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A new understanding in context of X-ray quantum crystallography (QCr) and the Kernel energy method (KEM)

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We offer a new understanding, at once obvious and also of importance. We suggest that if KEM is applied to Quantum Crystallography, it implies a new field of study. For huge molecular systems this would allow description of biological interactions using *Ab initio* quantum mechanical methodology. Crystallographic coordinates allow calculation of the complete quantum mechanics (QM) of crystallized biological molecules of any size. Any size envisions molecules of up to many hundreds of thousands of atoms in a biological complex. And, KEM has made this doable with any chemical model of any chosen accuracy. That is the new understanding within crystallography to which reference is made. We now recognize that KEM is capable of providing the entire quantum mechanics of crystallographic biological molecular systems. This because, given the X-ray structure the KEM formula delivers the energy E, and density matrices $\rho 2$, $\rho 1$, and the electron density ρ. The KEM formula, approximations to E, $\rho 2$, $\rho 1$, ρ, and the X-ray structure factors F (K) are expressed as follows:

$$E_0^{mol} = \sum_{I \le J \le n} E_{IJ} - (n-2) \sum_{I \le n} E_I \quad (1)$$

$$\rho_2 = \sum_{I \le J \le n}^{n} \rho_{2_{IJ}} - (n-2) \sum_{I=1}^{n} \rho_{2_I} \quad (2)$$

$$\rho_1 = \sum_{I \le J \le n}^{n} \rho_{1_{IJ}} - (n-2) \sum_{I=1}^{n} \rho_{1_I} \quad (3)$$

$$\rho = \sum_{I \le J \le n}^{n} \rho_{IJ} - (n-2) \sum_{I=1}^{n} \rho_I \quad (4)$$

$$F(K) = \int e^{iKr} \{ \sum_{I \le J \le n}^{n} \rho_{IJ} - (n-2) \sum_{I=1}^{n} \rho_I \} \, d^3r \quad (5)$$

On the right side of all above equations the first sums are over double kernel quantities and the second sums are over single kernel quantities. The energy and the 3 density matrices above, of proven accuracy, are sufficient for the complete ground state quantum mechanics of any molecular system, including the X-ray structure factors. The complete quantum algorithm here suggested, is as follows: (1) Recognize that the KEM formula delivers E, *London*ρ and F (K); (2) Given any crystal structure cut it into kernels; (3) Calculate the kernels in the chemical model most appropriate to the accuracy needed; (4) Calculate the full molecule energy E and the density matrices $\rho 2$, $\rho 1$, and ρ using the KEM formulas above; (5.) From the density matrices calculate any quantum mechanical property of interest for the whole molecule, including the –X-ray structure factors F (K).

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