

First-order hyperpolarizabilities of propellanes: Elucidating structure-property relationships

ELECTRONIC SUPPLEMENTARY INFORMATION

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Table S 1: Vectorial electronic and harmonic vibrational contributions to the first hyperpolarizability (in au) as computed using aug-cc-pVDZ basis set. The values obtained using 6-31+G basis set are shown in parentheses. Note that the sign differences observed for some compounds (e.g. **4** and **10**) are due to different orientation of the dipole moment vector (with an absolute value close to zero).

compound	$\beta_{ }^e$	$[\mu\alpha]_{ }^{(0,0)}$
1	196	(239)
2	218	(178)
3	246	(284)
4	-521	(-553)
5	112	(55)
6	247	(177)
7	534	(537)
8	212	(236)
9	251	(290)
10	449	(-489)
11	1198	(1367)
12	368	(405)
13	710	(811)
14	214	(231)
15	1087	(1326)
16	22	(-121)

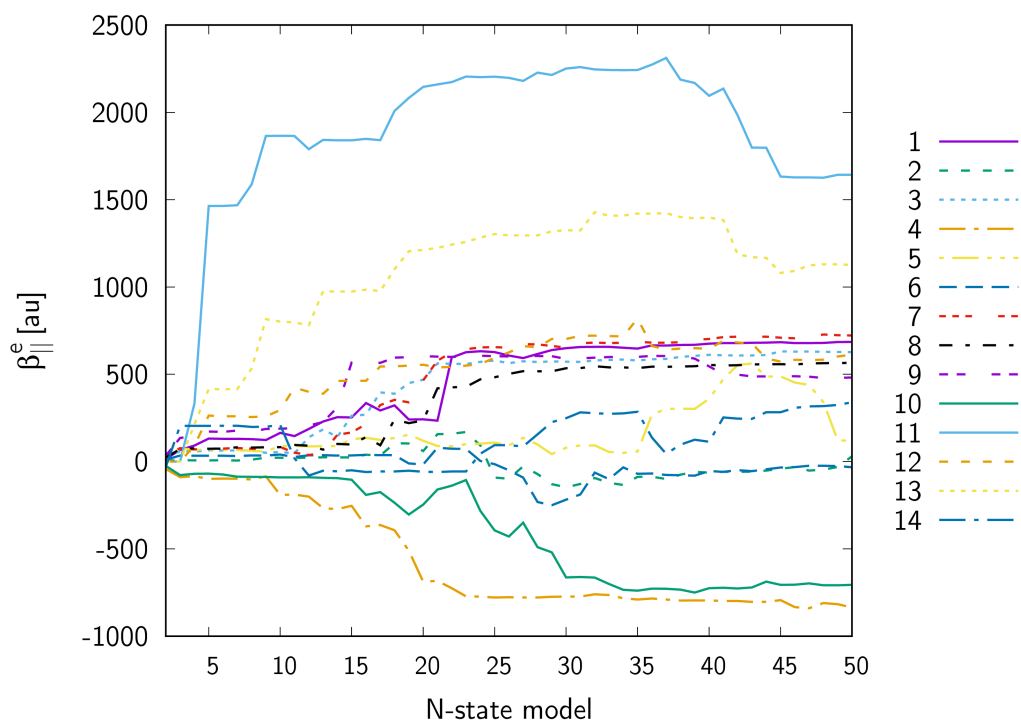


Figure S1: Convergence of the electronic first hyperpolarizability (in au) for **11-14** with the number of electronic states (N -state model accounts also for electronic ground state). Calculations were performed at CAM-B3LYP/6-31+G level of theory.