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Supporting information for article:

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Supporting Information

Extensive analysis of N—H...O hydrogen bonding in four classes of phosphorus compounds- a combined experimental and database study

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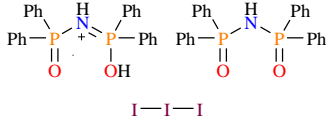
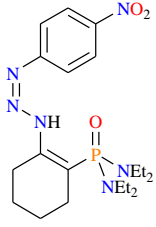
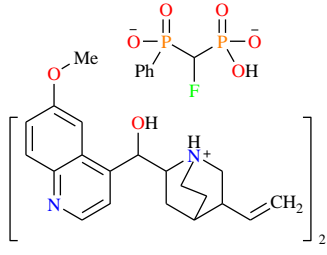
^dLaboratorio de Estudios Cristalográficos, IACT, CSIC-Universidad de Granada, Avda. de las Palmeras 4, 18100, Armilla, Granada, Spain

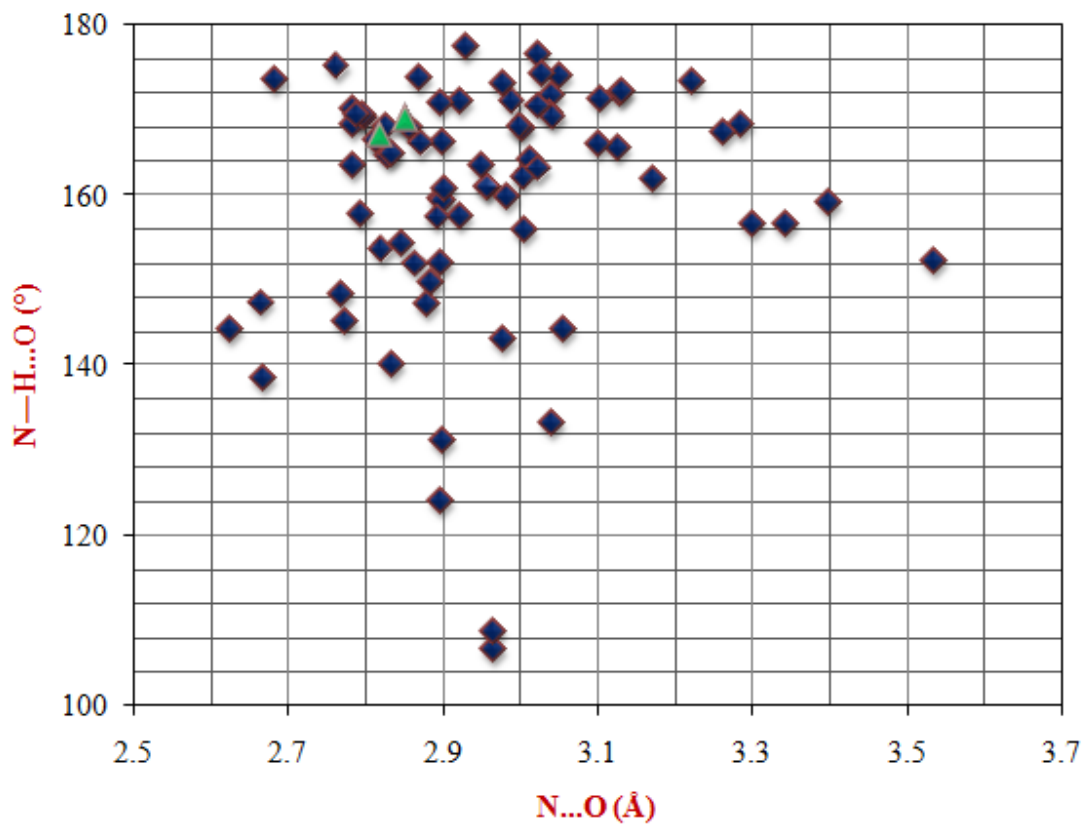
Correspondence e-mail: pourayoubi@um.ac.ir

Table S1 The chemical structures of the refcodes (arranged alphabetically) discussed in the text.

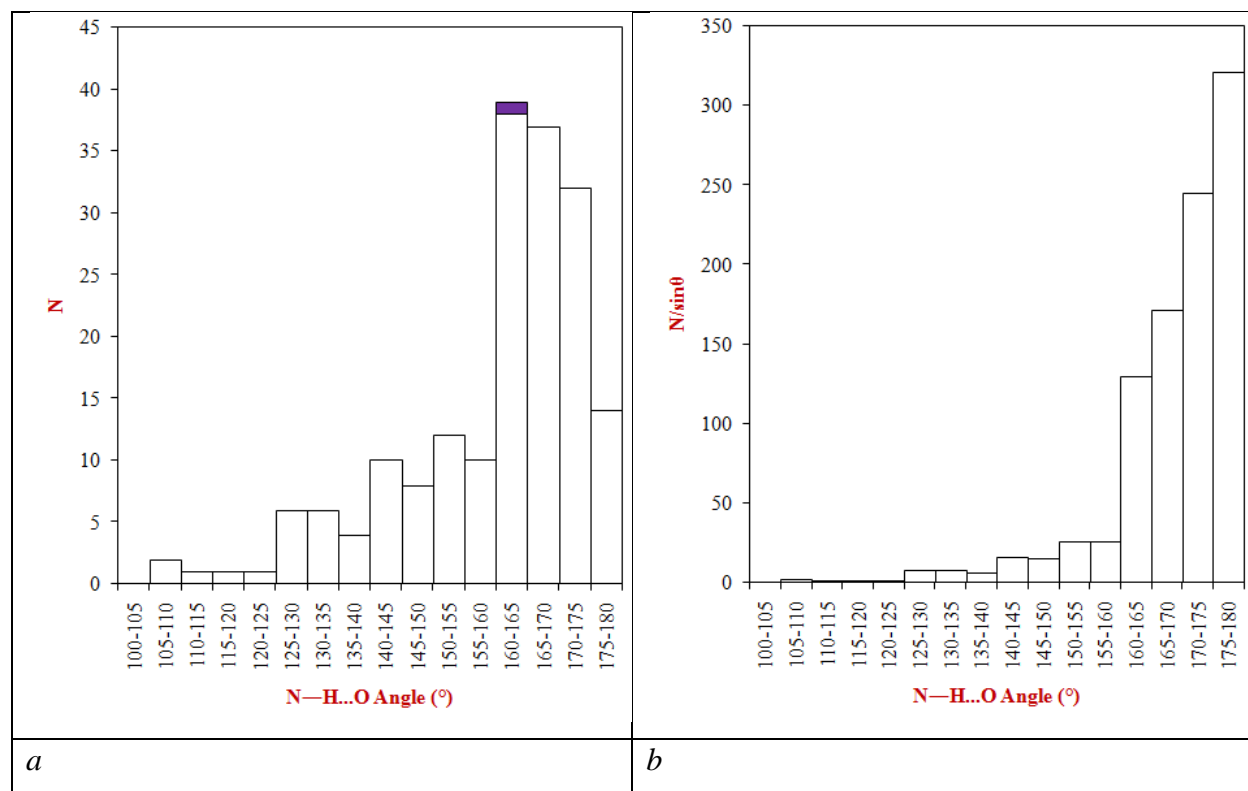
AFAYIQ		KUCKIE	<p>CH₃OH</p>
AQOHIY		PESGAW	
EZADEP	<p>CHCl₃</p>	PURZAF	
FAGBUK	<p>ClO₄</p>	ROJVET	
FAQREV	<p>Br</p>	ROLKUY	
FOYTUI	<p>2 H₂O</p>	TANZAL	
JICKEL		URESEQ	
KAWYIQ		VAWDUS	

Table S1 Continued.

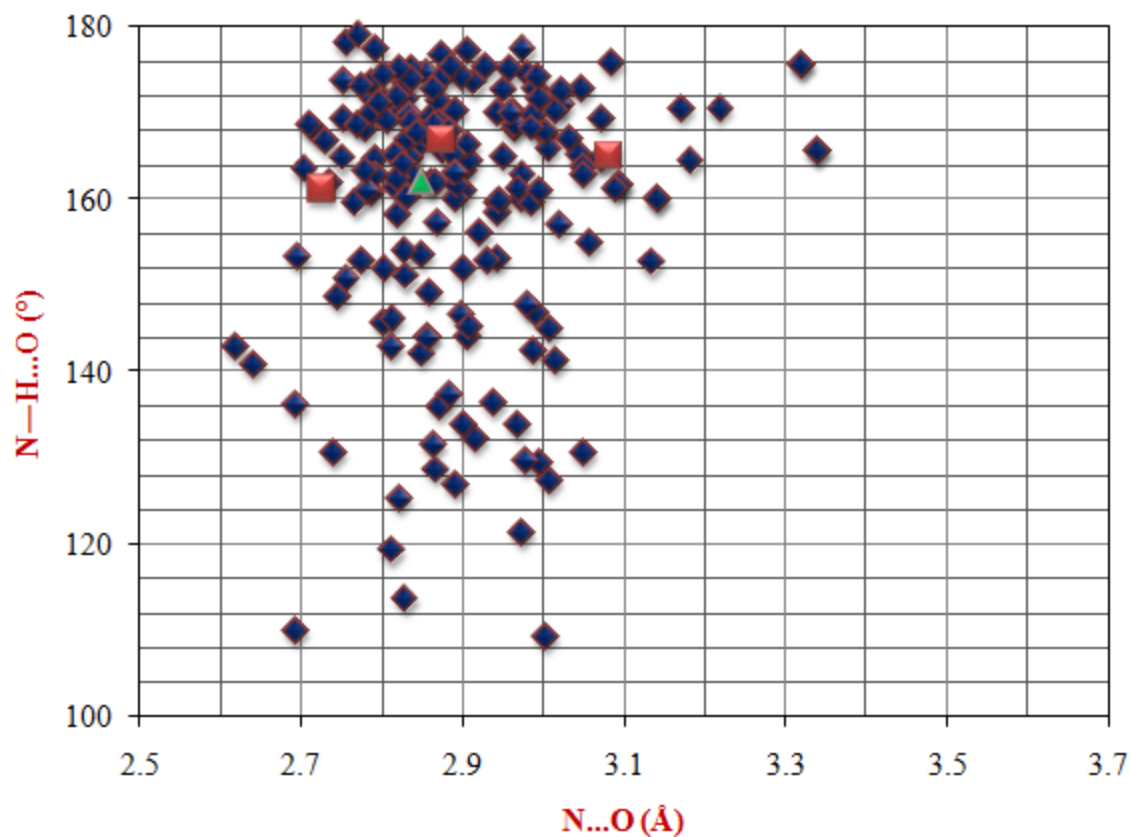
WINLEL	 <p>I—I—I</p>	YEDPIM10	
YUKMOG	 <p>Me—C(O)Me 1.5 H₂O</p>		

**Figure S1**

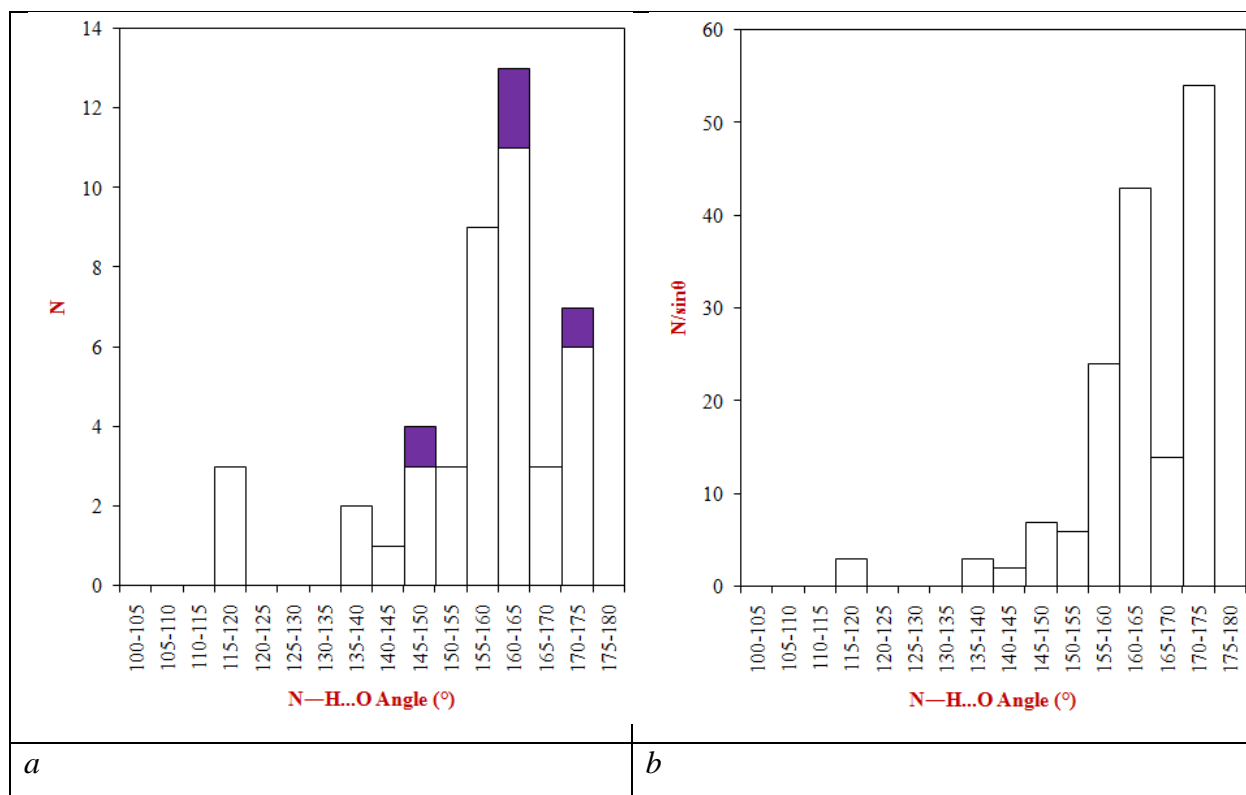
A scatterplot of N—H...O angles against N...O distances for (C)P(O)(N)₂ structures from a CSD search (dark blue squares), and including the data of structure (I) (green triangles).

**Figure S2**

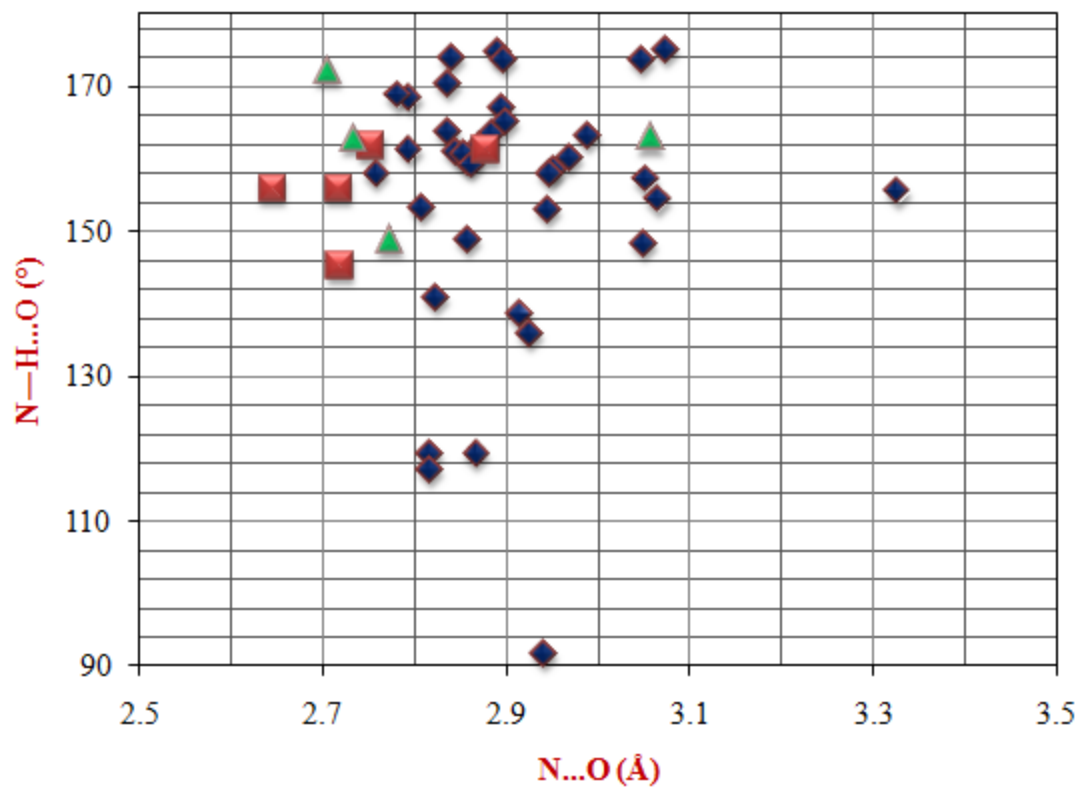
(a) A histogram of N—H...O angles for $(C)_2P(O)(N)$ structures from a CSD search, and including the N—H...O angle of structure (II) (purple part). (b) Histogram after ‘cone correction’, considering all of the data from CSD and structure (II) (the angular distribution is weighted by a correction factor of $1/\sin\theta$ to properly reflect angular preferences). The maximum population of N—H...O angles is between 160 and 165° and the N—H...O angle of structure (II) is also found in this region. The other important region in this family is within 165 and 170°. After cone correction, the maximum data are between 175 and 180°.

**Figure S3**

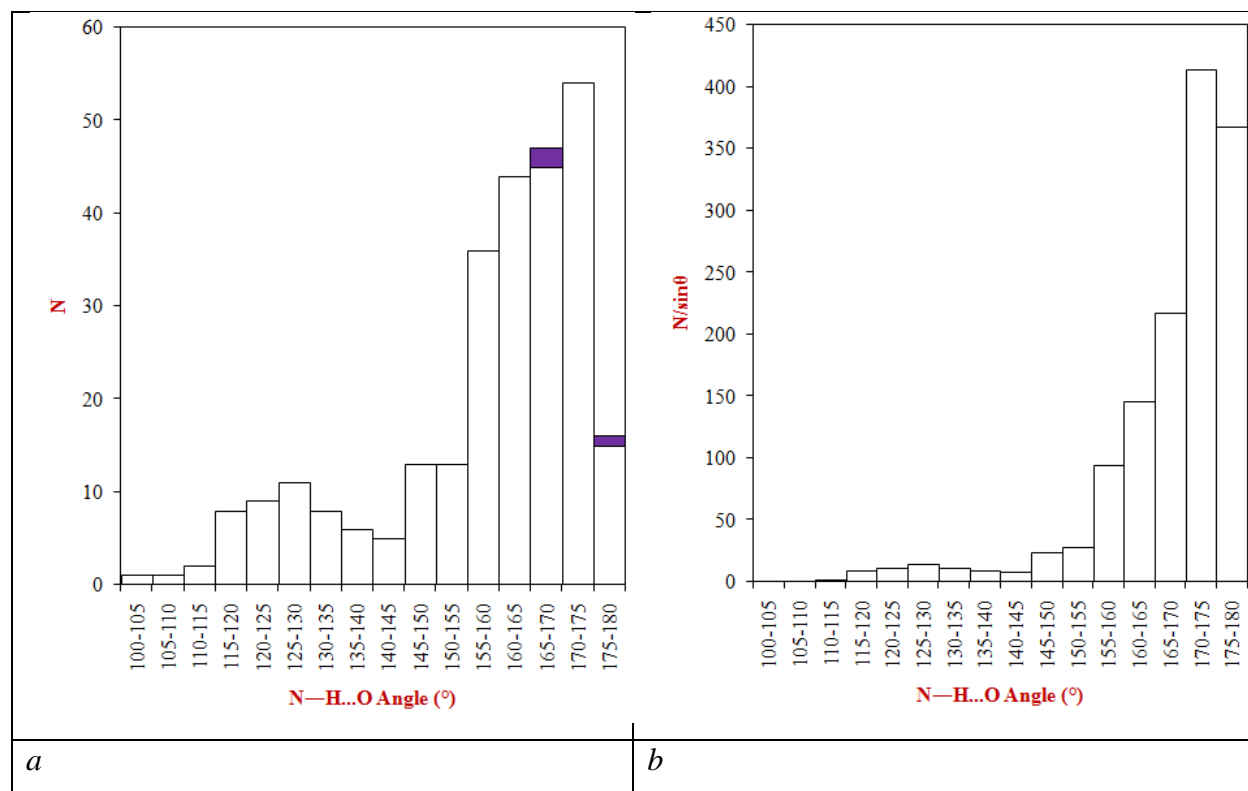
A scatterplot of N—H...O angles against N...O distances for $(C)_2P(O)(N)$ structures from a CSD search, and including one hit belonging to structure (II). The red and dark blue squares are related to the cation-anion and neutral structures, respectively. The one hit related to structure (II) is given as a green triangle.

**Figure S4**

(a) A histogram of N—H...O angles for (C)P(O)(O)(N) structures from a CSD search, and including the angle of structure (III) (purple part) [one hit with the angle of about 92° was excluded from the histogram]. (b) Histogram after ‘cone correction’, considering all of the data from CSD and structure (III) (the angular distribution is weighted by a correction factor of $1/\sin\theta$ to properly reflect angular preferences). The maximum population of N—H...O angles is between 160 and 165° and two of the N—H...O angles of structure (III) are also found in this region. After cone correction, the maximum data are between 170 and 175°.

**Figure S5**

A scatterplot of N—H...O angles against N...O distances for (C)P(O)(O)(N) structures from a CSD search, and including the data of structure (III). The red and dark blue squares are related to the cation-anion and neutral structures, respectively. The data related to structure (III) are given as green triangles.

**Figure S6**

(a) A histogram of N—H...O angles for $(C)_2P(O)(O)$ structures from a CSD search, and including the angles of structure (IV) (purple parts). (b) Histogram after ‘cone correction’, considering all of the data from CSD and structure (IV) (the angular distribution is weighted by a correction factor of $1/\sin\theta$ to properly reflect angular preferences). The maximum population of N—H...O angles is between 170 and 175°. After cone correction, the maximum data are also between 170 and 175°.