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Supporting information for article:

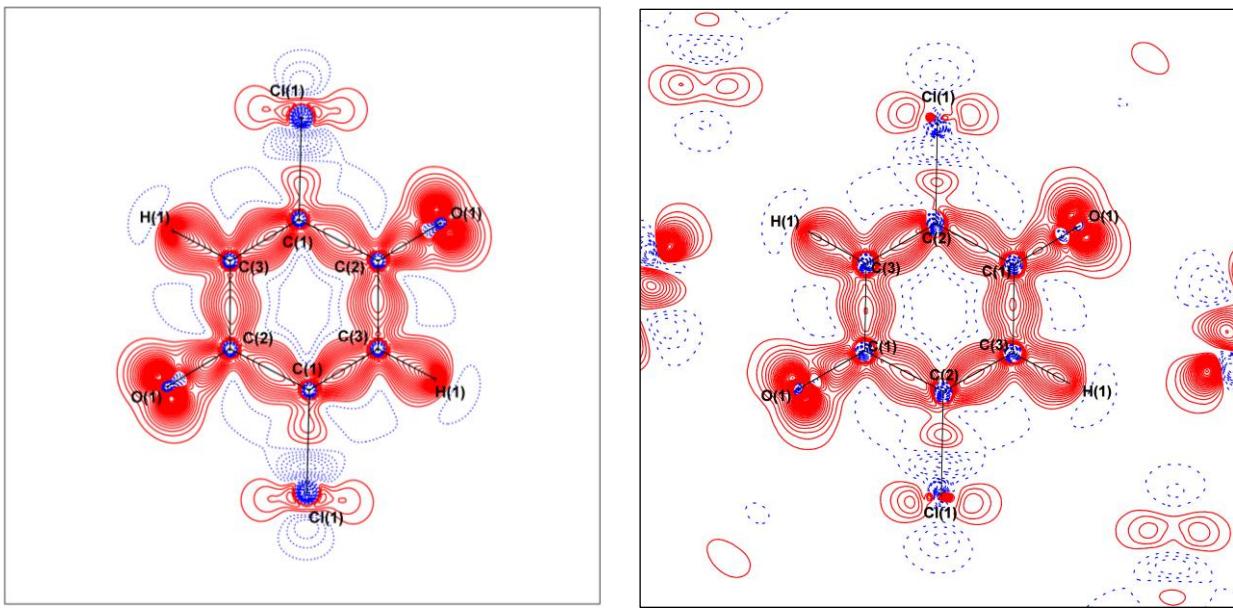
**Revisiting the Charge Density Analysis of 2,5-Dichloro-1,4-Benzoquinone at 20 K**

**Zhijie Chua, Bartosz Zarychta, Christopher G. Gianopoulos, Vladimir Zhurov and Alan Pinkerton**

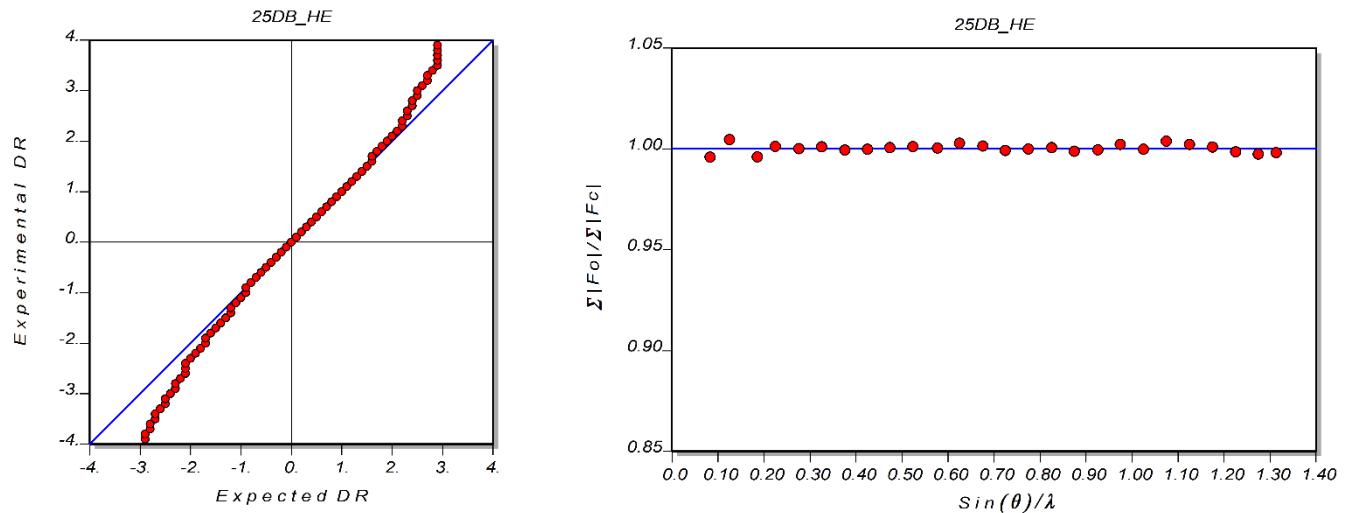
## Supplementary Material

### Contents

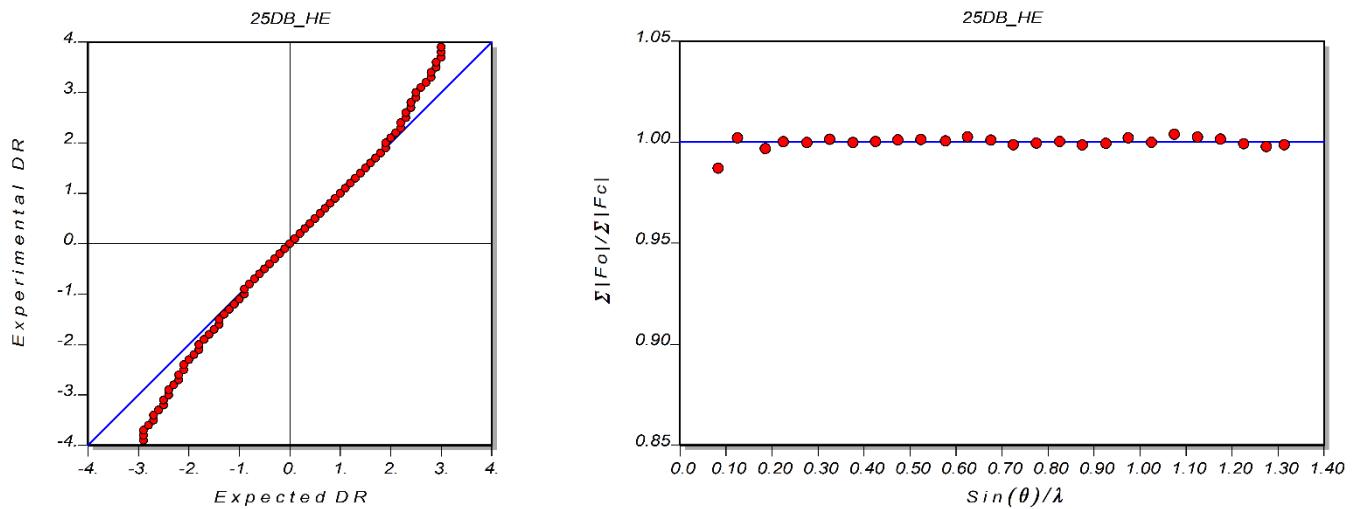
Figure S1: Static deformation map from theory	S2
Figure S2, S3: Normal probability plots and scale plots	S3
Figure S4: Fractal plots	S4
Figure S5, S6: Electrostatic potential isosurface maps	S5
Table S1: Properties of the intramolecular and intermolecular bond critical points	S6
Crystal09 calculations	S9
Multipole populations from theoretical structure factors	S15



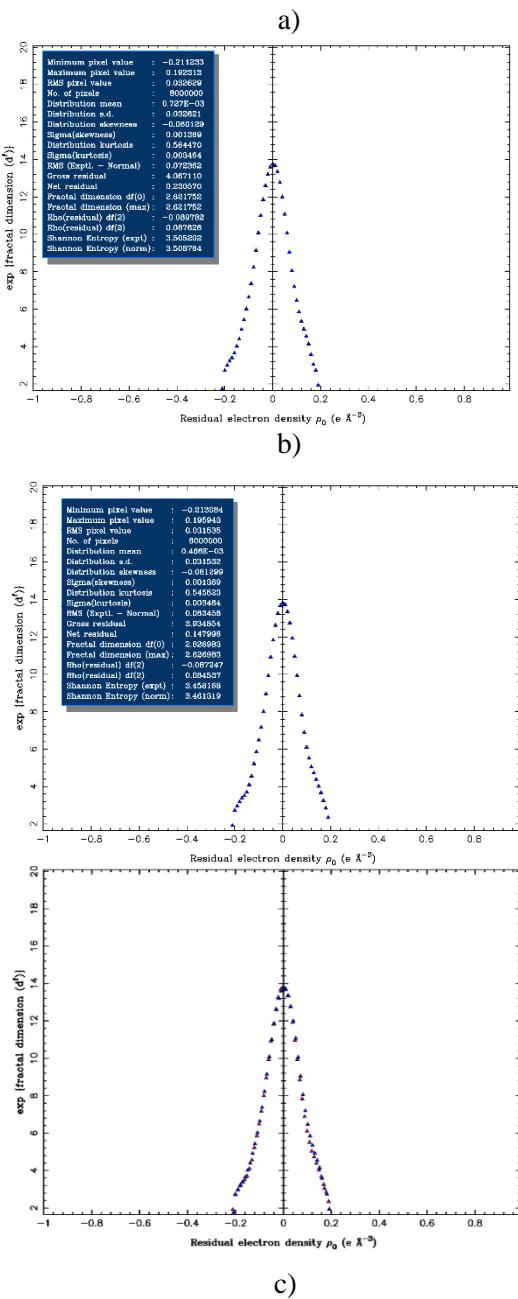
**Figure S1** Static deformation map from multipole refinement of theoretical structure factors (left) and direct calculations from wave functions (right). Contours are  $0.05 \text{ e}/\text{\AA}^3$ . Red solid contour lines denote positive charge density, blue dashed contours denote electron depletion.



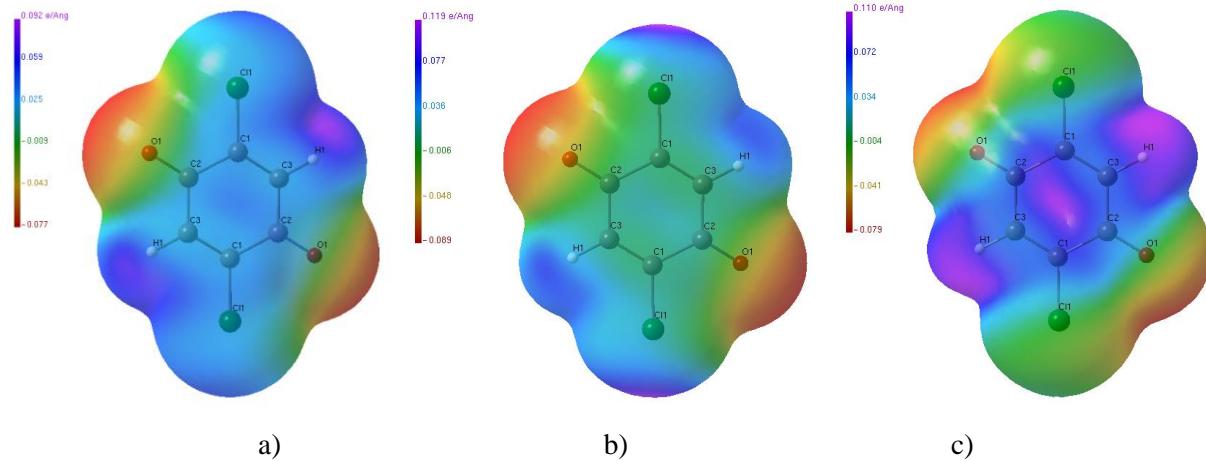
**Figure S2** Normal Probability plot(left) and scale plot averaged over  $0.05 \text{ \AA}^{-1}$  intervals (right ) for Model 1.



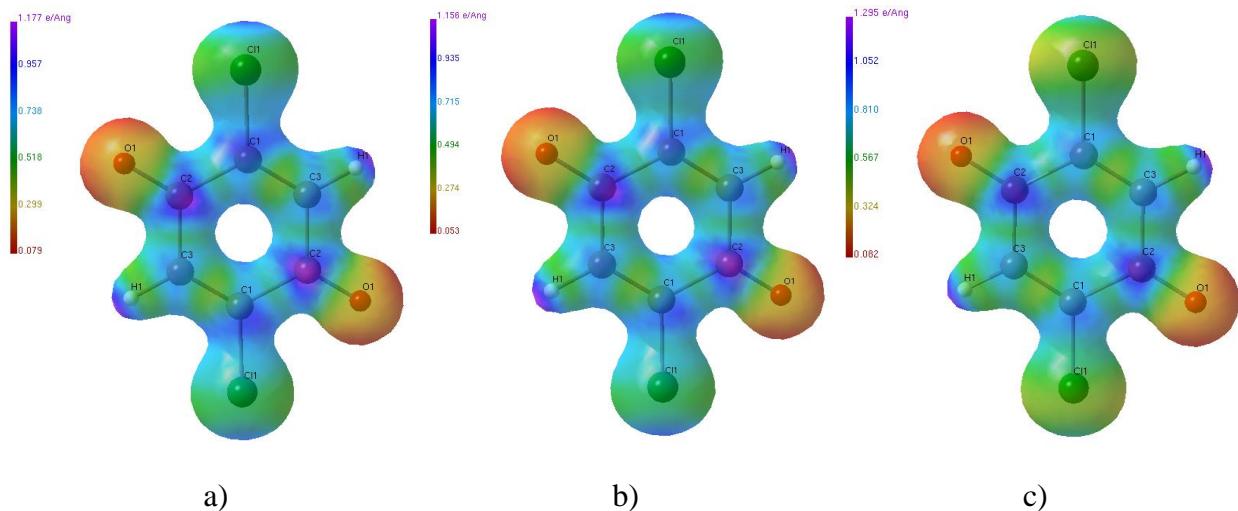
**Figure S3** Normal Probability plot(left) and scale plot averaged over  $0.05 \text{ \AA}^{-1}$  intervals (right ) for Model 2.



**Figure S4** Fractal plots for a) Model 1, b) Model 2, c) the overlay of a) on b).



**Figure S5** Electrostatic potential isosurface maps from experimental charge density refinements drawn at isosurface value of  $\pm 0.00675 \text{ e}\text{\AA}^{-1}$  for Model 1 (a), Model 2 (b) and TSF (c). Blue and red colours represent electropositive and electronegative regions respectively.



**Figure S6** Electrostatic potential isosurface maps from experimental charge density refinements drawn at isosurface value of  $\pm 0.5 \text{ e}\text{\AA}^{-3}$  for Model 1 (a), Model 2 (b) and TSF (c). Blue and red colours represent electropositive and electronegative regions respectively.

**Table S1** Properties of the Intramolecular and Intermolecular Bond Critical Points in DCBQ. 1<sup>st</sup> row: experimental multipole Model 1. 2<sup>nd</sup> row: experimental multipole Model 2. 3<sup>rd</sup> row: theoretical structure factors (TSF) multipole Model 2. 4<sup>th</sup> row: Wave functions from TOPOND

Bond	$\rho(r)$ (e/Å <sup>3</sup> )	$\nabla^2\rho(r)$ (e/Å <sup>5</sup> )	R <sub>ij</sub> (Å)	d <sub>1</sub> (Å)	d <sub>2</sub> (Å)	Hessian eigenvalues (e/Å <sup>5</sup> )	$\varepsilon$	g (au)	v (au)	h (au)	E (kJ/mol <sup>1</sup> )	
Intramolecular												
Cl(1) – C(1)	1.382	-3.04	1.711	0.943	0.769	-8.129	-7.911	12.999	0.028	0.1832	-0.3980	-0.2148
	1.413	-4.81	1.711	0.969	0.743	-8.018	-7.814	11.020	0.026	0.1788	-0.4076	-0.2287
	1.325	-2.75	1.711	0.929	0.783	-7.154	-6.580	10.988	0.087	0.1714	-0.3713	-0.1999
	1.397	-7.40	1.711	0.941	0.771	-7.808	-7.422	7.832	0.054	0.1568	-0.3904	-0.2336
O(1) – C(2)	2.855	-23.87	1.223	0.796	0.426	-27.873	-25.284	29.284	0.102	0.5194	-1.2865	-0.7671
	2.864	-24.49	1.223	0.795	0.428	-27.860	-25.374	28.743	0.098	0.5187	-1.2915	-0.7728
	2.777	-24.06	1.223	0.780	0.443	-25.100	-23.216	24.251	0.081	0.4874	-1.2244	-0.7370
	2.760	-15.78	1.223	0.796	0.427	-26.581	-24.508	35.305	0.084	0.5379	-1.2395	-0.7016
C(1) – C(2)	1.825	-15.47	1.497	0.755	0.742	-13.620	-12.289	10.439	0.108	0.2179	-0.5962	-0.3784
	1.823	-15.19	1.497	0.756	0.741	-13.680	-12.335	10.822	0.109	0.2190	-0.5956	-0.3766
	1.774	-13.41	1.497	0.754	0.743	-12.863	-11.377	10.830	0.131	0.2169	-0.5729	-0.3560
	1.788	-15.06	1.497	0.756	0.741	-13.327	-12.194	10.483	0.093	0.2097	-0.5757	-0.3660
C(1) – C(3)	2.336	-23.29	1.344	0.683	0.661	-18.113	-14.373	9.201	0.26	0.3291	-0.8997	-0.5706
	2.336	-23.02	1.344	0.683	0.661	-18.291	-14.458	9.731	0.265	0.3307	-0.9003	-0.5695
	2.287	-21.69	1.344	0.698	0.646	-17.394	-13.510	9.214	0.288	0.3230	-0.8709	-0.5480
	2.301	-23.33	1.344	0.696	0.648	-18.411	-14.050	9.133	0.311	0.3166	-0.8751	-0.5586
C(2) – C(3)	1.863	-15.57	1.475	0.748	0.727	-13.397	-12.644	10.468	0.059	0.2283	-0.6182	-0.3899
	1.861	-15.20	1.475	0.748	0.728	-13.466	-12.655	10.923	0.064	0.2304	-0.6186	-0.3881
	1.814	-13.82	1.475	0.754	0.721	-13.006	-11.545	10.729	0.127	0.2260	-0.5954	-0.3694
	1.829	-15.78	1.475	0.749	0.726	-13.495	-12.339	10.049	0.095	0.2167	-0.5971	-0.3804
C(3) – H(1)	1.861	-20.05	1.080	0.734	0.346	-18.838	-17.850	16.635	0.055	0.1968	-0.6016	-0.4048
	1.871	-20.51	1.080	0.731	0.349	-18.997	-18.101	16.586	0.05	0.1966	-0.6059	-0.4093

	1.896	-20.46	1.080	0.711	0.369	-18.254	-17.617	15.415	0.036	0.2046	-0.6214	-0.4168	
	1.937	-24.03	1.064	0.712	0.352	-19.448	-19.183	14.604	0.014	0.1924	-0.6340	-0.4416	
Intermolecular													
Cl(1) ... Cl(1) $-x + 1, y + 0.5, -z + 1.5$	0.032	0.39	3.694	1.828	1.867	-0.063	-0.050	0.499	0.277	0.0031	-0.0021	0.0009	2.8
	0.026	0.41	3.694	1.794	1.902	-0.052	-0.045	0.503	0.153	0.0031	-0.0019	0.0011	2.5
	0.035	0.41	3.694	1.813	1.882	-0.070	-0.053	0.531	0.325	0.0033	-0.0023	0.0010	3.0
	0.040	0.46	3.746	1.873	1.873	-0.096	-0.024	0.578	4.917	0.0037	-0.0027	0.0010	3.6
Cl(1) ... Cl(1) $-x + 1, -y, -z + 2$	0.020	0.24	3.984	1.992	1.992	-0.037	-0.024	0.296	0.496	0.0018	-0.0012	0.0006	1.5
	0.020	0.24	3.984	1.992	1.992	-0.037	-0.033	0.309	0.122	0.0018	-0.0012	0.0007	1.5
	0.023	0.25	3.984	1.992	1.992	-0.051	-0.042	0.343	0.201	0.0019	-0.0013	0.0006	1.7
	0.020	0.29	3.983	1.992	1.992	-0.048	-0.048	0.386	0.134	0.0022	-0.0014	0.0008	1.8
Cl(1) ... O(1) $-x + 1, y - 0.5, -z + 1.5$	0.066	0.87	3.041	1.604	1.437	-0.175	-0.167	1.209	0.043	0.0073	-0.0056	0.0017	7.3
	0.055	0.92	3.040	1.593	1.447	-0.162	-0.154	1.238	0.056	0.0073	-0.0051	0.0022	6.7
	0.064	0.89	3.040	1.618	1.423	-0.171	-0.155	1.217	0.107	0.0074	-0.0055	0.0019	7.2
	0.061	0.82	3.046	1.582	1.464	-0.145	-0.145	1.133	0.032	0.0068	-0.0051	0.0017	6.7
Cl(1) ... O(1) $x, y - 1, z$	0.032	0.40	3.465	1.853	1.614	-0.067	-0.062	0.533	0.08	0.0032	-0.0022	0.0010	2.9
	0.032	0.40	3.465	1.858	1.610	-0.075	-0.064	0.540	0.167	0.0032	-0.0022	0.0010	2.8
	0.031	0.42	3.465	1.883	1.582	-0.070	-0.062	0.555	0.125	0.0033	-0.0022	0.0011	2.9
	0.034	0.41	3.471	1.884	1.587	-0.072	-0.072	0.578	0.104	0.0033	-0.0023	0.0010	3.0
Cl(1) - C(1) $-x + 1, -y + 1, -z + 2$	0.043	0.43	3.507	1.809	1.700	-0.083	-0.051	0.562	0.637	0.0036	-0.0028	0.0008	3.6
	0.046	0.43	3.507	1.817	1.692	-0.089	-0.057	0.572	0.552	0.0037	-0.0029	0.0008	3.8
	0.041	0.43	3.507	1.860	1.653	-0.089	-0.020	0.541	3.479	0.0036	-0.0026	0.0009	3.5
	0.040	0.46	3.532	1.859	1.672	-0.072	-0.048	0.578	0.74	0.0037	-0.0027	0.0010	3.6
Cl(1) ... H(1) $x, -y + 0.5, z - 0.5$	0.047	0.57	2.965	1.770	1.228	-0.122	-0.072	0.759	0.7	0.0046	-0.0034	0.0012	4.5
	0.047	0.56	2.972	1.780	1.232	-0.119	-0.075	0.756	0.601	0.0046	-0.0034	0.0012	4.4
	0.043	0.56	2.972	1.803	1.185	-0.130	-0.078	0.768	0.671	0.0045	-0.0032	0.0013	4.2
	0.047	0.53	3.094	1.810	1.284	-0.120	-0.072	0.747	0.536	0.047	-0.0033	0.0011	4.3
O(1) ... C(2)	0.065	0.75	2.977	1.487	1.494	-0.158	-0.048	0.953	0.065	0.0064	-0.0051	0.0013	6.6
	0.065	0.76	2.977	1.488	1.494	-0.156	-0.046	0.957	0.065	0.0065	-0.0051	0.0014	6.7

$-x, y + 0.5, -z + 1.5$	0.059	0.64	2.977	1.487	1.493	-0.150	-0.100	0.890	0.059	0.0055	-0.0043	0.0012	5.7
	0.054	0.80	3.011	1.515	1.495	-0.145	-0.048	0.988	0.054	0.0064	-0.0046	0.0018	6.0
$O(1) \cdots H(1)$ $x, -y + 0.5, z - 0.5$	0.065	0.79	2.466	1.446	1.032	-0.217	-0.164	1.169	0.065	0.0067	-0.0052	0.0015	6.8
	0.062	0.78	2.463	1.452	1.020	-0.212	-0.155	1.150	0.062	0.0066	-0.0050	0.0015	6.6
	0.059	0.73	2.463	1.463	1.003	-0.185	-0.183	1.094	0.059	0.0060	-0.0046	0.0014	6.1
	0.061	0.72	2.489	1.482	1.007	-0.193	-0.193	1.109	0.061	0.0061	-0.0047	0.0014	6.2
$C(3) \cdots C(3)$ $-x, -y, -z + 2$	0.038	0.36	3.429	1.714	1.714	-0.090	-0.045	0.497	0.038	0.0030	-0.0023	0.0007	3.0
	0.036	0.35	3.429	1.714	1.714	-0.078	-0.048	0.481	0.036	0.0029	-0.0021	0.0008	2.8
	0.030	0.34	3.429	1.714	1.714	-0.084	-0.004	0.428	0.030	0.0027	-0.0019	0.0008	2.4
	0.034	0.36	3.512	1.756	1.756	-0.072	-0.024	0.458	0.034	0.0029	-0.0021	0.0008	2.7

## Crystal09 calculation for Model 1

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8 0.152959 0.706218 0.777334  
6 0.188671 0.384324 0.943392  
6 0.082172 0.611856 0.879242  
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KEEPsymm  
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0.1549730000D+03 0.7612690000D-01  
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0.1302900000D+02 0.6164620000D+00  
0.1827730000D+01 0.2210060000D+00  
0 1 3 4.0 1.00  
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0 3 1 0.0 1.0  
0.6 .1000000000D+01  
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1338. 0.008040  
255.4 0.053240  
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23.90 0.358100  
9.264 0.385500  
3.851 0.146800  
1.212 0.072800

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0 3 1 0. 1.  
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B3LYP  
XLGRID  
END  
SHRINK  
8 8  
LEVSHIFT

6 1  
TOLINTEG  
9 9 9 9 18  
EXCHSIZE  
15000000  
BIPOSIZE  
15000000  
MAXCYCLE  
150  
SCFDIR  
END  
+++ ENERGIES IN A.U. +++  
::: EXT EL-POLE -3.2227206234068E+03  
::: EXT EL-SPHEROPOLE 2.4987575187044E+01  
::: BIELET ZONE E-E 3.9661514972827E+03  
::: TOTAL E-E 7.6841844906298E+02  
::: TOTAL E-N + N-E -5.3780835693300E+03  
::: TOTAL N-N -4.1556608498718E+02  
::: KINETIC ENERGY 2.5965046590053E+03  
::: PSEUDO TOTAL ENERGY -2.4287265462488E+03  
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NUMERICALLY INTEGRATED DENSITY 176.0000169119  
TTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 15563.58 TCPU 15529.34  
CYC 27 ETOT(AU) -2.600856049081E+03 DETOT -7.57E-07 tst 1.01E-06 PX 8.96E-05  
== SCF ENDED - CONVERGENCE ON ENERGY E(AU) -2.6008560490812E+03 CYCLES 27  
ENERGY EXPRESSION=HARTREE+FOCK EXCH\*0.20000+(BECKE EXCH)\*0.80000+LYP CORR  
TOTAL ENERGY(DFT)(AU)( 27) -2.6008560490812E+03 DE-7.6E-07 tester 1.0E-06

## Crystal09 calculation for Model 2

CRYSTAL  
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6  
17 0.4150112 0.2666770 0.8662921  
8 0.152974 0.706209 0.777328  
6 0.1887007 0.3843001 0.9433806  
6 0.0821782 0.6118556 0.8792394  
6 0.1115040 0.2804081 1.0554846  
1 0.189028 0.116228 1.101329  
KEEPsymm  
ENDG  
1 4  
0 0 3 1. 1.  
33.8650000 0.0254938  
5.0947900 0.1903730  
1.1587900 0.8521610  
0 0 1 0. 1.  
0.3258400 1.0000000  
0 0 1 0. 1.  
0.1027410 1.0000000  
0 2 1 0. 1.  
0.7500000 1.0000000  
6 6  
0 0 6 2.0 1.00  
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0.4445530000D+02 0.2608010000D+00  
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0 1 1 0.0 1.00  
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0 1 1 0.0 1.00  
0.1455850000D+00 0.1000000000D+01 0.1000000000D+01  
0 3 1 0.0 1.0  
2.0 .1000000000D+01  
0 3 1 0.0 1.0  
0.6 .1000000000D+01  
8 6  
0 0 8 2.0 1.0  
8020. 0.001080  
1338. 0.008040  
255.4 0.053240  
69.22 0.168100  
23.90 0.358100  
9.264 0.385500  
3.851 0.146800  
1.212 0.072800

0 1 4 6. 1.0  
49.43 -0.008830 0.009580  
10.47 -0.091500 0.069600  
3.235 -0.040200 0.206500  
1.217 0.379000 0.347000  
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0 3 1 0. 1.  
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17 10  
0 0 7 2.0 1.0  
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1.8385832573 0.68636955368000  
0 0 1 0.0 1.0  
0.4498594500 1.0000000000000000  
0 0 1 0.0 1.0  
0.1363703100 1.0000000000000000  
0 2 5 6.0 1.0  
666.50423284 0.00236326638360  
157.64241690 0.01887930037400  
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18.536078105 0.25285612970000  
7.2940532777 0.43507154820000  
0 2 1 5.0 1.0  
2.80149164000 1.0000000000000000  
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0.73964278000 1.0000000000000000  
0 2 1 0.0 1.0  
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0 3 1 0.0 1.0  
0.23728440000 1.0000000000000000  
99 0  
END  
DFT  
B3LYP  
XLGRID  
END  
SHRINK  
8 8  
LEVSHIFT

6 1  
TOLINTEG  
9 9 9 9 18  
EXCHSIZE  
15000000  
BIPOSIZE  
15000000  
MAXCYCLE  
150  
SCFDIR  
END  
+++ ENERGIES IN A.U. +++  
::: EXT EL-POLE -3.2225932379095E+03  
::: EXT EL-SPHEROPOLE 2.4987101510045E+01  
::: BIELET ZONE E-E 3.9660084883136E+03  
::: TOTAL E-E 7.6840235191417E+02  
::: TOTAL E-N + N-E -5.3780486459923E+03  
::: TOTAL N-N -4.1558265488606E+02  
::: KINETIC ENERGY 2.5965019773644E+03  
::: PSEUDO TOTAL ENERGY -2.4287269715998E+03  
::: VIRIAL COEFFICIENT 1.0333865396917E+00  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 16789.76 TCPU 16789.31  
NUMERICALLY INTEGRATED DENSITY 176.0000514200  
TTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 16818.55 TCPU 16818.08  
CYC 27 ETOT(AU) -2.600856053975E+03 DETOT -7.56E-07 tst 1.01E-06 PX 8.84E-05  
== SCF ENDED - CONVERGENCE ON ENERGY E(AU) -2.6008560539754E+03 CYCLES 27  
ENERGY EXPRESSION=HARTREE+FOCK EXCH\*0.20000+(BECKE EXCH)\*0.80000+LYP CORR  
TOTAL ENERGY(DFT)(AU)( 27) -2.6008560539754E+03 DE-7.6E-07 tester 1.0E-06

Multipole populations from theoretical structure factors.

```

loop_
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_atom_rho_multipole_coeff_P20
_atom_rho_multipole_coeff_P21
_atom_rho_multipole_coeff_P2-1
_atom_rho_multipole_coeff_P22
_atom_rho_multipole_coeff_P2-2
_atom_rho_multipole_coeff_P30
_atom_rho_multipole_coeff_P31
_atom_rho_multipole_coeff_P3-1
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_atom_rho_multipole_coeff_P33
_atom_rho_multipole_coeff_P3-3
_atom_rho_multipole_coeff_P40
_atom_rho_multipole_coeff_P41
_atom_rho_multipole_coeff_P4-1
_atom_rho_multipole_coeff_P42
_atom_rho_multipole_coeff_P4-2
_atom_rho_multipole_coeff_P43
_atom_rho_multipole_coeff_P4-3
_atom_rho_multipole_coeff_P44
_atom_rho_multipole_coeff_P4-4
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_atom_rho_multipole_kappa_prime2
_atom_rho_multipole_kappa_prime3
_atom_rho_multipole_kappa_prime4
_atom_rho_multipole_radial_slater_n0
_atom_rho_multipole_radial_slater_zeta0
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_atom_rho_multipole_radial_slater_n2
_atom_rho_multipole_radial_slater_zeta2
_atom_rho_multipole_radial_slater_n3
_atom_rho_multipole_radial_slater_zeta3
_atom_rho_multipole_radial_slater_n4
_atom_rho_multipole_radial_slater_zeta4
CL(1) 6.536(9) 0.524(9) 0.0002(10) -0.0021(11) -0.0658(17)
-0.181(3) 0.0011(16) 0.0024(16) -0.0222(17) -0.0004(15)
0.120(5) 0.003(2) 0.002(2) 0.005(3) 0.003(3) -0.002(2) -0.005(2)
0.063(5) -0.001(3) 0.002(3) 0.001(3) 0.002(3) -0.001(3) 0.001(3) -0.001(2)
-0.000(3)
0.9853(7) 1.118(9) 1.446(15) 1.053(6) 0.777(11) 0.71(2)
4 3.9938571428571 4 3.9938571428571 4 3.9938571428571 4 3.9938571428571 4
3.9938571428571
O(1) 5.42(3) 0.70(3) 0.0005(8) -0.0010(9) -0.0766(16)
-0.0167(8) -0.0002(7) -0.0007(7) -0.1308(12) 0.0017(7)

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0.038(2) 0.0006(13) 0.0008(13) 0.0210(17) -0.0003(13) -0.0011(13) 0.0000(13)  
 0.012(2) 0.0017(18) 0.0012(18) 0.012(2) 0.0004(18) 0.0004(18) 0.0006(18)  
 -0.0011(16) -0.0011(16)  
 1.0075(14) 0.885(8) 1.095(10) 1.139(5) 0.89(2) 0.85(6)  
 2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974  
 C(1) 3.132(17) 0.896(15) 0.003(3) 0.083(6) -0.003(2)  
 -0.160(3) -0.001(2) 0.000(2) 0.006(2) -0.136(3)  
 -0.001(3) -0.021(3) 0.037(3) 0.002(3) 0.003(3) 0.257(3) 0.022(3)  
 0.006(5) 0.003(5) -0.004(5) -0.053(7) 0.020(6) 0.003(6) 0.004(6) 0.004(6)  
 0.016(8)  
 0.970(2) 1.127(5) 0.95(2) 0.874(4) 0.931(3) 0.693(14)  
 2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303  
 C(2) 3.065(17) 0.889(14) -0.014(3) -0.044(4) 0.005(2)  
 -0.298(3) -0.002(2) -0.001(2) -0.022(2) 0.088(3)  
 0.002(3) -0.006(3) -0.006(2) 0.001(2) 0.002(3) 0.312(4) -0.009(3)  
 0.075(6) 0.016(5) -0.011(5) 0.018(6) -0.008(6) -0.001(6) 0.006(5) 0.023(7)  
 0.055(7)  
 0.970(2) 1.127(5) 0.95(2) 0.874(4) 0.931(3) 0.693(14)  
 2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303  
 C(3) 2.982(17) 0.954(14) 0.006(3) -0.021(3) -0.005(3)  
 -0.199(3) 0.001(2) -0.003(2) 0.032(3) 0.043(2)  
 -0.003(3) 0.049(3) 0.020(2) -0.002(3) 0.004(3) 0.258(3) -0.008(3)  
 0.048(6) 0.000(5) 0.015(5) 0.022(6) -0.021(6) 0.010(6) 0.001(6) -0.086(8)  
 -0.061(7)  
 0.970(2) 1.127(5) 0.95(2) 0.874(4) 0.931(3) 0.693(14)  
 2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303  
 H(1) 0.903(4) 0 0.008(2) -0.011(3) 0.170(2)  
 0.048(3) 0.002(3) -0.010(3) -0.012(3) -0.000(3)  
 0 0 0 0 0 0 0  
 0 0 0 0 0 0 0 0  
 1.2 1.2 1.2 1.2 1.2 1.2  
 0 1.9154 1 1.9154 2 1.9154 3 1.9154 4 1.9154

loop\_

- \_atom\_local\_axes\_atom\_label
- \_atom\_local\_axes\_atom0
- \_atom\_local\_axes\_ax1
- \_atom\_local\_axes\_atom1
- \_atom\_local\_axes\_atom2
- \_atom\_local\_axes\_ax2

CL(1)	C(1)	Z	CL(1)	C(3)	Y
O(1)	C(2)	Z	O(1)	C(1)	Y
C(1)	C(2)	X	C(1)	C(3)	Y
C(2)	DUM0	X	C(2)	C(1)	Y
C(3)	C(1)	X	C(3)	DUM1	Y
H(1)	C(3)	Z	H(1)	DUM2	Y