

Supplementary Information

for the manuscript

Synthesis, Crystal Structures and Tautomerism in Novel Oximes

Based on Hydroxyalkylpyrazolones

Julio Belmar,^{*a} José Quezada, Claudio A. Jiménez^{*a}, Pau Díaz-Gallifa^b, Jorge Pasán^b and Catalina Ruiz-Pérez^b

^aDepartamento de Química Orgánica. Facultad de Ciencias Químicas. Universidad de Concepción.

Casilla 160-C, Concepción. Chile. Email: jbelmar@udec.cl, cjimenez@udec.cl

^bLaboratorio de Rayos X y Materiales Moleculares. Departamento de Física Fundamental II. Facultad de Física. Universidad de La Laguna. Avda. Astrofísico Francisco Sánchez s/n, E-38204 La Laguna. Spain.

Figure S1. Diastereomers of the oximino tautomer of compound **3**

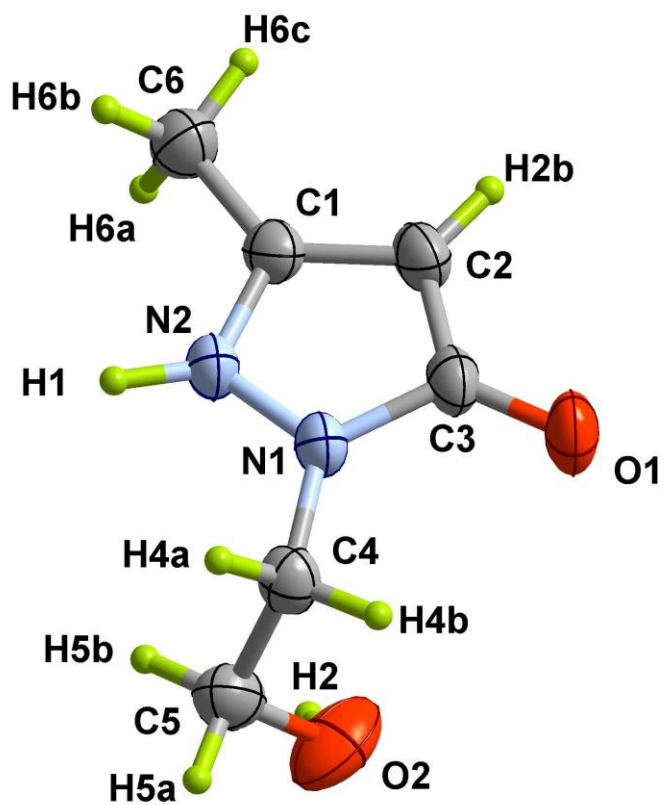
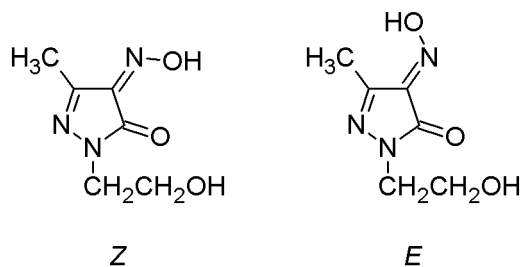


Figure S2. A view of the asymmetric unit of **1** together with the atom numbering scheme.

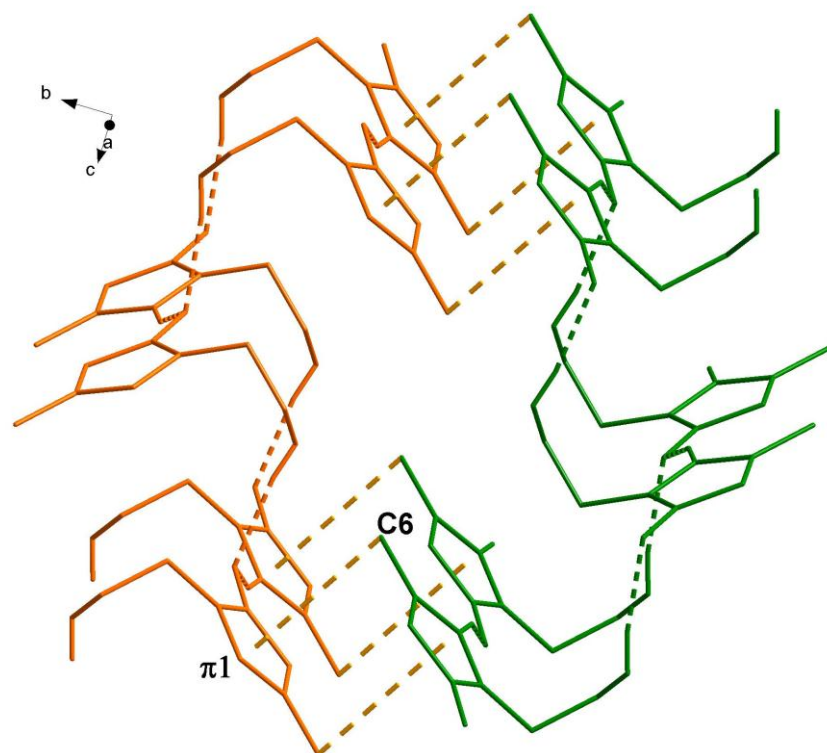


Figure S3. Supramolecular association of hydrogen bond layers (green and orange) mediated by CH... π interaction (yellow broken lines).

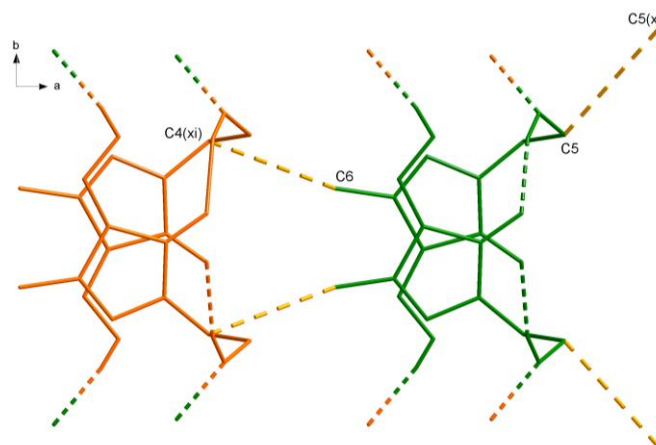


Figure S4. Layers of *ac*-plane of **3** projected on the *ab*-plane showing its connection to four adjacent molecules through CH₃...CH₃ hydrophobic type interactions (yellow broken lines)