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Bis(acetylacetonato)oxido(triphenylphosphine oxide)vanadium(IV)

Hui Chen, Youtao Si, Changneng Chen* and Qiutian Liu

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China
Correspondence e-mail: ccn@fjirsm.ac.cn

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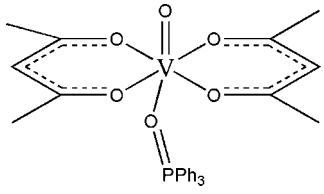
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.121; data-to-parameter ratio = 17.9.

In the structure of the title compound, $[V(C_5H_7O_2)_2O(C_{18}H_{15}OP)]$, the V atom adopts a slightly distorted octahedral geometry with its coordination completed by four O atoms of two acetylacetonate (acac) ligands, one oxo group and one O atom of the triphenylphosphine oxide ($OPPh_3$) ligand.

Related literature

For related literature, see: Hoshino *et al.* (2005); Mévellec *et al.* (2001); Rübenstahl *et al.* (1993); Shuter *et al.* (1995); Zhu *et al.* (1996); Caira & Gellatly (1980); Scott *et al.* (1992).



Experimental

Crystal data

$[V(C_5H_7O_2)_2O(C_{18}H_{15}OP)]$
M_r = 543.42
Triclinic, $P\overline{1}$
a = 10.153 (3) Å
b = 10.353 (3) Å
c = 13.407 (4) Å
α = 101.677 (2)°
β = 90.693 (5)°
γ = 106.688 (4)°
V = 1318.2 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 294 (2) K
0.28 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn70 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.860, T_{max} = 0.920
10251 measured reflections
5899 independent reflections
4756 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.121
S = 1.13
5899 reflections
329 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2106).

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supplementary materials

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Bis(acetylacetonato)oxido(triphenylphosphine oxide)vanadium(IV)

H. Chen, Y. Si, C. Chen and Q. Liu

Comment

The crystal consists of monomeric units of $VO(acac)_2(OPPh_3)$ packed together without contact significantly shorter than the sum of the van der Waals radii. Each V center is six-coordinated by four O atoms of two acac ligands, one oxo group and one O atom of $OPPh_3$ ligand to furnish a slightly distorted octahedral geometry. The four acac O atoms define the equatorial plane. The oxo group and the O atom from $OPPh_3$ ligand occupy the axial sites in a *trans* configuration. The V—$O_{(acac)}$ bond distances [1.9974 (13) Å-2.0085 (14) Å] are a little longer than those observed in $[VO(acac)_2]$ [1.966 (6) Å-1.986 (6) Å, Shuter *et al.*, 1995; Hoshino *et al.*, 2005] and the bond length of V—$O_{(OPPh3)}$ is 2.2586 (13) Å, significantly longer than those found in $[VOCl_2(OPPh_3)_2]$ [1.986 (5) Å and 2.002 (5) Å, Caira & Gellatly, 1980] and $[VCl_3(NPPh_3)(OPPh_3)]$(1.928 (6) Å, Rübenstahl *et al.*, 1993).

The presence of $OPPh_3$ ligand in the compound was unexpected since the original reactant was PPh_3. It has been shown in earlier studies that some metal oxo-complexes might react with PPh_3 to give rise to $OPPh_3$ due to their catalytic and redox properties (Scott *et al.*, 1992; Zhu *et al.*, 1996; Mévellec *et al.*, 2001). Thus, it was speculated that PPh_3 was oxidized to $OPPh_3$ by oxovanadium complex in this experiment.

Experimental

The title compound was obtained unintentionally when we attempted to synthesize vanadium coordination complexes containing 3,5-pyrazoledicarboxylato ligand (H_3pdc). To the mixture of H_3pdc (0.5 mmol), NaOH (1 mmol) and $VO(acac)_2$ (0.5 mmol) in 10 ml H_2O was added a $CHCl_3$ solution (5 ml) of PPh_3 (0.25 mmol). The resulting solution was allowed to stand at room temperature for six weeks to deposit green crystals of X-ray quality.

Refinement

H atoms bound to C atoms were located by geometry, and their positions and thermal parameters were constrained to ride on their parent atoms during the structure refinement.

Figures

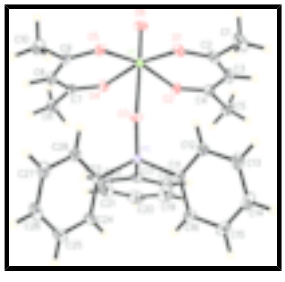


Fig. 1. The molecular structure of the title compound, showing atom labels and 20% probability ellipsoids for non-H atoms.

Bis(acetylacetonato)oxido(triphenylphosphine oxide)vanadium(IV)

Crystal data

$[V(C_5H_7O_2)_2O(C_{18}H_{15}OP)]$	$Z = 2$
$M_r = 543.42$	$F_{000} = 566$
Triclinic, $P\overline{1}$	$D_x = 1.369$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.153$ (3) Å	Cell parameters from 3761 reflections
$b = 10.353$ (3) Å	$\theta = 2.1$–27.5º
$c = 13.407$ (4) Å	$\mu = 0.48$ mm^{-1}
$\alpha = 101.677$ (2)º	$T = 294$ (2) K
$\beta = 90.693$ (5)º	Prism, green
$\gamma = 106.688$ (4)º	0.28 × 0.20 × 0.18 mm
$V = 1318.2$ (7) Å^3	

Data collection

Rigaku Saturn70 CCD diffractometer	5899 independent reflections
Radiation source: fine-focus sealed tube	4756 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 294$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 2.1$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 13$
$T_{min} = 0.860$, $T_{max} = 0.920$	$k = -13 \rightarrow 13$
10251 measured reflections	$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters constrained
$wR(F^2) = 0.121$	$w = 1/[\sigma^2(F_o^2) + (0.0785P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} = 0.001$
5899 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
329 parameters	$\Delta\rho_{min} = -0.54$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ 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}
V1	1.03517 (3)	0.82224 (3)	0.22396 (2)	0.02967 (11)
P1	0.67969 (4)	0.83817 (4)	0.24257 (3)	0.02730 (12)
O1	0.99298 (14)	0.67895 (14)	0.30948 (10)	0.0436 (3)
O2	0.92589 (13)	0.67788 (13)	0.10557 (9)	0.0400 (3)
O3	0.82442 (11)	0.83840 (13)	0.26469 (9)	0.0351 (3)
O4	1.02709 (13)	0.96524 (13)	0.14587 (9)	0.0362 (3)
O5	1.08719 (12)	0.96846 (13)	0.35241 (9)	0.0361 (3)
O6	1.18499 (13)	0.81385 (16)	0.19582 (11)	0.0494 (3)
C1	0.9215 (3)	0.4673 (3)	0.3614 (2)	0.0727 (8)
H1A	1.0123	0.4759	0.3885	0.109*
H1B	0.8748	0.3721	0.3322	0.109*
H1C	0.8705	0.5010	0.4153	0.109*
C2	0.9323 (2)	0.5508 (2)	0.27993 (16)	0.0455 (5)
C3	0.8760 (2)	0.4847 (2)	0.18191 (18)	0.0530 (5)
H3A	0.8369	0.3894	0.1692	0.064*
C4	0.87320 (19)	0.5503 (2)	0.10003 (15)	0.0413 (4)
C5	0.8031 (2)	0.4665 (2)	−0.00156 (18)	0.0592 (6)
H5A	0.7696	0.5239	−0.0370	0.089*
H5B	0.7272	0.3913	0.0089	0.089*
H5C	0.8678	0.4307	−0.0414	0.089*
C6	1.0415 (2)	1.1785 (2)	0.10245 (15)	0.0472 (5)
H6A	1.1270	1.1986	0.0705	0.071*
H6B	1.0256	1.2633	0.1359	0.071*
H6C	0.9674	1.1279	0.0516	0.071*
C7	1.04857 (17)	1.09364 (18)	0.17968 (13)	0.0327 (4)
C8	1.07829 (19)	1.15850 (19)	0.28267 (13)	0.0401 (4)
H8A	1.0870	1.2524	0.2998	0.048*
C9	1.09605 (17)	1.09559 (18)	0.36203 (13)	0.0340 (4)
C10	1.1309 (2)	1.1816 (2)	0.46922 (14)	0.0505 (5)
H10A	1.0637	1.1428	0.5132	0.076*
H10B	1.1304	1.2743	0.4695	0.076*
H10C	1.2207	1.1826	0.4933	0.076*
C11	0.55910 (16)	0.68625 (17)	0.27131 (12)	0.0304 (3)

C12	0.6134 (2)	0.60577 (19)	0.32063 (14)	0.0391 (4)
H12A	0.7083	0.6277	0.3338	0.047*
C13	0.5260 (3)	0.4921 (2)	0.35045 (18)	0.0571 (6)
H13A	0.5625	0.4384	0.3840	0.069*
C14	0.3867 (3)	0.4591 (2)	0.33060 (19)	0.0631 (6)
H14A	0.3287	0.3826	0.3504	0.076*
C15	0.3312 (2)	0.5391 (2)	0.28087 (18)	0.0569 (6)
H15A	0.2362	0.5162	0.2677	0.068*
C16	0.41669 (19)	0.6524 (2)	0.25089 (15)	0.0422 (4)
H16A	0.3797	0.7058	0.2174	0.051*
C17	0.63977 (17)	0.8411 (2)	0.11197 (13)	0.0352 (4)
C18	0.5849 (2)	0.7194 (2)	0.04015 (15)	0.0501 (5)
H18A	0.5602	0.6355	0.0606	0.060*
C19	0.5666 (3)	0.7217 (3)	−0.06184 (16)	0.0685 (7)
H19A	0.5292	0.6396	−0.1095	0.082*
C20	0.6035 (3)	0.8446 (4)	−0.09268 (18)	0.0713 (8)
H20A	0.5909	0.8457	−0.1613	0.086*
C21	0.6593 (3)	0.9662 (3)	−0.02260 (19)	0.0661 (7)
H21A	0.6855	1.0495	−0.0439	0.079*
C22	0.6762 (2)	0.9647 (2)	0.07985 (16)	0.0500 (5)
H22A	0.7124	1.0474	0.1273	0.060*
C23	0.64143 (17)	0.98229 (17)	0.32429 (13)	0.0312 (3)
C24	0.5175 (2)	1.0118 (2)	0.31082 (15)	0.0437 (4)
H24A	0.4564	0.9633	0.2544	0.052*
C25	0.4863 (2)	1.1131 (2)	0.38136 (18)	0.0561 (6)
H25A	0.4034	1.1324	0.3725	0.067*
C26	0.5757 (3)	1.1861 (2)	0.46471 (17)	0.0586 (6)
H26A	0.5531	1.2540	0.5120	0.070*
C27	0.6997 (3)	1.1587 (2)	0.47836 (16)	0.0553 (5)
H27A	0.7607	1.2082	0.5346	0.066*
C28	0.7323 (2)	1.0569 (2)	0.40744 (14)	0.0418 (4)
H28A	0.8158	1.0387	0.4160	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
V1	0.03094 (17)	0.03182 (17)	0.02627 (16)	0.01119 (12)	−0.00037 (11)	0.00367 (11)
P1	0.0250 (2)	0.0323 (2)	0.0259 (2)	0.01010 (16)	0.00204 (15)	0.00692 (16)
O1	0.0561 (8)	0.0432 (8)	0.0388 (7)	0.0234 (6)	0.0012 (6)	0.0130 (6)
O2	0.0475 (7)	0.0360 (7)	0.0329 (6)	0.0116 (5)	−0.0029 (5)	0.0007 (5)
O3	0.0262 (6)	0.0453 (7)	0.0358 (6)	0.0128 (5)	0.0023 (5)	0.0099 (5)
O4	0.0463 (7)	0.0355 (7)	0.0256 (6)	0.0104 (5)	0.0017 (5)	0.0067 (5)
O5	0.0389 (7)	0.0384 (7)	0.0272 (6)	0.0084 (5)	−0.0035 (5)	0.0033 (5)
O6	0.0390 (7)	0.0614 (9)	0.0501 (8)	0.0230 (6)	0.0053 (6)	0.0055 (7)
C1	0.109 (2)	0.0606 (15)	0.0722 (17)	0.0456 (15)	0.0271 (15)	0.0363 (13)
C2	0.0548 (12)	0.0396 (10)	0.0547 (12)	0.0276 (9)	0.0176 (9)	0.0182 (9)
C3	0.0662 (14)	0.0304 (10)	0.0608 (13)	0.0135 (9)	0.0143 (10)	0.0069 (9)
C4	0.0365 (9)	0.0378 (10)	0.0458 (10)	0.0131 (8)	0.0070 (8)	−0.0032 (8)

C5	0.0543 (13)	0.0488 (12)	0.0575 (13)	0.0070 (10)	0.0008 (10)	−0.0149 (10)
C6	0.0613 (13)	0.0421 (11)	0.0405 (10)	0.0155 (9)	0.0030 (9)	0.0138 (9)
C7	0.0303 (8)	0.0335 (9)	0.0334 (8)	0.0064 (7)	0.0058 (6)	0.0090 (7)
C8	0.0503 (11)	0.0301 (9)	0.0354 (9)	0.0074 (7)	0.0024 (8)	0.0036 (7)
C9	0.0284 (8)	0.0369 (9)	0.0293 (8)	0.0025 (7)	0.0028 (6)	0.0009 (7)
C10	0.0628 (13)	0.0468 (12)	0.0293 (9)	0.0048 (10)	0.0019 (9)	−0.0036 (8)
C11	0.0319 (8)	0.0315 (8)	0.0255 (7)	0.0081 (6)	0.0024 (6)	0.0028 (6)
C12	0.0424 (10)	0.0367 (9)	0.0388 (9)	0.0121 (8)	0.0007 (7)	0.0093 (8)
C13	0.0698 (15)	0.0438 (12)	0.0578 (13)	0.0088 (10)	−0.0015 (11)	0.0234 (10)
C14	0.0636 (15)	0.0494 (13)	0.0627 (14)	−0.0100 (11)	0.0071 (11)	0.0199 (11)
C15	0.0384 (11)	0.0588 (14)	0.0606 (14)	−0.0038 (9)	0.0048 (9)	0.0098 (11)
C16	0.0348 (9)	0.0454 (10)	0.0438 (10)	0.0079 (8)	0.0005 (7)	0.0094 (8)
C17	0.0304 (8)	0.0509 (10)	0.0290 (8)	0.0168 (7)	0.0053 (6)	0.0124 (7)
C18	0.0569 (12)	0.0578 (13)	0.0329 (10)	0.0144 (10)	0.0025 (8)	0.0074 (9)
C19	0.0749 (17)	0.094 (2)	0.0305 (11)	0.0219 (14)	−0.0027 (10)	0.0045 (12)
C20	0.0749 (17)	0.123 (3)	0.0339 (11)	0.0500 (17)	0.0091 (11)	0.0268 (14)
C21	0.0741 (16)	0.0909 (19)	0.0579 (15)	0.0409 (14)	0.0198 (12)	0.0467 (15)
C22	0.0551 (12)	0.0578 (13)	0.0453 (11)	0.0215 (10)	0.0105 (9)	0.0223 (10)
C23	0.0318 (8)	0.0304 (8)	0.0332 (8)	0.0102 (6)	0.0067 (6)	0.0089 (7)
C24	0.0405 (10)	0.0460 (11)	0.0486 (11)	0.0209 (8)	0.0008 (8)	0.0070 (9)
C25	0.0600 (13)	0.0589 (14)	0.0630 (14)	0.0375 (11)	0.0162 (11)	0.0140 (11)
C26	0.0888 (17)	0.0462 (12)	0.0477 (12)	0.0324 (12)	0.0226 (12)	0.0068 (10)
C27	0.0743 (15)	0.0441 (12)	0.0398 (11)	0.0125 (10)	−0.0013 (10)	−0.0009 (9)
C28	0.0427 (10)	0.0404 (10)	0.0401 (10)	0.0110 (8)	0.0003 (8)	0.0059 (8)

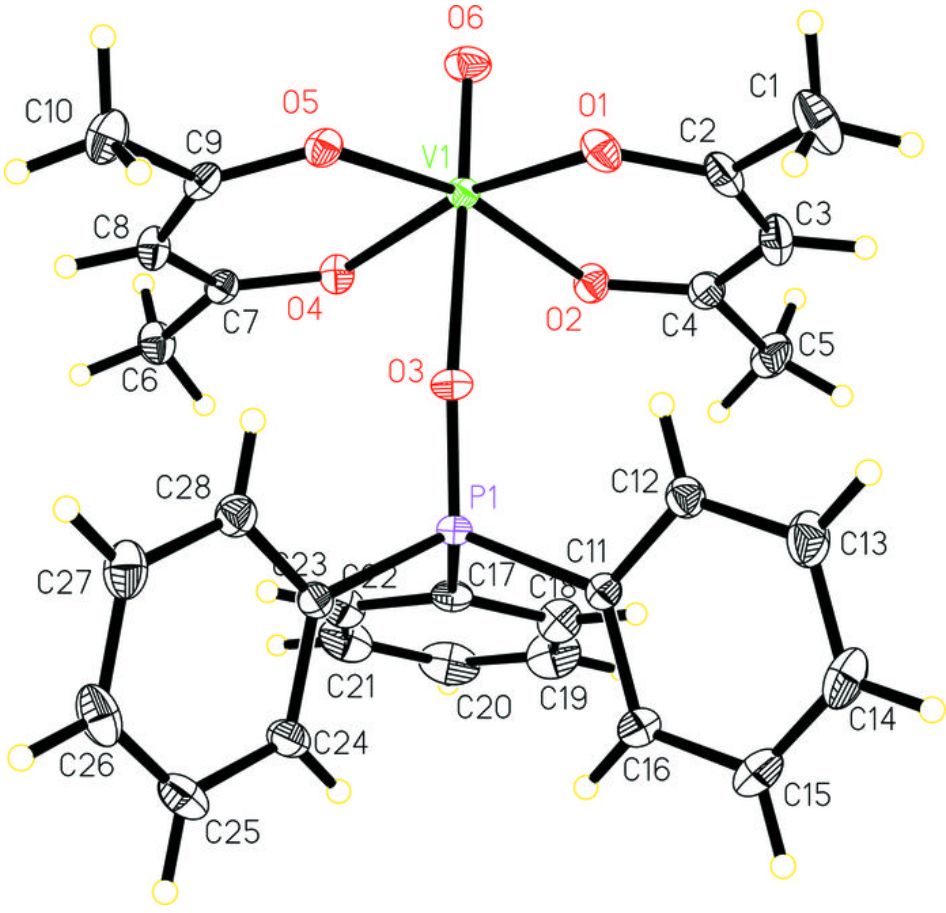
Geometric parameters (Å, °)

V1—O6	1.5937 (13)	C10—H10C	0.9600
V1—O4	1.9974 (13)	C11—C12	1.383 (2)
V1—O5	1.9999 (12)	C11—C16	1.396 (2)
V1—O1	2.0085 (14)	C12—C13	1.390 (3)
V1—O2	2.0072 (13)	C12—H12A	0.9300
V1—O3	2.2586 (13)	C13—C14	1.365 (4)
P1—O3	1.4948 (12)	C13—H13A	0.9300
P1—C17	1.8006 (18)	C14—C15	1.389 (3)
P1—C23	1.8052 (17)	C14—H14A	0.9300
P1—C11	1.8088 (17)	C15—C16	1.381 (3)
O1—C2	1.268 (2)	C15—H15A	0.9300
O2—C4	1.261 (2)	C16—H16A	0.9300
O4—C7	1.268 (2)	C17—C18	1.385 (3)
O5—C9	1.273 (2)	C17—C22	1.384 (3)
C1—C2	1.511 (3)	C18—C19	1.384 (3)
C1—H1A	0.9600	C18—H18A	0.9300
C1—H1B	0.9600	C19—C20	1.368 (4)
C1—H1C	0.9600	C19—H19A	0.9300
C2—C3	1.384 (3)	C20—C21	1.374 (4)
C3—C4	1.407 (3)	C20—H20A	0.9300
C3—H3A	0.9300	C21—C22	1.386 (3)
C4—C5	1.503 (3)	C21—H21A	0.9300

C5—H5A	0.9600	C22—H22A	0.9300
C5—H5B	0.9600	C23—C28	1.381 (3)
C5—H5C	0.9600	C23—C24	1.395 (2)
C6—C7	1.500 (3)	C24—C25	1.375 (3)
C6—H6A	0.9600	C24—H24A	0.9300
C6—H6B	0.9600	C25—C26	1.372 (3)
C6—H6C	0.9600	C25—H25A	0.9300
C7—C8	1.395 (2)	C26—C27	1.386 (3)
C8—C9	1.390 (3)	C26—H26A	0.9300
C8—H8A	0.9300	C27—C28	1.388 (3)
C9—C10	1.507 (2)	C27—H27A	0.9300
C10—H10A	0.9600	C28—H28A	0.9300
C10—H10B	0.9600		
O6—V1—O4	97.10 (7)	C8—C9—C10	119.21 (17)
O6—V1—O5	99.20 (6)	C9—C10—H10A	109.5
O4—V1—O5	89.73 (6)	C9—C10—H10B	109.5
O6—V1—O1	97.80 (7)	H10A—C10—H10B	109.5
O4—V1—O1	165.07 (5)	C9—C10—H10C	109.5
O5—V1—O1	88.84 (6)	H10A—C10—H10C	109.5
O6—V1—O2	98.11 (7)	H10B—C10—H10C	109.5
O4—V1—O2	88.28 (6)	C12—C11—C16	119.89 (17)
O5—V1—O2	162.69 (5)	C12—C11—P1	116.84 (13)
O1—V1—O2	88.67 (6)	C16—C11—P1	123.18 (14)
O6—V1—O3	178.95 (7)	C11—C12—C13	119.93 (19)
O4—V1—O3	82.22 (5)	C11—C12—H12A	120.0
O5—V1—O3	80.01 (5)	C13—C12—H12A	120.0
O1—V1—O3	82.89 (5)	C14—C13—C12	120.2 (2)
O2—V1—O3	82.68 (5)	C14—C13—H13A	119.9
O3—P1—C17	114.02 (7)	C12—C13—H13A	119.9
O3—P1—C23	111.29 (8)	C13—C14—C15	120.3 (2)
C17—P1—C23	108.27 (8)	C13—C14—H14A	119.9
O3—P1—C11	110.17 (8)	C15—C14—H14A	119.8
C17—P1—C11	107.56 (8)	C16—C15—C14	120.2 (2)
C23—P1—C11	105.08 (8)	C16—C15—H15A	119.9
C2—O1—V1	127.40 (13)	C14—C15—H15A	119.9
C4—O2—V1	128.54 (13)	C15—C16—C11	119.5 (2)
P1—O3—V1	155.14 (8)	C15—C16—H16A	120.3
C7—O4—V1	128.12 (11)	C11—C16—H16A	120.3
C9—O5—V1	126.73 (11)	C18—C17—C22	118.85 (18)
C2—C1—H1A	109.5	C18—C17—P1	120.72 (15)
C2—C1—H1B	109.5	C22—C17—P1	120.12 (15)
H1A—C1—H1B	109.5	C17—C18—C19	120.4 (2)
C2—C1—H1C	109.5	C17—C18—H18A	119.8
H1A—C1—H1C	109.5	C19—C18—H18A	119.8
H1B—C1—H1C	109.5	C20—C19—C18	120.2 (2)
O1—C2—C3	125.62 (19)	C20—C19—H19A	119.9
O1—C2—C1	115.3 (2)	C18—C19—H19A	119.9
C3—C2—C1	119.1 (2)	C21—C20—C19	120.2 (2)
C2—C3—C4	125.09 (19)	C21—C20—H20A	119.9

C2—C3—H3A	117.5	C19—C20—H20A	119.9
C4—C3—H3A	117.5	C20—C21—C22	119.9 (2)
O2—C4—C3	124.22 (18)	C20—C21—H21A	120.0
O2—C4—C5	116.27 (19)	C22—C21—H21A	120.0
C3—C4—C5	119.5 (2)	C17—C22—C21	120.4 (2)
C4—C5—H5A	109.5	C17—C22—H22A	119.8
C4—C5—H5B	109.5	C21—C22—H22A	119.8
H5A—C5—H5B	109.5	C28—C23—C24	119.53 (16)
C4—C5—H5C	109.5	C28—C23—P1	118.53 (13)
H5A—C5—H5C	109.5	C24—C23—P1	121.68 (14)
H5B—C5—H5C	109.5	C25—C24—C23	119.65 (19)
C7—C6—H6A	109.5	C25—C24—H24A	120.2
C7—C6—H6B	109.5	C23—C24—H24A	120.2
H6A—C6—H6B	109.5	C26—C25—C24	120.9 (2)
C7—C6—H6C	109.5	C26—C25—H25A	119.6
H6A—C6—H6C	109.5	C24—C25—H25A	119.6
H6B—C6—H6C	109.5	C25—C26—C27	120.00 (19)
O4—C7—C8	123.98 (16)	C25—C26—H26A	120.0
O4—C7—C6	116.74 (15)	C27—C26—H26A	120.0
C8—C7—C6	119.28 (16)	C28—C27—C26	119.5 (2)
C7—C8—C9	125.95 (17)	C28—C27—H27A	120.2
C7—C8—H8A	117.0	C26—C27—H27A	120.2
C9—C8—H8A	117.0	C23—C28—C27	120.39 (19)
O5—C9—C8	125.33 (16)	C23—C28—H28A	119.8
O5—C9—C10	115.46 (17)	C27—C28—H28A	119.8

Fig. 1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