FOUNDATIONS
ADVANCES

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Supporting information for article:

HgH2 meets relativistic quantum crystallography. How to teach relativity to a non-relativistic wavefunction

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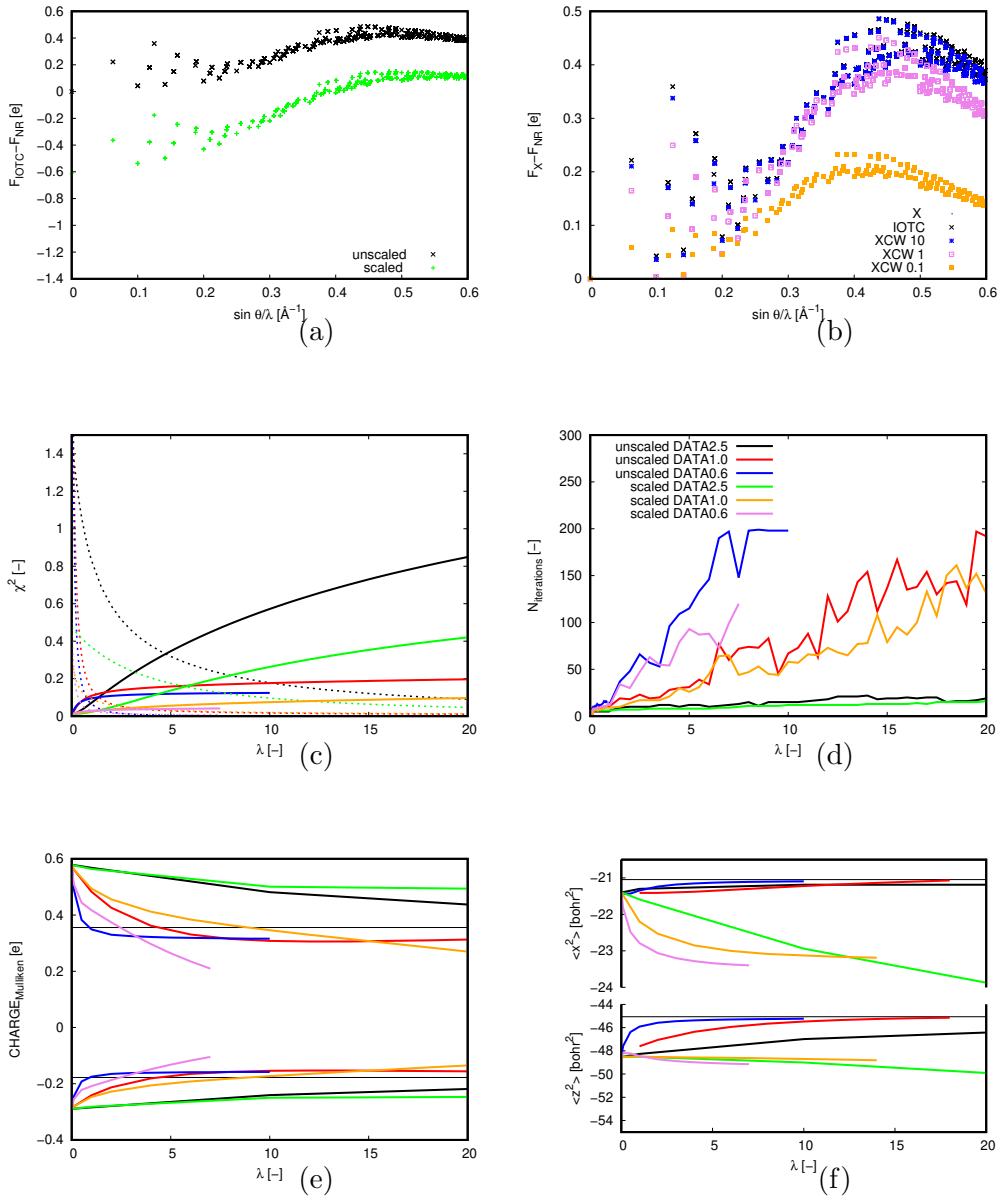
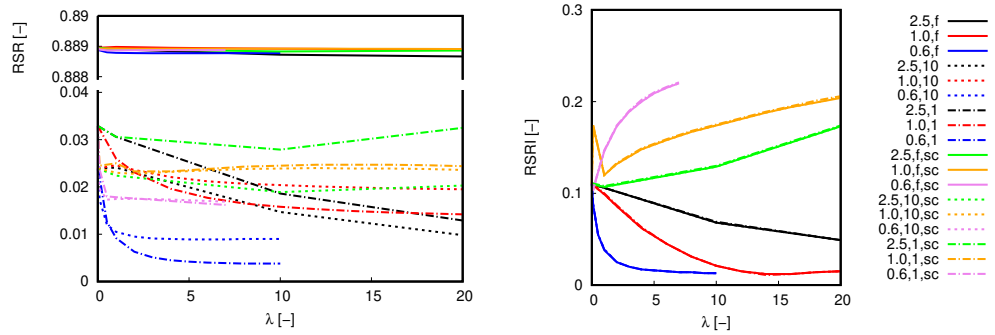


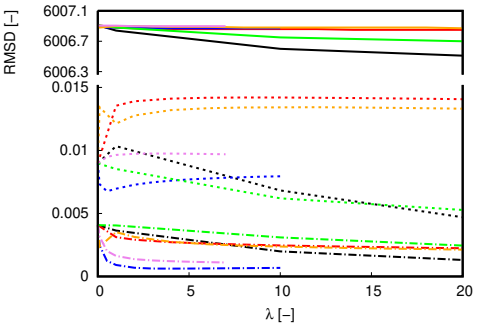
Fig. S1.
Low angle DATA0.6 results (a-b) and details of $\lambda < 20$ XCW fittings for DATA2.5 (c-f): (a) difference of IOTC and NR structure factor magnitudes of DATA0.6 for the unscaled (black crosses) and scaled (green plus signs) cases; (b) difference of IOTC and XCW structure factor magnitudes with NR ones for unscaled DATA0.6; (c) XCW fitting statistics χ^2 (dashed, left axis) and total energies (solid, arbitrary axis); (d) number of SCF iterations in the XCW fitting procedure (including the color legend which is valid for all sub-figures); (e) Mulliken charges with IOTC Hg (positive) and H (negative) as straight black lines; (f) $< x^2 >$ and $< z^2 >$ expectation values with IOTC $< x^2 >$ and $< z^2 >$ expectation values as straight black lines

IUCr macros version 2.1.10: 2016/01/28

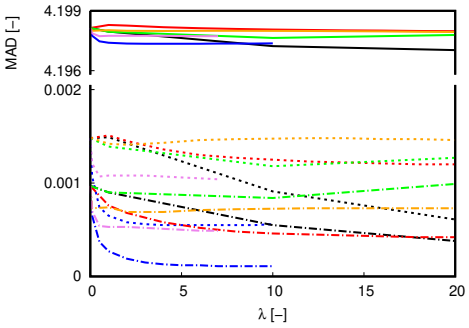


(a) RSR

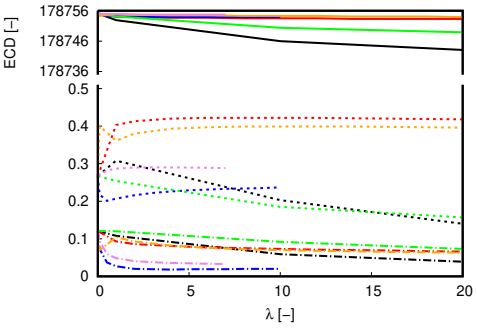
(b) RSRI



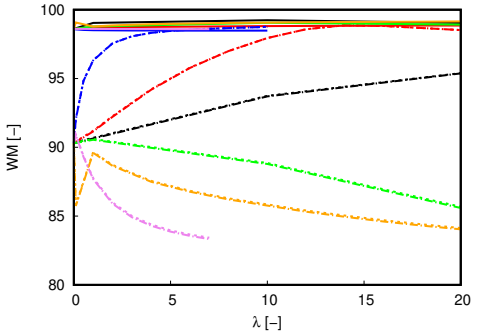
(c) RMSD



(d) MAD



(e) ECD



(f) WM

Fig. S2. Fitting statistics detail for $\lambda < 20$: (a) RSR; (b) RSRI; (c) RMSD; (d) MAD; (e) ECD; (f) WM similarity index. See the legend in the plot RSRI, where the first float is for the data resolution, the second value is for the electron density limit (f=no limit, 10=10.0$e.bohr^{-3}$,1=1.0$e.bohr^{-3}$) and sc denotes scaling during XCW fitting.