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Supporting information for article:

New refinement strategies for a pseudoatom databank – toward rapid electrostatic interaction energy estimations

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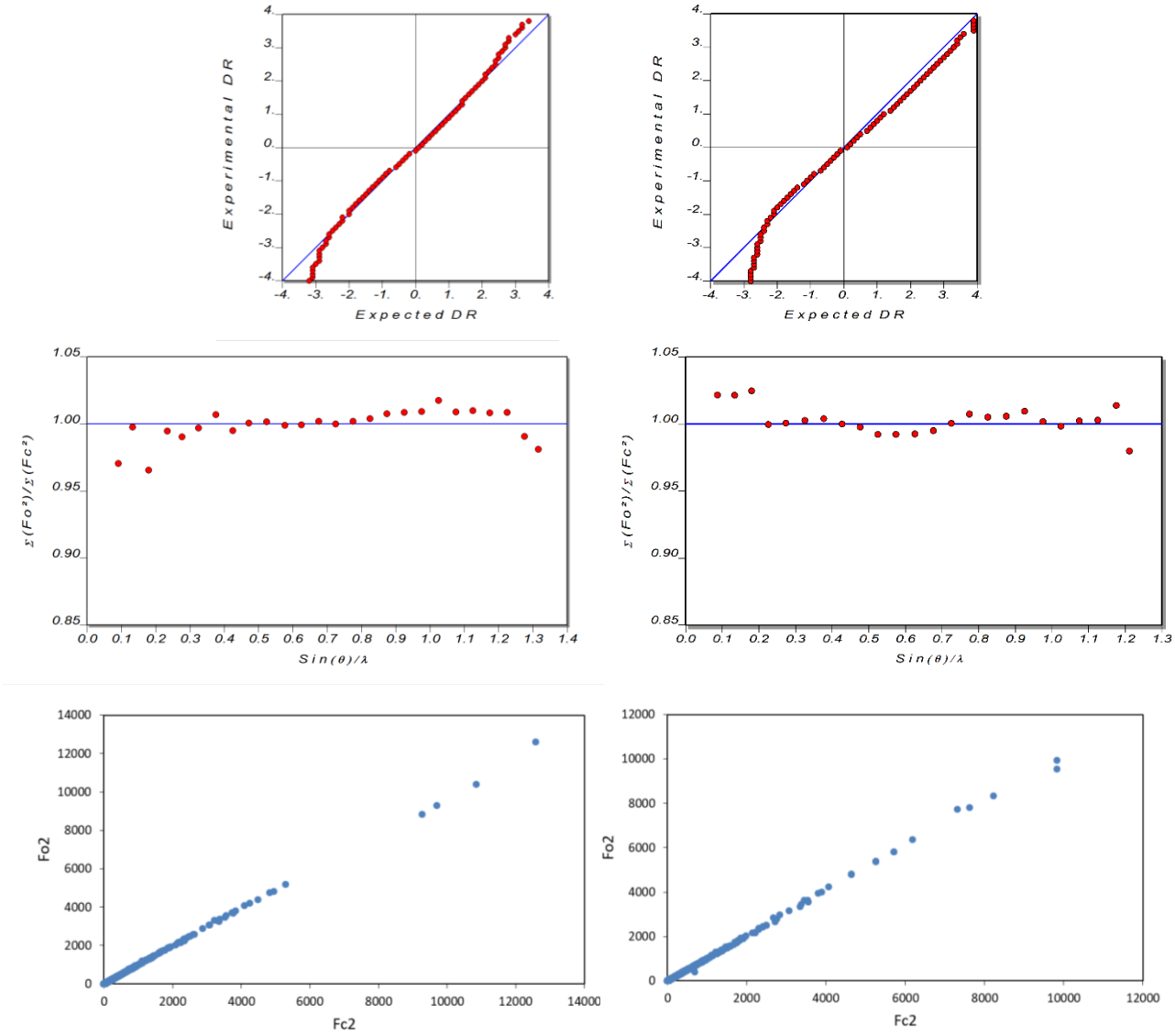

Figure 1S. Normal probability plots of F^2 residuals (top), scale plots (middle), and F_o^2 *vs.* F_c^2 plots from multipole model refinements for cyanuric acid dihydrate (left) and triptycene (right).

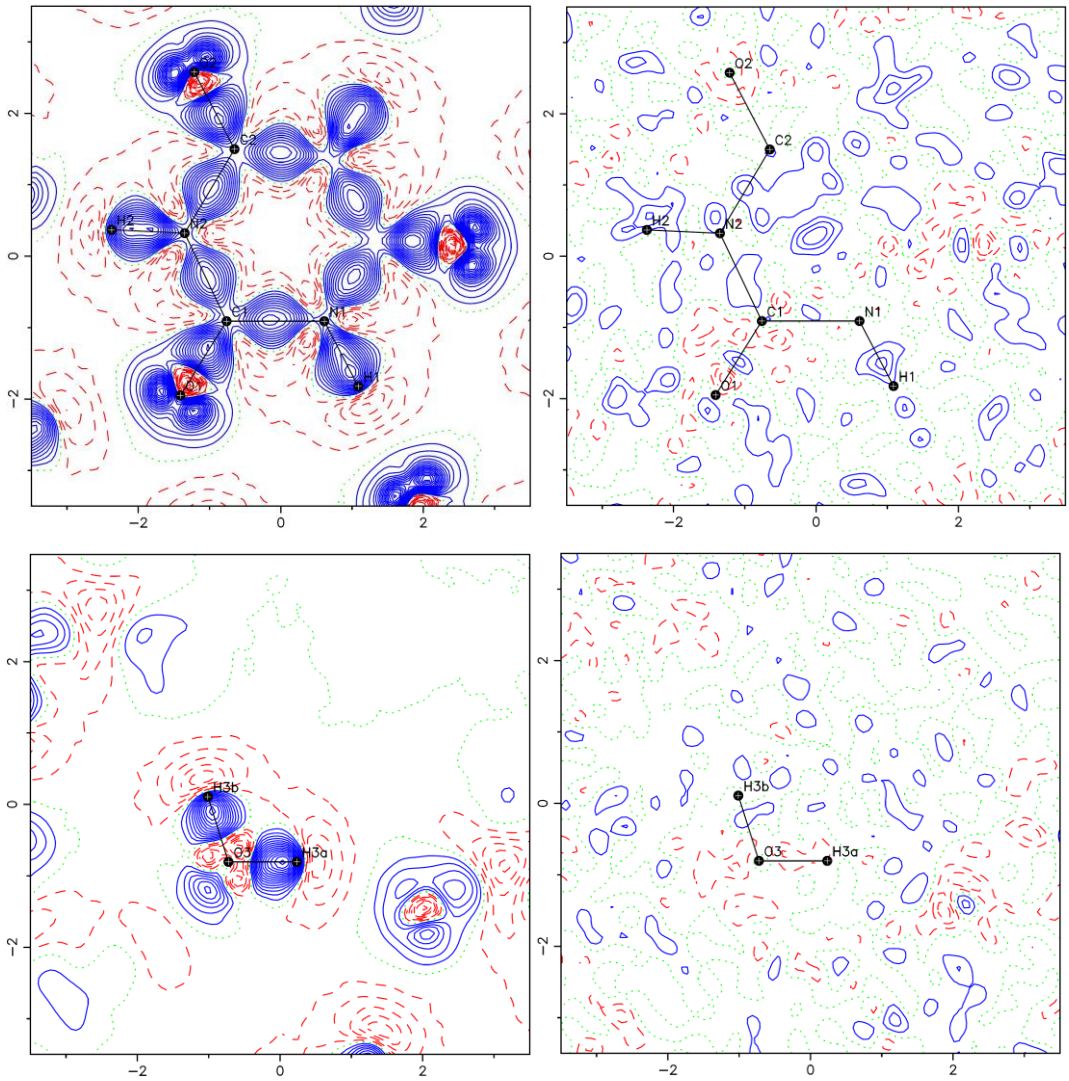

Figure 2S. Static deformation electron density (left) and residual electron density (right) Fourier maps computed for all data from multipole model refinement for cyanuric acid dihydrate. Contouring at 0.05 e·Å^{-3}; blue solid lines – positive values, red dashed lines – negative values.

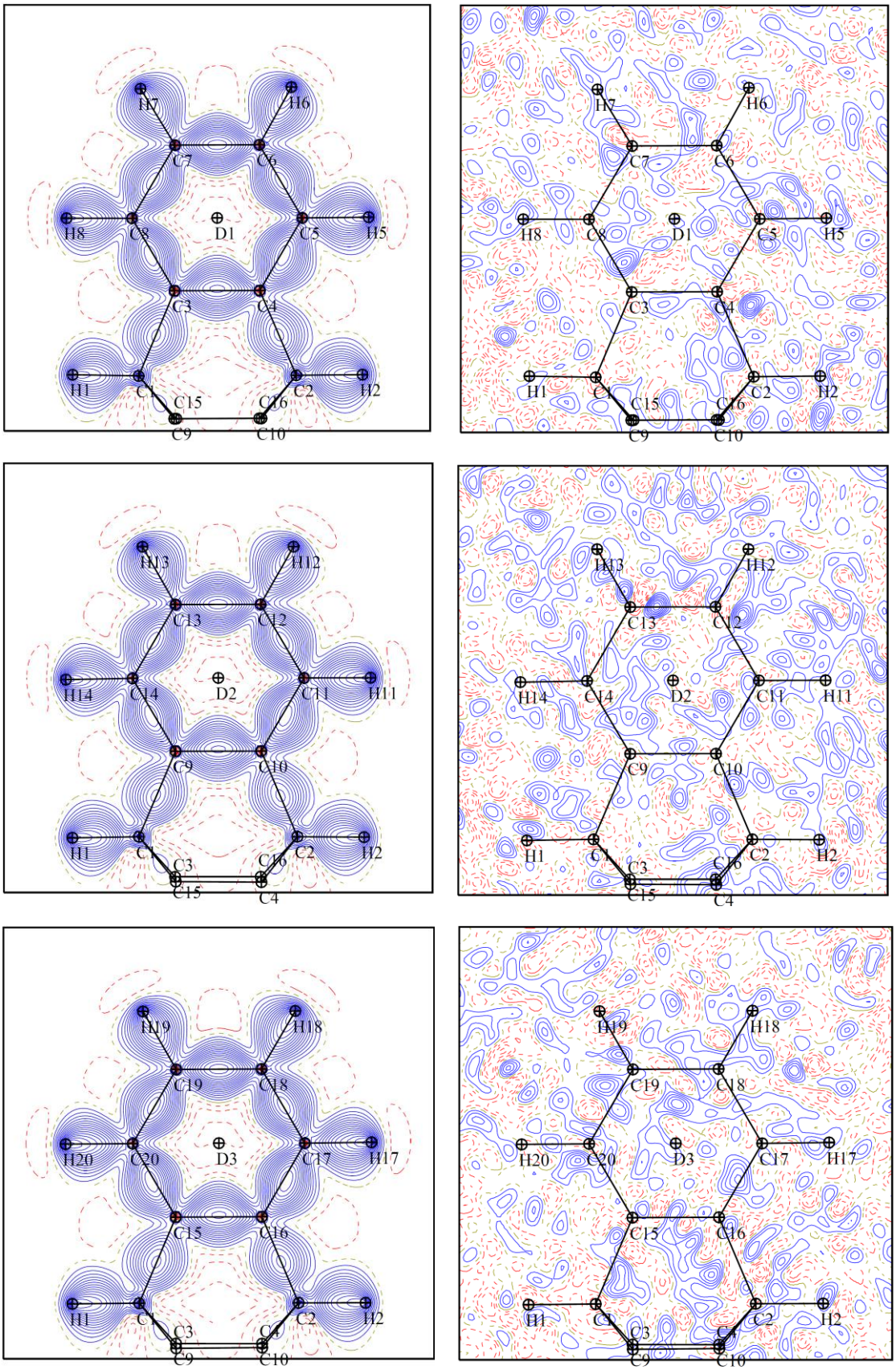

Figure 3S. Static deformation electron density (left) and residual electron density (right) Fourier maps computed for all data from multipole model refinement for triptycene. Contouring at 0.05 e·Å^{-3}; blue solid lines – positive values, red dashed lines – negative values.

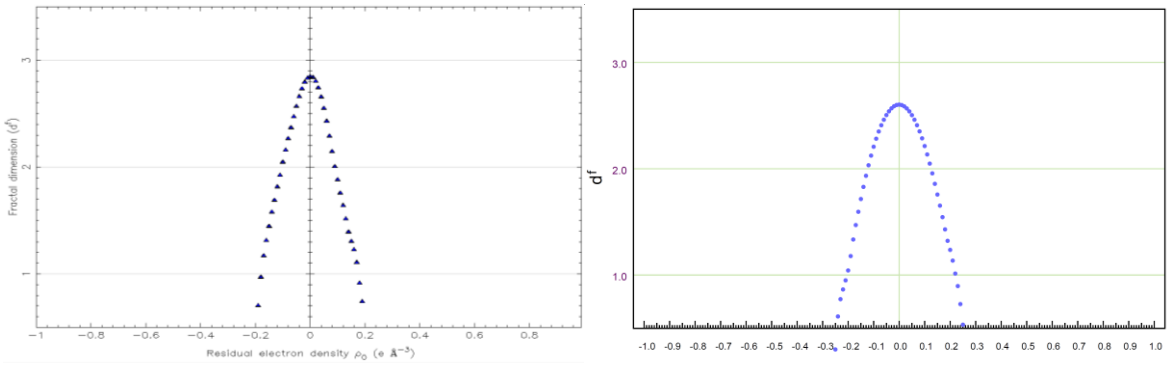

Figure 4S. Fractal dimension plots for residual electron density from multipole model refinement for cyanuric acid dihydrate (left) and triptycene (right).