Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information:

Challenging Compounds for Calculating Molecular Second Hyperpolarizabilities: the Triplet State of the Trimethylenemethane Diradical and Two Derivatives

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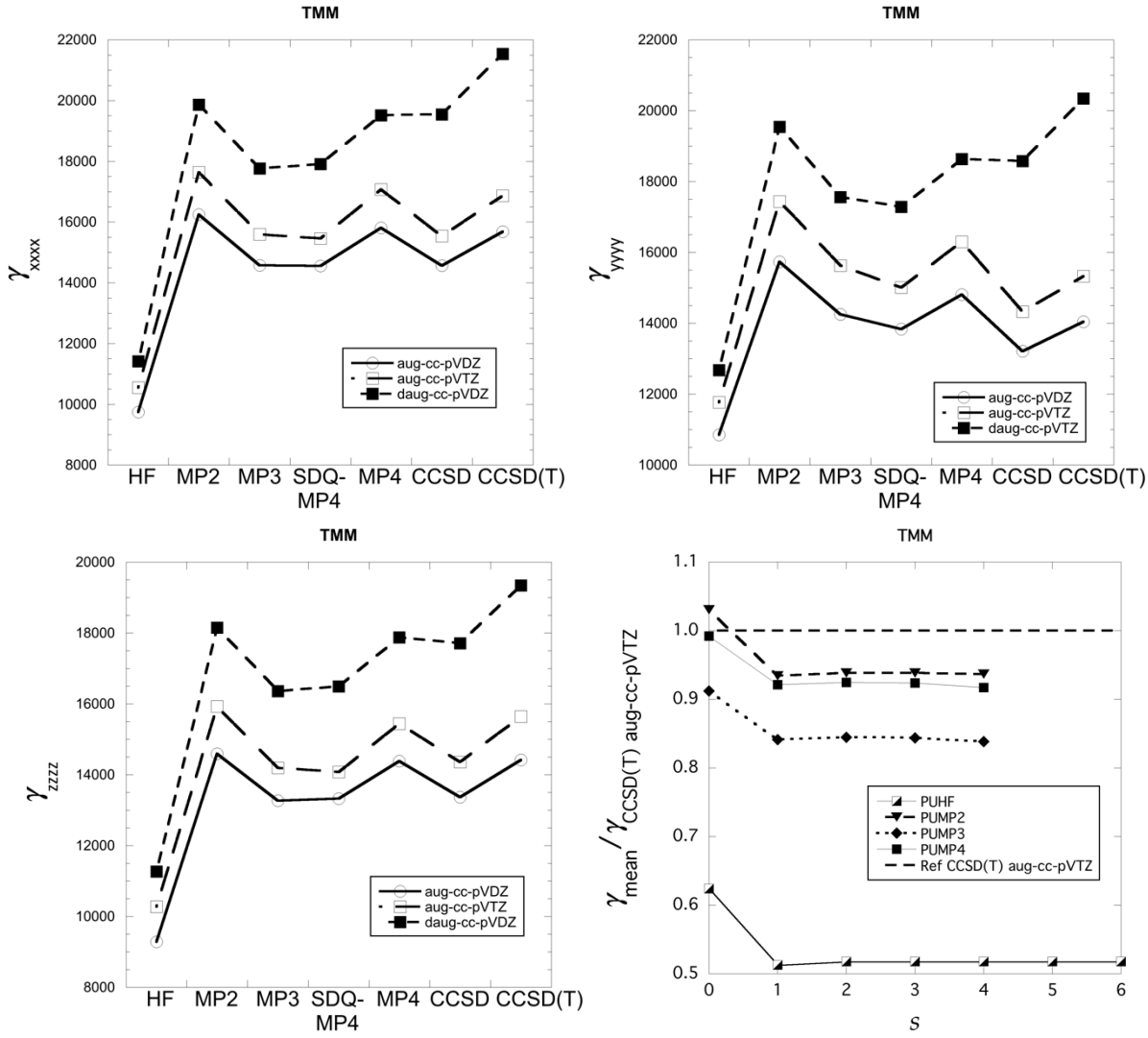

Figure S1. Basis set and electron correlation effects for wave function methods on the second hyperpolarizability of TMM. Lines are guides for the eyes. The three first figures compare wave function correlated schemes to UCCSD(T) results as a function of the basis set, for γ_{xxxx}, γ_{yyyy}, and γ_{zzzz} components whereas the last figure concentrates on Spin projected UHF, UMP2, UMP3, and UMP4 results obtained with the aug-cc-pVTZ basis set.

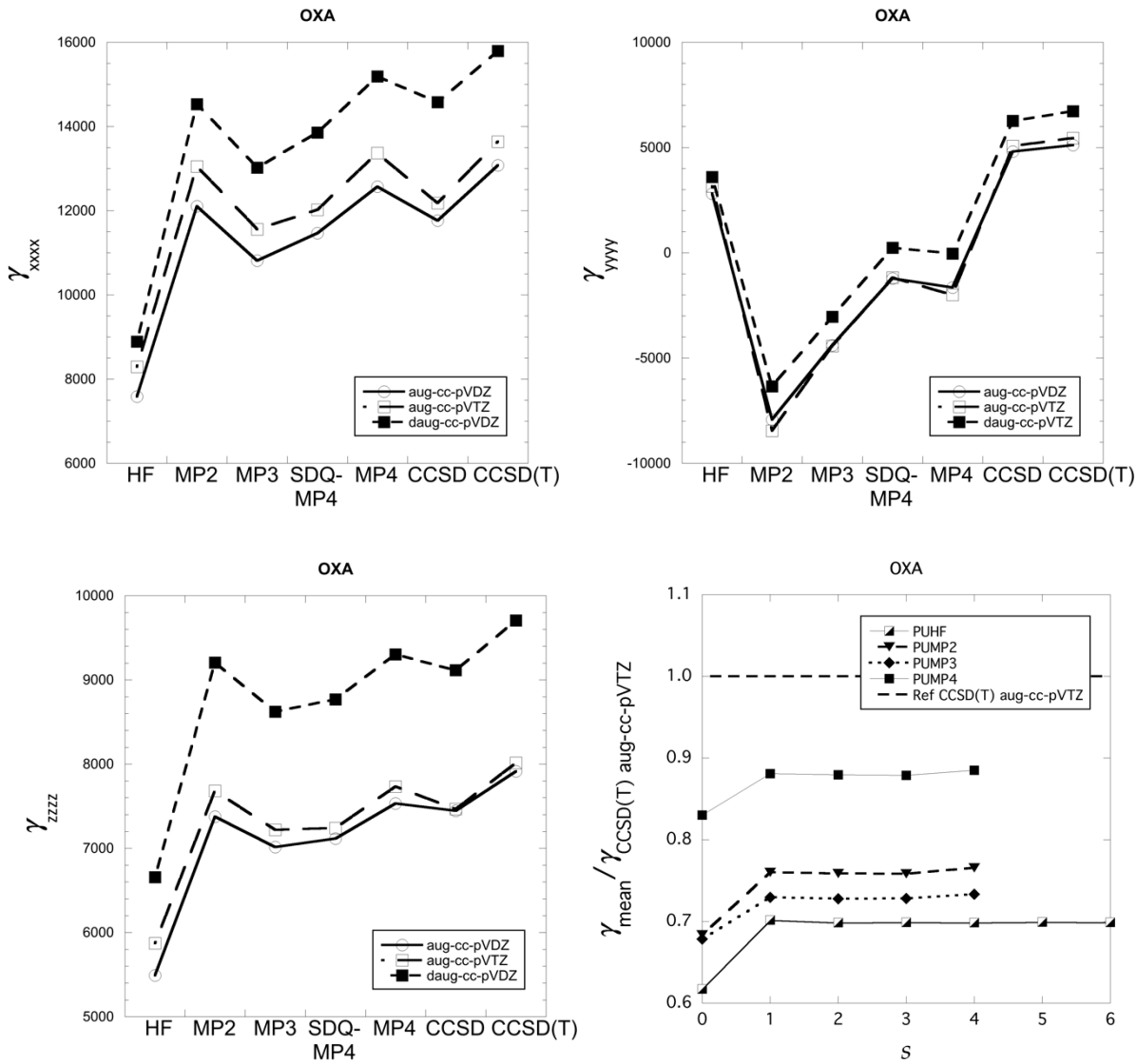

Figure S2. Basis set and electron correlation effects for wave function methods on the second hyperpolarizability of OXA. See Caption of Fig. S1 for more details.

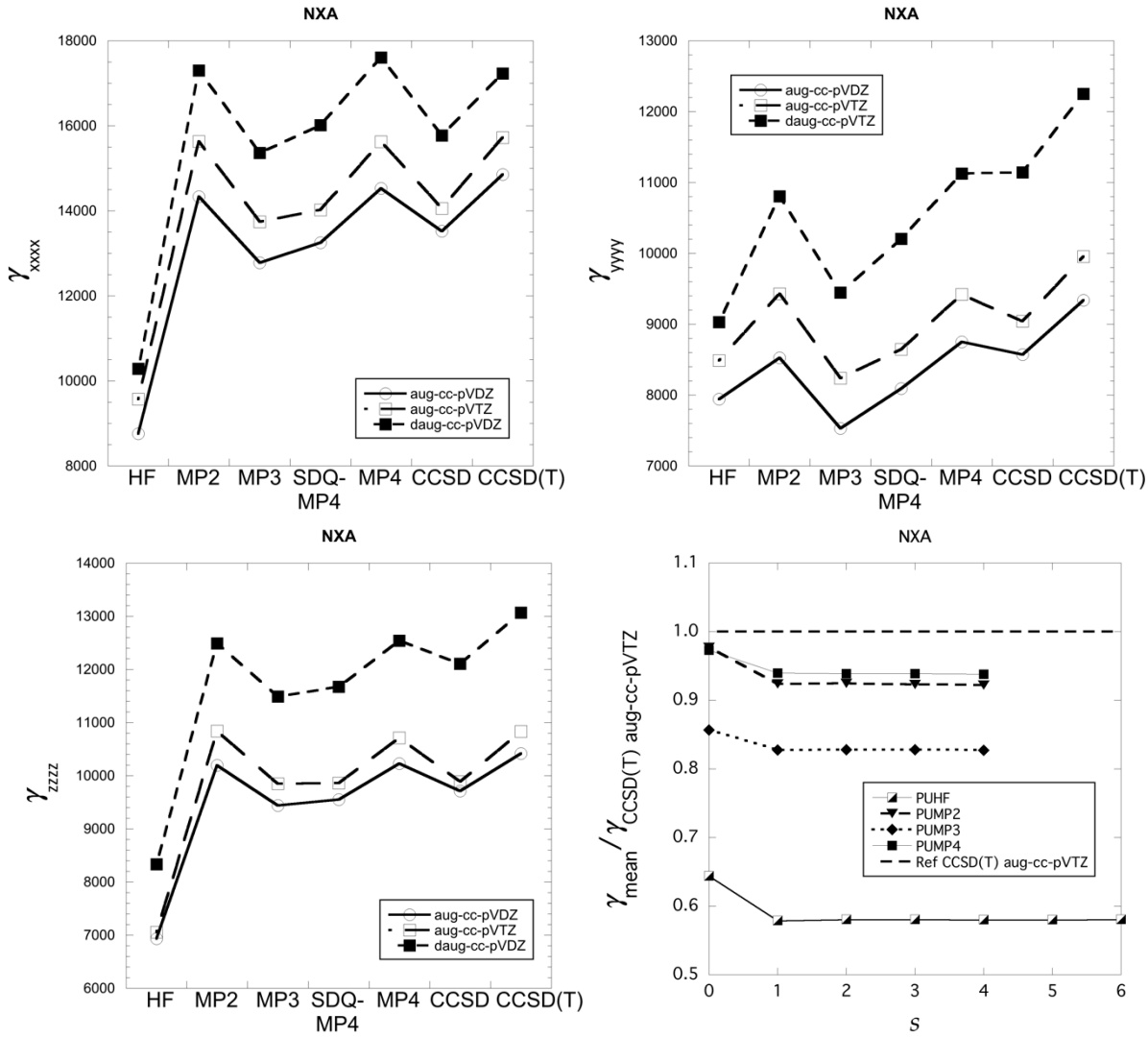

Figure S3. Basis set and electron correlation effects for wave function methods on the second hyperpolarizability of NXA. See Caption of Fig. S1 for more details.

Number of basis functions	TMM	OXA	NXA
aug-cc-pVDZ	146	128	137
aug-cc-pVTZ	322	276	299
d-aug-cc-pVDZ	206	180	193

Table S1. Number of basis set functions for the three compounds and the three basis sets considered in this study