

Supplementary Material (ESI) for New Journal of Chemistry  
This journal is (c) The Royal Society of Chemistry and  
The Centre National de la Recherche Scientifique, 2009

## **Supporting Information**

**for**

### **Three new co-crystals of hydroquinone: Crystal structures and Hirshfeld surface analysis of intermolecular interactions**

**Henrik F. Clausen,<sup>a</sup> Marie S. Chevallier,<sup>a</sup> Mark A. Spackman<sup>b</sup> and Bo B. Iversen<sup>\*a</sup>**

Bondlength [ $\text{\AA}$ ] of the hydroquinone entities in the structures **1**, **2** and **3**.

Compound	HQa(1)	HQb(1)	HQa(2)	HQa(3)	HQb(3)	HQc(3)	HQd(3)
Cx1-Ox1	1.3836(14)	1.3770(14)	1.366(2)	1.3829(16)	1.3816(15)	1.3824(14)	1.3747(15)
Cx1-Cx2	1.3865(18)	1.3868(18)	1.389(2)	1.3901(17)	1.3851(17)	1.3893(17)	1.3878(17)
Cx2-Cx3	1.3879(17)	1.3854(17)	1.386(3)	1.3849(18)	1.3921(17)	1.3894(17)	1.3867(18)
Cx3-Cx4	1.3869(16)	1.3916(16)	1.388(3)	1.3921(16)	1.3922(18)	1.3843(16)	1.3912(18)
Cx4-Cx5			1.390(3)	1.3902(18)			
Cx5-Cx6			1.383(3)	1.3874(18)			
Cx6-Cx1			1.390(3)	1.3896(16)			
Cx4-Ox4			1.375(2)	1.3691(16)			

Bondangles [ $^{\circ}$ ] of the hydroquinone entities in the structures **1**, **2** and **3**.

Compound	HQa(1)	HQb(1)	HQa(2)	HQa(3)	HQb(3)	HQc(3)	HQd(3)
Cx2-Cx1-Ox1	122.64(10)	122.34(10)	123.02(17)	122.52(10)	117.29(11)	122.36(10)	118.19(11)
Cx6-Cx1-Ox1	117.48(11)	117.88(11)	117.75(16)	117.60(11)	122.37(11)	117.26(10)	122.53(11)
Cx1-Cx2-Cx3	119.99(11)	120.12(10)	120.33(17)	119.97(11)	120.29(12)	119.31(11)	120.51(12)
Cx2-Cx3-Cx4	120.13(12)	120.11(12)	120.17(17)	120.33(11)	119.38(11)	120.33(11)	120.21(11)
Cx3-Cx4-Cx5	119.88(11)	119.77(11)	119.68(17)	119.57(12)	120.33(11)	120.36(11)	119.28(11)
Cx4-Cx5-Cx6			119.94(17)	120.16(11)			
Cx5-Cx6-Cx1			120.65(17)	120.08(11)			
Cx6-Cx1-Cx2			119.23(17)	119.88(11)			
Cx3-Cx4-Ox4			122.49(16)	117.47(11)			
Cx5-Cx4-Ox4			117.83(16)	122.94(11)			
Variation of angle	0.13	0.23	0.67	0.43	0.62	0.69	0.72

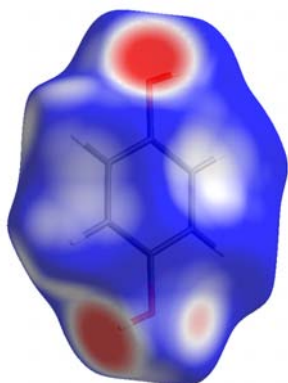
Supplementary Material (ESI) for New Journal of Chemistry

This journal is (c) The Royal Society of Chemistry and

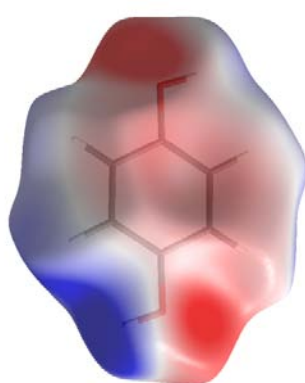
The Centre National de la Recherche Scientifique, 2009

a) Hirshfeld surface of HQa(**1**) with  $d_{\text{norm}}$  ranging from  $-0.5 \text{ \AA}$  (blue) to  $0.5 \text{ \AA}$  (red). b) The electrostatic potential plotted on the Hirshfeld surface of HQa(**1**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. c) The electrostatic potential plotted on an isosurface of the electron density of  $0.001 \text{ au}$  of HQa(**1**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region.

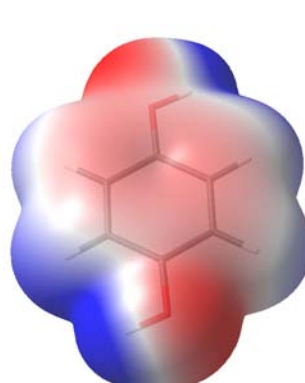
a)



b)

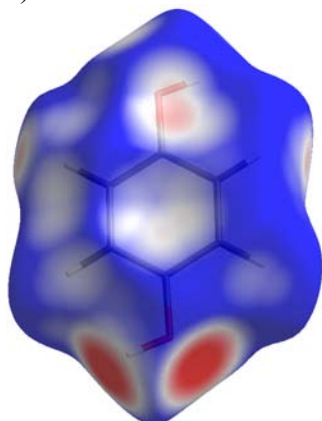


c)

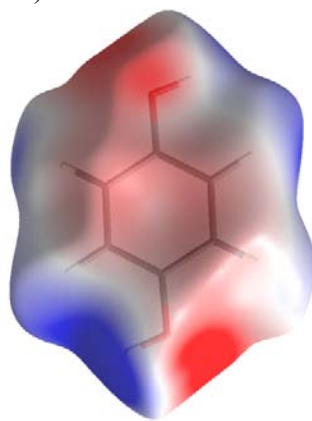


a) Hirshfeld surface of HQb(**1**) with  $d_{\text{norm}}$  ranging from  $-0.5 \text{ \AA}$  (blue) to  $0.5 \text{ \AA}$  (red). b) The electrostatic potential plotted on the Hirshfeld surface of HQb(**1**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. c) The electrostatic potential plotted on an isosurface of the electron density of  $0.001 \text{ au}$  of HQb(**1**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region.

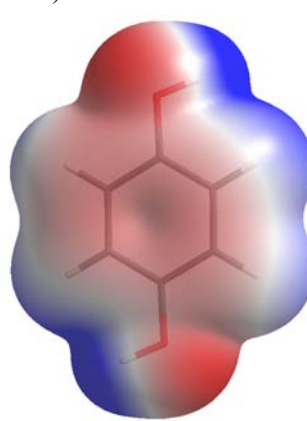
a)



b)



c)



Supplementary Material (ESI) for New Journal of Chemistry

This journal is (c) The Royal Society of Chemistry and

The Centre National de la Recherche Scientifique, 2009

a) Hirshfeld surface of propan-2-ol(**1**) with  $d_{\text{norm}}$  ranging from  $-0.5 \text{ \AA}$  (blue) to  $0.5 \text{ \AA}$  (red).

b) The electrostatic potential plotted on the Hirshfeld surface of propan-2-ol(**1**) with

values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. c) The electrostatic

potential plotted on an isosurface of the electron density of  $0.001 \text{ au}$  of propan-2-ol(**1**)

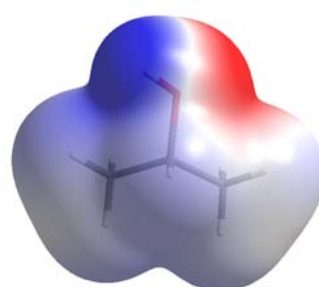
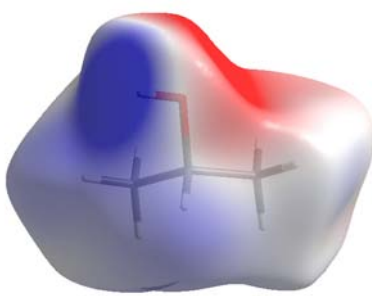
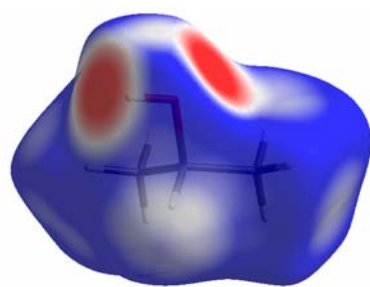
with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. d) Same as a) turned

$\sim 180^\circ$ . e) Same as b) turned  $\sim 180^\circ$ . f) Same as c) turned  $\sim 180^\circ$ .

a)

b)

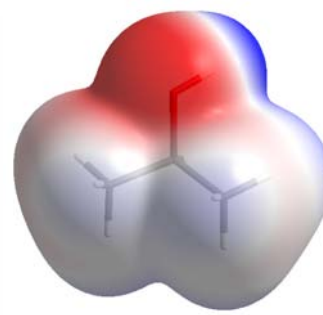
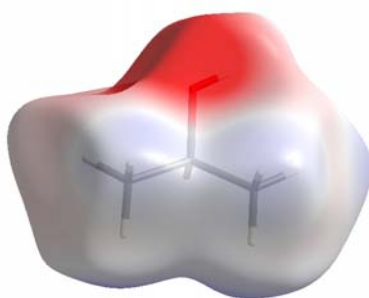
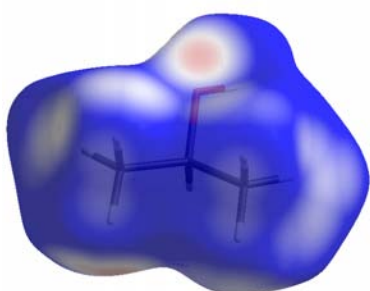
c)



d)

e)

f)



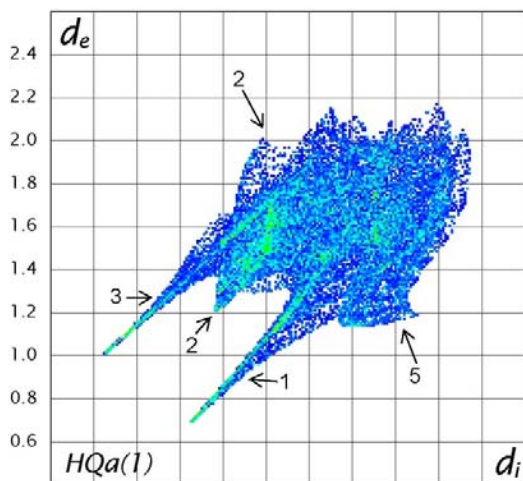
Supplementary Material (ESI) for New Journal of Chemistry

This journal is (c) The Royal Society of Chemistry and

The Centre National de la Recherche Scientifique, 2009

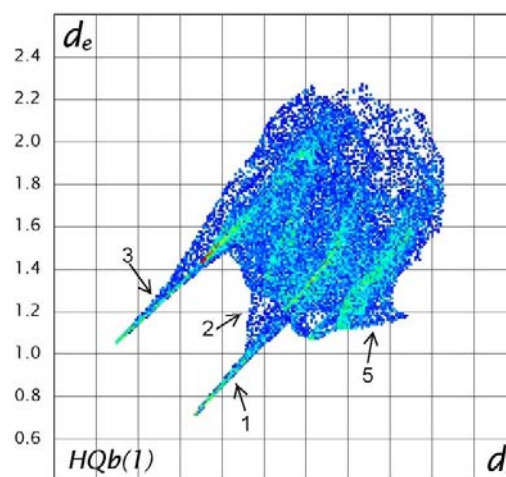
Fingerprint plots of the hydroquinone molecules a) HQa(1), b) HQb(1) and c) propan-2-ol(1) going from left to right. Close contacts are divided into 5 regions; 1 is O...H, 2 is H...H, 3 is H...O, 4 is H...C and 5 is C...H.

a)



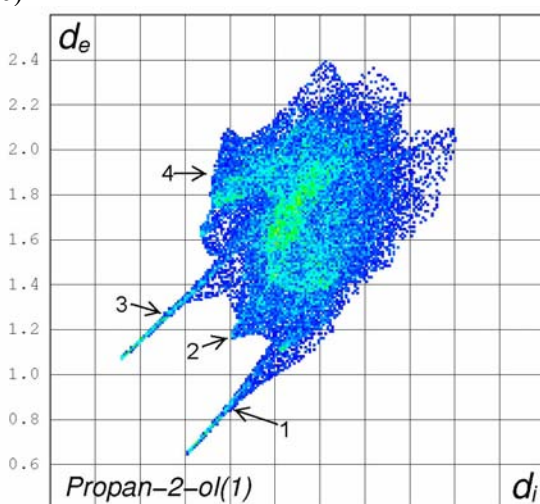
(A) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4

b)



(A) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4

c)



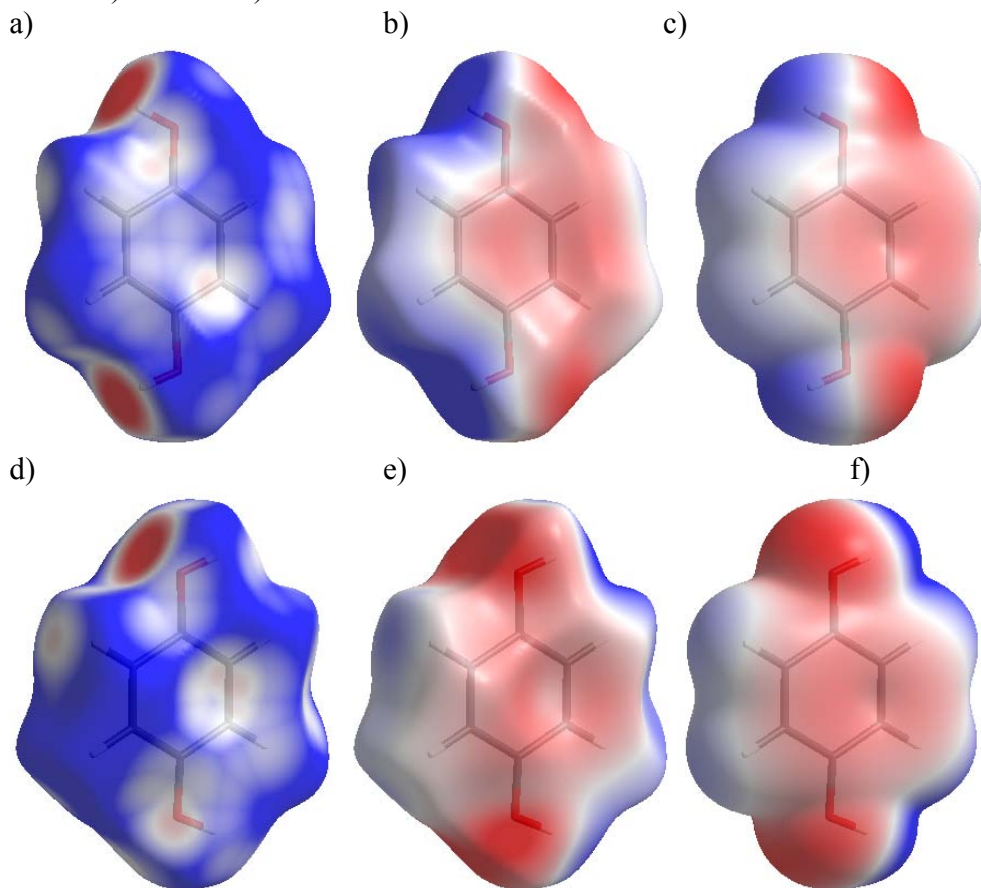
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4

Supplementary Material (ESI) for New Journal of Chemistry

This journal is (c) The Royal Society of Chemistry and

The Centre National de la Recherche Scientifique, 2009

a) Hirshfeld surface of HQa(2) with  $d_{\text{norm}}$  ranging from  $-0.5 \text{ \AA}$  (blue) to  $0.5 \text{ \AA}$  (red). b) The electrostatic potential plotted on the Hirshfeld surface of HQa(2) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. c) The electrostatic potential plotted on an isosurface of the electron density of  $0.001 \text{ au}$  of HQa(2) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. d) Same as a) turned  $\sim 180^\circ$ . e) Same as b) turned  $\sim 180^\circ$ . f) Same as c) turned  $\sim 180^\circ$ .

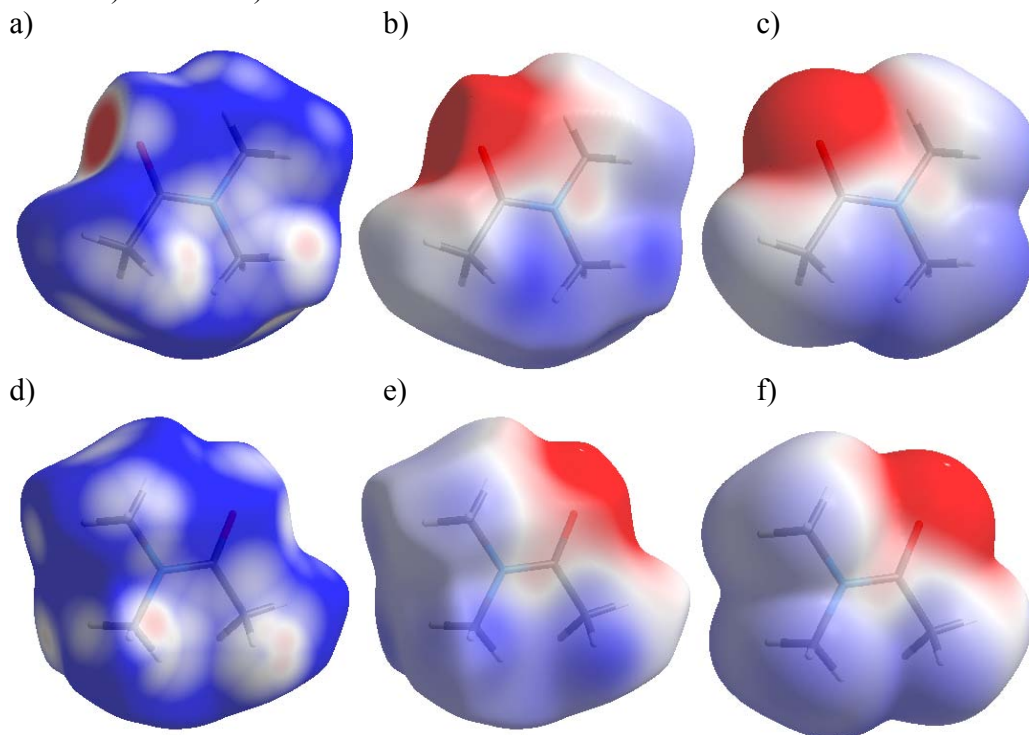


Supplementary Material (ESI) for New Journal of Chemistry

This journal is (c) The Royal Society of Chemistry and

The Centre National de la Recherche Scientifique, 2009

a) Hirshfeld surface of DMA with  $d_{\text{norm}}$  ranging from  $-0.5 \text{ \AA}$  (blue) to  $0.5 \text{ \AA}$  (red). b) The electrostatic potential plotted on the Hirshfeld surface of DMA with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. c) The electrostatic potential plotted on an isosurface of the electron density of  $0.001 \text{ au}$  of DMA with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. d) Same as a) turned  $\sim 180^\circ$ . e) Same as b) turned  $\sim 180^\circ$ . f) Same as c) turned  $\sim 180^\circ$ .



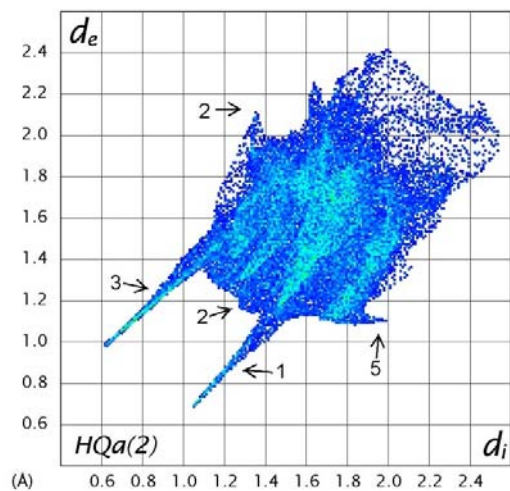
Supplementary Material (ESI) for New Journal of Chemistry

This journal is (c) The Royal Society of Chemistry and

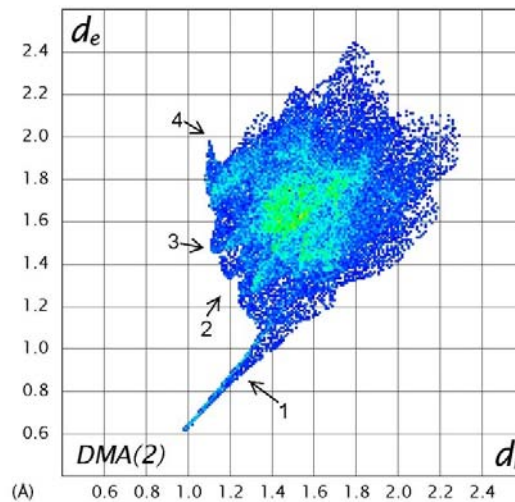
The Centre National de la Recherche Scientifique, 2009

Fingerprint plots of the hydroquinone molecules a) HQa(2) and b) DMA. Close contacts are divided into 5 regions; 1 is  $O\cdots H$ , 2 is  $H\cdots H$ , 3 is  $H\cdots O$ , 4 is  $H\cdots C$  and 5 is  $C\cdots H$ .

a)



b)





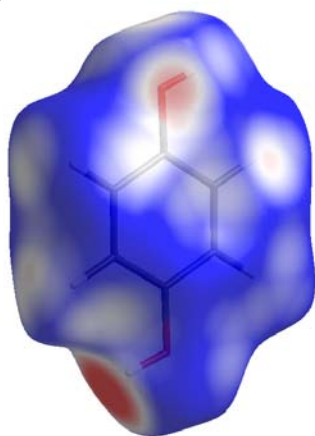
Supplementary Material (ESI) for New Journal of Chemistry

This journal is (c) The Royal Society of Chemistry and

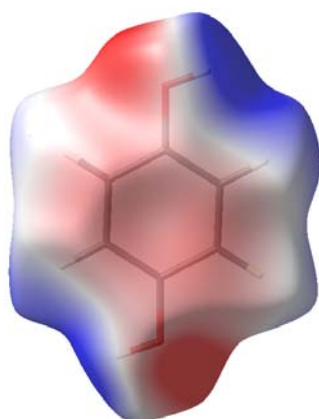
The Centre National de la Recherche Scientifique, 2009

a) Hirshfeld surface of HQa(**3**) with  $d_{\text{norm}}$  ranging from  $-0.5 \text{ \AA}$  (blue) to  $0.5 \text{ \AA}$  (red). b) The electrostatic potential plotted on the Hirshfeld surface of HQa(**3**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. c) The electrostatic potential plotted on an isosurface of the electron density of  $0.001 \text{ au}$  of HQa(**3**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. d) Same as a) turned  $\sim 180^\circ$ . e) Same as b) turned  $\sim 180^\circ$ . f) Same as c) turned  $\sim 180^\circ$ .

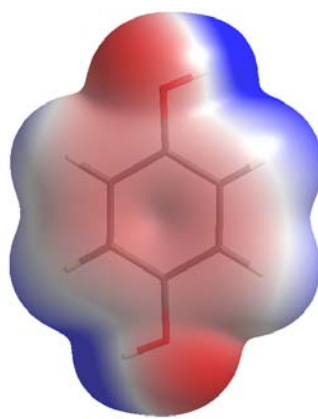
a)



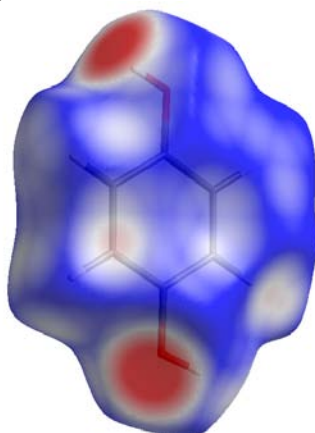
b)



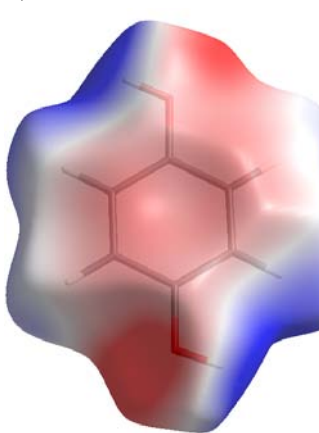
c)



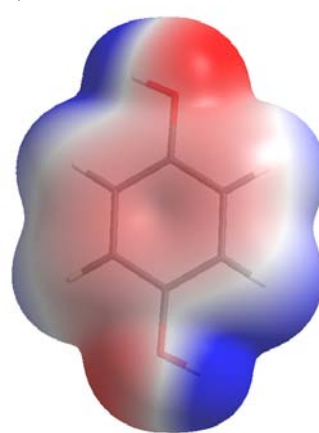
d)



e)

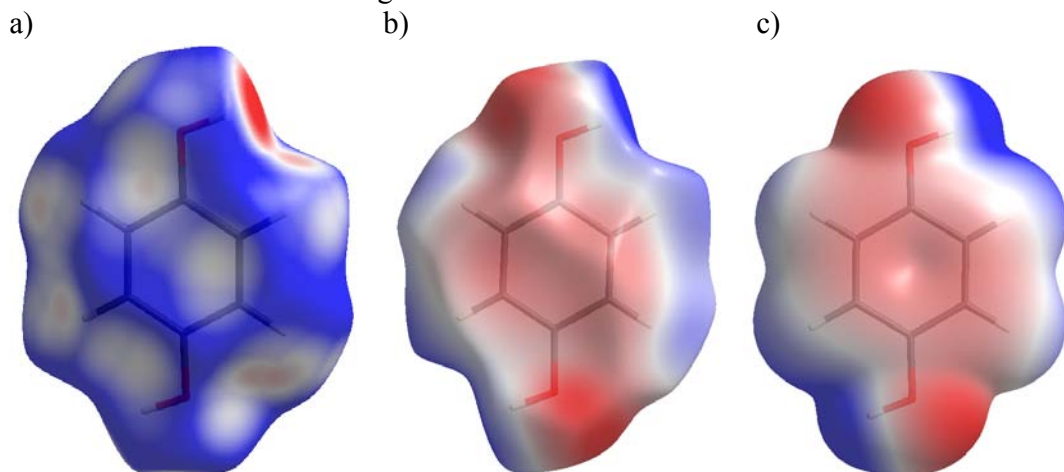


f)

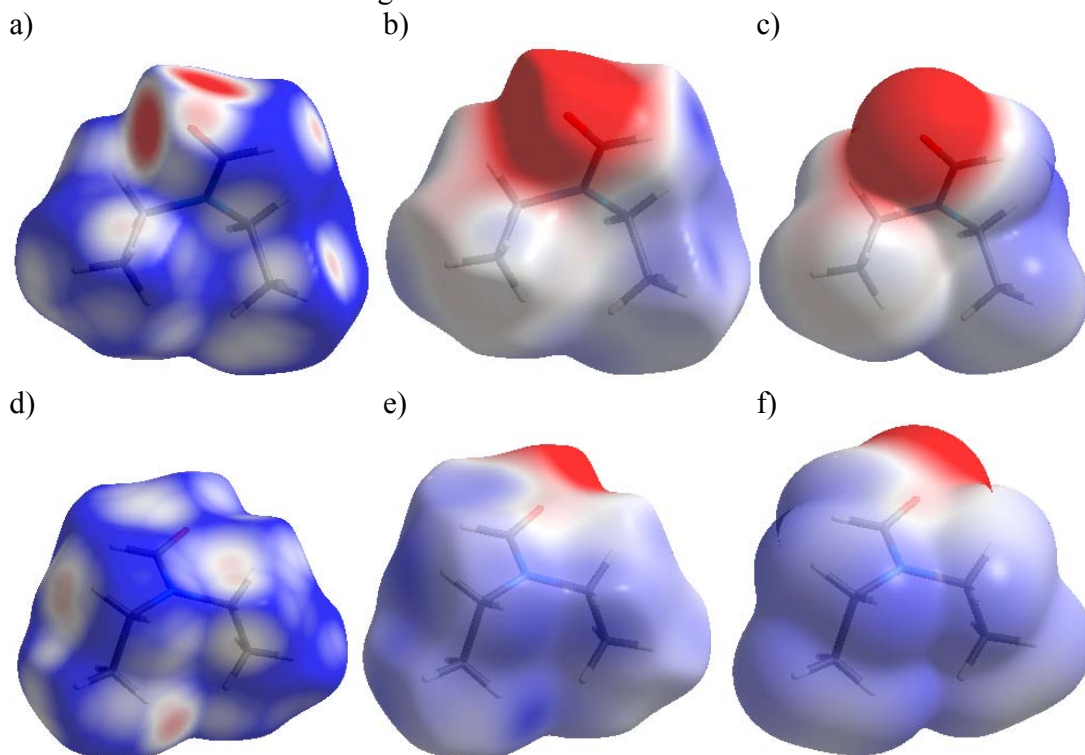




a) Hirshfeld surface of HQd(**3**) with  $d_{\text{norm}}$  ranging from  $-0.5 \text{ \AA}$  (blue) to  $0.5 \text{ \AA}$  (red). b) The electrostatic potential plotted on the Hirshfeld surface of HQd(**3**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. c) The electrostatic potential plotted on an isosurface of the electron density of  $0.001 \text{ au}$  of HQd(**3**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region.



a) Hirshfeld surface of DEF(**3**) with  $d_{\text{norm}}$  ranging from  $-0.5 \text{ \AA}$  (blue) to  $0.5 \text{ \AA}$  (red). b) The electrostatic potential plotted on the Hirshfeld surface of DEF(**3**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region. c) The electrostatic potential plotted on an isosurface of the electron density of  $0.001 \text{ au}$  of DEF(**3**) with values from  $0.05 \text{ a.u.}$  in the blue to  $-0.05 \text{ a.u.}$  in the red region.

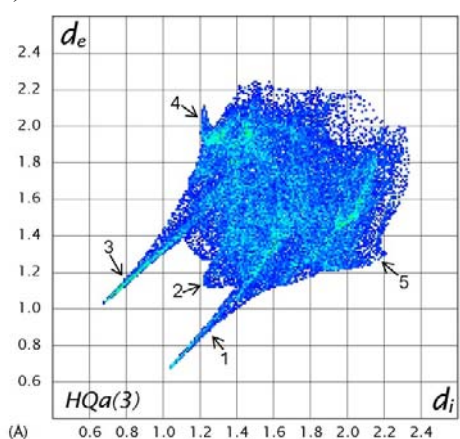


Fingerprint plots of the hydroquinone molecules a) HQa(3), b) HQb(3), c) HQc(3), d)

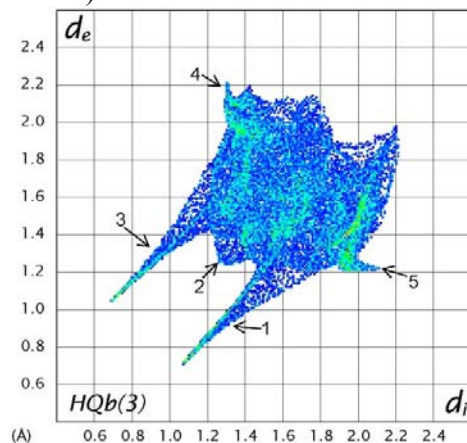
HQd(3) and e) DEF(3) going from left to right. Close contacts are divided into 5 regions;

1 is O...H, 2 is H...H, 3 is H...O, 4 is H...C and 5 is C...H.

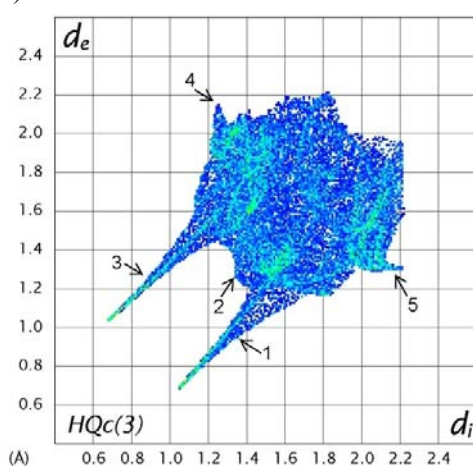
a)



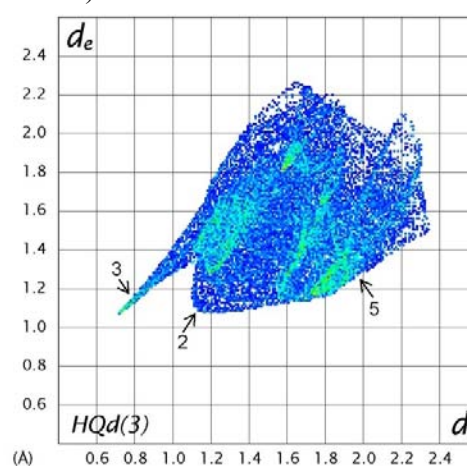
b)



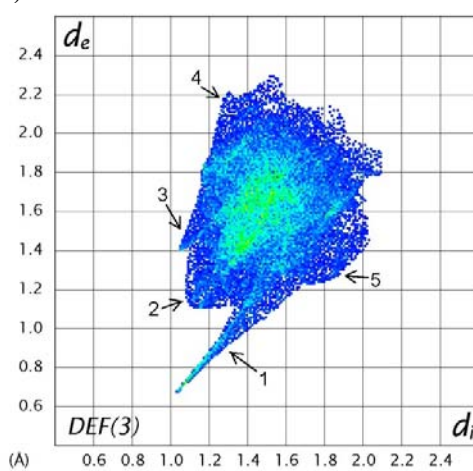
c)



d)



e)



Supplementary Material (ESI) for New Journal of Chemistry

This journal is (c) The Royal Society of Chemistry and

The Centre National de la Recherche Scientifique, 2009

Table of calculated dipole moments of **1**, **2** and **3** in Debye.

Molecule	Dipole moment / [Debye]	Conformation
HQa( <b>1</b> )	0	Trans
HQb( <b>1</b> )	0	Trans
Propan-2-ol( <b>1</b> )	1.662	
HQa( <b>2</b> )	2.7316	Cis
DMA( <b>2</b> )	4.2132	
HQa( <b>3</b> )	0.3215	Trans
HQb( <b>3</b> )	0	Trans
HQc( <b>3</b> )	0	Trans
HQd( <b>3</b> )	0	Trans
DEF( <b>3</b> )	4.3433	