Supporting Information

Halogen bonding in 2,5-dichloro-1,4-benzoquinone: Insights from experimental and theoretical charge density analysis

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Table S1. Topological features of all the covalent bonds of **1**. d_1 and d_2 are the distances from the CP to the first atom (A) and second atom (B) respectively. The interaction length, $R_{ij} = (d_1 + d_2)$. The values from periodic calculations using B3LYP 6-31G(*d,p*) method are given in italics.

Bond	R_{ij} (Å)	$\boldsymbol{\rho(r_b)}$ (eÅ^{-3})	$\boldsymbol{\nabla^2\rho(r_b)}$ (eÅ^{-5})	$\boldsymbol{d_1}$ (Å)	$\boldsymbol{d_2}$ (Å)	$\boldsymbol{\lambda_1}$	$\boldsymbol{\lambda_2}$	$\boldsymbol{\lambda_3}$	$\boldsymbol{\varepsilon}$
Cl1–C1	1.7102(2) *1.7101*	1.31(1) *1.35(1)*	–1.13(3) *–2.52(1)*	0.9307 *0.9420*	0.7795 *0.7682*	–7.85 *–7.78*	–7.03 *–7.17*	13.75 *12.43*	0.12 *0.08*
O1–C2	1.2204(3) *1.2204*	2.94(5) *2.77(1)*	–34.37(2) *–22.69(5)*	0.7706 *0.7916*	0.4499 *0.4289*	–29.11 *–24.66*	–25.91 *–22.90*	20.65 *24.87*	0.12 *0.08*
C1–C2	1.4960(3) *1.4960*	1.86(2) *1.77(1)*	–13.80(6) *–13.34(1)*	0.7318 *0.7511*	0.7643 *0.7451*	–14.04 *–12.74*	–11.88 *–11.04*	12.12 *10.44*	0.18 *0.15*
C2–C3	1.4762(3) *1.4762*	1.78(2) *1.79(1)*	–12.85(6) *–13.21(2)*	0.7544 *0.7640*	0.7219 *0.7121*	–13.63 *–12.82*	–11.55 *–11.25*	12.33 *10.86*	0.18 *0.14*
C3–H3	1.0830 *1.0830*	2.04(4) *1.89(1)*	–25.03(7) *–21.16(1)*	0.6934 *0.6884*	0.3896 *0.3946*	–20.31 *–17.61*	–18.71 *–16.95*	13.99 *13.39*	0.09 *0.04*

Table S2. Net atomic charges of **1** derived from multipolar refinements.

Atom	**Experiment (*e*)**	**Theory (*e*)**
Cl1	+0.14	+0.01
O1	–0.27	–0.13
C1	–0.22	–0.15
C2	+0.13	+0.01
C3	+0.28	+0.27
H3	–0.05	0.00