Electronic Supplementary Information (ESI) for:

Tautomeric transition between wobble A·C DNA base mispair and Watson-Crick-like A·C* mismatch: miscrostructural mechanism and biological significance

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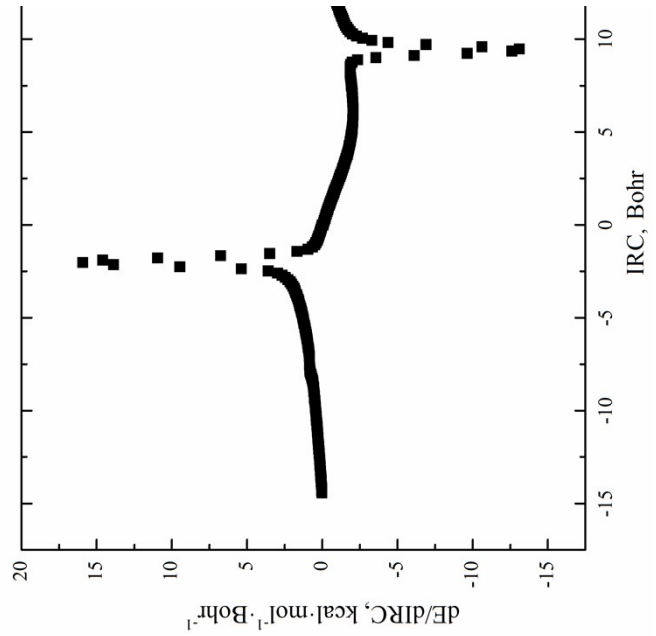

Fig. S1. Profile of the first derivative of the electronic energy with respect to the IRC (dE/dIRC) along the IRC of the A·C(w)↔A·C*(WC) tautomerisation *via* the sequential DPT obtained at the B3LYP/6-311++G(d,p) level of theory.

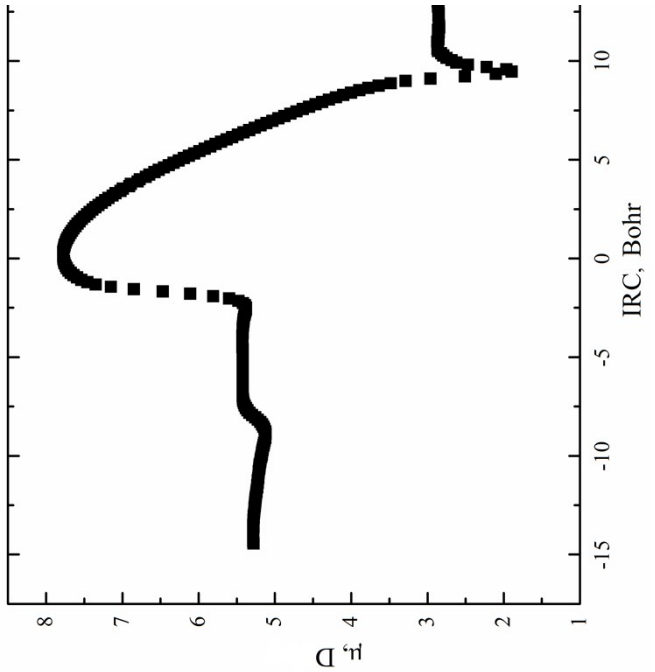

Fig. S2. Profile of the dipole moment μ along the IRC of the A·C(w)↔A·C*(WC) tautomerisation *via* the sequential DPT obtained at the B3LYP/6-311++G(d,p) level of theory.

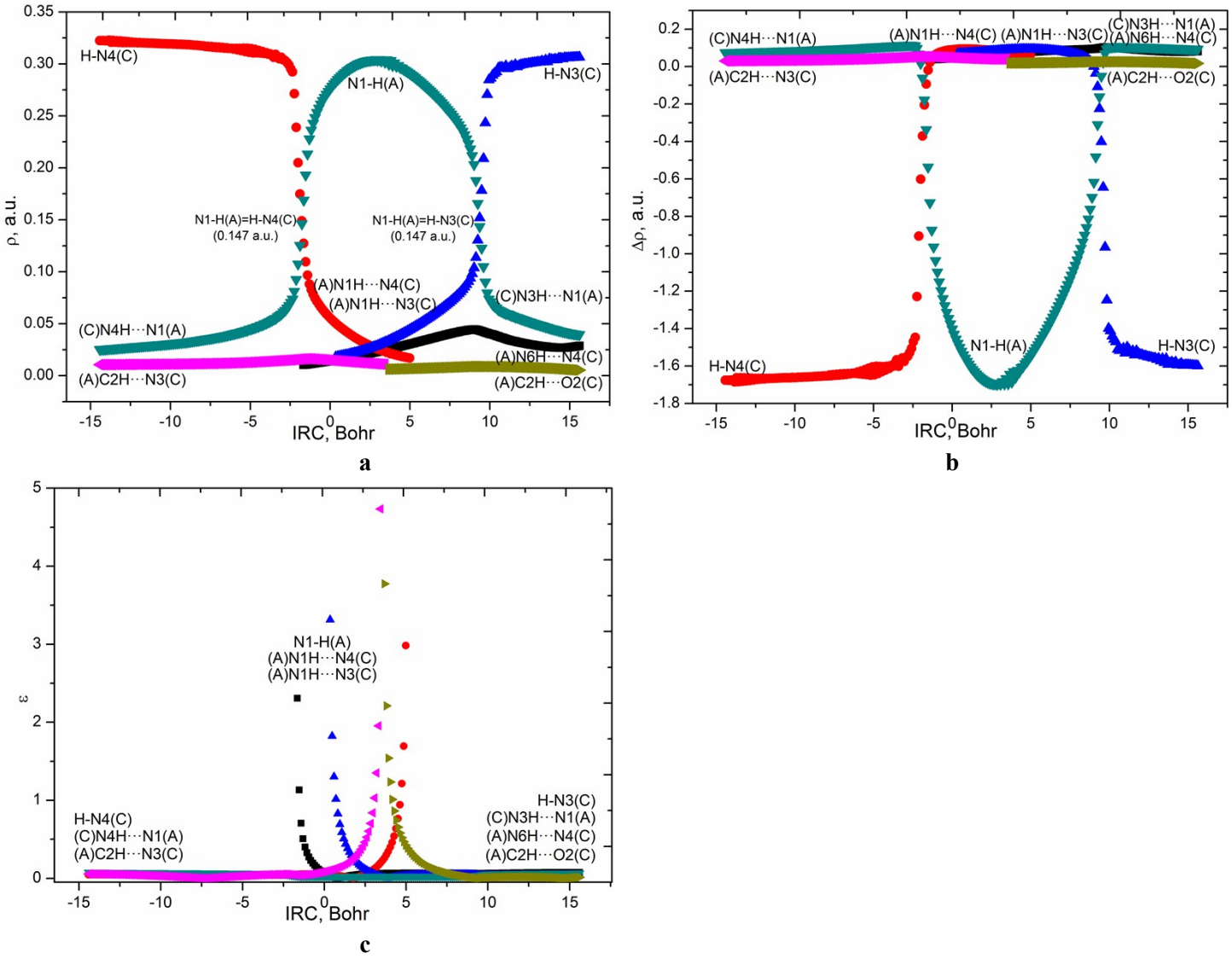

Fig. S3. Profiles of: (**a**) the electron density ρ; (**b**) the Laplacian of the electron density Δρ and (**c**) the ellipticity ε at the (3,-1) BCPs of the covalent and hydrogen bonds along the IRC of the A·C(w)↔A·C*(WC) tautomerisation *via* the sequential DPT obtained at the B3LYP/6-311++G(d,p) level of theory (see also Scheme 1, Fig. 3 and Tables 1, 4).

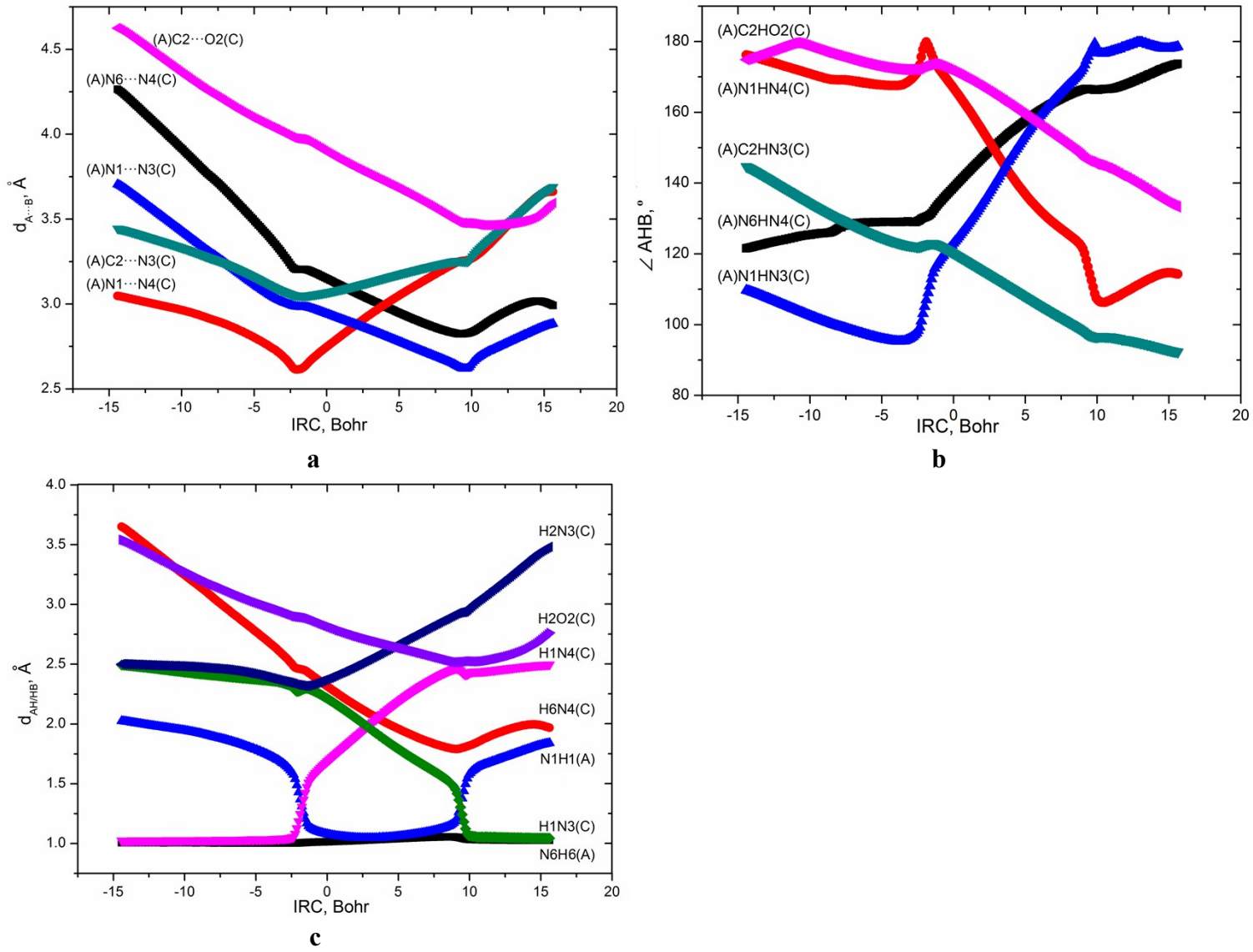

Fig. S4. Profiles of: (**a**) the distance $d_{A\cdots B}$ between the electronegative A and B atoms; (**b**) the distance $d_{AH/HB}$ between the hydrogen and electronegative A or B atoms and (**c**) the angle ∠AHB along the IRC of the A·C(w)↔A·C*(WC) tautomerisation *via* the sequential DPT obtained at the B3LYP/6-311++G(d,p) level of theory (see also Scheme 1, Fig. 3 and Tables 1, 4).