—H211 | 121.0 | B47—B411—H411 | 121.1 |
| B211—B212—B27 | 60.51 (18) | B411—B412—B47 | 60.43 (18) |
| B211—B212—B210 | 60.39 (19) | B411—B412—B410 | 59.90 (18) |
| B27—B212—B210 | 109.0 (2) | B47—B412—B410 | 108.6 (2) |
| B211—B212—B28 | 109.2 (2) | B411—B412—B49 | 107.3 (2) |
| B27—B212—B28 | 60.60 (17) | B47—B412—B49 | 108.1 (2) |
| B210—B212—B28 | 108.8 (2) | B410—B412—B49 | 59.57 (19) |
| B211—B212—B29 | 107.8 (2) | B411—B412—B48 | 109.3 (2) |
| B27—B212—B29 | 108.2 (2) | B47—B412—B48 | 60.87 (17) |

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|---|---|---|---|
| B210—B212—B29 | 59.65 (18) | B410—B412—B48 | 108.8 (2) |
| B28—B212—B29 | 60.09 (17) | B49—B412—B48 | 60.10 (18) |
| B211—B212—H212 | 121.3 | B411—B412—H412 | 121.6 |
| B27—B212—H212 | 121.1 | B47—B412—H412 | 121.2 |
| B210—B212—H212 | 121.3 | B410—B412—H412 | 121.6 |
| B28—B212—H212 | 121.0 | B49—B412—H412 | 122.4 |
| B29—B212—H212 | 122.2 | B48—B412—H412 | 120.7 |
| C1B—N1—C1A | 113.6 (2) | C1D—N2—C1C | 113.9 (2) |
| C1B—N1—B18 | 111.9 (2) | C1D—N2—B38 | 111.6 (2) |
| C1A—N1—B18 | 111.2 (2) | C1C—N2—B38 | 111.2 (2) |
| C1B—N1—H1 | 107 (2) | C1D—N2—H2 | 100 (2) |
| C1A—N1—H1 | 107 (2) | C1C—N2—H2 | 111 (2) |
| B18—N1—H1 | 105 (2) | B38—N2—H2 | 109 (2) |
| C2A—C1A—N1 | 115.6 (2) | C2C—C1C—N2 | 116.6 (2) |
| C2A—C1A—H1A1 | 108.4 | C2C—C1C—H1C1 | 108.1 |
| N1—C1A—H1A1 | 108.4 | N2—C1C—H1C1 | 108.1 |
| C2A—C1A—H1A2 | 108.4 | C2C—C1C—H1C2 | 108.1 |
| N1—C1A—H1A2 | 108.4 | N2—C1C—H1C2 | 108.1 |
| H1A1—C1A—H1A2 | 107.4 | H1C1—C1C—H1C2 | 107.3 |
| C7A—C2A—C3A | 119.3 (3) | C3C—C2C—C7C | 118.6 (3) |
| C7A—C2A—C1A | 119.8 (3) | C3C—C2C—C1C | 119.3 (3) |
| C3A—C2A—C1A | 120.9 (3) | C7C—C2C—C1C | 122.0 (3) |
| C4A—C3A—C2A | 120.0 (3) | C4C—C3C—C2C | 120.3 (3) |
| C4A—C3A—H3A | 120.0 | C4C—C3C—H3C | 119.8 |
| C2A—C3A—H3A | 120.0 | C2C—C3C—H3C | 119.8 |
| C3A—C4A—C5A | 120.6 (3) | C5C—C4C—C3C | 120.5 (3) |
| C3A—C4A—H4A | 119.7 | C5C—C4C—H4C | 119.7 |
| C5A—C4A—H4A | 119.7 | C3C—C4C—H4C | 119.7 |
| C6A—C5A—C4A | 119.5 (3) | C4C—C5C—C6C | 119.5 (3) |
| C6A—C5A—H5A | 120.3 | C4C—C5C—H5C | 120.3 |
| C4A—C5A—H5A | 120.3 | C6C—C5C—H5C | 120.3 |
| C5A—C6A—C7A | 120.5 (3) | C7C—C6C—C5C | 120.2 (3) |
| C5A—C6A—H6A | 119.7 | C7C—C6C—H6C | 119.9 |

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|---|---|---|---|
| C7A—C6A—H6A | 119.7 | C5C—C6C—H6C | 119.9 |
| C2A—C7A—C6A | 120.1 (3) | C6C—C7C—C2C | 120.8 (3) |
| C2A—C7A—H7A | 119.9 | C6C—C7C—H7C | 119.6 |
| C6A—C7A—H7A | 119.9 | C2C—C7C—H7C | 119.6 |
| N1—C1B—C2B | 116.9 (2) | C2D—C1D—N2 | 115.1 (2) |
| N1—C1B—H1B1 | 108.1 | C2D—C1D—H1D1 | 108.5 |
| C2B—C1B—H1B1 | 108.1 | N2—C1D—H1D1 | 108.5 |
| N1—C1B—H1B2 | 108.1 | C2D—C1D—H1D2 | 108.5 |
| C2B—C1B—H1B2 | 108.1 | N2—C1D—H1D2 | 108.5 |
| H1B1—C1B—H1B2 | 107.3 | H1D1—C1D—H1D2 | 107.5 |
| C3B—C2B—C7B | 119.0 (3) | C3D—C2D—C7D | 118.9 (3) |
| C3B—C2B—C1B | 123.4 (3) | C3D—C2D—C1D | 118.9 (3) |
| C7B—C2B—C1B | 117.4 (3) | C7D—C2D—C1D | 122.2 (3) |
| C2B—C3B—C4B | 120.4 (3) | C2D—C3D—C4D | 121.4 (3) |
| C2B—C3B—H3B | 119.8 | C2D—C3D—H3D | 119.3 |
| C4B—C3B—H3B | 119.8 | C4D—C3D—H3D | 119.3 |
| C5B—C4B—C3B | 120.1 (3) | C5D—C4D—C3D | 118.8 (3) |
| C5B—C4B—H4B | 120.0 | C5D—C4D—H4D | 120.6 |
| C3B—C4B—H4B | 120.0 | C3D—C4D—H4D | 120.6 |
| C6B—C5B—C4B | 119.6 (3) | C6D—C5D—C4D | 120.7 (3) |
| C6B—C5B—H5B | 120.2 | C6D—C5D—H5D | 119.6 |
| C4B—C5B—H5B | 120.2 | C4D—C5D—H5D | 119.6 |
| C5B—C6B—C7B | 120.5 (3) | C5D—C6D—C7D | 120.3 (3) |
| C5B—C6B—H6B | 119.8 | C5D—C6D—H6D | 119.8 |
| C7B—C6B—H6B | 119.8 | C7D—C6D—H6D | 119.8 |
| C6B—C7B—C2B | 120.4 (3) | C6D—C7D—C2D | 119.7 (3) |
| C6B—C7B—H7B | 119.8 | C6D—C7D—H7D | 120.2 |
| C2B—C7B—H7B | 119.8 | C2D—C7D—H7D | 120.2 |

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

Data collection:

(2) COLLECT (Hooft, 1998) and DENZO (Otwinowski & Minor, 1997)

(6) CrysAlis CCD, Oxford Diffraction Ltd., Version 1.171.29.8 (release 17-03-2006 CrysAlis171 .NET) (compiled Mar 17 2006,10:57:34)

(7) COLLECT (Hooft, 1998) and DENZO (Otwinowski & Minor, 1997)

(12) COLLECT (Hooft, 1998) and DENZO (Otwinowski & Minor, 1997)

Cell refinement:

(2) *COLLECT* and *DENZO*

(6) *CrysAlis CCD*, Oxford Diffraction Ltd., Version 1.171.29.8 (release 17-03-2006 CrysAlis171 .NET) (compiled Mar 17 2006,10:57:34)

(7) *COLLECT* and *DENZO*

(12) *COLLECT* and *DENZO*

Data reduction:

(2) *COLLECT* and *DENZO*

(6) *CrysAlis CCD*, Oxford Diffraction Ltd., Version 1.171.29.8 (release 17-03-2006 CrysAlis171 .NET) (compiled Mar 17 2006,10:57:34)

(7) *COLLECT* and *DENZO*

(12) *COLLECT* and *DENZO*

Program(s) used to solve structure:

(2) *SIR92* (Altomare *et al.*, 1994)

(6) *SIR92* (Altomare *et al.*, 1994)

(7) *SIR92* (Altomare *et al.*, 1994)

(12) *SIR92* (Altomare *et al.*, 1994)

Program(s) used to refine structure:

(2) *SHELXL97* (Sheldrick, 1997)

(6) *SHELXL97* (Sheldrick, 1997)

(7) *SHELXL97* (Sheldrick, 1997)

(12) *SHELXL97* (Sheldrick, 1997)

Molecular graphics:

(2) ?

(6) ?

(7) ?

(12) ?

Software used to prepare material for publication:

| | |
|---|---|
| (2) | ? |
| (6) | ? |
| (7) | ? |
| (12) | ? |

## References

## Figures