

# Tetraethylammonium tricarbonylchlorido(isoquinoline-1-carboxylato- $\kappa^2N,O$ )technetate(I)

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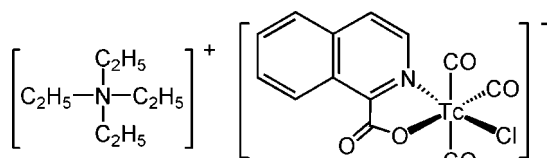
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Key indicators: single-crystal X-ray study;  $T = 193$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.028;  $wR$  factor = 0.067; data-to-parameter ratio = 23.0.

The asymmetric unit of the title compound,  $(C_8H_{20}N)[Tc(C_{10}H_6NO_2)Cl(CO)_3]$ , consists of two crystallographically independent technetium complexes related *via* a pseudo-inversion centre and two tetraethylammonium cations. The Tc atoms have slightly distorted octahedral coordination geometries, and they are linked with the cations by intermolecular  $C-H \cdots O$  and  $C-H \cdots Cl$  hydrogen-bonding contacts, forming two-dimensional columns, which lie approximately parallel to (001) in the crystal structure. The isoquinolate (isoquinoline-1-carboxylate) ligands link the columns by partial  $\pi-\pi$  stacking [centroid-centroid distance 4.3733 (11) Å], forming a three-dimensional network structure.

## Related literature

For related literature, see: Alberto *et al.* (1995, 1996); Waibel *et al.* (1999); Rattat *et al.* (2001); Marsh (1995); Marsh *et al.* (2002); Desiraju *et al.* (1991); Etter *et al.* (1990); Desiraju & Steiner, (1999); Bernstein *et al.* (1995); Steiner & Saenger, (1993).



## Experimental

### Crystal data

$(C_8H_{20}N)[Tc(C_{10}H_6NO_2)Cl(CO)_3]$   $\alpha = 102.878$  (12) $^\circ$   
 $M_r = 520.80$   $\beta = 109.624$  (12) $^\circ$   
 Triclinic,  $P\bar{1}$   $\gamma = 99.052$  (13) $^\circ$   
 $a = 11.7657$  (14) Å  $V = 2290.0$  (5) Å $^3$   
 $b = 12.7481$  (14) Å  $Z = 4$   
 $c = 17.1855$  (18) Å Mo  $K\alpha$  radiation

$\mu = 0.78$  mm $^{-1}$   
 $T = 193$  (2) K

0.77 × 0.48 × 0.19 mm

### Data collection

Stoe IPDS diffractometer  
 Absorption correction: numerical  
 (Coppens *et al.*, 1965)  
 $T_{min} = 0.670$ ,  $T_{max} = 0.828$

29670 measured reflections  
 12462 independent reflections  
 9515 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.058$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.067$   
 $S = 1.00$   
 12462 reflections

541 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 0.54$  e Å $^{-3}$   
 $\Delta\rho_{min} = -1.17$  e Å $^{-3}$

Table 1

Selected bond lengths (Å).

Tc1—C21	1.9045 (18)	Tc2—C22	1.9060 (19)
Tc1—C31	1.913 (2)	Tc2—C32	1.907 (2)
Tc1—C11	1.916 (2)	Tc2—C12	1.913 (2)
Tc1—O41	2.1293 (12)	Tc2—O42	2.1317 (12)
Tc1—N51	2.1778 (15)	Tc2—N52	2.1714 (15)
Tc1—Cl1	2.4822 (6)	Tc2—Cl2	2.4980 (6)

Table 2

Hydrogen-bond geometry (Å,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C151—H15A $\cdots$ O51	0.99	2.38	3.328 (2)	161
C171—H17A $\cdots$ O31 <sup>i</sup>	0.99	2.50	3.482 (3)	172
C191—H19B $\cdots$ O41	0.99	2.40	3.360 (2)	163
C192—H19C $\cdots$ O42 <sup>ii</sup>	0.99	2.56	3.507 (2)	160
C192—H19C $\cdots$ O52 <sup>ii</sup>	0.99	2.44	3.221 (2)	136
C202—H20E $\cdots$ Cl1 <sup>iii</sup>	0.98	2.81	3.786 (3)	177
C221—H22A $\cdots$ Cl1 <sup>iv</sup>	0.98	2.77	3.652 (2)	151

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

Data collection: *IPDS Software* (Stoe & Cie, 1997); cell refinement: *IPDS Software*; data reduction: *X-RED* (Stoe & Cie, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* and *PLUTON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2781).

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