Extrapolating DFT towards the complete basis set limit: Lessons from the PBE family of functionals

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Supplementary Material

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Additional supplemental files and archives in computer-readable form are available on Zenodo, see DOI: 10.5281/zenodo.4783007. An executable version of this archive is available on Binder.
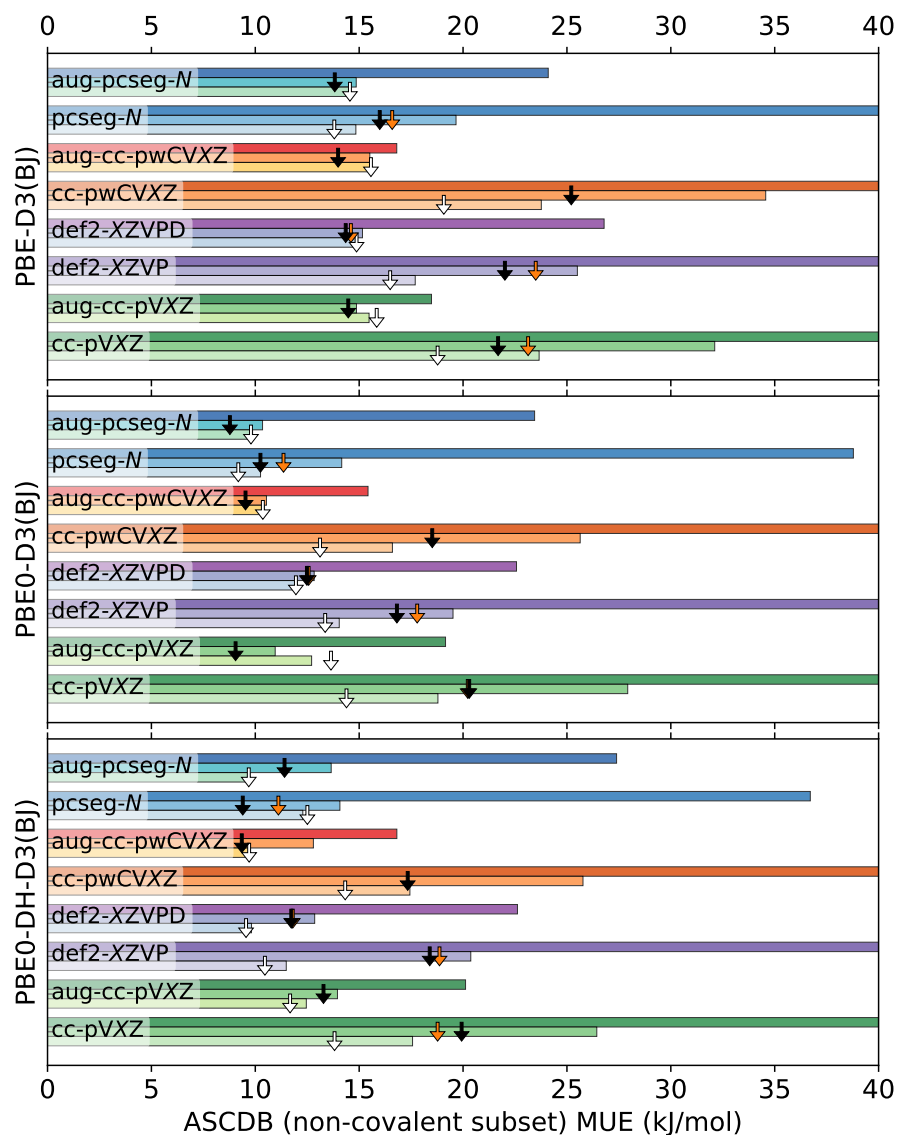
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Figure S1: The total of the mean unsigned errors in the non-covalent subset of the ASCDB database. Calculations with 2-, 3-, and 4-ζ basis sets shown as horizontal bars in ascending order. Results from the [2,3]-ζ and [3,4]-ζ extrapolations from current work are indicated by the black and white arrows, respectively. Comparison with previous [2,3]-ζ results (orange arrow) shown where available.
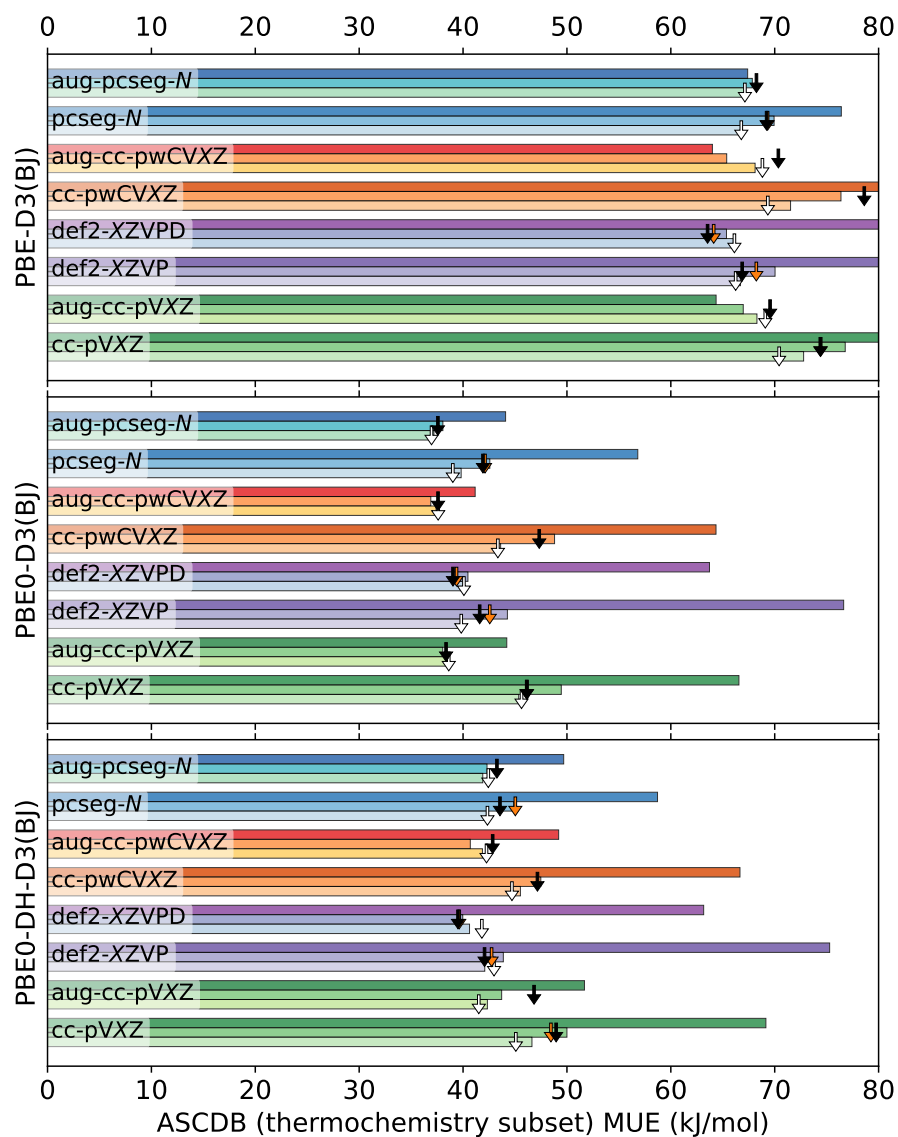
Figure S2: The total of the mean unsigned errors in the thermochemistry subset of the ASCDB database. Bars and symbols as in Fig. S1.
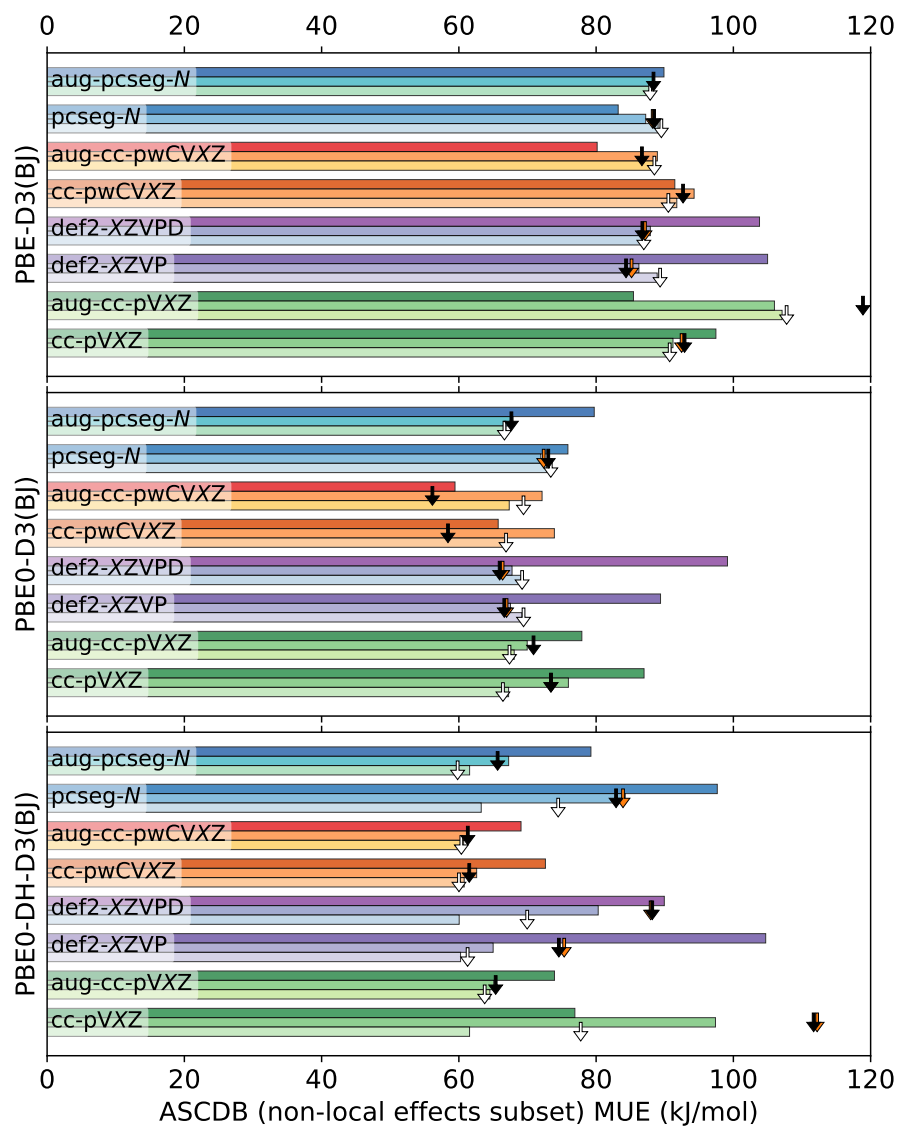
Figure S3: The total of the mean unsigned errors in the non-local subset of the ASCDB database. Bars and symbols as in Fig. S1.
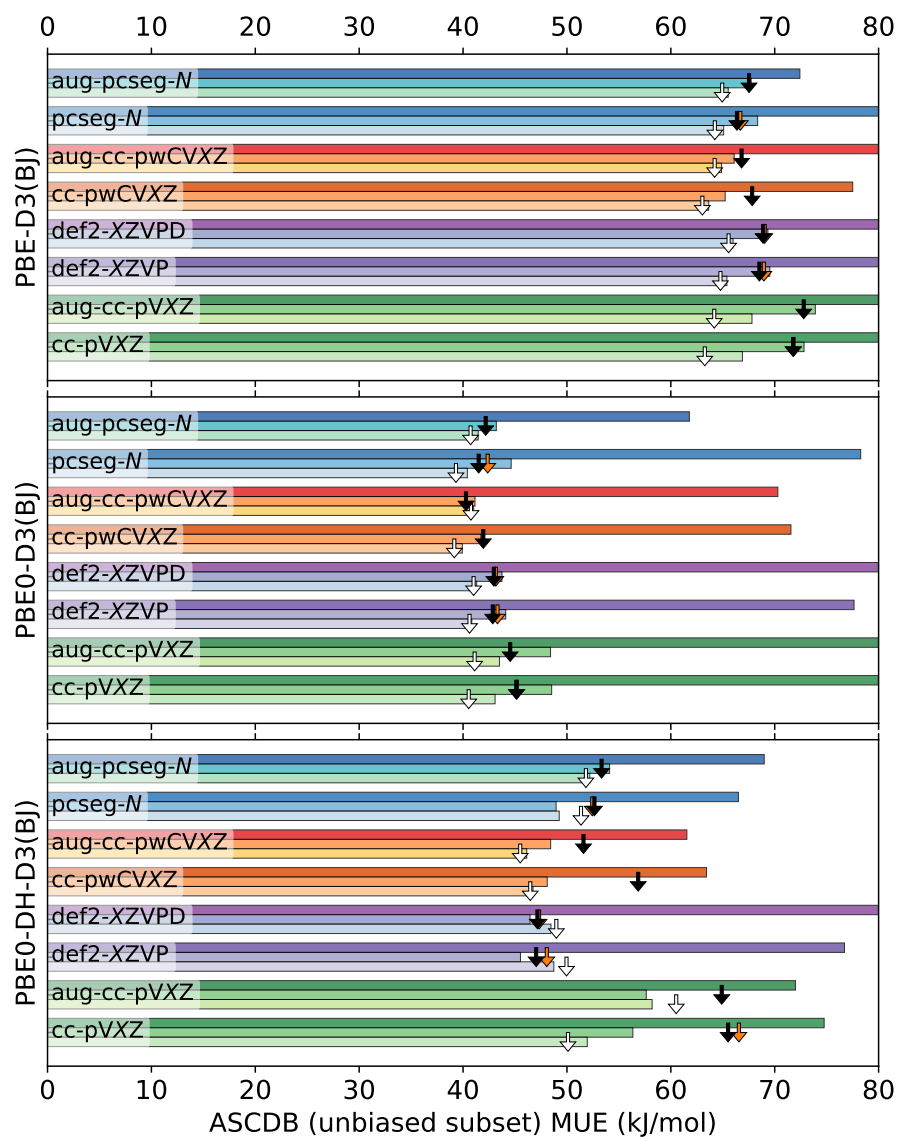
Figure S4: The total of the mean unsigned errors in the unbiased calculations subset of the ASCDB database. Bars and symbols as in Fig. S1.
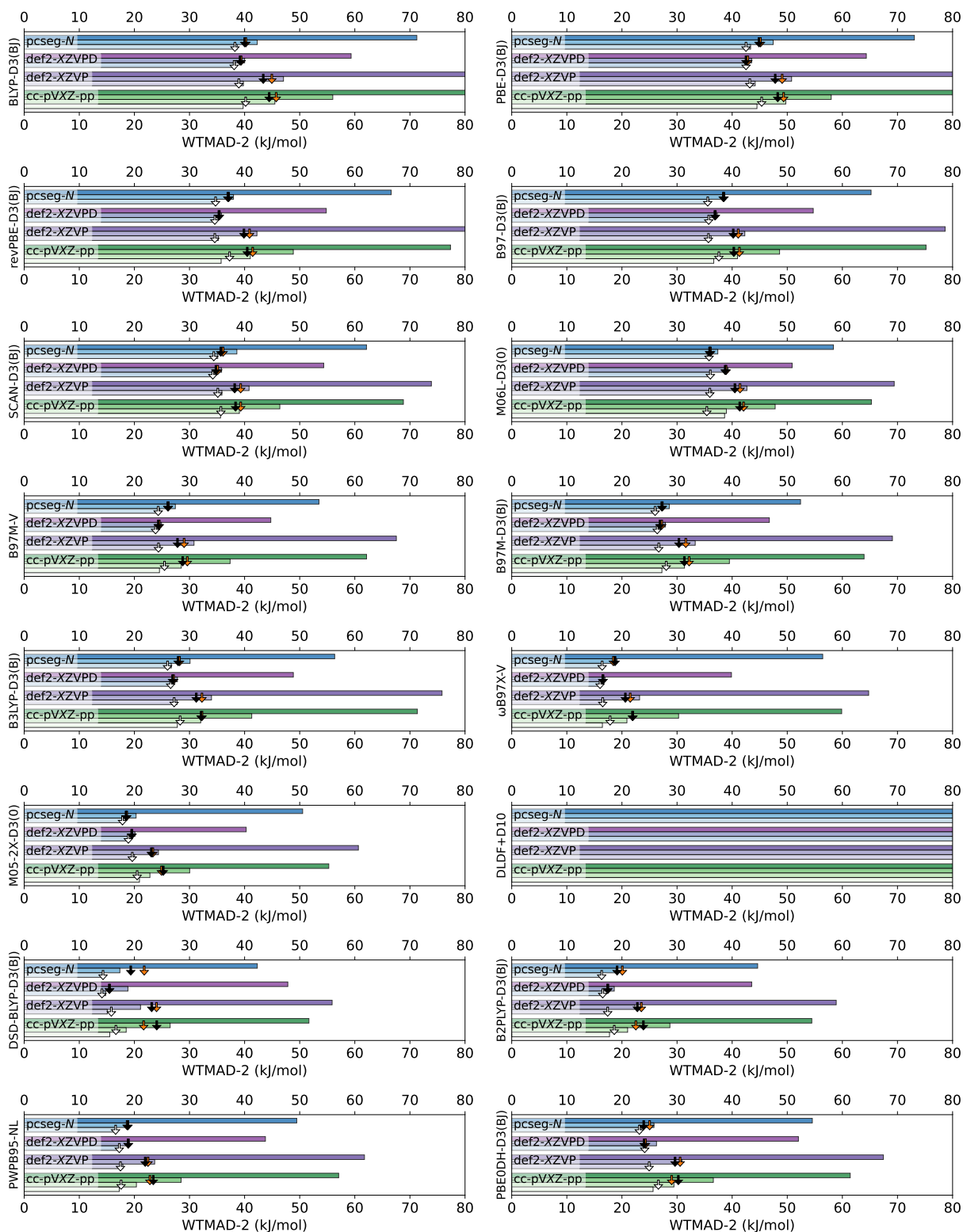
Figure S5: The WTMAD-2 measures of the diet100 subset of the GMTKN55 database. Bars and symbols as in Fig. S1. For the cc-pVXZ-pp basis sets, data from 2-, 3-, 4-, and 5-ζ basis sets shown.