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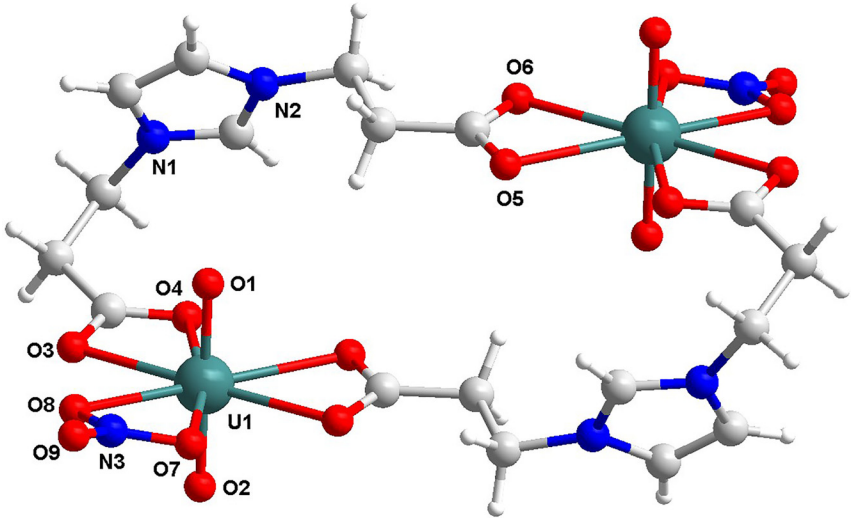
Crystal structure of *cyclo*-(bis(μ$_2$-3,3′-(1*H*-imidazole-3-ium-1,3-diyl)dipropionato-κ^4*O*,*O*′:*O*″,*O*‴)-dinitrato-κ^2*O*,*O*′-tetraoxido-diuranium(VI) $C_{18}H_{22}N_6O_{18}U_2$



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Abstract

$C_{18}H_{22}N_6O_{18}U_2$, monoclinic, *P*2/*c* (no. 13), *a* = 10.894(2) Å, *b* = 7.9674(16) Å, *c* = 16.787(3) Å, *β* = 100.823(2)°, *V* = 1399.1(5) Å^3, *Z* = 2, $R_{gt}(F)$ = 0.0307, w$R_{ref}(F^2)$ = 0.0728, *T* = 296(2) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.26 × 0.15 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	11.7 mm^{-1}
Diffractometer, scan mode:	*φ* and *ω*
θ_{max}, completeness:	27.6°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11,452, 3210, 0.058
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2720
$N(param)_{refined}$:	199
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

1 Source of materials

The zwitterionic ligand 3-(1-(2-carboxyethyl)-1*H*-imidazol-3-ium-3-yl)- propanoate (HL) was synthesized according to the literature [5]. A mixture of 0.504 g uranyl nitrate hexahydrate (1 mmol), 0.212 g (1 mmol) and 2 mL H_2O was added to a 25 mL Teflon-lined stainless steel autoclave at 373 K for 72 h. A large number of yellow needle crystals were obtained, washed with distilled water, and dried in air. Yield: 46% (based on HL).

2 Experimental details

The structure was solved by Direct Methods with the SHELXS-2018 program. All H-atoms from C and N atoms were

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2197 (6)	0.4682 (7)	0.5647 (3)	0.0223 (12)
C2	0.1764 (6)	0.3108 (7)	0.5177 (4)	0.0247 (13)
H2A	0.086651	0.322607	0.488050	0.030*
H2B	0.183559	0.219785	0.557120	0.030*
C3	0.2486 (6)	0.2619 (7)	0.4560 (4)	0.0224 (12)
H3A	0.336458	0.235255	0.485461	0.027*
H3B	0.209918	0.162653	0.425779	0.027*
C4	0.1401 (6)	0.4813 (8)	0.3475 (4)	0.0292 (14)
H4	0.055158	0.451616	0.340595	0.035*
C5	0.1820 (5)	0.6100 (8)	0.3114 (4)	0.0286 (14)
H5	0.131547	0.686150	0.274417	0.034*
C6	0.3486 (5)	0.4804 (7)	0.3909 (3)	0.0204 (12)
H6	0.432420	0.451372	0.418460	0.024*
C7	0.4015 (6)	0.7356 (7)	0.3217 (4)	0.0239 (13)
H7A	0.376975	0.760435	0.262756	0.029*
H7B	0.487400	0.689812	0.336351	0.029*
C8	0.4012 (6)	0.8980 (7)	0.3701 (4)	0.0256 (13)
H8A	0.323121	0.959372	0.344868	0.031*
H8B	0.401939	0.870476	0.426466	0.031*
C9	0.5129 (5)	1.0072 (7)	0.3720 (3)	0.0200 (12)
N1	0.2461 (4)	0.4009 (6)	0.3971 (3)	0.0187 (10)
N2	0.3135 (4)	0.6094 (6)	0.3387 (3)	0.0210 (10)
N3	0.0530 (5)	0.9775 (7)	0.6632 (3)	0.0309 (12)
O1	0.1982 (4)	0.8687 (5)	0.5245 (2)	0.0297 (10)
O2	0.3371 (5)	0.7329 (6)	0.7293 (3)	0.0361 (11)
O3	0.1426 (4)	0.5431 (5)	0.5969 (3)	0.0297 (10)
O4	0.3275 (4)	0.5315 (5)	0.5701 (2)	0.0252 (9)
O5	0.5208 (4)	1.1527 (5)	0.4018 (2)	0.0242 (9)
O6	0.6014 (4)	0.9485 (5)	0.3450 (3)	0.0301 (10)
O7	0.1627 (4)	1.0465 (5)	0.6748 (3)	0.0303 (10)
O8	0.0515 (4)	0.8213 (5)	0.6481 (3)	0.0340 (11)
O9	−0.0420 (5)	1.0548 (6)	0.6644 (3)	0.0451 (13)
U1	0.26867 (2)	0.79818 (3)	0.62644 (2)	0.01911 (8)

positioned with idealized geometry (U_{iso}(H) = 1.2U_{eq}(C)) using a riding model with C—H = 0.930, 0.969, and 0.970 Å.

3 Comment

The uranyl complexes based on zwitterionic ligands with 1,3-disubstituted imidazolium cations, such as 3-(carboxylatomethyl)-1*H*-imidazol-3-ium-1-yl)acetate, have been reported as one- and two-dimensional structures [6, 7]. Besides this, two zero-dimensional uranyl complexes based on 1-methyl-1*H*-imidazol-3-ium-3-yl)acetate have although been reported elsewhere [8, 9]. Herein we report the title uranyl complex based on 3-(1-(2-carboxyethyl)-1H-imidazol-3-ium-3-yl)-propanoate with longer aliphatic chain substituents.

The title uranyl complex crystallizes in the monoclinic space group *P*2/*c* (no. 13), consisting of two uranyl cations, two completely deprotonated zwitterionic ligands, and two nitrate anions, resulting in a cyclic struture (see the figure). Both crystallographically dependent uranylatoms are surrouded by two oxygen atoms from two zwitterionic ligands, two oxygen atoms from one nitrate and two oxygen atoms from themselves, generating an 8-coordinated polyhedron. All of the bond lengths are comparable with the reported similar results [6–9].

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