Abstract

1. Introduction

2. Experimental

2.1. Synthesis and crystallization

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

3. Results and discussion

Table 1

Experimental details

Crystal data	
Chemical formula	
M_r	408.29
Crystal system, space group	?, ?
Temperature (K)	293
a, b, c (Å)	10.2314 (2), 7.5215 (1), 24.5475 (4)
α, β, γ (°)	90, 97.921 (1), 90
V (Å^3)	1871.04 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.22
Crystal size (mm)	0.34 × 0.33 × 0.30
Data collection	
Diffractometer	?
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	43084, 4632, 3418
R_{int}	0.035
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.139, 1.05
No. of reflections	4632
No. of parameters	254
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.76, −0.71

Computer programs: SHELXT-2014 (Sheldrick, 2014), *SHELXL97* (Sheldrick, 1997), *ORTEP* for Windows (Farrugia, 2012), *WinGX* publication routines (Farrugia, 2012).

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supporting information

Computing details

Program(s) used to solve structure: SHELXT-2014 (Sheldrick, 2014); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP* for Windows (Farrugia, 2012); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 2012).

(shelx)

Crystal data

M_r = 408.29
a = 10.2314 (2) Å
b = 7.5215 (1) Å
c = 24.5475 (4) Å
α = 90°
β = 97.921 (1)°
γ = 90°
V = 1871.04 (5) Å^3
Z = 4
F(000) = 840
D_x = 1.449 Mg m^{-3}
Melting point: 0 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 0 reflections
θ = 0–0°
μ = 2.22 mm^{-1}
T = 293 K
0.34 × 0.33 × 0.30 mm

Data collection

Graphite monochromator
43084 measured reflections
4632 independent reflections
3418 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.3°, θ_{min} = 2.8°
h = −13→13
k = −10→9
l = −32→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.139
S = 1.05
4632 reflections
254 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 0.8381P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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) for (shelx)

	x	y	z	U_{iso}*/U_{eq}
Br1	0.96299 (4)	0.76868 (5)	0.231467 (13)	0.07914 (16)

O3	0.7709 (2)	0.9253 (2)	0.49427 (8)	0.0628 (5)
O1	0.4220 (2)	0.7071 (3)	0.36264 (9)	0.0721 (6)
O4	0.9149 (2)	0.7426 (2)	0.54317 (10)	0.0708 (6)
N1	0.6899 (2)	0.3122 (3)	0.47492 (9)	0.0533 (5)
O2	0.3495 (2)	0.4265 (3)	0.35881 (10)	0.0821 (7)
C11	0.7444 (2)	0.6165 (3)	0.48054 (8)	0.0430 (5)
C10	0.7649 (2)	0.4494 (3)	0.50023 (9)	0.0462 (5)
C3	0.7274 (2)	0.6808 (3)	0.37963 (9)	0.0447 (5)
C8	0.5516 (2)	0.5009 (3)	0.41607 (9)	0.0467 (5)
C7	0.6505 (2)	0.6517 (3)	0.42776 (9)	0.0443 (5)
C12	0.8083 (3)	0.7751 (3)	0.50617 (10)	0.0474 (5)
C9	0.5778 (2)	0.3377 (3)	0.43775 (10)	0.0491 (5)
C17	0.4314 (2)	0.5343 (4)	0.37711 (10)	0.0570 (6)
C6	0.8679 (3)	0.7322 (4)	0.29181 (10)	0.0548 (6)
C2	0.8128 (3)	0.5529 (4)	0.36496 (11)	0.0589 (6)
C1	0.8833 (3)	0.5779 (4)	0.32110 (12)	0.0645 (7)
C15	0.8595 (3)	0.3879 (4)	0.54869 (11)	0.0623 (7)
H15A	0.9482	0.3996	0.5406	0.093*
H15B	0.8421	0.2656	0.5563	0.093*
H15C	0.8486	0.4592	0.5802	0.093*
C5	0.7854 (3)	0.8629 (4)	0.30583 (13)	0.0679 (8)
C4	0.7164 (3)	0.8367 (4)	0.34961 (12)	0.0626 (7)
C16	0.4949 (3)	0.1735 (4)	0.42730 (14)	0.0656 (7)
H16A	0.4143	0.1883	0.4426	0.098*
H16B	0.5424	0.0732	0.4442	0.098*
H16C	0.4751	0.1539	0.3884	0.098*
C13	0.9757 (4)	0.8906 (4)	0.57496 (14)	0.0794 (9)
H13A	0.9669	0.998	0.5529	0.095*
H13B	1.0689	0.8672	0.5856	0.095*
C18	0.3173 (4)	0.7579 (6)	0.31924 (17)	0.0955 (13)
H18A	0.2444	0.675	0.3185	0.115*
H18B	0.2852	0.8753	0.327	0.115*
C19	0.3625 (5)	0.7592 (7)	0.26643 (19)	0.1165 (18)
H19A	0.4436	0.8247	0.2688	0.175*
H19B	0.2972	0.8145	0.24	0.175*
H19C	0.3769	0.6393	0.2552	0.175*
C14	0.9120 (5)	0.9147 (7)	0.62366 (19)	0.1271 (19)
H14A	0.8191	0.9333	0.613	0.191*
H14B	0.9493	1.0161	0.6439	0.191*
H14C	0.9253	0.8106	0.6464	0.191*
H7	0.601 (3)	0.766 (3)	0.4346 (10)	0.036 (6)*
H4	0.658 (3)	0.924 (5)	0.3589 (14)	0.079 (10)*
H1A	0.712 (3)	0.208 (4)	0.4866 (12)	0.055 (8)*
H5	0.775 (3)	0.970 (5)	0.2867 (15)	0.089 (11)*
H2	0.822 (3)	0.443 (4)	0.3841 (13)	0.069 (9)*
H1	0.941 (3)	0.490 (5)	0.3098 (14)	0.079 (10)*

Atomic displacement parameters (Å²) for (shelx)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0842 (3)	0.0994 (3)	0.0581 (2)	−0.01673 (17)	0.02506 (16)	0.00708 (15)

O3	0.0726 (12)	0.0443 (10)	0.0684 (11)	−0.0014 (8)	−0.0012 (9)	0.0019 (8)
O1	0.0599 (12)	0.0844 (15)	0.0671 (12)	0.0119 (10)	−0.0087 (10)	0.0120 (10)
O4	0.0808 (15)	0.0547 (11)	0.0687 (13)	−0.0008 (9)	−0.0189 (11)	−0.0065 (8)
N1	0.0597 (13)	0.0382 (11)	0.0610 (12)	0.0020 (9)	0.0050 (10)	0.0028 (9)
O2	0.0593 (12)	0.0995 (17)	0.0822 (15)	−0.0096 (12)	−0.0090 (10)	−0.0100 (13)
C11	0.0498 (12)	0.0414 (11)	0.0377 (10)	0.0023 (9)	0.0059 (8)	−0.0007 (8)
C10	0.0513 (12)	0.0455 (12)	0.0422 (11)	0.0036 (10)	0.0072 (9)	0.0012 (9)
C3	0.0466 (12)	0.0461 (12)	0.0397 (10)	0.0002 (9)	−0.0001 (8)	0.0024 (9)
C8	0.0441 (11)	0.0533 (13)	0.0433 (11)	0.0017 (10)	0.0086 (9)	−0.0054 (9)
C7	0.0504 (12)	0.0415 (11)	0.0405 (10)	0.0064 (9)	0.0050 (9)	0.0007 (9)
C12	0.0556 (14)	0.0461 (13)	0.0409 (11)	0.0004 (10)	0.0078 (10)	0.0005 (9)
C9	0.0501 (13)	0.0474 (13)	0.0518 (12)	−0.0026 (10)	0.0139 (10)	−0.0075 (10)
C17	0.0452 (13)	0.0780 (18)	0.0484 (13)	0.0039 (12)	0.0085 (10)	−0.0067 (12)
C6	0.0549 (14)	0.0682 (16)	0.0411 (12)	−0.0112 (12)	0.0060 (10)	0.0023 (10)
C2	0.0747 (17)	0.0513 (14)	0.0530 (14)	0.0113 (12)	0.0169 (12)	0.0092 (11)
C1	0.0752 (18)	0.0657 (17)	0.0557 (14)	0.0133 (14)	0.0201 (13)	0.0033 (12)
C15	0.0743 (18)	0.0535 (15)	0.0553 (14)	0.0072 (13)	−0.0046 (12)	0.0086 (11)
C5	0.0760 (19)	0.0635 (18)	0.0661 (17)	0.0052 (14)	0.0160 (14)	0.0242 (14)
C4	0.0680 (17)	0.0568 (16)	0.0650 (16)	0.0131 (13)	0.0158 (13)	0.0152 (13)
C16	0.0613 (16)	0.0547 (15)	0.0816 (19)	−0.0092 (13)	0.0130 (14)	−0.0072 (14)
C13	0.087 (2)	0.0659 (19)	0.078 (2)	−0.0103 (16)	−0.0155 (17)	−0.0090 (16)
C18	0.067 (2)	0.136 (4)	0.078 (2)	0.030 (2)	−0.0103 (18)	0.018 (2)
C19	0.088 (3)	0.176 (5)	0.082 (3)	0.014 (3)	0.001 (2)	0.043 (3)
C14	0.149 (4)	0.136 (4)	0.103 (3)	−0.060 (3)	0.040 (3)	−0.058 (3)

Geometric parameters (Å, º) for (shelx)

Br1—C6	1.901 (3)	C2—C1	1.389 (4)
O3—C12	1.215 (3)	C2—H2	0.95 (3)
O1—C17	1.347 (4)	C1—H1	0.95 (3)
O1—C18	1.454 (4)	C15—H15A	0.96
O4—C12	1.342 (3)	C15—H15B	0.96
O4—C13	1.449 (3)	C15—H15C	0.96
N1—C9	1.377 (3)	C5—C4	1.379 (4)
N1—C10	1.381 (3)	C5—H5	0.93 (4)
N1—H1A	0.85 (3)	C4—H4	0.94 (4)
O2—C17	1.207 (3)	C16—H16A	0.96
C11—C10	1.352 (3)	C16—H16B	0.96
C11—C12	1.461 (3)	C16—H16C	0.96
C11—C7	1.526 (3)	C13—C14	1.450 (6)
C10—C15	1.500 (3)	C13—H13A	0.97
C3—C2	1.380 (4)	C13—H13B	0.97
C3—C4	1.381 (4)	C18—C19	1.435 (6)
C3—C7	1.523 (3)	C18—H18A	0.97
C8—C9	1.350 (4)	C18—H18B	0.97
C8—C17	1.472 (3)	C19—H19A	0.96
C8—C7	1.521 (3)	C19—H19B	0.96
C7—H7	1.02 (2)	C19—H19C	0.96
C9—C16	1.500 (4)	C14—H14A	0.96
C6—C1	1.363 (4)	C14—H14B	0.96
C6—C5	1.371 (4)	C14—H14C	0.96

C17—O1—C18	117.8 (3)	C10—C15—H15B	109.5
C12—O4—C13	118.2 (2)	H15A—C15—H15B	109.5
C9—N1—C10	123.6 (2)	C10—C15—H15C	109.5
C9—N1—H1A	120 (2)	H15A—C15—H15C	109.5
C10—N1—H1A	116 (2)	H15B—C15—H15C	109.5
C10—C11—C12	124.5 (2)	C6—C5—C4	119.5 (3)
C10—C11—C7	120.9 (2)	C6—C5—H5	122 (2)
C12—C11—C7	114.58 (19)	C4—C5—H5	119 (2)
C11—C10—N1	119.0 (2)	C5—C4—C3	121.6 (3)
C11—C10—C15	128.4 (2)	C5—C4—H4	120 (2)
N1—C10—C15	112.6 (2)	C3—C4—H4	118 (2)
C2—C3—C4	117.4 (2)	C9—C16—H16A	109.5
C2—C3—C7	121.0 (2)	C9—C16—H16B	109.5
C4—C3—C7	121.5 (2)	H16A—C16—H16B	109.5
C9—C8—C17	120.9 (2)	C9—C16—H16C	109.5
C9—C8—C7	120.9 (2)	H16A—C16—H16C	109.5
C17—C8—C7	118.0 (2)	H16B—C16—H16C	109.5
C8—C7—C3	111.23 (18)	O4—C13—C14	109.4 (3)
C8—C7—C11	110.82 (19)	O4—C13—H13A	109.8
C3—C7—C11	110.58 (18)	C14—C13—H13A	109.8
C8—C7—H7	109.2 (14)	O4—C13—H13B	109.8
C3—C7—H7	108.9 (14)	C14—C13—H13B	109.8
C11—C7—H7	105.9 (14)	H13A—C13—H13B	108.2
O3—C12—O4	122.1 (2)	C19—C18—O1	111.5 (4)
O3—C12—C11	123.2 (2)	C19—C18—H18A	109.3
O4—C12—C11	114.6 (2)	O1—C18—H18A	109.3
C8—C9—N1	119.3 (2)	C19—C18—H18B	109.3
C8—C9—C16	127.2 (2)	O1—C18—H18B	109.3
N1—C9—C16	113.5 (2)	H18A—C18—H18B	108
O2—C17—O1	121.9 (3)	C18—C19—H19A	109.5
O2—C17—C8	127.0 (3)	C18—C19—H19B	109.5
O1—C17—C8	111.0 (2)	H19A—C19—H19B	109.5
C1—C6—C5	120.6 (3)	C18—C19—H19C	109.5
C1—C6—Br1	120.0 (2)	H19A—C19—H19C	109.5
C5—C6—Br1	119.4 (2)	H19B—C19—H19C	109.5
C3—C2—C1	121.5 (2)	C13—C14—H14A	109.5
C3—C2—H2	119.8 (19)	C13—C14—H14B	109.5
C1—C2—H2	118.6 (19)	H14A—C14—H14B	109.5
C6—C1—C2	119.3 (3)	C13—C14—H14C	109.5
C6—C1—H1	118 (2)	H14A—C14—H14C	109.5
C2—C1—H1	123 (2)	H14B—C14—H14C	109.5
C10—C15—H15A	109.5		

C12—C11—C10—N1	174.4 (2)	C17—C8—C9—N1	−178.7 (2)
C7—C11—C10—N1	−6.2 (3)	C7—C8—C9—N1	6.0 (3)
C12—C11—C10—C15	−4.0 (4)	C17—C8—C9—C16	−0.6 (4)
C7—C11—C10—C15	175.3 (2)	C7—C8—C9—C16	−175.8 (2)
C9—N1—C10—C11	−13.4 (4)	C10—N1—C9—C8	13.6 (4)
C9—N1—C10—C15	165.3 (2)	C10—N1—C9—C16	−164.9 (2)
C9—C8—C7—C3	101.2 (2)	C18—O1—C17—O2	−6.8 (4)

C17—C8—C7—C3	−74.2 (3)	C18—O1—C17—C8	172.6 (3)
C9—C8—C7—C11	−22.3 (3)	C9—C8—C17—O2	−3.4 (4)
C17—C8—C7—C11	162.4 (2)	C7—C8—C17—O2	171.9 (3)
C2—C3—C7—C8	−65.8 (3)	C9—C8—C17—O1	177.2 (2)
C4—C3—C7—C8	115.3 (3)	C7—C8—C17—O1	−7.5 (3)
C2—C3—C7—C11	57.8 (3)	C4—C3—C2—C1	−1.2 (4)
C4—C3—C7—C11	−121.1 (3)	C7—C3—C2—C1	179.9 (3)
C10—C11—C7—C8	22.4 (3)	C5—C6—C1—C2	1.0 (5)
C12—C11—C7—C8	−158.2 (2)	Br1—C6—C1—C2	−179.8 (2)
C10—C11—C7—C3	−101.4 (3)	C3—C2—C1—C6	0.0 (5)
C12—C11—C7—C3	77.9 (3)	C1—C6—C5—C4	−0.7 (5)
C13—O4—C12—O3	8.4 (4)	Br1—C6—C5—C4	−180.0 (2)
C13—O4—C12—C11	−173.3 (3)	C6—C5—C4—C3	−0.6 (5)
C10—C11—C12—O3	−165.5 (3)	C2—C3—C4—C5	1.5 (4)
C7—C11—C12—O3	15.2 (4)	C7—C3—C4—C5	−179.6 (3)
C10—C11—C12—O4	16.3 (4)	C12—O4—C13—C14	87.4 (4)
C7—C11—C12—O4	−163.1 (2)	C17—O1—C18—C19	−93.7 (4)