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# (Dibenzylacetone-$\kappa O$)(1,3-diphenylpropane-1,3-dionato-$\kappa^2 O,O'$)dioxouranium(VI)

**M. Alagar,[a] S. Kannan,[b] K. Rajagopal,[c] V. Venugopal,[b] R. V. Krishnakumar,[d] M. Subha Nandhini[e] and S. Natarajan[e]***

[a]Department of Physics, Ayya Nadar Janaki Ammal College, Sivakasi 626 123, India, [b]Fuel Chemistry Division, Bhabha Atomic Research Centre, Mumbai 400 085, India, [c]Department of Physics, Saraswathi Narayanan College, Madurai 625 022, India, [d]Department of Physics, Thiagarajar College, Madurai 625 009, India, and [e]Department of Physics, Madurai Kamaraj University, Madurai 625 021, India

Correspondence e-mail:
s_natarajan50@yahoo.com

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**Key indicators**

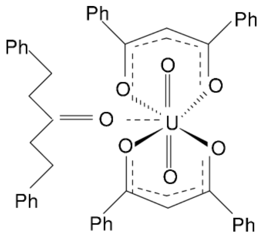
Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.031 Å
$R$ factor = 0.070
$wR$ factor = 0.267
Data-to-parameter ratio = 19.3

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

In the title compound, $[UO_2(C_{15}H_9O_2)_2(C_{17}H_{18}O)]$ or $[UO_2(DBM)_2(DBA)]$, where DBM is dibenzoyl methanate and DBA is dibenzylacetone, the $U^{VI}$ atom is coordinated by seven O atoms in a distorted pentagonal–bipyramidal geometry. The diphenylpropane-1,3-dionate system acts as a chelating ligand and coordinates through both of its ketonate O atoms, while the DBA ligand coordinates through the O atom. The average U—O distances for U—O(uranyl) [1.742 (2) Å], U—O(diketonate) [2.349 (2) Å] and U—O(DBA) [2.406 (2) Å] are within normal ranges. The DBA molecule retains its *trans–trans* geometry in the structure.

## Comment

An enhancement in the solvent extraction separation of the uranium(VI) ion from acid media using mixtures of $\beta$-diketones and neutral ligands has been well established (Ramakrishna & Patil, 1984). The organic phase adduct formation or the stability constants for these synergistic extractions mainly depend on the basicities and sizes of the neutral ligands used for a given $\beta$-diketone (Bhattacharya *et al.*, 2003). However, for a given neutral ligand, it depends mainly on the size of the $\beta$-diketone used (Batzar *et al.*, 1967). It is shown from the extraction (Batzar *et al.*, 1967; Pribilova *et al.*, 1981; Chakravortthy *et al.*, 1999), as well as spectroscopic data (Kannan, Venugopal, Pillai, Droege & Barnes, 1996; Kannan, 2000; Kannan *et al.*, 2001) that a given neutral ligand forms a stronger complex with $[UO_2(TTA)_2$ (HTTA = thenoyltrifluoroacetone) than with $[UO_2(DBM)_2]$ (HDBM = dibenzoyl methane). However, there are no X-ray structural studies to confirm these observations that the given neutral ligand forms a stronger complex (or shortened bond) with $[UO_2(TTA)_2]$ than with $[UO_2(DBM)_2]$.



(I)

In a continuation of our work on uranyl bis($\beta$-diketones) with neutral donor ligands (Rajagopal *et al.*, 2002; Alagar *et al.*, 2003), we report here the structure of the title compound, (I), $[UO_2(DBM)_2DBA]$ [DBA = $(C_6H_5CH{=}CH)_2CO$], to compare the observed U—O(DBA) bond distance with the reported bond distance of U—O(DBA) in $[UO_2(TTA)_2DBA]$

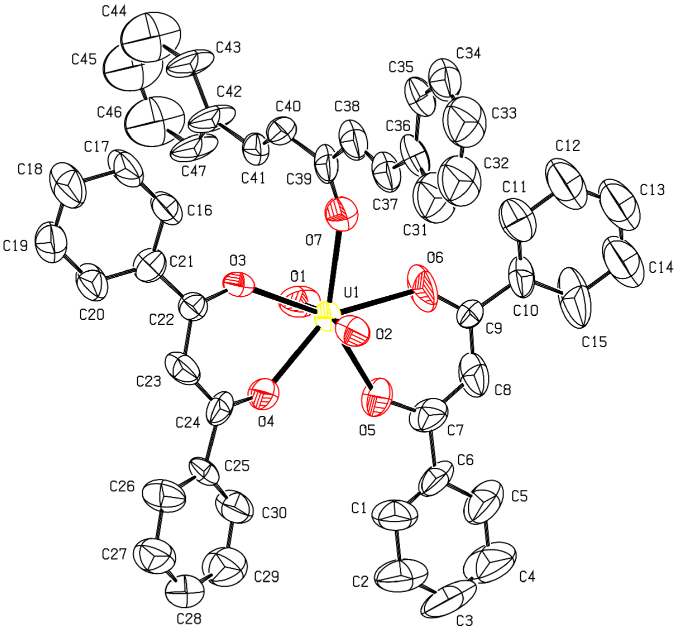


**Figure 1**
The molecular structure of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids.

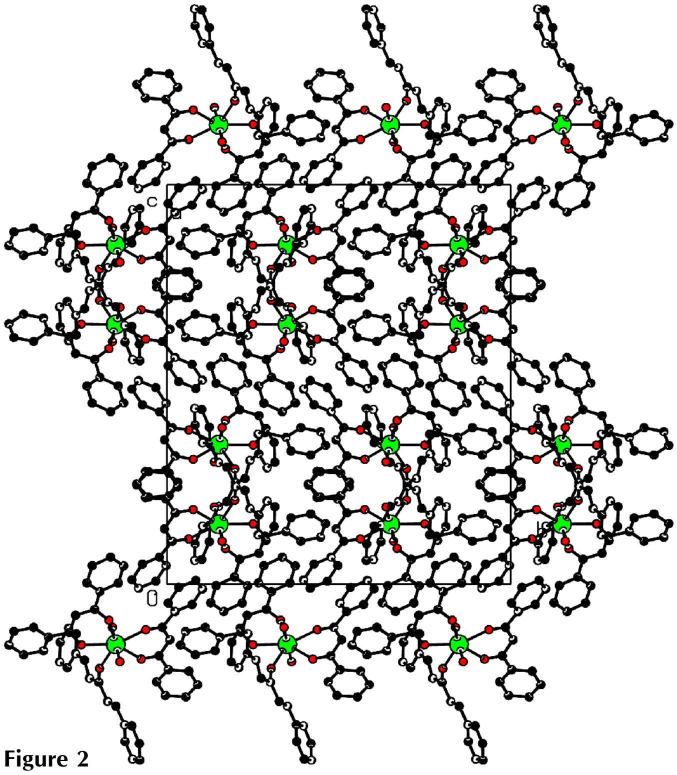


**Figure 2**
The packing of the molecules of (I), viewed down the *a* axis. H atoms have been omitted.

(Kannan, Venugopal, Pillai, Droege, Barnes & Schlempe, 1996).

The molecular structure of (I) with the atom numbering scheme is shown in Fig. 1. Selected bond distances and angles are listed in Table 1. The structure of the molecule shows that the U atom is surrounded by seven O atoms in a pentagonal bipyramidal geometry. Four O atoms of DBM and one O atom of DBA form a planar pentagon and two uranyl O atoms occupy the apices. The average U—O(uranyl) [1.742 (2) Å] (Alcock *et al.*, 1982)) and U—O(DBM) [2.349 (2) Å] (Taylor & Waugh, 1977; Kramer *et al.*, 1980; Kannan & Ferguson, 1997) distances are within normal ranges. The U—O(DBA) distance [2.406 (2) Å] is longer than that of $[UO_2(TTA)_2$-$(C_6H_5CH{=}CH)_2CO]$ [2.376 (6) Å; Kannan, Venugopal, Pillai, Droege & Barnes, 1996]. This shows clearly that the neutral ligand DBA forms a stronger complex (shortened bond) with $[UO_2(TTA)_2]$ than with $[UO_2(DBM)_2]$ (longer bond), which is also confirmed by the spectroscopic and extraction results. The DBA molecule retains its *trans–trans* geometry in the structure. Fig. 2 shows the crystal packing of (I) viewed down the *a* axis. The structure is stabilized by van der Waals interactions.

## Experimental

$[UO_2(DBM)_2DBA]$ was prepared according to the reported method (Kannan, Venugopal, Pillai, Droege, Barnes & Schlemper, 1996). Crystals suitable for the X-ray diffraction analysis were obtained from a chloroform/toluene mixture.

### Crystal data

$[UO_2(C_{15}H_9O_2)_2(C_{17}H_{18}O)]$
$M_r = 950.79$
Orthorhombic, *Pbca*
$a = 13.001$ (3) Å
$b = 23.211$ (3) Å
$c = 27.010$ (8) Å
$V = 8151$ (3) Å$^3$
$Z = 8$
$D_x = 1.550$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 2$–25°
$\mu = 4.03$ mm$^{-1}$
$T = 293$ (2) K
Thick plate, orange
0.30 × 0.24 × 0.15 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega$–$2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{\rm min} = 0.328$, $T_{\rm max} = 0.552$
7198 measured reflections
7148 independent reflections
3223 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\rm max} = 25.0°$
$h = -5 \rightarrow 15$
$k = -10 \rightarrow 27$
$l = -10 \rightarrow 32$
2 standard reflections every 100 reflections intensity decay: <1%

### Refinement

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.267$
$S = 1.03$
7148 reflections
370 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 334.1165P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 3.22$ e Å$^{-3}$
$\Delta\rho_{\rm min} = -2.38$ e Å$^{-3}$

**Table 1**
Selected bond distances (Å).

| | | | |
|---|---|---|---|
| U1—O2 | 1.723 (17) | U1—O3 | 2.358 (14) |
| U1—O1 | 1.760 (15) | U1—O6 | 2.399 (14) |
| U1—O4 | 2.315 (14) | U1—O7 | 2.406 (16) |
| U1—O5 | 2.322 (17) | | |

All the phenyl rings in the title compound (I) were refined as rigid hexagons of side 1.39 Å. In addition, atoms C13 and C14 were assigned the same anisotropic displacement parameters as C12 to obtain convergence during refinement. Similarly, C42 and C43 were assigned the parameters of C47, C37 those of C38, C33 and C32 those of C31, and C45 and C46 those of C44. All the H atoms were posi-

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tioned geometrically and were allowed to ride on their respective carrier atoms with C—H = 0.93 Å and $U_{iso} = 1.2U_{eq}(C)$. The highest peak and the deepest hole are located at (0.020, 0.049, 0.350) and (0.555, 0.123, 0.350), respectively, within the unit cell.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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