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X-ray crystallographic data for (±)-25:

Data Collection:

A clear, colorless crystal of molecular formula $C_{18}H_{20}O_3$ with approximate dimensions of 0.13 x 0.25 x 0.48 mm was obtained by recrystallization from acetone at 23 °C by slow evaporation. It was mounted on a glass fiber and placed in a goniometer head on an Enraf-Nonius CAD4 computer controlled kappa axis diffractometer equipped with a graphite monochromator using MoKa radiation ($\lambda = 0.71073$ Å).

Unit cell parameters and an orientation matrix for data collection were obtained by auto-indexing and least-squares refinement of 22 reflections in the range $2° < \Theta < 14°$. The crystal system was monoclinic with cell constants and calculated volume of: a = 11.388(3) Å, b = 10.536(2) Å, c = 13.154(4) Å, ß = 105.99(2)°, V = 1511(1) Å^3. From space group required extinctions and subsequent least squares refinement the space group was determined to be $P2_1/c$ (# 14). A total of 3014 unique reflections were collected at a temperature of 25±1 °C using the omega-2theta scan technique to a maximum 2Θ angle of 50.0°.

Data Reduction:

As a check on crystal and electronic stability two representative reflections were measured every 60 minutes. A linear decay correction was applied to the data. Lorentz, polarization, and no absorption corrections were made.

Structure Solution and Refinement:

The structure was solved with SHELX-86[1] using direct methods which revealed the positions of 21 atoms. HYDRO[2] was employed to locate the remaining hydrogens. Hydrogen atoms were included in the refinement but restrained to ride on the atom to which they were bonded. Anomalous dispersion effects were included in F_c[3]; the values

[1]Sheldrick, G. M. "SHELXS-86, Program for Crystal Structure Solution," University of Gottingen, 1986.
[2]Fair, C. K. "MolEN, An Interactive Structure Solution Procedure," Enraf-Nonius, Delft, The Netherlands (1990).
[3]Ibers, J. A.; Hamilton, W. C. *Acta Crystallogr.* **1964**, *17*, 781.

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for $\Delta f'$ and $\Delta f''$ were those of Cromer.[4] Only 1620 reflections having F_o greater than 3.0 times $\sigma(F_o)$ were used in the refinements. The final cycle of least-squares included 190 variable parameters and converged with a maximum parameter shift of 0.00 times its esd, and unweighted and weighted agreement factors of 0.0746 and 0.0748, respectively. The standard deviation of an observation of unit weight was 0.53. The largest peak in the final difference Fourier has a height of 0.31 e/Å^3 with an estimated error based on ΔF[5] of 0.07; Plots of $\sum w(|F_o|- |F_c|)^2$ versus $|F_o|$ reflection order in data collection, $\sin\Theta/\lambda$, and various classes of indices showed no unusual trends.

Scattering factors were taken from Cromer and Waber.[10] All calculations were performed on a MicroVAX computer using MolEN.[8]

Table of Crystallographic Data:

Formula	$C_{18}H_{20}O_3$
Formula Weight	284.36
Crystal dimensions, mm	0.13 x 0.25 x 0.48
Radiation Wavelength, Å	Mo, 0.71073
Temperature, °C	25 ± 1
Crystal System	monoclinic
Space Group	$P2_1/c$
a, Å	11.338 (3)
b, Å	10.536 (2)
c, Å	13.154
ß, deg	105.99 (2)
V, Å^3	1511 (1)
Z	4

[4]Cromer, D. T.; Waber, J. T. "International Tables for X-Ray Crystallography," Vol. IV, Knyoch, Birmingham, England (1974), Table 2.3.1.

[5]Cruickshank, D. W. J. *Acta. Crystallogr.* **1949**, *2*, 154.

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Density, g/cm^3	1.25
Absorption coeff., μ, cm^{-1}	0.8
Rel. transmission coeff.	0.000 - 0.000
Scan type	omega-2theta
Scan Rate, deg/min	5.49
Scan Width, deg	0.9 + 0.350tanΘ
hkl ranges, h	-13 to 13
hkl ranges, k	0 to 12
hkl ranges, l	-15 to 16
2Θ range, deg	2.0 - 50.0
Structure solution	Direct methods
No. of unique data	3014
No. of data used in refinement	1620
Weighting scheme, w	$4F_o^2/[\sigma(F_o)^2]^2$
No. of parameters refined	190
R[6]	0.0746
R_w[7]	0.0748
GOF	0.5
Largest shift/esd	0.00
High peak in diff map, e/Å^3	0.31 (6)

Table of Positional Parameters:

Atom	x	y	z	B (A^2)
O1	0.9197 (3)	0.2000 (3)	0.8090 (3)	3.34 (7)
O2	0.9412 (3)	0.0445 (3)	1.0958 (3)	3.25 (7)
O3	0.7900 (4)	0.0569 (4)	0.7260 (3)	4.39 (9)

[6] $R = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$

[7] $R_w = [\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2]^{1/2}$

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C1	0.9862 (4)	0.2590 (5)	0.9019 (4)	2.7 (1)
C2	1.0660 (5)	0.3526 (5)	0.8857 (4)	3.5 (1)
C3	1.1398 (5)	0.4141 (5)	0.9719 (4)	3.6 (1)
C4	1.1337 (5)	0.3852 (5)	1.0714 (4)	4.0 (1)
C5	1.0531 (5)	0.2931 (5)	1.0870 (4)	3.4 (1)
C6	0.9785 (4)	0.2287 (4)	1.0013 (4)	2.49 (9)
C7	0.8856 (4)	0.1336 (5)	1.0152 (4)	2.6 (1)
C8	0.8070 (4)	0.0775 (5)	0.9097 (4)	2.8 (1)
C9	0.8336 (4)	0.1051 (5)	0.8093 (4)	3.0 (1)
C10	0.8434 (5)	-0.0085 (6)	1.1312 (4)	4.1 (1)
C11	0.7485 (5)	0.0958 (5)	1.1244 (4)	3.5 (1)
C12	0.7669 (4)	0.1840 (5)	1.0372 (4)	2.7 (1)
C13	0.6991 (4)	0.1533 (5)	0.9243 (4)	2.9 (1)
C14	0.5990 (5)	0.1899 (5)	0.8550 (4)	3.5 (1)
C15	0.4983 (5)	0.2776 (5)	0.8691 (5)	4.0 (1)
C16	0.5333 (7)	0.4124 (6)	0.8501 (8)	9.2 (3)
C17	0.3793 (6)	0.2441 (7)	0.7891 (6)	6.9 (2)
C18	0.4787 (6)	0.2657 (8)	0.9782 (6)	7.6 (2)
H2	1.068	0.375	0.816	6.0*
H3	1.196	0.477	0.962	6.0*
H4	1.185	0.429	1.131	6.0*
H5	1.050	0.273	1.157	6.0*
H8	0.807	-0.077	1.087	6.0*
H10B	0.807	-0.012	0.900	6.0*
H10A	0.874	-0.038	1.202	6.0*
H11B	0.667	0.063	1.106	6.0*
H11A	0.764	0.139	1.190	6.0*

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H12	0.753	0.266	1.061	6.0*
H14	0.588	0.157	0.786	6.0*
H16A	0.472	0.470	0.858	10.0*
H16B	0.610	0.433	0.899	10.0*
H16C	0.541	0.418	0.780	10.0*
H17A	0.315	0.297	0.797	10.0*
H17B	0.390	0.254	0.720	10.0*
H17C	0.360	0.158	0.799	10.0*
H18A	0.415	0.321	0.985	10.0*
H18B	0.458	0.181	0.990	10.0*
H18C	0.553	0.288	1.029	10.0*

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $(4/3)*[a^2*B(1,1) + b^2*B(2,2) + c^2*B(3,3) + ab(\cos\gamma)*B(1,2) + ac(\cos\beta)*B(1,3) + bc(\cos\alpha)*B(2,3)]$.

Table of General Displacement Parameters — U

Atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
O1	0.054 (2)	0.039 (2)	0.033 (1)	-0.008 (2)	0.011 (1)	0.001 (2)
O2	0.042 (2)	0.038 (2)	0.044 (2)	0.006 (2)	0.013 (1)	0.014 (2)
O3	0.066 (2)	0.054 (2)	0.045 (2)	-0.007 (2)	0.012 (2)	-0.017 (2)
C1	0.036 (2)	0.029 (2)	0.038 (2)	0.005 (2)	0.009 (2)	-0.001 (2)
C2	0.051 (3)	0.037 (3)	0.046 (3)	0.001 (2)	0.017 (2)	0.007 (2)

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C3	0.047 (3)	0.034 (3)	0.062 (3)	-0.006 (2)	0.024 (2)
0.003 (3)					
C4	0.045 (3)	0.050 (3)	0.052 (3)	-0.014 (3)	0.008 (2)
-0.007 (3)					
C5	0.044 (3)	0.043 (3)	0.040 (2)	-0.001 (2)	0.010 (2)
0.002 (2)					
C6	0.034 (2)	0.025 (2)	0.034 (2)	0.004 (2)	0.008 (2)
0.004 (2)					
C7	0.032 (2)	0.029 (2)	0.037 (2)	0.002 (2)	0.008 (2)
0.004 (2)					
C8	0.039 (2)	0.023 (2)	0.044 (2)	0.003 (2)	0.012 (2)
-0.004 (2)					
C9	0.037 (2)	0.032 (3)	0.042 (2)	0.009 (2)	0.009 (2)
-0.003 (2)					
C10	0.059 (3)	0.048 (3)	0.058 (3)	0.005 (3)	0.032 (2)
0.011 (3)					
C11	0.050 (3)	0.043 (3)	0.042 (2)	-0.001 (3)	0.018 (2)
0.003 (2)					
C12	0.036 (2)	0.027 (2)	0.041 (2)	0.000 (2)	0.015 (2)
-0.000 (2)					
C13	0.034 (2)	0.026 (2)	0.048 (3)	-0.001 (2)	0.008 (2)
-0.007 (3)					
C14	0.042 (3)	0.036 (3)	0.051 (3)	-0.001 (2)	0.008 (2)
-0.007 (3)					
C15	0.035 (3)	0.043 (3)	0.066 (3)	0.006 (3)	0.000 (2)
-0.005 (3)					

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C16	0.085 (5)	0.037 (4)	0.231 (9)	0.015 (4)	0.052 (5)
-0.008 (5)					
C17	0.049 (3)	0.080 (5)	0.122 (6)	0.015 (4)	0.002 (4)
-0.009 (5)					
C18	0.083 (4)	0.104 (5)	0.109 (5)	0.046 (4)	0.042 (3)
-0.001 (5)					

The form of the anisotropic displacement parameter is: $\exp[-2\pi^2\{h^2a^2U(1,1) + k^2b^2U(2,2) + l^2c^2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)\}]$, where a, b, and c are reciprocal lattice constants.

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