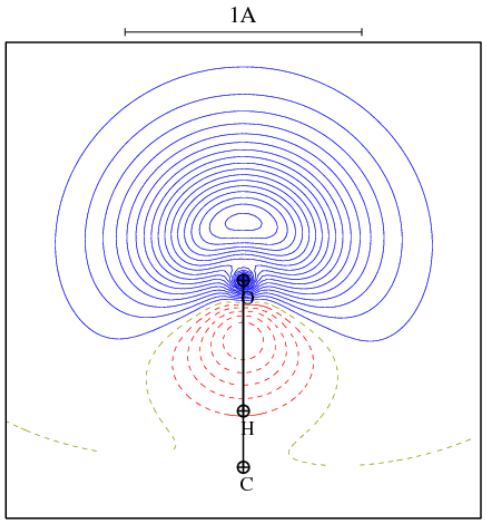
**Supplementary material.**

**Figure S1**

Example of another deformation of the experimental electron density in the lone pairs plane of a phenol group found in(±)-8'-benzhydryl-ideneamino-1,1'-binaphthyl-2-ol (Farrugia, L. J.; Kocovský, P.; Senn, H. M.; Vyskocil, S. *Acta Crystallogr*. 2009. B*65*, 757-769.)




Contours ±0.05e/Å$^3$. positive: solid blue lines. Negative: dashed red lines.

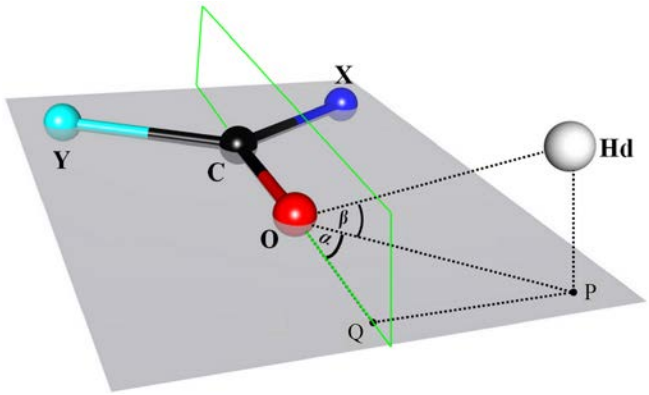



**Figure S2**: Diagram describing the $\alpha$ and $\beta$ angles obtainment for carbonyl.
P is the projection of Hd on the XYC=O plane containing the two lone pairs.
Q is the projection of H on the C=O line.

Distances and angles used from the Cambridge Structural Database:

- $OH_d$ = distance (O…Hd)
- $PH_d$ = distance( Hd , COH plane )
- (CO , $OH_d$) angle

Derived geometric data.

$OP = ( OH_d^2 - pH_d^2 )^{1/2}$

$OQ = \cos(CO,OH_d) * OH_d$

$\alpha$ = arccosine ( OQ / OP )

$\beta$ = arcsine ( $PH_d$ / $OH_d$ )

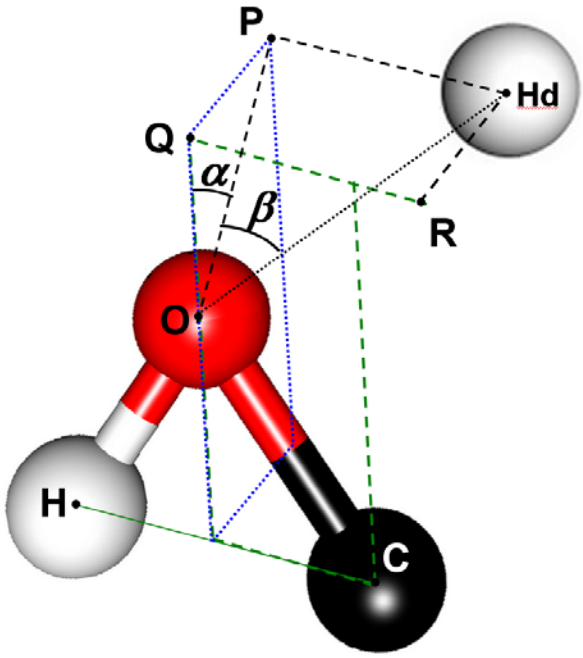



**Figure S3**:
Diagram describing the $\alpha$ and $\beta$ angles obtainment for hydroxyl group C-O-H.

R is the projection of $H_d$ on the COH plane.
Q is the projection on the inner bisecting line.
P is the projection on the COH bisecting plane containing the two electron lone pairs.

**Distances and angles used from the Cambridge Structural Database:**

- angles $COH_d$ COH
- distances $OH_d$ $CH_d$ CO
- distance to COH plane: PQ = $RH_d$

**Derived geometric data:**

OR = $(OH_d^2 - RH_d^2)^{1/2}$ as $ORH_d = 90°$
CR = $(CH_d^2 - RH_d^2)^{1/2}$ as $CRH_d = 90°$

Al-Kashi Theorem: COP = arcosine ( CO*CO + OR*OR – CR*CR ) / ( CO * OR )
COQ = 180 - COH / 2 as OQ is bisecting triangle COH.
COR + ROQ = COQ addition of angles
Then ROQ = COQ – COR = 180 – COH / 2 – COR
QR = OR * sin(ROQ) , QR = $PH_d$ is the distance to the electron lone pairs plane
OQ = $( OR^2 - QR^2 )^{1/2}$ as OQR=90°
$\beta$ = arcsine ( PHd / $OH_d$ ) $\alpha$ = arctan ( PQ / OQ )