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# The $\alpha$ polymorph of racemic tris(2,4-pentanedionato-$\kappa^2O,O'$)vanadium(III), redetermined at 120 K

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**Key indicators**

Single-crystal X-ray study
$T$ = 120 K
Mean $\sigma$(Wae) = 0.000 Å
$R$ factor = 0.058
$wR$ factor = 0.135
Data-to-parameter ratio = 18.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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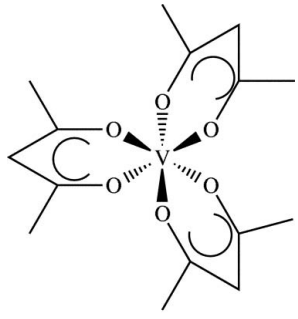
In the $\alpha$ polymorph of the title compound, $[V(C_5H_7O_2)_3]$, the molecules lie in general positions with no crystallographically imposed symmetry, but with approximate $D_3$ (32) molecular symmetry.

## Comment

The title compound, (I) (Fig. 1), crystallizes in two structurally characterized polymorphs, an orthorhombic form in space group *Pbca*, denoted $\alpha$, and a monoclinic form in space group $P2_1/n$, denoted $\beta$ (Morosin & Montgomery, 1969). The orthorhombic $\alpha$ form has been structurally characterized only at ambient temperature (Morosin & Montgomery, 1969; Filgueiras *et al.*, 2001), but neither report mentioned the molecular stereochemistry. We have now taken the opportunity to redetermine the structure of this phase using diffraction data collected at 120 K: the unit-cell dimensions and space group confirm that the same phase is present at 120 K as at ambient temperature.



(I)

In the $\alpha$ polymorph of compound (I) the molecules lie in general positions in space group *Pbca*, but the local molecular symmetry is very close to the ideal $D_3$ (32) expected for isolated molecules. Although the compound is racemic, the molecules are chiral, but the centrosymmetric space group accommodates equal numbers of the $\Lambda$ and $\Delta$ enantiomorphs: the selected reference molecule (Fig. 1) has $\Lambda$ configuration. The corresponding bond distances within the three independent ligands show some modest variation, as exemplified by the V—O and O—C distances (Table 1); likewise the ligand bite angles O—V—O within the rings show minor variation. While two of the three rings are effectively planar, that including atoms O11 and O13 shows a minor puckering, and this ring is best described as forming a boat conformer with a total puckering amplitude of 0.199 (2) Å, with the maximum displacement from the mean ring plane found for the V atom of 0.138 (2) Å.

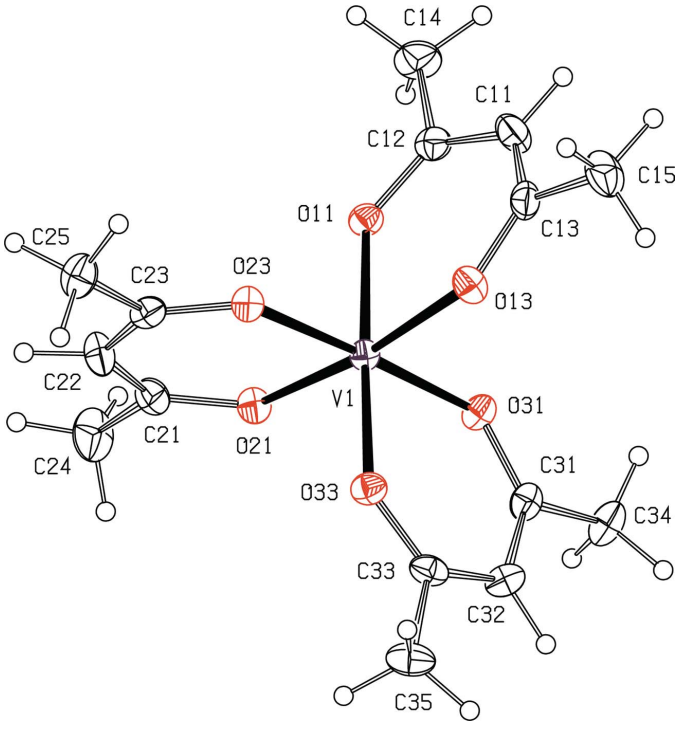



**Figure 1**
The Λ enantiomorph of compound (I) in the α polymorph, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Within each domain $0 < x < 0.5$ and $0.5 < x < 1.0$ there are four molecules, two of each enantiomer, with the Λ and Δ forms alternating, in chess-board fashion, on an approximately square grid (Fig. 2).

## Experimental

The title compound was prepared from $VO(CH_3COCHCOCH_3)_2$, according to the published procedure of Grdenić & Korpar-Čolig (1964), except that powdered tin was employed as the reducing agent rather than powdered zinc [m.p. 457 K; literature m.p. (Grdenić & Korpar-Čolig, 1964) 457 K].

*Crystal data*

$[V(C_5H_7O_2)_3]$
$M_r = 348.26$
Orthorhombic, *Pbca*
$a = 13.3920\ (7)$ Å
$b = 16.4043\ (6)$ Å
$c = 15.1901\ (10)$ Å
$V = 3337.1\ (3)$ Å$^3$
$Z = 8$
$D_x = 1.386$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3824 reflections
$\theta = 3.2$–$27.5°$
$\mu = 0.62$ mm$^{-1}$
$T = 120\ (2)$ K
Plate, brown
0.22 × 0.18 × 0.03 mm

*Data collection*

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.859$, $T_{max} = 0.982$
30601 measured reflections
3824 independent reflections
1876 reflections with $I > 2\sigma(I)$
$R_{int} = 0.174$
$\theta_{max} = 27.5°$
$h = -17 \rightarrow 17$
$k = -21 \rightarrow 21$
$l = -19 \rightarrow 18$

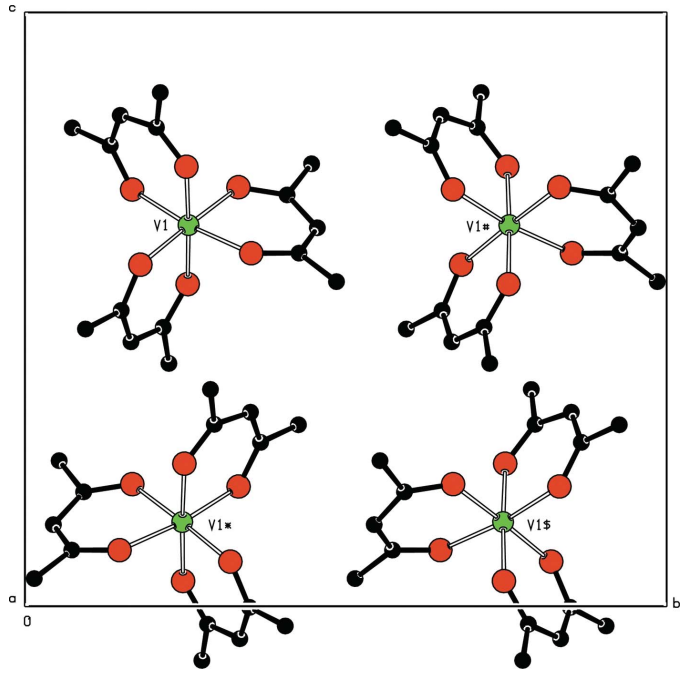



**Figure 2**
Projection on to (100) of the domain $0 < x < 0.5$ in the α polymorph of compound (I), showing the alternation of Λ and Δ enantiomorphs. For the sake of clarity, the H atoms have been omitted. Atoms marked with an asterisk (*), a hash (#) or a dollar sign ($) are at the symmetry positions $(x, \frac{1}{2} - y, -\frac{1}{2} + z)$, $(\frac{1}{2} - x, \frac{1}{2} + y, z)$ and $(\frac{1}{2} - x, 1 - y, -\frac{1}{2} + z)$, respectively.

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.135$
$S = 1.00$
3824 reflections
205 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.2837P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{min} = -0.47$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| V1—O11 | 1.998 (2) | C11—O11 | 1.272 (4) |
| V1—O13 | 1.983 (2) | C13—O13 | 1.279 (4) |
| V1—O21 | 1.971 (2) | C21—O21 | 1.283 (4) |
| V1—O23 | 2.006 (2) | C23—O23 | 1.263 (4) |
| V1—O31 | 1.986 (2) | C31—O31 | 1.271 (4) |
| V1—O33 | 1.959 (2) | C33—O33 | 1.284 (4) |
| | | | |
| O11—V1—O13 | 86.30 (10) | O31—V1—O33 | 88.74 (9) |
| O21—V1—O23 | 88.35 (9) | | |

All H atoms were located in difference maps, and then treated as riding atoms, with C—H distances 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for the ring CH atoms, and C—H distances 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl groups.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); soft-

ware used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. The authors thank the staff for all their help and advice.

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# supporting information

*Acta Cryst.* (2005). E**61**, m1326–m1328 [https://doi.org/10.1107/S1600536805018441]

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$M_r = 348.26$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 13.3920$ (7) Å
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$c = 15.1901$ (10) Å
$V = 3337.1$ (3) Å$^3$
$Z = 8$
$F(000) = 1456$
$D_x = 1.386$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3824 reflections
$\theta = 3.2$–27.5°
$\mu = 0.62$ mm$^{-1}$
$T = 120$ K
Plate, brown
0.22 × 0.18 × 0.03 mm

*Data collection*

Bruker–Nonius 95mm CCD camera on κ goniostat diffractometer
Radiation source: Bruker-Nonius FR91 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm$^{-1}$
π and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.859$, $T_{max} = 0.982$
30601 measured reflections
3824 independent reflections
1876 reflections with $I > 2\sigma(I)$
$R_{int} = 0.174$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -17 \rightarrow 17$
$k = -21 \rightarrow 21$
$l = -19 \rightarrow 18$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.135$
$S = 1.00$
3824 reflections
205 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.2837P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{min} = -0.47$ e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| V1 | 0.27195 (4) | 0.25489 (3) | 0.64183 (3) | 0.02443 (18) |

| | | | | |
|---|---|---|---|---|
| O11 | 0.18295 (16) | 0.33275 (14) | 0.70562 (13) | 0.0298 (6) |
| O13 | 0.34058 (17) | 0.35266 (14) | 0.59448 (14) | 0.0325 (6) |
| O21 | 0.19802 (16) | 0.16706 (13) | 0.70173 (14) | 0.0302 (6) |
| O23 | 0.37185 (15) | 0.25153 (14) | 0.74014 (14) | 0.0289 (5) |
| O31 | 0.17568 (16) | 0.25354 (14) | 0.54240 (13) | 0.0298 (5) |
| O33 | 0.35710 (16) | 0.17987 (14) | 0.57521 (15) | 0.0311 (6) |
| C11 | 0.1690 (3) | 0.4085 (2) | 0.6926 (2) | 0.0333 (9) |
| C12 | 0.2281 (3) | 0.4557 (2) | 0.6374 (2) | 0.0424 (10) |
| C13 | 0.3122 (3) | 0.4271 (2) | 0.5946 (2) | 0.0351 (9) |
| C14 | 0.0859 (3) | 0.4467 (2) | 0.7451 (3) | 0.0495 (11) |
| C15 | 0.3795 (3) | 0.4855 (2) | 0.5466 (3) | 0.0515 (12) |
| C21 | 0.2160 (3) | 0.1329 (2) | 0.7760 (2) | 0.0353 (9) |
| C22 | 0.2988 (3) | 0.1485 (2) | 0.8267 (3) | 0.0396 (10) |
| C23 | 0.3745 (2) | 0.2049 (2) | 0.8063 (2) | 0.0302 (8) |
| C24 | 0.1377 (3) | 0.0738 (3) | 0.8056 (3) | 0.0565 (12) |
| C25 | 0.4643 (3) | 0.2109 (2) | 0.8651 (2) | 0.0414 (10) |
| C31 | 0.1806 (3) | 0.2154 (2) | 0.4697 (2) | 0.0306 (9) |
| C32 | 0.2614 (3) | 0.1652 (2) | 0.4453 (2) | 0.0351 (9) |
| C33 | 0.3428 (3) | 0.1500 (2) | 0.4981 (2) | 0.0325 (9) |
| C34 | 0.0925 (3) | 0.2243 (2) | 0.4089 (2) | 0.0407 (10) |
| C35 | 0.4259 (3) | 0.0943 (2) | 0.4668 (3) | 0.0453 (10) |
| H12 | 0.2096 | 0.5110 | 0.6286 | 0.051* |
| H14A | 0.0265 | 0.4119 | 0.7423 | 0.074* |
| H14B | 0.0701 | 0.5005 | 0.7207 | 0.074* |
| H14C | 0.1069 | 0.4527 | 0.8066 | 0.074* |
| H15A | 0.4405 | 0.4941 | 0.5809 | 0.077* |
| H15B | 0.3450 | 0.5377 | 0.5387 | 0.077* |
| H15C | 0.3967 | 0.4629 | 0.4888 | 0.077* |
| H22 | 0.3055 | 0.1188 | 0.8801 | 0.047* |
| H24A | 0.0730 | 0.1016 | 0.8090 | 0.085* |
| H24B | 0.1553 | 0.0524 | 0.8638 | 0.085* |
| H24C | 0.1334 | 0.0287 | 0.7634 | 0.085* |
| H25A | 0.5127 | 0.1688 | 0.8489 | 0.062* |
| H25B | 0.4438 | 0.2031 | 0.9265 | 0.062* |
| H25C | 0.4949 | 0.2648 | 0.8585 | 0.062* |
| H32 | 0.2595 | 0.1404 | 0.3888 | 0.042* |
| H34A | 0.0439 | 0.1811 | 0.4213 | 0.061* |
| H34B | 0.1149 | 0.2200 | 0.3477 | 0.061* |
| H34C | 0.0611 | 0.2776 | 0.4183 | 0.061* |
| H35A | 0.4906 | 0.1200 | 0.4784 | 0.068* |
| H35B | 0.4188 | 0.0847 | 0.4034 | 0.068* |
| H35C | 0.4221 | 0.0423 | 0.4982 | 0.068* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| V1 | 0.0213 (3) | 0.0267 (3) | 0.0253 (3) | 0.0004 (3) | 0.0020 (2) | 0.0012 (3) |
| O11 | 0.0275 (14) | 0.0328 (15) | 0.0292 (13) | 0.0027 (11) | 0.0039 (11) | −0.0025 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O13 | 0.0265 (15) | 0.0313 (15) | 0.0397 (15) | 0.0002 (11) | 0.0071 (11) | 0.0062 (12) |
| O21 | 0.0240 (14) | 0.0321 (14) | 0.0344 (14) | −0.0060 (11) | −0.0020 (11) | 0.0026 (12) |
| O23 | 0.0237 (13) | 0.0328 (14) | 0.0301 (12) | −0.0023 (12) | −0.0002 (10) | 0.0028 (12) |
| O31 | 0.0219 (13) | 0.0413 (14) | 0.0263 (12) | 0.0029 (12) | 0.0021 (10) | −0.0020 (12) |
| O33 | 0.0272 (14) | 0.0334 (14) | 0.0328 (13) | 0.0030 (11) | −0.0003 (11) | −0.0042 (11) |
| C11 | 0.030 (2) | 0.036 (2) | 0.034 (2) | 0.0041 (18) | −0.0074 (17) | −0.0050 (18) |
| C12 | 0.049 (3) | 0.029 (2) | 0.049 (2) | 0.007 (2) | 0.001 (2) | 0.009 (2) |
| C13 | 0.041 (2) | 0.037 (2) | 0.028 (2) | −0.0016 (19) | −0.0065 (17) | 0.0070 (17) |
| C14 | 0.041 (3) | 0.053 (3) | 0.054 (2) | 0.018 (2) | 0.004 (2) | −0.011 (2) |
| C15 | 0.059 (3) | 0.038 (2) | 0.058 (3) | −0.012 (2) | 0.003 (2) | 0.015 (2) |
| C21 | 0.037 (2) | 0.030 (2) | 0.039 (2) | −0.0023 (18) | 0.0025 (18) | 0.0054 (17) |
| C22 | 0.039 (3) | 0.038 (2) | 0.041 (2) | −0.0022 (19) | −0.0074 (18) | 0.0146 (19) |
| C23 | 0.025 (2) | 0.036 (2) | 0.030 (2) | 0.0050 (17) | −0.0022 (16) | −0.0060 (18) |
| C24 | 0.054 (3) | 0.060 (3) | 0.056 (3) | −0.028 (2) | 0.002 (2) | 0.019 (2) |
| C25 | 0.028 (2) | 0.058 (3) | 0.037 (2) | 0.0038 (19) | −0.0062 (17) | 0.004 (2) |
| C31 | 0.026 (2) | 0.039 (2) | 0.027 (2) | −0.0084 (18) | 0.0018 (16) | 0.0032 (17) |
| C32 | 0.032 (2) | 0.041 (2) | 0.032 (2) | −0.0017 (19) | 0.0025 (17) | −0.0097 (17) |
| C33 | 0.032 (2) | 0.024 (2) | 0.042 (2) | −0.0025 (17) | 0.0081 (18) | −0.0029 (17) |
| C34 | 0.030 (2) | 0.065 (3) | 0.027 (2) | −0.0012 (19) | −0.0008 (16) | 0.0005 (18) |
| C35 | 0.038 (3) | 0.039 (2) | 0.060 (3) | 0.0076 (19) | 0.004 (2) | −0.015 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| V1—O11 | 1.998 (2) | C21—C22 | 1.375 (5) |
| V1—O13 | 1.983 (2) | C21—C24 | 1.497 (5) |
| V1—O21 | 1.971 (2) | C22—C23 | 1.407 (5) |
| V1—O23 | 2.006 (2) | C22—H22 | 0.95 |
| V1—O31 | 1.986 (2) | C23—C25 | 1.502 (4) |
| V1—O33 | 1.959 (2) | C24—H24A | 0.98 |
| C11—O11 | 1.272 (4) | C24—H24B | 0.98 |
| C13—O13 | 1.279 (4) | C24—H24C | 0.98 |
| C21—O21 | 1.283 (4) | C25—H25A | 0.98 |
| C23—O23 | 1.263 (4) | C25—H25B | 0.98 |
| C31—O31 | 1.271 (4) | C25—H25C | 0.98 |
| C33—O33 | 1.284 (4) | C31—C32 | 1.409 (5) |
| C11—C12 | 1.387 (5) | C31—C34 | 1.506 (5) |
| C11—C14 | 1.507 (5) | C32—C33 | 1.377 (5) |
| C12—C13 | 1.383 (5) | C32—H32 | 0.95 |
| C12—H12 | 0.95 | C33—C35 | 1.516 (5) |
| C13—C15 | 1.504 (5) | C34—H34A | 0.98 |
| C14—H14A | 0.98 | C34—H34B | 0.98 |
| C14—H14B | 0.98 | C34—H34C | 0.98 |
| C14—H14C | 0.98 | C35—H35A | 0.98 |
| C15—H15A | 0.98 | C35—H35B | 0.98 |
| C15—H15B | 0.98 | C35—H35C | 0.98 |
| C15—H15C | 0.98 | | |
| | | | |
| O33—V1—O21 | 94.10 (10) | C21—C22—C23 | 125.5 (3) |

| | | | |
|---|---|---|---|
| O33—V1—O13 | 92.92 (10) | C21—C22—H22 | 117.3 |
| O21—V1—O13 | 172.45 (10) | C23—C22—H22 | 117.3 |
| O21—V1—O31 | 90.96 (9) | O23—C23—C22 | 123.6 (3) |
| O13—V1—O31 | 91.96 (10) | O23—C23—C25 | 117.1 (3) |
| O33—V1—O11 | 177.91 (9) | C22—C23—C25 | 119.3 (3) |
| O21—V1—O11 | 86.78 (9) | C23—O23—V1 | 128.9 (2) |
| O11—V1—O13 | 86.30 (10) | C21—C24—H24A | 109.5 |
| O31—V1—O11 | 89.35 (9) | C21—C24—H24B | 109.5 |
| O33—V1—O23 | 88.80 (9) | H24A—C24—H24B | 109.5 |
| O21—V1—O23 | 88.35 (9) | C21—C24—H24C | 109.5 |
| O31—V1—O33 | 88.74 (9) | H24A—C24—H24C | 109.5 |
| O13—V1—O23 | 89.03 (9) | H24B—C24—H24C | 109.5 |
| O31—V1—O23 | 177.39 (10) | C23—C25—H25A | 109.5 |
| O11—V1—O23 | 93.12 (9) | C23—C25—H25B | 109.5 |
| O11—C11—C12 | 123.7 (3) | H25A—C25—H25B | 109.5 |
| O11—C11—C14 | 115.6 (3) | C23—C25—H25C | 109.5 |
| C12—C11—C14 | 120.6 (3) | H25A—C25—H25C | 109.5 |
| C11—O11—V1 | 129.5 (2) | H25B—C25—H25C | 109.5 |
| C13—C12—C11 | 124.0 (3) | O31—C31—C32 | 123.8 (3) |
| C13—C12—H12 | 118.0 | O31—C31—C34 | 116.4 (3) |
| C11—C12—H12 | 118.0 | C32—C31—C34 | 119.8 (3) |
| O13—C13—C12 | 124.5 (3) | C31—O31—V1 | 129.2 (2) |
| O13—C13—C15 | 115.4 (3) | C33—C32—C31 | 124.1 (3) |
| C12—C13—C15 | 120.0 (4) | C33—C32—H32 | 117.9 |
| C13—O13—V1 | 129.3 (2) | C31—C32—H32 | 117.9 |
| C11—C14—H14A | 109.5 | O33—C33—C32 | 125.4 (3) |
| C11—C14—H14B | 109.5 | O33—C33—C35 | 114.0 (3) |
| H14A—C14—H14B | 109.5 | C32—C33—C35 | 120.5 (3) |
| C11—C14—H14C | 109.5 | C33—O33—V1 | 128.7 (2) |
| H14A—C14—H14C | 109.5 | C31—C34—H34A | 109.5 |
| H14B—C14—H14C | 109.5 | C31—C34—H34B | 109.5 |
| C13—C15—H15A | 109.5 | H34A—C34—H34B | 109.5 |
| C13—C15—H15B | 109.5 | C31—C34—H34C | 109.5 |
| H15A—C15—H15B | 109.5 | H34A—C34—H34C | 109.5 |
| C13—C15—H15C | 109.5 | H34B—C34—H34C | 109.5 |
| H15A—C15—H15C | 109.5 | C33—C35—H35A | 109.5 |
| H15B—C15—H15C | 109.5 | C33—C35—H35B | 109.5 |
| O21—C21—C22 | 124.2 (3) | H35A—C35—H35B | 109.5 |
| O21—C21—C24 | 114.6 (3) | C33—C35—H35C | 109.5 |
| C22—C21—C24 | 121.2 (3) | H35A—C35—H35C | 109.5 |
| C21—O21—V1 | 129.2 (2) | H35B—C35—H35C | 109.5 |

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| C12—C11—O11—V1 | −11.0 (5) | C21—C22—C23—O23 | 4.2 (6) |
| C14—C11—O11—V1 | 172.0 (2) | C21—C22—C23—C25 | −175.6 (4) |
| O21—V1—O11—C11 | −166.3 (3) | C22—C23—O23—V1 | −5.6 (5) |
| O13—V1—O11—C11 | 16.7 (3) | C25—C23—O23—V1 | 174.2 (2) |
| O31—V1—O11—C11 | −75.3 (3) | O33—V1—O23—C23 | −92.0 (3) |
| O23—V1—O11—C11 | 105.5 (3) | O21—V1—O23—C23 | 2.1 (3) |

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| O11—C11—C12—C13 | −4.1 (6) | O13—V1—O23—C23 | 175.1 (3) |
| C14—C11—C12—C13 | 172.7 (3) | O11—V1—O23—C23 | 88.8 (3) |
| C11—C12—C13—O13 | 6.3 (6) | C32—C31—O31—V1 | −1.0 (5) |
| C11—C12—C13—C15 | −171.3 (3) | C34—C31—O31—V1 | 177.4 (2) |
| C12—C13—O13—V1 | 6.8 (5) | O33—V1—O31—C31 | −0.2 (3) |
| C15—C13—O13—V1 | −175.5 (2) | O21—V1—O31—C31 | −94.2 (3) |
| O33—V1—O13—C13 | 163.6 (3) | O13—V1—O31—C31 | 92.7 (3) |
| O31—V1—O13—C13 | 74.8 (3) | O11—V1—O31—C31 | 179.0 (3) |
| O11—V1—O13—C13 | −14.5 (3) | O31—C31—C32—C33 | 1.8 (6) |
| O23—V1—O13—C13 | −107.6 (3) | C34—C31—C32—C33 | −176.6 (3) |
| C22—C21—O21—V1 | −5.2 (5) | C31—C32—C33—O33 | −1.1 (6) |
| C24—C21—O21—V1 | 174.0 (3) | C31—C32—C33—C35 | 179.3 (3) |
| O33—V1—O21—C21 | 91.9 (3) | C32—C33—O33—V1 | −0.3 (5) |
| O31—V1—O21—C21 | −179.3 (3) | C35—C33—O33—V1 | 179.3 (2) |
| O11—V1—O21—C21 | −90.0 (3) | O21—V1—O33—C33 | 91.6 (3) |
| O23—V1—O21—C21 | 3.2 (3) | O13—V1—O33—C33 | −91.1 (3) |
| O21—C21—C22—C23 | 1.4 (6) | O31—V1—O33—C33 | 0.8 (3) |
| C24—C21—C22—C23 | −177.6 (4) | O23—V1—O33—C33 | 179.9 (3) |