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Supporting information for article:

A method to estimate statistical errors of properties derived from charge density modeling

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Supplementary Materials.

Estimating errors of derived properties in charge density analyses

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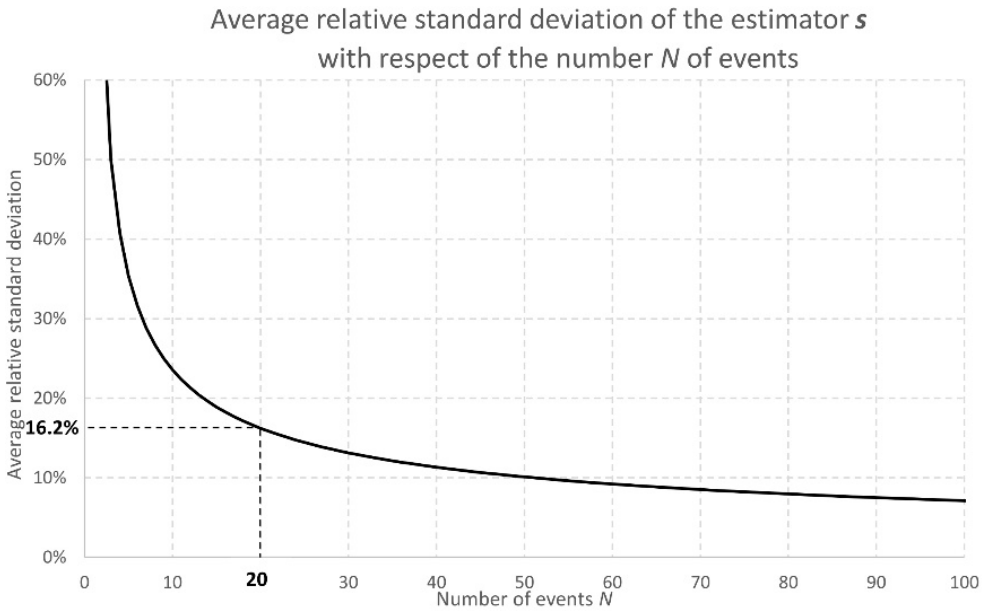

Figure Sup1. Plot of the relative standard deviation (equation (16)) of the SSD value as a function of the number *N* of deviating models.

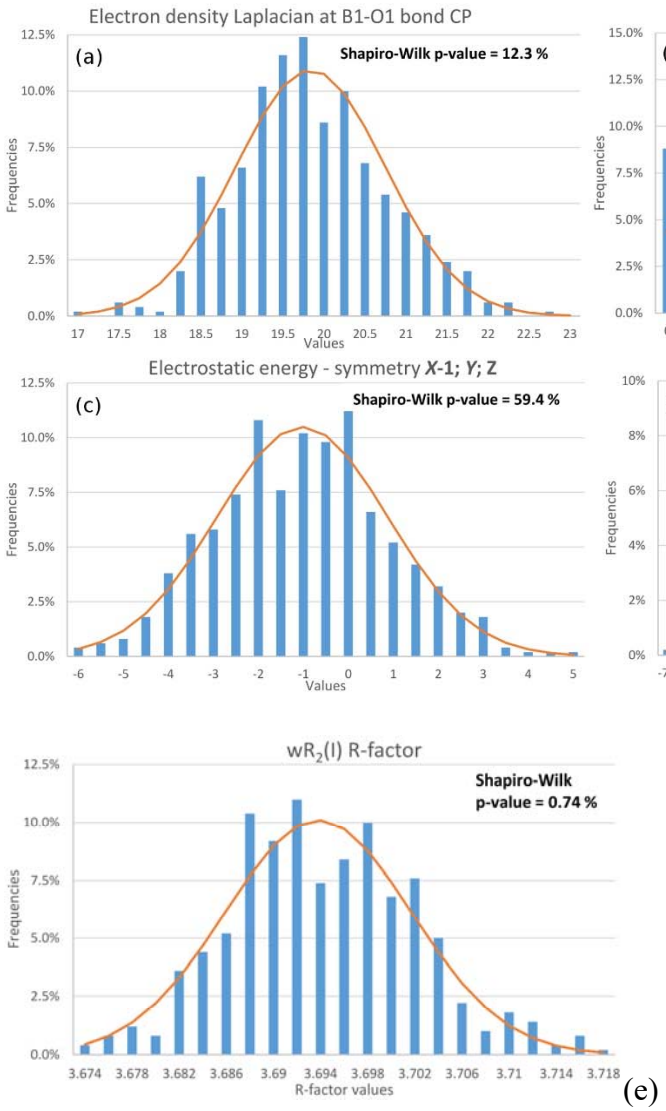

Figure Sup2.
Population histograms for different properties deduced from 500 perturbed models: electron density Laplacian (a) and ellipticity (b) at CP of B1-O1 bond, electrostatic interaction energies between reference and neighboring molecules (c) and (d). Ideal Gaussian distributions are defined considering sample average and SSD value, and superimposed. Shapiro-Wilk test *P*-value are also given.

(e) *R*-factor values $wR^2(I)$.

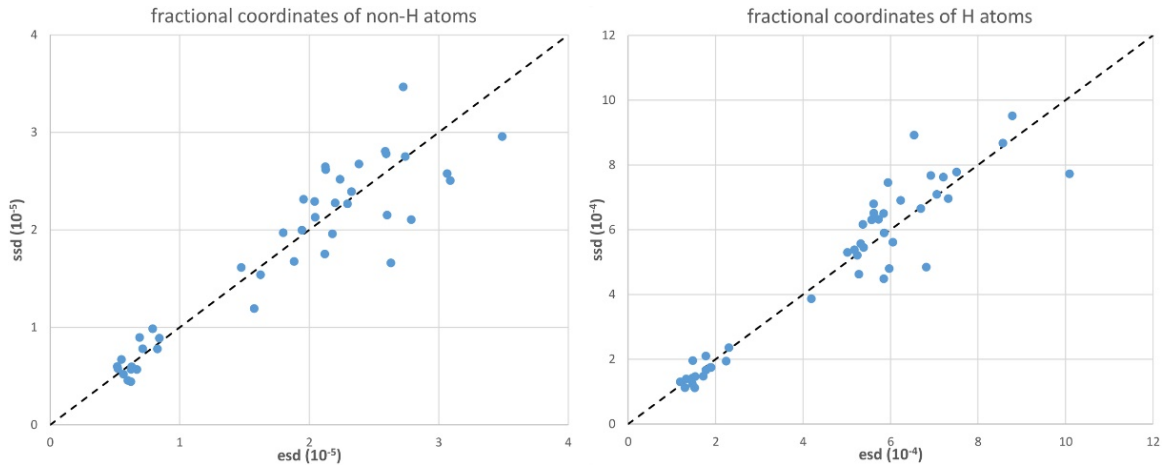

Figure Sup3. Scatterplot of e.s.d. (sigmaX) and SSD values for the fractional coordinates of the non-H atoms (left) and the H atoms (right) of the $C_{11}H_{15}BO_2$ molecule.

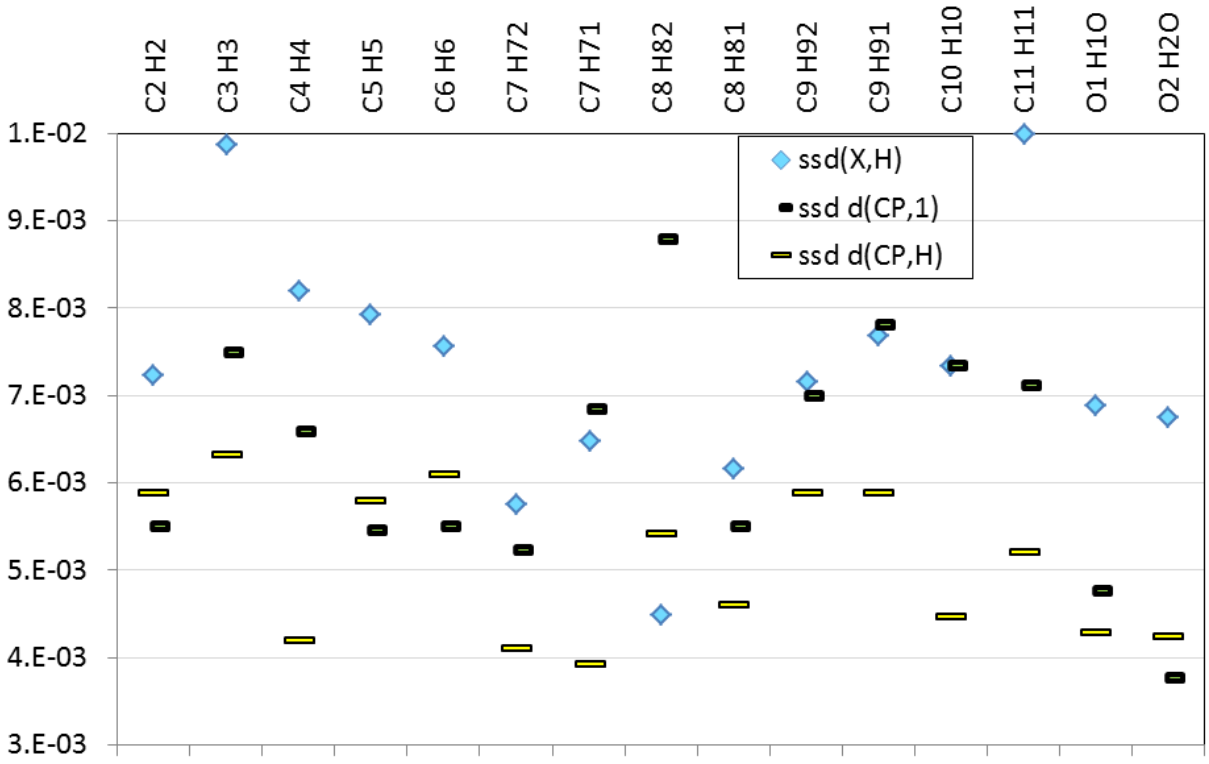

Figure Sup4. Plot of SSD values of X…CP and H…CP distances for all X-H covalent bonds. The SSD and e.s.d. (sigma) of the X-H bond distances are also shown.

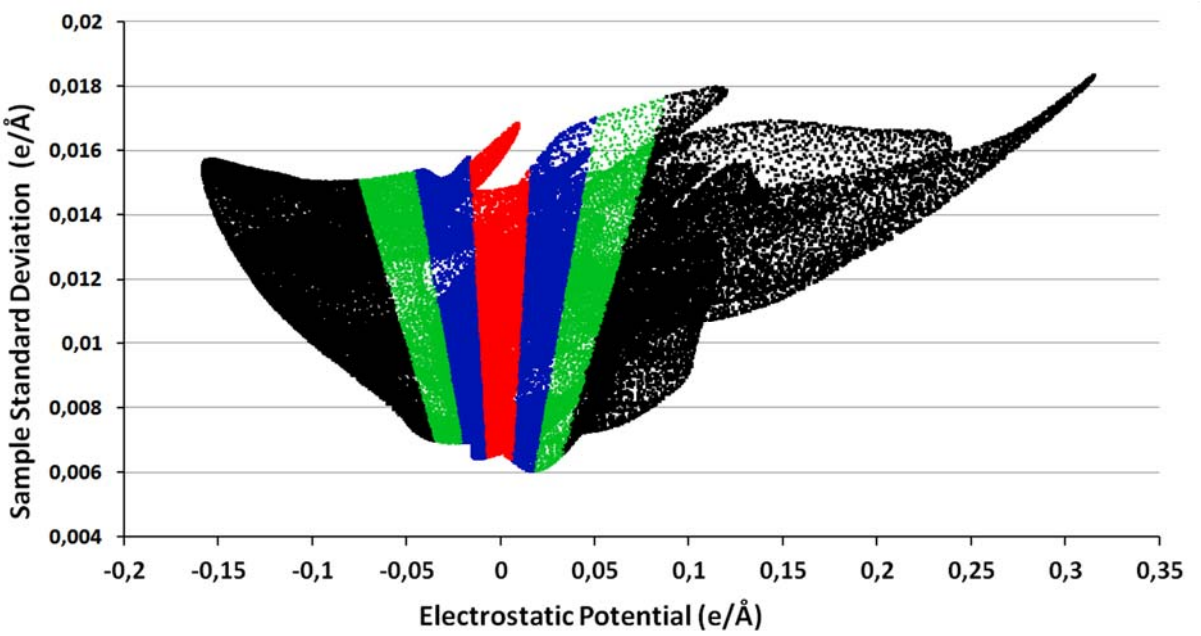

Figure Sup5. Sample standard deviation SSD(φ) plotted versus the electrostatic potential values φ on ~70k points defining the 0.001*au* electron density iso-surface of BOH2 compound. Dots are colored according to the signal over noise ratio $s=|\varphi/\mathrm{SSD}(\varphi)|$. Black : $s \geq 5$; green : $3 \leq s < 5$; blue : $1 \leq s < 3$ and red : $s < 1$.

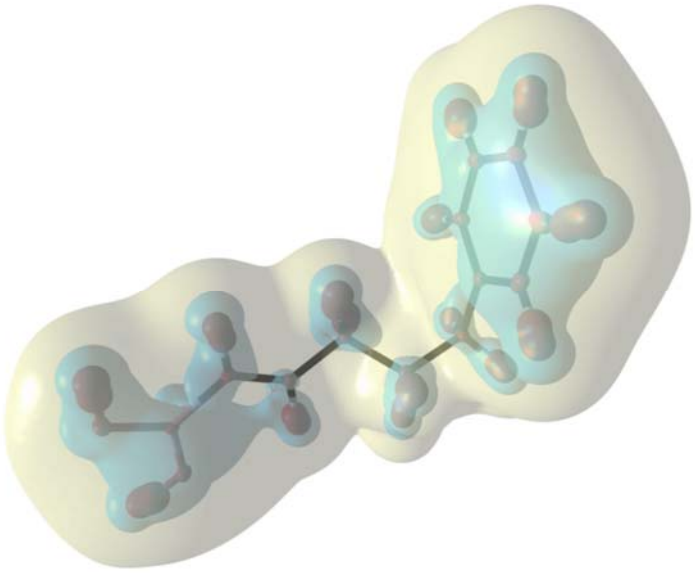

Figure Sup6. SSD(φ) iso-contour surfaces of 0.04 (inner, red), 0.02 (intermediate, blue) and 0.01 e/Å (outer, yellow).

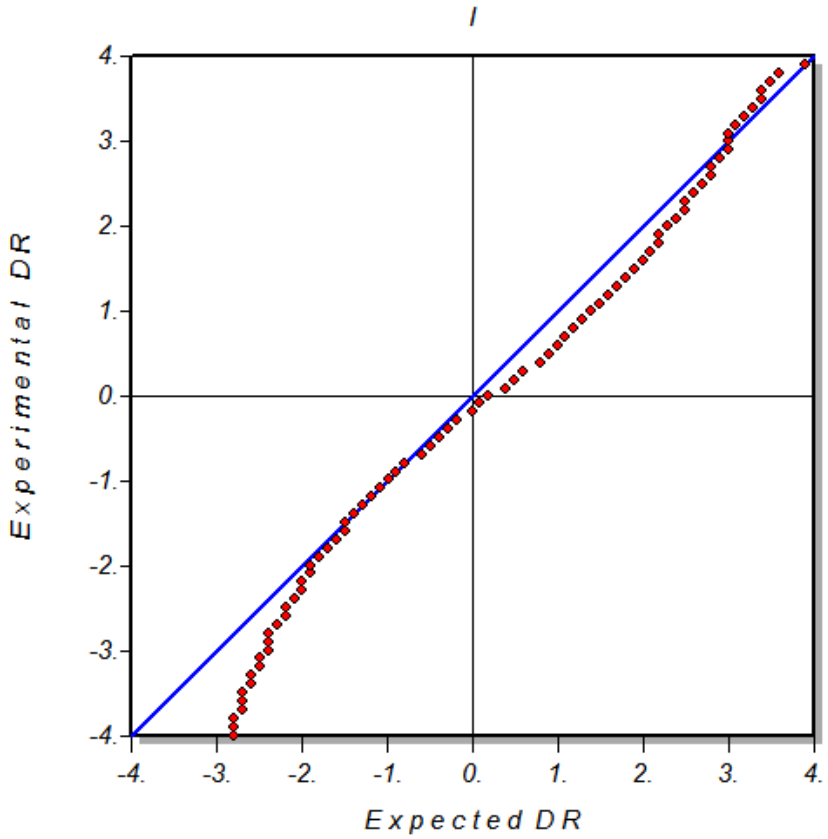

Figure Sup7. Normal probability plots of (F^2_o-F^2_c) using program XDRKplot (Zhurov, Zhurova & Pinkerton, J. Appl. Cryst. (2008). 41, 340–349). The weighting scheme used is $\sigma^2 = [\sigma(F^2)]^2$.

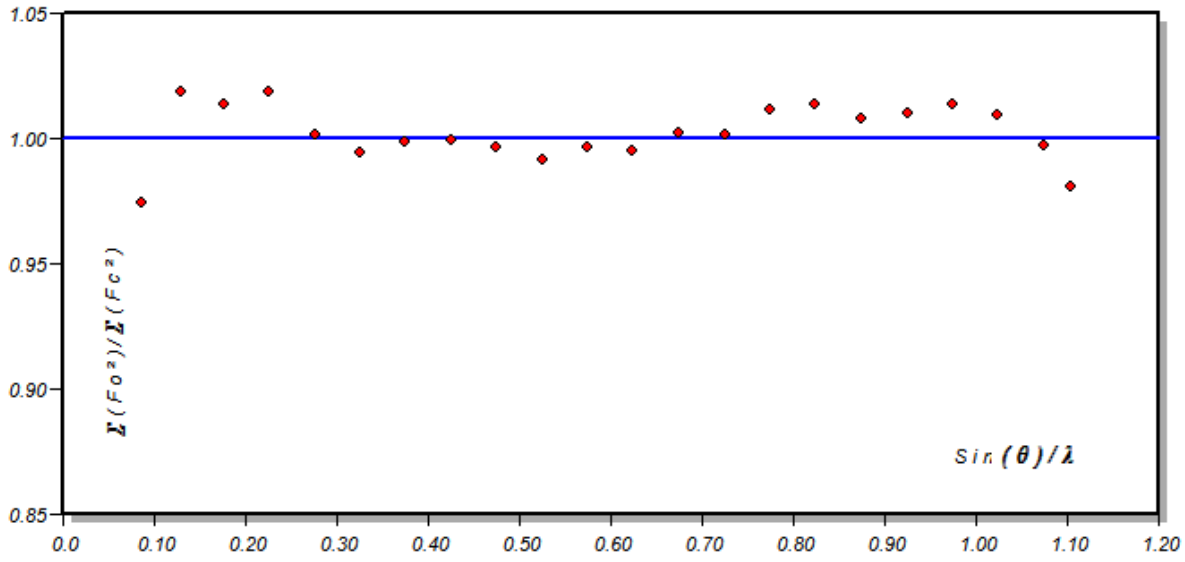

Figure Sup8. Variation of scale factor, Σ (Fo^2)/ Σ (Fc^2), with respect to resolution for the BOH molecule.

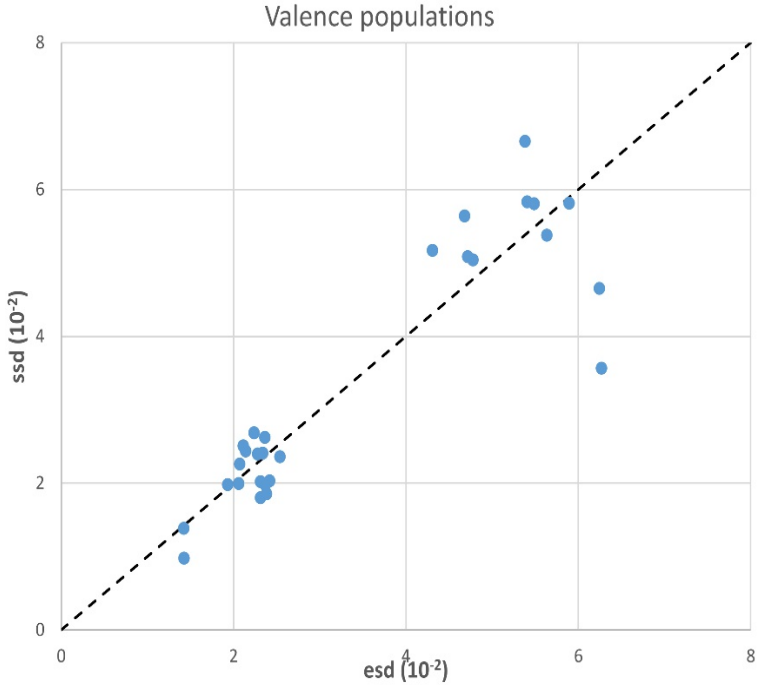

Figure Sup9.

Scatterplot e.s.d. vs. SSD values for the P_{val} parameters of the $C_{11}H_{15}BO_2$ molecule model.

Table Sup1.

λ_1, λ_2, λ_3 eigenvalues of the Hessian matrix $\partial^2\rho/\partial x_i \partial x_j$ at the bond critical points of BOH2 molecule.

Atom A	Atom B	λ_1	SSD	λ_2	SSD	λ_3	SSD
B1	C11	-10.51	0.23	-9.64	0.19	13.34	0.77
B1	O1	-12.78	0.21	-12.76	0.20	45.35	0.59
B1	O2	-13.00	0.25	-12.59	0.27	43.07	0.56
C1	C2	-16.50	0.16	-13.77	0.20	10.96	0.42
C1	C6	-16.80	0.19	-13.60	0.15	10.64	0.41
C1	C7	-11.30	0.16	-11.08	0.12	10.92	0.27
C2	C3	-16.11	0.22	-13.42	0.15	10.41	0.43
C3	C4	-17.10	0.16	-13.99	0.13	10.82	0.52
C4	C5	-16.72	0.13	-13.80	0.12	9.84	0.30
C5	C6	-16.16	0.16	-12.97	0.16	9.60	0.30
C7	C8	-10.34	0.10	-9.38	0.08	9.81	0.17
C8	C9	-10.32	0.11	-8.99	0.14	9.38	0.14
C9	C10	-11.80	0.13	-10.06	0.13	8.64	0.19
C10	C11	-17.78	0.16	-13.33	0.13	9.54	0.32
C1	H10	-16.03	0.15	-14.79	0.18	14.05	0.25
C1	H11	-16.07	0.20	-15.58	0.18	16.97	0.41
C2	H2	-17.48	0.26	-16.59	0.25	18.54	0.52
C3	H3	-17.95	0.27	-17.00	0.28	18.24	0.59
C4	H4	-16.40	0.24	-15.66	0.25	15.62	0.43
C5	H5	-17.46	0.26	-16.40	0.28	16.16	0.43
C6	H6	-17.59	0.20	-16.65	0.22	17.05	0.55
C7	H71	-14.97	0.22	-14.52	0.22	15.97	0.47
C7	H72	-15.19	0.21	-14.48	0.19	15.39	0.36
C8	H81	-15.19	0.26	-14.50	0.27	15.07	0.43
C8	H82	-15.49	0.19	-15.04	0.27	15.62	0.55
C9	H91	-14.22	0.23	-12.99	0.24	13.18	0.48
C9	H92	-13.47	0.17	-13.16	0.14	14.80	0.40
H1	O1	-38.14	0.99	-37.91	0.98	44.90	1.55
H2	O2	-38.82	0.86	-37.97	0.85	45.74	1.33