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Crystal structure of the (1*R*,2*S*,5*R*) diastereomer of acoltremon, $C_{18}H_{27}NO_2$, from synchrotron powder diffraction data and density functional theory calculations

Jacob K. Salazar,[a] James A. Kaduk,[b,c]* Anja Dosen[d] and Thomas N. Blanton[d]

[a]North Central College, Department of Chemistry, 131 S. Loomis St., Naperville IL 60540, USA, [b]North Central College, Department of Physics, 131 S. Loomis St., Naperville IL 60540, USA, [c]Illinois Institute of Technology, Department of Chemistry, 3101 S. Dearborn St., Chicago IL 60616, USA, and [d]ICDD, 12 Campus Blvd., Newtown Square, PA 19073-3273, USA. *Correspondence e-mail: kaduk@polycrystallography.com

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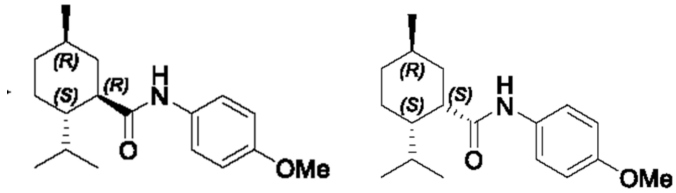
The crystal structure of the (1*R*,2*S*,5*R*) diastereomer of acoltremon [systematic name: (1*R*,2*S*,5*R*)-2-isopropyl-*N*-(4-methoxyphenyl)-5-methylcyclohexane-1-carboxamide], $C_{18}H_{27}NO_2$, has been solved and refined using synchrotron X-ray powder diffraction data, and optimized using density functional theory techniques. Acoltremon crystallizes in space group $P2_12_12_1$ and the crystal structure consists of corrugated layers lying parallel to the *bc* plane. N—H···O hydrogen bonds link the molecules into chains propagating along the *a*-axis direction, with graph-set descriptor $C_1^1(4)$.

1. Chemical context

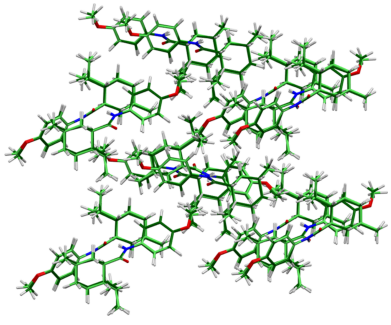
Acoltremon, $C_{18}H_{27}NO_2$ (sold under the brand name Tryptyr in the United States, and also known as AR-15512) is used to treat dry-eye syndrome. It is administered as a preservative free dilute solution in eye drops for the purpose of increasing basal tears production. The systematic name (CAS Registry Number 68489-09-8) is (1*R*,2*S*,5*R*)-*N*-(4-methoxyphenyl)-5-methyl-2-propan-2-ylcyclohexane-1-carboxamide.



AR-15512 **4**

A crystal structure of acoltremon at 100 K has been reported (Rodriguez-Arévalo *et al.*, 2021), but it is of the (1*S*,2*S*,5*R*) diastereomer, **4**, and not the active pharmaceutical. We are unaware of any published powder diffraction data on the (1*R*,2*S*,5*R*) diastereomer.

This work was carried out as part of a project (Kaduk *et al.*, 2014) to determine the crystal structures of large-volume commercial pharmaceuticals, and includes depositing high-quality powder diffraction data for them in the Powder Diffraction File (Kabekkodu *et al.*, 2024).



2. Structural commentary

The dispersion-corrected *VASP* calculations indicate that the structure of the (1*R*,2*S*,5*R*) diastereomer determined here is

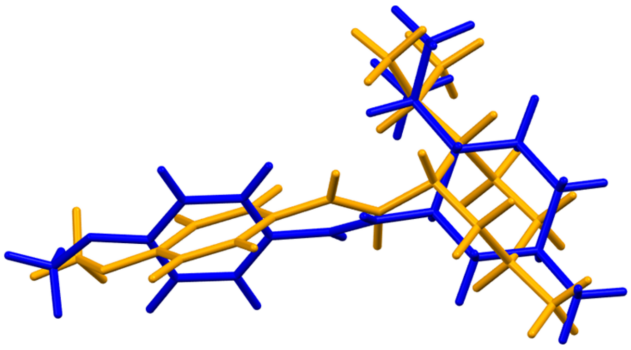


Figure 1
Comparison of the (1*R*,2*S*,5*R*) diastereomer characterized in this study (blue) to the (1*S*,2*S*,5*R*) diastereomer characterized by Rodriguez-Arévalo *et al.* (2021; orange). The root-mean-square Cartesian displacement is 1.206 Å.

23.3 kcal mol^{-1} lower in energy than that of the (1*S*,2*S*,5*R*) diastereomer determined by Rodriguez-Arévalo *et al.* (2021) (see Table 5 in the supporting information). As expected, the molecules are quite different (Fig. 1), with a root-mean-square Cartesian displacement of 1.206 Å.

The root-mean-square difference of the non-H atoms in the Rietveld-refined and *VASP*-optimized structures of acoltremon, calculated using the *Mercury* (Macrae *et al.*, 2020) CSD-Materials/Search/Crystal Packing Similarity tool is 0.133 Å (Fig. 2); the structures are essentially identical. The root-mean-square Cartesian displacement of the non-H atoms

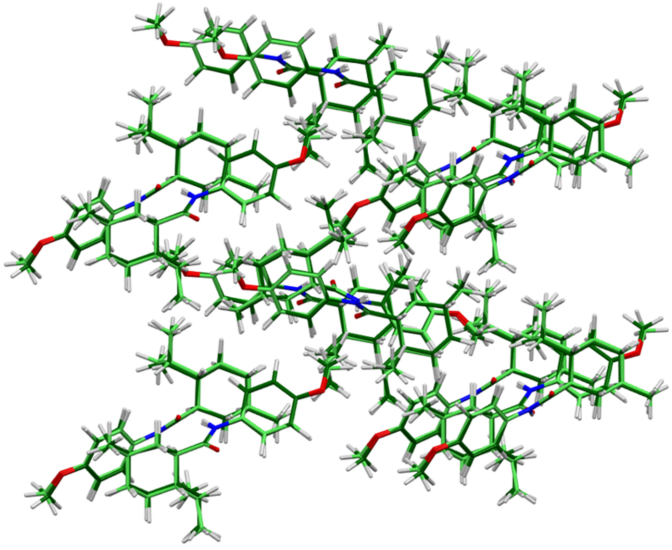


Figure 2
Comparison of the Rietveld-refined (colored by atom type) and *VASP*-optimized (pale green) structures of acoltremon, calculated using the *Mercury* CSD-Materials/Search/Crystal Packing Similarity tool. The root-mean-square Cartesian displacement is 0.133 Å.

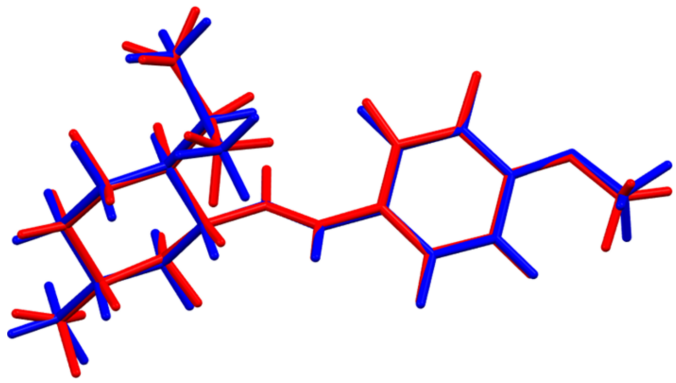


Figure 3
Comparison of the refined structure of acoltremon (red) to the *VASP*-optimized structure (blue). The comparison was generated using the *Mercury* Calculate/Molecule Overlay tool; the root-mean-square Cartesian displacement is 0.108 Å.

in the refined and optimized structures, calculated using the *Mercury* Calculate/molecule overlay tool, is 0.108 Å (Fig. 3). The agreements are within the normal range for correct structures (van de Streek & Neumann, 2014). The asymmetric unit is illustrated in Fig. 4. The remaining discussion will emphasize the *VASP*-optimized structure.

All the bond distances, bond angles, and torsion angles fall within the normal ranges indicated by a *Mercury* Mogul geometry check (Macrae *et al.*, 2020). Quantum chemical geometry optimization of the isolated acoltremon molecule (DFT/B3LYP/6-31G*/water) using *Spartan '24* (Wavefunction, 2025) indicated that the observed conformation lies 2.7 kcal mol^{-1} above a local minimum, which has a similar overall conformation (r.m.s. displacement = 0.338 Å); the difference is mainly in the orientation of the phenyl ring. Similarly, the observed conformation of the (1*S*,2*S*,5*R*) diastereomer lies 3.4 kcal mol^{-1} higher in energy than a local minimum, which differs more (r.m.s. displacement = 0.653 Å), mainly in the orientations of the isopropyl, methyl, and phenyl groups. These single-molecule calculations indicate that the diaster-

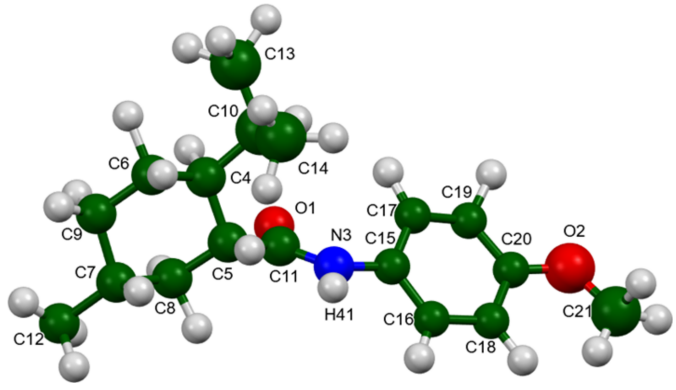


Figure 4
The asymmetric unit of acoltremon, with the atom numbering. The atoms are represented by 50% probability spheroids.

Table 1
Hydrogen-bond geometry (Å, °) for *VASP*-optimized acoltremon.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*	Mulliken overlap	H-bond energy
N3—H41···O1^{i}	1.04	1.80	2.836	175	0.064	5.8
C5—H23···O1^{i}	1.10	2.47	3.428	145	0.014	–
C13—H35···O2	1.10	2.61	3.594	148	0.010	–
C10—H31···C11^{ii}	1.11	2.50	2.991	106	0.012	–

Symmetry codes: (i) $-x-1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+\frac{5}{2}, -y-\frac{1}{2}, -z+1$.

Table 2
Hydrogen-bond geometry (Å, °) for *VASP*-optimized (1*S*,2*S*,5*R*) diastereomer.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*	Mulliken overlap	H-bond energy
N1—H1*N*···O1^{i}	1.03	1.89	2.922	176	0.048	5.1
C18—H18*B*···O1^{ii}	1.10	2.30	3.383	169	0.022	
C10—H10···O1^{iii}	1.10	2.48	3.466	149	0.016	
C9–H9*B*···O2	1.10	2.61	3.526	140	0.011	
C3–H00*F*···C11	1.11	2.55	2.963	101	0.011	

Symmetry codes: (i) $-x+1, y+\frac{3}{2}, -z+\frac{3}{2}$; (ii) $x+\frac{5}{2}, -y-\frac{1}{2}, -z+1$; (iii) $-x-1, y+\frac{3}{2}, -z+\frac{3}{2}$.

eomer of this study is 2.4 kcal mol^{-1} more stable than the other one.

3. Supramolecular features

A view down the *a* axis of the crystal structure (Fig. 5) shows the molecules clearly, but a view down the *c* axis (Fig. 6) makes it clear that the structure consists of corrugated layers lying parallel to the *bc* plane. The *Mercury* aromatics analyser indicates only extremely weak phenyl–phenyl interactions, with distances $\geq$ 8.56 Å. The mean Miller plane of the molecule is approximately (721).

Analysis of the contributions to the total crystal energy of the structure using the forcite module of *Materials Studio* (Dassault Systèmes, 2025) indicated that bond, angle, and torsion distortion terms contribute about equally to the intramolecular energy. The intermolecular energy is dominated by van der Waals attractions, which in this force field based analysis include hydrogen bonds. The hydrogen bonds are better discussed using the results of the DFT calculation.

The hydrogen bonds are summarized in Tables 1 and 2. In both the (1*R*,2*S*,5*R*) diastereomer studied here and the (1*S*,2*S*,5*R*) diastereomer of Rodriguez-Arévalo *et al.* (2021), the amino and carbonyl groups link the molecules into chains (Fig. 7) propagating along the *a*-axis direction, with graph-set descriptor (Etter, 1990; Bernstein *et al.*, 1995; Motherwell *et al.*, 2000) $C_1^1(4)$. These chains link the corrugated layers. However, the patterns of C—H···O and C—H···C hydrogen bonds are almost completely different between the two diastereomers.

The volume enclosed by the Hirshfeld surface of acoltremon (Fig. 9; Spackman *et al.*, 2021) is 424.36 Å^3, 98.31% of 1/4 of the unit-cell volume. The packing density is thus typical.

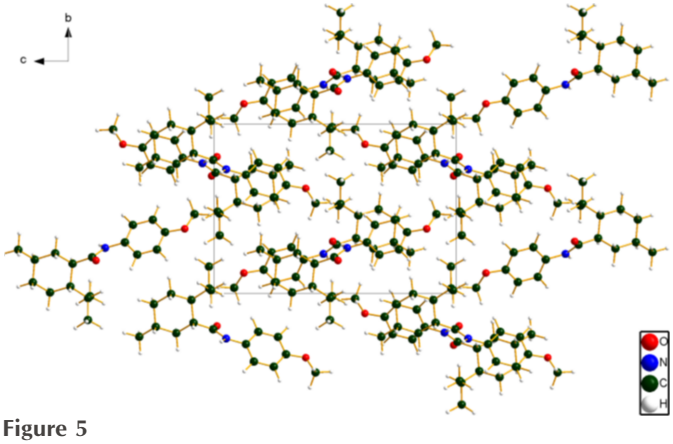


Figure 5
The unit-cell packing of acoltremon, viewed down the *a*-axis direction.

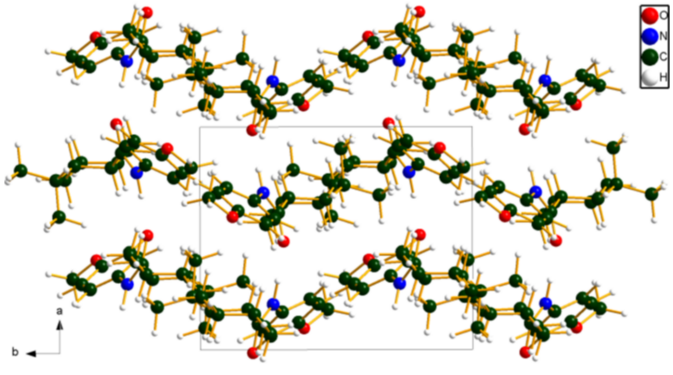


Figure 6
The unit-cell packing of acoltremon, viewed down the *c*-axis direction.

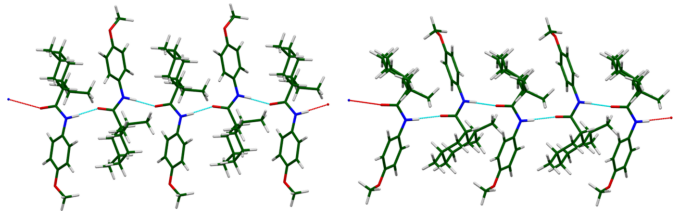


Figure 7
The hydrogen bond chains in the (1*R*,2*S*,5*R*) diastereomer characterized in this study (left) and the (1*S*,2*S*,5*R*) diastereomer (right) characterized by Rodríguez-Arévalo *et al.* (2021). In each case the crystallographic *a* axis is horizontal.

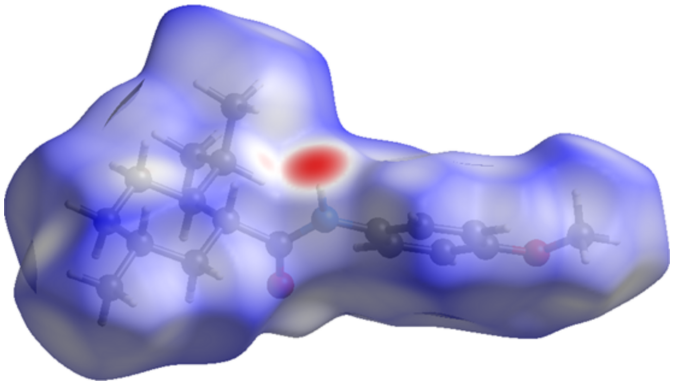


Figure 8
The Hirshfeld surface of acoltremon. Intermolecular contacts longer than the sums of the van der Waals radii are colored blue, and contacts shorter than the sums of the radii are colored red. Contacts equal to the sums of radii are white.

The only significant close contacts (red in Fig. 8) involve the hydrogen bonds. The volume/non-hydrogen atom is larger than normal, at 20.5 Å^3.

The Bravais–Friedel–Donnay–Harker (Bravais, 1866; Friedel, 1907; Donnay & Harker, 1937) algorithm suggests that we might expect isotropic morphology for acoltremon. A second-order spherical harmonic model for preferred orientation was included. The texture index was 1.034, indicating that the preferred orientation was slight in this rotated capillary specimen.

4. Database survey

A reduced cell search in the Cambridge Structural Database (CSD 2026.1.0; Groom *et al.*, 2016), combined with the chemistry C, H, N, and O only, yielded 22 hits, but no structures for acoltremon or its derivatives.

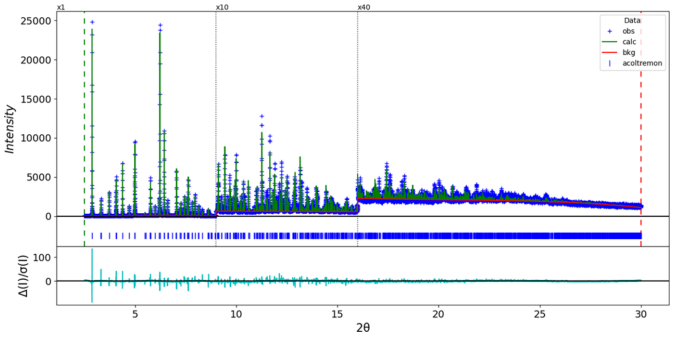


Figure 9
The Rietveld plot for acoltremon. The blue crosses represent the observed data points, and the green line is the calculated pattern. The cyan curve is the normalized error plot, and the red line is the background curve. The blue tick marks indicate the peak positions. The vertical scale has been multiplied by a factor of 10× for $2\theta > 9.0°$ and by a factor of 40× for $2\theta > 16.0°$.

Table 3
Experimental details.

	acoltremon_2
Crystal data	
Chemical formula	$C_{18}H_{27}NO_2$
M_r	289.42
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	295
a, b, c (Å)	9.320220 (15), 11.39111 (3), 16.26284 (4)
V (Å^3)	1726.59 (1)
Z	4
Radiation type	Synchrotron, λ = 0.46873 Å
μ (mm^{-1})	0.005
Specimen shape, size (mm)	Cylinder, 2.0 × 1.5
Data collection	
Diffractometer	11-BM, APS
Specimen mounting	Kapton capillary
Data collection mode	Transmission
Scan method	Step
2θ values (°)	$2\theta_{min}$ = 0.510, $2\theta_{max}$ = 49.995, $2\theta_{step}$ = 0.001
Refinement	
R factors and goodness of fit	R_p = 0.113, R_{wp} = 0.133, R_{exp} = 0.038, $R(F^2)$ = 0.10052, χ^2 = 12.888
No. of parameters	83
No. of restraints	53
$(\Delta/\sigma)_{max}$	1.712

Computer programs: *GSAS-II* (Toby & Von Dreele, 2013) and *DIAMOND* (Brandenburg & Putz, 2025).

5. Synthesis and crystallization

Acoltremon is a commercial reagent and was purchased from TargetMol (Batch #141432) and used as-received.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The white powder was packed into a 1.5 mm diameter Kapton capillary, and rotated during the measurement at ∼50 Hz. The powder pattern was measured at 295 K at beam line 11-BM (Lee *et al.*, 2008; Wang *et al.*, 2008; Antao *et al.*, 2008) of the Advanced Photon Source at Argonne National Laboratory using a wavelength of 0.4687342 Å from 0.5–50° 2θ with a step size of 0.001° and a counting time of 0.1 sec step^{-1}. The high-resolution powder diffraction data were collected using twelve silicon crystal analyzers that allow for high angular resolution, high precision, and accurate peak positions. A mixture of silicon (NIST SRM 640c) and alumina (NIST SRM 676a) standards (ratio Al_2O_3:Si = 2:1 by weight) was used to calibrate the instrument and refine the monochromatic wavelength used in the experiment.

The pattern was indexed on a primitive orthorhombic unit cell with a = 9.32059, b = 11.39187, c = 16.25977 Å, V = 1727.5 Å^3, and Z = 4 using *N-TREOR* as incorporated into *EXPO2014* (Altomare *et al.*, 2013). The suggested space group was $P2_12_12_1$, which was confirmed by successful solution and refinement of the structure.

The *a*, *b*, and *c* lattice parameters at 298 K were 2.0% larger, 9.7% larger, and 7.0% smaller than those reported at 100 K. Refinement was started using the fractional coordinates of Rodriguez-Arévalo *et al.* (2021), before we realized that they were for a different diastereomer. The refinement changed the chiralities to result in the enantiomer of the correct diastereomer.

To make a cleaner narrative, the molecular structure of (1*R*,2*S*,5*R*)-acoltremon was downloaded from PubChem (Kim *et al.*, 2023) as Conformer3D_COMPOUND_CID_11266244.sdf. It was converted to a *.mol2 file using *Mercury* (Macrae *et al.*, 2020). The structure was solved using Monte Carlo simulated annealing techniques as implemented in *EXPO2014* (Altomare *et al.*, 2013).

Rietveld refinement was carried out using *GSAS-II* (Toby & Von Dreele, 2013). Only the 2.5–30.0° portion of the pattern was included in the refinements (d_{min} = 0.905 Å). The μR value was fixed at 0.00, calculated using the 11-BM website (https://11bm.xray.aps.anl.gov/absorb/). All non-H bond distances and angles were subjected to restraints, based on a *Mercury* Mogul geometry check (Sykes *et al.*, 2011; Bruno *et al.*, 2004). The Mogul average and standard deviation for each quantity were used as the restraint parameters. The aromatic ring was restrained to be planar. The restraints contributed 4.0% to the overall χ^2. The hydrogen atoms were included in calculated positions, which were recalculated during the refinement using *Materials Studio* (Dassault Systèmes, 2024). The U_{iso}(H) values were grouped by chemical similarity. The peak profiles were described using an isotropic microstrain model, with the strain fixed at 10 ppm. The background was modeled using a six-term shifted Chebyshev polynomial, with a peak at 6.17° to model the scattering from the Kapton capillary and any amorphous component of the sample.

The final refinement of 83 variables using 27,501 observations and 53 restraints yielded the residuals R_{wp} = 0.1352 and GOF = 3.59. The largest peak (0.13 Å from C15) and hole (1.19 Å from C10) in the difference Fourier map are 1.07 (16) and −0.67 (16) e Å^{-3}, respectively. The final Rietveld plot is shown in Fig. 9. The largest features in the normalized error plot are in the positions and shapes of some of the strong low-angle peaks, and may indicate a change in the specimen during the measurement.

The crystal structures of both diastereomers were optimized (fixed experimental unit cells) with density functional theory techniques using *VASP* (Kresse & Furthmüller, 1996) through the *MedeA* graphical interface (Materials Design, 2024). The calculations were carried out on 32 cores of a 144-core (768 Gb memory) HPE Superdome Flex 280 Linux server at North Central College. The calculation used the GGA-PBE functional, a plane wave cutoff energy of 400.0 eV, and a *k*-point spacing of 0.5 Å^{-1} leading to a 2 × 2 × 1 mesh. To permit comparison of the energies and lattice parameters of the two diastereomers, dispersion-corrected DFT calculations were also carried out using *VASP*, incorporating the DFT-D3 approach of Grimme and allowing the lattice parameters to optimize. Single-point density functional theory calculations (fixed experimental cell) and population analysis were carried out using *CRYSTAL23* (Erba *et al.*, 2023). (fixed experimental cell) and population analysis were carried out using *CRYSTAL17* (Dovesi *et al.*, 2018). The basis sets for the H, C, N and O atoms in the calculation were those of Gatti *et al.* (1994). The calculations were run on a 3.5 GHz PC using 8 *k*-points and the B3LYP functional.

Acknowledgements

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supporting information

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Crystal structure of the (1*R*,2*S*,5*R*) diastereomer of acoltremon, $C_{18}H_{27}NO_2$, from synchrotron powder diffraction data and density functional theory calculations

Jacob K. Salazar, James A. Kaduk, Anja Dosen and Thomas N. Blanton

Computing details

(1*R*,2*S*,5*R*)-2-Isopropyl-*N*-(4-methoxyphenyl)-5-methylcyclohexane-1-carboxamide (acoltremon_2)

Crystal data

$C_{18}H_{27}NO_2$
M_r = 289.42
Orthorhombic, $P2_12_12_1$
a = 9.320220 (15) Å
b = 11.39111 (3) Å
c = 16.26284 (4) Å
V = 1726.59 (1) Å^3
Z = 4
D_x = 1.113 Mg m^{-3}
Synchrotron radiation, λ = 0.46873 Å
T = 295 K
cylinder, 2.0 × 1.5 mm

Data collection

11-BM, APS diffractometer
Specimen mounting: Kapton capillary
Data collection mode: transmission
Scan method: step
$2\theta_{min}$ = 0.510°, $2\theta_{max}$ = 49.995°, $2\theta_{step}$ = 0.001°

Refinement

Least-squares matrix: full
R_p = 0.113
R_{wp} = 0.133
R_{exp} = 0.038
$R(F^2)$ = 0.10052
49486 data points
Profile function: Finger-Cox-Jephcoat function parameters U, V, W, X, Y, SH/L: peak variance(Gauss) = Utan(Th)^2+Vtan(Th)+W: peak HW(Lorentz) = X/cos(Th)+Ytan(Th); SH/L = S/L+H/L U, V, W in (centideg)^2, X & Y in centideg 2.543, -0.174, 0.052, 0.000, 0.000, 0.002,
83 parameters
53 restraints
16 constraints
Weighting scheme based on measured s.u.'s
$(\Delta/\sigma)_{max}$ = 1.712
Background function: Background function: "chebyschev-1" function with 6 terms: 47.29(16), -6.65(24), -12.59(16), 2.79(16), -3.99(17), -0.00(16), Background peak parameters: pos, int, sig, gam: 6.167(16), 1.122(32)e4, 1.24(5)e4, 0.100,
Preferred orientation correction: Simple spherical harmonic correction Order = 2 Coefficients: 0:0:C(2,0) = 0.290(5); 0:0:C(2,2) = 0.295(3)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.0060 (5)	0.3097 (4)	0.5123 (3)	0.0774 (13)*
O2	0.9044 (5)	0.1119 (5)	0.8745 (3)	0.122 (2)*

N3	0.7965 (5)	0.2314 (5)	0.5481 (3)	0.0774 (13)*
C4	0.8275 (6)	0.4484 (4)	0.4087 (3)	0.0785 (11)*
C5	0.8154 (5)	0.3208 (4)	0.4181 (3)	0.0785 (11)*
C6	0.7586 (6)	0.4837 (5)	0.3279 (4)	0.0785 (11)*
C7	0.8365 (6)	0.2953 (5)	0.2633 (3)	0.0785 (11)*
C8	0.8992 (6)	0.2713 (5)	0.3472 (4)	0.0785 (11)*
C9	0.8316 (7)	0.4299 (6)	0.2550 (3)	0.0785 (11)*
C10	0.7665 (7)	0.5165 (6)	0.4855 (4)	0.124 (2)*
C11	0.8833 (5)	0.2836 (5)	0.4956 (3)	0.0774 (13)*
C12	0.9335 (7)	0.2360 (6)	0.1913 (3)	0.0785 (11)*
C13	0.7878 (7)	0.6442 (7)	0.4737 (4)	0.124 (2)*
C14	0.5992 (7)	0.5117 (7)	0.4841 (5)	0.124 (2)*
C15	0.8281 (7)	0.2023 (6)	0.6291 (3)	0.0637 (11)*
C16	0.7831 (7)	0.0934 (5)	0.6598 (3)	0.0637 (11)*
C17	0.8947 (7)	0.2790 (4)	0.6808 (4)	0.0637 (11)*
C18	0.8106 (7)	0.0608 (5)	0.7419 (4)	0.0637 (11)*
C19	0.9405 (6)	0.2401 (5)	0.7600 (4)	0.0637 (11)*
C20	0.8859 (7)	0.1368 (6)	0.7939 (3)	0.0637 (11)*
C21	0.8311 (7)	0.0201 (7)	0.9119 (4)	0.122 (2)*
H22	0.94662	0.47012	0.40403	0.0942*
H23	0.69849	0.29161	0.41551	0.0942*
H24	0.76261	0.58335	0.32187	0.0942*
H25	0.64173	0.45417	0.32732	0.0942*
H26	0.72280	0.25865	0.26023	0.0942*
H27	1.01186	0.31027	0.34713	0.0942*
H28	0.90827	0.17223	0.35567	0.0942*
H29	0.77023	0.45365	0.19669	0.0942*
H30	0.94572	0.46530	0.25046	0.0942*
H31	0.81334	0.48356	0.54600	0.1482*
H32	1.05097	0.26012	0.20108	0.0942*
H33	0.92100	0.13649	0.19352	0.0942*
H34	0.89651	0.26980	0.12882	0.0942*
H35	0.68069	0.69145	0.48081	0.1482*
H36	0.83250	0.66107	0.40953	0.1482*
H37	0.86659	0.67839	0.52166	0.1482*
H38	0.56192	0.41944	0.50089	0.1482*
H39	0.55441	0.57720	0.53046	0.1482*
H40	0.55903	0.53493	0.41992	0.1482*
H41	0.69380	0.20820	0.53000	0.0928*
H42	0.72320	0.02953	0.61815	0.0764*
H43	0.91356	0.37362	0.66070	0.0764*
H44	0.77148	−0.02757	0.76598	0.0764*
H45	1.02243	0.29354	0.79616	0.0764*
H46	0.91141	−0.04652	0.93674	0.1460*
H47	0.75825	−0.02427	0.86494	0.1460*
H48	0.76348	0.05576	0.96470	0.1460*

Geometric parameters (Å, º)

O1—C11	1.213 (4)	C15—N3	1.391 (4)
O2—C20	1.352 (5)	C15—C16	1.402 (5)
O2—C21	1.389 (7)	C15—C17	1.362 (4)
N3—C11	1.317 (5)	C16—C15	1.402 (5)
N3—C15	1.391 (4)	C16—C18	1.410 (4)
N3—H41	1.035 (4)	C16—H42	1.140 (4)
C4—C5	1.465 (5)	C17—C15	1.362 (4)
C4—C6	1.517 (5)	C17—C19	1.428 (5)
C4—C10	1.575 (5)	C17—H43	1.139 (4)
C4—H22	1.140 (5)	C18—C16	1.410 (4)
C5—C4	1.465 (5)	C18—C20	1.399 (5)
C5—C8	1.502 (4)	C18—H44	1.140 (4)
C5—C11	1.472 (4)	C19—C17	1.428 (5)
C5—H23	1.140 (5)	C19—C20	1.395 (5)
C6—C4	1.517 (5)	C19—H45	1.140 (4)
C6—C9	1.498 (5)	C20—O2	1.352 (5)
C6—H24	1.141 (6)	C20—C18	1.399 (5)
C6—H25	1.140 (6)	C20—C19	1.395 (5)
C7—C8	1.509 (6)	C21—O2	1.389 (7)
C7—C9	1.540 (6)	C21—H46	1.139 (8)
C7—C12	1.626 (6)	C21—H47	1.140 (7)
C7—H26	1.140 (6)	C21—H48	1.140 (7)
C8—C5	1.502 (4)	H22—C4	1.140 (5)
C8—C7	1.509 (6)	H23—C5	1.140 (5)
C8—H27	1.140 (6)	H24—C6	1.141 (6)
C8—H28	1.140 (6)	H25—C6	1.140 (6)
C9—C6	1.498 (5)	H26—C7	1.140 (6)
C9—C7	1.540 (6)	H27—C8	1.140 (6)
C9—H29	1.140 (5)	H28—C8	1.140 (6)
C9—H30	1.140 (6)	H29—C9	1.140 (5)
C10—C4	1.575 (5)	H30—C9	1.140 (6)
C10—C13	1.481 (8)	H31—C10	1.140 (6)
C10—C14	1.561 (6)	H32—C12	1.140 (7)
C10—H31	1.140 (6)	H33—C12	1.140 (7)
C11—O1	1.213 (4)	H34—C12	1.140 (6)
C11—N3	1.317 (5)	H35—C13	1.140 (7)
C11—C5	1.472 (4)	H36—C13	1.140 (7)
C12—C7	1.626 (6)	H37—C13	1.140 (7)
C12—H32	1.140 (7)	H38—C14	1.140 (7)
C12—H33	1.140 (7)	H39—C14	1.140 (7)
C12—H34	1.140 (6)	H40—C14	1.140 (7)
C13—C10	1.481 (8)	H41—N3	1.035 (4)
C13—H35	1.140 (7)	H42—C16	1.140 (4)
C13—H36	1.140 (7)	H43—C17	1.139 (4)
C13—H37	1.140 (7)	H44—C18	1.140 (4)
C14—C10	1.561 (6)	H45—C19	1.140 (4)

C14—H38	1.140 (7)	H46—C21	1.139 (8)
C14—H39	1.140 (7)	H47—C21	1.140 (7)
C14—H40	1.140 (7)	H48—C21	1.140 (7)
C20—O2—C21	121.3 (5)	H32—C12—H33	109.5 (5)
C11—N3—C15	126.2 (4)	H32—C12—H34	109.5 (5)
C11—N3—H41	119.9 (4)	H33—C12—H34	109.4 (5)
C15—N3—H41	113.8 (5)	C10—C13—H35	109.4 (6)
C5—C4—C6	108.7 (4)	C10—C13—H36	109.4 (6)
C5—C4—H22	107.3 (4)	H35—C13—H36	109.5 (6)
C6—C4—H22	107.3 (5)	C10—C13—H37	109.5 (7)
C4—C5—C8	104.6 (4)	H35—C13—H37	109.5 (6)
C4—C5—C11	110.0 (3)	H36—C13—H37	109.5 (5)
C8—C5—C11	109.0 (4)	C10—C14—H38	109.4 (6)
C4—C5—H23	111.1 (4)	C10—C14—H39	109.5 (6)
C8—C5—H23	111.0 (4)	H38—C14—H39	109.5 (6)
C11—C5—H23	111.0 (4)	C10—C14—H40	109.4 (5)
C4—C6—C9	112.7 (4)	H38—C14—H40	109.5 (6)
C4—C6—H24	108.9 (5)	H39—C14—H40	109.5 (6)
C9—C6—H24	108.9 (5)	N3—C15—C16	119.0 (5)
C4—C6—H25	109.5 (5)	N3—C15—C17	121.9 (5)
C9—C6—H25	107.9 (5)	C16—C15—C17	119.0 (3)
H24—C6—H25	108.9 (4)	C15—C16—C18	121.0 (3)
C8—C7—C9	105.7 (4)	C15—C16—H42	120.0 (5)
C8—C7—H26	109.5 (5)	C18—C16—H42	119.0 (5)
C9—C7—H26	109.4 (5)	C15—C17—C19	119.6 (3)
C5—C8—C7	115.1 (4)	C15—C17—H43	120.0 (5)
C5—C8—H27	109.5 (5)	C19—C17—H43	120.4 (5)
C7—C8—H27	106.5 (5)	C16—C18—C20	120.1 (3)
C5—C8—H28	108.5 (5)	C16—C18—H44	119.9 (5)
C7—C8—H28	108.4 (5)	C20—C18—H44	120.0 (5)
H27—C8—H28	108.5 (4)	C17—C19—C20	120.6 (3)
C6—C9—C7	110.5 (4)	C17—C19—H45	120.0 (6)
C6—C9—H29	109.5 (5)	C20—C19—H45	119.4 (6)
C7—C9—H29	108.9 (5)	O2—C20—C18	121.3 (5)
C6—C9—H30	109.3 (6)	O2—C20—C19	120.9 (5)
C7—C9—H30	109.3 (5)	C18—C20—C19	117.8 (3)
H29—C9—H30	109.3 (4)	O2—C21—H46	109.5 (6)
C13—C10—C14	99.6 (5)	O2—C21—H47	109.4 (5)
C13—C10—H31	112.5 (6)	H46—C21—H47	109.5 (7)
C14—C10—H31	112.5 (6)	O2—C21—H48	109.4 (7)
O1—C11—N3	123.0 (4)	H46—C21—H48	109.5 (5)
O1—C11—C5	121.7 (3)	H47—C21—H48	109.5 (6)
N3—C11—C5	114.9 (3)		

(acoltremon_2_VASP)

Crystal data

$C_{18}H_{27}NO_2$
M_r = 289.42
Orthorhombic, $P2_12_12_1$
a = 9.32022 Å
b = 11.39111 Å
c = 16.26284 Å
V = 1726.59 Å^3
Z = 4

Data collection

$h = \rightarrow$
$k = \rightarrow$
$l = \rightarrow$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	B_{iso}*/B_{eq}
O1	1.01413	0.30651	0.51100	
O2	0.90354	0.11941	0.87778	
N3	0.79574	0.23233	0.54912	
C4	0.82622	0.46054	0.40507	
C5	0.81815	0.32519	0.41433	
C6	0.76351	0.49545	0.32138	
C7	0.84080	0.30145	0.25810	
C8	0.89693	0.26450	0.34276	
C9	0.84152	0.43556	0.25010	
C10	0.76145	0.52847	0.47885	
C11	0.88472	0.28716	0.49524	
C12	0.92763	0.24298	0.18986	
C13	0.80650	0.65778	0.47776	
C14	0.59804	0.51763	0.48653	
C15	0.83074	0.19945	0.63072	
C16	0.77289	0.09627	0.66346	
C17	0.91421	0.27182	0.68170	
C18	0.79465	0.06595	0.74578	
C19	0.93765	0.24165	0.76324	
C20	0.87726	0.13914	0.79624	
C21	0.81861	0.03231	0.91816	
H22	0.94183	0.48270	0.40418	
H23	0.70449	0.29852	0.41349	
H24	0.76879	0.59126	0.31368	
H25	0.64871	0.47176	0.31927	
H26	0.72797	0.27240	0.25317	
H27	1.01212	0.28588	0.34672	
H28	0.88899	0.16829	0.34954	
H29	0.79251	0.46137	0.19103	
H30	0.95403	0.46632	0.24810	
H31	0.80890	0.48978	0.53495	
H32	1.04086	0.27042	0.19257	
H33	0.92576	0.14661	0.19508	
H34	0.88640	0.26639	0.12866	

H35	0.75606	0.70558	0.42664
H36	0.92354	0.66743	0.47264
H37	0.77364	0.70176	0.53494
H38	0.56228	0.42571	0.48786
H39	0.56132	0.55978	0.54368
H40	0.54279	0.56176	0.43530
H41	0.69185	0.21534	0.52992
H42	0.70813	0.03924	0.62428
H43	0.95775	0.35348	0.65753
H44	0.74655	−0.01411	0.76994
H45	0.99958	0.29888	0.80367
H46	0.84877	0.03673	0.98317
H47	0.84234	−0.05661	0.89556
H48	0.70326	0.05132	0.91125

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H41···O1^{i}	1.04	1.80	2.836	175
C5—H23···O1^{i}	1.10	2.47	3.428	145
C13—H35···O2	1.10	2.61	3.594	148
C10—H31···C11^{ii}	1.11	2.50	2.991	106

Symmetry codes: (i) −*x*−1, *y*+1/2, −*z*+3/2; (ii) *x*+5/2, −*y*−1/2, −*z*+1.

(Molecules_100K_VASP)

Crystal data

$C_{18}H_{27}NO_2$
M_r = 289.42
$P2_12_12_1$
a = 9.13710 Å
b = 10.38210 Å
c = 17.48930 Å
α = 90°
β = 90°
γ = 90°
V = 1659.07 Å^3
Z = 4

Data collection

h = →
k = →
l = →

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.8885	0.6624	0.5105	?
O2	0.9034	0.0242	0.8026	?
N1	0.6836	0.7769	0.5428	?
C1	0.4621	0.4887	0.5510	?
C2	0.6165	0.2918	0.5384	?
C3	0.6132	0.4381	0.5276	?
C4	0.6568	0.4789	0.4455	?
C5	0.7971	0.4126	0.4174	?
C6	0.8423	0.4550	0.3372	?

C7	0.8627	0.6007	0.3317	?
C8	0.9099	0.6428	0.2520	?
C9	0.7217	0.6676	0.3564	?
C10	0.6655	0.6279	0.4362	?
C11	0.7566	0.6895	0.4990	?
C12	0.7420	0.8372	0.6090	?
C13	0.8065	0.7644	0.6670	?
C14	0.8608	0.8232	0.7329	?
C15	0.8508	0.9571	0.7411	?
C16	0.7842	0.0306	0.6835	?
C17	0.7303	0.9709	0.6182	?
C18	0.9601	0.9513	0.8652	?
H1N	0.5786	0.8009	0.5264	?
H1A	0.4530	0.5939	0.5468	?
H1B	0.4372	0.4617	0.6104	?
H1C	0.3768	0.4467	0.5142	?
H2A	0.5461	0.2438	0.4959	?
H2B	0.5744	0.2658	0.5953	?
H2C	0.7273	0.2517	0.5331	?
H00F	0.6953	0.4796	0.5671	?
H4	0.5669	0.4483	0.4070	?
H5A	0.8866	0.4336	0.4578	?
H5B	0.7817	0.3074	0.4178	?
H6A	0.9438	0.4055	0.3201	?
H6B	0.7577	0.4254	0.2955	?
H7	0.9499	0.6281	0.3720	?
H8A	0.8272	0.6157	0.2090	?
H8B	0.0141	0.5972	0.2357	?
H8C	0.9255	0.7478	0.2491	?
H9A	0.6348	0.6435	0.3149	?
H9B	0.7337	0.7731	0.3539	?
H10	0.5539	0.6665	0.4413	?
H13	0.8143	0.6603	0.6610	?
H14	0.9108	0.7635	0.7769	?
H16	0.7757	0.1346	0.6910	?
H17	0.6780	0.0285	0.5738	?
H18A	0.8752	0.8875	0.8892	?
H18B	0.9948	0.0218	0.9082	?
H18C	0.0551	0.8926	0.8477	?

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1	1.03	1.89	2.922	176
C18—H18*B*···O1	1.10	2.30	3.383	169
C10—H10···O1	1.10	2.48	3.466	149
C9—H9*B*···O2	1.10	2.61	3.526	140
C3—H00*F*···C11	1.11	2.55	2.963	101