crystals

MDPI

Article,

Investigating Differences and Similarities between Betaxolol Polymorphs

Supplementary Materials

Table S1. Cell parameters of **BE_IV** at 200 and 300 K.

T(K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å³)
200	9.366(1)	19.802(7)	19.980(3)	102.55(1)	3617(2)
300	9.393(2)	20.094(3)	20.027(3)	101.91(2)	3699(1)

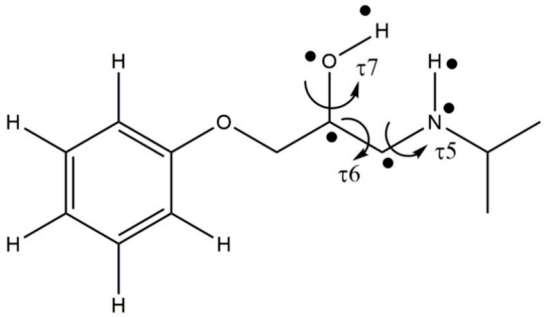
Table S2. Selected dihedral angles of BE_I and BE_IV (S enantiomer).

Dihedral angle (°)	BE_IV	BE_I (ROKNUB)
τ_1	−178,7(2)	171
τ_2	−178,2(2)	−161
τ_3	58,6(3)	−62
τ_4	169,6(2)	176
τ_5	43(2)	81
τ_6	−66,3(3)	−62
τ_7	−163(2)	135

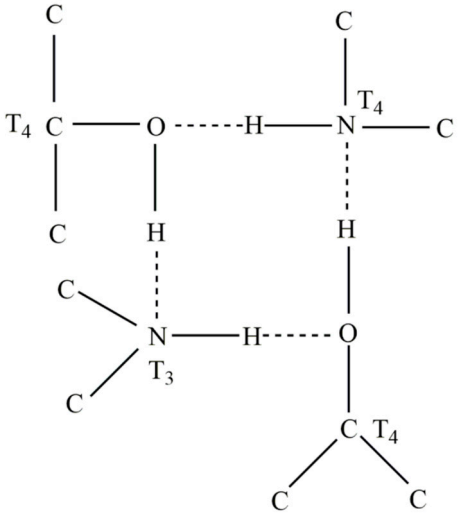
Table S3. Selected intermolecular interactions in **BE_I** (ROKNUB refcode in the Cambridge. Structural Database).

	X···Y (Å	H···Y(Å)	X-H···Y (°)
O2-H2o···N1[1]	2.862	2.04	174
N1-H1n···O2[2]	3.380	2.56	161

[1] =1 − x,2-y,1 − z; [2] = −x,2 − y, −z.



Scheme S1. Molecular sketch showing the dihedral angles definition for the ethanolamine fragment.



Scheme S2. Fragment searched in the CSD for the R4, 4(8) pattern.

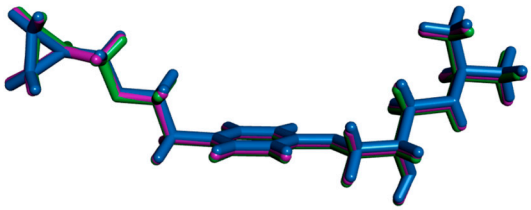


Figure S1. Superimposition of the betaxolol molecule in **BE_IV** at 100 (blue), 200 (green) and 300 K (pink).

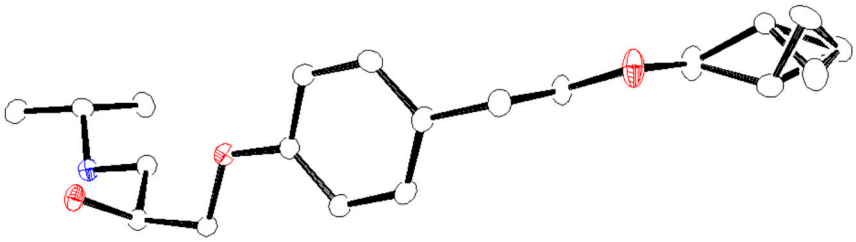


Figure S2. Ortep-3 view of the betaxolol moiety in the asymmetric unit of **BE_IV** showing the double position of the cyclopropylmethoxy fragment. (ellipsoid probability 20%, hydrogen atoms have been omitted for the sake of clarity).

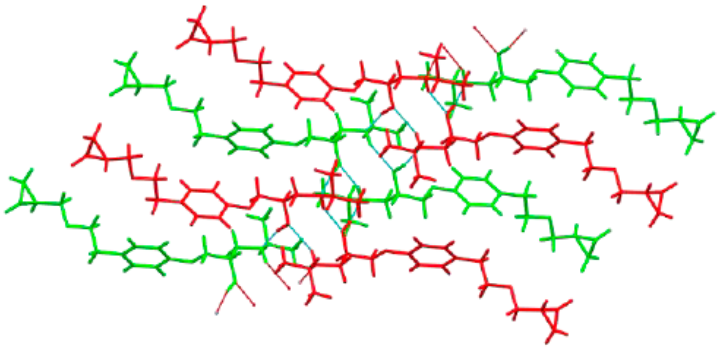


Figure S3. View of the crystal packing of **BE_IV** along the *a* axis direction highlighting the facing betaxolol chains held together by the OH...N hydrogen bonds. For sake of clarity only the set of coordinates having the highest occupancy factor has been reported.

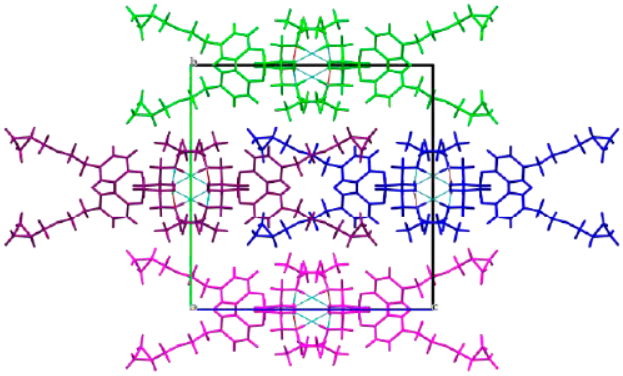


Figure S4. View of the crystal packing of **BE_IV** (different color codes have been used to identify R and S enantiomers). For sake of clarity only the set of coordinates having the highest occupancy factor has been reported.

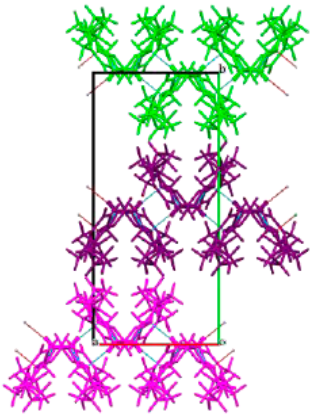


Figure S5. View of the crystal packing of **BE_IV** along the *c* axis direction highlighting the zig-zag arrangement of the alternating R and S betaxolol molecules within each chain. For sake of clarity for cyclopropylmethoxy the model having the highest occupancy factor was shown.