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# Poly[[diaquabis($\mu_4$-benzene-1,3-dicarboxylato)($\mu_3$-benzene-1,3-dicarboxylato)dierbium(III)] monohydrate]

**Wen-Dong Song,[a] De-Yun Ma[b] and Chao-Hua Zhang[c]***

[a]College of Science, Guang Dong Ocean University, Zhan Jiang 524088, People's Republic of China, [b]College of Chemistry, South China University of Technology, GuangZhou 510640, People's Republic of China, and [c]School of Food Science and Technology, Guang Dong Ocean Unversity, Zhan Jiang 524088, People's Republic of China
Correspondence e-mail: songwd60@126.com

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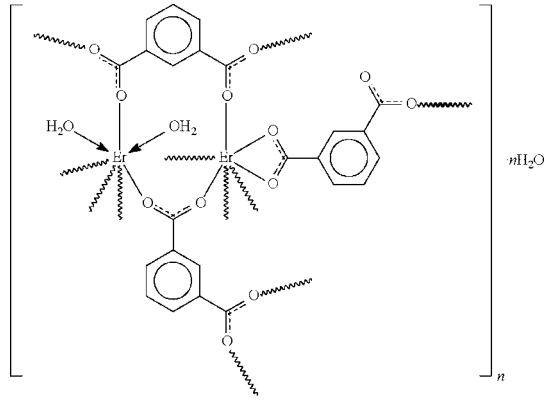
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; disorder in main residue; $R$ factor = 0.019; $wR$ factor = 0.045; data-to-parameter ratio = 14.3.

The title erbium coordination polymer, $\{[Er_2(C_8H_4O_4)_3(H_2O)_2]\cdot H_2O\}_n$, was obtained by the hydrothermal reaction of $ErCl_3$ with benzene-1,3-dicarboxylic acid (1,3-BDC) in alkaline aqueous solution. Each of the two crystallographically independent $Er^{III}$ ions is seven-coordinate and has a distorted pentagonal–bipyramidal geometry. One Er centre is coordinated by seven O atoms from six 1,3-BDC ligands and the other Er centre is surrounded by five O atoms from five 1,3-BDC ligands and two water molecules. The bridging ligands, which have two different coordination modes, link the metal centres to form a three-dimensional network with channels parallel to the $b$ axis in which solvent water molecules are located. The crystal structure is stabilized by intra- and intermolecular O—H···O hydrogen-bonding interactions. One benzene ring and the solvent water molecule are independently disordered over two positions each, with occupancy ratios of 0.595 (2):0.405 (2) and 0.661 (1):0.339 (1), respectively.

## Related literature

For related literature, see: Bourne *et al.* (2001); Zhang *et al.* (2003). *PLATON* (Spek, 2003) was used for the analysis of voids in the structure.




## Experimental

### Crystal data

$[Er_2(C_8H_4O_4)_3(H_2O)_2]\cdot H_2O$
$M_r$ = 880.90
Monoclinic, $P2_1/c$
$a$ = 10.5553 (2) Å
$b$ = 14.9526 (3) Å
$c$ = 17.4798 (3) Å
$\beta$ = 103.908 (1)°
$V$ = 2677.94 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 6.30 mm$^{-1}$
$T$ = 293 (2) K
0.25 × 0.19 × 0.16 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.248, $T_{max}$ = 0.369
33045 measured reflections
6127 independent reflections
5579 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.045
$S$ = 1.06
6127 reflections
429 parameters
68 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.74 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.75 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1*WB*—H2*WB*···O12$^{i}$ | 0.817 (10) | 2.54 (5) | 3.019 (7) | 118 (5) |
| O1*WB*—H1*WB*···O10$^{ii}$ | 0.813 (10) | 2.071 (19) | 2.709 (6) | 135 (3) |
| O3*W*—H6*W*···O1*WB* | 0.822 (10) | 2.00 (3) | 2.742 (7) | 150 (5) |
| O2*W*—H3*W*···O1*WB* | 0.817 (10) | 2.13 (3) | 2.837 (8) | 144 (4) |
| O2*W*—H4*W*···O3$^{iii}$ | 0.819 (10) | 2.002 (11) | 2.820 (3) | 176 (5) |
| O1*WA*—H2*WA*···O12$^{i}$ | 0.822 (10) | 2.54 (5) | 3.087 (14) | 125 (5) |
| O1*WA*—H1*WA*···O10$^{ii}$ | 0.825 (10) | 2.071 (19) | 2.862 (14) | 160 (4) |
| O3*W*—H6*W*···O1*WA* | 0.822 (10) | 1.93 (3) | 2.702 (14) | 157 (5) |
| O2*W*—H3*W*···O1*WA* | 0.817 (10) | 2.80 (4) | 3.429 (16) | 135 (4) |
| O3*W*—H5*W*···O1 | 0.819 (10) | 1.881 (14) | 2.692 (3) | 170 (5) |

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x+1, y, z$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); 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: ZL2067).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2826-m2827 [ **doi:10.1107/S1600536807051975** ]

# Poly[[diaquabis($\mu_4$-benzene-1,3-dicarboxylato)($\mu_3$-benzene-1,3-dicarboxylato)dierbium(III)] monohydrate]

**W.-D. Song, D.-Y. Ma and C.-H. Zhang**

## Comment

As a building block, benzene-1,3-dicarboxylic acid (1,3-BDC) is an excellent candidate for the construction of supramolecular complexes (Bourne *et al.*, 2001; Zhang *et al.*, 2003). Recently, we obtained the title coordination polymer by the reaction of $ErCl_3$ with benzene-1,3-dicarboxylic acid in alkaline aqueous solution, and its crystal structure is reported here.

Each of the two crystallographically independent $Er^{III}$ centres is seven-coordinate and has a distorted pentagonal bipyramidal geometry: one Er centre is coordinated by seven oxygen atoms from six 1,3-BDC ligands, and the other Er centre is surrounded by five oxygen atoms from five 1,3-BDC ligands and two water molecules (Fig. 1). The adjacent Er···Er separations are 4.448 (4) and 4.965 (5) Å, respectively. The dianionic ligands cross-link the metal ions to form a three-dimensional network with channels running along the *c* axis hosting an uncoordinated disordered water molecule (Fig. 2). The title compound exhibits two types of large voids that seem to be partially filled by diffuse solvent (no corrections for this were applied to the dataset). The larger of the voids has a volume of of 142.3 $Å^3$ (5.3% of the unit cell volume) and is located in close proximity to a disordered phenyl ring of one of the 1,3-BDC ligands. The large void thus gives the phenyl ring additional degrees of freedom which can be seen as a likely cause of the disorder of the phenyl ring. The second type of void in the structure (75.6 $Å^3$, 2.8% of the unit cell volume) is located close to the disordered water solvate molecule (see refinement section for details). These water molecules are hydrogen bonded to coordinated water molecules and carboxylate units that all form a hydrogen bonded chain parallel to the *b* axis (Table 1).

## Experimental

A mixture of $ErCl_3$ (0.5 mmol, 0.186 g), benzenedicarboxylic acid (0.75 mmol, 0.125 g), NaOH (1.5 mmol; 0.06 g) and $H_2O$ (10 ml) was placed in a 20 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K $h^{-1}$. The crystals obtained were washed with water and dryed in air.

## Refinement

Two types of large apparently unfilled voids are found in the unit cell of the title compound. Their volumes were calculated using *PLATON* (Spek, 2003) as 142.3 and 75.6 $Å^3$ (5.3% and 2.8% of the unit cell volume), respectively. The larger void is located close to one of phenyl rings of the 1,3-BDC ligands, giving it enough room to rotate around the C—C bond connecting the ring which may result in the disorder; the smaller unfilled void is located close to a disordered water solvate molecule. Based on these observations, one of the phenyl rings and the lattice water molecule were split into two positions. The occupancy ratios refined to 0.595 (2) to 0.405 (2) and 0.661 (1) to 0.339 (1), respectively. Due to the significant overlap of the disordered atoms the following restraints were applied: The phenyl ring C11 C12 C13 C14 C15 C16 and its disordered counterpart were each restrained to be flat and its equivalent bond distances were restrained to be the same within a standard

deviation of 0.01 Å. All water H atoms were tentatively located in difference density Fourier maps and were refined with O—H distance restraints of 0.82 (1) Å and with $U_{iso}$(H) = 1.5$U_{eq}$(O). The hydrogen atoms of the disordered water molecule were set to have each the same coordinates for both disordered $H_2O$ molecules. Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C).

**Figures**

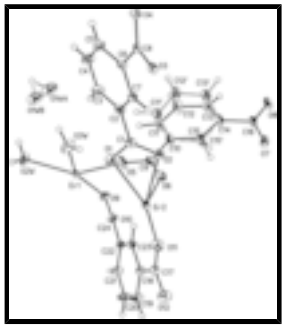

Fig. 1. The molecular structure showing the atomic-numbering scheme and displacement ellipsoids drawn at the 30% probability level.

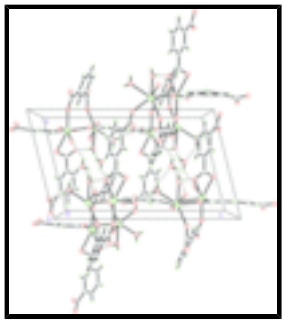

Fig. 2. The molecular packing showing the intra/intermolecular hydrogen bonding interactions as broken lines. The minor moiety of the disordered phenyl rings and water molecules were omitted for clarity.

**Poly[[diaquabis(μ4-benzene-1,3-dicarboxylato)(μ3-benzene-1,3- dicarboxylato)dierbium(III)] monohydrate]**

*Crystal data*

| | |
|---|---|
| $[Er_2(C_8H_4O_4)_3(H_2O)_2]\cdot H_2O$ | $F_{000}$ = 1672 |
| $M_r$ = 880.90 | $D_x$ = 2.185 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 6000 reflections |
| $a$ = 10.5553 (2) Å | θ = 1.7–28.0º |
| $b$ = 14.9526 (3) Å | μ = 6.30 mm$^{-1}$ |
| $c$ = 17.4798 (3) Å | $T$ = 293 (2) K |
| β = 103.9080 (10)º | Block, red |
| $V$ = 2677.94 (9) Å$^3$ | 0.25 × 0.19 × 0.16 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII area-detector diffractometer | 6127 independent reflections |

| | |
|---|---|
| Radiation source: fine-focus sealed tube | 5579 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.028$ |
| $T = 293(2)$ K | $\theta_{max} = 27.5^{o}$ |
| φ and ω scans | $\theta_{min} = 1.8^{o}$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -13\rightarrow13$ |
| $T_{min} = 0.248$, $T_{max} = 0.369$ | $k = -18\rightarrow19$ |
| 33045 measured reflections | $l = -22\rightarrow22$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.019$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.045$ | $w = 1/[\sigma^2(F_o^2) + (0.0206P)^2 + 2.4501P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.06$ | $(\Delta/\sigma)_{max} = 0.002$ |
| 6127 reflections | $\Delta\rho_{max} = 0.74$ e Å$^{-3}$ |
| 429 parameters | $\Delta\rho_{min} = -0.75$ e Å$^{-3}$ |
| 68 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.4248 (3) | 0.86190 (19) | 0.39035 (18) | 0.0260 (6) | |
| C2 | 0.5658 (3) | 0.8382 (2) | 0.41007 (18) | 0.0265 (6) | |
| C3 | 0.6091 (3) | 0.7605 (2) | 0.3798 (2) | 0.0345 (7) | |
| H3 | 0.5493 | 0.7234 | 0.3468 | 0.041* | |
| C4 | 0.7393 (3) | 0.7386 (2) | 0.3985 (2) | 0.0414 (9) | |
| H4 | 0.7672 | 0.6862 | 0.3790 | 0.050* | |
| C5 | 0.8288 (3) | 0.7944 (2) | 0.44620 (19) | 0.0329 (7) | |
| H5 | 0.9170 | 0.7798 | 0.4581 | 0.039* | |

| | | | | | |
|---|---|---|---|---|---|
| C6 | 0.7880 (3) | 0.87251 (19) | 0.47671 (17) | 0.0231 (6) | |
| C7 | 0.6560 (3) | 0.8938 (2) | 0.45889 (17) | 0.0232 (6) | |
| H7 | 0.6279 | 0.9454 | 0.4796 | 0.028* | |
| C8 | 0.8849 (3) | 0.9284 (2) | 0.53231 (16) | 0.0228 (6) | |
| C9 | 0.1432 (3) | 0.7014 (2) | 0.37867 (17) | 0.0261 (6) | |
| C10 | 0.1544 (4) | 0.6373 (2) | 0.44503 (19) | 0.0356 (8) | |
| C11 | 0.1555 (11) | 0.5435 (4) | 0.4307 (4) | 0.043 (2) | 0.595 (17) |
| H11 | 0.1552 | 0.5225 | 0.3806 | 0.051* | 0.595 (17) |
| C12 | 0.1570 (14) | 0.4837 (4) | 0.4916 (4) | 0.053 (3) | 0.595 (17) |
| H12 | 0.1670 | 0.4228 | 0.4837 | 0.064* | 0.595 (17) |
| C13 | 0.1438 (13) | 0.5141 (4) | 0.5636 (4) | 0.043 (2) | 0.595 (17) |
| H13 | 0.1346 | 0.4734 | 0.6022 | 0.052* | 0.595 (17) |
| C14 | 0.1441 (4) | 0.6070 (2) | 0.57907 (19) | 0.0406 (9) | |
| C15 | 0.1481 (17) | 0.6677 (5) | 0.5196 (4) | 0.020 (3) | 0.595 (17) |
| H15 | 0.1466 | 0.7288 | 0.5294 | 0.024* | 0.595 (17) |
| C12' | 0.241 (2) | 0.4969 (8) | 0.5074 (6) | 0.057 (4) | 0.405 (17) |
| H12' | 0.2761 | 0.4402 | 0.5047 | 0.069* | 0.405 (17) |
| C13' | 0.2122 (17) | 0.5254 (7) | 0.5762 (6) | 0.045 (3) | 0.405 (17) |
| H13' | 0.2377 | 0.4908 | 0.6215 | 0.054* | 0.405 (17) |
| C11' | 0.2174 (15) | 0.5528 (6) | 0.4422 (7) | 0.046 (3) | 0.405 (17) |
| H11' | 0.2424 | 0.5356 | 0.3969 | 0.055* | 0.405 (17) |
| C15' | 0.124 (2) | 0.6645 (8) | 0.5149 (6) | 0.023 (5) | 0.405 (17) |
| H15' | 0.0898 | 0.7213 | 0.5185 | 0.028* | 0.405 (17) |
| C16 | 0.1198 (3) | 0.6381 (2) | 0.65529 (17) | 0.0277 (6) | |
| C17 | −0.1653 (3) | 0.9341 (2) | 0.26831 (18) | 0.0266 (6) | |
| C18 | −0.2393 (3) | 0.86014 (19) | 0.22034 (18) | 0.0255 (6) | |
| C19 | −0.3618 (3) | 0.8754 (2) | 0.1715 (2) | 0.0376 (8) | |
| H19 | −0.3973 | 0.9327 | 0.1679 | 0.045* | |
| C20 | −0.4318 (3) | 0.8064 (2) | 0.1280 (2) | 0.0441 (9) | |
| H20 | −0.5135 | 0.8175 | 0.0949 | 0.053* | |
| C21 | −0.3796 (3) | 0.7207 (2) | 0.1339 (2) | 0.0343 (7) | |
| H21 | −0.4271 | 0.6739 | 0.1057 | 0.041* | |
| C22 | −0.2561 (3) | 0.70480 (19) | 0.18197 (18) | 0.0252 (6) | |
| C23 | −0.1856 (3) | 0.77463 (19) | 0.22438 (17) | 0.0238 (6) | |
| H23 | −0.1023 | 0.7643 | 0.2556 | 0.029* | |
| C24 | −0.2007 (3) | 0.6126 (2) | 0.18770 (17) | 0.0249 (6) | |
| Er1 | 0.123252 (11) | 0.638620 (8) | 0.184714 (7) | 0.01869 (4) | |
| Er2 | 0.165788 (12) | 0.917258 (8) | 0.343349 (7) | 0.01900 (4) | |
| O1 | 0.3531 (2) | 0.83950 (16) | 0.32336 (13) | 0.0330 (5) | |
| O2 | 0.3765 (2) | 0.90475 (15) | 0.43797 (13) | 0.0344 (5) | |
| O3 | 0.85407 (19) | 1.00772 (14) | 0.54583 (11) | 0.0250 (4) | |
| O4 | 0.9920 (2) | 0.89345 (16) | 0.56502 (12) | 0.0325 (5) | |
| O5 | 0.1421 (3) | 0.67059 (18) | 0.31182 (13) | 0.0471 (7) | |
| O6 | 0.1334 (2) | 0.78295 (14) | 0.39261 (13) | 0.0342 (5) | |
| O7 | 0.0848 (2) | 0.71862 (14) | 0.65904 (13) | 0.0323 (5) | |
| O8 | 0.1330 (3) | 0.58356 (15) | 0.71069 (13) | 0.0393 (6) | |
| O9 | −0.0799 (2) | 0.60084 (16) | 0.20490 (14) | 0.0366 (5) | |
| O10 | −0.2784 (2) | 0.54756 (14) | 0.17309 (14) | 0.0338 (5) | |
| O11 | −0.0531 (2) | 0.91931 (17) | 0.30952 (15) | 0.0400 (6) | |

| | | | | | |
|---|---|---|---|---|---|
| O12 | −0.2207 (2) | 1.00858 (15) | 0.26555 (15) | 0.0430 (6) | |
| O2W | 0.2469 (2) | 0.60998 (19) | 0.09076 (15) | 0.0402 (6) | |
| H3W | 0.3236 (16) | 0.595 (3) | 0.103 (3) | 0.060* | |
| H4W | 0.221 (4) | 0.580 (3) | 0.0511 (16) | 0.060* | |
| O3W | 0.3326 (2) | 0.6988 (2) | 0.22505 (18) | 0.0520 (8) | |
| H5W | 0.347 (5) | 0.743 (2) | 0.254 (2) | 0.078* | |
| H6W | 0.398 (3) | 0.668 (3) | 0.227 (3) | 0.078* | |
| O1WA | 0.5067 (13) | 0.5632 (10) | 0.2455 (10) | 0.0634 (18) | 0.339 (12) |
| H1WA | 0.5571 (14) | 0.549 (4) | 0.2180 (16) | 0.095* | 0.339 (12) |
| H2WA | 0.459 (5) | 0.520 (2) | 0.2300 (15) | 0.095* | 0.339 (12) |
| O1WB | 0.4793 (6) | 0.5556 (5) | 0.1995 (5) | 0.0634 (18) | 0.661 (12) |
| H1WB | 0.5571 (14) | 0.549 (4) | 0.2180 (16) | 0.095* | 0.661 (12) |
| H2WB | 0.459 (5) | 0.520 (2) | 0.2300 (15) | 0.095* | 0.661 (12) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0277 (16) | 0.0197 (14) | 0.0283 (16) | −0.0009 (12) | 0.0022 (13) | −0.0013 (12) |
| C2 | 0.0262 (15) | 0.0262 (15) | 0.0246 (15) | 0.0017 (12) | 0.0013 (12) | −0.0026 (12) |
| C3 | 0.0336 (17) | 0.0279 (17) | 0.0358 (18) | 0.0034 (13) | −0.0039 (14) | −0.0105 (14) |
| C4 | 0.041 (2) | 0.0354 (19) | 0.044 (2) | 0.0154 (15) | 0.0030 (16) | −0.0146 (16) |
| C5 | 0.0262 (16) | 0.0369 (18) | 0.0332 (17) | 0.0119 (14) | 0.0026 (13) | −0.0051 (14) |
| C6 | 0.0215 (14) | 0.0260 (15) | 0.0207 (14) | 0.0034 (11) | 0.0030 (11) | 0.0033 (11) |
| C7 | 0.0250 (15) | 0.0216 (14) | 0.0224 (14) | 0.0028 (11) | 0.0045 (12) | −0.0020 (11) |
| C8 | 0.0228 (14) | 0.0307 (16) | 0.0159 (13) | 0.0029 (12) | 0.0067 (11) | 0.0021 (11) |
| C9 | 0.0286 (15) | 0.0296 (16) | 0.0198 (14) | 0.0007 (12) | 0.0053 (12) | 0.0041 (12) |
| C10 | 0.065 (2) | 0.0231 (16) | 0.0209 (15) | 0.0101 (15) | 0.0143 (15) | 0.0026 (12) |
| C11 | 0.083 (6) | 0.026 (3) | 0.023 (3) | 0.003 (3) | 0.020 (4) | −0.002 (2) |
| C12 | 0.106 (7) | 0.019 (3) | 0.038 (4) | 0.007 (4) | 0.025 (4) | −0.002 (3) |
| C13 | 0.080 (6) | 0.022 (3) | 0.032 (4) | 0.005 (3) | 0.022 (4) | 0.005 (2) |
| C14 | 0.081 (3) | 0.0238 (16) | 0.0207 (16) | 0.0138 (17) | 0.0187 (17) | 0.0028 (13) |
| C15 | 0.022 (5) | 0.014 (4) | 0.022 (4) | 0.004 (3) | 0.002 (3) | −0.001 (3) |
| C12' | 0.097 (9) | 0.041 (6) | 0.040 (5) | 0.024 (6) | 0.029 (6) | 0.002 (4) |
| C13' | 0.073 (8) | 0.034 (5) | 0.030 (5) | 0.015 (5) | 0.018 (5) | 0.014 (4) |
| C11' | 0.075 (8) | 0.037 (5) | 0.030 (5) | 0.017 (5) | 0.021 (5) | 0.002 (4) |
| C15' | 0.026 (9) | 0.024 (6) | 0.019 (6) | 0.001 (4) | 0.003 (4) | −0.002 (4) |
| C16 | 0.0399 (18) | 0.0247 (15) | 0.0180 (14) | −0.0029 (13) | 0.0059 (13) | −0.0032 (12) |
| C17 | 0.0295 (16) | 0.0238 (15) | 0.0258 (15) | −0.0083 (12) | 0.0053 (13) | −0.0003 (12) |
| C18 | 0.0254 (15) | 0.0211 (14) | 0.0289 (16) | −0.0035 (11) | 0.0045 (12) | −0.0014 (12) |
| C19 | 0.0329 (18) | 0.0197 (16) | 0.053 (2) | 0.0064 (13) | −0.0043 (16) | −0.0024 (14) |
| C20 | 0.0330 (19) | 0.0287 (18) | 0.057 (2) | 0.0042 (14) | −0.0153 (16) | −0.0053 (17) |
| C21 | 0.0303 (17) | 0.0240 (16) | 0.0433 (19) | −0.0023 (13) | −0.0014 (14) | −0.0088 (14) |
| C22 | 0.0270 (15) | 0.0203 (14) | 0.0304 (16) | 0.0014 (12) | 0.0112 (12) | 0.0012 (12) |
| C23 | 0.0198 (14) | 0.0232 (15) | 0.0288 (15) | 0.0001 (11) | 0.0065 (12) | 0.0023 (12) |
| C24 | 0.0321 (17) | 0.0214 (14) | 0.0248 (15) | 0.0051 (12) | 0.0138 (13) | 0.0019 (12) |
| Er1 | 0.01977 (7) | 0.01790 (7) | 0.01744 (7) | −0.00041 (4) | 0.00257 (5) | 0.00048 (5) |
| Er2 | 0.02283 (7) | 0.01816 (7) | 0.01542 (7) | −0.00301 (5) | 0.00344 (5) | −0.00120 (5) |
| O1 | 0.0238 (11) | 0.0396 (13) | 0.0324 (12) | −0.0005 (9) | 0.0003 (9) | −0.0148 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O2 | 0.0303 (12) | 0.0374 (13) | 0.0319 (12) | 0.0081 (10) | 0.0007 (10) | −0.0122 (10) |
| O3 | 0.0265 (11) | 0.0291 (11) | 0.0182 (10) | −0.0003 (9) | 0.0029 (8) | −0.0022 (8) |
| O4 | 0.0247 (11) | 0.0443 (13) | 0.0248 (11) | 0.0077 (10) | −0.0016 (9) | 0.0003 (10) |
| O5 | 0.079 (2) | 0.0455 (15) | 0.0171 (11) | −0.0018 (14) | 0.0119 (12) | 0.0012 (10) |
| O6 | 0.0466 (14) | 0.0240 (12) | 0.0356 (12) | 0.0014 (10) | 0.0168 (11) | 0.0102 (9) |
| O7 | 0.0494 (14) | 0.0213 (11) | 0.0296 (12) | −0.0020 (10) | 0.0162 (10) | −0.0068 (9) |
| O8 | 0.0684 (17) | 0.0319 (13) | 0.0176 (11) | −0.0004 (11) | 0.0105 (11) | 0.0037 (9) |
| O9 | 0.0314 (13) | 0.0375 (13) | 0.0462 (14) | 0.0111 (10) | 0.0199 (11) | 0.0119 (11) |
| O10 | 0.0384 (13) | 0.0187 (11) | 0.0455 (14) | 0.0026 (9) | 0.0125 (11) | −0.0041 (10) |
| O11 | 0.0293 (13) | 0.0465 (15) | 0.0396 (14) | −0.0114 (11) | −0.0010 (11) | −0.0036 (11) |
| O12 | 0.0498 (15) | 0.0200 (12) | 0.0528 (16) | −0.0052 (10) | −0.0001 (12) | −0.0092 (11) |
| O2W | 0.0273 (12) | 0.0592 (17) | 0.0346 (14) | −0.0048 (12) | 0.0086 (11) | −0.0237 (12) |
| O3W | 0.0266 (13) | 0.0621 (19) | 0.0632 (18) | −0.0064 (12) | 0.0028 (12) | −0.0415 (15) |
| O1WA | 0.036 (3) | 0.066 (3) | 0.092 (5) | 0.005 (2) | 0.024 (4) | 0.008 (4) |
| O1WB | 0.036 (3) | 0.066 (3) | 0.092 (5) | 0.005 (2) | 0.024 (4) | 0.008 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—O2 | 1.251 (4) | C18—C19 | 1.386 (4) |
| C1—O1 | 1.277 (4) | C18—C23 | 1.393 (4) |
| C1—C2 | 1.488 (4) | C19—C20 | 1.386 (5) |
| C1—Er2 | 2.784 (3) | C19—H19 | 0.9300 |
| C2—C7 | 1.391 (4) | C20—C21 | 1.390 (5) |
| C2—C3 | 1.398 (4) | C20—H20 | 0.9300 |
| C3—C4 | 1.374 (5) | C21—C22 | 1.391 (4) |
| C3—H3 | 0.9300 | C21—H21 | 0.9300 |
| C4—C5 | 1.380 (5) | C22—C23 | 1.388 (4) |
| C4—H4 | 0.9300 | C22—C24 | 1.491 (4) |
| C5—C6 | 1.395 (4) | C23—H23 | 0.9300 |
| C5—H5 | 0.9300 | C24—O9 | 1.250 (4) |
| C6—C7 | 1.390 (4) | C24—O10 | 1.258 (4) |
| C6—C8 | 1.487 (4) | Er1—O7$^{i}$ | 2.199 (2) |
| C7—H7 | 0.9300 | Er1—O5 | 2.234 (2) |
| C8—O4 | 1.252 (3) | Er1—O4$^{ii}$ | 2.266 (2) |
| C8—O3 | 1.268 (3) | Er1—O12$^{iii}$ | 2.273 (2) |
| C9—O6 | 1.253 (4) | Er1—O9 | 2.325 (2) |
| C9—O5 | 1.253 (4) | Er1—O3W | 2.333 (2) |
| C9—C10 | 1.487 (4) | Er1—O2W | 2.370 (2) |
| C10—C15 | 1.397 (6) | Er2—O11 | 2.243 (2) |
| C10—C15' | 1.397 (8) | Er2—O6 | 2.243 (2) |
| C10—C11 | 1.424 (6) | Er2—O8$^{i}$ | 2.261 (2) |
| C10—C11' | 1.434 (8) | Er2—O3$^{iv}$ | 2.2913 (19) |
| C11—C12 | 1.388 (7) | Er2—O10$^{v}$ | 2.336 (2) |
| C11—H11 | 0.9300 | Er2—O1 | 2.390 (2) |
| C12—C13 | 1.376 (7) | Er2—O2 | 2.439 (2) |
| C12—H12 | 0.9300 | O3—Er2$^{iv}$ | 2.2913 (19) |
| C13—C14 | 1.415 (6) | O4—Er1$^{vi}$ | 2.266 (2) |

| | | | |
|---|---|---|---|
| C13—H13 | 0.9300 | O7—Er1$^{vii}$ | 2.199 (2) |
| C14—C15' | 1.389 (8) | O8—Er2$^{vii}$ | 2.261 (2) |
| C14—C15 | 1.389 (6) | O10—Er2$^{iii}$ | 2.336 (2) |
| C14—C13' | 1.422 (8) | O12—Er1$^{v}$ | 2.273 (2) |
| C14—C16 | 1.491 (4) | O2W—H3W | 0.817 (10) |
| C15—H15 | 0.9300 | O2W—H4W | 0.819 (10) |
| C12'—C13' | 1.376 (9) | O3W—H5W | 0.819 (10) |
| C12'—C11' | 1.388 (9) | O3W—H6W | 0.822 (10) |
| C12'—H12' | 0.9300 | O1WA—H1WA | 0.825 (10) |
| C13'—H13' | 0.9300 | O1WA—H2WA | 0.822 (10) |
| C11'—H11' | 0.9300 | O1WA—H1WB | 0.825 (10) |
| C15'—H15' | 0.9300 | O1WA—H2WB | 0.822 (10) |
| C16—O8 | 1.248 (4) | O1WB—H1WA | 0.813 (10) |
| C16—O7 | 1.265 (4) | O1WB—H2WA | 0.817 (10) |
| C17—O11 | 1.249 (4) | O1WB—H1WB | 0.813 (10) |
| C17—O12 | 1.254 (4) | O1WB—H2WB | 0.817 (10) |
| C17—C18 | 1.490 (4) | | |
| O2—C1—O1 | 119.9 (3) | C23—C22—C21 | 119.9 (3) |
| O2—C1—C2 | 120.8 (3) | C23—C22—C24 | 120.6 (3) |
| O1—C1—C2 | 119.3 (3) | C21—C22—C24 | 119.6 (3) |
| O2—C1—Er2 | 61.10 (16) | C22—C23—C18 | 120.3 (3) |
| O1—C1—Er2 | 58.93 (15) | C22—C23—H23 | 119.9 |
| C2—C1—Er2 | 174.7 (2) | C18—C23—H23 | 119.9 |
| C7—C2—C3 | 119.4 (3) | O9—C24—O10 | 121.1 (3) |
| C7—C2—C1 | 119.9 (3) | O9—C24—C22 | 120.4 (3) |
| C3—C2—C1 | 120.7 (3) | O10—C24—C22 | 118.4 (3) |
| C4—C3—C2 | 120.5 (3) | O7$^{i}$—Er1—O5 | 87.89 (9) |
| C4—C3—H3 | 119.7 | O7$^{i}$—Er1—O4$^{ii}$ | 88.57 (9) |
| C2—C3—H3 | 119.7 | O5—Er1—O4$^{ii}$ | 148.43 (9) |
| C3—C4—C5 | 120.0 (3) | O7$^{i}$—Er1—O12$^{iii}$ | 162.37 (9) |
| C3—C4—H4 | 120.0 | O5—Er1—O12$^{iii}$ | 83.04 (10) |
| C5—C4—H4 | 120.0 | O4$^{ii}$—Er1—O12$^{iii}$ | 107.00 (9) |
| C4—C5—C6 | 120.5 (3) | O7$^{i}$—Er1—O9 | 97.76 (8) |
| C4—C5—H5 | 119.7 | O5—Er1—O9 | 76.46 (10) |
| C6—C5—H5 | 119.7 | O4$^{ii}$—Er1—O9 | 72.98 (8) |
| C7—C6—C5 | 119.5 (3) | O12$^{iii}$—Er1—O9 | 94.78 (9) |
| C7—C6—C8 | 120.9 (3) | O7$^{i}$—Er1—O3W | 78.59 (10) |
| C5—C6—C8 | 119.5 (3) | O5—Er1—O3W | 76.44 (10) |
| C6—C7—C2 | 120.1 (3) | O4$^{ii}$—Er1—O3W | 133.26 (9) |
| C6—C7—H7 | 120.0 | O12$^{iii}$—Er1—O3W | 84.59 (10) |
| C2—C7—H7 | 120.0 | O9—Er1—O3W | 152.77 (9) |
| O4—C8—O3 | 123.4 (3) | O7$^{i}$—Er1—O2W | 98.02 (9) |
| O4—C8—C6 | 117.9 (3) | O5—Er1—O2W | 142.72 (10) |
| O3—C8—C6 | 118.7 (3) | O4$^{ii}$—Er1—O2W | 68.79 (8) |
| O6—C9—O5 | 123.8 (3) | O12$^{iii}$—Er1—O2W | 80.58 (10) |

| | | | |
|---|---|---|---|
| O6—C9—C10 | 118.1 (3) | O9—Er1—O2W | 138.00 (9) |
| O5—C9—C10 | 118.1 (3) | O3W—Er1—O2W | 68.87 (9) |
| C15—C10—C11 | 119.2 (5) | O11—Er2—O6 | 82.59 (9) |
| C15'—C10—C11 | 117.0 (6) | O11—Er2—O8$^{i}$ | 80.53 (9) |
| C15—C10—C11' | 116.4 (6) | O6—Er2—O8$^{i}$ | 112.88 (8) |
| C15'—C10—C11' | 119.5 (7) | O11—Er2—O3$^{iv}$ | 85.32 (8) |
| C15—C10—C9 | 120.3 (4) | O6—Er2—O3$^{iv}$ | 93.46 (8) |
| C15'—C10—C9 | 120.2 (4) | O8$^{i}$—Er2—O3$^{iv}$ | 147.91 (8) |
| C11—C10—C9 | 120.0 (4) | O11—Er2—O10$^{v}$ | 118.58 (8) |
| C11'—C10—C9 | 119.4 (5) | O6—Er2—O10$^{v}$ | 157.37 (9) |
| C12—C11—C10 | 120.0 (6) | O8$^{i}$—Er2—O10$^{v}$ | 80.53 (8) |
| C12—C11—H11 | 120.0 | O3$^{iv}$—Er2—O10$^{v}$ | 81.27 (8) |
| C10—C11—H11 | 120.0 | O11—Er2—O1 | 143.48 (8) |
| C13—C12—C11 | 120.2 (6) | O6—Er2—O1 | 80.12 (8) |
| C13—C12—H12 | 119.9 | O8$^{i}$—Er2—O1 | 77.04 (9) |
| C11—C12—H12 | 119.9 | O3$^{iv}$—Er2—O1 | 127.49 (7) |
| C12—C13—C14 | 120.2 (6) | O10$^{v}$—Er2—O1 | 85.68 (8) |
| C12—C13—H13 | 119.9 | O11—Er2—O2 | 153.31 (9) |
| C14—C13—H13 | 119.9 | O6—Er2—O2 | 82.50 (8) |
| C15'—C14—C13 | 117.5 (6) | O8$^{i}$—Er2—O2 | 125.81 (9) |
| C15—C14—C13 | 119.9 (5) | O3$^{iv}$—Er2—O2 | 73.63 (7) |
| C15'—C14—C13' | 119.0 (6) | O10$^{v}$—Er2—O2 | 74.89 (8) |
| C15—C14—C13' | 115.3 (6) | O1—Er2—O2 | 53.87 (7) |
| C15'—C14—C16 | 120.1 (5) | O11—Er2—C1 | 163.29 (9) |
| C15—C14—C16 | 120.5 (4) | O6—Er2—C1 | 81.38 (9) |
| C13—C14—C16 | 119.0 (4) | O8$^{i}$—Er2—C1 | 101.46 (9) |
| C13'—C14—C16 | 119.8 (5) | O3$^{iv}$—Er2—C1 | 100.30 (8) |
| C14—C15—C10 | 120.1 (6) | O10$^{v}$—Er2—C1 | 77.99 (8) |
| C14—C15—H15 | 119.9 | O1—Er2—C1 | 27.23 (8) |
| C10—C15—H15 | 119.9 | O2—Er2—C1 | 26.69 (8) |
| C13'—C12'—C11' | 119.8 (10) | C1—O1—Er2 | 93.85 (17) |
| C13'—C12'—H12' | 120.1 | C1—O2—Er2 | 92.22 (18) |
| C11'—C12'—H12' | 120.1 | C8—O3—Er2$^{iv}$ | 134.08 (18) |
| C12'—C13'—C14 | 121.1 (8) | C8—O4—Er1$^{vi}$ | 142.64 (19) |
| C12'—C13'—H13' | 119.5 | C9—O5—Er1 | 169.8 (2) |
| C14—C13'—H13' | 119.5 | C9—O6—Er2 | 140.3 (2) |
| C12'—C11'—C10 | 119.8 (9) | C16—O7—Er1$^{vii}$ | 153.1 (2) |
| C12'—C11'—H11' | 120.1 | C16—O8—Er2$^{vii}$ | 139.5 (2) |
| O8—C16—O7 | 124.1 (3) | C24—O9—Er1 | 148.6 (2) |
| O8—C16—C14 | 118.5 (3) | C24—O10—Er2$^{iii}$ | 110.14 (18) |
| O7—C16—C14 | 117.3 (3) | C17—O11—Er2 | 158.2 (2) |
| O11—C17—O12 | 123.3 (3) | C17—O12—Er1$^{v}$ | 125.5 (2) |
| O11—C17—C18 | 119.3 (3) | Er1—O2W—H3W | 123 (3) |
| O12—C17—C18 | 117.4 (3) | Er1—O2W—H4W | 124 (3) |

| | | | |
|---|---|---|---|
| C19—C18—C23 | 119.3 (3) | H3W—O2W—H4W | 100 (4) |
| C19—C18—C17 | 120.6 (3) | Er1—O3W—H5W | 121 (3) |
| C23—C18—C17 | 120.1 (3) | Er1—O3W—H6W | 122 (4) |
| C20—C19—C18 | 120.7 (3) | H5W—O3W—H6W | 113 (5) |
| C20—C19—H19 | 119.6 | H1WA—O1WA—H2WA | 92 (5) |
| C18—C19—H19 | 119.6 | H2WA—O1WA—H1WB | 92 (5) |
| C19—C20—C21 | 119.7 (3) | H1WA—O1WA—H2WB | 92 (5) |
| C19—C20—H20 | 120.1 | H1WB—O1WA—H2WB | 92 (5) |
| C21—C20—H20 | 120.1 | H1WA—O1WB—H2WA | 93 (5) |
| C20—C21—C22 | 120.0 (3) | H2WA—O1WB—H1WB | 93 (5) |
| C20—C21—H21 | 120.0 | H1WA—O1WB—H2WB | 93 (5) |
| C22—C21—H21 | 120.0 | H1WB—O1WB—H2WB | 93 (5) |

Symmetry codes: (i) $x$, $-y+3/2$, $z-1/2$; (ii) $x-1$, $-y+3/2$, $z-1/2$; (iii) $-x$, $y-1/2$, $-z+1/2$; (iv) $-x+1$, $-y+2$, $-z+1$; (v) $-x$, $y+1/2$, $-z+1/2$; (vi) $x+1$, $-y+3/2$, $z+1/2$; (vii) $x$, $-y+3/2$, $z+1/2$.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1WB—H2WB···O12$^{iii}$ | 0.817 (10) | 2.54 (5) | 3.019 (7) | 118 (5) |
| O1WB—H1WB···O10$^{viii}$ | 0.813 (10) | 2.071 (19) | 2.709 (6) | 135 (3) |
| O3W—H6W···O1WB | 0.822 (10) | 2.00 (3) | 2.742 (7) | 150 (5) |
| O2W—H3W···O1WB | 0.817 (10) | 2.13 (3) | 2.837 (8) | 144 (4) |
| O2W—H4W···O3$^{ix}$ | 0.819 (10) | 2.002 (11) | 2.820 (3) | 176 (5) |
| O1WA—H2WA···O12$^{iii}$ | 0.822 (10) | 2.54 (5) | 3.087 (14) | 125 (5) |
| O1WA—H1WA···O10$^{viii}$ | 0.825 (10) | 2.071 (19) | 2.862 (14) | 160 (4) |
| O3W—H6W···O1WA | 0.822 (10) | 1.93 (3) | 2.702 (14) | 157 (5) |
| O2W—H3W···O1WA | 0.817 (10) | 2.80 (4) | 3.429 (16) | 135 (4) |
| O3W—H5W···O1 | 0.819 (10) | 1.881 (14) | 2.692 (3) | 170 (5) |

Symmetry codes: (iii) $-x$, $y-1/2$, $-z+1/2$; (viii) $x+1$, $y$, $z$; (ix) $-x+1$, $y-1/2$, $-z+1/2$.

**Fig. 1**

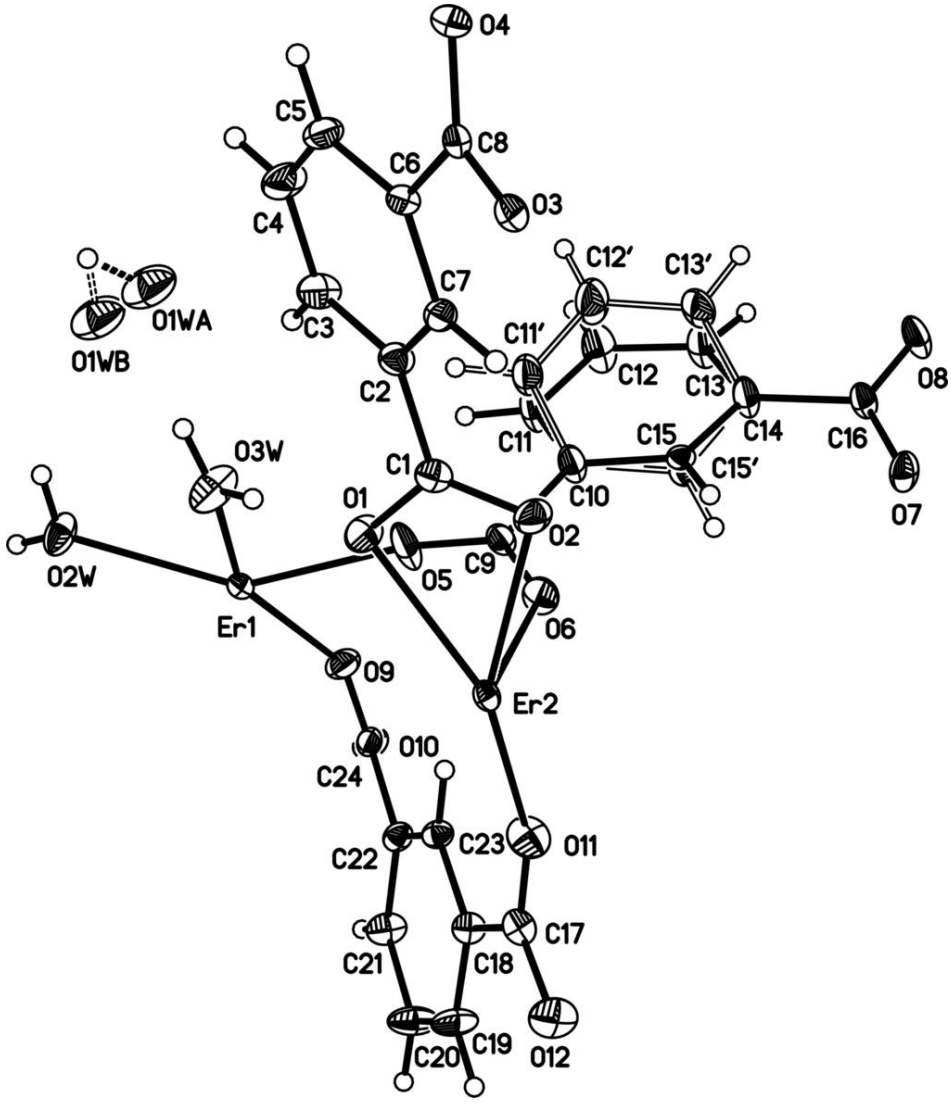
O4
C5
C8
C6
O3
C4
C12′
C13′
C7
O1WA
C3
C11′
O1WB
C12
C13
O8
C2
C11
C15
C14
C16
O3W
C1
C15′
C10
O7
O1
O2
O2W
C9
O5
O6
Er1
O9
Er2
O10
C24
C22
C23
O11
C17
C21
C18
C20
C19
O12

**Fig. 2**