

# Tetraethylammonium bromidotricarbonyl[3,5,7-tribromotropolonato(1-)- $\kappa^2O,O'$ ]rhenate(I)

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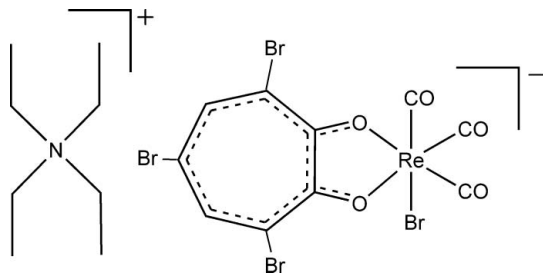
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.017;  $wR$  factor = 0.037; data-to-parameter ratio = 19.9.

In the salt  $(C_8H_{20}N)[ReBr(C_7H_2Br_3O_2)(CO)_3]$ , the bromidotricarbonyl(tribromotropolonato)rhenate(I) anion interacts with adjacent anions through intermolecular bromido-bromido interactions [3.2675 (5)–3.4962 (4) Å]. The  $Re^I$  atom shows octahedral coordination. The crystal structure also involves  $C-H \cdots O$  and  $C-H \cdots Br$  interactions.

## Related literature

For general background, see: Merlau *et al.* (2001); Abou-Hamdan *et al.* (1998); Keefe *et al.* (2003); Mines *et al.* (2002); Sun & Lees (2002). For related structures of diketonato complexes, see: Brasey *et al.* (2004); Crous *et al.* (2005); Roodt *et al.* (2003).



## Experimental

### Crystal data

$(C_8H_{20}N)[ReBr(C_7H_2Br_3O_2)(CO)_3]$   $\gamma = 112.888$  (1) $^\circ$   
 $M_r = 838.21$   $V = 1191.34$  (8) Å<sup>3</sup>  
 Triclinic,  $P\bar{1}$   $Z = 2$   
 $a = 8.9520$  (3) Å Mo  $K\alpha$  radiation  
 $b = 10.0667$  (3) Å  $\mu = 11.84$  mm<sup>-1</sup>  
 $c = 15.3855$  (7) Å  $T = 100$  (2) K  
 $\alpha = 108.391$  (2) $^\circ$   $0.29 \times 0.11 \times 0.06$  mm  
 $\beta = 92.198$  (2) $^\circ$

### Data collection

Bruker APEXII area-detector diffractometer 39168 measured reflections  
 Absorption correction: multi-scan (SADABS; Bruker, 1998) 5202 independent reflections  
 $T_{min} = 0.242$ ,  $T_{max} = 0.481$  4815 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.037$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$  262 parameters  
 $wR(F^2) = 0.037$  H-atom parameters constrained  
 $S = 1.05$   $\Delta\rho_{max} = 1.07$  e Å<sup>-3</sup>  
 5202 reflections  $\Delta\rho_{min} = -0.94$  e Å<sup>-3</sup>

Table 1

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C18-H18C \cdots O8^i$	0.96	2.49	3.423 (3)	164
$C4-H4 \cdots O8^{ii}$	0.93	2.54	3.449 (3)	167
$C11-H11B \cdots Br3^{iii}$	0.97	2.86	3.765 (3)	155

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

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT-Plus (Bruker, 2004); data reduction: SAINT-Plus and XPREP (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg & Putz, 2006); 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: NG2352).

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**supplementary materials**

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## Tetraethylammonium bromidotricarbonyl[3,5,7-tribromotropolonato(1-)- $\kappa^2O,O'$ ]rhenate(I)

M. Schutte, H. G. Visser and G. Steyl

### Comment

The title compound, (I), is presented as an example of a *fac*-Re<sup>I</sup>(CO)<sub>3</sub> fragment containing the highly substituted 3,5,7-tribromotropolonato moiety, see Figure 1. These rhenium systems are commonly employed in catalysis [Merlau *et al.*, 2001; Abou-Hamdan *et al.*, 1998], sensing devices [Keefe *et al.*, 2003; Mines *et al.*, 2002] and building blocks in self-assembled metallomacrocycles [Sun & Lees, 2002]. A closely related derivative of 3-hydroxy-1,2,4-benzotriazine-4-one [Brasey *et al.*, 2004] have been reported.

The title complex crystallizes in the asymmetric unit with two independent ionic fragments. The effect of the small bite angle of the tribromotropolonato moiety can be observed from the slightly distorted octahedral geometry around the Re<sup>I</sup> metal centre, see Table 1.

An interesting observation in the title complex is the effect of weak intermolecular hydrogen bonding contacts between the cationic [NEt<sub>4</sub>]<sup>+</sup> and anionic [ReBr(CO)<sub>3</sub>TropBr<sub>3</sub>]<sup>-</sup> moieties, see Table 2. This solid state ordering is further enhanced through Br·Br interactions between pairs of the brominated tropolonato moieties, Br3·Br7 [*x*, 1 + *y*, *z*] 3.2675 (5)%A 168.4 (1)% and Br7·Br3 [*x*, -1 + *y*, *z*] 3.2675 (5)%A 166.2 (1)% respectively. The bromido ligand on the metal centre is also involved in Br·Br interactions with the brominated tropolonato ligand, Br5·Br1 [2 - *x*, 1 - *y*, 1 - *z*] 3.4962 (4)%A 165.1 (1)%.

### Experimental

The title complex was synthesized from the literature procedure [Brasey *et al.*, 2004].

### Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95Å and with  $U_{iso}(H) = 1.2$  times  $U_{eq}(C \text{ aromatic})$ .

### Figures

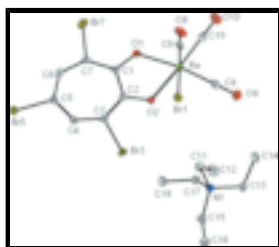


Fig. 1. : Representation of the title compound (I), showing the numbering scheme and displacement ellipsoids (50% probability). Hydrogen atoms omitted for clarity.

## Tetraethylammonium bromidotricarbonyl[3,5,7-tribromotropolonato(1-)- $\kappa^2 O, O'$ ]rhenate(I)

### Crystal data

$(C_8H_{20}N)[ReBr(C_7H_2Br_3O_2)(CO)_3]$	$Z = 2$
$M_r = 838.21$	$F_{000} = 784$
Triclinic, $P\bar{1}$	$D_x = 2.337 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 8.9520 (3) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 10.0667 (3) \text{ \AA}$	Cell parameters from 7112 reflections
$c = 15.3855 (7) \text{ \AA}$	$\theta = 2.5\text{--}28.3^\circ$
$\alpha = 108.391 (2)^\circ$	$\mu = 11.84 \text{ mm}^{-1}$
$\beta = 92.198 (2)^\circ$	$T = 100 (2) \text{ K}$
$\gamma = 112.888 (1)^\circ$	Cuboid, red
$V = 1191.34 (8) \text{ \AA}^3$	$0.29 \times 0.11 \times 0.06 \text{ mm}$

### Data collection

Bruker APEXII area-detector diffractometer	5202 independent reflections
Radiation source: fine-focus sealed tube	4815 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.037$
Detector resolution: $512 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 27.0^\circ$
$T = 100(2) \text{ K}$	$\theta_{\text{min}} = 2.3^\circ$
$\varphi$ and $\omega$ scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$k = -12 \rightarrow 12$
$T_{\text{min}} = 0.242$ , $T_{\text{max}} = 0.481$	$l = -19 \rightarrow 19$
39168 measured reflections	

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.017$	H-atom parameters constrained
$wR(F^2) = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.0118P)^2 + 1.3206P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
5202 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
262 parameters	$\Delta\rho_{\text{max}} = 1.07 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.94 \text{ e \AA}^{-3}$
	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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Re	0.532795 (13)	0.457269 (11)	0.769936 (7)	0.01223 (4)
Br1	0.83966 (3)	0.63718 (3)	0.855160 (18)	0.01689 (6)
Br7	0.72937 (5)	0.08570 (3)	0.56481 (2)	0.03019 (8)
O1	0.6335 (2)	0.3195 (2)	0.67748 (12)	0.0150 (4)
O2	0.6044 (2)	0.5569 (2)	0.66630 (12)	0.0136 (4)
C1	0.6785 (3)	0.3535 (3)	0.60665 (17)	0.0124 (5)
C2	0.6665 (3)	0.4926 (3)	0.60184 (17)	0.0124 (5)
O9	0.4074 (2)	0.6863 (2)	0.88511 (14)	0.0226 (4)
O8	0.1777 (2)	0.2494 (2)	0.66949 (14)	0.0259 (5)
O10	0.4645 (3)	0.3058 (2)	0.91674 (14)	0.0283 (5)
C3	0.7218 (3)	0.5592 (3)	0.53385 (18)	0.0136 (5)
C7	0.7331 (3)	0.2587 (3)	0.53904 (18)	0.0148 (5)
C9	0.4556 (3)	0.5991 (3)	0.84268 (18)	0.0162 (6)
C4	0.7840 (3)	0.5125 (3)	0.45567 (17)	0.0144 (5)
H4	0.8115	0.5777	0.4217	0.017*
C10	0.4905 (3)	0.3636 (3)	0.86116 (19)	0.0175 (6)
C8	0.3129 (3)	0.3267 (3)	0.70577 (18)	0.0164 (6)
C6	0.7882 (3)	0.2677 (3)	0.45755 (18)	0.0155 (5)
H6	0.8130	0.1871	0.4233	0.019*
C5	0.8111 (3)	0.3809 (3)	0.42055 (17)	0.0142 (5)
Br5	0.90032 (3)	0.35922 (3)	0.308775 (18)	0.01785 (6)
Br3	0.70316 (4)	0.74797 (3)	0.554539 (18)	0.02090 (7)
N1	0.1588 (3)	0.8844 (2)	0.13098 (15)	0.0137 (4)
C13	0.2088 (3)	0.8280 (3)	0.03798 (18)	0.0151 (5)
H13A	0.2937	0.7940	0.0474	0.018*
H13B	0.1142	0.7387	-0.0039	0.018*
C11	0.3016 (3)	1.0234 (3)	0.19990 (19)	0.0202 (6)
H11A	0.3313	1.1077	0.1768	0.024*
H11B	0.2648	1.0547	0.2583	0.024*
C12	0.4542 (4)	0.9999 (4)	0.2193 (2)	0.0267 (7)
H12A	0.5376	1.0939	0.2636	0.040*
H12B	0.4944	0.9720	0.1624	0.040*
H12C	0.4278	0.9189	0.2442	0.040*

## supplementary materials

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C17	0.0210 (3)	0.9313 (3)	0.11604 (18)	0.0161 (6)
H17A	-0.0681	0.8443	0.0689	0.019*
H17B	0.0618	1.0145	0.0919	0.019*
C16	-0.0599 (3)	0.6199 (3)	0.1175 (2)	0.0205 (6)
H16A	-0.0858	0.5435	0.1461	0.031*
H16B	-0.0524	0.5752	0.0537	0.031*
H16C	-0.1451	0.6558	0.1201	0.031*
C15	0.1032 (3)	0.7543 (3)	0.16911 (19)	0.0185 (6)
H15A	0.1875	0.7159	0.1674	0.022*
H15B	0.0949	0.7961	0.2339	0.022*
C18	-0.0482 (4)	0.9838 (3)	0.20244 (19)	0.0215 (6)
H18A	-0.1343	1.0112	0.1868	0.032*
H18B	0.0381	1.0720	0.2491	0.032*
H18C	-0.0920	0.9015	0.2261	0.032*
C14	0.2724 (4)	0.9454 (3)	-0.00897 (19)	0.0208 (6)
H14A	0.3007	0.8996	-0.0670	0.031*
H14B	0.3684	1.0331	0.0308	0.031*
H14C	0.1884	0.9778	-0.0206	0.031*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Re	0.01471 (6)	0.01303 (6)	0.00992 (6)	0.00557 (4)	0.00251 (4)	0.00571 (4)
Br1	0.01523 (13)	0.01916 (13)	0.01356 (13)	0.00593 (11)	0.00087 (10)	0.00433 (11)
Br7	0.0631 (2)	0.02116 (15)	0.01990 (15)	0.02841 (16)	0.01035 (15)	0.01089 (12)
O1	0.0228 (10)	0.0132 (9)	0.0120 (9)	0.0087 (8)	0.0028 (8)	0.0069 (8)
O2	0.0185 (10)	0.0135 (9)	0.0128 (9)	0.0088 (8)	0.0046 (8)	0.0067 (7)
C1	0.0129 (13)	0.0099 (12)	0.0122 (13)	0.0029 (10)	-0.0015 (10)	0.0041 (10)
C2	0.0116 (13)	0.0105 (12)	0.0118 (13)	0.0027 (10)	-0.0028 (10)	0.0028 (10)
O9	0.0237 (11)	0.0221 (10)	0.0227 (11)	0.0113 (9)	0.0061 (9)	0.0066 (9)
O8	0.0210 (12)	0.0282 (11)	0.0203 (11)	-0.0006 (10)	-0.0023 (9)	0.0131 (9)
O10	0.0381 (13)	0.0338 (12)	0.0223 (11)	0.0163 (11)	0.0096 (10)	0.0201 (10)
C3	0.0175 (14)	0.0092 (12)	0.0138 (13)	0.0065 (11)	-0.0003 (11)	0.0031 (10)
C7	0.0188 (14)	0.0102 (12)	0.0162 (14)	0.0065 (11)	-0.0002 (11)	0.0056 (11)
C9	0.0159 (14)	0.0201 (14)	0.0135 (13)	0.0062 (12)	0.0022 (11)	0.0092 (11)
C4	0.0167 (14)	0.0145 (13)	0.0102 (13)	0.0037 (11)	0.0006 (10)	0.0058 (11)
C10	0.0175 (14)	0.0182 (14)	0.0163 (14)	0.0086 (12)	0.0021 (11)	0.0045 (12)
C8	0.0212 (15)	0.0183 (14)	0.0119 (13)	0.0058 (12)	0.0044 (11)	0.0111 (11)
C6	0.0174 (14)	0.0145 (13)	0.0132 (13)	0.0085 (11)	0.0001 (11)	0.0015 (11)
C5	0.0137 (13)	0.0186 (13)	0.0080 (12)	0.0055 (11)	0.0015 (10)	0.0036 (10)
Br5	0.02020 (14)	0.02090 (14)	0.01201 (13)	0.00902 (12)	0.00518 (11)	0.00470 (11)
Br3	0.04105 (18)	0.01303 (13)	0.01313 (13)	0.01459 (13)	0.00591 (12)	0.00633 (11)
N1	0.0157 (11)	0.0131 (11)	0.0106 (11)	0.0054 (9)	-0.0005 (9)	0.0034 (9)
C13	0.0171 (14)	0.0169 (13)	0.0113 (13)	0.0084 (11)	0.0024 (11)	0.0037 (11)
C11	0.0202 (15)	0.0169 (14)	0.0129 (14)	0.0014 (12)	-0.0006 (11)	0.0007 (11)
C12	0.0192 (16)	0.0290 (16)	0.0213 (16)	0.0021 (13)	-0.0026 (12)	0.0068 (13)
C17	0.0212 (14)	0.0151 (13)	0.0151 (14)	0.0104 (12)	0.0045 (11)	0.0060 (11)
C16	0.0194 (15)	0.0137 (13)	0.0277 (16)	0.0056 (12)	0.0065 (12)	0.0080 (12)

C15	0.0222 (15)	0.0177 (14)	0.0176 (14)	0.0080 (12)	0.0028 (12)	0.0096 (12)
C18	0.0271 (16)	0.0228 (15)	0.0205 (15)	0.0138 (13)	0.0102 (12)	0.0104 (12)
C14	0.0238 (16)	0.0256 (15)	0.0181 (15)	0.0133 (13)	0.0091 (12)	0.0099 (12)

*Geometric parameters (Å, °)*

Re—C9	1.894 (3)	N1—C15	1.519 (3)
Re—C8	1.897 (3)	C13—C14	1.513 (4)
Re—C10	1.898 (3)	C13—H13A	0.9700
Re—O2	2.1322 (17)	C13—H13B	0.9700
Re—O1	2.1411 (18)	C11—C12	1.508 (4)
Re—Br1	2.6270 (3)	C11—H11A	0.9700
Br7—C7	1.893 (2)	C11—H11B	0.9700
O1—C1	1.276 (3)	C12—H12A	0.9600
O2—C2	1.276 (3)	C12—H12B	0.9600
C1—C7	1.416 (4)	C12—H12C	0.9600
C1—C2	1.470 (3)	C17—C18	1.518 (4)
C2—C3	1.419 (4)	C17—H17A	0.9700
O9—C9	1.156 (3)	C17—H17B	0.9700
O8—C8	1.150 (3)	C16—C15	1.513 (4)
O10—C10	1.161 (3)	C16—H16A	0.9600
C3—C4	1.370 (4)	C16—H16B	0.9600
C3—Br3	1.900 (2)	C16—H16C	0.9600
C7—C6	1.381 (4)	C15—H15A	0.9700
C4—C5	1.383 (4)	C15—H15B	0.9700
C4—H4	0.9300	C18—H18A	0.9600
C6—C5	1.379 (4)	C18—H18B	0.9600
C6—H6	0.9300	C18—H18C	0.9600
C5—Br5	1.909 (3)	C14—H14A	0.9600
N1—C11	1.511 (3)	C14—H14B	0.9600
N1—C17	1.515 (3)	C14—H14C	0.9600
N1—C13	1.518 (3)		
C9—Re—C8	88.62 (12)	C14—C13—H13A	108.4
C9—Re—C10	86.86 (11)	N1—C13—H13A	108.4
C8—Re—C10	88.99 (11)	C14—C13—H13B	108.4
C9—Re—O2	98.38 (9)	N1—C13—H13B	108.4
C8—Re—O2	95.05 (9)	H13A—C13—H13B	107.5
C10—Re—O2	173.44 (9)	C12—C11—N1	115.6 (2)
C9—Re—O1	171.81 (9)	C12—C11—H11A	108.4
C8—Re—O1	93.43 (10)	N1—C11—H11A	108.4
C10—Re—O1	101.08 (9)	C12—C11—H11B	108.4
O2—Re—O1	73.56 (6)	N1—C11—H11B	108.4
C9—Re—Br1	92.28 (8)	H11A—C11—H11B	107.4
C8—Re—Br1	178.69 (8)	C11—C12—H12A	109.5
C10—Re—Br1	92.00 (8)	C11—C12—H12B	109.5
O2—Re—Br1	83.89 (5)	H12A—C12—H12B	109.5
O1—Re—Br1	85.55 (5)	C11—C12—H12C	109.5
C1—O1—Re	117.78 (15)	H12A—C12—H12C	109.5
C2—O2—Re	118.07 (15)	H12B—C12—H12C	109.5



## supplementary materials

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O1—C1—C7	120.2 (2)	N1—C17—C18	115.0 (2)
O1—C1—C2	115.1 (2)	N1—C17—H17A	108.5
C7—C1—C2	124.7 (2)	C18—C17—H17A	108.5
O2—C2—C3	119.7 (2)	N1—C17—H17B	108.5
O2—C2—C1	115.3 (2)	C18—C17—H17B	108.5
C3—C2—C1	125.0 (2)	H17A—C17—H17B	107.5
C4—C3—C2	132.3 (2)	C15—C16—H16A	109.5
C4—C3—Br3	113.97 (19)	C15—C16—H16B	109.5
C2—C3—Br3	113.70 (18)	H16A—C16—H16B	109.5
C6—C7—C1	132.4 (2)	C15—C16—H16C	109.5
C6—C7—Br7	113.58 (19)	H16A—C16—H16C	109.5
C1—C7—Br7	114.01 (19)	H16B—C16—H16C	109.5
O9—C9—Re	178.3 (2)	C16—C15—N1	114.9 (2)
C3—C4—C5	128.5 (2)	C16—C15—H15A	108.5
C3—C4—H4	115.8	N1—C15—H15A	108.5
C5—C4—H4	115.8	C16—C15—H15B	108.5
O10—C10—Re	179.8 (2)	N1—C15—H15B	108.5
O8—C8—Re	177.7 (2)	H15A—C15—H15B	107.5
C5—C6—C7	128.3 (2)	C17—C18—H18A	109.5
C5—C6—H6	115.9	C17—C18—H18B	109.5
C7—C6—H6	115.9	H18A—C18—H18B	109.5
C6—C5—C4	128.5 (2)	C17—C18—H18C	109.5
C6—C5—Br5	116.31 (19)	H18A—C18—H18C	109.5
C4—C5—Br5	115.13 (19)	H18B—C18—H18C	109.5
C11—N1—C17	108.3 (2)	C13—C14—H14A	109.5
C11—N1—C13	111.1 (2)	C13—C14—H14B	109.5
C17—N1—C13	108.73 (19)	H14A—C14—H14B	109.5
C11—N1—C15	109.1 (2)	C13—C14—H14C	109.5
C17—N1—C15	111.3 (2)	H14A—C14—H14C	109.5
C13—N1—C15	108.26 (19)	H14B—C14—H14C	109.5
C14—C13—N1	115.4 (2)		
C8—Re—O1—C1	91.20 (19)	O1—C1—C7—Br7	0.4 (3)
C10—Re—O1—C1	-179.16 (19)	C2—C1—C7—Br7	-178.69 (19)
O2—Re—O1—C1	-3.06 (17)	C2—C3—C4—C5	-0.2 (5)
Br1—Re—O1—C1	-87.99 (17)	Br3—C3—C4—C5	-179.2 (2)
C9—Re—O2—C2	179.53 (18)	C1—C7—C6—C5	2.7 (5)
C8—Re—O2—C2	-91.12 (19)	Br7—C7—C6—C5	-177.6 (2)
O1—Re—O2—C2	0.97 (17)	C7—C6—C5—C4	-0.3 (5)
Br1—Re—O2—C2	88.11 (17)	C7—C6—C5—Br5	176.9 (2)
Re—O1—C1—C7	-174.73 (18)	C3—C4—C5—C6	-2.7 (5)
Re—O1—C1—C2	4.5 (3)	C3—C4—C5—Br5	180.0 (2)
Re—O2—C2—C3	-177.45 (18)	C11—N1—C13—C14	-58.5 (3)
Re—O2—C2—C1	0.9 (3)	C17—N1—C13—C14	60.6 (3)
O1—C1—C2—O2	-3.6 (3)	C15—N1—C13—C14	-178.4 (2)
C7—C1—C2—O2	175.6 (2)	C17—N1—C11—C12	-176.8 (2)
O1—C1—C2—C3	174.7 (2)	C13—N1—C11—C12	-57.5 (3)
C7—C1—C2—C3	-6.1 (4)	C15—N1—C11—C12	61.8 (3)
O2—C2—C3—C4	-176.0 (3)	C11—N1—C17—C18	-61.8 (3)
C1—C2—C3—C4	5.8 (5)	C13—N1—C17—C18	177.3 (2)

O2—C2—C3—Br3	3.0 (3)	C15—N1—C17—C18	58.2 (3)
C1—C2—C3—Br3	-175.16 (19)	C11—N1—C15—C16	168.0 (2)
O1—C1—C7—C6	-179.8 (3)	C17—N1—C15—C16	48.5 (3)
C2—C1—C7—C6	1.1 (5)	C13—N1—C15—C16	-70.9 (3)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C18—H18C $\cdots$ O8 <sup>i</sup>	0.96	2.49	3.423 (3)	164
C4—H4 $\cdots$ O8 <sup>ii</sup>	0.93	2.54	3.449 (3)	167
C11—H11B $\cdots$ Br3 <sup>iii</sup>	0.97	2.86	3.765 (3)	155

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

Fig. 1

