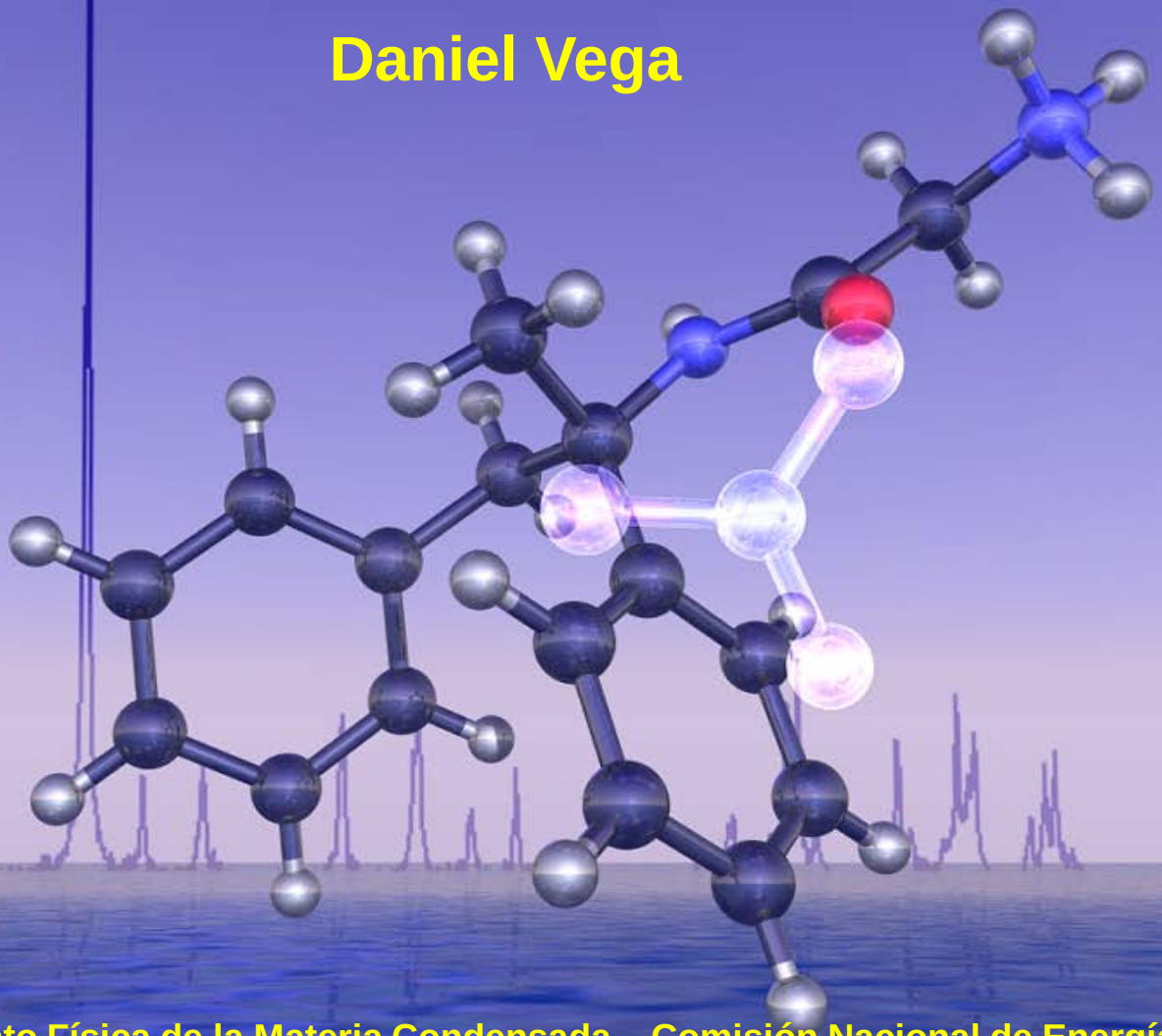
Difracción de Rayos X

Los mejores anteojos para ver polimorfismo

Daniel Vega

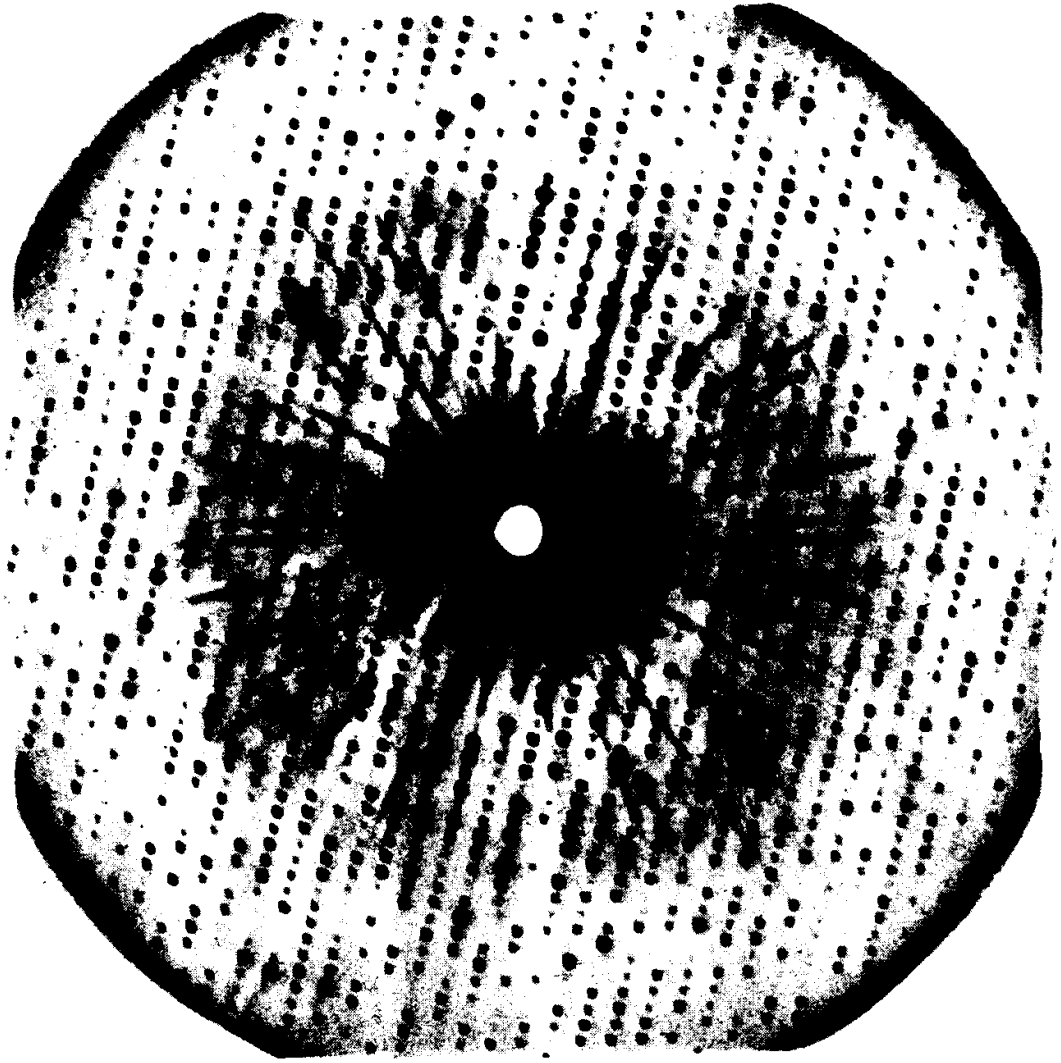


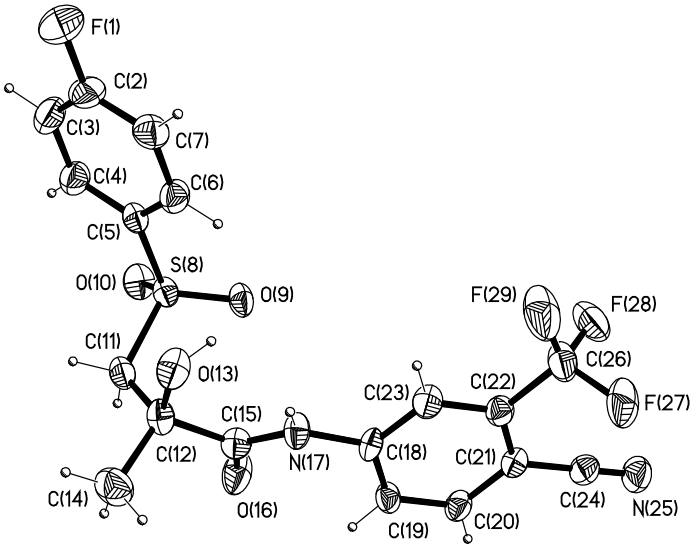
Departamento Física de la Materia Condensada – Comisión Nacional de Energía Atómica

Escuela de Ciencia y Tecnología - UNSAM

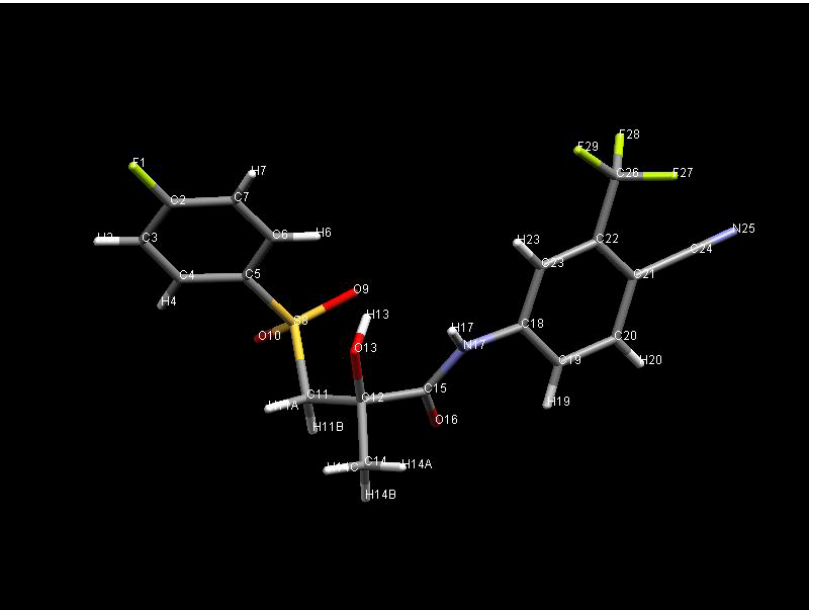
Difractómetro de Monocristales

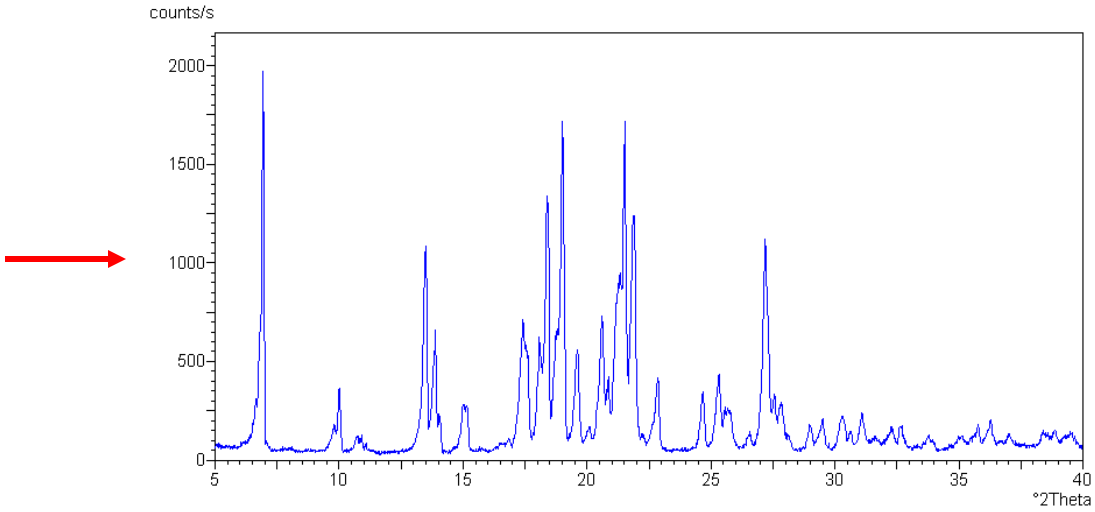
Resultado Monocristales



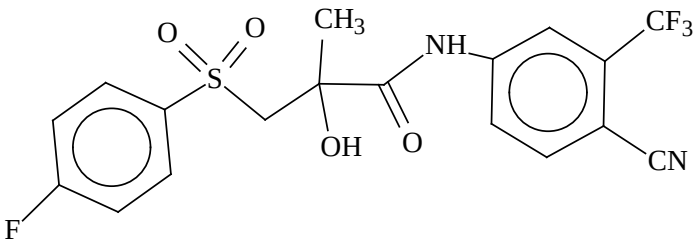


Cálculo de difractograma

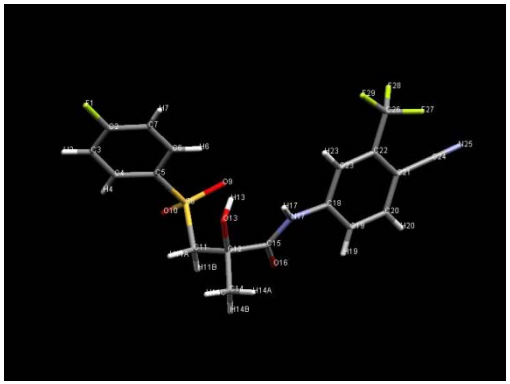




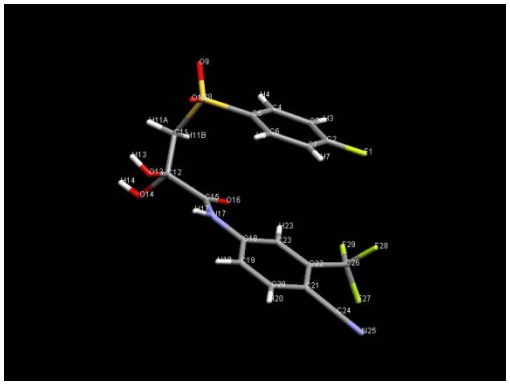
Bicalutamida



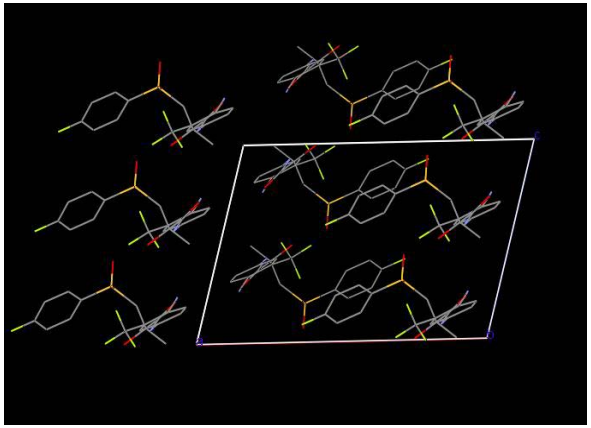
Forma I



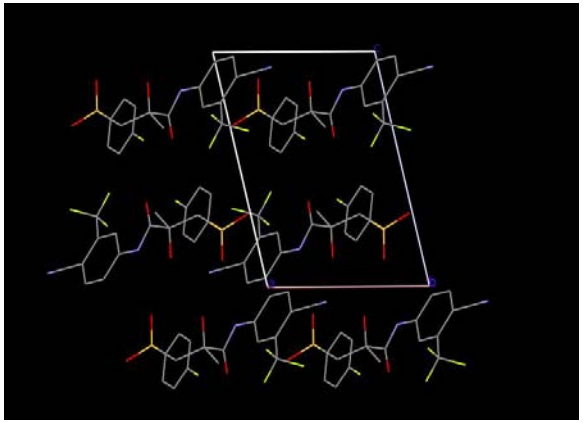
Forma II



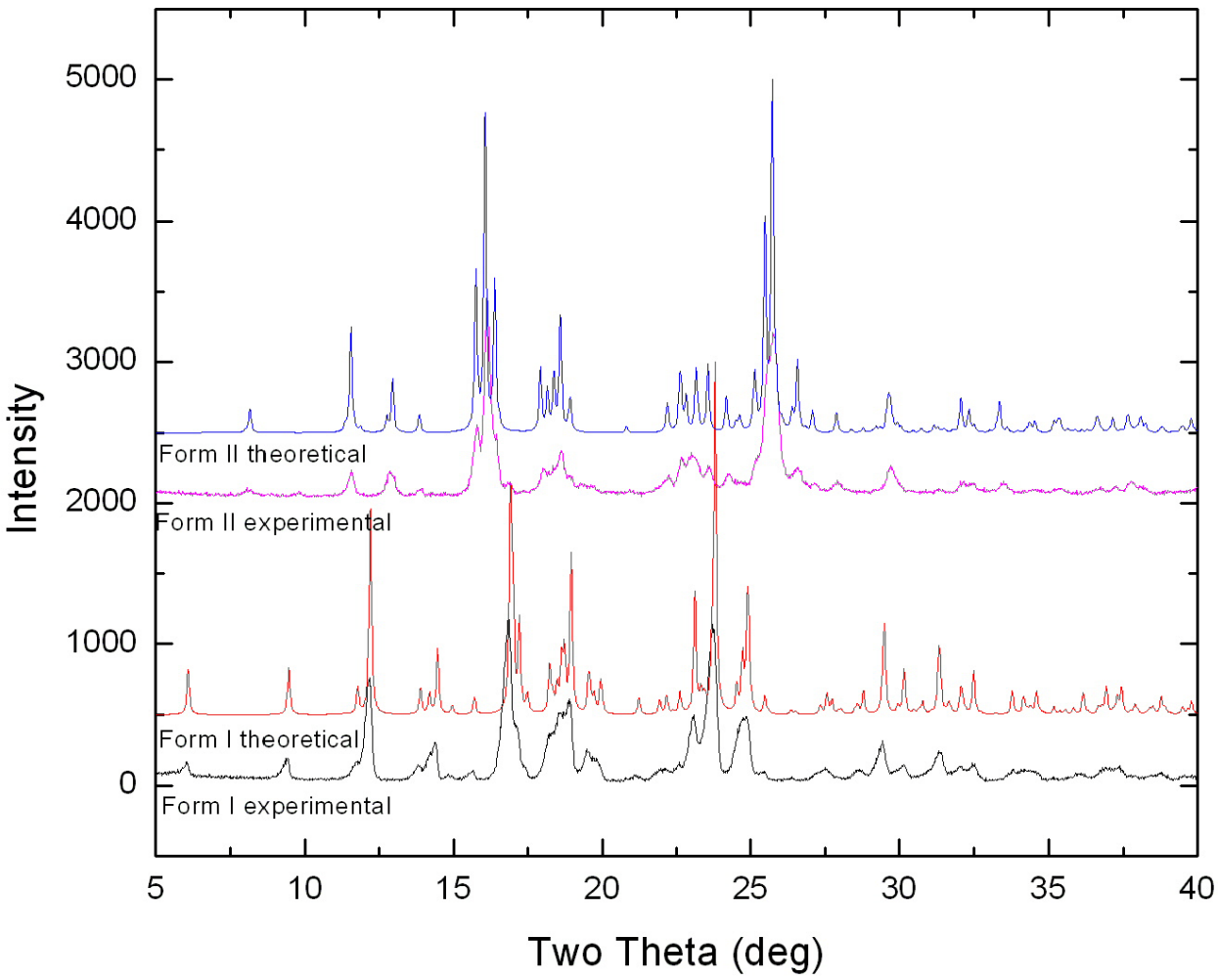
Empaquetamiento Forma I



Empaquetamiento Forma II



Bicalutamida



Clorhidrato de Venlafaxina

-"1-[2-(Dimethylamino)-1-(4-methoxyphenyl)ethylcyclohexanol hydrochloride (Venlafaxine Hydrochloride)"
D.Vega, D. Fernandez, G. Echeverría. Acta Cryst. (2000) C56, 1009-1010.

Ortorrómbico → Bloques → Forma I

-"A monoclinic polymorph of Venlafaxine Hydrochloride"
A. Sivalakshmidevi, K. Vyas, S. Mahender Rao, G. Om Reddy. Acta Cryst. (2002) E58, o1072-o1074.

Monoclínico → Agujas → Forma II

Clorhidrato de Venlafaxina

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

1-[2-(1-Hydroxycyclohexyl)-2-(4-methoxyphenyl)ethyl]dimethylammonium chloride (venlafaxine hydrochloride)

Daniel Vega,[a]* Daniel Fernández[b] and Gustavo Echeverría[c]

[a]Departamento de Física, Comisión Nacional de Energía Atómica, Buenos Aires, Argentina, [b]Escuela de Ciencia y Tecnología, Universidad Nacional de General San Martín, Buenos Aires, Argentina, and [c]LANADI, Departamento de Física, Universidad Nacional de La Plata, La Plata, Argentina
Correspondence e-mail: vega@cnea.gov.ar

Received 11 April 2000
Accepted 8 May 2000

The crystal structure of racemic venlafaxine hydrochloride, $C_{17}H_{28}NO_2^+\cdot Cl^-$, consists of two types of parallel chains formed by translated venlafaxine$^+$ cations, hydrogen bonded by Cl^- anions, and characterized by the opposite chirality of their constituent molecules. These chains organize in two different types of broad layers of opposite handedness, related by a glide plane.

Comment

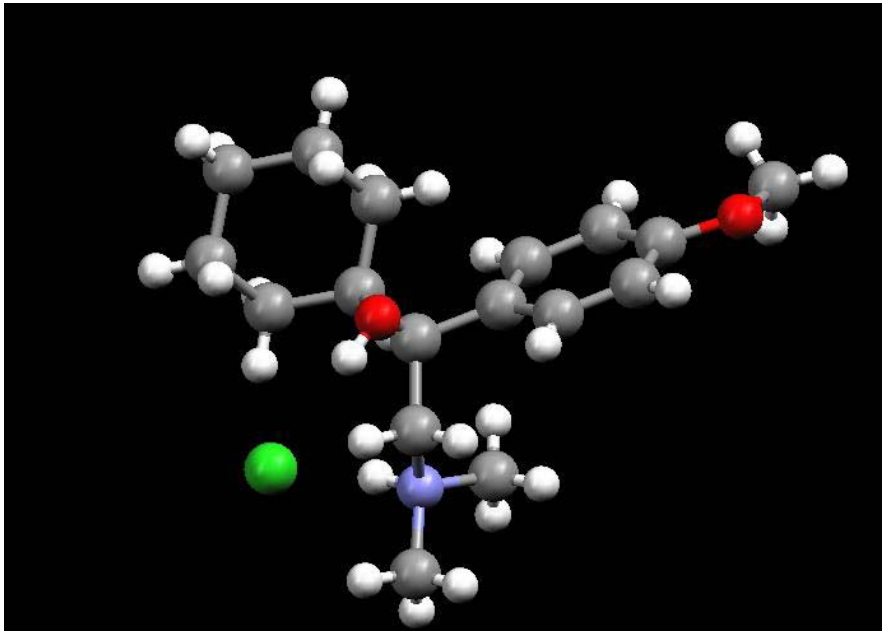
KIDGUZ; it was deposited as supplementary material for a paper by Yardley *et al.* (1990), but in the final publication this structure is not actually described].

Two different crystalline forms of the racemic venlafaxine hydrochloride derivative could be identified by X-ray powder methods, while single crystals of only one of them could be obtained (hereafter VHCl). Its X-ray structure determination was carried out in order to study its molecular conformation and to compare it with VHBr.

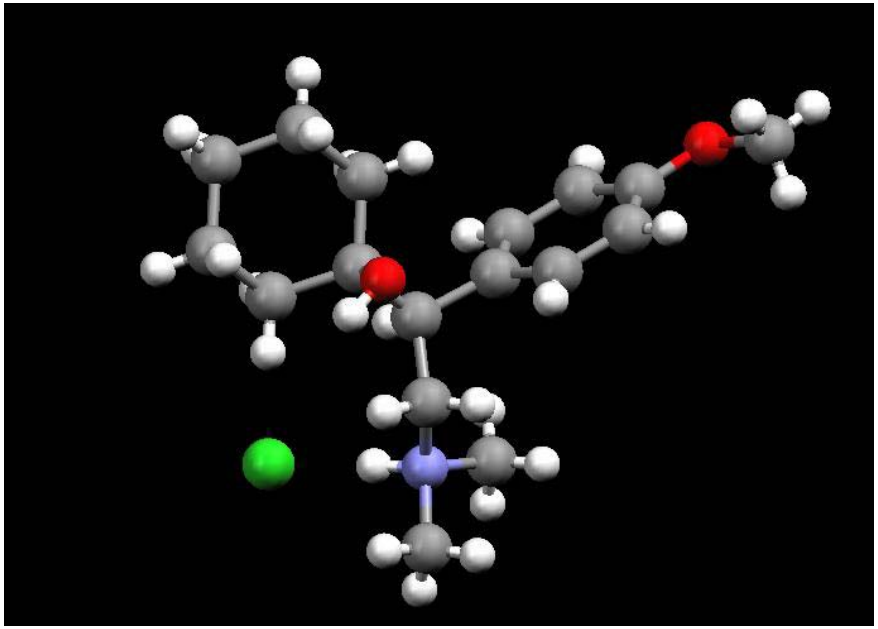
The asymmetric unit of the title compound (Fig. 1) consists of a $C_{17}H_{28}NO_2^+$ cation and a Cl^- anion. The dimethylammonium N atom, N1, shows quaternary character due to proton transfer from HCl and consequently bears the positive charge in the molecular cation. The N1 bond angles range from 107 to 114° (see Table 1) confirming the tetrahedral bond configuration. The hexanolic ring adopts a chair conformation, with C8, C10, C11 and C13 defining a plane (mean deviation 0.004 Å), and C9 and C12 being 0.645 (5) and −0.661 (5) Å out of the plane, respectively.

The comparison of both the VHCl and VHBr structures shows no significant differences between the relevant geometric parameters except for a torsion angle at the methoxy substituent and differences expected due to the unequal size of the halogen anion. A least-squares fit, using the facilities provided by *XP* in the *SHELXTL/PC* package (Sheldrick, 1991), gave an r.m.s. deviation of 0.05 Å. The maximum deviations occur at the halogen (0.11 Å) and C17 (0.14 Å) locations. C17 is the C atom of the methoxy substituent of the benzene and the location difference is evidence of the dissimilarity between the C3—C4—O1—C17 torsion angle in VHCl [−10.9 (7)°] and the corresponding one in VHBr (−0.5°).

Clorhidrato de Venlafaxina

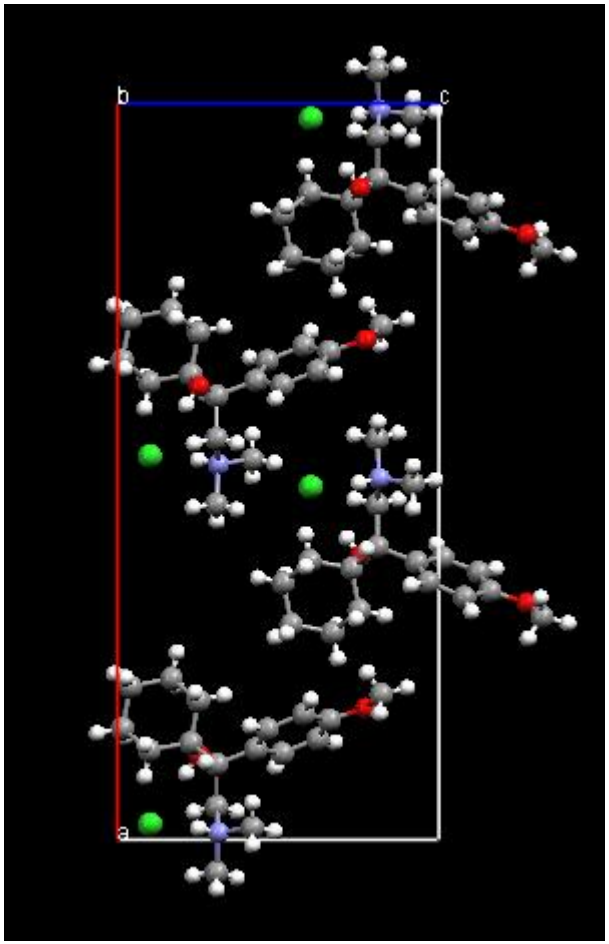


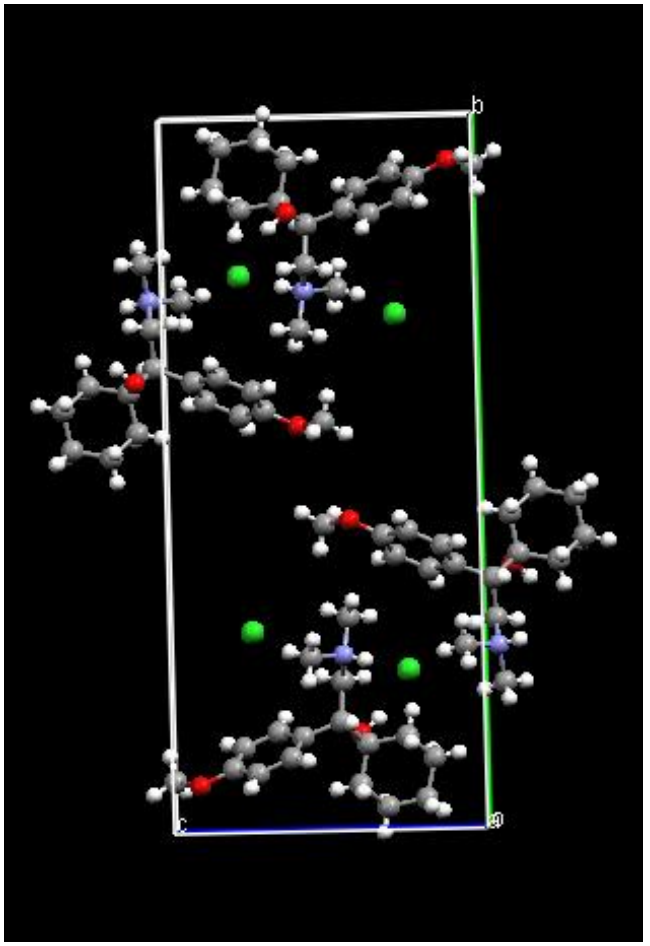
Forma I



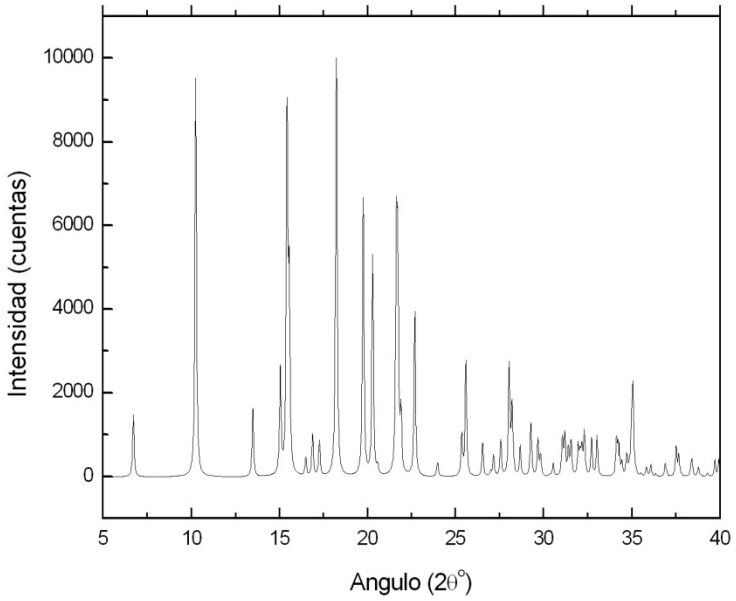
Forma II

Clorhidrato de Venlafaxina

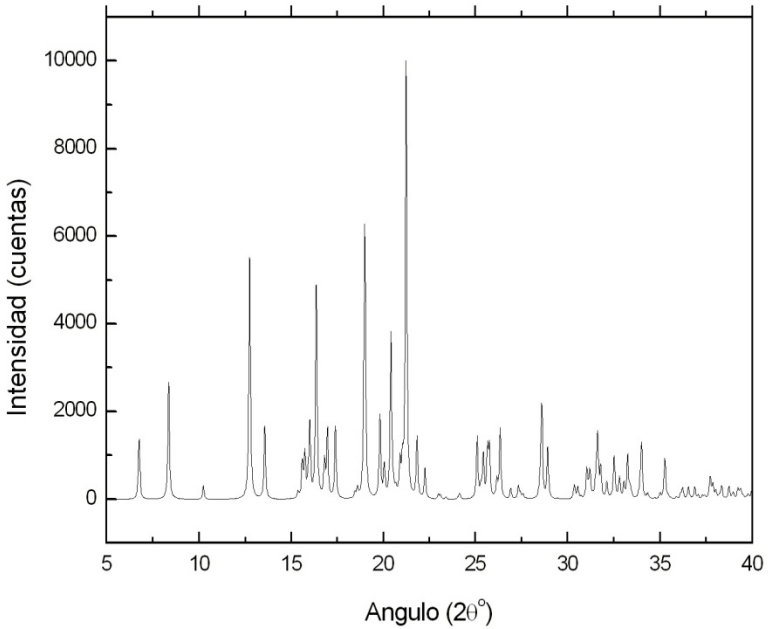




Clorhidrato de Venlafaxina



Forma I



Forma II

Clorhidrato de Venlafaxina