†Crystal and molecular structure of 5-[2-(4-methoxyphenyl)ethyl]-1,2,3-oxadiazole 3-oxide (2a)

Abstract

We present the crystal and molecular structure of 5-[2-(4-methoxyphenyl)ethyl]-1,2,3-oxadiazole 3-oxide (**2a**)

Comment

The study of the titled structure was undertaken to establish its three dimensional structure. Geometries are tabulated below. All diagrams and calculations were performed using maXus (Bruker Nonius, Delft & MacScience, Japan).

Experimental

Crystal data

$C_{11}H_{12}N_2O_3$
$C_{11}H_{12}N_2O_3$
$M_r = 220.228$
Monoclinic
$P2_1/c$
a = 5.6130 (4)Å
b = 8.9250 (5)Å
c = 22.154 (2)Å
$\alpha = 90.00°$
$\beta = 95.563$ (3)°
$\gamma = 90.00°$
V = 1104.60 (13)Å^3

Z = 4
$D_x = 1.324$ Mg m^{-3}
Density measured by: not measured
fine-focus sealed tube
Mo $K\alpha$ radiation
$\lambda = 0.71073$
$\mu = 0.098$ mm^{-1}
T = 298 K
plate
Colourless
Crystal source:Local laboratory

Data collection

DIP Image plate
IP
Absorption correction: none
1973 measured reflections
1863 independent reflections
1417 observed reflections

Criterion: >2sigma(I)
$\theta_{max} = 25.78°$
h = 0 → 6
k = 0 → 10
l = -26 → 26

Refinement

Refinement on F^2
fullmatrix least squares refinement
R(all) = 0.0674
R(gt) = 0.0538
wR(ref) = 0.1580
wR(gt)= 0.1412
S(ref) = 1.065

1863 reflections
145 parameters
0 restraints
Only coordinates of H atoms refined
Calculated weights calc
$\Delta/\sigma_{max} = 0.000$
$\Delta\rho_{max} = 0.168$eÅ^3
$\Delta\rho_{min} = -0.305$eÅ^3

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†*Prepared by maXus*

Extinction correction: none
Atomic scattering factors from International

Tables Vol C Tables 4.2.6.8 and 6.1.1.4

Data collection: DIP Image plate
Cell refinement: Scalepack(HKL)
Data reduction: maXus (Mackay et al., 1999)
Program(s) used to refine structure: *SHELXL*-97 (Sheldrick, 1997)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters ($Å^2$)*
$U_{eq} = 1/3 \sum_i \sum_j U_{ij} a_i^* a_j^* \boldsymbol{a}_i . \boldsymbol{a}_j$.

	x	y	z	U_{eq}	Occ
N1	0.2762 (3)	0.17174 (19)	0.51164 (8)	0.0784 (5)	1
C2	0.8731 (4)	-0.0575 (2)	0.18234 (8)	0.0697 (5)	1
O3	1.0095 (3)	-0.08965 (19)	0.13600 (6)	0.0922 (5)	1
C4	0.6115 (4)	-0.0120 (2)	0.28184 (9)	0.0724 (5)	1
C5	0.2837 (4)	0.1031 (2)	0.45599 (9)	0.0737 (5)	1
C6	0.4670 (4)	0.1648 (2)	0.43143 (9)	0.0726 (5)	1
C7	0.9407 (4)	-0.1268 (2)	0.23726 (9)	0.0785 (6)	1
O8	0.5675 (3)	0.26679 (19)	0.47131 (8)	0.1000 (6)	1
C9	0.5465 (4)	0.0547 (2)	0.22634 (10)	0.0798 (6)	1
C10	0.6751 (4)	0.0341 (2)	0.17703 (9)	0.0764 (6)	1
O11	0.1291 (3)	0.14538 (19)	0.55044 (7)	0.1003 (6)	1
C12	0.5798 (4)	0.1449 (2)	0.37425 (9)	0.0783 (6)	1
C13	0.8125 (4)	-0.1031 (2)	0.28604 (9)	0.0776 (6)	1
C14	0.4740 (4)	0.0163 (3)	0.33594 (10)	0.0849 (6)	1
C15	0.9760 (6)	-0.0029 (3)	0.08279 (11)	0.1055 (8)	1
N16	0.4443 (4)	0.2703 (2)	0.52256 (9)	0.0999 (6)	1
H5	0.1497	0.0168	0.4432	0.088	1
H7	1.0767	-0.1924	0.2415	0.094	1
H9	0.4054	0.1160	0.2214	0.096	1
H10	0.6288	0.0842	0.1394	0.092	1
H12A	0.5624	0.2348	0.3504	0.094	1
H12B	0.7467	0.1232	0.3837	0.094	1
H13	0.8642	-0.1512	0.3238	0.093	1
H14A	0.3117	0.0417	0.3220	0.102	1
H14B	0.4756	-0.0726	0.3604	0.102	1
H15A	1.0821	-0.0378	0.0543	0.127	1
H15B	1.0097	0.1004	0.0923	0.127	1
H15C	0.8133	-0.0125	0.0654	0.127	1

Table 2. *Anisotropic displacement parameters ($Å^2$)*

	U_{11}	U_{12}	U_{13}	U_{22}	U_{23}	U_{33}
N1	0.0870 (13)	0.0062 (9)	0.0180 (9)	0.0727 (10)	0.0007 (8)	0.0774 (10)
C2	0.0723 (12)	-0.0003 (9)	0.0069 (9)	0.0687 (11)	-0.0031 (8)	0.0680 (11)
O3	0.1005 (12)	0.0220 (9)	0.0208 (8)	0.1011 (11)	0.0025 (7)	0.0773 (9)
C4	0.0704 (13)	-0.0137 (9)	0.0106 (9)	0.0723 (12)	-0.0049 (8)	0.0752 (12)
C5	0.0769 (13)	0.0007 (9)	0.0126 (9)	0.0683 (11)	-0.0002 (9)	0.0770 (12)
C6	0.0744 (13)	0.0010 (9)	0.0085 (9)	0.0658 (11)	-0.0010 (8)	0.0777 (12)
C7	0.0737 (13)	0.0092 (10)	0.0031 (10)	0.0811 (13)	0.0051 (9)	0.0799 (13)
O8	0.1053 (12)	-0.0291 (9)	0.0266 (9)	0.1013 (12)	-0.0220 (8)	0.0966 (11)
C9	0.0746 (13)	0.0114 (10)	0.0082 (10)	0.0797 (13)	0.0007 (10)	0.0853 (14)

C10	0.0820 (14)	0.0101 (10)	0.0034 (10)	0.0744 (12)	0.0057 (9)	0.0718 (12)
O11	0.1161 (14)	-0.0030 (9)	0.0390 (10)	0.0974 (12)	-0.0042 (8)	0.0930 (11)
C12	0.0774 (13)	-0.0061 (10)	0.0177 (10)	0.0745 (12)	-0.0008 (9)	0.0850 (13)
C13	0.0790 (14)	-0.0051 (10)	0.0014 (9)	0.0823 (13)	0.0092 (9)	0.0704 (11)
C14	0.0810 (15)	-0.0184 (11)	0.0182 (11)	0.0949 (15)	-0.0082 (10)	0.0809 (13)
C15	0.130 (2)	0.0091 (16)	0.0361 (14)	0.1083 (18)	0.0093 (13)	0.0826 (15)
N16	0.1118 (16)	-0.0216 (12)	0.0246 (11)	0.1001 (14)	-0.0195 (10)	0.0907 (13)

Table 3 . *Geometric parameters (Å, °)*

N1—O11	1.270 (2)	C9—C10	1.379 (3)
N1—N16	1.295 (3)	C12—C14	1.514 (3)
N1—C5	1.381 (3)	C5—H5	1.0942
C2—O3	1.369 (2)	C7—H7	0.9600
C2—C10	1.376 (3)	C9—H9	0.9599
C2—C7	1.384 (3)	C10—H10	0.9600
O3—C15	1.408 (3)	C12—H12A	0.9601
C4—C9	1.383 (3)	C12—H12B	0.9600
C4—C13	1.387 (3)	C13—H13	0.9600
C4—C14	1.508 (3)	C14—H14A	0.9600
C5—C6	1.329 (3)	C14—H14B	0.9599
C6—O8	1.353 (2)	C15—H15A	0.9601
C6—C12	1.481 (3)	C15—H15B	0.9601
C7—C13	1.371 (3)	C15—H15C	0.9600
O8—N16	1.386 (3)		
O11—N1—N16	120.59 (18)	C13—C7—H7	119.3
O11—N1—C5	126.86 (19)	C2—C7—H7	120.4
N16—N1—C5	112.54 (18)	C10—C9—H9	118.3
O3—C2—C10	124.48 (18)	C4—C9—H9	119.4
O3—C2—C7	116.10 (18)	C2—C10—H10	120.0
C10—C2—C7	119.40 (19)	C9—C10—H10	120.5
C2—O3—C15	118.28 (18)	C6—C12—H12A	110.0
C9—C4—C13	117.06 (19)	C14—C12—H12A	108.2
C9—C4—C14	121.6 (2)	C6—C12—H12B	109.1
C13—C4—C14	121.35 (19)	C14—C12—H12B	106.9
C6—C5—N1	105.85 (19)	H12A—C12—H12B	109.5
C5—C6—O8	107.59 (18)	C7—C13—H13	118.7
C5—C6—C12	135.45 (19)	C4—C13—H13	119.8
O8—C6—C12	116.95 (18)	C4—C14—H14A	109.1
C13—C7—C2	120.3 (2)	C12—C14—H14A	108.0
C6—O8—N16	109.88 (16)	C4—C14—H14B	109.4
C10—C9—C4	122.3 (2)	C12—C14—H14B	109.2
C2—C10—C9	119.47 (19)	H14A—C14—H14B	109.5
C6—C12—C14	113.16 (17)	O3—C15—H15A	109.3
C7—C13—C4	121.53 (19)	O3—C15—H15B	109.7
C4—C14—C12	111.65 (17)	H15A—C15—H15B	109.5
N1—N16—O8	104.13 (17)	O3—C15—H15C	109.3
C6—C5—H5	136.6	H15A—C15—H15C	109.5
N1—C5—H5	117.6	H15B—C15—H15C	109.5

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