Supporting Information: A New Method to Analyze and Understand Molecular Linear and Nonlinear Responses via Field-Induced Functions. A Straightforward Alternative to Sum-Over-States (SOS) Analysis

Nicolás Otero,† Panaghiotis Karamanis,‡ and Marcos Mandado*,†

†*Department of Physical Chemistry, University of Vigo, As Lagoas-Marcosende s/n, 36310. Vigo, Spain*

‡*Équipe Chimie-Physique (ECP), Institut des Sciences Analytiques et de Physico-chimie pour l'Environnement et les Materiaux (IPREM) UMR 5254, Technopole Helioparc, 2 avenue du President Pierre Angot, 64053. Pau Cedex 09, France)*

E-mail: mandado@uvigo.es

Contents

1 Detailed description of the electronic supporting information

This electronic supporting information (ESI) contains two kinds of information:

- Plots with the representations of the variation of a component of the polarizability, α, or one of the 1st hyperpolarizability, β, with respect to the number of molecular orbitals (MOs) or excited states, depending on the approach considered. If it is not said otherwise, the principal axis is considered along z direction.

  Each figure is formed by four subfigures, except N_2 molecule, whose full β tensor is zero. Subfigures (a) and (c) were obtained by means of our field-induced orbital (FIO) decomposition and summed over the number of MOs. For α, three approaches were considered: coupled perturbed Kohn-Sham (CPKS), coupled perturbed Hartree-Fock (CPHF) and uncoupled perturbed Hartree-Fock (UPHF). In the case of β, only CPKS and CPHF approaches were taken into account.

  The values shown in subfigures (b) and (d) were computed through the TDDFT and CIS *sum over states* method (SOS) as implemented in Multiwfn.[S1] In the case of larger molecules, the number of excited states considered to compute the (hyper)polarizabilities were truncated to a value of 1500.

  In addition to the four subfigures and caused by the enormous number of states and MOs, subfigures (e) and (f) of benzene derivatives, the series of molecules based on CN−C≡C−H as well as H−C≡C−CF_3 are also included with a shorten range on the x axis to observe the most important variations.

  The plots were obtained at CAM-B3LYP and HF approaches combined in both cases with 6-311G(d,p) and 6-311++G(d,p) basis sets for the optimized structures. The FIOs and SOS results of these basis sets are included in the corresponding subsections, as can be seen in the table of contents. Since the FIOs and TDDFT-SOS approaches are independent of the functional to be considered, CAM-B3LYP was employed due to the well-known results obtained in calculations of (hyper)polarizabilities.[S2–S6] The first derivative of the density matrices with respect to an uniform electric field was obtained analytically from the corresponding Gaussian calculations.[S7] On the contrary, the second derivative was computed by the symmetric numerical definition of the finite field (FF) approach with an electric field strength of 0.001 au.

In all cases, the recomputed total values of the corresponding component are included in plots (a)–(d).

- Outputs from our either TDDFT (CAM-B3LYP) or CIS calculations of the molecules commented in the main text of the work, *i.e.*, the following set of molecules are shown: $\mathbf{HHe^+}$ (Subsections 3.1.2 and 3.1.3), **HF** (Subsections 5.1.2 and 5.1.3), $\mathbf{H_2O}$ (Subsections 7.1.2 and 7.1.3), $\mathbf{H_2S}$ (Subsections 8.1.2 and 8.1.3), **p-nitroaniline** (Subsections 16.1.2 and 16.1.3), **m-nitroaniline** (Subsections **??** and **??**) and **p-methoxy-nitrobenzene** (Subsections 18.1.2 and 18.1.3). These outputs, considering the aforementioned two basis sets, are formed by a truncated set of excited states (except HHe^+, the full number of excited states was printed) adequate to represent the most important contributions to recover the final SOS value (see the corresponding figures of the same section and read the main text of the work). The symmetry determined by Gaussian 09 (`symm`), the energy (`Exc.E`), the oscillator strength (`Osc.Strength`), the transition dipole moment (`f`) and $\langle S^2 \rangle$ (`<S**2>`) are included together with the main excited configurations ordered by the five first largest and the five first lowest CI coefficients. In the last line of each excited state, the number of nonnegligible excited configurations with respect to the CI coefficient (`#CIs`), as well as the number of positive (`#CIs>0`) and negative (`#CIs<0`) values considered to obtain the SOS plots are shown.

References

(S1) Lu, T.; Chen, F. Multiwfn: A multifunctional wavefunction analyzer. *J. Comput. Chem.* **2012**, *33*, 580–592.

(S2) Yanai, T.; Tew, D. P.; Handy, N. C. A new hybrid exchange–correlation functional using the Coulomb-attenuating method (CAM-B3LYP). *Chem. Phys. Lett.* **2004**, *393*, 51–57.

(S3) Xenides, D.; Karamanis, P.; Pouchan, C. A critical analysis of the performance of new generation functionals on the calculation of the (hyper) polarizabilities of clusters of varying stoichiometry: Test case the Si_mGe_n ($m + n = 7$, $n = 0 - 7$) clusters. *Chem. Phys. Lett.* **2010**, *498*, 134–139.

(S4) Karamanis, P.; Pouchan, C.; Weatherford, C. A.; Gutsev, G. L. Evolution of properties in prolate $(GaAs)_n$ clusters. *J. Phys. Chem. C* **2011**, *115*, 97–107.

(S5) Karamanis, P.; Marchal, R.; Carbonniére, P.; Pouchan, C. Doping-enhanced hyperpolarizabilities of silicon clusters: A global ab initio and density functional theory study of $Si_{10}(Li, Na, K)_n$ ($n = 1, 2$) clusters. *J. Chem. Phys.* **2011**, *135*, 044511.

(S6) Karamanis, P. The importance of the DFT method on the computation of the second hyperpolarizability of semiconductor clusters of increasing size: A critical analysis on prolate aluminum phosphide clusters. *Int. J. Quantum Chem.* **2012**, *112*, 2115–2125.

(S7) Otero, N.; Alsenoy, C. V.; Pouchan, C.; Karamanis, P. Hirshfeld-based intrinsic polarizability density representations as a tool to analyze molecular polarizability. *J. Comput. Chem.* **2015**, *36*, 1831–1843.

2 Molecular polarizability and 1st hyperpolarizability tensor components

Table S1: Tensor components of polarizability α of the molecules considered in this work. 1 CAM-B3LYP/6-311G**, 2 CAM-B3LYP/6-311++G*, 3 HF/6-311G**, 4 HF/6-311++G**

Molecule	Level	α_{XX}	α_{XY}	α_{YY}	α_{XZ}	α_{YZ}	α_{ZZ}
HHe^+	1	0.62	0.00	0.62	0.00	0.00	1.62
	2	0.62	0.00	0.62	0.00	0.00	1.63
	3	0.60	0.00	0.60	0.00	0.00	1.46
	4	0.60	0.00	0.60	0.00	0.00	1.46
N_2	1	6.05	0.00	6.05	0.00	0.00	13.66
	2	7.81	0.00	7.81	0.00	0.00	15.23
	3	5.73	0.00	5.73	0.00	0.00	13.68
	4	7.00	0.00	7.00	0.00	0.00	14.66
CO	1	8.61	0.00	8.61	0.00	0.00	13.04
	2	9.92	0.00	9.92	0.00	0.00	15.27
	3	8.23	0.00	8.23	0.00	0.00	12.45
	4	9.06	0.00	9.06	0.00	0.00	14.01
LiF	1	7.33	0.00	7.33	0.00	0.00	8.08
	2	7.31	0.00	7.31	0.00	0.00	9.31
	3	4.84	0.00	4.84	0.00	0.00	5.64
	4	5.17	0.00	5.17	0.00	0.00	6.58
HF	1	1.82	0.00	1.82	0.00	0.00	4.58
	2	2.82	0.00	2.82	0.00	0.00	5.05
	3	1.70	0.00	1.70	0.00	0.00	4.15
	4	2.32	0.00	2.32	0.00	0.00	4.42

Continued on next page

Table S1 – *Continued from previous page*

Molecule	Level	α_{XX}	α_{XY}	α_{YY}	α_{XZ}	α_{YZ}	α_{ZZ}
HCl	1	6.82	0.00	6.82	0.00	0.00	13.32
	2	9.43	0.00	9.43	0.00	0.00	13.48
	3	6.56	0.00	6.56	0.00	0.00	12.82
	4	8.70	0.00	8.70	0.00	0.00	12.95
H_2O	1	4.02	0.00	7.66	0.00	0.00	5.83
	2	6.81	0.00	8.21	0.00	0.00	6.76
	3	3.77	0.00	7.08	0.00	0.00	5.28
	4	5.50	0.00	7.42	0.00	0.00	5.85
H_2S	1	11.59	0.00	18.52	0.00	0.00	17.27
	2	19.27	0.00	18.64	0.00	0.00	17.31
	3	11.24	0.00	18.19	0.00	0.00	16.15
	4	17.99	0.00	18.31	0.00	0.00	16.17
NH_3	1	10.18	0.00	10.18	0.00	0.00	7.89
	2	10.95	0.00	10.95	0.00	0.00	12.89
	3	9.65	0.00	9.65	0.00	0.00	7.38
	4	10.19	0.00	10.19	0.00	0.00	10.70
F−CC−H	1	10.43	0.00	10.43	0.00	0.00	30.09
	2	13.09	0.00	13.09	0.00	0.00	32.28
	3	10.21	0.00	10.21	0.00	0.00	28.49
	4	12.51	0.00	12.51	0.00	0.00	29.96
$HCCCF_3$	1	20.33	0.00	20.33	0.00	0.00	43.04
	2	25.83	0.00	25.83	0.00	0.00	47.35
	3	18.88	0.00	18.88	0.00	0.00	39.89
	4	42.88	0.00	23.26	0.00	0.00	23.26

Continued on next page

Table S1 – *Continued from previous page*

Molecule	Level	α_{XX}	α_{XY}	α_{YY}	α_{XZ}	α_{YZ}	α_{ZZ}
CN−CC−H	1	15.74	0.00	15.74	0.00	0.00	63.21
	2	18.53	0.00	18.53	0.00	0.00	65.17
	3	15.50	0.00	15.50	0.00	0.00	59.87
	4	18.04	0.00	18.04	0.00	0.00	63.11
CN−CC−CC−H	1	22.20	0.00	22.20	0.00	0.00	135.18
	2	26.54	0.00	26.54	0.00	0.00	142.87
	3	22.03	0.00	22.03	0.00	0.00	121.44
	4	25.87	0.00	25.87	0.00	0.00	126.60
CN−CC−CC−CC−H	1	28.56	0.00	28.56	0.00	0.00	236.59
	2	34.28	0.00	34.28	0.00	0.00	247.52
	3	28.46	0.00	28.46	0.00	0.00	201.60
	4	33.62	0.00	33.62	0.00	0.00	208.47
p−cyanoaniline	1	37.39	−0.31	138.11	0.00	0.00	81.57
	2	51.43	0.17	147.59	0.00	0.00	86.80
	3	37.25	−0.51	126.22	0.00	0.00	78.37
	4	50.36	−0.09	133.04	0.00	0.00	83.05
p−cyanoaniline	1	81.57	0.00	37.39	0.00	−0.31	138.11
	2	86.80	0.00	51.43	0.00	0.17	147.59
	3	78.37	0.00	37.25	0.00	−0.51	126.22
	4	83.05	0.00	50.36	0.00	−0.09	133.04
p−nitroaniline	1	91.94	0.00	36.12	0.00	0.25	131.30
	2	98.17	0.00	50.40	0.00	−0.20	143.48
	3	88.50	0.00	35.99	0.00	0.44	115.25
	4	93.83	0.00	49.25	0.00	0.05	122.90

Continued on next page

Table S1 – *Continued from previous page*

Molecule	Level	α_{XX}	α_{XY}	α_{YY}	α_{XZ}	α_{YZ}	α_{ZZ}
m−nitroaniline	1	95.68	18.61	44.15	−1.38	−12.71	109.43
	2						
	3	78.01	27.89	57.77	2.74	−12.20	98.47
	4						
p−methoxy−nitrobenzene	1	44.02	0.00	96.90	0.00	2.02	137.08
	2	56.62	0.00	103.91	0.00	1.37	147.44
	3	43.18	0.00	93.02	0.00	2.07	122.03
	4	55.18	0.00	98.91	0.00	1.81	128.82

Table S2: Nonzero tensor components of the 1st hyperpolarizability β of the molecules considered in this work. 1 CAM-B3LYP/6-311G**, 2 CAM-B3LYP/6-311++G*, 3 HF/6-311G**, 4 HF/6-311++G**

Molecule	Level	β_{XXX}	β_{XXY}	β_{XYY}	β_{YYY}	β_{XXZ}	β_{XYZ}	β_{YYZ}	β_{XZZ}	β_{YZZ}
Molecule	Level	β_{XXX}	β_{XXY}	β_{XYY}	β_{YYY}	β_{XXZ}	β_{XYZ}	β_{YYZ}	β_{XZZ}	β_{YZZ}
HHe^{+}	1	0.00	0.00	0.00	0.00	0.12	0.00	0.12	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.12	0.00	0.12	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.11	0.00	0.11	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.12	0.00	0.12	0.00	0.00
CO	1	0.00	0.00	0.00	0.00	−0.64	0.00	−0.64	0.00	0.00
	2	0.00	0.00	0.00	0.00	4.05	0.00	4.05	0.00	0.00
	3	0.00	0.00	0.00	0.00	−1.06	0.00	−1.06	0.00	0.00
	4	0.00	0.00	0.00	0.00	1.98	0.00	1.98	0.00	0.00
LiF	1	0.00	0.00	0.00	0.00	73.27	0.00	73.27	0.00	0.00
	2	0.00	0.00	0.00	0.00	50.88	0.00	50.88	0.00	0.00
	3	0.00	0.00	0.00	0.00	32.53	0.00	32.53	0.00	0.00
	4	0.00	0.00	0.00	0.00	22.48	0.00	22.48	0.00	0.00
HF	1	0.00	0.00	0.00	0.00	2.42	0.00	2.42	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.28	0.00	0.28	0.00	0.00

Continued o

Table S2 – *Continued from previous page*

Molecule	Level	β_{XXX}	β_{XXY}	β_{XYY}	β_{YYY}	β_{XXZ}	β_{XYZ}	β_{YYZ}	β_{XZZ}	β_{YZZ}
	3	0.00	0.00	0.00	0.00	1.55	0.00	1.55	0.00	0.00
	4	0.00	0.00	0.00	0.00	−0.05	0.00	−0.05	0.00	0.00
HCl	1	0.00	0.00	0.00	0.00	7.57	0.00	7.57	0.00	0.00
	2	0.00	0.00	0.00	0.00	−0.75	0.00	−0.75	0.00	0.00
	3	0.00	0.00	0.00	0.00	5.27	0.00	5.27	0.00	0.00
	4	0.00	0.00	0.00	0.00	−1.48	0.00	−1.48	0.00	0.00
H_2O	1	0.00	0.00	0.00	0.00	4.41	0.00	18.81	0.00	0.00
	2	0.00	0.00	0.00	0.00	3.04	0.00	17.76	0.00	0.00
	3	0.00	0.00	0.00	0.00	2.63	0.00	15.71	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.04	0.00	14.49	0.00	0.00
H_2S	1	0.00	0.00	0.00	0.00	6.76	0.00	17.74	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.16	0.00	30.68	0.00	0.00
	3	0.00	0.00	0.00	0.00	3.91	0.00	19.92	0.00	0.00
	4	0.00	0.00	0.00	0.00	−2.40	0.00	29.41	0.00	0.00
NH_3	1	0.00	20.36	0.00	−20.36	15.50	0.00	15.50	0.00	0.00
	2	0.00	16.26	0.00	−16.24	0.90	0.00	0.90	0.00	0.00
	3	0.00	18.34	0.00	−18.34	12.44	0.00	12.44	0.00	0.00

Continued o

Table S2 – *Continued from previous page*

Molecule	Level	β_{XXX}	β_{XXY}	β_{XYY}	β_{YYY}	β_{XXZ}	β_{XYZ}	β_{YYZ}	β_{XZZ}	β_{YZZ}
	4	0.00	15.57	0.00	−15.57	2.99	0.00	2.99	0.00	0.00
F−CC−H	1	0.00	0.00	0.00	0.00	1.28	0.00	1.28	0.00	0.00
	2	0.00	0.00	0.00	0.00	13.29	0.00	13.29	0.00	0.00
	3	0.00	0.00	0.00	0.00	−0.05	0.00	−0.05	0.00	0.00
	4	0.00	0.00	0.00	0.00	7.95	0.00	7.95	0.00	0.00
$HCCCF_3$	1	0.00	−3.96	0.00	3.96	−16.42	0.00	−16.42	0.00	0.00
	2	0.00	−9.46	0.00	9.45	−11.65	0.00	−11.64	0.00	0.00
	3	0.00	−2.71	0.00	2.71	−11.78	0.00	−11.78	0.00	0.00
	4	0.00	−3.43	−7.02	3.43	−8.42	0.00	−8.42	0.00	7.02
CN−CC−H	1	0.00	0.00	0.00	0.00	9.45	0.00	9.45	0.00	0.00
	2	0.00	0.00	0.00	0.00	9.23	0.00	9.23	0.00	0.00
	3	0.00	0.00	0.00	0.00	10.16	0.00	10.16	0.00	0.00
	4	0.00	0.00	0.00	0.00	11.58	0.00	11.58	0.00	0.00
CN−CC−CC−H	1	0.00	0.00	0.00	0.00	12.16	0.00	12.16	0.00	0.00
	2	0.00	0.00	0.00	0.00	17.70	0.00	17.70	0.00	0.00
	3	0.00	0.00	0.00	0.00	12.58	0.00	12.58	0.00	0.00
	4	0.00	0.00	0.00	0.00	17.46	0.00	17.46	0.00	0.00

Continued o

Table S2 – *Continued from previous page*

Molecule	Level	β_{XXX}	β_{XXY}	β_{XYY}	β_{YYY}	β_{XXZ}	β_{XYZ}	β_{YYZ}	β_{XZZ}	β_{YZZ}
CN−CC−CC−CC−H	1	0.00	0.00	0.00	0.00	14.11	0.00	14.11	0.00	0.00
	2	0.00	0.00	0.00	0.00	24.09	0.00	24.09	0.00	0.00
	3	0.00	0.00	0.00	0.00	14.15	0.00	14.15	0.00	0.00
	4	0.00	0.00	0.00	0.00	21.85	0.00	21.85	0.00	0.00
p−cyanoaniline	1	0.00	4.22	0.00	3.63	−94.92	0.00	−14.54	0.00	28.60
	2	0.00	3.20	0.00	9.11	−84.28	0.00	−44.47	0.00	7.34
	3	0.00	4.44	0.00	3.42	−100.81	0.00	−14.12	0.00	23.41
	4	0.00	4.48	0.00	9.30	−96.13	0.00	−31.04	0.00	5.61
p−nitroaniline	1	0.00	−3.71	0.00	−3.22	−143.65	0.00	−15.50	0.00	−28.53
	2	0.00	−2.31	0.00	−7.68	−142.01	0.00	−60.12	0.00	−10.54
	3	0.00	−4.04	0.00	−3.18	−165.83	0.00	−10.48	0.00	−22.73
	4	0.00	−3.50	0.00	−8.39	−174.41	0.00	−37.66	0.00	−7.14
m−nitroaniline	1	−17.72	−31.14	−50.88	−87.01	13.48	33.60	74.67	−57.98	16.35
	2									
	3	−47.85	−44.53	−43.13	−49.85	20.89	21.95	16.41	−33.82	11.14
	4									
p−methoxy−nitrobenzene	1	0.00	−33.44	0.00	7.09	−37.53	0.00	−113.23	0.00	−82.49

Continued o

Table S2 – *Continued from previous page*

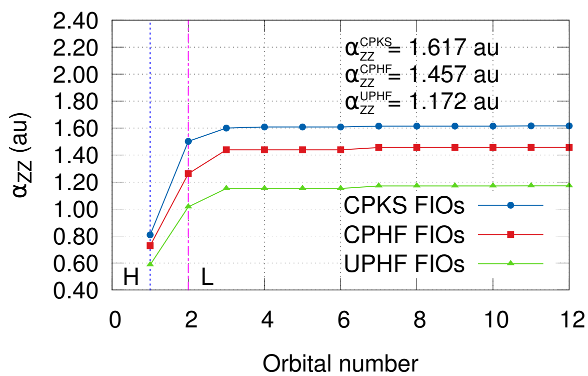
Molecule	Level	β_{XXX}	β_{XXY}	β_{XYY}	β_{YYY}	β_{XXZ}	β_{XYZ}	β_{YYZ}	β_{XZZ}	β_{YZZ}
	2	0.00	−30.04	0.00	2.45	−39.28	0.00	−110.52	0.00	−105.12
	3	0.00	−26.81	0.00	9.20	−26.03	0.00	−136.73	0.00	−61.17
	4	0.00	−21.62	0.00	9.85	−28.48	0.00	−140.21	0.00	−71.73

3 HHe^+

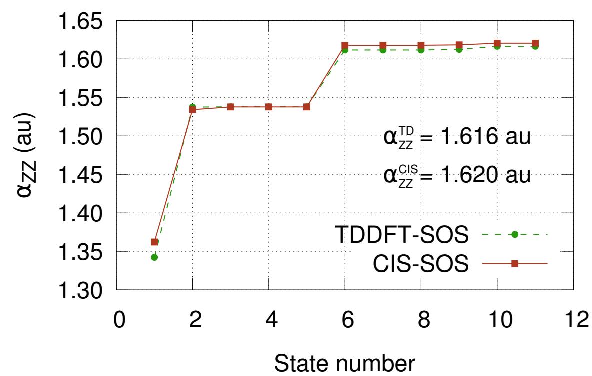
3.1 6-311G(d,p)

3.1.1 Plots

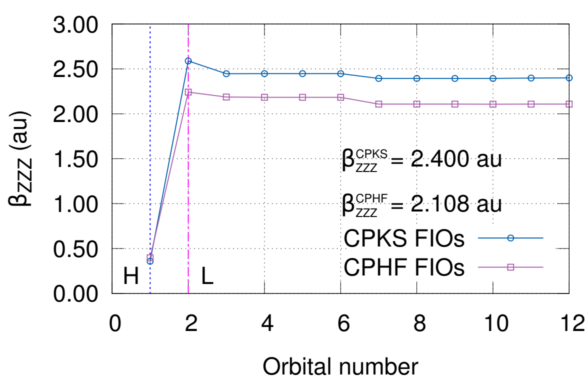
Figure S1: For HHe^+ molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S1a and S1c) or states (SOS approaches, in Plots S1b and S1d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.04 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



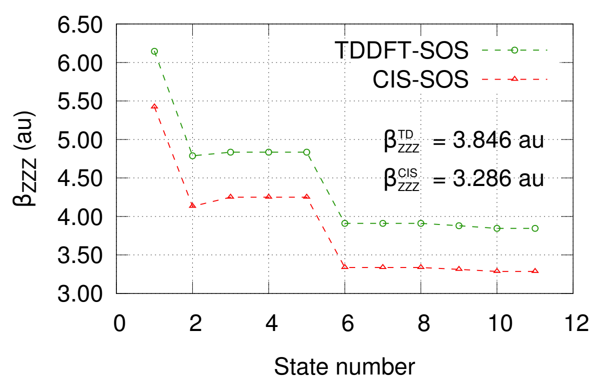
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

3.1.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-SG   25.3777         48.86    0.3892    0.000
          max(1)=        1 ->  2         0.70588
          max(2)=        1 ->  7         0.01962
          max(3)=        1 -> 11        -0.00521
          max(4)=        1 -> 10        -0.00607
          max(5)=        1 -> 12        -0.00815
          min(1)=        1 ->  4        -0.05874
          min(2)=        1 ->  3        -0.02041
          min(3)=        1 -> 12        -0.00815
          min(4)=        1 -> 10        -0.00607
          min(5)=        1 -> 11        -0.00521
          #CIs=7 #CIs>0=2 #CIs<0=5

2        Singlet-SG   32.8423         37.75    0.0947    0.000
          max(1)=        1 ->  3         0.70684
          max(2)=        1 ->  2         0.02014
          max(3)=        1 -> 10         0.00422
          max(4)=        1 -> 12        -0.00125
          max(5)=        1 ->  4        -0.00287
          min(1)=        1 ->  7        -0.01227
          min(2)=        1 -> 11        -0.00600
          min(3)=        1 ->  4        -0.00287
          min(4)=        1 -> 12        -0.00125
          min(5)=        1 -> 10         0.00422
          #CIs=7 #CIs>0=3 #CIs<0=4

3        Singlet-SG   46.8246         26.48    0.0004    0.000
          max(1)=        1 ->  4         0.70534
          max(2)=        1 ->  2         0.06098
          max(3)=        1 ->  7         0.00683
          max(4)=        1 ->  3         0.00130
          max(5)=        1 -> 11        -0.01096
          min(1)=        1 -> 10        -0.01534
          min(2)=        1 -> 12        -0.01193
          min(3)=        1 -> 11        -0.01096
          min(4)=        1 ->  3         0.00130
          min(5)=        1 ->  7         0.00683
          #CIs=7 #CIs>0=4 #CIs<0=3

4        Singlet-?Sym   49.6261         24.98    0.6477    0.000
          max(1)=        1 ->  5         0.68562
          max(2)=        1 ->  6         0.17112
          max(3)=        1 ->  8         0.03117
          max(4)=        1 ->  9         0.00778
          max(5)=        1 ->  4         0.70534
          min(1)=        1 ->  9         0.00778
          min(2)=        1 ->  8         0.03117
          min(3)=        1 ->  6         0.17112
          min(4)=        1 ->  5         0.68562
          min(5)=        1 -> 10        -0.01534
          #CIs=4 #CIs>0=4 #CIs<0=0

5        Singlet-?Sym   49.6261         24.98    0.6477    0.000
          max(1)=        1 ->  6         0.68562
          max(2)=        1 ->  9         0.03117
          max(3)=        1 ->  8        -0.00778
          max(4)=        1 ->  5        -0.17112
          max(5)=        1 ->  5         0.68562
          min(1)=        1 ->  5        -0.17112
          min(2)=        1 ->  8        -0.00778
          min(3)=        1 ->  9         0.03117
          min(4)=        1 ->  6         0.68562
          min(5)=        1 ->  9         0.00778
          #CIs=4 #CIs>0=2 #CIs<0=2

6        Singlet-SG   62.9858         19.68    0.1317    0.000
          max(1)=        1 ->  7         0.70660
          max(2)=        1 ->  3         0.01341
          max(3)=        1 -> 11         0.00424
          max(4)=        1 -> 12         0.00210
          max(5)=        1 ->  4        -0.00606
          min(1)=        1 -> 10        -0.02235
```

```
        min(2)=        1 ->  2        -0.02114
        min(3)=        1 ->  4        -0.00606
        min(4)=        1 -> 12         0.00210
        min(5)=        1 -> 11         0.00424
        #CIs=7 #CIs>0=4 #CIs<0=3

7     Singlet-?Sym   67.8741         18.27    0.0646    0.000
        max(1)=        1 ->  8         0.70122
        max(2)=        1 ->  6         0.00392
        max(3)=        1 ->  5        -0.03213
        max(4)=        1 ->  9        -0.08553
        max(5)=        1 ->  7         0.70660
        min(1)=        1 ->  9        -0.08553
        min(2)=        1 ->  5        -0.03213
        min(3)=        1 ->  6         0.00392
        min(4)=        1 ->  8         0.70122
        min(5)=        1 -> 10        -0.02235
        #CIs=4 #CIs>0=2 #CIs<0=2

8     Singlet-?Sym   67.8741         18.27    0.0646    0.000
        max(1)=        1 ->  9         0.70122
        max(2)=        1 ->  8         0.08553
        max(3)=        1 ->  5        -0.00392
        max(4)=        1 ->  6        -0.03213
        max(5)=        1 ->  8         0.70122
        min(1)=        1 ->  6        -0.03213
        min(2)=        1 ->  5        -0.00392
        min(3)=        1 ->  8         0.08553
        min(4)=        1 ->  9         0.70122
        min(5)=        1 ->  9        -0.08553
        #CIs=4 #CIs>0=2 #CIs<0=2

9     Singlet-SG   77.1426         16.07    0.0019    0.000
        max(1)=        1 -> 10         0.70618
        max(2)=        1 ->  7         0.02284
        max(3)=        1 ->  4         0.01452
        max(4)=        1 ->  2         0.00667
        max(5)=        1 -> 12        -0.00146
        min(1)=        1 -> 11        -0.02345
        min(2)=        1 ->  3        -0.00411
        min(3)=        1 -> 12        -0.00146
        min(4)=        1 ->  2         0.00667
        min(5)=        1 ->  4         0.01452
        #CIs=7 #CIs>0=4 #CIs<0=3

10    Singlet-SG   96.1022         12.90    0.0172    0.000
        max(1)=        1 -> 11         0.70657
        max(2)=        1 -> 10         0.02337
        max(3)=        1 ->  4         0.01134
        max(4)=        1 ->  2         0.00711
        max(5)=        1 ->  3         0.00569
        min(1)=        1 -> 12        -0.01013
        min(2)=        1 ->  7        -0.00336
        min(3)=        1 ->  3         0.00569
        min(4)=        1 ->  2         0.00711
        min(5)=        1 ->  4         0.01134
        #CIs=7 #CIs>0=5 #CIs<0=2

11    Singlet-SG  190.6269          6.50    0.0000    0.000
        max(1)=        1 -> 12         0.70701
        max(2)=        1 ->  4         0.01214
        max(3)=        1 ->  2         0.01028
        max(4)=        1 -> 11         0.00999
        max(5)=        1 -> 10         0.00163
        min(1)=        1 ->  7        -0.00194
        min(2)=        1 ->  3         0.00107
        min(3)=        1 -> 10         0.00163
        min(4)=        1 -> 11         0.00999
        min(5)=        1 ->  2         0.01028
        #CIs=7 #CIs>0=6 #CIs<0=1
```

3.1.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_
1     Singlet-SG   27.3850         45.27    0.4599    0.000
        max(1)=        1 ->  2         0.69064
```

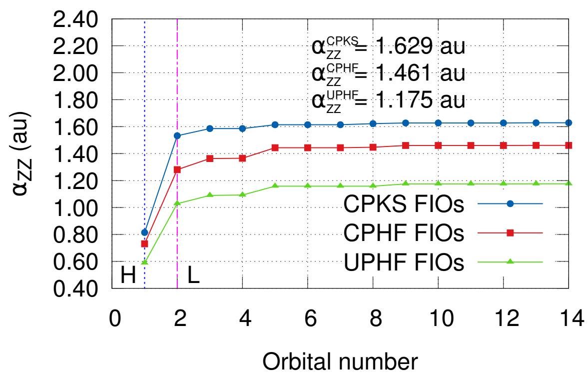
```
        max(2)=      1 ->  3        0.15138
        max(3)=      1 ->  4        0.00085
        max(4)=      1 -> 11       -0.00083
        max(5)=      1 -> 10       -0.00419
        min(1)=      1 ->  7       -0.00761
        min(2)=      1 -> 12       -0.00534
        min(3)=      1 -> 10       -0.00419
        min(4)=      1 -> 11       -0.00083
        min(5)=      1 ->  4        0.00085
        #CIs=7 #CIs>0=3 #CIs<0=4

2       Singlet-SG   35.3079        35.12    0.0965    0.000
        max(1)=      1 ->  3        0.68769
        max(2)=      1 -> 11        0.00673
        max(3)=      1 -> 12        0.00078
        max(4)=      1 -> 10       -0.01229
        max(5)=      1 ->  7       -0.02391
        min(1)=      1 ->  2       -0.15098
        min(2)=      1 ->  4       -0.05936
        min(3)=      1 ->  7       -0.02391
        min(4)=      1 -> 10       -0.01229
        min(5)=      1 -> 12        0.00078
        #CIs=7 #CIs>0=3 #CIs<0=4

3       Singlet-SG   48.2215        25.71    0.0038    0.000
        max(1)=      1 ->  4        0.70452
        max(2)=      1 ->  3        0.05741
        max(3)=      1 -> 11        0.01036
        max(4)=      1 -> 12       -0.00016
        max(5)=      1 -> 10       -0.00303
        min(1)=      1 ->  2       -0.01354
        min(2)=      1 ->  7       -0.00763
        min(3)=      1 -> 10       -0.00303
        min(4)=      1 -> 12       -0.00016
        min(5)=      1 -> 11        0.01036
        #CIs=7 #CIs>0=3 #CIs<0=4

4       Singlet-?Sym   50.2671        24.67    0.7000    0.000
        max(1)=      1 ->  5        0.59801
        max(2)=      1 ->  8        0.01161
        max(3)=      1 ->  9       -0.01844
        max(4)=      1 ->  6       -0.37670
        max(5)=      1 ->  4        0.70452
        min(1)=      1 ->  6       -0.37670
        min(2)=      1 ->  9       -0.01844
        min(3)=      1 ->  8        0.01161
        min(4)=      1 ->  5        0.59801
        min(5)=      1 ->  2       -0.01354
        #CIs=4 #CIs>0=2 #CIs<0=2

5       Singlet-?Sym   50.2671        24.67    0.7000    0.000
        max(1)=      1 ->  6        0.59801
        max(2)=      1 ->  5        0.37670
        max(3)=      1 ->  9       -0.01161
        max(4)=      1 ->  8       -0.01844
        max(5)=      1 ->  5        0.59801
        min(1)=      1 ->  8       -0.01844
        min(2)=      1 ->  9       -0.01161
        min(3)=      1 ->  5        0.37670
        min(4)=      1 ->  6        0.59801
        min(5)=      1 ->  6       -0.37670
        #CIs=4 #CIs>0=2 #CIs<0=2

6       Singlet-SG   64.5538        19.21    0.1502    0.000
        max(1)=      1 ->  7        0.70500
        max(2)=      1 ->  3        0.02445
        max(3)=      1 -> 11        0.02297
        max(4)=      1 ->  4        0.00516
        max(5)=      1 ->  2        0.00216
        min(1)=      1 -> 10       -0.04254
        min(2)=      1 -> 12       -0.00179
        min(3)=      1 ->  2        0.00216
        min(4)=      1 ->  4        0.00516
        min(5)=      1 -> 11        0.02297
        #CIs=7 #CIs>0=5 #CIs<0=2

7       Singlet-?Sym   69.9228        17.73    0.0531    0.000
        max(1)=      1 ->  9        0.53751
        max(2)=      1 ->  5        0.01657
        max(3)=      1 ->  6       -0.01415
        max(4)=      1 ->  8       -0.45891
        max(5)=      1 ->  7        0.70500
```

```
        min(1)=      1 ->  8       -0.45891
        min(2)=      1 ->  6       -0.01415
        min(3)=      1 ->  5        0.01657
        min(4)=      1 ->  9        0.53751
        min(5)=      1 -> 10       -0.04254
        #CIs=4 #CIs>0=2 #CIs<0=2

8    Singlet-?Sym   69.9228        17.73    0.0531    0.000
        max(1)=      1 ->  8        0.53751
        max(2)=      1 ->  9        0.45891
        max(3)=      1 ->  6        0.01657
        max(4)=      1 ->  5        0.01415
        max(5)=      1 ->  9        0.53751
        min(1)=      1 ->  5        0.01415
        min(2)=      1 ->  6        0.01657
        min(3)=      1 ->  9        0.45891
        min(4)=      1 ->  8        0.53751
        min(5)=      1 ->  8       -0.45891
        #CIs=4 #CIs>0=4 #CIs<0=0

9    Singlet-SG   79.7245        15.55    0.0013    0.000
        max(1)=      1 -> 10        0.70491
        max(2)=      1 ->  7        0.04303
        max(3)=      1 ->  3        0.01496
        max(4)=      1 -> 12        0.00432
        max(5)=      1 ->  4        0.00278
        min(1)=      1 -> 11       -0.03170
        min(2)=      1 ->  2        0.00147
        min(3)=      1 ->  4        0.00278
        min(4)=      1 -> 12        0.00432
        min(5)=      1 ->  3        0.01496
        #CIs=7 #CIs>0=6 #CIs<0=1

10   Singlet-SG  100.0171        12.40    0.0099    0.000
        max(1)=      1 -> 11        0.70591
        max(2)=      1 -> 10        0.03320
        max(3)=      1 ->  2        0.00245
        max(4)=      1 -> 12        0.00040
        max(5)=      1 ->  3       -0.00734
        min(1)=      1 ->  7       -0.02067
        min(2)=      1 ->  4       -0.00982
        min(3)=      1 ->  3       -0.00734
        min(4)=      1 -> 12        0.00040
        min(5)=      1 ->  2        0.00245
        #CIs=7 #CIs>0=4 #CIs<0=3

11   Singlet-SG  195.2285         6.35    0.0002    0.000
        max(1)=      1 -> 12        0.70707
        max(2)=      1 ->  2        0.00538
        max(3)=      1 ->  7        0.00150
        max(4)=      1 ->  3        0.00038
        max(5)=      1 ->  4        0.00024
        min(1)=      1 -> 10       -0.00445
        min(2)=      1 -> 11       -0.00016
        min(3)=      1 ->  4        0.00024
        min(4)=      1 ->  3        0.00038
        min(5)=      1 ->  7        0.00150
        #CIs=7 #CIs>0=5 #CIs<0=2
```

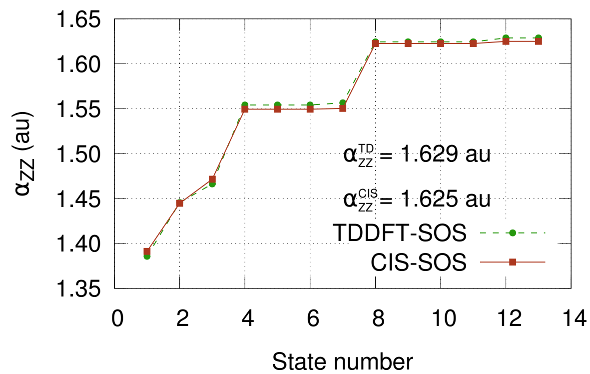
3.2 6-311G++(d,p)

3.2.1 Plots

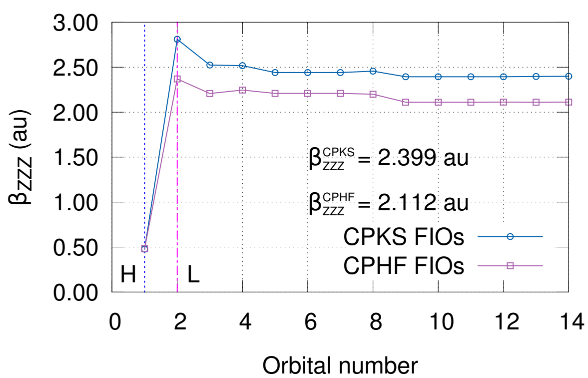
Figure S2: For HHe^+ molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S2a and S2c) or states (SOS approaches, in Plots S2b and S2d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.01 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



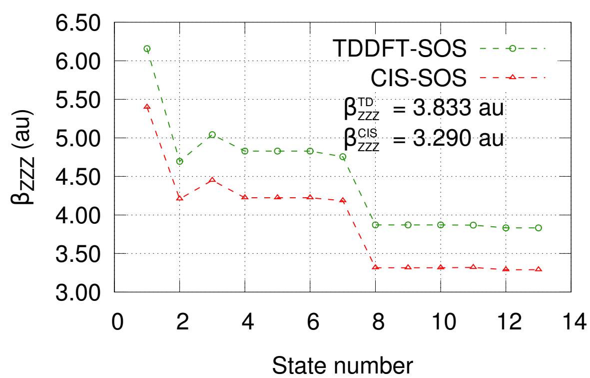
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

3.2.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1       Singlet-SG   25.1296         49.34    0.3939    0.000
        max(1)=        1 ->  2          0.70332
        max(2)=        1 ->  9          0.02163
        max(3)=        1 ->  5          0.01447
        max(4)=        1 -> 12         -0.00201
        max(5)=        1 -> 13         -0.00342
        min(1)=        1 ->  4         -0.05371
        min(2)=        1 ->  3         -0.05257
        min(3)=        1 ->  8         -0.03704
        min(4)=        1 -> 14         -0.00709
        min(5)=        1 -> 13         -0.00342
        #CIs=9 #CIs>0=3 #CIs<0=6

2       Singlet-SG   30.6326         40.47    0.0252    0.000
        max(1)=        1 ->  3          0.70046
        max(2)=        1 ->  4          0.06388
        max(3)=        1 ->  2          0.05598
        max(4)=        1 ->  5          0.04451
        max(5)=        1 -> 12         -0.00111
        min(1)=        1 ->  8         -0.01699
        min(2)=        1 ->  9         -0.00620
        min(3)=        1 -> 13         -0.00407
        min(4)=        1 -> 14         -0.00290
        min(5)=        1 -> 12         -0.00111
        #CIs=9 #CIs>0=4 #CIs<0=5

3       Singlet-SG   34.7510         35.68    0.0113    0.000
        max(1)=        1 ->  4          0.70028
        max(2)=        1 ->  2          0.05004
        max(3)=        1 ->  9          0.00912
        max(4)=        1 -> 12         -0.00367
        max(5)=        1 -> 13         -0.00392
        min(1)=        1 ->  3         -0.06453
        min(2)=        1 ->  5         -0.05487
        min(3)=        1 ->  8         -0.02113
        min(4)=        1 -> 14         -0.00632
        min(5)=        1 -> 13         -0.00392
        #CIs=9 #CIs>0=3 #CIs<0=6

4       Singlet-SG   38.2925         32.38    0.0580    0.000
        max(1)=        1 ->  5          0.70329
        max(2)=        1 ->  4          0.05189
        max(3)=        1 ->  8          0.01362
        max(4)=        1 -> 12          0.00803
        max(5)=        1 -> 14          0.00137
        min(1)=        1 ->  3         -0.04807
        min(2)=        1 ->  2         -0.01391
        min(3)=        1 ->  9         -0.01248
        min(4)=        1 -> 13         -0.00457
        min(5)=        1 -> 14          0.00137
        #CIs=9 #CIs>0=5 #CIs<0=4

5       Singlet-?Sym   49.6273         24.98    0.6480    0.000
        max(1)=        1 ->  6          0.58275
        max(2)=        1 -> 11          0.02657
        max(3)=        1 -> 10         -0.01822
        max(4)=        1 ->  7         -0.39970
        max(5)=        1 ->  5          0.70329
        min(1)=        1 ->  7         -0.39970
        min(2)=        1 -> 10         -0.01822
        min(3)=        1 -> 11          0.02657
        min(4)=        1 ->  6          0.58275
        min(5)=        1 ->  3         -0.04807
        #CIs=4 #CIs>0=2 #CIs<0=2

6       Singlet-?Sym   49.6273         24.98    0.6480    0.000
        max(1)=        1 ->  7          0.58275
        max(2)=        1 ->  6          0.39970
        max(3)=        1 -> 10          0.02657
        max(4)=        1 -> 11          0.01822
        max(5)=        1 ->  6          0.58275
        min(1)=        1 -> 11          0.01822
        min(2)=        1 -> 10          0.02657
        min(3)=        1 ->  6          0.39970
        min(4)=        1 ->  7          0.58275
        min(5)=        1 ->  7         -0.39970
        #CIs=4 #CIs>0=4 #CIs<0=0

7       Singlet-SG   54.0800         22.93    0.0032    0.000
        max(1)=        1 ->  8          0.70582
```

```
max(2)=     1 ->  2     0.04125
max(3)=     1 ->  4     0.01935
max(4)=     1 ->  9     0.01682
max(5)=     1 ->  3     0.01352
min(1)=     1 ->  5    -0.01333
min(2)=     1 -> 14    -0.01019
min(3)=     1 -> 13    -0.00972
min(4)=     1 -> 12    -0.00861
min(5)=     1 ->  3     0.01352
#CIs=9 #CIs>0=5 #CIs<0=4

8   Singlet-SG   64.0602   19.35   0.1254   0.000
max(1)=     1 ->  9     0.70608
max(2)=     1 ->  5     0.01421
max(3)=     1 ->  3     0.00753
max(4)=     1 -> 13     0.00678
max(5)=     1 -> 14     0.00307
min(1)=     1 -> 12    -0.02742
min(2)=     1 ->  2    -0.02419
min(3)=     1 ->  8    -0.01586
min(4)=     1 ->  4    -0.00683
min(5)=     1 -> 14     0.00307
#CIs=9 #CIs>0=5 #CIs<0=4

9   Singlet-?Sym   67.8710   18.27   0.0651   0.000
max(1)=     1 -> 10     0.69698
max(2)=     1 -> 11     0.11508
max(3)=     1 ->  6    -0.00529
max(4)=     1 ->  7    -0.03202
max(5)=     1 ->  9     0.70608
min(1)=     1 ->  7    -0.03202
min(2)=     1 ->  6    -0.00529
min(3)=     1 -> 11     0.11508
min(4)=     1 -> 10     0.69698
min(5)=     1 -> 12    -0.02742
#CIs=4 #CIs>0=2 #CIs<0=2

10  Singlet-?Sym   67.8710   18.27   0.0651   0.000
max(1)=     1 -> 11     0.69698
max(2)=     1 ->  7     0.00529
max(3)=     1 ->  6    -0.03202
max(4)=     1 -> 10    -0.11508
max(5)=     1 -> 10     0.69698
min(1)=     1 -> 10    -0.11508
min(2)=     1 ->  6    -0.03202
min(3)=     1 ->  7     0.00529
min(4)=     1 -> 11     0.69698
min(5)=     1 ->  7    -0.03202
#CIs=4 #CIs>0=2 #CIs<0=2

11  Singlet-SG   81.6646   15.18   0.0000   0.000
max(1)=     1 -> 12     0.70620
max(2)=     1 ->  9     0.02804
max(3)=     1 ->  8     0.00742
max(4)=     1 ->  4     0.00289
max(5)=     1 ->  2     0.00201
min(1)=     1 -> 13    -0.01945
min(2)=     1 ->  5    -0.00788
min(3)=     1 -> 14    -0.00016
min(4)=     1 ->  3     0.00158
min(5)=     1 ->  2     0.00201
#CIs=9 #CIs>0=6 #CIs<0=3

12  Singlet-SG   97.3985   12.73   0.0185   0.000
max(1)=     1 -> 13     0.70669
max(2)=     1 -> 12     0.01962
max(3)=     1 ->  8     0.00999
max(4)=     1 ->  2     0.00511
max(5)=     1 ->  4     0.00491
min(1)=     1 -> 14    -0.00857
min(2)=     1 ->  9    -0.00577
min(3)=     1 ->  3     0.00334
min(4)=     1 ->  5     0.00400
min(5)=     1 ->  4     0.00491
#CIs=9 #CIs>0=7 #CIs<0=2

13  Singlet-SG  194.5931    6.37   0.0000   0.000
max(1)=     1 -> 14     0.70703
max(2)=     1 ->  8     0.01027
max(3)=     1 ->  2     0.00937
max(4)=     1 -> 13     0.00846
max(5)=     1 ->  4     0.00666
```

```
min(1)=        1 ->  9        -0.00279
min(2)=        1 ->  5        -0.00189
min(3)=        1 -> 12         0.00036
min(4)=        1 ->  3         0.00218
min(5)=        1 ->  4         0.00666
#CIs=9 #CIs>0=7 #CIs<0=2
```

3.2.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-SG   27.2151         45.56    0.4638    0.000
        max(1)=        1 ->  2         0.68603
        max(2)=        1 ->  4         0.03846
        max(3)=        1 -> 13        -0.00033
        max(4)=        1 -> 12        -0.00190
        max(5)=        1 ->  9        -0.00389
        min(1)=        1 ->  3        -0.14286
        min(2)=        1 ->  5        -0.08511
        min(3)=        1 ->  8        -0.01384
        min(4)=        1 -> 14        -0.00462
        min(5)=        1 ->  9        -0.00389
        #CIs=9 #CIs>0=2 #CIs<0=7

2        Singlet-SG   33.4779         37.03    0.0270    0.000
        max(1)=        1 ->  3         0.64369
        max(2)=        1 ->  4         0.22561
        max(3)=        1 ->  2         0.13717
        max(4)=        1 ->  5         0.12136
        max(5)=        1 ->  8         0.03399
        min(1)=        1 -> 13        -0.00281
        min(2)=        1 -> 14        -0.00215
        min(3)=        1 -> 12         0.00259
        min(4)=        1 ->  9         0.00699
        min(5)=        1 ->  8         0.03399
        #CIs=9 #CIs>0=7 #CIs<0=2

3        Singlet-SG   38.1164         32.53    0.0175    0.000
        max(1)=        1 ->  4         0.65507
        max(2)=        1 ->  8         0.04347
        max(3)=        1 -> 13         0.00254
        max(4)=        1 -> 14        -0.00334
        max(5)=        1 -> 12        -0.00595
        min(1)=        1 ->  3        -0.18050
        min(2)=        1 ->  5        -0.16569
        min(3)=        1 ->  2        -0.09407
        min(4)=        1 ->  9        -0.00754
        min(5)=        1 -> 12        -0.00595
        #CIs=9 #CIs>0=3 #CIs<0=6

4        Singlet-SG   41.4654         29.90    0.0604    0.000
        max(1)=        1 ->  5         0.66948
        max(2)=        1 ->  4         0.12336
        max(3)=        1 ->  2         0.03956
        max(4)=        1 ->  8         0.03758
        max(5)=        1 ->  9         0.02596
        min(1)=        1 ->  3        -0.18026
        min(2)=        1 -> 13        -0.00917
        min(3)=        1 -> 14         0.00045
        min(4)=        1 -> 12         0.01865
        min(5)=        1 ->  9         0.02596
        #CIs=9 #CIs>0=7 #CIs<0=2

5        Singlet-?Sym   50.2689         24.66    0.7008    0.000
        max(1)=        1 ->  6         0.56957
        max(2)=        1 -> 10         0.01283
        max(3)=        1 -> 11        -0.01746
        max(4)=        1 ->  7        -0.41848
        max(5)=        1 ->  5         0.66948
        min(1)=        1 ->  7        -0.41848
        min(2)=        1 -> 11        -0.01746
        min(3)=        1 -> 10         0.01283
        min(4)=        1 ->  6         0.56957
        min(5)=        1 ->  3        -0.18026
        #CIs=4 #CIs>0=2 #CIs<0=2

6        Singlet-?Sym   50.2689         24.66    0.7008    0.000
```

```
        max(1)=      1 ->  7       0.56957
        max(2)=      1 ->  6       0.41848
        max(3)=      1 -> 11      -0.01283
        max(4)=      1 -> 10      -0.01746
        max(5)=      1 ->  6       0.56957
        min(1)=      1 -> 10      -0.01746
        min(2)=      1 -> 11      -0.01283
        min(3)=      1 ->  6       0.41848
        min(4)=      1 ->  7       0.56957
        min(5)=      1 ->  7      -0.41848
        #CIs=4 #CIs>0=2 #CIs<0=2

7     Singlet-SG   55.4610      22.36   0.0011   0.000
        max(1)=      1 ->  8       0.70363
        max(2)=      1 -> 13       0.01144
        max(3)=      1 ->  2       0.01060
        max(4)=      1 ->  9       0.00999
        max(5)=      1 -> 14       0.00250
        min(1)=      1 ->  4      -0.05715
        min(2)=      1 ->  5      -0.03340
        min(3)=      1 ->  3      -0.01315
        min(4)=      1 -> 12       0.00112
        min(5)=      1 -> 14       0.00250
        #CIs=9 #CIs>0=6 #CIs<0=3

8     Singlet-SG   65.8644      18.82   0.1411   0.000
        max(1)=      1 ->  9       0.70507
        max(2)=      1 -> 13       0.02621
        max(3)=      1 ->  4       0.00118
        max(4)=      1 ->  2      -0.00012
        max(5)=      1 ->  3      -0.00226
        min(1)=      1 -> 12      -0.03697
        min(2)=      1 ->  5      -0.02612
        min(3)=      1 ->  8      -0.01155
        min(4)=      1 -> 14      -0.00266
        min(5)=      1 ->  3      -0.00226
        #CIs=9 #CIs>0=3 #CIs<0=6

9     Singlet-?Sym   69.9154      17.73   0.0538   0.000
        max(1)=      1 -> 10       0.67884
        max(2)=      1 -> 11       0.19673
        max(3)=      1 ->  7       0.02081
        max(4)=      1 ->  6       0.00603
        max(5)=      1 ->  9       0.70507
        min(1)=      1 ->  6       0.00603
        min(2)=      1 ->  7       0.02081
        min(3)=      1 -> 11       0.19673
        min(4)=      1 -> 10       0.67884
        min(5)=      1 -> 12      -0.03697
        #CIs=4 #CIs>0=4 #CIs<0=0

10    Singlet-?Sym   69.9154      17.73   0.0538   0.000
        max(1)=      1 -> 11       0.67884
        max(2)=      1 ->  6       0.02081
        max(3)=      1 ->  7      -0.00603
        max(4)=      1 -> 10      -0.19673
        max(5)=      1 -> 10       0.67884
        min(1)=      1 -> 10      -0.19673
        min(2)=      1 ->  7      -0.00603
        min(3)=      1 ->  6       0.02081
        min(4)=      1 -> 11       0.67884
        min(5)=      1 ->  6       0.00603
        #CIs=4 #CIs>0=2 #CIs<0=2

11    Singlet-SG   84.3348      14.70   0.0001   0.000
        max(1)=      1 -> 12       0.70522
        max(2)=      1 ->  9       0.03721
        max(3)=      1 -> 14       0.00281
        max(4)=      1 ->  4       0.00166
        max(5)=      1 ->  3       0.00035
        min(1)=      1 -> 13      -0.02834
        min(2)=      1 ->  5      -0.02154
        min(3)=      1 ->  8      -0.00207
        min(4)=      1 ->  2      -0.00057
        min(5)=      1 ->  3       0.00035
        #CIs=9 #CIs>0=5 #CIs<0=4

12    Singlet-SG  101.3328      12.24   0.0110   0.000
        max(1)=      1 -> 13       0.70589
        max(2)=      1 -> 12       0.02994
        max(3)=      1 ->  5       0.01038
        max(4)=      1 ->  2       0.00152
```

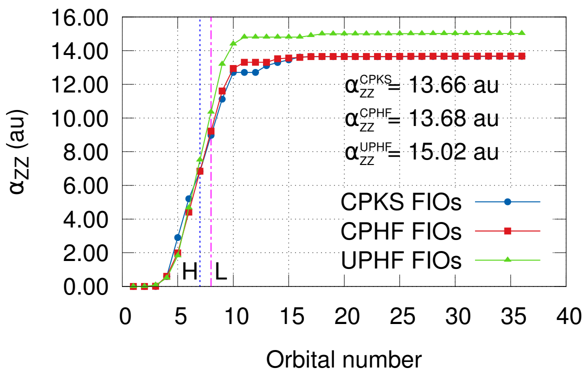
```
        max(5)=        1 ->  3          0.00111
        min(1)=        1 ->  9         -0.02446
        min(2)=        1 ->  8         -0.01060
        min(3)=        1 ->  3          0.00111
        min(4)=        1 ->  4          0.00111
        min(5)=        1 ->  2          0.00152
        #CIs=8 #CIs>0=6 #CIs<0=2

13      Singlet-SG  199.0088         6.23     0.0000     0.000
        max(1)=        1 -> 14          0.70707
        max(2)=        1 ->  2          0.00439
        max(3)=        1 ->  4          0.00416
        max(4)=        1 ->  9          0.00241
        max(5)=        1 ->  3          0.00033
        min(1)=        1 -> 12         -0.00299
        min(2)=        1 ->  8         -0.00233
        min(3)=        1 ->  5         -0.00129
        min(4)=        1 -> 13          0.00018
        min(5)=        1 ->  3          0.00033
        #CIs=9 #CIs>0=6 #CIs<0=3
```

4 N_2

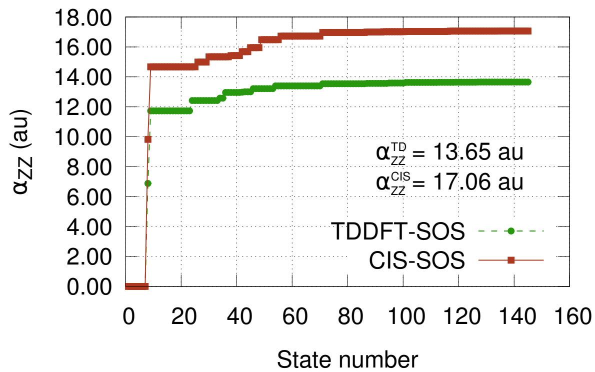
4.1 6-311G(d,p)

4.1.1 Plots

Figure S3: For N_2 molecule and 6-311G(d,p) basis set, plots of variation of α_{ZZ} with respect to the number of orbitals (FIO decomposition presented in this work, in Figure ZZZ) or states (SOS approach, in Figure S3a). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. Recomputed values of α_{ZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.

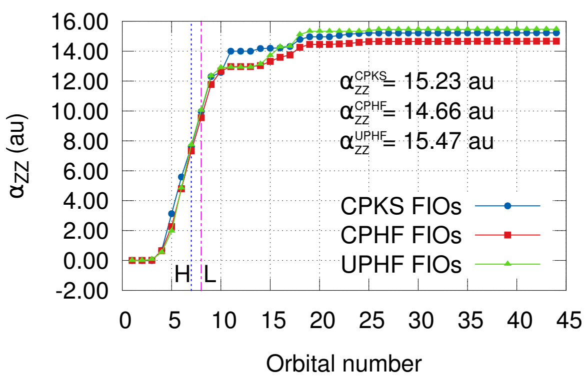


(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

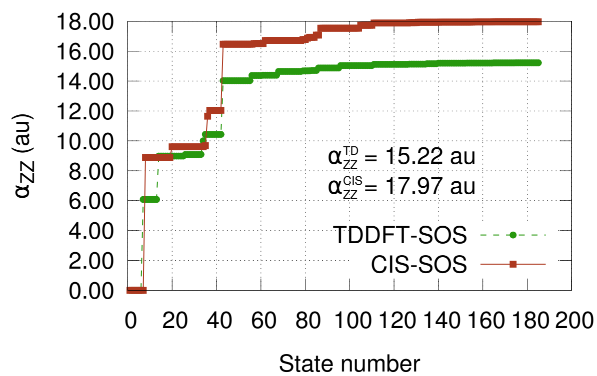
4.2 6-311++G(d,p)

4.2.1 Plots

Figure S4: For N_2 molecule and 6-311++G(d,p) basis set, plots of variation of α_{ZZ} with respect to the number of orbitals (FIO decomposition presented in this work, in Figure ZZZ) or states (SOS approach, in Figure S4a). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. Recomputed values of α_{ZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



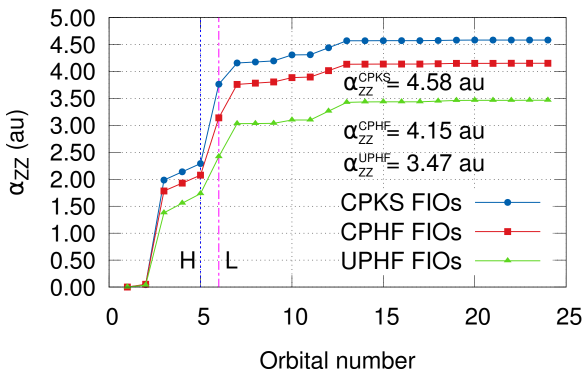
(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

5 HF

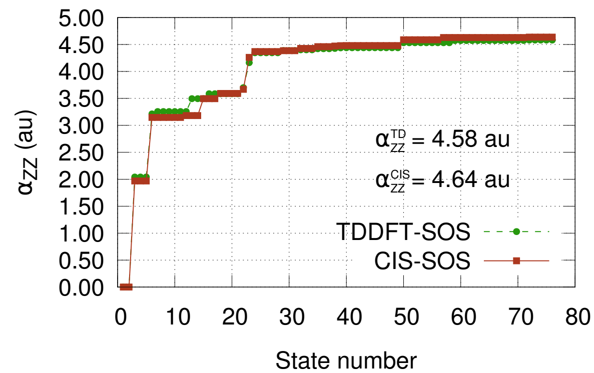
5.1 6-311G(d,p)

5.1.1 Plots

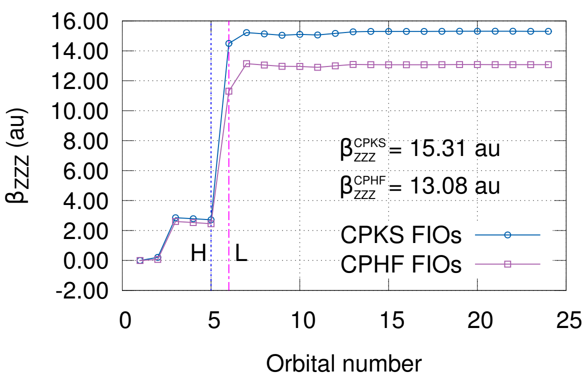
Figure S5: For HF molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S5a and S5c) or states (SOS approaches, in Plots S5b and S5d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.02 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



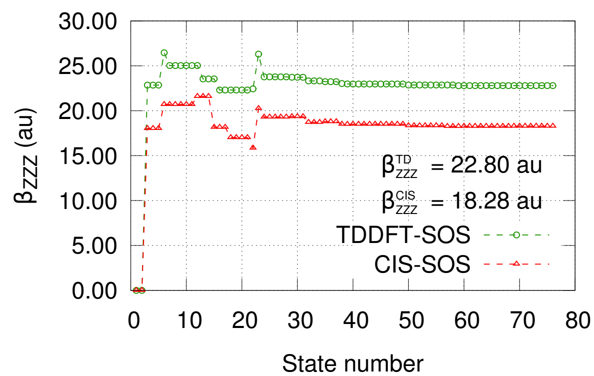
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

5.1.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-?Sym    9.7484        127.18    0.0196    0.000
         max(1)=        5 ->  6         0.70013
         max(2)=        5 ->  7         0.05593
         max(3)=        5 -> 11         0.00895
         max(4)=        4 -> 17         0.00353
         max(5)=        5 -> 16         0.00353
         min(1)=        4 ->  6        -0.08111
         min(2)=        5 -> 10        -0.01210
         min(3)=        4 ->  7        -0.00648
         min(4)=        2 ->  9        -0.00395
         min(5)=        2 -> 19        -0.00188
         #CIs=36 #CIs>0=19 #CIs<0=17

2        Singlet-?Sym    9.7484        127.18    0.0196    0.000
         max(1)=        4 ->  6         0.70013
         max(2)=        5 ->  6         0.08111
         max(3)=        4 ->  7         0.05593
         max(4)=        4 -> 11         0.00895
         max(5)=        5 ->  7         0.00648
         min(1)=        4 -> 10        -0.01210
         min(2)=        2 ->  8        -0.00395
         min(3)=        4 -> 16        -0.00353
         min(4)=        2 -> 18        -0.00188
         min(5)=        4 -> 20        -0.00186
         #CIs=36 #CIs>0=17 #CIs<0=19

3        Singlet-SG   14.2483         87.02    0.1866    0.000
         max(1)=        3 ->  6         0.70537
         max(2)=        4 ->  8         0.03354
         max(3)=        5 ->  9         0.03354
         max(4)=        3 -> 11         0.01300
         max(5)=        2 -> 11         0.01211
         min(1)=        3 ->  7        -0.02865
         min(2)=        2 -> 14        -0.00293
         min(3)=        2 -> 20        -0.00183
         min(4)=        2 -> 10        -0.00114
         min(5)=        3 -> 23        -0.00071
         #CIs=24 #CIs>0=16 #CIs<0=8

4        Singlet-?Sym   19.1128         64.87    0.0380    0.000
         max(1)=        4 ->  7         0.65596
         max(2)=        5 ->  7         0.25691
         max(3)=        5 -> 17         0.00522
         max(4)=        2 -> 12         0.00518
         max(5)=        3 -> 18         0.00240
         min(1)=        4 ->  6        -0.05264
         min(2)=        5 ->  6        -0.02062
         min(3)=        4 -> 10        -0.01632
         min(4)=        4 -> 14        -0.01092
         min(5)=        3 -> 12        -0.00821
         #CIs=37 #CIs>0=17 #CIs<0=20

5        Singlet-?Sym   19.1128         64.87    0.0380    0.000
         max(1)=        5 ->  7         0.65596
         max(2)=        4 ->  6         0.02062
         max(3)=        4 -> 10         0.00639
         max(4)=        4 -> 17         0.00522
         max(5)=        5 -> 16         0.00522
         min(1)=        4 ->  7        -0.25691
         min(2)=        5 ->  6        -0.05264
         min(3)=        5 -> 10        -0.01632
         min(4)=        5 -> 14        -0.01092
         min(5)=        3 -> 13        -0.00821
         #CIs=37 #CIs>0=19 #CIs<0=18

6        Singlet-SG   24.8444         49.90    0.3252    0.000
         max(1)=        3 ->  7         0.69678
         max(2)=        4 ->  8         0.07887
         max(3)=        5 ->  9         0.07887
         max(4)=        4 -> 12         0.03505
         max(5)=        5 -> 13         0.03505
         min(1)=        2 -> 14        -0.00837
```

```
        min(2)=        4 -> 18        -0.00807
        min(3)=        5 -> 19        -0.00807
        min(4)=        3 -> 20        -0.00445
        min(5)=        3 -> 15        -0.00239
        #CIs=25 #CIs>0=16 #CIs<0=9

7       Singlet-SG   31.7579        39.04    0.0200    0.000
        max(1)=        2 ->  6         0.69080
        max(2)=        2 ->  7         0.02635
        max(3)=        3 -> 11         0.02229
        max(4)=        4 -> 12         0.01501
        max(5)=        5 -> 13         0.01501
        min(1)=        4 ->  8        -0.10235
        min(2)=        5 ->  9        -0.10235
        min(3)=        3 -> 10        -0.01609
        min(4)=        4 -> 18        -0.00780
        min(5)=        5 -> 19        -0.00780
        #CIs=25 #CIs>0=13 #CIs<0=12

8       Singlet-?Sym   33.2149        37.33    0.0000    0.000
        max(1)=        5 ->  8         0.50001
        max(2)=        5 -> 22         0.00357
        max(3)=        4 -> 19         0.00026
        max(4)=        5 -> 12         0.00022
        max(5)=        4 -> 13        -0.00022
        min(1)=        4 ->  9        -0.50001
        min(2)=        4 -> 21        -0.00357
        min(3)=        5 -> 18        -0.00026
        min(4)=        4 -> 13        -0.00022
        min(5)=        5 -> 12         0.00022
        #CIs=8 #CIs>0=4 #CIs<0=4

9       Singlet-?Sym   33.5752        36.93    0.0000    0.000
        max(1)=        4 ->  9         0.49999
        max(2)=        5 ->  8         0.49999
        max(3)=        4 -> 21         0.00348
        max(4)=        5 -> 22         0.00348
        max(5)=        2 -> 17         0.00256
        min(1)=        4 -> 19        -0.00012
        min(2)=        5 -> 18        -0.00012
        min(3)=        4 -> 13        -0.00011
        min(4)=        5 -> 12        -0.00011
        min(5)=        5 ->  9        -0.00001
        #CIs=12 #CIs>0=7 #CIs<0=5

10      Singlet-?Sym   33.5752        36.93    0.0000    0.000
        max(1)=        4 ->  8         0.49999
        max(2)=        4 -> 22         0.00348
        max(3)=        5 -> 19         0.00012
        max(4)=        5 -> 13         0.00011
        max(5)=        4 ->  9        -0.00001
        min(1)=        5 ->  9        -0.49999
        min(2)=        5 -> 21        -0.00348
        min(3)=        2 -> 16        -0.00256
        min(4)=        3 -> 16        -0.00126
        min(5)=        4 -> 18        -0.00012
        #CIs=12 #CIs>0=4 #CIs<0=8

11      Singlet-?Sym   34.6083        35.82    0.0004    0.000
        max(1)=        5 -> 10         0.70260
        max(2)=        5 ->  7         0.01815
        max(3)=        5 ->  6         0.01069
        max(4)=        5 -> 14         0.00742
        max(5)=        4 -> 17         0.00561
        min(1)=        3 ->  9        -0.05751
        min(2)=        4 -> 10        -0.04755
        min(3)=        3 -> 13        -0.01150
        min(4)=        2 ->  9        -0.00870
        min(5)=        5 -> 15        -0.00464
        #CIs=36 #CIs>0=18 #CIs<0=18

12      Singlet-?Sym   34.6083        35.82    0.0004    0.000
        max(1)=        4 -> 10         0.70260
        max(2)=        5 -> 10         0.04755
        max(3)=        4 ->  7         0.01815
        max(4)=        4 ->  6         0.01069
        max(5)=        4 -> 14         0.00742
        min(1)=        3 ->  8        -0.05751
        min(2)=        3 -> 12        -0.01150
        min(3)=        2 ->  8        -0.00870
        min(4)=        4 -> 16        -0.00561
        min(5)=        4 -> 15        -0.00464
```

```
          #CIs=36 #CIs>0=21 #CIs<0=15

13     Singlet-SG   37.0885        33.43    0.1478    0.000
          max(1)=        3 -> 10         0.52121
          max(2)=        2 ->  7         0.10466
          max(3)=        3 ->  7         0.06640
          max(4)=        3 ->  6         0.02774
          max(5)=        2 -> 11         0.02669
          min(1)=        4 ->  8        -0.31905
          min(2)=        5 ->  9        -0.31905
          min(3)=        2 ->  6        -0.08795
          min(4)=        2 -> 14        -0.00782
          min(5)=        3 -> 15        -0.00628
          #CIs=26 #CIs>0=15 #CIs<0=11

14     Singlet-?Sym   37.4368        33.12    0.0010    0.000
          max(1)=        3 ->  9         0.70452
          max(2)=        5 -> 10         0.05715
          max(3)=        4 -> 17         0.00543
          max(4)=        5 -> 16         0.00543
          max(5)=        3 -> 19         0.00455
          min(1)=        3 -> 13        -0.01455
          min(2)=        5 -> 11        -0.00788
          min(3)=        2 ->  9        -0.00740
          min(4)=        2 -> 13        -0.00370
          min(5)=        5 -> 20        -0.00153
          #CIs=28 #CIs>0=17 #CIs<0=11

15     Singlet-?Sym   37.4368        33.12    0.0010    0.000
          max(1)=        3 ->  8         0.70452
          max(2)=        4 -> 10         0.05715
          max(3)=        5 -> 17         0.00543
          max(4)=        3 -> 18         0.00455
          max(5)=        3 -> 22         0.00446
          min(1)=        3 -> 12        -0.01455
          min(2)=        4 -> 11        -0.00788
          min(3)=        2 ->  8        -0.00740
          min(4)=        4 -> 16        -0.00543
          min(5)=        2 -> 12        -0.00370
          #CIs=28 #CIs>0=14 #CIs<0=14

16     Singlet-SG   41.0629        30.19    0.0690    0.000
          max(1)=        2 ->  7         0.67483
          max(2)=        3 -> 11         0.06680
          max(3)=        2 -> 11         0.00524
          max(4)=        3 ->  7         0.00470
          max(5)=        4 -> 22         0.00198
          min(1)=        3 -> 10        -0.18857
          min(2)=        2 ->  6        -0.04316
          min(3)=        4 ->  8        -0.03670
          min(4)=        5 ->  9        -0.03670
          min(5)=        4 -> 18        -0.00650
          #CIs=26 #CIs>0=7 #CIs<0=19

17     Singlet-?Sym   43.6287        28.42    0.2384    0.000
          max(1)=        5 -> 11         0.70330
          max(2)=        4 -> 11         0.04835
          max(3)=        3 -> 13         0.04384
          max(4)=        3 ->  9         0.00823
          max(5)=        3 -> 19         0.00359
          min(1)=        2 ->  9        -0.03136
          min(2)=        5 ->  6        -0.00890
          min(3)=        2 -> 13        -0.00477
          min(4)=        5 -> 20        -0.00454
          min(5)=        2 ->  8        -0.00216
          #CIs=36 #CIs>0=17 #CIs<0=19

18     Singlet-?Sym   43.6287        28.42    0.2384    0.000
          max(1)=        4 -> 11         0.70330
          max(2)=        3 -> 12         0.04384
          max(3)=        3 ->  8         0.00823
          max(4)=        3 -> 18         0.00359
          max(5)=        5 -> 17         0.00326
          min(1)=        5 -> 11        -0.04835
          min(2)=        2 ->  8        -0.03136
          min(3)=        4 ->  6        -0.00890
          min(4)=        2 -> 12        -0.00477
          min(5)=        4 -> 20        -0.00454
          #CIs=36 #CIs>0=17 #CIs<0=19

19     Singlet-?Sym   45.5255        27.23    0.0000    0.000
          max(1)=        4 -> 13         0.49999
```

```
          max(2)=        5 -> 12         0.49999
          max(3)=        3 -> 17         0.00086
          max(4)=        2 -> 17         0.00085
          max(5)=        5 -> 13         0.00075
          min(1)=        4 -> 19        -0.00318
          min(2)=        5 -> 18        -0.00318
          min(3)=        4 -> 12        -0.00075
          min(4)=        4 -> 21        -0.00001
          min(5)=        5 -> 22        -0.00001
          #CIs=12 #CIs>0=7 #CIs<0=5

20       Singlet-?Sym   45.5255         27.23    0.0000    0.000
          max(1)=        4 -> 12         0.49999
          max(2)=        5 -> 19         0.00318
          max(3)=        4 -> 13         0.00075
          max(4)=        5 -> 12         0.00075
          max(5)=        4 ->  8         0.00010
          min(1)=        5 -> 13        -0.49999
          min(2)=        4 -> 18        -0.00318
          min(3)=        3 -> 16        -0.00086
          min(4)=        2 -> 16        -0.00085
          min(5)=        5 ->  9        -0.00010
          #CIs=12 #CIs>0=6 #CIs<0=6

21       Singlet-?Sym   45.5781         27.20    0.0000    0.000
          max(1)=        5 -> 12         0.49999
          max(2)=        4 -> 19         0.00391
          max(3)=        4 -> 21         0.00026
          max(4)=        4 ->  9         0.00022
          max(5)=        5 ->  8        -0.00022
          min(1)=        4 -> 13        -0.49999
          min(2)=        5 -> 18        -0.00391
          min(3)=        5 -> 22        -0.00026
          min(4)=        5 ->  8        -0.00022
          min(5)=        4 ->  9         0.00022
          #CIs=8 #CIs>0=4 #CIs<0=4

22       Singlet-SG   46.1756         26.85    0.1086    0.000
          max(1)=        3 -> 11         0.35181
          max(2)=        2 -> 11         0.12650
          max(3)=        3 ->  7         0.08663
          max(4)=        3 -> 14         0.04823
          max(5)=        3 ->  6         0.03473
          min(1)=        3 -> 10        -0.31846
          min(2)=        4 ->  8        -0.27020
          min(3)=        5 ->  9        -0.27020
          min(4)=        4 -> 12        -0.19263
          min(5)=        5 -> 13        -0.19263
          #CIs=26 #CIs>0=13 #CIs<0=13

23       Singlet-SG   47.4801         26.11    0.4714    0.000
          max(1)=        3 -> 11         0.41253
          max(2)=        4 -> 12         0.39957
          max(3)=        5 -> 13         0.39957
          max(4)=        4 -> 18         0.01712
          max(5)=        5 -> 19         0.01712
          min(1)=        3 -> 14        -0.05195
          min(2)=        2 -> 10        -0.04999
          min(3)=        2 ->  7        -0.04505
          min(4)=        3 ->  7        -0.03926
          min(5)=        2 ->  6        -0.02861
          #CIs=25 #CIs>0=15 #CIs<0=10
```

5.1.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-?Sym   12.0824        102.62    0.0238    0.000
          max(1)=        5 ->  6         0.53959
          max(2)=        5 ->  7         0.13179
          max(3)=        5 -> 11         0.03502
          max(4)=        4 -> 10         0.02682
          max(5)=        5 -> 15         0.00971
          min(1)=        4 ->  6        -0.42020
          min(2)=        4 ->  7        -0.10263
          min(3)=        5 -> 10        -0.03444
          min(4)=        4 -> 11        -0.02727
```

```
        min(5)=     5 -> 14      -0.01179
        #states=34 #states>0=16 #states<0=18

2   Singlet-?Sym  12.0824    102.62  0.0238  0.000
        max(1)=     4 ->  6       0.53959
        max(2)=     5 ->  6       0.42020
        max(3)=     4 ->  7       0.13179
        max(4)=     5 ->  7       0.10263
        max(5)=     4 -> 11       0.03502
        min(1)=     4 -> 10      -0.03444
        min(2)=     5 -> 10      -0.02682
        min(3)=     4 -> 14      -0.01179
        min(4)=     5 -> 14      -0.00918
        min(5)=     4 -> 23      -0.00311
        #states=34 #states>0=21 #states<0=13

3   Singlet-SG  16.4027    75.59  0.2385  0.000
        max(1)=     3 ->  6       0.69825
        max(2)=     3 ->  7       0.07072
        max(3)=     4 ->  8       0.05015
        max(4)=     5 ->  9       0.05015
        max(5)=     3 -> 11       0.04267
        min(1)=     3 -> 10      -0.00654
        min(2)=     2 ->  6      -0.00604
        min(3)=     2 -> 14      -0.00566
        min(4)=     3 -> 23      -0.00179
        min(5)=     2 -> 23      -0.00155
        #states=24 #states>0=19 #states<0=5

4   Singlet-?Sym  21.6414    57.29  0.0565  0.000
        max(1)=     5 ->  7       0.56812
        max(2)=     4 ->  6       0.09466
        max(3)=     4 -> 10       0.03425
        max(4)=     4 -> 14       0.02557
        max(5)=     5 -> 15       0.01263
        min(1)=     4 ->  7      -0.37572
        min(2)=     5 ->  6      -0.14313
        min(3)=     5 -> 10      -0.05179
        min(4)=     5 -> 14      -0.03867
        min(5)=     3 -> 13      -0.00879
        #states=36 #states>0=17 #states<0=19

5   Singlet-?Sym  21.6414    57.29  0.0565  0.000
        max(1)=     4 ->  7       0.56812
        max(2)=     5 ->  7       0.37572
        max(3)=     4 -> 15       0.01263
        max(4)=     5 -> 15       0.00835
        max(5)=     2 -> 12       0.00763
        min(1)=     4 ->  6      -0.14313
        min(2)=     5 ->  6      -0.09466
        min(3)=     4 -> 10      -0.05179
        min(4)=     4 -> 14      -0.03867
        min(5)=     5 -> 10      -0.03425
        #states=36 #states>0=17 #states<0=19

6   Singlet-SG  27.0282    45.87  0.3872  0.000
        max(1)=     3 ->  7       0.68277
        max(2)=     4 ->  8       0.10281
        max(3)=     5 ->  9       0.10281
        max(4)=     4 -> 12       0.03791
        max(5)=     5 -> 13       0.03791
        min(1)=     3 ->  6      -0.08600
        min(2)=     3 -> 10      -0.02836
        min(3)=     2 ->  7      -0.02226
        min(4)=     3 -> 14      -0.01898
        min(5)=     4 -> 19      -0.00846
        #states=24 #states>0=14 #states<0=10

7   Singlet-?Sym  34.1898    36.26  0.0000  0.000
        max(1)=     5 ->  8       0.49975
        max(2)=     5 -> 22       0.01482
        max(3)=     5 -> 12       0.00500
        max(4)=     4 -> 18       0.00063
        max(5)=     5 -> 19      -0.00063
        min(1)=     4 ->  9      -0.49975
        min(2)=     4 -> 21      -0.01482
        min(3)=     4 -> 13      -0.00500
        min(4)=     5 -> 19      -0.00063
        min(5)=     4 -> 18       0.00063
        #states=8 #states>0=4 #states<0=4

8   Singlet-?Sym  34.5435    35.89  0.0000  0.000
```

max(1)= 5 -> 9 0.49980
max(2)= 5 -> 21 0.01358
max(3)= 5 -> 13 0.00344
max(4)= 2 -> 17 0.00333
max(5)= 3 -> 17 0.00067
min(1)= 4 -> 8 -0.49980
min(2)= 4 -> 22 -0.01358
min(3)= 4 -> 12 -0.00344
min(4)= 5 -> 18 -0.00066
min(5)= 4 -> 19 0.00066
#states=10 #states>0=6 #states<0=4

9 Singlet-?Sym 34.5435 35.89 0.0000 0.000
max(1)= 4 -> 9 0.49980
max(2)= 5 -> 8 0.49980
max(3)= 4 -> 21 0.01358
max(4)= 5 -> 22 0.01358
max(5)= 4 -> 13 0.00344
min(1)= 2 -> 16 -0.00333
min(2)= 3 -> 16 -0.00067
min(3)= 4 -> 18 -0.00066
min(4)= 5 -> 19 -0.00066
min(5)= 4 -> 13 0.00344
#states=10 #states>0=6 #states<0=4

10 Singlet-?Sym 36.1022 34.34 0.0014 0.000
max(1)= 5 -> 10 0.62498
max(2)= 4 -> 10 0.31508
max(3)= 5 -> 7 0.06394
max(4)= 5 -> 11 0.03841
max(5)= 4 -> 7 0.03223
min(1)= 3 -> 9 -0.03369
min(2)= 3 -> 8 -0.01699
min(3)= 3 -> 13 -0.01257
min(4)= 5 -> 15 -0.01026
min(5)= 3 -> 12 -0.00634
#states=35 #states>0=21 #states<0=14

11 Singlet-?Sym 36.1022 34.34 0.0014 0.000
max(1)= 4 -> 10 0.62498
max(2)= 4 -> 7 0.06394
max(3)= 4 -> 11 0.03841
max(4)= 4 -> 6 0.02249
max(5)= 3 -> 9 0.01699
min(1)= 5 -> 10 -0.31508
min(2)= 3 -> 8 -0.03369
min(3)= 5 -> 7 -0.03223
min(4)= 5 -> 11 -0.01936
min(5)= 3 -> 12 -0.01257
#states=35 #states>0=18 #states<0=17

12 Singlet-SG 38.0466 32.59 0.0230 0.000
max(1)= 2 -> 6 0.53808
max(2)= 3 -> 10 0.25213
max(3)= 2 -> 7 0.14849
max(4)= 3 -> 7 0.08412
max(5)= 2 -> 11 0.03692
min(1)= 4 -> 8 -0.23618
min(2)= 5 -> 9 -0.23618
min(3)= 2 -> 14 -0.01129
min(4)= 2 -> 10 -0.00979
min(5)= 4 -> 19 -0.00574
#states=25 #states>0=13 #states<0=12

13 Singlet-?Sym 38.5159 32.19 0.0001 0.000
max(1)= 3 -> 8 0.69780
max(2)= 3 -> 9 0.10225
max(3)= 4 -> 10 0.03564
max(4)= 4 -> 11 0.02616
max(5)= 3 -> 22 0.01715
min(1)= 2 -> 12 -0.01288
min(2)= 2 -> 19 -0.00511
min(3)= 4 -> 6 -0.00402
min(4)= 2 -> 13 -0.00189
min(5)= 4 -> 20 -0.00109
#states=33 #states>0=24 #states<0=9

14 Singlet-?Sym 38.5159 32.19 0.0001 0.000
max(1)= 3 -> 9 0.69780
max(2)= 5 -> 10 0.03564
max(3)= 5 -> 11 0.02616
max(4)= 3 -> 21 0.01715

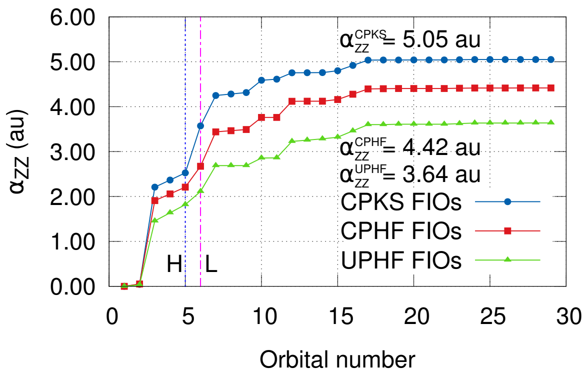
```
max(5)=   2 ->  9    0.00592
min(1)=   3 ->  8   -0.10225
min(2)=   2 -> 13   -0.01288
min(3)=   4 -> 10   -0.00522
min(4)=   2 -> 18   -0.00511
min(5)=   5 -> 17   -0.00421
#states=33 #states>0=16 #states<0=17

15   Singlet-SG   38.8694   31.90   0.2130   0.000
max(1)=   3 -> 10    0.49289
max(2)=   3 ->  7    0.08178
max(3)=   2 -> 10    0.04860
max(4)=   3 ->  6    0.02090
max(5)=   3 -> 14    0.02041
min(1)=   2 ->  6   -0.40590
min(2)=   4 ->  8   -0.19908
min(3)=   5 ->  9   -0.19908
min(4)=   2 ->  7   -0.05090
min(5)=   3 -> 15   -0.01043
#states=23 #states>0=14 #states<0=9

16   Singlet-?Sym   45.1100   27.48   0.2896   0.000
max(1)=   5 -> 11    0.70043
max(2)=   2 ->  9    0.02993
max(3)=   3 -> 13    0.02980
max(4)=   5 -> 15    0.02857
max(5)=   4 -> 16    0.00348
min(1)=   5 ->  6   -0.04560
min(2)=   4 -> 11   -0.04529
min(3)=   5 -> 10   -0.04034
min(4)=   3 ->  9   -0.02493
min(5)=   5 ->  7   -0.01206
#states=31 #states>0=13 #states<0=18

17   Singlet-?Sym   45.1100   27.48   0.2896   0.000
max(1)=   4 -> 11    0.70043
max(2)=   5 -> 11    0.04529
max(3)=   2 ->  8    0.02993
max(4)=   3 -> 12    0.02980
max(5)=   4 -> 15    0.02857
min(1)=   4 ->  6   -0.04560
min(2)=   4 -> 10   -0.04034
min(3)=   3 ->  8   -0.02493
min(4)=   4 ->  7   -0.01206
min(5)=   4 -> 20   -0.01188
#states=31 #states>0=14 #states<0=17

18   Singlet-SG   47.2064   26.26   0.0982   0.000
max(1)=   2 ->  7    0.62911
max(2)=   4 -> 12    0.08063
max(3)=   5 -> 13    0.08063
max(4)=   3 ->  7    0.03327
max(5)=   2 -> 11    0.01882
min(1)=   2 ->  6   -0.19425
min(2)=   3 -> 10   -0.17280
min(3)=   4 ->  8   -0.09351
min(4)=   5 ->  9   -0.09351
min(5)=   2 -> 10   -0.04884
#states=25 #states>0=13 #states<0=12

19   Singlet-?Sym   48.4145   25.61   0.0000   0.000
max(1)=   5 -> 13    0.49976
max(2)=   4 -> 19    0.01496
max(3)=   4 ->  8    0.00346
max(4)=   4 -> 22    0.00015
max(5)=   2 -> 17   -0.00011
min(1)=   4 -> 12   -0.49976
min(2)=   5 -> 18   -0.01496
min(3)=   5 ->  9   -0.00346
min(4)=   3 -> 17   -0.00072
min(5)=   5 -> 21   -0.00015
#states=12 #states>0=4 #states<0=8

20   Singlet-?Sym   48.4145   25.61   0.0000   0.000
max(1)=   4 -> 13    0.49976
max(2)=   5 -> 12    0.49976
max(3)=   3 -> 16    0.00072
max(4)=   5 -> 13    0.00012
max(5)=   2 -> 16    0.00011
min(1)=   4 -> 18   -0.01496
min(2)=   5 -> 19   -0.01496
min(3)=   4 ->  9   -0.00346
```

```
        min(4)=        5 ->  8        -0.00346
        min(5)=        4 -> 21        -0.00015
        #states=12 #states>0=5 #states<0=7

21      Singlet-?Sym   48.5122         25.56    0.0000    0.000
        max(1)=        5 -> 12         0.49972
        max(2)=        4 -> 18         0.01595
        max(3)=        4 ->  9         0.00501
        max(4)=        4 -> 21         0.00045
        max(5)=        5 -> 22        -0.00045
        min(1)=        4 -> 13        -0.49972
        min(2)=        5 -> 19        -0.01595
        min(3)=        5 ->  8        -0.00501
        min(4)=        5 -> 22        -0.00045
        min(5)=        4 -> 21         0.00045
        #states=8 #states>0=4 #states<0=4

22      Singlet-SG   48.8362         25.39    0.0809    0.000
        max(1)=        3 -> 11         0.66958
        max(2)=        2 -> 10         0.03031
        max(3)=        3 -> 15         0.02673
        max(4)=        2 -> 11         0.01561
        max(5)=        3 ->  7         0.01530
        min(1)=        4 -> 12        -0.12835
        min(2)=        5 -> 13        -0.12835
        min(3)=        3 -> 10        -0.08210
        min(4)=        4 ->  8        -0.05871
        min(5)=        5 ->  9        -0.05871
        #states=26 #states>0=13 #states<0=13

23      Singlet-?Sym   50.5029         24.55    0.6813    0.000
        max(1)=        4 -> 12         0.42459
        max(2)=        5 -> 13         0.42459
        max(3)=        3 -> 11         0.21226
        max(4)=        4 ->  8         0.15236
        max(5)=        5 ->  9         0.15236
        min(1)=        3 ->  7        -0.09358
        min(2)=        3 -> 14        -0.08157
        min(3)=        2 -> 11        -0.06761
        min(4)=        2 -> 10        -0.04123
        min(5)=        3 ->  6        -0.03072
        #states=26 #states>0=15 #states<0=11
```

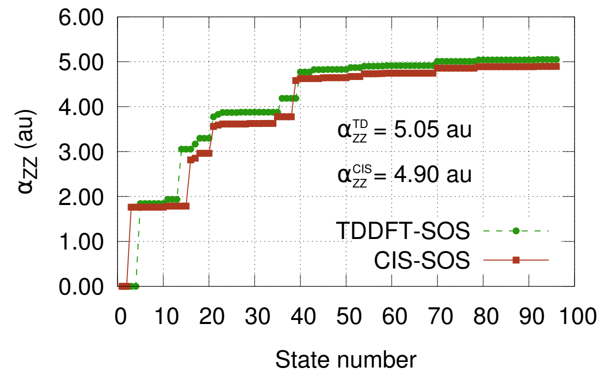
5.2 6-311++G(d,p)

5.2.1 Plots

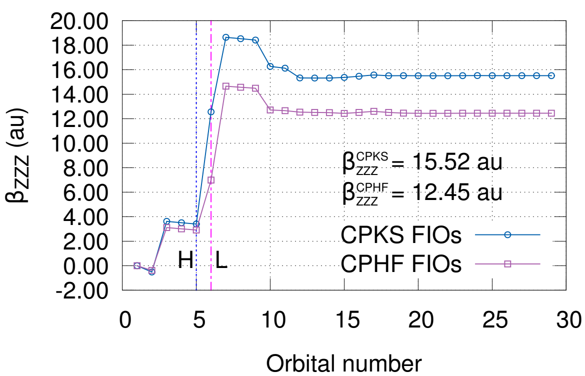
Figure S6: For HF molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S6a and S6c) or states (SOS approaches, in Plots S6b and S6d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.01 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



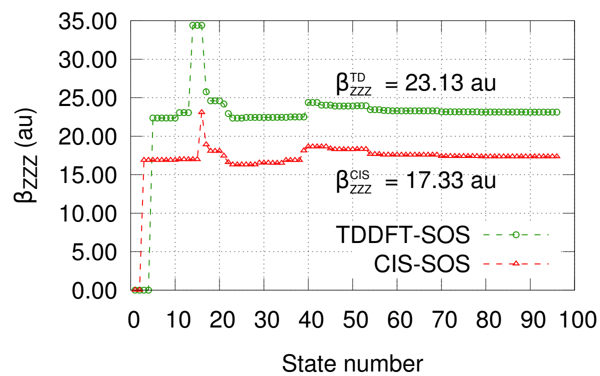
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

5.2.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-?Sym    9.5784        129.44    0.0302    0.000
         max(1)=        5 ->  6         0.56118
         max(2)=        4 ->  6         0.39106
         max(3)=        5 ->  7         0.13820
         max(4)=        4 ->  7         0.09630
         max(5)=        5 -> 11         0.03273
         min(1)=        5 -> 12        -0.02299
         min(2)=        4 -> 12        -0.01602
         min(3)=        5 -> 15        -0.00525
         min(4)=        4 -> 15        -0.00366
         min(5)=        2 -> 13        -0.00248
         #CIs=46 #CIs>0=23 #CIs<0=23

2        Singlet-?Sym    9.5784        129.44    0.0302    0.000
         max(1)=        4 ->  6         0.56118
         max(2)=        4 ->  7         0.13820
         max(3)=        4 -> 11         0.03273
         max(4)=        4 -> 10         0.03139
         max(5)=        5 -> 12         0.01602
         min(1)=        5 ->  6        -0.39106
         min(2)=        5 ->  7        -0.09630
         min(3)=        4 -> 12        -0.02299
         min(4)=        5 -> 11        -0.02281
         min(5)=        5 -> 10        -0.02187
         #CIs=46 #CIs>0=24 #CIs<0=22

3        Singlet-?Sym   13.2757         93.39    0.0161    0.000
         max(1)=        4 ->  7         0.59902
         max(2)=        5 ->  7         0.31328
         max(3)=        3 -> 17         0.00278
         max(4)=        4 -> 21         0.00174
         max(5)=        5 -> 22         0.00174
         min(1)=        4 ->  6        -0.14512
         min(2)=        4 -> 10        -0.09015
         min(3)=        5 ->  6        -0.07589
         min(4)=        4 -> 12        -0.06714
         min(5)=        5 -> 10        -0.04715
         #CIs=46 #CIs>0=23 #CIs<0=23

4        Singlet-?Sym   13.2757         93.39    0.0161    0.000
         max(1)=        5 ->  7         0.59902
         max(2)=        4 ->  6         0.07589
         max(3)=        4 -> 10         0.04715
         max(4)=        4 -> 12         0.03511
         max(5)=        4 -> 15         0.00482
         min(1)=        4 ->  7        -0.31328
         min(2)=        5 ->  6        -0.14512
         min(3)=        5 -> 10        -0.09015
         min(4)=        5 -> 12        -0.06714
         min(5)=        5 -> 15        -0.00921
         #CIs=46 #CIs>0=22 #CIs<0=24

5        Singlet-SG   13.5686         91.38    0.1527    0.000
         max(1)=        3 ->  6         0.68540
         max(2)=        4 ->  8         0.09770
         max(3)=        5 ->  9         0.09770
         max(4)=        3 ->  7         0.08276
         max(5)=        3 -> 10         0.04809
         min(1)=        2 -> 12        -0.00588
         min(2)=        4 -> 17        -0.00316
         min(3)=        5 -> 16        -0.00316
         min(4)=        2 -> 15        -0.00314
         min(5)=        3 -> 15        -0.00280
         #CIs=32 #CIs>0=19 #CIs<0=13

6        Singlet-?Sym   15.0780         82.23    0.0000    0.000
         max(1)=        5 ->  8         0.49967
         max(2)=        5 -> 14         0.01782
         max(3)=        5 -> 17         0.00529
         max(4)=        5 -> 26         0.00034
         max(5)=        4 -> 24         0.00003
         min(1)=        4 ->  9        -0.49967
         min(2)=        4 -> 13        -0.01782
         min(3)=        4 -> 16        -0.00529
         min(4)=        4 -> 27        -0.00034
         min(5)=        5 -> 23        -0.00003
         #CIs=10 #CIs>0=5 #CIs<0=5

7        Singlet-?Sym   15.1837         81.66    0.0000    0.000
         max(1)=        4 ->  9         0.49978
```

```
        max(2)=        5 ->  8         0.49978
        max(3)=        4 -> 13         0.01406
        max(4)=        5 -> 14         0.01406
        max(5)=        4 -> 16         0.00458
        min(1)=        4 -> 24        -0.00002
        min(2)=        5 -> 23        -0.00002
        min(3)=        4 -> 27         0.00051
        min(4)=        5 -> 26         0.00051
        min(5)=        3 -> 22         0.00083
        #CIs=12 #CIs>0=10 #CIs<0=2

8       Singlet-?Sym   15.1837         81.66    0.0000    0.000
        max(1)=        4 ->  8         0.49978
        max(2)=        4 -> 14         0.01406
        max(3)=        4 -> 17         0.00458
        max(4)=        2 -> 21         0.00199
        max(5)=        3 -> 21         0.00083
        min(1)=        5 ->  9        -0.49978
        min(2)=        5 -> 13        -0.01406
        min(3)=        5 -> 16        -0.00458
        min(4)=        5 -> 27        -0.00051
        min(5)=        4 -> 23        -0.00002
        #CIs=12 #CIs>0=7 #CIs<0=5

9       Singlet-?Sym   15.6619         79.16    0.0309    0.000
        max(1)=        5 -> 10         0.65417
        max(2)=        4 -> 10         0.24426
        max(3)=        5 ->  7         0.08336
        max(4)=        4 ->  7         0.03112
        max(5)=        5 -> 15         0.01138
        min(1)=        5 ->  6        -0.05631
        min(2)=        4 ->  6        -0.02102
        min(3)=        5 -> 11        -0.01997
        min(4)=        5 -> 12        -0.01377
        min(5)=        4 -> 11        -0.00746
        #CIs=47 #CIs>0=16 #CIs<0=31

10      Singlet-?Sym   15.6619         79.16    0.0309    0.000
        max(1)=        4 -> 10         0.65417
        max(2)=        4 ->  7         0.08336
        max(3)=        5 ->  6         0.02102
        max(4)=        4 -> 15         0.01138
        max(5)=        5 -> 11         0.00746
        min(1)=        5 -> 10        -0.24426
        min(2)=        4 ->  6        -0.05631
        min(3)=        5 ->  7        -0.03112
        min(4)=        4 -> 11        -0.01997
        min(5)=        4 -> 12        -0.01377
        #CIs=47 #CIs>0=25 #CIs<0=22

11      Singlet-?Sym   16.4171         75.52    0.0115    0.000
        max(1)=        4 ->  8         0.39821
        max(2)=        5 ->  9         0.39821
        max(3)=        3 ->  7         0.36890
        max(4)=        3 -> 11         0.02117
        max(5)=        2 -> 12         0.00980
        min(1)=        3 ->  6        -0.14835
        min(2)=        3 -> 10        -0.14758
        min(3)=        3 -> 12        -0.04469
        min(4)=        3 -> 15        -0.02312
        min(5)=        2 ->  7        -0.01835
        #CIs=34 #CIs>0=8 #CIs<0=26

12      Singlet-?Sym   18.2404         67.97    0.0924    0.000
        max(1)=        4 -> 11         0.69518
        max(2)=        5 -> 11         0.10727
        max(3)=        3 ->  8         0.05108
        max(4)=        4 -> 10         0.01910
        max(5)=        4 -> 12         0.01572
        min(1)=        4 ->  6        -0.04058
        min(2)=        4 -> 15        -0.01356
        min(3)=        5 ->  6        -0.00626
        min(4)=        3 -> 17        -0.00440
        min(5)=        2 -> 14        -0.00284
        #CIs=47 #CIs>0=22 #CIs<0=25

13      Singlet-?Sym   18.2404         67.97    0.0924    0.000
        max(1)=        5 -> 11         0.69518
        max(2)=        3 ->  9         0.05108
        max(3)=        5 -> 10         0.01910
        max(4)=        5 -> 12         0.01572
        max(5)=        4 ->  6         0.00626
```

```
        min(1)=        4 -> 11        -0.10727
        min(2)=        5 ->  6        -0.04058
        min(3)=        5 -> 15        -0.01356
        min(4)=        3 ->  8        -0.00788
        min(5)=        3 -> 16        -0.00440
        #CIs=47 #CIs>0=25 #CIs<0=22

14      Singlet-SG   18.5639         66.79    0.1732    0.000
        max(1)=        3 ->  7         0.58095
        max(2)=        3 -> 10         0.23673
        max(3)=        3 -> 12         0.03949
        max(4)=        4 -> 14         0.03630
        max(5)=        5 -> 13         0.03630
        min(1)=        4 ->  8        -0.22540
        min(2)=        5 ->  9        -0.22540
        min(3)=        3 -> 11        -0.03182
        min(4)=        3 ->  6        -0.02141
        min(5)=        2 -> 12        -0.01690
        #CIs=33 #CIs>0=19 #CIs<0=14

15      Singlet-?Sym   18.8792         65.67    0.0014    0.000
        max(1)=        3 ->  8         0.70473
        max(2)=        3 -> 14         0.01951
        max(3)=        3 -> 17         0.00878
        max(4)=        4 -> 10         0.00439
        max(5)=        3 -> 23         0.00235
        min(1)=        4 -> 11        -0.05198
        min(2)=        3 ->  9        -0.01326
        min(3)=        2 ->  8        -0.00249
        min(4)=        4 -> 15        -0.00237
        min(5)=        4 -> 18        -0.00177
        #CIs=43 #CIs>0=23 #CIs<0=20

16      Singlet-?Sym   18.8792         65.67    0.0014    0.000
        max(1)=        3 ->  9         0.70473
        max(2)=        3 -> 13         0.01951
        max(3)=        3 ->  8         0.01326
        max(4)=        3 -> 16         0.00878
        max(5)=        5 -> 10         0.00439
        min(1)=        5 -> 11        -0.05198
        min(2)=        2 ->  9        -0.00249
        min(3)=        5 -> 15        -0.00237
        min(4)=        5 -> 21        -0.00234
        min(5)=        5 -> 18        -0.00177
        #CIs=43 #CIs>0=21 #CIs<0=22

17      Singlet-SG   19.9758         62.07    0.0203    0.000
        max(1)=        3 -> 10         0.64226
        max(2)=        4 ->  8         0.15845
        max(3)=        5 ->  9         0.15845
        max(4)=        3 -> 11         0.09867
        max(5)=        2 -> 12         0.00754
        min(1)=        3 ->  7        -0.12997
        min(2)=        3 ->  6        -0.07934
        min(3)=        3 -> 12        -0.05143
        min(4)=        4 -> 14        -0.03507
        min(5)=        5 -> 13        -0.03507
        #CIs=34 #CIs>0=13 #CIs<0=21

18      Singlet-SG   21.9019         56.61    0.0283    0.000
        max(1)=        3 -> 11         0.69699
        max(2)=        3 ->  7         0.02726
        max(3)=        3 -> 12         0.02201
        max(4)=        2 ->  6         0.02033
        max(5)=        2 ->  7         0.01850
        min(1)=        3 -> 10        -0.07745
        min(2)=        4 ->  8        -0.04874
        min(3)=        5 ->  9        -0.04874
        min(4)=        3 ->  6        -0.02803
        min(5)=        2 -> 12        -0.00687
        #CIs=33 #CIs>0=21 #CIs<0=12

19      Singlet-?Sym   22.5967         54.87    0.0250    0.000
        max(1)=        4 -> 12         0.59791
        max(2)=        5 -> 12         0.36723
        max(3)=        4 ->  7         0.06976
        max(4)=        5 ->  7         0.04284
        max(5)=        4 -> 15         0.01263
        min(1)=        4 -> 11        -0.01271
        min(2)=        4 -> 19        -0.01107
        min(3)=        5 -> 11        -0.00781
        min(4)=        3 -> 17        -0.00683
```

```
        min(5)=      5 -> 19        -0.00680
        #CIs=46 #CIs>0=27 #CIs<0=19

20    Singlet-?Sym   22.5967        54.87    0.0250    0.000
        max(1)=      5 -> 12         0.59791
        max(2)=      5 ->  7         0.06976
        max(3)=      5 -> 15         0.01263
        max(4)=      2 ->  9         0.01024
        max(5)=      5 ->  6         0.00794
        min(1)=      4 -> 12        -0.36723
        min(2)=      4 ->  7        -0.04284
        min(3)=      5 -> 11        -0.01271
        min(4)=      5 -> 19        -0.01107
        min(5)=      4 -> 15        -0.00775
        #CIs=46 #CIs>0=24 #CIs<0=22

21    Singlet-SG   28.0003        44.28    0.1677    0.000
        max(1)=      3 -> 12         0.69279
        max(2)=      4 ->  8         0.04307
        max(3)=      5 ->  9         0.04307
        max(4)=      3 -> 10         0.02267
        max(5)=      4 -> 17         0.02231
        min(1)=      4 -> 14        -0.06640
        min(2)=      5 -> 13        -0.06640
        min(3)=      2 ->  6        -0.06520
        min(4)=      2 -> 10        -0.03705
        min(5)=      2 ->  7        -0.02746
        #CIs=33 #CIs>0=15 #CIs<0=18

22    Singlet-SG   31.5816        39.26    0.0249    0.000
        max(1)=      2 ->  6         0.69172
        max(2)=      2 ->  7         0.09990
        max(3)=      3 -> 12         0.06033
        max(4)=      2 -> 10         0.02592
        max(5)=      4 ->  8         0.02170
        min(1)=      4 -> 14        -0.04758
        min(2)=      5 -> 13        -0.04758
        min(3)=      3 -> 15        -0.02596
        min(4)=      3 -> 11        -0.01921
        min(5)=      4 -> 17        -0.01828
        #CIs=33 #CIs>0=13 #CIs<0=20

23    Singlet-SG   35.2070        35.22    0.0229    0.000
        max(1)=      2 ->  7         0.68655
        max(2)=      4 ->  8         0.01356
        max(3)=      5 ->  9         0.01356
        max(4)=      3 -> 18         0.01188
        max(5)=      3 -> 12         0.00803
        min(1)=      2 -> 10        -0.11122
        min(2)=      2 ->  6        -0.09972
        min(3)=      2 -> 12        -0.04923
        min(4)=      2 -> 11        -0.03786
        min(5)=      4 -> 14        -0.01987
        #CIs=32 #CIs>0=8 #CIs<0=24

24    Singlet-?Sym   37.0121        33.50    0.0164    0.000
        max(1)=      2 ->  8         0.68553
        max(2)=      3 -> 17         0.01537
        max(3)=      2 -> 14         0.01383
        max(4)=      4 -> 21         0.00817
        max(5)=      5 -> 22         0.00817
        min(1)=      2 ->  9        -0.16898
        min(2)=      3 -> 14        -0.01642
        min(3)=      4 -> 15        -0.01635
        min(4)=      4 -> 18        -0.01217
        min(5)=      4 -> 12        -0.01178
        #CIs=47 #CIs>0=25 #CIs<0=22

25    Singlet-?Sym   37.0121        33.50    0.0164    0.000
        max(1)=      2 ->  9         0.68553
        max(2)=      2 ->  8         0.16898
        max(3)=      3 -> 16         0.01537
        max(4)=      2 -> 13         0.01383
        max(5)=      4 -> 22         0.00817
        min(1)=      3 -> 13        -0.01642
        min(2)=      5 -> 15        -0.01635
        min(3)=      5 -> 18        -0.01217
        min(4)=      5 -> 12        -0.01178
        min(5)=      5 -> 21        -0.00817
        #CIs=47 #CIs>0=26 #CIs<0=21

26    Singlet-SG   37.4162        33.14    0.0010    0.000
```

```
max(1)=    2 -> 10     0.69005
max(2)=    2 ->  7     0.09841
max(3)=    3 -> 12     0.02113
max(4)=    4 ->  8     0.01193
max(5)=    5 ->  9     0.01193
min(1)=    4 -> 14    -0.07067
min(2)=    5 -> 13    -0.07067
min(3)=    2 ->  6    -0.05244
min(4)=    3 -> 15    -0.01965
min(5)=    3 ->  7    -0.01064
#CIs=34 #CIs>0=17 #CIs<0=17

27   Singlet-SG   39.8666   31.10   0.0044   0.000
max(1)=    2 -> 11     0.69972
max(2)=    2 -> 12     0.03729
max(3)=    2 ->  7     0.02974
max(4)=    3 -> 10     0.00959
max(5)=    2 -> 18     0.00497
min(1)=    4 -> 14    -0.05116
min(2)=    5 -> 13    -0.05116
min(3)=    2 ->  6    -0.03258
min(4)=    4 -> 17    -0.02218
min(5)=    5 -> 16    -0.02218
#CIs=33 #CIs>0=13 #CIs<0=20

28   Singlet-?Sym   41.8623   29.62   0.0000   0.000
max(1)=    4 -> 13     0.49947
max(2)=    5 ->  8     0.01793
max(3)=    4 -> 16     0.01420
max(4)=    4 -> 27     0.00364
max(5)=    5 -> 23     0.00128
min(1)=    5 -> 14    -0.49947
min(2)=    4 ->  9    -0.01793
min(3)=    5 -> 17    -0.01420
min(4)=    5 -> 26    -0.00364
min(5)=    4 -> 24    -0.00128
#CIs=10 #CIs>0=5 #CIs<0=5

29   Singlet-?Sym   42.0714   29.47   0.0000   0.000
max(1)=    4 -> 13     0.49975
max(2)=    5 -> 14     0.49975
max(3)=    4 -> 16     0.00601
max(4)=    5 -> 17     0.00601
max(5)=    4 -> 27     0.00356
min(1)=    4 ->  9    -0.01412
min(2)=    5 ->  8    -0.01412
min(3)=    4 -> 24    -0.00099
min(4)=    5 -> 23    -0.00099
min(5)=    3 -> 22     0.00114
#CIs=12 #CIs>0=8 #CIs<0=4

30   Singlet-?Sym   42.0714   29.47   0.0000   0.000
max(1)=    5 -> 13     0.49975
max(2)=    4 ->  8     0.01412
max(3)=    5 -> 16     0.00601
max(4)=    5 -> 27     0.00356
max(5)=    4 -> 23     0.00099
min(1)=    4 -> 14    -0.49975
min(2)=    5 ->  9    -0.01412
min(3)=    4 -> 17    -0.00601
min(4)=    4 -> 26    -0.00356
min(5)=    2 -> 21    -0.00201
#CIs=12 #CIs>0=5 #CIs<0=7

31   Singlet-?Sym   43.4895   28.51   0.0018   0.000
max(1)=    5 -> 15     0.58358
max(2)=    4 -> 15     0.39205
max(3)=    3 -> 16     0.01818
max(4)=    3 -> 17     0.01221
max(5)=    5 -> 11     0.01217
min(1)=    3 -> 13    -0.05338
min(2)=    3 -> 14    -0.03586
min(3)=    5 -> 12    -0.01262
min(4)=    5 -> 10    -0.01083
min(5)=    4 -> 12    -0.00848
#CIs=46 #CIs>0=29 #CIs<0=17

32   Singlet-?Sym   43.4895   28.51   0.0018   0.000
max(1)=    4 -> 15     0.58358
max(2)=    3 -> 13     0.03586
max(3)=    3 -> 17     0.01818
max(4)=    4 -> 11     0.01217
```

```
        max(5)=    2 ->  8      0.01202
        min(1)=    5 -> 15     -0.39205
        min(2)=    3 -> 14     -0.05338
        min(3)=    4 -> 12     -0.01262
        min(4)=    3 -> 16     -0.01221
        min(5)=    4 -> 10     -0.01083
        #CIs=46 #CIs>0=24 #CIs<0=22

33    Singlet-SG   44.3180     27.98   0.0000   0.000
        max(1)=    2 -> 12      0.64836
        max(2)=    4 -> 14      0.17401
        max(3)=    5 -> 13      0.17401
        max(4)=    2 ->  7      0.06048
        max(5)=    2 -> 10      0.03196
        min(1)=    3 -> 15     -0.11051
        min(2)=    3 -> 18     -0.02780
        min(3)=    2 -> 11     -0.01301
        min(4)=    2 -> 19     -0.01013
        min(5)=    2 -> 18     -0.00901
        #CIs=34 #CIs>0=23 #CIs<0=11

34    Singlet-?Sym   46.0076     26.95   0.0141   0.000
        max(1)=    3 -> 14      0.70034
        max(2)=    3 -> 17      0.06914
        max(3)=    4 -> 15      0.06144
        max(4)=    2 ->  8      0.01662
        max(5)=    4 -> 21      0.00797
        min(1)=    3 ->  8     -0.02005
        min(2)=    3 -> 13     -0.00839
        min(3)=    2 -> 14     -0.00703
        min(4)=    4 -> 19     -0.00687
        min(5)=    4 -> 12     -0.00451
        #CIs=41 #CIs>0=23 #CIs<0=18

35    Singlet-?Sym   46.0076     26.95   0.0141   0.000
        max(1)=    3 -> 13      0.70034
        max(2)=    3 -> 16      0.06914
        max(3)=    5 -> 15      0.06144
        max(4)=    2 ->  9      0.01662
        max(5)=    3 -> 14      0.00839
        min(1)=    3 ->  9     -0.02005
        min(2)=    5 -> 21     -0.00797
        min(3)=    2 -> 13     -0.00703
        min(4)=    5 -> 19     -0.00687
        min(5)=    5 -> 12     -0.00451
        #CIs=41 #CIs>0=26 #CIs<0=15

36    Singlet-SG   46.0142     26.94   0.2948   0.000
        max(1)=    3 -> 15      0.49866
        max(2)=    2 -> 12      0.25054
        max(3)=    3 ->  7      0.03128
        max(4)=    2 -> 18      0.02582
        max(5)=    3 ->  6      0.01620
        min(1)=    4 -> 14     -0.29831
        min(2)=    5 -> 13     -0.29831
        min(3)=    3 -> 12     -0.05786
        min(4)=    2 -> 11     -0.04490
        min(5)=    2 -> 10     -0.04298
        #CIs=33 #CIs>0=14 #CIs<0=19

37    Singlet-?Sym   46.4005     26.72   0.0000   0.000
        max(1)=    4 -> 16      0.49993
        max(2)=    5 -> 17      0.49993
        max(3)=    4 -> 24      0.00303
        max(4)=    5 -> 23      0.00303
        max(5)=    4 -> 27      0.00115
        min(1)=    4 -> 13     -0.00614
        min(2)=    5 -> 14     -0.00614
        min(3)=    4 ->  9     -0.00441
        min(4)=    5 ->  8     -0.00441
        min(5)=    3 -> 22     -0.00054
        #CIs=12 #CIs>0=6 #CIs<0=6

38    Singlet-?Sym   46.4005     26.72   0.0000   0.000
        max(1)=    5 -> 16      0.49993
        max(2)=    4 -> 14      0.00614
        max(3)=    4 ->  8      0.00441
        max(4)=    5 -> 24      0.00303
        max(5)=    5 -> 27      0.00115
        min(1)=    4 -> 17     -0.49993
        min(2)=    5 -> 13     -0.00614
        min(3)=    5 ->  9     -0.00441
```

```
          min(4)=        4 -> 23        -0.00303
          min(5)=        4 -> 26        -0.00115
          #CIs=12 #CIs>0=7 #CIs<0=5

39        Singlet-?Sym   46.4344        26.70    0.0000    0.000
          max(1)=        4 -> 16         0.49976
          max(2)=        5 -> 14         0.01437
          max(3)=        5 ->  8         0.00477
          max(4)=        4 -> 24         0.00368
          max(5)=        4 -> 27         0.00135
          min(1)=        5 -> 17        -0.49976
          min(2)=        4 -> 13        -0.01437
          min(3)=        4 ->  9        -0.00477
          min(4)=        5 -> 23        -0.00368
          min(5)=        5 -> 26        -0.00135
          #CIs=10 #CIs>0=5 #CIs<0=5

40        Singlet-?Sym   47.7941        25.94    0.6017    0.000
          max(1)=        4 -> 17         0.45504
          max(2)=        5 -> 16         0.45504
          max(3)=        2 -> 12         0.03458
          max(4)=        3 ->  7         0.02273
          max(5)=        3 -> 18         0.02161
          min(1)=        3 -> 15        -0.18122
          min(2)=        4 -> 14        -0.14689
          min(3)=        5 -> 13        -0.14689
          min(4)=        3 -> 12        -0.05964
          min(5)=        3 -> 19        -0.05207
          #CIs=34 #CIs>0=18 #CIs<0=16

41        Singlet-?Sym   50.8965        24.36    0.3830    0.000
          max(1)=        3 -> 17         0.59677
          max(2)=        3 -> 16         0.36549
          max(3)=        4 -> 19         0.01624
          max(4)=        5 -> 19         0.00995
          max(5)=        4 -> 12         0.00823
          min(1)=        3 -> 14        -0.05625
          min(2)=        4 -> 18        -0.05329
          min(3)=        3 -> 13        -0.03445
          min(4)=        5 -> 18        -0.03264
          min(5)=        4 -> 15        -0.02262
          #CIs=48 #CIs>0=23 #CIs<0=25
```

5.2.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1         Singlet-?Sym   11.9145       104.06    0.0300    0.000
          max(1)=        5 ->  6         0.52373
          max(2)=        5 ->  7         0.30641
          max(3)=        5 -> 11         0.11227
          max(4)=        5 -> 10         0.06641
          max(5)=        4 -> 12         0.05477
          min(1)=        4 ->  6        -0.26468
          min(2)=        4 ->  7        -0.15485
          min(3)=        5 -> 12        -0.10838
          min(4)=        4 -> 11        -0.05674
          min(5)=        4 -> 10        -0.03356
          #CIs=44 #CIs>0=21 #CIs<0=23

2         Singlet-?Sym   11.9145       104.06    0.0300    0.000
          max(1)=        4 ->  6         0.52373
          max(2)=        4 ->  7         0.30641
          max(3)=        5 ->  6         0.26468
          max(4)=        5 ->  7         0.15485
          max(5)=        4 -> 11         0.11227
          min(1)=        4 -> 12        -0.10838
          min(2)=        5 -> 12        -0.05477
          min(3)=        4 -> 15        -0.02697
          min(4)=        5 -> 15        -0.01363
          min(5)=        4 -> 19        -0.01297
          #CIs=44 #CIs>0=29 #CIs<0=15

3         Singlet-SG   15.7111        78.91    0.1958    0.000
          max(1)=        3 ->  6         0.60306
          max(2)=        3 ->  7         0.26720
          max(3)=        4 ->  9         0.13778
```

```
        max(4)=      5 ->  8        0.13778
        max(5)=      3 -> 11        0.11576
        min(1)=      3 -> 12       -0.05736
        min(2)=      3 -> 15       -0.01597
        min(3)=      2 ->  7       -0.01411
        min(4)=      2 ->  6       -0.00498
        min(5)=      2 -> 19       -0.00458
        #CIs=30 #CIs>0=21 #CIs<0=9

4       Singlet-?Sym   15.7979       78.48    0.0261    0.000
        max(1)=      5 ->  7        0.55625
        max(2)=      4 ->  7        0.04469
        max(3)=      5 -> 20        0.00696
        max(4)=      3 -> 16        0.00371
        max(5)=      4 -> 22        0.00185
        min(1)=      5 ->  6       -0.33730
        min(2)=      5 -> 10       -0.20533
        min(3)=      5 -> 12       -0.17067
        min(4)=      5 -> 15       -0.04318
        min(5)=      4 ->  6       -0.02709
        #CIs=41 #CIs>0=17 #CIs<0=24

5       Singlet-?Sym   15.7979       78.48    0.0261    0.000
        max(1)=      4 ->  7        0.55625
        max(2)=      5 ->  6        0.02709
        max(3)=      5 -> 10        0.01650
        max(4)=      5 -> 12        0.01371
        max(5)=      4 -> 20        0.00696
        min(1)=      4 ->  6       -0.33730
        min(2)=      4 -> 10       -0.20533
        min(3)=      4 -> 12       -0.17067
        min(4)=      5 ->  7       -0.04469
        min(5)=      4 -> 15       -0.04318
        #CIs=41 #CIs>0=23 #CIs<0=18

6       Singlet-?Sym   17.2784       71.76    0.0000    0.000
        max(1)=      5 ->  9        0.49683
        max(2)=      5 -> 14        0.05371
        max(3)=      5 -> 17        0.01621
        max(4)=      5 -> 27        0.00329
        max(5)=      4 -> 24        0.00013
        min(1)=      4 ->  8       -0.49683
        min(2)=      4 -> 13       -0.05371
        min(3)=      4 -> 16       -0.01621
        min(4)=      4 -> 26       -0.00329
        min(5)=      5 -> 23       -0.00013
        #CIs=10 #CIs>0=5 #CIs<0=5

7       Singlet-?Sym   17.2989       71.67    0.0000    0.000
        max(1)=      4 ->  8        0.49736
        max(2)=      5 ->  9        0.49736
        max(3)=      4 -> 13        0.04884
        max(4)=      5 -> 14        0.04884
        max(5)=      4 -> 16        0.01529
        min(1)=      2 -> 22       -0.00166
        min(2)=      4 ->  9       -0.00070
        min(3)=      3 -> 22       -0.00027
        min(4)=      4 -> 24       -0.00019
        min(5)=      5 -> 23       -0.00019
        #CIs=14 #CIs>0=9 #CIs<0=5

8       Singlet-?Sym   17.2989       71.67    0.0000    0.000
        max(1)=      5 ->  8        0.49736
        max(2)=      5 -> 13        0.04884
        max(3)=      5 -> 16        0.01529
        max(4)=      5 -> 26        0.00282
        max(5)=      2 -> 21        0.00166
        min(1)=      4 ->  9       -0.49736
        min(2)=      4 -> 14       -0.04884
        min(3)=      4 -> 17       -0.01529
        min(4)=      4 -> 27       -0.00282
        min(5)=      4 ->  8       -0.00070
        #CIs=14 #CIs>0=7 #CIs<0=7

9       Singlet-?Sym   18.1234       68.41    0.0314    0.000
        max(1)=      5 -> 10        0.66525
        max(2)=      5 ->  7        0.12381
        max(3)=      5 -> 11        0.06687
        max(4)=      5 -> 18        0.03270
        max(5)=      5 -> 15        0.03232
        min(1)=      5 ->  6       -0.18092
        min(2)=      5 -> 12       -0.04824
```

```
         min(3)=        5 -> 21        -0.00408
         min(4)=        4 -> 10        -0.00379
         min(5)=        5 -> 19        -0.00280
         #CIs=31 #CIs>0=17 #CIs<0=14

10       Singlet-?Sym   18.1234          68.41    0.0314    0.000
         max(1)=        4 -> 10         0.66525
         max(2)=        4 ->  7         0.12381
         max(3)=        4 -> 11         0.06687
         max(4)=        4 -> 18         0.03270
         max(5)=        4 -> 15         0.03232
         min(1)=        4 ->  6        -0.18092
         min(2)=        4 -> 12        -0.04824
         min(3)=        4 -> 19        -0.00280
         min(4)=        4 -> 25        -0.00105
         min(5)=        5 ->  6        -0.00103
         #CIs=31 #CIs>0=22 #CIs<0=9

11       Singlet-?Sym   18.6919          66.33    0.0039    0.000
         max(1)=        4 ->  9         0.36939
         max(2)=        5 ->  8         0.36939
         max(3)=        3 ->  7         0.30592
         max(4)=        2 -> 12         0.01600
         max(5)=        4 -> 14         0.01134
         min(1)=        3 ->  6        -0.28933
         min(2)=        3 -> 10        -0.19081
         min(3)=        3 -> 12        -0.10075
         min(4)=        3 -> 15        -0.04466
         min(5)=        2 ->  7        -0.01668
         #CIs=31 #CIs>0=10 #CIs<0=21

12       Singlet-?Sym   20.7628          59.71    0.0525    0.000
         max(1)=        5 -> 11         0.53783
         max(2)=        3 ->  8         0.41629
         max(3)=        3 -> 13         0.04214
         max(4)=        5 -> 12         0.02634
         max(5)=        5 -> 18         0.02127
         min(1)=        4 -> 11        -0.10691
         min(2)=        3 ->  9        -0.08275
         min(3)=        5 ->  6        -0.07307
         min(4)=        5 -> 10        -0.07215
         min(5)=        5 ->  7        -0.06087
         #CIs=43 #CIs>0=21 #CIs<0=22

13       Singlet-?Sym   20.7628          59.71    0.0525    0.000
         max(1)=        4 -> 11         0.53783
         max(2)=        3 ->  9         0.41629
         max(3)=        5 -> 11         0.10691
         max(4)=        3 ->  8         0.08275
         max(5)=        3 -> 14         0.04214
         min(1)=        4 ->  6        -0.07307
         min(2)=        4 -> 10        -0.07215
         min(3)=        4 ->  7        -0.06087
         min(4)=        4 -> 15        -0.03193
         min(5)=        5 ->  6        -0.01453
         #CIs=43 #CIs>0=28 #CIs<0=15

14       Singlet-?Sym   20.9412          59.21    0.0439    0.000
         max(1)=        3 ->  9         0.47181
         max(2)=        5 -> 11         0.22691
         max(3)=        4 ->  6         0.04261
         max(4)=        3 -> 14         0.04137
         max(5)=        4 ->  7         0.03615
         min(1)=        4 -> 11        -0.35287
         min(2)=        3 ->  8        -0.30340
         min(3)=        5 ->  6        -0.02740
         min(4)=        3 -> 13        -0.02660
         min(5)=        5 ->  7        -0.02326
         #CIs=44 #CIs>0=23 #CIs<0=21

15       Singlet-?Sym   20.9412          59.21    0.0439    0.000
         max(1)=        3 ->  8         0.47181
         max(2)=        3 ->  9         0.30340
         max(3)=        5 ->  6         0.04261
         max(4)=        3 -> 13         0.04137
         max(5)=        5 ->  7         0.03615
         min(1)=        5 -> 11        -0.35287
         min(2)=        4 -> 11        -0.22691
         min(3)=        5 -> 12        -0.01739
         min(4)=        5 -> 18        -0.01524
         min(5)=        4 -> 12        -0.01119
         #CIs=44 #CIs>0=27 #CIs<0=17
```

```
16    Singlet-SG   21.1870   58.52   0.2080   0.000
      max(1)=   3 ->  7    0.52266
      max(2)=   3 -> 10    0.29800
      max(3)=   4 -> 14    0.03320
      max(4)=   5 -> 13    0.03320
      max(5)=   3 -> 15    0.02683
      min(1)=   4 ->  9   -0.21817
      min(2)=   5 ->  8   -0.21817
      min(3)=   3 ->  6   -0.18874
      min(4)=   3 -> 12   -0.04468
      min(5)=   2 -> 12   -0.01017
      #CIs=32 #CIs>0=20 #CIs<0=12

17    Singlet-SG   22.1522   55.97   0.0082   0.000
      max(1)=   3 -> 10    0.58476
      max(2)=   4 ->  9    0.19111
      max(3)=   5 ->  8    0.19111
      max(4)=   3 -> 11    0.13729
      max(5)=   2 -> 12    0.01959
      min(1)=   3 ->  7   -0.21739
      min(2)=   3 ->  6   -0.10687
      min(3)=   3 -> 12   -0.04714
      min(4)=   4 -> 14   -0.03978
      min(5)=   5 -> 13   -0.03978
      #CIs=30 #CIs>0=13 #CIs<0=17

18    Singlet-SG   24.3185   50.98   0.0292   0.000
      max(1)=   3 -> 11    0.68114
      max(2)=   3 -> 18    0.03006
      max(3)=   3 -> 12    0.02777
      max(4)=   4 -> 14    0.01805
      max(5)=   5 -> 13    0.01805
      min(1)=   3 -> 10   -0.14011
      min(2)=   3 ->  6   -0.07064
      min(3)=   4 ->  9   -0.05794
      min(4)=   5 ->  8   -0.05794
      min(5)=   3 ->  7   -0.02786
      #CIs=31 #CIs>0=18 #CIs<0=13

19    Singlet-?Sym   25.2680   49.07   0.0272   0.000
      max(1)=   5 -> 12    0.66461
      max(2)=   5 ->  7    0.21985
      max(3)=   4 -> 12    0.06741
      max(4)=   5 -> 19    0.04840
      max(5)=   5 -> 15    0.04231
      min(1)=   3 -> 16   -0.00948
      min(2)=   5 -> 20   -0.00686
      min(3)=   4 -> 22   -0.00629
      min(4)=   3 -> 24   -0.00431
      min(5)=   5 -> 11   -0.00397
      #CIs=43 #CIs>0=26 #CIs<0=17

20    Singlet-?Sym   25.2680   49.07   0.0272   0.000
      max(1)=   4 -> 12    0.66461
      max(2)=   4 ->  7    0.21985
      max(3)=   4 -> 19    0.04840
      max(4)=   4 -> 15    0.04231
      max(5)=   4 ->  6    0.01222
      min(1)=   5 -> 12   -0.06741
      min(2)=   5 ->  7   -0.02230
      min(3)=   3 -> 17   -0.00948
      min(4)=   4 -> 20   -0.00686
      min(5)=   4 -> 21   -0.00629
      #CIs=43 #CIs>0=20 #CIs<0=23

21    Singlet-SG   30.4963   40.66   0.2501   0.000
      max(1)=   3 -> 12    0.67977
      max(2)=   3 ->  7    0.09924
      max(3)=   4 ->  9    0.06274
      max(4)=   5 ->  8    0.06274
      max(5)=   3 -> 10    0.03869
      min(1)=   4 -> 14   -0.08800
      min(2)=   5 -> 13   -0.08800
      min(3)=   2 -> 10   -0.01804
      min(4)=   2 -> 18   -0.01759
      min(5)=   2 ->  6   -0.01605
      #CIs=32 #CIs>0=15 #CIs<0=17

22    Singlet-SG   38.2279   32.43   0.0194   0.000
      max(1)=   2 ->  6    0.60203
      max(2)=   2 ->  7    0.32218
```

```
        max(3)=        2 -> 11         0.10171
        max(4)=        2 -> 10         0.06264
        max(5)=        3 ->  7         0.01055
        min(1)=        2 -> 12        -0.09953
        min(2)=        4 -> 14        -0.05109
        min(3)=        5 -> 13        -0.05109
        min(4)=        4 -> 17        -0.03419
        min(5)=        5 -> 16        -0.03419
        #CIs=32 #CIs>0=14 #CIs<0=18

23      Singlet-SG   42.0036         29.52    0.0192    0.000
        max(1)=        2 ->  7         0.57611
        max(2)=        4 ->  9         0.01274
        max(3)=        5 ->  8         0.01274
        max(4)=        3 -> 10         0.01250
        max(5)=        3 ->  7         0.00911
        min(1)=        2 ->  6        -0.32206
        min(2)=        2 -> 10        -0.17300
        min(3)=        2 -> 12        -0.16783
        min(4)=        4 -> 17        -0.03956
        min(5)=        5 -> 16        -0.03956
        #CIs=32 #CIs>0=9 #CIs<0=23

24      Singlet-?Sym   43.5292         28.48    0.0000    0.000
        max(1)=        5 -> 14         0.49317
        max(2)=        5 -> 17         0.05902
        max(3)=        4 ->  8         0.05534
        max(4)=        5 -> 27         0.01491
        max(5)=        4 -> 24         0.00373
        min(1)=        4 -> 13        -0.49317
        min(2)=        4 -> 16        -0.05902
        min(3)=        5 ->  9        -0.05534
        min(4)=        4 -> 26        -0.01491
        min(5)=        5 -> 23        -0.00373
        #CIs=10 #CIs>0=5 #CIs<0=5

25      Singlet-?Sym   43.5482         28.47    0.0187    0.000
        max(1)=        2 ->  9         0.61668
        max(2)=        2 ->  8         0.33351
        max(3)=        2 -> 14         0.05847
        max(4)=        3 -> 17         0.03289
        max(5)=        2 -> 13         0.03162
        min(1)=        4 -> 15        -0.03279
        min(2)=        3 -> 14        -0.01831
        min(3)=        5 -> 15        -0.01774
        min(4)=        4 -> 11        -0.01409
        min(5)=        4 -> 18        -0.00994
        #CIs=46 #CIs>0=21 #CIs<0=25

26      Singlet-?Sym   43.5482         28.47    0.0187    0.000
        max(1)=        2 ->  8         0.61668
        max(2)=        2 -> 13         0.05847
        max(3)=        3 -> 16         0.03289
        max(4)=        4 -> 15         0.01774
        max(5)=        2 -> 16         0.01267
        min(1)=        2 ->  9        -0.33351
        min(2)=        5 -> 15        -0.03279
        min(3)=        2 -> 14        -0.03162
        min(4)=        3 -> 13        -0.01831
        min(5)=        3 -> 17        -0.01779
        #CIs=46 #CIs>0=22 #CIs<0=24

27      Singlet-?Sym   43.7371         28.35    0.0000    0.000
        max(1)=        4 -> 13         0.49404
        max(2)=        5 -> 14         0.49404
        max(3)=        4 -> 16         0.05619
        max(4)=        5 -> 17         0.05619
        max(5)=        4 -> 26         0.01376
        min(1)=        4 ->  8        -0.05033
        min(2)=        5 ->  9        -0.05033
        min(3)=        4 -> 14        -0.00494
        min(4)=        4 -> 24        -0.00365
        min(5)=        5 -> 23        -0.00365
        #CIs=20 #CIs>0=10 #CIs<0=10

28      Singlet-?Sym   43.7371         28.35    0.0000    0.000
        max(1)=        5 -> 13         0.49404
        max(2)=        5 -> 16         0.05619
        max(3)=        4 ->  9         0.05033
        max(4)=        5 -> 26         0.01376
        max(5)=        4 -> 23         0.00365
        min(1)=        4 -> 14        -0.49404
```

```
        min(2)=        4 -> 17        -0.05619
        min(3)=        5 ->  8        -0.05033
        min(4)=        4 -> 27        -0.01376
        min(5)=        4 -> 13        -0.00494
        #CIs=20 #CIs>0=9 #CIs<0=11

29      Singlet-SG   44.3839         27.93    0.0107    0.000
        max(1)=        2 -> 10         0.65724
        max(2)=        2 ->  7         0.09934
        max(3)=        2 -> 11         0.06909
        max(4)=        3 -> 15         0.03702
        max(5)=        2 -> 15         0.03142
        min(1)=        2 ->  6        -0.15705
        min(2)=        4 -> 14        -0.10467
        min(3)=        5 -> 13        -0.10467
        min(4)=        2 -> 12        -0.05324
        min(5)=        3 -> 10        -0.02027
        #CIs=32 #CIs>0=15 #CIs<0=17

30      Singlet-?Sym   45.2872         27.38    0.0015    0.000
        max(1)=        5 -> 15         0.69676
        max(2)=        5 -> 11         0.03763
        max(3)=        2 ->  8         0.03419
        max(4)=        5 -> 18         0.02796
        max(5)=        5 ->  7         0.02605
        min(1)=        5 -> 12        -0.05371
        min(2)=        3 -> 13        -0.05278
        min(3)=        5 -> 10        -0.04635
        min(4)=        4 -> 15        -0.02539
        min(5)=        5 -> 20        -0.01536
        #CIs=41 #CIs>0=20 #CIs<0=21

31      Singlet-?Sym   45.2872         27.38    0.0015    0.000
        max(1)=        4 -> 15         0.69676
        max(2)=        4 -> 11         0.03763
        max(3)=        2 ->  9         0.03419
        max(4)=        4 -> 18         0.02796
        max(5)=        4 ->  7         0.02605
        min(1)=        4 -> 12        -0.05371
        min(2)=        3 -> 14        -0.05278
        min(3)=        4 -> 10        -0.04635
```

```
        min(4)=        4 -> 20        -0.01536
        min(5)=        5 -> 12        -0.00196
        #CIs=41 #CIs>0=30 #CIs<0=11

32      Singlet-SG   46.8521         26.46    0.0025    0.000
        max(1)=        2 -> 11         0.68763
        max(2)=        2 -> 12         0.04870
        max(3)=        2 -> 18         0.02444
        max(4)=        3 -> 10         0.01646
        max(5)=        2 -> 20         0.00519
        min(1)=        2 -> 10        -0.09090
        min(2)=        2 ->  6        -0.08807
        min(3)=        3 -> 15        -0.04482
        min(4)=        2 ->  7        -0.03966
        min(5)=        2 -> 15        -0.03861
        #CIs=32 #CIs>0=9 #CIs<0=23

33      Singlet-?Sym   47.6919         26.00    0.0117    0.000
        max(1)=        3 -> 13         0.66569
        max(2)=        3 -> 14         0.19729
        max(3)=        3 -> 16         0.09241
        max(4)=        5 -> 15         0.04525
        max(5)=        3 -> 17         0.02739
        min(1)=        3 ->  8        -0.06443
        min(2)=        3 ->  9        -0.01909
        min(3)=        5 -> 21        -0.00675
        min(4)=        5 -> 12        -0.00616
        min(5)=        2 -> 24        -0.00571
        #CIs=43 #CIs>0=28 #CIs<0=15

34      Singlet-?Sym   47.6919         26.00    0.0117    0.000
        max(1)=        3 -> 14         0.66569
        max(2)=        3 -> 17         0.09241
        max(3)=        4 -> 15         0.04525
        max(4)=        2 -> 17         0.02205
        max(5)=        4 -> 18         0.02129
        min(1)=        3 -> 13        -0.19729
        min(2)=        3 ->  9        -0.06443
        min(3)=        3 -> 16        -0.02739
        min(4)=        5 -> 15        -0.01341
        min(5)=        2 -> 16        -0.00653
```

```
#CIs=43 #CIs>0=24 #CIs<0=19

35  Singlet-SG   47.7102   25.99   0.1516   0.000
    max(1)=   3 -> 15    0.52662
    max(2)=   3 -> 19    0.03383
    max(3)=   3 ->  7    0.03330
    max(4)=   3 -> 11    0.03280
    max(5)=   3 -> 18    0.02923
    min(1)=   4 -> 14   -0.28466
    min(2)=   5 -> 13   -0.28466
    min(3)=   2 -> 10   -0.12197
    min(4)=   4 -> 17   -0.09935
    min(5)=   5 -> 16   -0.09935
    #CIs=33 #CIs>0=14 #CIs<0=19

36  Singlet-?Sym   48.9219   25.34   0.0000   0.000
    max(1)=   4 -> 16    0.49637
    max(2)=   5 -> 17    0.49637
    max(3)=   4 -> 24    0.01447
    max(4)=   5 -> 23    0.01447
    max(5)=   4 -> 26    0.00335
    min(1)=   4 -> 13   -0.05743
    min(2)=   5 -> 14   -0.05743
    min(3)=   4 ->  8   -0.00963
    min(4)=   5 ->  9   -0.00963
    min(5)=   3 -> 22   -0.00082
    #CIs=12 #CIs>0=6 #CIs<0=6

37  Singlet-?Sym   48.9219   25.34   0.0000   0.000
    max(1)=   5 -> 16    0.49637
    max(2)=   4 -> 14    0.05743
    max(3)=   5 -> 24    0.01447
    max(4)=   4 ->  9    0.00963
    max(5)=   5 -> 26    0.00335
    min(1)=   4 -> 17   -0.49637
    min(2)=   5 -> 13   -0.05743
    min(3)=   4 -> 23   -0.01447
    min(4)=   5 ->  8   -0.00963
    min(5)=   4 -> 27   -0.00335
    #CIs=12 #CIs>0=7 #CIs<0=5

38  Singlet-?Sym   49.0153   25.29   0.0000   0.000
    max(1)=   5 -> 17    0.49598
    max(2)=   4 -> 13    0.06044
    max(3)=   5 -> 23    0.01545
    max(4)=   4 ->  8    0.00967
    max(5)=   5 -> 27    0.00377
    min(1)=   4 -> 16   -0.49598
    min(2)=   5 -> 14   -0.06044
    min(3)=   4 -> 24   -0.01545
    min(4)=   5 ->  9   -0.00967
    min(5)=   4 -> 26   -0.00377
    #CIs=10 #CIs>0=5 #CIs<0=5

39  Singlet-?Sym   50.6494   24.48   0.9291   0.000
    max(1)=   4 -> 17    0.40917
    max(2)=   5 -> 16    0.40917
    max(3)=   2 -> 12    0.28695
    max(4)=   2 ->  7    0.12930
    max(5)=   3 -> 19    0.05461
    min(1)=   4 -> 14   -0.16281
    min(2)=   5 -> 13   -0.16281
    min(3)=   3 -> 12   -0.06142
    min(4)=   2 -> 10   -0.04661
    min(5)=   2 -> 11   -0.02511
    #CIs=32 #CIs>0=17 #CIs<0=15

40  Singlet-SG   51.3252   24.16   0.0531   0.000
    max(1)=   2 -> 12    0.58096
    max(2)=   3 -> 15    0.18145
    max(3)=   2 ->  7    0.17257
    max(4)=   4 -> 14    0.10663
    max(5)=   5 -> 13    0.10663
    min(1)=   4 -> 17   -0.18363
    min(2)=   5 -> 16   -0.18363
    min(3)=   3 -> 19   -0.02596
    min(4)=   3 -> 18   -0.02488
    min(5)=   2 -> 18   -0.01056
    #CIs=32 #CIs>0=21 #CIs<0=11

41  Singlet-?Sym   53.2054   23.30   0.4536   0.000
    max(1)=   3 -> 16    0.54376
```

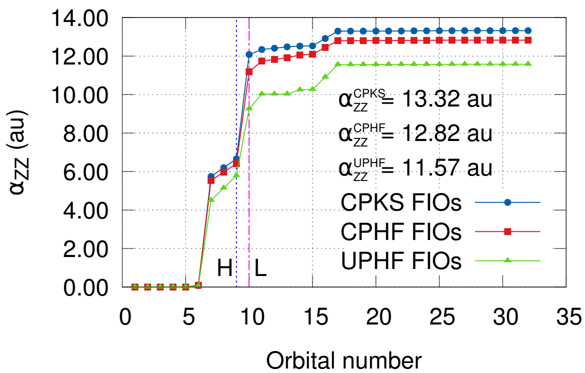
```
max(2)=         3 -> 17          0.43157
max(3)=         2 -> 13          0.03149
max(4)=         2 -> 14          0.02499
max(5)=         5 -> 21          0.01432
min(1)=         3 -> 13         -0.07121
min(2)=         3 -> 14         -0.05651
min(3)=         5 -> 18         -0.04060
min(4)=         2 ->  8         -0.03482
min(5)=         4 -> 18         -0.03222
#CIs=44 #CIs>0=19 #CIs<0=25
```

6 HCl

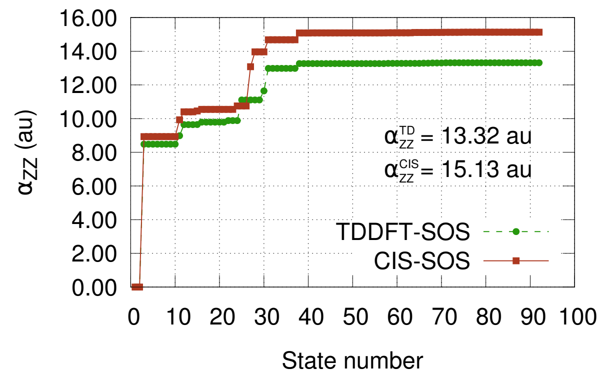
6.1 6-311G(d,p)

6.1.1 Plots

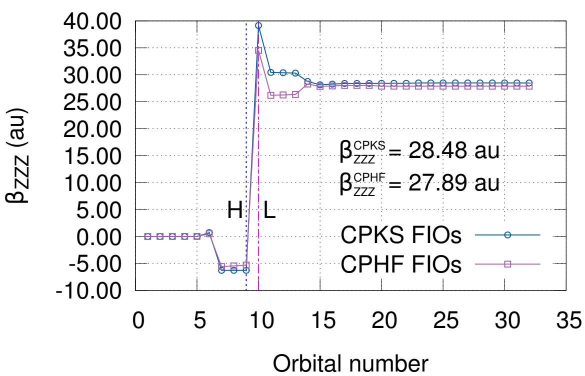
Figure S7: For HCl molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S7a and S7c) or states (SOS approaches, in Plots S7b and S7d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.01 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



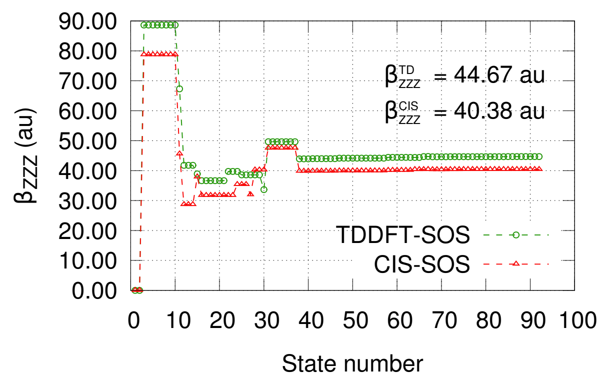
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

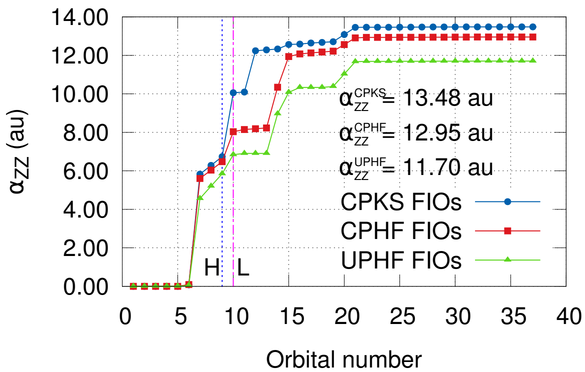


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

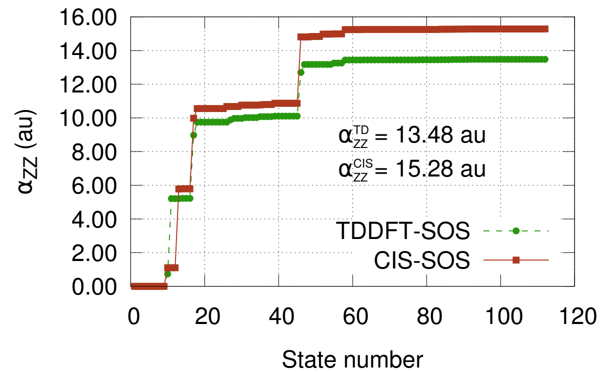
6.2 6-311++G(d,p)

6.2.1 Plots

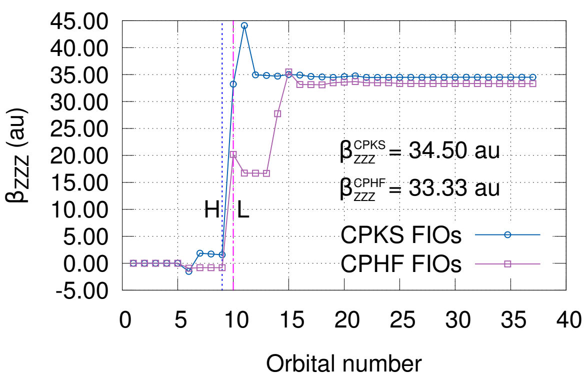
Figure S8: For HCl molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S8a and S8c) or states (SOS approaches, in Plots S8b and S8d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.06 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



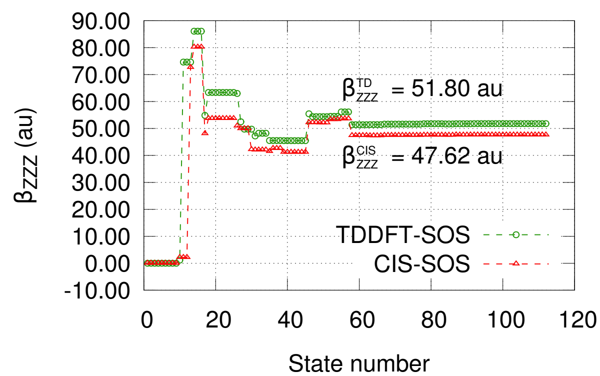
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



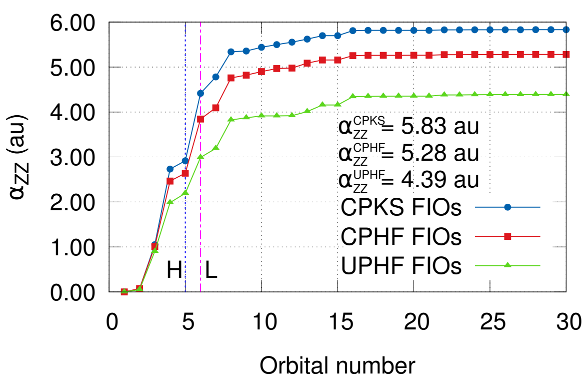
(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

7 H_2O

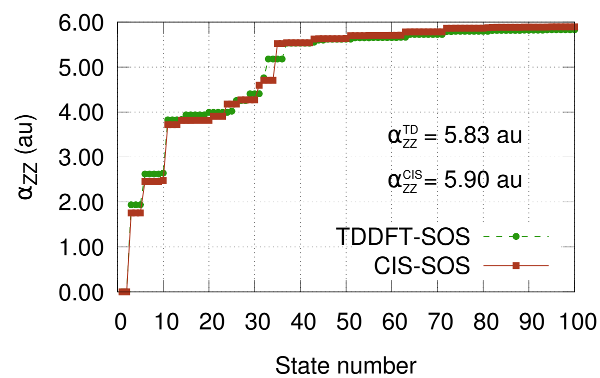
7.1 6-311G(d,p)

7.1.1 Plots

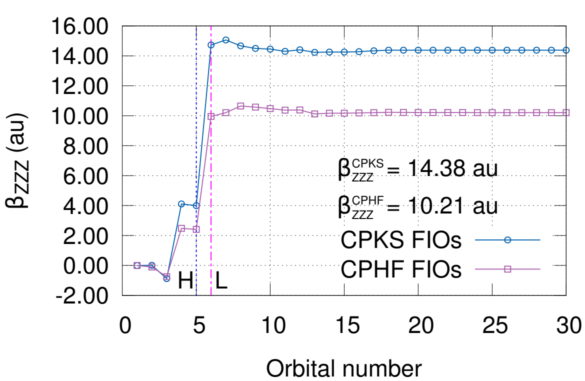
Figure S9: For H_2O molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S9a and S9c) or states (SOS approaches, in Plots S9b and S9d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.02 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



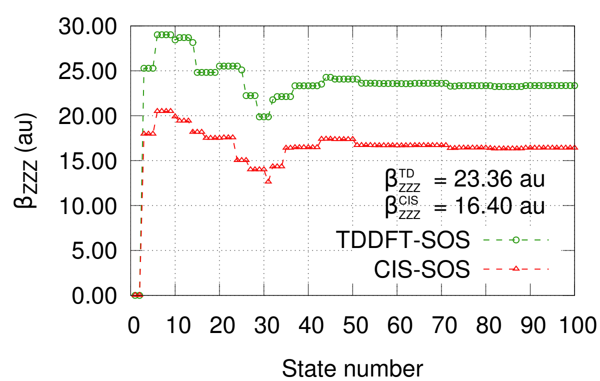
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

7.1.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-B1    7.4450        166.53    0.0265    0.000
          max(1)=        5 ->  6          0.70615
          max(2)=        5 -> 10          0.01679
          max(3)=        2 -> 11          0.00495
          max(4)=        5 -> 25          0.00396
          max(5)=        2 -> 22          0.00187
          min(1)=        5 ->  9         -0.03581
          min(2)=        5 -> 13         -0.00974
          min(3)=        3 -> 23         -0.00333
          min(4)=        5 -> 14         -0.00314
          min(5)=        4 -> 22         -0.00306
          #states=21 #states>0=12 #states<0=9

2        Singlet-A2    9.3956        131.96    0.0000    0.000
          max(1)=        5 ->  7          0.70282
          max(2)=        5 ->  8          0.07139
          max(3)=        5 -> 12          0.03137
          max(4)=        2 -> 15          0.00328
          max(5)=        5 -> 21          0.00186
          min(1)=        3 -> 11         -0.00287
          min(2)=        5 -> 18         -0.00189
          min(3)=        4 -> 15          0.00005
          min(4)=        3 -> 22          0.00023
          min(5)=        3 -> 27          0.00029
          #states=16 #states>0=14 #states<0=2

3        Singlet-A1    9.7608        127.02    0.0831    0.000
          max(1)=        4 ->  6          0.70407
          max(2)=        2 ->  6          0.01169
          max(3)=        2 -> 10          0.00301
          max(4)=        2 -> 19          0.00177
          max(5)=        2 -> 24          0.00141
          min(1)=        3 ->  7         -0.05111
          min(2)=        3 ->  8         -0.02584
          min(3)=        4 ->  9         -0.02436
          min(4)=        5 -> 11         -0.02154
          min(5)=        4 -> 13         -0.01319
          #states=32 #states>0=13 #states<0=19

4        Singlet-B2   11.7572        105.45    0.0493    0.000
          max(1)=        4 ->  7          0.70420
          max(2)=        4 -> 12          0.03096
          max(3)=        3 ->  9          0.02523
          max(4)=        4 ->  8          0.02167
          max(5)=        5 -> 15          0.00949
          min(1)=        3 ->  6         -0.04529
          min(2)=        2 ->  7         -0.01200
          min(3)=        2 ->  8         -0.00448
          min(4)=        3 -> 13         -0.00342
          min(5)=        3 -> 19         -0.00315
          #states=28 #states>0=15 #states<0=13

5        Singlet-B2   13.6671         90.72    0.2301    0.000
          max(1)=        3 ->  6          0.70410
          max(2)=        4 ->  7          0.04683
          max(3)=        3 -> 10          0.01555
          max(4)=        2 ->  8          0.00900
          max(5)=        2 -> 12          0.00728
          min(1)=        4 ->  8         -0.04276
          min(2)=        3 ->  9         -0.00787
          min(3)=        3 -> 13         -0.00786
          min(4)=        2 ->  7         -0.00427
          min(5)=        3 -> 20         -0.00268
          #states=28 #states>0=14 #states<0=14

6        Singlet-A1   16.4798         75.23    0.0836    0.000
          max(1)=        3 ->  7          0.69406
          max(2)=        4 ->  9          0.07754
          max(3)=        4 ->  6          0.05067
          max(4)=        2 ->  6          0.02311
          max(5)=        2 -> 10          0.00505
          min(1)=        5 -> 11         -0.08145
```

```
        min(2)=        4 -> 10        -0.05991
        min(3)=        2 -> 13        -0.01796
        min(4)=        2 ->  9        -0.01170
        min(5)=        4 -> 14        -0.00820
        #states=32 #states>0=13 #states<0=19

7       Singlet-A2   16.4823         75.22    0.0000    0.000
        max(1)=        5 ->  8         0.70335
        max(2)=        5 -> 17         0.00551
        max(3)=        2 -> 15         0.00402
        max(4)=        3 -> 16         0.00152
        max(5)=        4 -> 23         0.00146
        min(1)=        5 ->  7        -0.07148
        min(2)=        5 -> 18        -0.01292
        min(3)=        3 -> 11        -0.00279
        min(4)=        5 -> 21         0.00007
        min(5)=        5 -> 12         0.00027
        #states=16 #states>0=13 #states<0=3

8       Singlet-B1   18.2693         67.86    0.1098    0.000
        max(1)=        5 ->  9         0.70462
        max(2)=        5 ->  6         0.03664
        max(3)=        3 -> 15         0.01952
        max(4)=        5 -> 14         0.01511
        max(5)=        4 -> 22         0.00784
        min(1)=        5 -> 10        -0.03669
        min(2)=        4 -> 16        -0.01422
        min(3)=        2 -> 11        -0.01195
        min(4)=        4 -> 11        -0.00983
        min(5)=        5 -> 25        -0.00862
        #states=21 #states>0=10 #states<0=11

9       Singlet-B2   19.5924         63.28    0.1626    0.000
        max(1)=        4 ->  8         0.69023
        max(2)=        3 ->  9         0.13979
        max(3)=        3 ->  6         0.04498
        max(4)=        5 -> 15         0.02937
        max(5)=        3 -> 14         0.01653
        min(1)=        2 ->  7        -0.02841
        min(2)=        4 ->  7        -0.02381
        min(3)=        3 -> 13        -0.01183
        min(4)=        3 -> 19        -0.01154
        min(5)=        2 -> 12        -0.00636
        #states=29 #states>0=16 #states<0=13

10      Singlet-A1   20.1903         61.41    0.0037    0.000
        max(1)=        4 ->  9         0.69335
        max(2)=        3 ->  8         0.09678
        max(3)=        5 -> 11         0.04687
        max(4)=        4 ->  6         0.02446
        max(5)=        4 -> 10         0.02086
        min(1)=        3 ->  7        -0.07088
        min(2)=        2 ->  6        -0.03485
        min(3)=        4 -> 19        -0.00907
        min(4)=        3 -> 18        -0.00638
        min(5)=        2 -> 10        -0.00439
        #states=33 #states>0=18 #states<0=15

11      Singlet-A1   24.0479         51.56    0.3084    0.000
        max(1)=        3 ->  8         0.68778
        max(2)=        2 ->  6         0.02708
        max(3)=        4 -> 13         0.02354
        max(4)=        4 ->  6         0.01822
        max(5)=        5 -> 22         0.00870
        min(1)=        5 -> 11        -0.10529
        min(2)=        4 ->  9        -0.08643
        min(3)=        4 -> 10        -0.06761
        min(4)=        4 -> 14        -0.04153
        min(5)=        5 -> 16        -0.03280
        #states=34 #states>0=17 #states<0=17

12      Singlet-B2   25.3359         48.94    0.4482    0.000
        max(1)=        3 ->  9         0.68990
        max(2)=        2 ->  7         0.02512
        max(3)=        2 -> 18         0.01090
        max(4)=        4 -> 17         0.01027
        max(5)=        3 -> 19         0.00553
        min(1)=        4 ->  8        -0.13780
        min(2)=        5 -> 15        -0.05403
        min(3)=        3 -> 10        -0.03554
        min(4)=        3 -> 14        -0.02565
        min(5)=        4 ->  7        -0.01947
```

```
        #states=29 #states>0=11 #states<0=18

13      Singlet-B1   26.3281       47.09    0.0043    0.000
        max(1)=       5 -> 10       0.70251
        max(2)=       5 ->  9       0.03551
        max(3)=       5 -> 14       0.01435
        max(4)=       5 -> 13       0.01142
        max(5)=       3 -> 15       0.01069
        min(1)=       4 -> 11      -0.06565
        min(2)=       5 ->  6      -0.01448
        min(3)=       4 -> 16      -0.01123
        min(4)=       2 -> 11      -0.00628
        min(5)=       5 -> 20      -0.00469
        #states=21 #states>0=13 #states<0=8

14      Singlet-A1   26.8026       46.26    0.0023    0.000
        max(1)=       2 ->  6       0.55788
        max(2)=       5 -> 11       0.40820
        max(3)=       3 ->  8       0.02606
        max(4)=       3 ->  7       0.01543
        max(5)=       5 -> 22       0.00590
        min(1)=       4 -> 10      -0.14000
        min(2)=       2 ->  9      -0.03125
        min(3)=       4 -> 14      -0.01544
        min(4)=       2 -> 13      -0.01275
        min(5)=       4 -> 13      -0.01143
        #states=34 #states>0=19 #states<0=15

15      Singlet-A1   27.7605       44.66    0.0361    0.000
        max(1)=       4 -> 10       0.45111
        max(2)=       2 ->  6       0.38926
        max(3)=       3 -> 12       0.05436
        max(4)=       4 ->  9       0.03237
        max(5)=       2 ->  9       0.01766
        min(1)=       5 -> 11      -0.37344
        min(2)=       3 ->  8      -0.02482
        min(3)=       3 ->  7      -0.02093
        min(4)=       4 ->  6      -0.01708
        min(5)=       4 -> 14      -0.01236
        #states=33 #states>0=19 #states<0=14

16      Singlet-B1   28.5426       43.44    0.0004    0.000
        max(1)=       4 -> 11       0.70385
        max(2)=       5 -> 10       0.06474
        max(3)=       5 ->  9       0.01298
        max(4)=       3 -> 15       0.00754
        max(5)=       4 -> 22       0.00601
        min(1)=       2 -> 11      -0.00748
        min(2)=       5 -> 13      -0.00654
        min(3)=       4 -> 16      -0.00487
        min(4)=       5 -> 20      -0.00393
        min(5)=       5 -> 25      -0.00340
        #states=21 #states>0=12 #states<0=9

17      Singlet-A2   29.1471       42.54    0.0000    0.000
        max(1)=       5 -> 12       0.70607
        max(2)=       5 -> 26       0.00594
        max(3)=       5 -> 29       0.00309
        max(4)=       4 -> 15       0.00279
        max(5)=       5 -> 21       0.00213
        min(1)=       5 ->  7      -0.03122
        min(2)=       3 -> 11      -0.01859
        min(3)=       5 -> 18      -0.00901
        min(4)=       5 ->  8      -0.00368
        min(5)=       3 -> 16      -0.00133
        #states=15 #states>0=8 #states<0=7

18      Singlet-B2   29.1639       42.51    0.0249    0.000
        max(1)=       2 ->  7       0.70262
        max(2)=       2 ->  8       0.04474
        max(3)=       4 ->  8       0.03021
        max(4)=       5 -> 15       0.02864
        max(5)=       3 -> 10       0.02379
        min(1)=       3 -> 13      -0.03709
        min(2)=       3 ->  9      -0.01426
        min(3)=       3 -> 24      -0.00479
        min(4)=       3 -> 19      -0.00293
        min(5)=       4 -> 21      -0.00257
        #states=29 #states>0=19 #states<0=10

19      Singlet-B2   31.2720       39.65    0.0552    0.000
        max(1)=       4 -> 12       0.70364
```

```
        max(2)=       3 ->  9        0.00621
        max(3)=       4 -> 26        0.00557
        max(4)=       4 -> 21        0.00257
        max(5)=       4 -> 29        0.00248
        min(1)=       3 -> 10       -0.05643
        min(2)=       4 ->  7       -0.03140
        min(3)=       2 ->  8       -0.02077
        min(4)=       4 -> 18       -0.00909
        min(5)=       3 -> 13       -0.00785
        #states=29 #states>0=12 #states<0=17

20      Singlet-A1   32.2158        38.49    0.0254    0.000
        max(1)=       4 -> 10        0.44285
        max(2)=       5 -> 11        0.31756
        max(3)=       3 ->  8        0.08835
        max(4)=       3 ->  7        0.08007
        max(5)=       3 -> 18        0.01510
        min(1)=       3 -> 12       -0.38580
        min(2)=       2 ->  6       -0.14060
        min(3)=       2 ->  9       -0.10601
        min(4)=       4 -> 13       -0.07796
        min(5)=       2 -> 13       -0.04564
        #states=34 #states>0=13 #states<0=21

21      Singlet-A2   32.5557        38.08    0.0000    0.000
        max(1)=       3 -> 11        0.70682
        max(2)=       5 -> 12        0.01868
        max(3)=       3 -> 16        0.00515
        max(4)=       3 -> 27        0.00474
        max(5)=       2 -> 15        0.00408
        min(1)=       5 -> 21       -0.00040
        min(2)=       2 -> 23       -0.00013
        min(3)=       5 -> 17       -0.00008
        min(4)=       5 -> 26        0.00015
        min(5)=       5 -> 29        0.00021
        #states=16 #states>0=13 #states<0=3

22      Singlet-B2   32.6057        38.03    0.0715    0.000
        max(1)=       3 -> 10        0.70183
        max(2)=       4 -> 12        0.05425
        max(3)=       3 ->  9        0.03306
        max(4)=       3 -> 19        0.00651
        max(5)=       2 -> 12        0.00643
        min(1)=       2 ->  8       -0.04556
        min(2)=       5 -> 15       -0.02289
        min(3)=       2 ->  7       -0.01922
        min(4)=       3 ->  6       -0.01537
        min(5)=       4 ->  8       -0.00929
        #states=28 #states>0=13 #states<0=15

23      Singlet-B1   35.3546        35.07    0.2780    0.000
        max(1)=       5 -> 13        0.70377
        max(2)=       4 -> 16        0.01793
        max(3)=       5 ->  6        0.00925
        max(4)=       4 -> 11        0.00800
        max(5)=       5 -> 20        0.00343
        min(1)=       5 -> 14       -0.05491
        min(2)=       3 -> 15       -0.02904
        min(3)=       2 -> 11       -0.01841
        min(4)=       5 -> 10       -0.00858
        min(5)=       2 -> 16       -0.00635
        #states=20 #states>0=9 #states<0=11

24      Singlet-B2   36.4613        34.00    0.0132    0.000
        max(1)=       2 ->  8        0.70193
        max(2)=       3 -> 10        0.04063
        max(3)=       4 -> 12        0.02309
        max(4)=       3 ->  9        0.01872
        max(5)=       3 -> 19        0.01043
        min(1)=       2 ->  7       -0.04660
        min(2)=       3 -> 13       -0.04061
        min(3)=       5 -> 15       -0.02747
        min(4)=       3 ->  6       -0.01090
        min(5)=       2 -> 12       -0.00575
        #states=29 #states>0=16 #states<0=13

25      Singlet-A1   36.7454        33.74    0.0155    0.000
        max(1)=       4 -> 13        0.45863
        max(2)=       2 ->  9        0.37355
        max(3)=       2 ->  6        0.05708
        max(4)=       4 -> 14        0.04690
        max(5)=       2 -> 13        0.02161
```

```
        min(1)=      3 -> 12       -0.36537
        min(2)=      4 -> 10       -0.07242
        min(3)=      5 -> 11       -0.06040
        min(4)=      3 ->  8       -0.03184
        min(5)=      2 -> 10       -0.02044
        #states=34 #states>0=18 #states<0=16

26   Singlet-A1   37.7280     32.86    0.1525    0.000
        max(1)=      2 ->  9        0.51484
        max(2)=      3 ->  8        0.01380
        max(3)=      2 ->  6        0.01327
        max(4)=      2 -> 10        0.01316
        max(5)=      3 -> 18        0.00515
        min(1)=      4 -> 13       -0.47829
        min(2)=      3 -> 12       -0.07042
        min(3)=      4 -> 10       -0.02153
        min(4)=      5 -> 16       -0.01458
        min(5)=      4 ->  9       -0.00910
        #states=34 #states>0=16 #states<0=18

27   Singlet-B1   39.9174     31.06    0.1543    0.000
        max(1)=      5 -> 14        0.70186
        max(2)=      5 -> 13        0.05138
        max(3)=      4 -> 16        0.03444
        max(4)=      5 -> 20        0.00563
        max(5)=      5 ->  6        0.00309
        min(1)=      3 -> 15       -0.05544
        min(2)=      5 ->  9       -0.01411
        min(3)=      5 -> 10       -0.01302
        min(4)=      2 -> 16       -0.00800
        min(5)=      5 -> 24       -0.00635
        #states=21 #states>0=10 #states<0=11

28   Singlet-B2   41.0057     30.24    0.1354    0.000
        max(1)=      3 -> 13        0.50218
        max(2)=      5 -> 15        0.49075
        max(3)=      2 ->  8        0.04624
        max(4)=      3 ->  9        0.03435
        max(5)=      3 -> 10        0.01399
        min(1)=      3 -> 14       -0.05363
        min(2)=      4 ->  8       -0.01843
        min(3)=      4 -> 18       -0.00602
        min(4)=      4 ->  7       -0.00452
        min(5)=      2 -> 12       -0.00221
        #states=27 #states>0=18 #states<0=9

29   Singlet-A1   41.5677     29.83    0.1166    0.000
        max(1)=      3 -> 12        0.43955
        max(2)=      2 ->  9        0.28204
        max(3)=      5 -> 11        0.24599
        max(4)=      4 -> 10        0.23623
        max(5)=      4 -> 13        0.22929
        min(1)=      2 -> 13       -0.15527
        min(2)=      4 -> 14       -0.12715
        min(3)=      2 ->  6       -0.10825
        min(4)=      4 ->  9       -0.04234
        min(5)=      2 -> 14       -0.03711
        #states=34 #states>0=16 #states<0=18

30   Singlet-B2   41.7356     29.71    0.2993    0.000
        max(1)=      3 -> 13        0.49106
        max(2)=      3 -> 14        0.11443
        max(3)=      2 ->  7        0.04167
        max(4)=      4 -> 18        0.03530
        max(5)=      4 ->  8        0.03363
        min(1)=      5 -> 15       -0.48759
        min(2)=      2 -> 12       -0.03995
        min(3)=      3 ->  9       -0.02908
        min(4)=      3 -> 19       -0.02258
        min(5)=      4 -> 17       -0.01930
        #states=29 #states>0=15 #states<0=14

31   Singlet-A2   42.5653     29.13    0.0000    0.000
        max(1)=      4 -> 15        0.70702
        max(2)=      4 -> 23        0.00788
        max(3)=      3 -> 16        0.00465
        max(4)=      5 -> 21        0.00433
        max(5)=      2 -> 23        0.00263
        min(1)=      2 -> 15       -0.00344
        min(2)=      5 -> 12       -0.00287
        min(3)=      3 -> 11       -0.00231
        min(4)=      5 -> 18       -0.00197
```

```
min(5)=        3 -> 22       -0.00088
#states=16 #states>0=8 #states<0=8

32      Singlet-A1   43.0050         28.83    0.2949    0.000
min(5)=        3 -> 22       -0.00088
max(1)=        4 -> 14        0.65511
max(2)=        3 -> 12        0.07714
max(3)=        4 -> 10        0.06582
max(4)=        5 -> 11        0.05746
max(5)=        3 ->  8        0.04229
min(1)=        5 -> 16       -0.21775
min(2)=        2 -> 10       -0.05573
min(3)=        2 -> 13       -0.05376
min(4)=        4 ->  9       -0.02003
min(5)=        3 -> 17       -0.01494
#states=34 #states>0=19 #states<0=15

33      Singlet-A1   46.1901         26.84    0.4031    0.000
max(1)=        2 -> 10        0.61488
max(2)=        2 -> 13        0.05756
max(3)=        4 ->  9        0.01346
max(4)=        2 -> 14        0.01293
max(5)=        4 -> 13        0.01091
min(1)=        5 -> 16       -0.33361
min(2)=        3 -> 12       -0.04863
min(3)=        4 -> 14       -0.03980
min(4)=        4 -> 10       -0.03068
min(5)=        5 -> 11       -0.02834
#states=34 #states>0=20 #states<0=14

34      Singlet-B1   46.3378         26.76    0.3301    0.000
max(1)=        2 -> 11        0.68852
max(2)=        3 -> 15        0.14998
max(3)=        5 -> 13        0.02656
max(4)=        5 -> 19        0.01564
max(5)=        5 -> 14        0.01143
min(1)=        4 -> 16       -0.04529
min(2)=        5 -> 20       -0.01266
min(3)=        5 -> 25       -0.00640
min(4)=        5 ->  6       -0.00352
min(5)=        5 -> 24       -0.00331
#states=21 #states>0=15 #states<0=6

35      Singlet-B2   46.6248         26.59    0.4669    0.000
max(1)=        3 -> 14        0.69181
max(2)=        5 -> 15        0.11017
max(3)=        2 -> 12        0.06058
max(4)=        3 ->  9        0.02927
max(5)=        3 -> 19        0.02577
min(1)=        3 -> 13       -0.03756
min(2)=        4 -> 18       -0.03331
min(3)=        4 ->  8       -0.02828
min(4)=        2 ->  7       -0.01462
min(5)=        5 -> 23       -0.01454
#states=29 #states>0=14 #states<0=15

36      Singlet-B1   47.1570         26.29    0.0698    0.000
max(1)=        3 -> 15        0.58822
max(2)=        4 -> 16        0.37646
max(3)=        5 -> 14        0.02667
max(4)=        5 -> 13        0.01396
max(5)=        2 -> 22        0.00588
min(1)=        2 -> 11       -0.10346
min(2)=        5 -> 19       -0.02000
min(3)=        5 ->  9       -0.01160
min(4)=        4 -> 22       -0.01026
min(5)=        5 -> 10       -0.00410
#states=20 #states>0=11 #states<0=9
```

7.1.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1       Singlet-B1    9.1435        135.60    0.0334    0.000
max(1)=        5 ->  6        0.69518
max(2)=        5 -> 10        0.05494
max(3)=        5 -> 25        0.00722
```

```
        max(4)=        5 -> 19          0.00552
        max(5)=        5 -> 24          0.00356
        min(1)=        5 ->  9         -0.10597
        min(2)=        5 -> 13         -0.04558
        min(3)=        5 -> 14         -0.01226
        min(4)=        5 -> 20         -0.00711
        min(5)=        4 -> 22         -0.00503
        #states=20 #states>0=9 #states<0=11

2       Singlet-A2   10.9976        112.74    0.0000    0.000
        max(1)=        5 ->  7          0.67657
        max(2)=        5 ->  8          0.17849
        max(3)=        5 -> 12          0.09969
        max(4)=        5 -> 21          0.00613
        max(5)=        5 -> 29          0.00465
        min(1)=        5 -> 18         -0.01808
        min(2)=        3 -> 11         -0.00342
        min(3)=        2 -> 23         -0.00233
        min(4)=        4 -> 15         -0.00054
        min(5)=        4 -> 23         -0.00027
        #states=16 #states>0=10 #states<0=6

3       Singlet-A1   11.6285        106.62    0.1068    0.000
        max(1)=        4 ->  6          0.69628
        max(2)=        4 -> 10          0.01680
        max(3)=        4 -> 19          0.00583
        max(4)=        3 -> 18          0.00353
        max(5)=        2 -> 19          0.00296
        min(1)=        4 ->  9         -0.08738
        min(2)=        4 -> 13         -0.04633
        min(3)=        3 ->  7         -0.04312
        min(4)=        5 -> 11         -0.03734
        min(5)=        3 ->  8         -0.03001
        #states=31 #states>0=10 #states<0=21

4       Singlet-B2   13.4601         92.11    0.0774    0.000
        max(1)=        4 ->  7          0.69007
        max(2)=        4 ->  8          0.11713
        max(3)=        4 -> 12          0.09317
        max(4)=        3 ->  9          0.02572
        max(5)=        5 -> 15          0.01164
        min(1)=        2 ->  7         -0.01435
        min(2)=        4 -> 18         -0.00906
        min(3)=        3 -> 19         -0.00604
        min(4)=        2 ->  8         -0.00597
        min(5)=        2 -> 18         -0.00540
        #states=28 #states>0=17 #states<0=11

5       Singlet-B2   15.1582         81.79    0.2558    0.000
        max(1)=        3 ->  6          0.69771
        max(2)=        3 -> 10          0.05047
        max(3)=        4 ->  7          0.00692
        max(4)=        3 -> 19          0.00438
        max(5)=        5 -> 15          0.00434
        min(1)=        3 ->  9         -0.08306
        min(2)=        4 ->  8         -0.03719
        min(3)=        3 -> 13         -0.03667
        min(4)=        2 ->  7         -0.02717
        min(5)=        3 -> 20         -0.00886
        #states=27 #states>0=14 #states<0=13

6       Singlet-A1   18.1618         68.27    0.1038    0.000
        max(1)=        3 ->  7          0.68186
        max(2)=        3 ->  8          0.08424
        max(3)=        4 ->  9          0.06440
        max(4)=        4 ->  6          0.04995
        max(5)=        3 -> 12          0.04112
        min(1)=        5 -> 11         -0.11005
        min(2)=        4 -> 10         -0.08070
        min(3)=        2 -> 13         -0.02116
        min(4)=        4 -> 14         -0.01121
        min(5)=        4 -> 13         -0.00981
        #states=32 #states>0=14 #states<0=18

7       Singlet-A2   18.3499         67.57    0.0000    0.000
        max(1)=        5 ->  8          0.68094
        max(2)=        5 -> 12          0.02015
        max(3)=        5 -> 17          0.01640
        max(4)=        2 -> 15          0.00592
        max(5)=        5 -> 29          0.00344
        min(1)=        5 ->  7         -0.18393
        min(2)=        5 -> 18         -0.04149
```

```
        min(3)=      3 -> 11      -0.00457
        min(4)=      2 -> 23      -0.00179
        min(5)=      5 -> 26      -0.00082
        #states=15 #states>0=10 #states<0=5

8    Singlet-B1   20.2860      61.12   0.1541   0.000
        max(1)=      5 ->  9       0.68891
        max(2)=      5 ->  6       0.11412
        max(3)=      5 -> 14       0.02534
        max(4)=      3 -> 15       0.02465
        max(5)=      4 -> 22       0.01113
        min(1)=      5 -> 10      -0.09559
        min(2)=      5 -> 19      -0.02832
        min(3)=      4 -> 16      -0.01626
        min(4)=      2 -> 11      -0.01490
        min(5)=      5 -> 25      -0.01030
        #states=21 #states>0=12 #states<0=9

9    Singlet-B2   21.5272      57.59   0.2114   0.000
        max(1)=      4 ->  8       0.67789
        max(2)=      3 ->  9       0.13310
        max(3)=      3 ->  6       0.05162
        max(4)=      5 -> 15       0.03412
        max(5)=      3 -> 14       0.02330
        min(1)=      4 ->  7      -0.12491
        min(2)=      4 -> 18      -0.02601
        min(3)=      2 ->  7      -0.02316
        min(4)=      3 -> 13      -0.01782
        min(5)=      3 -> 19      -0.01612
        #states=28 #states>0=16 #states<0=12

10   Singlet-A1   22.3378      55.50   0.0065   0.000
        max(1)=      4 ->  9       0.68979
        max(2)=      4 ->  6       0.09055
        max(3)=      5 -> 11       0.07695
        max(4)=      3 ->  8       0.05313
        max(5)=      4 -> 14       0.01915
        min(1)=      3 ->  7      -0.06763
        min(2)=      4 -> 19      -0.03185
        min(3)=      2 ->  6      -0.02035
        min(4)=      4 -> 10      -0.00954
        min(5)=      3 -> 18      -0.00817
        #states=32 #states>0=19 #states<0=13

11   Singlet-A1   25.6809      48.28   0.3664   0.000
        max(1)=      3 ->  8       0.67337
        max(2)=      2 ->  9       0.03073
        max(3)=      3 -> 12       0.02558
        max(4)=      4 -> 13       0.01546
        max(5)=      4 ->  6       0.01047
        min(1)=      5 -> 11      -0.14822
        min(2)=      3 ->  7      -0.11290
        min(3)=      4 -> 10      -0.05653
        min(4)=      4 ->  9      -0.04766
        min(5)=      4 -> 14      -0.04454
        #states=31 #states>0=14 #states<0=17

12   Singlet-B2   27.0060      45.91   0.5800   0.000
        max(1)=      3 ->  9       0.67812
        max(2)=      3 ->  6       0.08248
        max(3)=      2 ->  7       0.04611
        max(4)=      2 ->  8       0.03192
        max(5)=      2 -> 12       0.02255
        min(1)=      4 ->  8      -0.13319
        min(2)=      3 -> 10      -0.08283
        min(3)=      5 -> 15      -0.05735
        min(4)=      4 -> 12      -0.02643
        min(5)=      3 -> 19      -0.01851
        #states=27 #states>0=12 #states<0=15

13   Singlet-B1   27.2615      45.48   0.0033   0.000
        max(1)=      5 -> 10       0.69414
        max(2)=      5 ->  9       0.10012
        max(3)=      5 -> 14       0.03855
        max(4)=      5 -> 13       0.03081
        max(5)=      5 -> 19       0.01715
        min(1)=      4 -> 11      -0.05686
        min(2)=      5 ->  6      -0.03750
        min(3)=      4 -> 16      -0.01272
        min(4)=      5 -> 20      -0.00870
        min(5)=      2 -> 11      -0.00357
        #states=21 #states>0=13 #states<0=8
```

14 Singlet-A1 28.2577 43.88 0.0348 0.000

max(1)= 5 -> 11 0.52721

max(2)= 3 -> 8 0.07978

max(3)= 2 -> 6 0.05201

max(4)= 4 -> 6 0.03192

max(5)= 3 -> 7 0.02822

min(1)= 4 -> 10 -0.44913

min(2)= 4 -> 9 -0.07043

min(3)= 3 -> 12 -0.04264

min(4)= 2 -> 9 -0.03126

min(5)= 4 -> 13 -0.02101

#states=32 #states>0=14 #states<0=18

15 Singlet-B1 29.3023 42.31 0.0020 0.000

max(1)= 4 -> 11 0.70379

max(2)= 5 -> 10 0.05384

max(3)= 5 -> 13 0.02516

max(4)= 4 -> 27 0.01977

max(5)= 5 -> 9 0.01682

min(1)= 2 -> 22 -0.00480

min(2)= 2 -> 16 -0.00368

min(3)= 5 -> 20 -0.00182

min(4)= 5 -> 25 -0.00170

min(5)= 5 -> 24 -0.00143

#states=20 #states>0=15 #states<0=5

16 Singlet-A2 30.8203 40.23 0.0000 0.000

max(1)= 5 -> 12 0.69802

max(2)= 5 -> 26 0.02110

max(3)= 5 -> 29 0.01102

max(4)= 5 -> 21 0.01074

max(5)= 2 -> 15 0.00323

min(1)= 5 -> 7 -0.09158

min(2)= 5 -> 8 -0.04745

min(3)= 5 -> 18 -0.03045

min(4)= 3 -> 11 -0.02195

min(5)= 2 -> 23 -0.00255

#states=16 #states>0=6 #states<0=10

17 Singlet-A1 32.1386 38.58 0.0020 0.000

max(1)= 2 -> 6 0.60273

max(2)= 4 -> 10 0.28259

max(3)= 5 -> 11 0.15393

max(4)= 3 -> 8 0.07180

max(5)= 3 -> 7 0.05580

min(1)= 2 -> 9 -0.10806

min(2)= 3 -> 12 -0.08806

min(3)= 2 -> 13 -0.04101

min(4)= 4 -> 14 -0.02765

min(5)= 5 -> 16 -0.01880

#states=33 #states>0=21 #states<0=12

18 Singlet-B2 32.9175 37.67 0.0662 0.000

max(1)= 4 -> 12 0.69403

max(2)= 2 -> 7 0.07541

max(3)= 2 -> 12 0.02083

max(4)= 4 -> 26 0.01833

max(5)= 4 -> 29 0.01056

min(1)= 4 -> 7 -0.08737

min(2)= 4 -> 8 -0.03599

min(3)= 3 -> 10 -0.03290

min(4)= 4 -> 18 -0.03150

min(5)= 2 -> 8 -0.01558

#states=25 #states>0=12 #states<0=13

19 Singlet-A2 33.7332 36.75 0.0000 0.000

max(1)= 3 -> 11 0.70597

max(2)= 3 -> 16 0.02493

max(3)= 5 -> 12 0.02242

max(4)= 3 -> 27 0.01668

max(5)= 2 -> 15 0.01003

min(1)= 2 -> 23 -0.00610

min(2)= 4 -> 15 -0.00465

min(3)= 5 -> 7 -0.00081

min(4)= 5 -> 29 -0.00013

min(5)= 5 -> 26 -0.00011

#states=16 #states>0=11 #states<0=5

20 Singlet-B2 33.9624 36.51 0.0927 0.000

max(1)= 3 -> 10 0.65878

max(2)= 2 -> 7 0.23906

max(3)= 3 -> 9 0.06643
max(4)= 2 -> 12 0.04028
max(5)= 3 -> 14 0.02538
min(1)= 3 -> 6 -0.03125
min(2)= 3 -> 13 -0.01754
min(3)= 5 -> 15 -0.00884
min(4)= 3 -> 20 -0.00816
min(5)= 2 -> 18 -0.00727
#states=28 #states>0=16 #states<0=12

21 Singlet-A1 34.4238 36.02 0.0476 0.000
max(1)= 3 -> 12 0.42831
max(2)= 2 -> 6 0.32214
max(3)= 2 -> 9 0.04064
max(4)= 4 -> 9 0.02431
max(5)= 4 -> 14 0.02087
min(1)= 4 -> 10 -0.34337
min(2)= 5 -> 11 -0.25990
min(3)= 3 -> 8 -0.11649
min(4)= 3 -> 7 -0.09233
min(5)= 3 -> 18 -0.02545
#states=33 #states>0=20 #states<0=13

22 Singlet-B2 34.5364 35.90 0.0024 0.000
max(1)= 2 -> 7 0.63055
max(2)= 2 -> 8 0.16759
max(3)= 2 -> 12 0.06511
max(4)= 5 -> 15 0.06019
max(5)= 4 -> 8 0.03692
min(1)= 3 -> 10 -0.22620
min(2)= 3 -> 9 -0.07412
min(3)= 4 -> 12 -0.07274
min(4)= 3 -> 13 -0.03724
min(5)= 2 -> 18 -0.00980
#states=28 #states>0=16 #states<0=12

23 Singlet-B1 36.5430 33.93 0.3422 0.000
max(1)= 5 -> 13 0.70240
max(2)= 5 -> 6 0.04567
max(3)= 2 -> 11 0.03321
max(4)= 5 -> 20 0.02217
max(5)= 4 -> 16 0.01432
min(1)= 3 -> 15 -0.02827
min(2)= 5 -> 10 -0.02638
min(3)= 4 -> 11 -0.02333
min(4)= 5 -> 9 -0.01633
min(5)= 5 -> 25 -0.01609
#states=21 #states>0=10 #states<0=11

24 Singlet-A1 38.6227 32.10 0.1823 0.000
max(1)= 4 -> 13 0.68243
max(2)= 4 -> 14 0.06061
max(3)= 4 -> 6 0.04244
max(4)= 2 -> 6 0.03135
max(5)= 2 -> 10 0.03108
min(1)= 3 -> 12 -0.13386
min(2)= 4 -> 10 -0.07313
min(3)= 5 -> 11 -0.04533
min(4)= 3 -> 8 -0.02165
min(5)= 4 -> 25 -0.01294
#states=33 #states>0=22 #states<0=11

25 Singlet-B2 41.7617 29.69 0.0071 0.000
max(1)= 2 -> 8 0.68256
max(2)= 3 -> 10 0.04830
max(3)= 4 -> 12 0.03401
max(4)= 2 -> 12 0.02331
max(5)= 5 -> 15 0.01912
min(1)= 2 -> 7 -0.16609
min(2)= 2 -> 18 -0.03097
min(3)= 4 -> 17 -0.01476
min(4)= 3 -> 6 -0.01196
min(5)= 3 -> 9 -0.01089
#states=28 #states>0=16 #states<0=12

26 Singlet-B1 42.0235 29.50 0.1561 0.000
max(1)= 5 -> 14 0.70071
max(2)= 2 -> 11 0.03494
max(3)= 4 -> 16 0.03492
max(4)= 5 -> 20 0.01183
max(5)= 5 -> 6 0.01042
min(1)= 3 -> 15 -0.05856

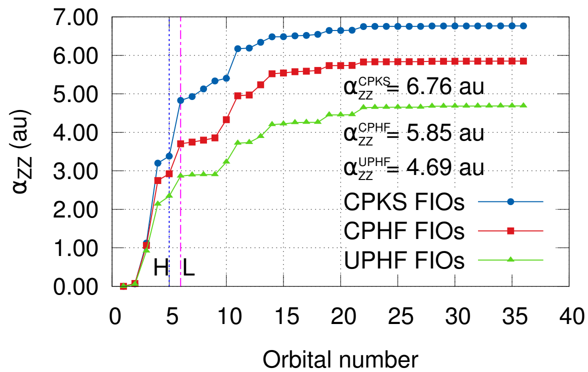
```
        min(2)=        5 -> 10        -0.03304
        min(3)=        5 ->  9        -0.02867
        min(4)=        5 -> 24        -0.02765
        min(5)=        2 -> 16        -0.00874
        #states=21 #states>0=9 #states<0=12

27      Singlet-A1   42.1927         29.39    0.0734    0.000
        max(1)=        2 ->  9         0.54454
        max(2)=        2 ->  6         0.15166
        max(3)=        4 -> 14         0.08151
        max(4)=        5 -> 16         0.04288
        max(5)=        2 -> 13         0.03024
        min(1)=        3 -> 12        -0.34801
        min(2)=        4 -> 10        -0.12503
        min(3)=        5 -> 11        -0.11016
        min(4)=        4 -> 13        -0.10997
        min(5)=        2 -> 10        -0.07825
        #states=32 #states>0=15 #states<0=17

28      Singlet-B2   42.6650         29.06    0.0658    0.000
        max(1)=        3 -> 13         0.62289
        max(2)=        5 -> 15         0.32791
        max(3)=        2 -> 12         0.04011
        max(4)=        3 ->  6         0.03196
        max(5)=        3 -> 20         0.02091
        min(1)=        3 -> 14        -0.01060
        min(2)=        3 -> 25        -0.00644
        min(3)=        4 ->  8        -0.00507
        min(4)=        4 ->  7        -0.00289
        min(5)=        2 ->  8        -0.00155
        #states=29 #states>0=20 #states<0=9

29      Singlet-B2   43.9053         28.24    0.4593    0.000
        max(1)=        5 -> 15         0.60140
        max(2)=        3 ->  9         0.05190
        max(3)=        3 -> 19         0.02666
        max(4)=        4 -> 17         0.02440
        max(5)=        3 -> 10         0.01691
        min(1)=        3 -> 13        -0.31918
        min(2)=        3 -> 14        -0.15346
        min(3)=        2 ->  7        -0.05055
        min(4)=        4 ->  8        -0.04507
        min(5)=        4 -> 18        -0.03734
        #states=29 #states>0=13 #states<0=16

30      Singlet-A2   44.8333         27.65    0.0000    0.000
        max(1)=        4 -> 15         0.70546
        max(2)=        4 -> 23         0.02901
        max(3)=        3 -> 11         0.00592
        max(4)=        2 -> 23         0.00589
        max(5)=        5 -> 21         0.00578
        min(1)=        2 -> 15        -0.02964
        min(2)=        3 -> 16        -0.02206
        min(3)=        5 -> 12        -0.00231
        min(4)=        5 -> 18        -0.00173
        min(5)=        3 -> 22        -0.00158
        #states=16 #states>0=10 #states<0=6

31      Singlet-A1   45.0818         27.50    0.2982    0.000
        max(1)=        4 -> 14         0.47648
        max(2)=        2 -> 13         0.07653
        max(3)=        2 ->  6         0.04783
        max(4)=        5 -> 22         0.02402
        max(5)=        2 -> 20         0.01195
        min(1)=        2 ->  9        -0.34241
        min(2)=        3 -> 12        -0.25008
        min(3)=        5 -> 11        -0.16084
        min(4)=        4 -> 10        -0.15815
        min(5)=        5 -> 16        -0.11879
        #states=33 #states>0=18 #states<0=15

32      Singlet-A1   45.7819         27.08    0.1032    0.000
        max(1)=        4 -> 14         0.44738
        max(2)=        3 -> 12         0.29431
        max(3)=        2 ->  9         0.25822
        max(4)=        5 -> 11         0.19824
        max(5)=        4 -> 10         0.17814
        min(1)=        5 -> 16        -0.22536
        min(2)=        2 -> 13        -0.09773
        min(3)=        2 ->  6        -0.04880
        min(4)=        4 ->  9        -0.03835
        min(5)=        2 -> 14        -0.02401
```

```
#states=32 #states>0=16 #states<0=16

33   Singlet-B2   48.5010   25.56   0.6210   0.000
     max(1)=   3 -> 14    0.67999
     max(2)=   5 -> 15    0.12960
     max(3)=   2 -> 12    0.08822
     max(4)=   4 -> 17    0.04585
     max(5)=   3 -> 19    0.02988
     min(1)=   3 -> 13   -0.06053
     min(2)=   2 -> 17   -0.04136
     min(3)=   4 ->  8   -0.03682
     min(4)=   4 -> 18   -0.03179
     min(5)=   2 ->  7   -0.03020
     #states=28 #states>0=13 #states<0=15

34   Singlet-B1   48.9576   25.32   0.6080   0.000
     max(1)=   3 -> 15    0.64380
     max(2)=   2 -> 11    0.25506
     max(3)=   4 -> 16    0.12313
     max(4)=   2 -> 16    0.04626
     max(5)=   5 -> 14    0.03417
     min(1)=   5 -> 19   -0.02506
     min(2)=   5 ->  9   -0.01912
     min(3)=   4 -> 22   -0.01893
     min(4)=   4 -> 11   -0.00794
     min(5)=   5 -> 10   -0.00645
     #states=20 #states>0=14 #states<0=6

35   Singlet-A1   49.6651   24.96   0.9053   0.000
     max(1)=   5 -> 16    0.60968
     max(2)=   4 -> 14    0.19094
     max(3)=   3 -> 12    0.08274
     max(4)=   4 -> 10    0.06910
     max(5)=   3 -> 18    0.05888
     min(1)=   2 -> 10   -0.25123
     min(2)=   2 -> 13   -0.07250
     min(3)=   4 -> 19   -0.02658
     min(4)=   3 -> 17   -0.02650
     min(5)=   4 ->  9   -0.02388
     #states=33 #states>0=16 #states<0=17

36   Singlet-B1   50.4783   24.56   0.2298   0.000
     max(1)=   2 -> 11    0.54624
     max(2)=   2 -> 16    0.02227
     max(3)=   4 -> 22    0.01636
     max(4)=   2 -> 27    0.01540
     max(5)=   5 ->  9    0.00624
     min(1)=   4 -> 16   -0.42598
     min(2)=   3 -> 15   -0.13474
     min(3)=   5 -> 13   -0.02236
     min(4)=   5 -> 14   -0.01666
     min(5)=   3 -> 23   -0.01037
     #states=20 #states>0=10 #states<0=10
```

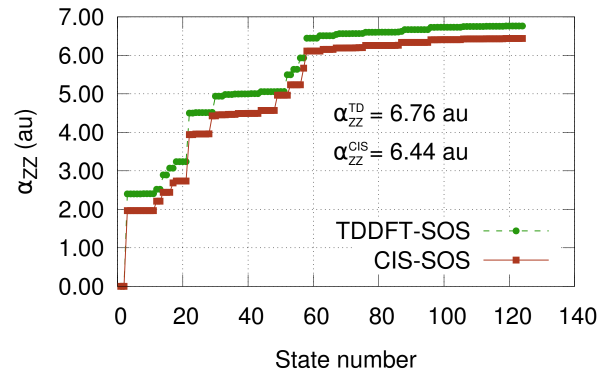
7.2 6-311++G(d,p)

7.2.1 Plots

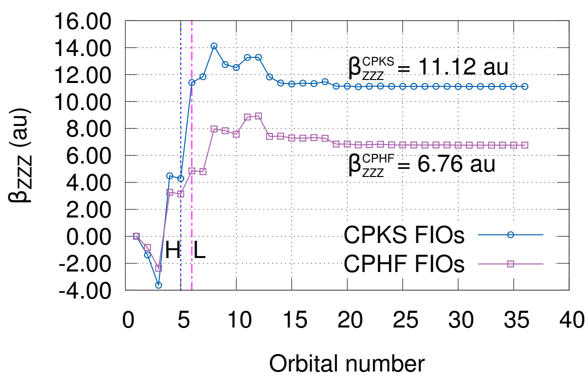
Figure S10: For H_2O molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S10a and S10c) or states (SOS approaches, in Plots S10b and S10d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.01 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



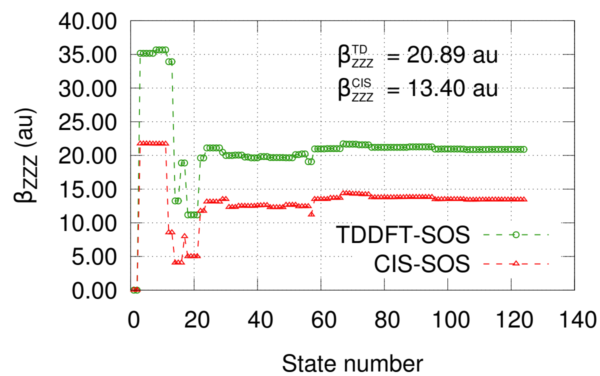
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

7.2.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-B1    7.0656        175.48    0.0430    0.000
         max(1)=        5 ->  6         0.69164
         max(2)=        5 ->  9         0.02286
         max(3)=        5 -> 16         0.00818
         max(4)=        2 -> 17         0.00446
         max(5)=        5 -> 31         0.00316
         min(1)=        5 ->  8        -0.14018
         min(2)=        5 -> 13        -0.03766
         min(3)=        5 -> 15        -0.01357
         min(4)=        4 -> 10        -0.00353
         min(5)=        3 -> 29        -0.00260
         #CIs=24 #CIs>0=15 #CIs<0=9

2        Singlet-A2    8.6960        142.58    0.0000    0.000
         max(1)=        5 ->  7         0.68100
         max(2)=        5 -> 11         0.14949
         max(3)=        5 -> 12         0.11540
         max(4)=        5 -> 18         0.00966
         max(5)=        2 -> 20         0.00197
         min(1)=        5 -> 14        -0.02226
         min(2)=        3 -> 10        -0.00261
         min(3)=        3 -> 17        -0.00148
         min(4)=        5 -> 32        -0.00065
         min(5)=        4 -> 20         0.00009
         #CIs=19 #CIs>0=15 #CIs<0=4

3        Singlet-A1    9.1679        135.24    0.0909    0.000
         max(1)=        4 ->  6         0.69150
         max(2)=        4 ->  9         0.05192
         max(3)=        3 -> 14         0.01310
         max(4)=        2 ->  9         0.00593
         max(5)=        2 -> 16         0.00377
         min(1)=        4 ->  8        -0.10644
         min(2)=        5 -> 10        -0.06702
         min(3)=        4 -> 13        -0.04911
         min(4)=        3 -> 11        -0.02173
         min(5)=        3 ->  7        -0.01263
         #CIs=42 #CIs>0=18 #CIs<0=24

4        Singlet-B2   10.7886        114.92    0.0220    0.000
         max(1)=        4 ->  7         0.69084
         max(2)=        4 -> 12         0.11322
         max(3)=        4 -> 11         0.09718
         max(4)=        3 ->  8         0.01419
         max(5)=        3 -> 15         0.01030
         min(1)=        2 -> 11        -0.00694
         min(2)=        3 ->  6        -0.00615
         min(3)=        2 ->  7        -0.00548
         min(4)=        3 -> 19        -0.00384
         min(5)=        3 ->  9        -0.00355
         #CIs=34 #CIs>0=17 #CIs<0=17

5        Singlet-B1   11.3098        109.63    0.0135    0.000
         max(1)=        5 ->  8         0.61707
         max(2)=        5 ->  9         0.31795
         max(3)=        5 ->  6         0.11232
         max(4)=        5 -> 15         0.03812
         max(5)=        3 -> 20         0.00328
         min(1)=        5 -> 13        -0.05807
         min(2)=        5 -> 16        -0.02629
         min(3)=        2 -> 10        -0.00579
         min(4)=        5 -> 19        -0.00305
         min(5)=        4 -> 10        -0.00149
         #CIs=25 #CIs>0=12 #CIs<0=13

6        Singlet-A2   11.6120        106.77    0.0000    0.000
         max(1)=        5 -> 11         0.68564
         max(2)=        5 -> 18         0.00691
         max(3)=        2 -> 20         0.00282
         max(4)=        5 -> 24         0.00274
         max(5)=        5 -> 12         0.00157
         min(1)=        5 ->  7        -0.15347
         min(2)=        5 -> 14        -0.07909
         min(3)=        3 -> 10        -0.00732
         min(4)=        3 -> 17        -0.00117
         min(5)=        5 -> 32        -0.00044
         #CIs=19 #CIs>0=14 #CIs<0=5

7        Singlet-B1   11.8022        105.05    0.0041    0.000
         max(1)=        5 ->  9         0.62946
```

```
max(2)=     4 -> 10     0.03259
max(3)=     2 -> 10     0.00942
max(4)=     4 -> 22     0.00487
max(5)=     4 -> 17     0.00454
min(1)=     5 ->  8    -0.30783
min(2)=     5 ->  6    -0.08343
min(3)=     5 -> 15    -0.02764
min(4)=     5 -> 21    -0.00965
min(5)=     5 -> 16    -0.00793
#CIs=25 #CIs>0=11 #CIs<0=14

8    Singlet-A1   12.0620   102.79   0.0003   0.000
max(1)=     5 -> 10     0.65817
max(2)=     4 ->  9     0.16900
max(3)=     4 ->  8     0.14652
max(4)=     4 ->  6     0.06805
max(5)=     4 -> 15     0.01365
min(1)=     3 ->  7    -0.07841
min(2)=     3 -> 11    -0.04695
min(3)=     3 -> 12    -0.04549
min(4)=     4 -> 13    -0.03117
min(5)=     4 -> 16    -0.02145
#CIs=42 #CIs>0=17 #CIs<0=25

9    Singlet-B2   13.0950    94.68   0.1017   0.000
max(1)=     3 ->  6     0.68118
max(2)=     4 ->  7     0.02655
max(3)=     4 -> 14     0.02207
max(4)=     3 -> 16     0.00659
max(5)=     4 -> 12     0.00530
min(1)=     4 -> 11    -0.13326
min(2)=     3 ->  8    -0.12410
min(3)=     3 -> 13    -0.03958
min(4)=     2 -> 14    -0.00697
min(5)=     2 ->  7    -0.00589
#CIs=35 #CIs>0=22 #CIs<0=13

10   Singlet-B1   13.4847    91.94   0.0043   0.000
max(1)=     4 -> 10     0.69627
max(2)=     5 -> 13     0.11539
max(3)=     4 -> 17     0.02519
max(4)=     5 ->  8     0.02209
max(5)=     5 ->  6     0.01483
min(1)=     5 ->  9    -0.02346
min(2)=     5 -> 15    -0.00582
min(3)=     5 -> 16    -0.00465
min(4)=     4 -> 22    -0.00297
min(5)=     5 -> 25    -0.00249
#CIs=26 #CIs>0=14 #CIs<0=12

11   Singlet-A2   13.5756    91.33   0.0000   0.000
max(1)=     5 -> 12     0.69638
max(2)=     5 -> 18     0.03155
max(3)=     2 -> 20     0.00131
max(4)=     5 -> 24     0.00105
max(5)=     5 -> 23     0.00070
min(1)=     5 ->  7    -0.11265
min(2)=     5 -> 11    -0.02965
min(3)=     5 -> 14    -0.02148
min(4)=     3 -> 10    -0.00598
min(5)=     3 -> 17    -0.00171
#CIs=19 #CIs>0=13 #CIs<0=6

12   Singlet-A1   13.6771    90.65   0.0098   0.000
max(1)=     4 ->  8     0.62303
max(2)=     3 ->  7     0.12860
max(3)=     4 ->  6     0.11331
max(4)=     3 -> 11     0.06724
max(5)=     4 -> 15     0.04742
min(1)=     4 ->  9    -0.26220
min(2)=     5 -> 10    -0.06239
min(3)=     4 -> 13    -0.03142
min(4)=     3 -> 14    -0.02107
min(5)=     2 ->  6    -0.01224
#CIs=41 #CIs>0=26 #CIs<0=15

13   Singlet-B1   13.9251    89.04   0.2295   0.000
max(1)=     5 -> 13     0.69411
max(2)=     5 ->  6     0.04408
max(3)=     5 ->  8     0.04008
max(4)=     5 ->  9     0.03321
max(5)=     2 -> 10     0.00825
```

```
        min(1)=     4 -> 10     -0.11588
        min(2)=     3 -> 20     -0.00829
        min(3)=     4 -> 17     -0.00549
        min(4)=     2 -> 17     -0.00266
        min(5)=     5 -> 16     -0.00254
        #CIs=26 #CIs>0=13 #CIs<0=13

14    Singlet-A1   14.0017     88.55    0.0329    0.000
        max(1)=     4 ->  9      0.58843
        max(2)=     3 ->  7      0.30091
        max(3)=     4 ->  8      0.16055
        max(4)=     3 -> 11      0.10152
        max(5)=     3 -> 12      0.08715
        min(1)=     5 -> 10     -0.13441
        min(2)=     4 ->  6     -0.02044
        min(3)=     3 -> 14     -0.01773
        min(4)=     4 -> 15     -0.00766
        min(5)=     2 ->  6     -0.00742
        #CIs=43 #CIs>0=25 #CIs<0=18

15    Singlet-B2   14.0754     88.09    0.1941    0.000
        max(1)=     4 -> 11      0.68254
        max(2)=     3 ->  6      0.14328
        max(3)=     3 ->  8      0.03412
        max(4)=     3 -> 15      0.03244
        max(5)=     5 -> 20      0.01551
        min(1)=     4 ->  7     -0.09217
        min(2)=     4 -> 14     -0.02779
        min(3)=     3 -> 13     -0.02701
        min(4)=     4 -> 12     -0.02574
        min(5)=     3 ->  9     -0.02356
        #CIs=35 #CIs>0=17 #CIs<0=18

16    Singlet-A1   15.4623     80.18    0.0190    0.000
        max(1)=     3 ->  7      0.57066
        max(2)=     5 -> 10      0.14238
        max(3)=     3 -> 14      0.02853
        max(4)=     4 -> 15      0.01668
        max(5)=     2 ->  6      0.00983
        min(1)=     4 -> 13     -0.28149
        min(2)=     4 ->  8     -0.18966
        min(3)=     4 ->  9     -0.18768
        min(4)=     3 -> 11     -0.03757
        min(5)=     5 -> 17     -0.03005
        #CIs=41 #CIs>0=12 #CIs<0=29

17    Singlet-B2   15.5247     79.86    0.0042    0.000
        max(1)=     4 -> 12      0.69625
        max(2)=     4 -> 18      0.03145
        max(3)=     3 ->  9      0.01360
        max(4)=     4 -> 11      0.00900
        max(5)=     2 -> 14      0.00268
        min(1)=     4 ->  7     -0.11596
        min(2)=     4 -> 14     -0.01951
        min(3)=     3 -> 13     -0.01010
        min(4)=     2 -> 11     -0.00717
        min(5)=     3 -> 19     -0.00186
        #CIs=35 #CIs>0=20 #CIs<0=15

18    Singlet-A1   15.8050     78.45    0.0187    0.000
        max(1)=     4 -> 13      0.64318
        max(2)=     3 ->  7      0.24176
        max(3)=     5 -> 10      0.08461
        max(4)=     4 ->  6      0.05523
        max(5)=     3 -> 14      0.01957
        min(1)=     4 ->  9     -0.10020
        min(2)=     4 ->  8     -0.05266
        min(3)=     3 -> 12     -0.04434
        min(4)=     3 -> 11     -0.04188
        min(5)=     4 -> 16     -0.02236
        #CIs=43 #CIs>0=17 #CIs<0=26

19    Singlet-B2   17.4650     70.99    0.0202    0.000
        max(1)=     3 ->  8      0.55587
        max(2)=     3 ->  9      0.42179
        max(3)=     3 ->  6      0.08974
        max(4)=     3 -> 15      0.02027
        max(5)=     2 -> 11      0.00993
        min(1)=     3 -> 13     -0.04292
        min(2)=     4 -> 11     -0.03631
        min(3)=     3 -> 16     -0.02610
        min(4)=     4 -> 14     -0.02418
```

```
        min(5)=       4 -> 12       -0.01091
        #CIs=35 #CIs>0=14 #CIs<0=21

20      Singlet-A2   17.5250        70.75    0.0000    0.000
        max(1)=       3 -> 10        0.70641
        max(2)=       3 -> 17        0.02690
        max(3)=       5 -> 14        0.01239
        max(4)=       5 -> 11        0.00898
        max(5)=       5 -> 12        0.00697
        min(1)=       5 -> 18       -0.00213
        min(2)=       5 -> 24       -0.00087
        min(3)=       4 -> 20       -0.00015
        min(4)=       5 -> 32        0.00008
        min(5)=       5 -> 23        0.00010
        #CIs=18 #CIs>0=15 #CIs<0=3

21      Singlet-B2   18.0920        68.53    0.2259    0.000
        max(1)=       3 ->  9        0.56528
        max(2)=       4 -> 11        0.05752
        max(3)=       4 -> 14        0.04931
        max(4)=       5 -> 20        0.01222
        max(5)=       4 -> 18        0.00590
        min(1)=       3 ->  8       -0.41187
        min(2)=       3 ->  6       -0.06941
        min(3)=       2 -> 14       -0.00990
        min(4)=       3 -> 15       -0.00868
        min(5)=       4 -> 12       -0.00862
        #CIs=36 #CIs>0=19 #CIs<0=17

22      Singlet-A1   18.4329        67.26    0.1931    0.000
        max(1)=       3 -> 11        0.66976
        max(2)=       5 -> 10        0.05992
        max(3)=       4 -> 15        0.03792
        max(4)=       2 ->  9        0.02021
        max(5)=       4 ->  6        0.01630
        min(1)=       3 -> 12       -0.18873
        min(2)=       4 ->  8       -0.07682
        min(3)=       4 ->  9       -0.04611
        min(4)=       5 -> 17       -0.03060
        min(5)=       4 -> 16       -0.02777
        #CIs=42 #CIs>0=17 #CIs<0=25

23      Singlet-B2   19.6757        63.01    0.0093    0.000
        max(1)=       3 -> 13        0.70202
        max(2)=       3 ->  6        0.04877
        max(3)=       4 -> 14        0.04441
        max(4)=       3 ->  8        0.03327
        max(5)=       3 ->  9        0.02172
        min(1)=       2 ->  7       -0.01917
        min(2)=       2 -> 11       -0.01135
        min(3)=       3 -> 16       -0.00612
        min(4)=       3 -> 15       -0.00505
        min(5)=       4 -> 24       -0.00454
        #CIs=36 #CIs>0=22 #CIs<0=14

24      Singlet-A1   20.4158        60.73    0.0023    0.000
        max(1)=       3 -> 12        0.66605
        max(2)=       3 -> 11        0.15716
        max(3)=       5 -> 10        0.08316
        max(4)=       4 -> 15        0.05918
        max(5)=       2 ->  6        0.04360
        min(1)=       4 ->  8       -0.07218
        min(2)=       4 ->  9       -0.06693
        min(3)=       5 -> 17       -0.06213
        min(4)=       4 -> 16       -0.04766
        min(5)=       3 ->  7       -0.03684
        #CIs=43 #CIs>0=17 #CIs<0=26

25      Singlet-A2   20.6769        59.96    0.0000    0.000
        max(1)=       5 -> 14        0.70166
        max(2)=       5 -> 11        0.08102
        max(3)=       5 -> 12        0.02532
        max(4)=       5 -> 27        0.00207
        max(5)=       5 ->  7        0.00089
        min(1)=       5 -> 24       -0.01531
        min(2)=       3 -> 10       -0.01361
        min(3)=       5 -> 23       -0.00462
        min(4)=       2 -> 20       -0.00418
        min(5)=       5 -> 18       -0.00409
        #CIs=19 #CIs>0=7 #CIs<0=12

26      Singlet-B1   22.2915        55.62    0.0437    0.000
```

```
          max(1)=        5 -> 15         0.70375
          max(2)=        3 -> 20         0.01885
          max(3)=        5 -> 21         0.01033
          max(4)=        5 ->  9         0.00756
          max(5)=        4 -> 28         0.00736
          min(1)=        5 ->  8        -0.04895
          min(2)=        2 -> 10        -0.02729
          min(3)=        5 -> 16        -0.02487
          min(4)=        4 -> 22        -0.01332
          min(5)=        5 -> 19        -0.01326
          #CIs=26 #CIs>0=13 #CIs<0=13

27     Singlet-B2   23.5321         52.69    0.0937    0.000
          max(1)=        4 -> 14         0.69115
          max(2)=        3 ->  8         0.05384
          max(3)=        4 -> 11         0.03163
          max(4)=        2 ->  7         0.02634
          max(5)=        2 -> 12         0.02287
          min(1)=        3 -> 15        -0.11070
          min(2)=        3 -> 13        -0.04548
          min(3)=        5 -> 20        -0.03452
          min(4)=        3 ->  9        -0.02616
          min(5)=        4 -> 18        -0.01290
          #CIs=36 #CIs>0=17 #CIs<0=19

28     Singlet-A1   24.2153         51.20    0.0000    0.000
          max(1)=        4 -> 15         0.69087
          max(2)=        2 ->  8         0.04154
          max(3)=        5 -> 17         0.02851
          max(4)=        4 ->  9         0.02817
          max(5)=        4 -> 16         0.01398
          min(1)=        3 -> 14        -0.08550
          min(2)=        2 ->  6        -0.07527
          min(3)=        3 -> 11        -0.04622
          min(4)=        4 ->  8        -0.03836
          min(5)=        3 -> 12        -0.03810
          #CIs=43 #CIs>0=20 #CIs<0=23

29     Singlet-A1   26.6660         46.50    0.0018    0.000
          max(1)=        2 ->  6         0.68062
          max(2)=        5 -> 17         0.06049
          max(3)=        4 -> 15         0.05628
          max(4)=        3 -> 18         0.03052
          max(5)=        4 -> 16         0.02993
          min(1)=        3 -> 14        -0.13429
          min(2)=        2 ->  8        -0.07799
          min(3)=        3 -> 12        -0.03442
          min(4)=        2 -> 13        -0.03160
          min(5)=        3 -> 11        -0.02429
          #CIs=42 #CIs>0=23 #CIs<0=19

30     Singlet-A1   28.0269         44.24    0.1489    0.000
          max(1)=        3 -> 14         0.67325
          max(2)=        2 ->  6         0.11931
          max(3)=        5 -> 17         0.09799
          max(4)=        4 -> 15         0.08717
          max(5)=        4 -> 16         0.08316
          min(1)=        2 ->  9        -0.05739
          min(2)=        4 -> 19        -0.03710
          min(3)=        5 -> 10        -0.02311
          min(4)=        3 ->  7        -0.01165
          min(5)=        4 ->  6        -0.01067
          #CIs=42 #CIs>0=27 #CIs<0=15

31     Singlet-B2   28.1815         43.99    0.0104    0.000
          max(1)=        2 ->  7         0.69014
          max(2)=        2 -> 11         0.11997
          max(3)=        2 -> 12         0.08383
          max(4)=        3 -> 13         0.02229
          max(5)=        5 -> 20         0.01823
          min(1)=        4 -> 14        -0.02827
          min(2)=        3 -> 19        -0.01307
          min(3)=        4 -> 24        -0.00683
          min(4)=        2 -> 14        -0.00596
          min(5)=        3 -> 21        -0.00495
          #CIs=35 #CIs>0=20 #CIs<0=15

32     Singlet-B2   29.1611         42.52    0.2181    0.000
          max(1)=        3 -> 15         0.69228
          max(2)=        4 -> 14         0.10962
          max(3)=        3 -> 19         0.01872
          max(4)=        2 -> 14         0.01758
```

```
        max(5)=       2 -> 12        0.01287
        min(1)=       5 -> 20       -0.06585
        min(2)=       2 -> 11       -0.03616
        min(3)=       3 -> 16       -0.03299
        min(4)=       4 -> 18       -0.02836
        min(5)=       4 -> 11       -0.02567
        #CIs=36 #CIs>0=16 #CIs<0=20

33      Singlet-A1   31.0251         39.96    0.0189    0.000
        max(1)=       2 ->  9        0.50775
        max(2)=       2 ->  8        0.48135
        max(3)=       2 ->  6        0.04451
        max(4)=       3 -> 14        0.02177
        max(5)=       4 -> 21        0.02010
        min(1)=       2 -> 13       -0.06626
        min(2)=       5 -> 17       -0.03361
        min(3)=       3 -> 18       -0.01986
        min(4)=       4 -> 19       -0.01932
        min(5)=       2 -> 16       -0.01669
        #CIs=41 #CIs>0=19 #CIs<0=22

34      Singlet-B1   31.0404         39.94    0.0142    0.000
        max(1)=       2 -> 10        0.70335
        max(2)=       5 -> 15        0.02498
        max(3)=       2 -> 17        0.01805
        max(4)=       3 -> 20        0.01732
        max(5)=       4 -> 28        0.00653
        min(1)=       5 -> 16       -0.05427
        min(2)=       4 -> 17       -0.01899
        min(3)=       5 -> 19       -0.01674
        min(4)=       4 -> 22       -0.01368
        min(5)=       5 -> 25       -0.01011
        #CIs=26 #CIs>0=14 #CIs<0=12

35      Singlet-B2   31.1819         39.76    0.0149    0.000
        max(1)=       2 -> 11        0.69297
        max(2)=       3 -> 15        0.04061
        max(3)=       3 -> 13        0.00939
        max(4)=       4 -> 12        0.00818
        max(5)=       3 -> 16        0.00701
        min(1)=       2 ->  7       -0.11893
        min(2)=       2 -> 14       -0.05116
        min(3)=       2 -> 12       -0.02835
        min(4)=       3 ->  9       -0.01142
        min(5)=       3 -> 19       -0.01000
        #CIs=36 #CIs>0=16 #CIs<0=20

36      Singlet-A1   31.2155         39.72    0.0052    0.000
        max(1)=       2 ->  8        0.48330
        max(2)=       2 ->  6        0.07753
        max(3)=       2 -> 15        0.03221
        max(4)=       5 -> 10        0.02209
        max(5)=       2 -> 16        0.00798
        min(1)=       2 ->  9       -0.48189
        min(2)=       5 -> 17       -0.12505
        min(3)=       2 -> 13       -0.06967
        min(4)=       4 -> 16       -0.05388
        min(5)=       3 -> 14       -0.04433
        #CIs=42 #CIs>0=17 #CIs<0=25

37      Singlet-B1   32.4479         38.21    0.0142    0.000
        max(1)=       5 -> 16        0.70243
        max(2)=       2 -> 10        0.05137
        max(3)=       5 -> 15        0.02635
        max(4)=       5 -> 21        0.02185
        max(5)=       5 ->  8        0.01975
        min(1)=       4 -> 17       -0.03193
        min(2)=       4 -> 22       -0.01620
        min(3)=       5 -> 19       -0.01409
        min(4)=       5 -> 25       -0.01100
        min(5)=       5 ->  6       -0.00410
        #CIs=26 #CIs>0=16 #CIs<0=10

38      Singlet-A1   33.0038         37.57    0.0017    0.000
        max(1)=       2 -> 13        0.68721
        max(2)=       2 ->  8        0.06590
        max(3)=       2 ->  6        0.05231
        max(4)=       2 ->  9        0.01416
        max(5)=       2 -> 21        0.01130
        min(1)=       5 -> 17       -0.13902
        min(2)=       4 -> 16       -0.02383
        min(3)=       2 -> 15       -0.01242
```

```
min(4)=        2 -> 16        -0.00477
min(5)=        3 -> 14        -0.00464
#CIs=41 #CIs>0=23 #CIs<0=18

39   Singlet-B2   33.1201   37.43   0.0247   0.000
max(1)=        2 -> 12         0.69911
max(2)=        5 -> 20         0.02937
max(3)=        3 -> 16         0.02180
max(4)=        2 -> 18         0.02088
max(5)=        4 -> 18         0.01152
min(1)=        2 ->  7        -0.08959
min(2)=        3 -> 19        -0.01843
min(3)=        4 -> 14        -0.01818
min(4)=        2 -> 14        -0.01467
min(5)=        3 -> 21        -0.00984
#CIs=36 #CIs>0=19 #CIs<0=17

40   Singlet-A2   33.7225   36.77   0.0000   0.000
max(1)=        5 -> 18         0.70618
max(2)=        5 -> 24         0.00677
max(3)=        5 -> 14         0.00629
max(4)=        4 -> 20         0.00435
max(5)=        5 -> 35         0.00314
min(1)=        5 -> 12        -0.03253
min(2)=        5 -> 11        -0.00695
min(3)=        5 -> 32        -0.00639
min(4)=        3 -> 17        -0.00615
min(5)=        5 ->  7        -0.00278
#CIs=18 #CIs>0=9 #CIs<0=9

41   Singlet-A1   34.0157   36.45   0.0040   0.000
max(1)=        4 -> 16         0.49937
max(2)=        3 -> 18         0.04544
max(3)=        2 -> 15         0.02644
max(4)=        4 ->  9         0.01845
max(5)=        4 -> 19         0.01842
min(1)=        5 -> 17        -0.48584
min(2)=        2 -> 13        -0.07454
min(3)=        2 ->  8        -0.06545
min(4)=        3 -> 12        -0.01306
min(5)=        5 -> 22        -0.00944
#CIs=42 #CIs>0=25 #CIs<0=17

42   Singlet-B1   35.4521   34.97   0.0039   0.000
max(1)=        4 -> 17         0.70538
max(2)=        5 -> 16         0.02975
max(3)=        2 -> 10         0.02052
max(4)=        3 -> 20         0.00947
max(5)=        5 -> 15         0.00740
min(1)=        4 -> 10        -0.02562
min(2)=        5 -> 19        -0.01421
min(3)=        5 -> 25        -0.00616
min(4)=        4 -> 22        -0.00592
min(5)=        2 -> 17        -0.00464
#CIs=26 #CIs>0=13 #CIs<0=13

43   Singlet-B2   35.7803   34.65   0.0613   0.000
max(1)=        4 -> 18         0.70366
max(2)=        2 -> 14         0.02139
max(3)=        3 -> 15         0.02050
max(4)=        4 -> 14         0.01553
max(5)=        3 -> 19         0.01126
min(1)=        5 -> 20        -0.03337
min(2)=        3 -> 16        -0.03210
min(3)=        4 -> 12        -0.03179
min(4)=        4 -> 11        -0.01158
min(5)=        3 -> 21        -0.00842
#CIs=36 #CIs>0=14 #CIs<0=22

44   Singlet-A1   37.5457   33.02   0.0323   0.000
max(1)=        4 -> 16         0.41222
max(2)=        5 -> 17         0.35178
max(3)=        2 ->  8         0.07722
max(4)=        2 -> 13         0.07503
max(5)=        3 -> 12         0.05513
min(1)=        3 -> 18        -0.39272
min(2)=        2 -> 15        -0.12480
min(3)=        3 -> 14        -0.08672
min(4)=        4 -> 21        -0.08143
min(5)=        2 ->  9        -0.05149
#CIs=43 #CIs>0=20 #CIs<0=23
```

```
45   Singlet-B2   38.5945   32.12   0.0351   0.000
     max(1)=   3 -> 16    0.69627
     max(2)=   2 -> 14    0.04436
     max(3)=   4 -> 18    0.02423
     max(4)=   3 -> 15    0.02209
     max(5)=   3 ->  9    0.01842
     min(1)=   5 -> 20   -0.10355
     min(2)=   2 -> 12   -0.01691
     min(3)=   3 -> 25   -0.00895
     min(4)=   5 -> 29   -0.00581
     min(5)=   2 -> 11   -0.00513
     #CIs=35 #CIs>0=21 #CIs<0=14

46   Singlet-A2   39.4993   31.39   0.0000   0.000
     max(1)=   3 -> 17    0.70647
     max(2)=   4 -> 20    0.00927
     max(3)=   5 -> 18    0.00629
     max(4)=   3 -> 33    0.00532
     max(5)=   2 -> 20    0.00429
     min(1)=   3 -> 10   -0.02688
     min(2)=   5 -> 14   -0.00138
     min(3)=   5 -> 24   -0.00136
     min(4)=   2 -> 29   -0.00080
     min(5)=   5 -> 27   -0.00069
     #CIs=18 #CIs>0=11 #CIs<0=7

47   Singlet-B1   40.1338   30.89   0.0075   0.000
     max(1)=   5 -> 19    0.70576
     max(2)=   3 -> 20    0.02474
     max(3)=   2 -> 10    0.01663
     max(4)=   5 -> 15    0.01360
     max(5)=   4 -> 17    0.01259
     min(1)=   4 -> 22   -0.01680
     min(2)=   2 -> 17   -0.00763
     min(3)=   5 -> 13   -0.00665
     min(4)=   5 -> 25   -0.00662
     min(5)=   5 -> 21   -0.00489
     #CIs=26 #CIs>0=16 #CIs<0=10

48   Singlet-B2   40.4690   30.64   0.0014   0.000
     max(1)=   2 -> 14    0.69266
     max(2)=   5 -> 20    0.12263
     max(3)=   2 -> 11    0.05122
     max(4)=   3 -> 19    0.03177
     max(5)=   3 -> 21    0.01376
     min(1)=   3 -> 16   -0.02499
     min(2)=   4 -> 18   -0.01663
     min(3)=   4 -> 23   -0.00809
     min(4)=   3 ->  8   -0.00765
     min(5)=   3 -> 15   -0.00739
     #CIs=36 #CIs>0=20 #CIs<0=16

49   Singlet-A1   41.2289   30.07   0.0012   0.000
     max(1)=   2 -> 15    0.56383
     max(2)=   4 -> 19    0.11671
     max(3)=   4 -> 21    0.09107
     max(4)=   2 ->  9    0.02576
     max(5)=   3 -> 14    0.02202
     min(1)=   3 -> 18   -0.37659
     min(2)=   4 -> 16   -0.08335
     min(3)=   5 -> 17   -0.07448
     min(4)=   2 ->  8   -0.05965
     min(5)=   2 -> 16   -0.01841
     #CIs=43 #CIs>0=21 #CIs<0=22

50   Singlet-B2   41.7194   29.72   0.5302   0.000
     max(1)=   5 -> 20    0.67217
     max(2)=   3 -> 19    0.11765
     max(3)=   3 -> 16    0.10033
     max(4)=   3 -> 15    0.06251
     max(5)=   4 -> 14    0.04309
     min(1)=   2 -> 14   -0.11772
     min(2)=   2 -> 12   -0.03085
     min(3)=   3 -> 25   -0.02362
     min(4)=   2 -> 11   -0.01857
     min(5)=   4 -> 11   -0.01815
     #CIs=36 #CIs>0=18 #CIs<0=18

51   Singlet-A2   42.6302   29.08   0.0000   0.000
     max(1)=   4 -> 20    0.70696
     max(2)=   4 -> 29    0.00786
     max(3)=   3 -> 22    0.00383
```

```
        max(4)=     5 -> 27      0.00372
        max(5)=     2 -> 29      0.00263
        min(1)=     3 -> 17     -0.00923
        min(2)=     5 -> 18     -0.00446
        min(3)=     2 -> 20     -0.00364
        min(4)=     3 -> 28     -0.00089
        min(5)=     5 -> 11     -0.00020
        #CIs=19 #CIs>0=13 #CIs<0=6

52    Singlet-A1   42.7663     28.99    0.3607    0.000
        max(1)=     4 -> 19      0.56600
        max(2)=     4 -> 21      0.13569
        max(3)=     5 -> 22      0.12699
        max(4)=     3 -> 14      0.05355
        max(5)=     4 -> 15      0.02704
        min(1)=     2 -> 15     -0.29279
        min(2)=     3 -> 18     -0.17426
        min(3)=     5 -> 17     -0.10626
        min(4)=     4 -> 16     -0.10144
        min(5)=     2 -> 13     -0.03243
        #CIs=43 #CIs>0=22 #CIs<0=21

53    Singlet-B1   43.7573     28.33    0.1145    0.000
        max(1)=     5 -> 21      0.69212
        max(2)=     4 -> 22      0.05676
        max(3)=     5 -> 19      0.01071
        max(4)=     2 -> 10      0.00865
        max(5)=     5 ->  9      0.00562
        min(1)=     3 -> 20     -0.12990
        min(2)=     5 -> 16     -0.01665
        min(3)=     2 -> 17     -0.01244
        min(4)=     2 -> 22     -0.01132
        min(5)=     5 -> 13     -0.00623
        #CIs=25 #CIs>0=11 #CIs<0=14

54    Singlet-A1   44.5993     27.80    0.1259    0.000
        max(1)=     4 -> 21      0.41260
        max(2)=     2 -> 21      0.04761
        max(3)=     2 ->  6      0.03356
        max(4)=     5 -> 28      0.02047
        max(5)=     4 -> 15      0.01940
        min(1)=     4 -> 19     -0.32640
        min(2)=     3 -> 18     -0.28620
        min(3)=     2 -> 15     -0.23623
        min(4)=     5 -> 22     -0.19379
        min(5)=     5 -> 17     -0.14837
        #CIs=43 #CIs>0=19 #CIs<0=24

55    Singlet-B2   47.0241     26.37    0.3558    0.000
        max(1)=     3 -> 19      0.69344
        max(2)=     3 -> 25      0.02654
        max(3)=     2 -> 12      0.02362
        max(4)=     5 -> 29      0.02103
        max(5)=     4 -> 11      0.01362
        min(1)=     5 -> 20     -0.11068
        min(2)=     4 -> 24     -0.03698
        min(3)=     2 -> 18     -0.03028
        min(4)=     4 -> 14     -0.03028
        min(5)=     3 -> 15     -0.02499
        #CIs=35 #CIs>0=18 #CIs<0=17

56    Singlet-A1   47.2714     26.23    0.2965    0.000
        max(1)=     5 -> 22      0.39363
        max(2)=     2 -> 21      0.08596
        max(3)=     2 ->  6      0.03560
        max(4)=     4 ->  8      0.02839
        max(5)=     2 -> 19      0.02639
        min(1)=     4 -> 21     -0.37873
        min(2)=     3 -> 18     -0.25834
        min(3)=     4 -> 19     -0.21687
        min(4)=     5 -> 17     -0.17170
        min(5)=     4 -> 16     -0.13721
        #CIs=43 #CIs>0=21 #CIs<0=22

57    Singlet-B1   47.3841     26.17    0.1902    0.000
        max(1)=     3 -> 20      0.62026
        max(2)=     4 -> 22      0.32582
        max(3)=     5 -> 21      0.08981
        max(4)=     5 -> 25      0.01873
        max(5)=     2 -> 17      0.00921
        min(1)=     5 -> 15     -0.01313
        min(2)=     5 -> 19     -0.01227
```

```
          min(3)=        5 -> 16        -0.01145
          min(4)=        4 -> 28        -0.01091
          min(5)=        2 -> 10        -0.00900
          #CIs=26 #CIs>0=14 #CIs<0=12

58     Singlet-A1   47.9076        25.88    0.5313    0.000
          max(1)=        5 -> 22         0.53441
          max(2)=        4 -> 21         0.38508
          max(3)=        4 -> 16         0.11178
          max(4)=        3 -> 18         0.11138
          max(5)=        5 -> 17         0.10545
          min(1)=        4 -> 19        -0.08636
          min(2)=        3 -> 14        -0.07030
          min(3)=        3 -> 24        -0.06036
          min(4)=        2 -> 21        -0.05737
          min(5)=        2 -> 19        -0.04030
          #CIs=43 #CIs>0=23 #CIs<0=20

59     Singlet-B2   49.5809        25.01    0.0571    0.000
          max(1)=        3 -> 21         0.70602
          max(2)=        3 -> 15         0.01107
          max(3)=        5 -> 20         0.01099
          max(4)=        2 -> 12         0.01002
          max(5)=        4 -> 18         0.00934
          min(1)=        2 -> 18        -0.01892
          min(2)=        2 -> 14        -0.01674
          min(3)=        3 -> 13        -0.01336
          min(4)=        4 -> 24        -0.00861
          min(5)=        4 -> 23        -0.00630
          #CIs=36 #CIs>0=18 #CIs<0=18

60     Singlet-B1   49.7636        24.91    1.0406    0.000
          max(1)=        4 -> 22         0.62129
          max(2)=        5 -> 15         0.02381
          max(3)=        5 -> 16         0.02359
          max(4)=        5 -> 19         0.02200
          max(5)=        2 -> 10         0.02083
          min(1)=        3 -> 20        -0.30623
          min(2)=        5 -> 21        -0.10925
          min(3)=        5 -> 25        -0.05403
          min(4)=        2 -> 17        -0.05347
          min(5)=        5 -> 31        -0.01513
          #CIs=26 #CIs>0=14 #CIs<0=12
```

7.2.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___    Exc.E Osc._Strength   ___f___ _<S**2>_

1      Singlet-B1    8.7596       141.54    0.0459    0.000
          max(1)=        5 ->  6         0.62825
          max(2)=        5 -> 10         0.28394
          max(3)=        5 -> 16         0.03734
          max(4)=        5 -> 31         0.00598
          max(5)=        5 -> 30         0.00246
          min(1)=        5 -> 13        -0.11236
          min(2)=        5 ->  8        -0.07639
          min(3)=        5 -> 15        -0.06447
          min(4)=        5 -> 21        -0.01729
          min(5)=        4 ->  9        -0.01212
          #CIs=23 #CIs>0=8 #CIs<0=15

2      Singlet-A2   10.4507       118.64    0.0000    0.000
          max(1)=        5 ->  7         0.60811
          max(2)=        5 -> 11         0.20221
          max(3)=        5 -> 17         0.04983
          max(4)=        5 -> 24         0.01332
          max(5)=        5 -> 35         0.00357
          min(1)=        5 -> 12        -0.27743
          min(2)=        5 -> 14        -0.09814
          min(3)=        5 -> 32        -0.00334
          min(4)=        3 -> 18        -0.00240
          min(5)=        2 -> 29        -0.00173
          #CIs=18 #CIs>0=9 #CIs<0=9

3      Singlet-A1   11.0021       112.69    0.1071    0.000
          max(1)=        4 ->  6         0.63565
```

```
        max(2)=     4 -> 10      0.25113
        max(3)=     4 -> 16      0.01739
        max(4)=     3 -> 14      0.01514
        max(5)=     3 -> 12      0.01127
        min(1)=     4 -> 13     -0.12227
        min(2)=     5 ->  9     -0.11528
        min(3)=     4 -> 15     -0.04943
        min(4)=     5 -> 18     -0.02191
        min(5)=     4 -> 21     -0.01857
        #CIs=40 #CIs>0=15 #CIs<0=25

4    Singlet-B2   12.6684     97.87    0.0363    0.000
        max(1)=     4 ->  7      0.63875
        max(2)=     4 -> 11      0.13686
        max(3)=     4 -> 17      0.04438
        max(4)=     3 ->  6      0.01718
        max(5)=     3 -> 15      0.01369
        min(1)=     4 -> 12     -0.25881
        min(2)=     4 -> 14     -0.05847
        min(3)=     2 -> 11     -0.01115
        min(4)=     2 ->  7     -0.00633
        min(5)=     3 -> 19     -0.00587
        #CIs=34 #CIs>0=22 #CIs<0=12

5    Singlet-B1   12.8836     96.23    0.0149    0.000
        max(1)=     5 ->  8      0.58332
        max(2)=     5 ->  6      0.20488
        max(3)=     5 -> 15      0.07595
        max(4)=     5 -> 25      0.00777
        max(5)=     3 -> 20      0.00309
        min(1)=     5 -> 10     -0.30898
        min(2)=     5 -> 13     -0.09950
        min(3)=     5 -> 16     -0.07870
        min(4)=     4 ->  9     -0.01301
        min(5)=     5 -> 19     -0.00819
        #CIs=23 #CIs>0=12 #CIs<0=11

6    Singlet-A2   13.4466     92.20    0.0000    0.000
        max(1)=     5 -> 11      0.59031
        max(2)=     5 -> 17      0.03236
        max(3)=     5 -> 24      0.01770
        max(4)=     5 -> 23      0.00384
        max(5)=     2 -> 20      0.00373
        min(1)=     5 ->  7     -0.30191
        min(2)=     5 -> 14     -0.18242
        min(3)=     5 -> 12     -0.16008
        min(4)=     3 ->  9     -0.00832
        min(5)=     3 -> 18     -0.00221
        #CIs=17 #CIs>0=9 #CIs<0=8

7    Singlet-A1   13.5680     91.38    0.0000    0.000
        max(1)=     5 ->  9      0.64194
        max(2)=     4 ->  8      0.21415
        max(3)=     4 ->  6      0.13264
        max(4)=     3 -> 12      0.07246
        max(5)=     5 -> 18      0.04609
        min(1)=     3 ->  7     -0.06950
        min(2)=     4 -> 13     -0.05154
        min(3)=     4 -> 10     -0.05098
        min(4)=     3 -> 11     -0.04809
        min(5)=     4 -> 16     -0.04084
        #CIs=40 #CIs>0=19 #CIs<0=21

8    Singlet-B1   13.7253     90.33    0.0028    0.000
        max(1)=     5 -> 10      0.54474
        max(2)=     5 ->  8      0.36545
        max(3)=     4 ->  9      0.01396
        max(4)=     2 ->  9      0.00619
        max(5)=     4 -> 22      0.00579
        min(1)=     5 ->  6     -0.22749
        min(2)=     5 -> 15     -0.09445
        min(3)=     5 -> 13     -0.08680
        min(4)=     5 -> 21     -0.03115
        min(5)=     3 -> 20     -0.00753
        #CIs=23 #CIs>0=10 #CIs<0=13

9    Singlet-B2   14.7596     84.00    0.1622    0.000
        max(1)=     3 ->  6      0.63000
        max(2)=     3 -> 10      0.27294
        max(3)=     3 -> 16      0.03319
        max(4)=     4 -> 14      0.03221
        max(5)=     2 -> 12      0.01593
```

```
        min(1)=     3 -> 13     -0.10156
        min(2)=     3 ->  8     -0.09205
        min(3)=     4 -> 11     -0.06495
        min(4)=     3 -> 15     -0.04971
        min(5)=     2 ->  7     -0.01485
        #CIs=32 #CIs>0=16 #CIs<0=16

10   Singlet-B1   14.9661    82.84   0.0090   0.000
        max(1)=     4 ->  9      0.68307
        max(2)=     5 -> 13      0.15723
        max(3)=     4 -> 18      0.07561
        max(4)=     5 ->  6      0.04301
        max(5)=     5 ->  8      0.02926
        min(1)=     5 -> 15     -0.00824
        min(2)=     5 -> 16     -0.00811
        min(3)=     2 -> 28     -0.00230
        min(4)=     2 -> 22     -0.00155
        min(5)=     5 -> 31     -0.00138
        #CIs=23 #CIs>0=15 #CIs<0=8

11   Singlet-A2   15.4066    80.47   0.0000   0.000
        max(1)=     5 -> 12      0.61191
        max(2)=     5 -> 11      0.28172
        max(3)=     5 ->  7      0.19743
        max(4)=     5 -> 14      0.03333
        max(5)=     5 -> 32      0.00278
        min(1)=     5 -> 17     -0.07776
        min(2)=     5 -> 24     -0.00666
        min(3)=     5 -> 35     -0.00234
        min(4)=     5 -> 27     -0.00122
        min(5)=     5 -> 23     -0.00080
        #CIs=19 #CIs>0=11 #CIs<0=8

12   Singlet-A1   15.5618    79.67   0.0269   0.000
        max(1)=     4 ->  8      0.57809
        max(2)=     3 ->  7      0.27203
        max(3)=     3 -> 11      0.12373
        max(4)=     3 -> 17      0.04115
        max(5)=     4 ->  6      0.02522
        min(1)=     3 -> 12     -0.17389
        min(2)=     5 ->  9     -0.15136
        min(3)=     4 -> 10     -0.10060
        min(4)=     3 -> 14     -0.06389
        min(5)=     4 -> 13     -0.06292
        #CIs=41 #CIs>0=21 #CIs<0=20

13   Singlet-B1   15.7335    78.80   0.2358   0.000
        max(1)=     5 -> 13      0.66537
        max(2)=     5 ->  8      0.11575
        max(3)=     5 ->  6      0.09714
        max(4)=     5 -> 10      0.06988
        max(5)=     5 -> 21      0.02661
        min(1)=     4 ->  9     -0.16392
        min(2)=     5 -> 15     -0.02624
        min(3)=     4 -> 18     -0.01546
        min(4)=     3 -> 20     -0.00964
        min(5)=     5 -> 16     -0.00954
        #CIs=25 #CIs>0=14 #CIs<0=11

14   Singlet-A1   15.7372    78.78   0.0256   0.000
        max(1)=     4 -> 10      0.61650
        max(2)=     4 ->  8      0.17460
        max(3)=     3 -> 12      0.03133
        max(4)=     5 ->  9      0.02985
        max(5)=     3 -> 14      0.01904
        min(1)=     4 ->  6     -0.25581
        min(2)=     4 -> 15     -0.11425
        min(3)=     3 ->  7     -0.06418
        min(4)=     4 -> 13     -0.05068
        min(5)=     3 -> 11     -0.03187
        #CIs=40 #CIs>0=15 #CIs<0=25

15   Singlet-B2   15.9655    77.66   0.1960   0.000
        max(1)=     4 -> 11      0.63282
        max(2)=     3 ->  6      0.07824
        max(3)=     3 -> 15      0.03434
        max(4)=     4 -> 17      0.03209
        max(5)=     5 -> 20      0.01834
        min(1)=     4 ->  7     -0.21697
        min(2)=     4 -> 12     -0.15568
        min(3)=     4 -> 14     -0.13131
        min(4)=     3 -> 13     -0.02863
```

```
          min(5)=        3 ->  8        -0.01830
          #CIs=34 #CIs>0=20 #CIs<0=14

16    Singlet-B2   17.3383        71.51    0.0078    0.000
          max(1)=        4 -> 12         0.62464
          max(2)=        4 -> 11         0.23694
          max(3)=        4 ->  7         0.21147
          max(4)=        4 -> 14         0.04462
          max(5)=        3 ->  6         0.01592
          min(1)=        4 -> 17        -0.07803
          min(2)=        3 -> 10        -0.01703
          min(3)=        4 -> 24        -0.00764
          min(4)=        3 ->  8        -0.00527
          min(5)=        2 ->  7        -0.00513
          #CIs=34 #CIs>0=17 #CIs<0=17

17    Singlet-A1   17.5348        70.71    0.0339    0.000
          max(1)=        4 -> 13         0.40651
          max(2)=        4 ->  8         0.24658
          max(3)=        4 ->  6         0.07958
          max(4)=        3 -> 12         0.06108
          max(5)=        4 -> 21         0.03034
          min(1)=        3 ->  7        -0.49006
          min(2)=        5 ->  9        -0.12969
          min(3)=        4 -> 10        -0.05437
          min(4)=        4 -> 15        -0.02547
          min(5)=        3 -> 14        -0.01832
          #CIs=41 #CIs>0=26 #CIs<0=15

18    Singlet-A1   17.6965        70.06    0.0067    0.000
          max(1)=        4 -> 13         0.55292
          max(2)=        3 ->  7         0.38995
          max(3)=        4 -> 10         0.12599
          max(4)=        5 ->  9         0.10510
          max(5)=        4 ->  6         0.07262
          min(1)=        4 ->  8        -0.07216
          min(2)=        5 -> 18        -0.02929
          min(3)=        4 -> 15        -0.02700
          min(4)=        4 -> 16        -0.02532
          min(5)=        3 -> 17        -0.02259
          #CIs=41 #CIs>0=14 #CIs<0=27

19    Singlet-A2   19.1457        64.76    0.0000    0.000
          max(1)=        3 ->  9         0.70306
          max(2)=        3 -> 18         0.07278
          max(3)=        5 -> 14         0.01330
          max(4)=        5 -> 11         0.01184
          max(5)=        3 -> 22         0.00346
          min(1)=        5 -> 12        -0.00607
          min(2)=        5 -> 17        -0.00354
          min(3)=        2 -> 29        -0.00273
          min(4)=        5 ->  7        -0.00200
          min(5)=        5 -> 24        -0.00164
          #CIs=18 #CIs>0=11 #CIs<0=7

20    Singlet-B2   19.1730        64.67    0.0189    0.000
          max(1)=        3 ->  8         0.56403
          max(2)=        3 ->  6         0.22703
          max(3)=        3 -> 15         0.06856
          max(4)=        2 -> 11         0.01950
          max(5)=        3 -> 25         0.00519
          min(1)=        3 -> 10        -0.33970
          min(2)=        3 -> 16        -0.06965
          min(3)=        3 -> 13        -0.06051
          min(4)=        4 -> 11        -0.02918
          min(5)=        4 -> 14        -0.01775
          #CIs=33 #CIs>0=12 #CIs<0=21

21    Singlet-B2   19.9832        62.04    0.2440    0.000
          max(1)=        3 -> 10         0.53455
          max(2)=        3 ->  8         0.40143
          max(3)=        4 -> 11         0.05526
          max(4)=        4 -> 14         0.03717
          max(5)=        2 -> 12         0.02623
          min(1)=        3 ->  6        -0.18860
          min(2)=        3 -> 13        -0.07845
          min(3)=        3 -> 15        -0.07263
          min(4)=        3 -> 21        -0.01982
          min(5)=        3 -> 19        -0.01230
          #CIs=34 #CIs>0=19 #CIs<0=15

22    Singlet-A1   20.4429        60.65    0.2268    0.000
```

```
max(1)=   3 -> 11   0.68186
max(2)=   5 ->  9   0.07609
max(3)=   4 -> 10   0.05693
max(4)=   4 -> 15   0.02959
max(5)=   2 ->  8   0.02204
min(1)=   4 ->  8  -0.08372
min(2)=   3 -> 14  -0.08321
min(3)=   3 ->  7  -0.07509
min(4)=   5 -> 18  -0.04105
min(5)=   4 -> 16  -0.03452
#CIs=38 #CIs>0=19 #CIs<0=19

23   Singlet-B2   21.5936   57.42   0.0146   0.000
max(1)=   3 -> 13   0.68816
max(2)=   3 ->  6   0.09417
max(3)=   3 ->  8   0.08007
max(4)=   3 -> 10   0.06493
max(5)=   4 -> 14   0.05304
min(1)=   3 -> 15  -0.02446
min(2)=   4 -> 12  -0.01946
min(3)=   3 -> 16  -0.01646
min(4)=   2 ->  7  -0.01594
min(5)=   2 -> 11  -0.01132
#CIs=34 #CIs>0=21 #CIs<0=13

24   Singlet-A1   22.3774   55.41   0.0038   0.000
max(1)=   3 -> 12   0.66336
max(2)=   3 ->  7   0.13470
max(3)=   4 ->  8   0.09661
max(4)=   5 -> 18   0.07963
max(5)=   4 -> 16   0.05954
min(1)=   5 ->  9  -0.09606
min(2)=   4 -> 10  -0.05992
min(3)=   4 -> 15  -0.05554
min(4)=   4 -> 13  -0.04185
min(5)=   3 -> 17  -0.03172
#CIs=38 #CIs>0=24 #CIs<0=14

25   Singlet-A2   22.6302   54.79   0.0000   0.000
max(1)=   5 -> 14   0.67160
max(2)=   5 -> 11   0.17631
max(3)=   5 -> 27   0.00309
max(4)=   2 -> 29   0.00193
max(5)=   3 -> 18   0.00032
min(1)=   5 -> 12  -0.12071
min(2)=   5 -> 24  -0.04651
min(3)=   5 -> 17  -0.02464
min(4)=   3 ->  9  -0.01695
min(5)=   5 -> 23  -0.01273
#CIs=17 #CIs>0=5 #CIs<0=12

26   Singlet-B1   24.5042   50.60   0.0603   0.000
max(1)=   5 -> 15   0.68640
max(2)=   5 -> 10   0.14307
max(3)=   5 -> 25   0.03245
max(4)=   3 -> 20   0.02433
max(5)=   5 -> 21   0.01642
min(1)=   5 -> 16  -0.06138
min(2)=   5 -> 19  -0.02465
min(3)=   5 ->  8  -0.02375
min(4)=   2 ->  9  -0.01869
min(5)=   4 -> 22  -0.01563
#CIs=26 #CIs>0=14 #CIs<0=12

27   Singlet-B2   25.6603   48.32   0.1368   0.000
max(1)=   4 -> 14   0.67300
max(2)=   4 -> 11   0.12166
max(3)=   3 -> 19   0.02661
max(4)=   2 -> 17   0.01065
max(5)=   2 -> 23   0.00927
min(1)=   4 -> 12  -0.09940
min(2)=   3 -> 15  -0.09057
min(3)=   3 -> 10  -0.07164
min(4)=   3 -> 13  -0.05417
min(5)=   5 -> 20  -0.04144
#CIs=35 #CIs>0=13 #CIs<0=22

28   Singlet-A1   26.6329   46.55   0.0014   0.000
max(1)=   4 -> 15   0.68371
max(2)=   4 -> 10   0.12677
max(3)=   3 -> 12   0.06187
max(4)=   5 -> 18   0.05178
```

```
max(5)=      4 -> 25     0.03802
min(1)=      3 -> 14    -0.05265
min(2)=      3 -> 11    -0.04027
min(3)=      5 ->  9    -0.02890
min(4)=      2 ->  6    -0.02531
min(5)=      2 -> 10    -0.02402
#CIs=41 #CIs>0=25 #CIs<0=16

29   Singlet-A1   29.8738   41.50   0.1879   0.000
max(1)=      3 -> 14     0.67362
max(2)=      5 -> 18     0.10998
max(3)=      3 -> 11     0.10357
max(4)=      4 -> 16     0.08018
max(5)=      4 -> 15     0.05176
min(1)=      3 -> 12    -0.05647
min(2)=      4 -> 19    -0.04197
min(3)=      2 ->  6    -0.03766
min(4)=      5 ->  9    -0.03354
min(5)=      3 -> 24    -0.02298
#CIs=41 #CIs>0=20 #CIs<0=21

30   Singlet-B2   31.0714   39.90   0.3134   0.000
max(1)=      3 -> 15     0.67968
max(2)=      3 -> 10     0.11095
max(3)=      4 -> 14     0.09533
max(4)=      2 -> 11     0.03544
max(5)=      3 -> 25     0.02414
min(1)=      5 -> 20    -0.06814
min(2)=      3 -> 16    -0.06393
min(3)=      4 -> 17    -0.04064
min(4)=      2 -> 14    -0.03912
min(5)=      2 -> 12    -0.02993
#CIs=35 #CIs>0=14 #CIs<0=21

31   Singlet-A1   32.0963   38.63   0.0133   0.000
max(1)=      2 ->  6     0.63250
max(2)=      2 -> 10     0.25262
max(3)=      5 -> 18     0.11731
max(4)=      4 -> 16     0.05076
max(5)=      4 -> 15     0.02899
min(1)=      2 -> 13    -0.09101
min(2)=      2 ->  8    -0.07473
min(3)=      2 -> 15    -0.05155
min(4)=      5 ->  9    -0.01481
min(5)=      3 -> 12    -0.00787
#CIs=40 #CIs>0=25 #CIs<0=15

32   Singlet-B1   33.7190   36.77   0.0231   0.000
max(1)=      5 -> 16     0.69503
max(2)=      5 ->  8     0.07297
max(3)=      5 -> 15     0.06835
max(4)=      5 -> 21     0.04478
max(5)=      3 -> 20     0.01845
min(1)=      4 -> 18    -0.03435
min(2)=      5 -> 10    -0.03166
min(3)=      5 -> 19    -0.02252
min(4)=      2 ->  9    -0.02200
min(5)=      5 -> 25    -0.01923
#CIs=25 #CIs>0=13 #CIs<0=12

33   Singlet-B2   33.7757   36.71   0.0051   0.000
max(1)=      2 ->  7     0.62408
max(2)=      2 -> 11     0.19587
max(3)=      5 -> 20     0.03739
max(4)=      2 -> 17     0.03603
max(5)=      4 -> 17     0.02389
min(1)=      2 -> 12    -0.24456
min(2)=      2 -> 14    -0.07528
min(3)=      3 -> 15    -0.03298
min(4)=      4 -> 14    -0.01900
min(5)=      3 -> 19    -0.01492
#CIs=33 #CIs>0=20 #CIs<0=13

34   Singlet-A1   35.2181   35.20   0.0045   0.000
max(1)=      5 -> 18     0.50657
max(2)=      2 -> 10     0.06044
max(3)=      2 ->  8     0.02961
max(4)=      4 -> 10     0.02261
max(5)=      5 -> 22     0.01503
min(1)=      4 -> 16    -0.46822
min(2)=      2 ->  6    -0.07725
min(3)=      4 ->  8    -0.05520
```

```
        min(4)=        5 ->  9        -0.04700
        min(5)=        4 -> 15        -0.04417
        #CIs=41 #CIs>0=15 #CIs<0=26

35      Singlet-A2   35.2394        35.18    0.0000    0.000
        max(1)=        5 -> 17         0.69875
        max(2)=        5 -> 12         0.09127
        max(3)=        5 -> 14         0.04491
        max(4)=        5 -> 24         0.02428
        max(5)=        5 -> 35         0.01103
        min(1)=        5 -> 32        -0.02214
        min(2)=        5 ->  7        -0.00764
        min(3)=        5 -> 23        -0.00494
        min(4)=        5 -> 11        -0.00440
        min(5)=        3 -> 18        -0.00405
        #CIs=19 #CIs>0=9 #CIs<0=10

36      Singlet-B1   36.3011        34.15    0.0120    0.000
        max(1)=        2 ->  9         0.70076
        max(2)=        2 -> 18         0.07258
        max(3)=        3 -> 20         0.02840
        max(4)=        5 -> 15         0.02030
        max(5)=        5 -> 16         0.01944
        min(1)=        5 -> 19        -0.02955
        min(2)=        5 -> 13        -0.01969
        min(3)=        4 -> 22        -0.01891
        min(4)=        5 -> 25        -0.00675
        min(5)=        5 -> 26        -0.00375
        #CIs=25 #CIs>0=15 #CIs<0=10

37      Singlet-A1   36.3670        34.09    0.0146    0.000
        max(1)=        2 ->  8         0.54910
        max(2)=        2 ->  6         0.21403
        max(3)=        2 -> 15         0.07624
        max(4)=        3 -> 14         0.02803
        max(5)=        5 -> 22         0.02250
        min(1)=        2 -> 10        -0.35381
        min(2)=        2 -> 13        -0.08652
        min(3)=        4 -> 16        -0.06861
        min(4)=        2 -> 16        -0.06769
        min(5)=        4 -> 19        -0.03761
        #CIs=41 #CIs>0=17 #CIs<0=24

38      Singlet-B2   36.7336        33.75    0.0025    0.000
        max(1)=        2 -> 11         0.60576
        max(2)=        5 -> 20         0.03480
        max(3)=        2 -> 17         0.02424
        max(4)=        4 -> 17         0.01709
        max(5)=        2 -> 24         0.01095
        min(1)=        2 ->  7        -0.27770
        min(2)=        2 -> 14        -0.16780
        min(3)=        2 -> 12        -0.15289
        min(4)=        3 -> 15        -0.03692
        min(5)=        4 -> 14        -0.01345
        #CIs=34 #CIs>0=18 #CIs<0=16

39      Singlet-B1   36.7426        33.74    0.0034    0.000
        max(1)=        4 -> 18         0.70094
        max(2)=        5 -> 16         0.03300
        max(3)=        5 -> 21         0.02603
        max(4)=        4 -> 33         0.02090
        max(5)=        4 -> 22         0.00959
        min(1)=        4 ->  9        -0.07683
        min(2)=        2 ->  9        -0.01632
        min(3)=        2 -> 22        -0.00614
        min(4)=        2 -> 28        -0.00459
        min(5)=        5 -> 25        -0.00272
        #CIs=25 #CIs>0=15 #CIs<0=10

40      Singlet-A1   36.8413        33.65    0.0009    0.000
        max(1)=        2 -> 10         0.48932
        max(2)=        2 ->  8         0.42051
        max(3)=        4 -> 16         0.18502
        max(4)=        5 -> 18         0.05012
        max(5)=        4 ->  8         0.01275
        min(1)=        2 ->  6        -0.17958
        min(2)=        2 -> 15        -0.10338
        min(3)=        3 -> 17        -0.03379
        min(4)=        3 -> 12        -0.02664
        min(5)=        3 -> 14        -0.02294
        #CIs=41 #CIs>0=20 #CIs<0=21
```

```
41    Singlet-B2   37.3220    33.22   0.0788   0.000
      max(1)=    4 -> 17    0.69084
      max(2)=    4 -> 12    0.08905
      max(3)=    4 -> 14    0.04788
      max(4)=    3 -> 15    0.02994
      max(5)=    4 -> 24    0.02886
      min(1)=    2 -> 12   -0.06707
      min(2)=    2 -> 11   -0.04041
      min(3)=    2 ->  7   -0.03286
      min(4)=    5 -> 20   -0.03012
      min(5)=    3 -> 16   -0.02383
      #CIs=34 #CIs>0=18 #CIs<0=16

42    Singlet-A1   38.6380    32.09   0.0004   0.000
      max(1)=    2 -> 13    0.65792
      max(2)=    2 ->  6    0.10789
      max(3)=    2 ->  8    0.08301
      max(4)=    3 -> 17    0.08141
      max(5)=    2 -> 10    0.06139
      min(1)=    4 -> 16   -0.14605
      min(2)=    5 -> 18   -0.11390
      min(3)=    2 -> 15   -0.03051
      min(4)=    2 -> 16   -0.01659
      min(5)=    5 -> 22   -0.00695
      #CIs=40 #CIs>0=22 #CIs<0=18

43    Singlet-B2   38.7323    32.01   0.0186   0.000
      max(1)=    2 -> 12    0.61562
      max(2)=    2 -> 11    0.24977
      max(3)=    2 ->  7    0.17607
      max(4)=    4 -> 17    0.07587
      max(5)=    2 -> 14    0.03229
      min(1)=    3 -> 16   -0.10873
      min(2)=    2 -> 17   -0.07037
      min(3)=    5 -> 20   -0.04642
      min(4)=    3 ->  8   -0.02409
      min(5)=    3 -> 10   -0.01045
      #CIs=35 #CIs>0=18 #CIs<0=17

44    Singlet-A1   39.7527    31.19   0.0544   0.000
      max(1)=    3 -> 17    0.44723
      max(2)=    2 -> 10    0.17107
      max(3)=    3 -> 14    0.11480
      max(4)=    3 -> 12    0.08843
      max(5)=    2 -> 15    0.05726
      min(1)=    4 -> 16   -0.33921
      min(2)=    5 -> 18   -0.28845
      min(3)=    2 -> 13   -0.19975
      min(4)=    2 ->  6   -0.02528
      min(5)=    4 -> 19   -0.02193
      #CIs=43 #CIs>0=20 #CIs<0=23

45    Singlet-B2   40.2449    30.81   0.0363   0.000
      max(1)=    3 -> 16    0.67925
      max(2)=    2 -> 12    0.08501
      max(3)=    3 -> 15    0.06213
      max(4)=    3 ->  8    0.06127
      max(5)=    2 -> 14    0.04825
      min(1)=    5 -> 20   -0.12247
      min(2)=    3 -> 10   -0.03104
      min(3)=    3 -> 19   -0.02494
      min(4)=    3 -> 25   -0.01723
      min(5)=    2 -> 23   -0.01113
      #CIs=33 #CIs>0=22 #CIs<0=11

46    Singlet-A2   41.1640    30.12   0.0000   0.000
      max(1)=    3 -> 18    0.70202
      max(2)=    3 -> 22    0.02970
      max(3)=    3 -> 33    0.01811
      max(4)=    2 -> 20    0.01617
      max(5)=    5 -> 17    0.00505
      min(1)=    3 ->  9   -0.07295
      min(2)=    4 -> 20   -0.01673
      min(3)=    2 -> 29   -0.00612
      min(4)=    5 -> 14   -0.00225
      min(5)=    5 -> 24   -0.00196
      #CIs=19 #CIs>0=11 #CIs<0=8

47    Singlet-B1   41.8180    29.65   0.0008   0.000
      max(1)=    5 -> 19    0.70008
      max(2)=    5 -> 21    0.07691
      max(3)=    2 ->  9    0.02496
```

```
max(4)=     5 -> 30     0.02382
max(5)=     5 -> 15     0.02338
min(1)=     5 -> 13    -0.02516
min(2)=     4 -> 22    -0.01895
min(3)=     5 -> 31    -0.00968
min(4)=     4 -> 18    -0.00468
min(5)=     2 -> 28    -0.00075
#CIs=26 #CIs>0=19 #CIs<0=7

48   Singlet-B2   43.8497   28.27   0.6294   0.000
max(1)=     5 -> 20     0.67056
max(2)=     3 -> 19     0.14827
max(3)=     3 -> 16     0.10714
max(4)=     3 -> 15     0.07597
max(5)=     2 -> 12     0.06606
min(1)=     3 -> 25    -0.02200
min(2)=     2 -> 11    -0.01317
min(3)=     4 -> 11    -0.01310
min(4)=     3 -> 10    -0.01190
min(5)=     2 -> 24    -0.01105
#CIs=35 #CIs>0=23 #CIs<0=12

49   Singlet-A1   44.4780   27.88   0.3529   0.000
max(1)=     4 -> 19     0.54294
max(2)=     4 -> 21     0.28533
max(3)=     5 -> 22     0.10177
max(4)=     2 -> 15     0.05775
max(5)=     3 -> 14     0.04971
min(1)=     3 -> 17    -0.25462
min(2)=     4 -> 16    -0.13944
min(3)=     5 -> 18    -0.12350
min(4)=     4 -> 13    -0.03786
min(5)=     2 -> 13    -0.03007
#CIs=43 #CIs>0=24 #CIs<0=19

50   Singlet-A2   44.8370   27.65   0.0000   0.000
max(1)=     4 -> 20     0.70534
max(2)=     4 -> 29     0.02893
max(3)=     3 -> 18     0.01829
max(4)=     2 -> 29     0.00567
max(5)=     5 -> 27     0.00497
min(1)=     2 -> 20    -0.02901
min(2)=     3 -> 22    -0.01984
min(3)=     5 -> 17    -0.00404
min(4)=     3 -> 28    -0.00155
min(5)=     5 -> 12    -0.00091
#CIs=19 #CIs>0=12 #CIs<0=7

51   Singlet-B1   44.9045   27.61   0.1799   0.000
max(1)=     5 -> 21     0.68550
max(2)=     4 -> 22     0.05002
max(3)=     2 -> 18     0.03913
max(4)=     5 -> 10     0.02225
max(5)=     5 -> 26     0.01838
min(1)=     3 -> 20    -0.12507
min(2)=     5 -> 19    -0.07038
min(3)=     5 -> 16    -0.04001
min(4)=     5 -> 13    -0.03376
min(5)=     4 -> 18    -0.02401
#CIs=26 #CIs>0=11 #CIs<0=15

52   Singlet-B2   45.9796   26.97   0.0095   0.000
max(1)=     2 -> 14     0.67546
max(2)=     2 -> 11     0.16138
max(3)=     3 -> 15     0.01766
max(4)=     4 -> 23     0.01378
max(5)=     3 -> 10     0.01057
min(1)=     2 -> 12    -0.10786
min(2)=     3 -> 16    -0.04498
min(3)=     2 -> 24    -0.03800
min(4)=     2 -> 17    -0.02782
min(5)=     4 -> 17    -0.02396
#CIs=35 #CIs>0=17 #CIs<0=18

53   Singlet-A1   46.2190   26.83   0.2598   0.000
max(1)=     2 -> 15     0.35197
max(2)=     4 -> 21     0.26330
max(3)=     2 -> 10     0.14142
max(4)=     2 -> 25     0.02856
max(5)=     5 -> 28     0.02179
min(1)=     4 -> 19    -0.36965
min(2)=     3 -> 17    -0.30946
```

```
        min(3)=     5 -> 22     -0.13103
        min(4)=     4 -> 16     -0.12079
        min(5)=     5 -> 18     -0.12025
        #CIs=43 #CIs>0=15 #CIs<0=28

54   Singlet-A1  47.2925     26.22   0.0000   0.000
        max(1)=     2 -> 15      0.46747
        max(2)=     5 -> 22      0.23390
        max(3)=     4 -> 19      0.11667
        max(4)=     2 -> 10      0.09411
        max(5)=     2 -> 25      0.02660
        min(1)=     4 -> 21     -0.44386
        min(2)=     3 -> 17     -0.04212
        min(3)=     2 -> 16     -0.03702
        min(4)=     5 -> 28     -0.02029
        min(5)=     2 -> 19     -0.02012
        #CIs=41 #CIs>0=21 #CIs<0=20

55   Singlet-B2  48.8593     25.38   0.5023   0.000
        max(1)=     3 -> 19      0.68478
        max(2)=     2 -> 23      0.04075
        max(3)=     3 -> 25      0.03362
        max(4)=     5 -> 29      0.01928
        max(5)=     4 -> 11      0.01174
        min(1)=     5 -> 20     -0.13906
        min(2)=     4 -> 14     -0.04404
        min(3)=     2 -> 12     -0.03880
        min(4)=     4 -> 24     -0.03616
        min(5)=     4 -> 23     -0.03296
        #CIs=36 #CIs>0=18 #CIs<0=18

56   Singlet-B1  49.3378     25.13   0.4700   0.000
        max(1)=     3 -> 20      0.66290
        max(2)=     4 -> 22      0.20740
        max(3)=     5 -> 21      0.09872
        max(4)=     2 -> 18      0.04911
        max(5)=     2 -> 22      0.03564
        min(1)=     5 -> 15     -0.02663
        min(2)=     2 ->  9     -0.02621
        min(3)=     5 -> 19     -0.02558
        min(4)=     4 -> 28     -0.02424
        min(5)=     5 -> 16     -0.01731
        #CIs=25 #CIs>0=16 #CIs<0=9

57   Singlet-A1  50.0322     24.78   0.4859   0.000
        max(1)=     5 -> 22      0.46561
        max(2)=     2 -> 21      0.04067
        max(3)=     3 -> 12      0.02742
        max(4)=     2 -> 10      0.02302
        max(5)=     4 ->  8      0.02256
        min(1)=     2 -> 15     -0.31405
        min(2)=     3 -> 17     -0.25054
        min(3)=     4 -> 19     -0.19490
        min(4)=     5 -> 18     -0.18599
        min(5)=     4 -> 16     -0.13515
        #CIs=41 #CIs>0=18 #CIs<0=23

58   Singlet-A1  50.7723     24.42   0.5155   0.000
        max(1)=     5 -> 22      0.43907
        max(2)=     4 -> 21      0.35649
        max(3)=     3 -> 17      0.22464
        max(4)=     5 -> 18      0.17803
        max(5)=     4 -> 16      0.17007
        min(1)=     3 -> 14     -0.08888
        min(2)=     4 -> 19     -0.07601
        min(3)=     3 -> 24     -0.06889
        min(4)=     2 -> 21     -0.06757
        min(5)=     4 -> 15     -0.04139
        #CIs=42 #CIs>0=21 #CIs<0=21

59   Singlet-B2  51.1934     24.22   0.0677   0.000
        max(1)=     3 -> 21      0.70073
        max(2)=     2 -> 17      0.07312
        max(3)=     3 -> 19      0.02049
        max(4)=     3 -> 26      0.01697
        max(5)=     3 -> 10      0.01441
        min(1)=     3 -> 13     -0.03992
        min(2)=     3 -> 16     -0.01375
        min(3)=     4 -> 24     -0.01175
        min(4)=     3 -> 30     -0.01132
        min(5)=     2 -> 14     -0.00923
        #CIs=34 #CIs>0=18 #CIs<0=16
```

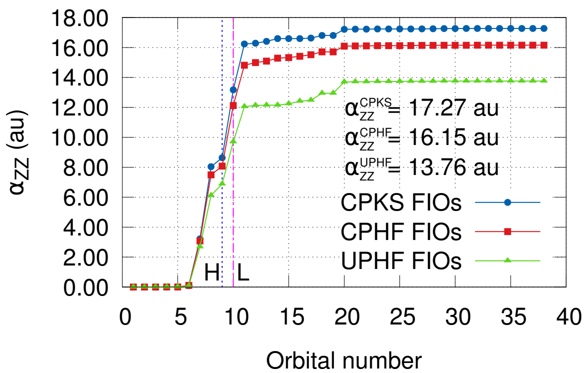
								min(1)=	3 -> 20	-0.18318
60	Singlet-B1		52.1627		23.77	1.0346	0.000	min(2)=	2 -> 18	-0.09098
		max(1)=		4 -> 22		0.66714		min(3)=	5 -> 21	-0.07206
		max(2)=		2 -> 9		0.03462		min(4)=	5 -> 25	-0.05107
		max(3)=		5 -> 19		0.03070		min(5)=	2 -> 22	-0.02926
		max(4)=		5 -> 15		0.03017		#CIs=25 #CIs>0=10 #CIs<0=15		
		max(5)=		5 -> 16		0.02095				

8 H_2S

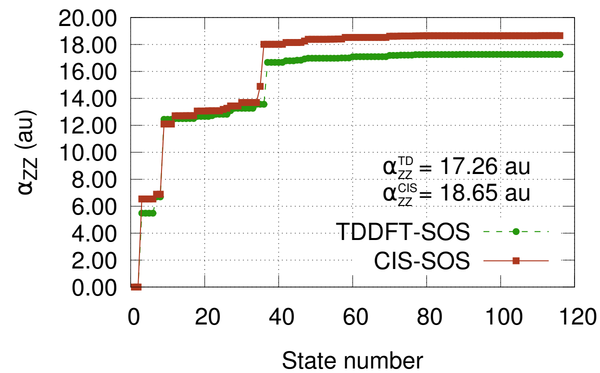
8.1 6-311G(d,p)

8.1.1 Plots

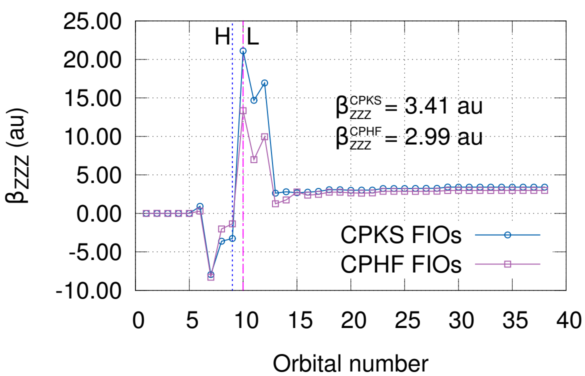
Figure S11: For H_2S molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S11a and S11c) or states (SOS approaches, in Plots S11b and S11d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.02 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



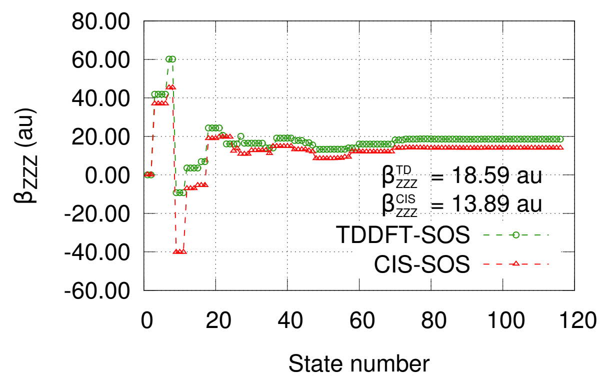
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

8.1.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-A2    6.1367        202.04    0.0000    0.000
       max(1)=        9 -> 11         0.70435
       max(2)=        9 -> 12         0.01945
       max(3)=        6 -> 19         0.00681
       max(4)=        8 -> 19         0.00487
       max(5)=        9 -> 27         0.00433
       min(1)=        9 -> 16        -0.06033
       min(2)=        9 -> 22        -0.00621
       min(3)=        7 -> 14        -0.00595
       min(4)=        8 -> 24        -0.00203
       min(5)=        9 -> 23        -0.00147
       #states=18 #states>0=7 #states<0=11

2        Singlet-B1    6.6231        187.20    0.0300    0.000
       max(1)=        9 -> 10         0.70574
       max(2)=        9 -> 13         0.03158
       max(3)=        9 -> 21         0.01189
       max(4)=        6 -> 20         0.00537
       max(5)=        6 -> 14         0.00458
       min(1)=        9 -> 17        -0.02781
       min(2)=        9 -> 15        -0.02244
       min(3)=        7 -> 19        -0.01261
       min(4)=        8 -> 20        -0.01088
       min(5)=        6 -> 25        -0.00237
       #states=24 #states>0=15 #states<0=9

3        Singlet-A1    9.6042        129.09    0.2275    0.000
       max(1)=        8 -> 10         0.69458
       max(2)=        7 -> 16         0.02000
       max(3)=        8 -> 18         0.00994
       max(4)=        6 -> 10         0.00497
       max(5)=        9 -> 20         0.00479
       min(1)=        7 -> 11        -0.11848
       min(2)=        9 -> 14        -0.04780
       min(3)=        8 -> 15        -0.02088
       min(4)=        8 -> 17        -0.01946
       min(5)=        6 -> 13        -0.00962
       #states=38 #states>0=18 #states<0=20

4        Singlet-A2    9.9884        124.13    0.0000    0.000
       max(1)=        9 -> 12         0.70624
       max(2)=        9 -> 22         0.01446
       max(3)=        9 -> 27         0.00631
       max(4)=        6 -> 19         0.00130
       max(5)=        9 -> 33         0.00092
       min(1)=        9 -> 16        -0.02251
       min(2)=        9 -> 11        -0.02132
       min(3)=        9 -> 23        -0.00530
       min(4)=        7 -> 14        -0.00178
       min(5)=        9 -> 31        -0.00140
       #states=18 #states>0=8 #states<0=10

5        Singlet-B2   10.0186        123.75    0.1793    0.000
       max(1)=        8 -> 11         0.68078
       max(2)=        7 -> 15         0.06911
       max(3)=        9 -> 19         0.05056
       max(4)=        8 -> 12         0.01396
       max(5)=        7 -> 13         0.01266
       min(1)=        7 -> 10        -0.17246
       min(2)=        7 -> 18        -0.02942
       min(3)=        6 -> 12        -0.01983
       min(4)=        6 -> 11        -0.01752
       min(5)=        8 -> 16        -0.00745
       #states=32 #states>0=13 #states<0=19

6        Singlet-B1   10.4787        118.32    0.0018    0.000
       max(1)=        9 -> 13         0.70295
       max(2)=        8 -> 20         0.01254
       max(3)=        9 -> 26         0.00918
       max(4)=        7 -> 19         0.00867
       max(5)=        9 -> 17         0.00596
       min(1)=        9 -> 15        -0.06523
```

min(2)= 9 -> 10 -0.03329

min(3)= 8 -> 14 -0.01451

min(4)= 6 -> 14 -0.00557

min(5)= 9 -> 18 -0.00470

#states=24 #states>0=9 #states<0=15

7 Singlet-A1 11.6289 106.62 0.0737 0.000

max(1)= 9 -> 14 0.61895

max(2)= 6 -> 10 0.03172

max(3)= 7 -> 16 0.00892

max(4)= 6 -> 13 0.00629

max(5)= 7 -> 23 0.00425

min(1)= 7 -> 11 -0.27824

min(2)= 8 -> 13 -0.16962

min(3)= 7 -> 12 -0.09646

min(4)= 9 -> 20 -0.01636

min(5)= 8 -> 18 -0.01285

#states=38 #states>0=17 #states<0=21

8 Singlet-B2 12.0005 103.32 0.6273 0.000

max(1)= 7 -> 10 0.67641

max(2)= 8 -> 11 0.16647

max(3)= 8 -> 12 0.08854

max(4)= 7 -> 13 0.07661

max(5)= 8 -> 16 0.02615

min(1)= 6 -> 12 -0.02424

min(2)= 7 -> 18 -0.01118

min(3)= 6 -> 16 -0.01006

min(4)= 7 -> 17 -0.00643

min(5)= 7 -> 21 -0.00473

#states=31 #states>0=15 #states<0=16

9 Singlet-A1 12.5786 98.57 0.4102 0.000

max(1)= 7 -> 11 0.60443

max(2)= 9 -> 14 0.20389

max(3)= 8 -> 10 0.11705

max(4)= 8 -> 15 0.10692

max(5)= 9 -> 20 0.03894

min(1)= 8 -> 13 -0.25663

min(2)= 6 -> 13 -0.02392

min(3)= 6 -> 17 -0.01535

min(4)= 8 -> 26 -0.01105

min(5)= 6 -> 18 -0.00936

#states=37 #states>0=18 #states<0=19

10 Singlet-B2 12.8738 96.31 0.0017 0.000

max(1)= 8 -> 12 0.69998

max(2)= 8 -> 22 0.01414

max(3)= 8 -> 27 0.00623

max(4)= 6 -> 12 0.00507

max(5)= 7 -> 30 0.00196

min(1)= 7 -> 10 -0.07937

min(2)= 8 -> 16 -0.03786

min(3)= 8 -> 11 -0.03488

min(4)= 6 -> 11 -0.02195

min(5)= 7 -> 13 -0.01772

#states=32 #states>0=14 #states<0=18

11 Singlet-B1 13.8437 89.56 0.1843 0.000

max(1)= 8 -> 14 0.53160

max(2)= 6 -> 14 0.01835

max(3)= 9 -> 18 0.01185

max(4)= 6 -> 20 0.00908

max(5)= 9 -> 21 0.00544

min(1)= 9 -> 15 -0.46366

min(2)= 9 -> 13 -0.03214

min(3)= 7 -> 19 -0.02046

min(4)= 8 -> 20 -0.01625

min(5)= 9 -> 10 -0.01399

#states=24 #states>0=15 #states<0=9

12 Singlet-A1 13.9451 88.91 0.0047 0.000

max(1)= 8 -> 13 0.59095

max(2)= 9 -> 14 0.19051

max(3)= 7 -> 11 0.15729

max(4)= 8 -> 15 0.10214

max(5)= 8 -> 10 0.04891

min(1)= 7 -> 12 -0.27337

min(2)= 8 -> 17 -0.01889

min(3)= 6 -> 17 -0.01885

min(4)= 7 -> 22 -0.01405

min(5)= 7 -> 27 -0.00716

```
        #states=38 #states>0=20 #states<0=18

13      Singlet-B1   14.1832        87.42    0.2250    0.000
        max(1)=        9 -> 15         0.52432
        max(2)=        8 -> 14         0.46534
        max(3)=        9 -> 13         0.05775
        max(4)=        8 -> 20         0.04483
        max(5)=        7 -> 19         0.04155
        min(1)=        6 -> 14        -0.02960
        min(2)=        9 -> 21        -0.02388
        min(3)=        9 -> 18        -0.01792
        min(4)=        6 -> 20        -0.00930
        min(5)=        9 -> 30        -0.00580
        #states=24 #states>0=11 #states<0=13

14      Singlet-A2   15.1065        82.07    0.0000    0.000
        max(1)=        9 -> 16         0.70316
        max(2)=        9 -> 11         0.05995
        max(3)=        7 -> 14         0.03194
        max(4)=        9 -> 12         0.02405
        max(5)=        9 -> 22         0.01650
        min(1)=        9 -> 27        -0.00944
        min(2)=        6 -> 19        -0.00574
        min(3)=        8 -> 19        -0.00331
        min(4)=        9 -> 31        -0.00254
        min(5)=        6 -> 24        -0.00074
        #states=18 #states>0=13 #states<0=5

15      Singlet-B2   15.7316        78.81    0.0116    0.000
        max(1)=        7 -> 13         0.69939
        max(2)=        6 -> 12         0.01545
        max(3)=        7 -> 18         0.01182
        max(4)=        7 -> 21         0.00913
        max(5)=        7 -> 26         0.00771
        min(1)=        7 -> 10        -0.07038
        min(2)=        7 -> 15        -0.04752
        min(3)=        6 -> 11        -0.03661
        min(4)=        8 -> 16        -0.02901
        min(5)=        8 -> 11        -0.02597
        #states=30 #states>0=15 #states<0=15

16      Singlet-A1   16.0085        77.45    0.0009    0.000
        max(1)=        7 -> 12         0.57083
        max(2)=        8 -> 15         0.35091
        max(3)=        8 -> 13         0.17185
        max(4)=        9 -> 14         0.12202
        max(5)=        6 -> 10         0.04200
        min(1)=        8 -> 18        -0.03258
        min(2)=        9 -> 20        -0.03232
        min(3)=        8 -> 17        -0.03155
        min(4)=        7 -> 11        -0.03142
        min(5)=        7 -> 16        -0.02785
        #states=38 #states>0=20 #states<0=18

17      Singlet-A2   16.2374        76.36    0.0000    0.000
        max(1)=        7 -> 14         0.70622
        max(2)=        8 -> 19         0.00674
        max(3)=        7 -> 28         0.00559
        max(4)=        9 -> 11         0.00308
        max(5)=        6 -> 19         0.00217
        min(1)=        9 -> 16        -0.03229
        min(2)=        7 -> 25        -0.01078
        min(3)=        8 -> 24        -0.00266
        min(4)=        9 -> 22        -0.00226
        min(5)=        9 -> 31        -0.00055
        #states=18 #states>0=11 #states<0=7

18      Singlet-A1   17.0906        72.55    0.0194    0.000
        max(1)=        8 -> 15         0.58020
        max(2)=        6 -> 17         0.04129
        max(3)=        8 -> 21         0.02503
        max(4)=        6 -> 15         0.01573
        max(5)=        9 -> 28         0.01180
        min(1)=        7 -> 12        -0.29133
        min(2)=        8 -> 13        -0.15155
        min(3)=        9 -> 14        -0.12753
        min(4)=        7 -> 11        -0.11240
        min(5)=        6 -> 10        -0.11115
        #states=38 #states>0=15 #states<0=23

19      Singlet-B2   18.0971        68.51    0.0232    0.000
        max(1)=        8 -> 16         0.61322
```

```
max(2)=    6 -> 11    0.04170
max(3)=    8 -> 11    0.03744
max(4)=    8 -> 12    0.03230
max(5)=    7 -> 17    0.01941
min(1)=    7 -> 15   -0.34197
min(2)=    9 -> 19   -0.03225
min(3)=    7 -> 10   -0.02769
min(4)=    6 -> 16   -0.01199
min(5)=    7 -> 21   -0.01034
#states=31 #states>0=23 #states<0=8

20  Singlet-B2  19.5598  63.39  0.0830  0.000
max(1)=    7 -> 15    0.58455
max(2)=    8 -> 16    0.32830
max(3)=    7 -> 18    0.05383
max(4)=    7 -> 13    0.03794
max(5)=    6 -> 12    0.03001
min(1)=    9 -> 19   -0.16164
min(2)=    6 -> 11   -0.12849
min(3)=    8 -> 11   -0.05179
min(4)=    7 -> 17   -0.03429
min(5)=    7 -> 10   -0.01490
#states=32 #states>0=19 #states<0=13

21  Singlet-B2  20.3042  61.06  0.0094  0.000
max(1)=    6 -> 11    0.68751
max(2)=    7 -> 15    0.13685
max(3)=    7 -> 13    0.04474
max(4)=    6 -> 12    0.03842
max(5)=    9 -> 19    0.03037
min(1)=    7 -> 17   -0.04419
min(2)=    6 -> 16   -0.02137
min(3)=    7 -> 10   -0.01536
min(4)=    7 -> 18   -0.01416
min(5)=    9 -> 24   -0.01097
#states=32 #states>0=17 #states<0=15

22  Singlet-A1  20.5496  60.33  0.0112  0.000
max(1)=    6 -> 10    0.50437
max(2)=    9 -> 20    0.10029
max(3)=    8 -> 18    0.06266
max(4)=    8 -> 21    0.01715
max(5)=    7 -> 22    0.01384
min(1)=    7 -> 16   -0.47757
min(2)=    7 -> 12   -0.03569
min(3)=    9 -> 14   -0.03327
min(4)=    6 -> 15   -0.02372
min(5)=    8 -> 13   -0.01713
#states=38 #states>0=15 #states<0=23

23  Singlet-A1  21.2525  58.34  0.0214  0.000
max(1)=    7 -> 16    0.49341
max(2)=    6 -> 10    0.47400
max(3)=    8 -> 15    0.10782
max(4)=    7 -> 22    0.04069
max(5)=    8 -> 21    0.03142
min(1)=    9 -> 14   -0.07346
min(2)=    9 -> 20   -0.05997
min(3)=    8 -> 13   -0.05383
min(4)=    7 -> 12   -0.05275
min(5)=    8 -> 18   -0.04297
#states=38 #states>0=19 #states<0=19

24  Singlet-B1  21.8636  56.71  0.3016  0.000
max(1)=    9 -> 17    0.67575
max(2)=    9 -> 18    0.19922
max(3)=    9 -> 10    0.02422
max(4)=    6 -> 14    0.01559
max(5)=    9 -> 32    0.00271
min(1)=    8 -> 20   -0.04252
min(2)=    7 -> 19   -0.02921
min(3)=    9 -> 15   -0.01561
min(4)=    8 -> 14   -0.00465
min(5)=    9 -> 30   -0.00454
#states=24 #states>0=12 #states<0=12

25  Singlet-B1  22.2070  55.83  0.0836  0.000
max(1)=    9 -> 18    0.67695
max(2)=    8 -> 20    0.03182
max(3)=    7 -> 19    0.03053
max(4)=    9 -> 15    0.02227
max(5)=    9 -> 26    0.00924
```

```
        min(1)=     9 -> 17     -0.19484
        min(2)=     6 -> 14     -0.03095
        min(3)=     9 -> 21     -0.01205
        min(4)=     9 -> 10     -0.00936
        min(5)=     9 -> 29     -0.00813
        #states=23 #states>0=12 #states<0=11

26   Singlet-B2   23.7240      52.26   0.1220   0.000
        max(1)=     6 -> 12      0.66374
        max(2)=     9 -> 19      0.23393
        max(3)=     8 -> 16      0.01576
        max(4)=     7 -> 10      0.01525
        max(5)=     7 -> 15      0.00961
        min(1)=     6 -> 11     -0.05142
        min(2)=     7 -> 17     -0.03099
        min(3)=     6 -> 16     -0.01705
        min(4)=     7 -> 13     -0.00840
        min(5)=     6 -> 23     -0.00388
        #states=30 #states>0=14 #states<0=16

27   Singlet-A1   24.1684      51.30   0.0713   0.000
        max(1)=     6 -> 13      0.66567
        max(2)=     9 -> 20      0.21278
        max(3)=     7 -> 16      0.02262
        max(4)=     8 -> 15      0.00974
        max(5)=     7 -> 11      0.00833
        min(1)=     8 -> 17     -0.09676
        min(2)=     6 -> 10     -0.02571
        min(3)=     8 -> 18     -0.01770
        min(4)=     8 -> 13     -0.01367
        min(5)=     7 -> 12     -0.01223
        #states=37 #states>0=17 #states<0=20

28   Singlet-A1   24.5575      50.49   0.0459   0.000
        max(1)=     8 -> 17      0.69727
        max(2)=     6 -> 13      0.09223
        max(3)=     6 -> 15      0.04423
        max(4)=     9 -> 20      0.03082
        max(5)=     8 -> 13      0.02263
        min(1)=     8 -> 18     -0.01368
        min(2)=     8 -> 21     -0.01333
        min(3)=     6 -> 17     -0.01203
        min(4)=     7 -> 11     -0.01009
        min(5)=     8 -> 29     -0.00957
        #states=38 #states>0=23 #states<0=15

29   Singlet-A1   24.7506      50.09   0.0000   0.000
        max(1)=     9 -> 20      0.49323
        max(2)=     7 -> 16      0.03197
        max(3)=     8 -> 29      0.00782
        max(4)=     7 -> 12      0.00622
        max(5)=     6 -> 18      0.00606
        min(1)=     8 -> 18     -0.47452
        min(2)=     6 -> 13     -0.17269
        min(3)=     7 -> 11     -0.01531
        min(4)=     7 -> 22     -0.01018
        min(5)=     6 -> 15     -0.01010
        #states=38 #states>0=19 #states<0=19

30   Singlet-B1   24.9203      49.75   0.0307   0.000
        max(1)=     6 -> 14      0.69740
        max(2)=     8 -> 20      0.08917
        max(3)=     7 -> 19      0.04966
        max(4)=     9 -> 15      0.02526
        max(5)=     9 -> 18      0.01986
        min(1)=     9 -> 21     -0.04497
        min(2)=     9 -> 17     -0.01376
        min(3)=     6 -> 25     -0.00751
        min(4)=     6 -> 20     -0.00558
        min(5)=     9 -> 10     -0.00209
        #states=23 #states>0=12 #states<0=11

31   Singlet-B2   25.4755      48.67   0.1569   0.000
        max(1)=     9 -> 19      0.56675
        max(2)=     7 -> 18      0.34208
        max(3)=     7 -> 15      0.08740
        max(4)=     8 -> 16      0.07374
        max(5)=     7 -> 17      0.02337
        min(1)=     6 -> 12     -0.20767
        min(2)=     8 -> 11     -0.04970
        min(3)=     8 -> 22     -0.04715
        min(4)=     6 -> 11     -0.02610
```

```
min(5)=        7 -> 21        -0.02543
#states=32 #states>0=17 #states<0=15

32   Singlet-A2   26.7526    46.34   0.0000   0.000
max(1)=        8 -> 19         0.70688
max(2)=        9 -> 16         0.00406
max(3)=        9 -> 33         0.00140
max(4)=        9 -> 31         0.00038
max(5)=        7 -> 28         0.00036
min(1)=        8 -> 24        -0.01287
min(2)=        6 -> 19        -0.00908
min(3)=        7 -> 14        -0.00658
min(4)=        9 -> 22        -0.00466
min(5)=        9 -> 11        -0.00458
#states=18 #states>0=8 #states<0=10

33   Singlet-B2   26.8165    46.23   0.0452   0.000
max(1)=        7 -> 17         0.70232
max(2)=        7 -> 15         0.04531
max(3)=        6 -> 12         0.03676
max(4)=        6 -> 11         0.03374
max(5)=        6 -> 16         0.02727
min(1)=        7 -> 18        -0.02880
min(2)=        8 -> 11        -0.01260
min(3)=        7 -> 26        -0.00957
min(4)=        9 -> 24        -0.00946
min(5)=        8 -> 27        -0.00576
#states=31 #states>0=16 #states<0=15

34   Singlet-A1   27.1740    45.63   0.0998   0.000
max(1)=        6 -> 15         0.68058
max(2)=        6 -> 13         0.03474
max(3)=        6 -> 10         0.02516
max(4)=        7 -> 11         0.02156
max(5)=        9 -> 14         0.01439
min(1)=        8 -> 18        -0.13433
min(2)=        9 -> 20        -0.09980
min(3)=        7 -> 16        -0.04832
min(4)=        8 -> 17        -0.04678
min(5)=        6 -> 17        -0.03046
#states=38 #states>0=18 #states<0=20

35   Singlet-B1   27.9258    44.40   0.1019   0.000
max(1)=        8 -> 20         0.61956
max(2)=        9 -> 21         0.18128
max(3)=        9 -> 17         0.02993
max(4)=        7 -> 24         0.00588
max(5)=        9 -> 30         0.00514
min(1)=        7 -> 19        -0.28231
min(2)=        6 -> 14        -0.04621
min(3)=        9 -> 15        -0.01943
min(4)=        9 -> 13        -0.01017
min(5)=        6 -> 20        -0.00921
#states=24 #states>0=12 #states<0=12

36   Singlet-B2   29.0272    42.71   0.1140   0.000
max(1)=        6 -> 16         0.66893
max(2)=        7 -> 18         0.19743
max(3)=        6 -> 12         0.04546
max(4)=        6 -> 11         0.03486
max(5)=        8 -> 11         0.02117
min(1)=        9 -> 19        -0.07958
min(2)=        7 -> 15        -0.04690
min(3)=        8 -> 16        -0.02622
min(4)=        7 -> 17        -0.01932
min(5)=        7 -> 30        -0.00900
#states=32 #states>0=16 #states<0=16

37   Singlet-A1   29.2152    42.44   1.1948   0.000
max(1)=        8 -> 18         0.48614
max(2)=        9 -> 20         0.41615
max(3)=        6 -> 15         0.17512
max(4)=        7 -> 16         0.11052
max(5)=        8 -> 15         0.07562
min(1)=        6 -> 13        -0.12333
min(2)=        7 -> 22        -0.11234
min(3)=        8 -> 21        -0.10008
min(4)=        7 -> 11        -0.07222
min(5)=        8 -> 10        -0.02790
#states=38 #states>0=23 #states<0=15
```

8.1.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-A2    6.5858        188.26    0.0000    0.000
          max(1)=        9 -> 11         0.68473
          max(2)=        9 -> 16         0.15654
          max(3)=        9 -> 22         0.01734
          max(4)=        7 -> 14         0.00533
          max(5)=        7 -> 20         0.00230
          min(1)=        9 -> 12        -0.07773
          min(2)=        9 -> 28        -0.01399
          min(3)=        9 -> 23        -0.00575
          min(4)=        6 -> 24        -0.00478
          min(5)=        6 -> 19        -0.00109
          #states=17 #states>0=10 #states<0=7

2        Singlet-B1    7.3651        168.34    0.0293    0.000
          max(1)=        9 -> 10         0.69679
          max(2)=        9 -> 13         0.05818
          max(3)=        9 -> 21         0.00753
          max(4)=        9 -> 26         0.00566
          max(5)=        9 -> 29         0.00506
          min(1)=        9 -> 15        -0.07391
          min(2)=        9 -> 17        -0.06890
          min(3)=        8 -> 20        -0.01783
          min(4)=        7 -> 19        -0.01594
          min(5)=        8 -> 14        -0.01013
          #states=22 #states>0=14 #states<0=8

3        Singlet-A1   10.4995        118.09    0.3246    0.000
          max(1)=        8 -> 10         0.68556
          max(2)=        7 -> 11         0.05393
          max(3)=        7 -> 12         0.03096
          max(4)=        7 -> 16         0.02463
          max(5)=        8 -> 18         0.00874
          min(1)=        9 -> 14        -0.12854
          min(2)=        8 -> 15        -0.06941
          min(3)=        8 -> 17        -0.05471
          min(4)=        6 -> 13        -0.02563
          min(5)=        8 -> 21        -0.01313
          #states=36 #states>0=20 #states<0=16

4        Singlet-A2   10.6850        116.04    0.0000    0.000
          max(1)=        9 -> 12         0.69713
          max(2)=        9 -> 11         0.09295
          max(3)=        9 -> 22         0.03202
          max(4)=        9 -> 28         0.01743
          max(5)=        9 -> 23         0.01093
          min(1)=        9 -> 16        -0.06207
          min(2)=        8 -> 19        -0.00429
          min(3)=        6 -> 19        -0.00422
          min(4)=        7 -> 20        -0.00136
          min(5)=        7 -> 27        -0.00045
          #states=16 #states>0=10 #states<0=6

5        Singlet-B2   10.8617        114.15    0.3294    0.000
          max(1)=        8 -> 11         0.68080
          max(2)=        7 -> 10         0.10204
          max(3)=        8 -> 16         0.09296
          max(4)=        7 -> 18         0.04348
          max(5)=        6 -> 12         0.02506
          min(1)=        7 -> 15        -0.07779
          min(2)=        8 -> 12        -0.06554
          min(3)=        9 -> 19        -0.05814
          min(4)=        7 -> 13        -0.02140
          min(5)=        7 -> 21        -0.01613
          #states=30 #states>0=15 #states<0=15

6        Singlet-B1   11.1118        111.58    0.0028    0.000
          max(1)=        9 -> 13         0.69731
          max(2)=        9 -> 26         0.02083
          max(3)=        9 -> 29         0.01391
          max(4)=        9 -> 21         0.01318
          max(5)=        7 -> 19         0.00973
          min(1)=        9 -> 15        -0.08998
          min(2)=        9 -> 10        -0.06723
          min(3)=        9 -> 18        -0.00870
```

```
min(4)=        6 -> 20        -0.00619
min(5)=        6 -> 14        -0.00349
#states=21 #states>0=10 #states<0=11

7    Singlet-A1   12.2558        101.16    0.0237    0.000
max(1)=        9 -> 14         0.62332
max(2)=        7 -> 11         0.22171
max(3)=        8 -> 10         0.10470
max(4)=        7 -> 16         0.04615
max(5)=        6 -> 10         0.02881
min(1)=        8 -> 13        -0.18241
min(2)=        7 -> 12        -0.11430
min(3)=        7 -> 22        -0.01541
min(4)=        8 -> 21        -0.01539
min(5)=        9 -> 20        -0.01534
#states=33 #states>0=14 #states<0=19

8    Singlet-B2   12.8484         96.50    0.6319    0.000
max(1)=        7 -> 10         0.64037
max(2)=        8 -> 12         0.23951
max(3)=        7 -> 13         0.13566
max(4)=        6 -> 11         0.01482
max(5)=        9 -> 19         0.01473
min(1)=        8 -> 11        -0.07216
min(2)=        7 -> 15        -0.05929
min(3)=        6 -> 12        -0.05095
min(4)=        7 -> 17        -0.04315
min(5)=        6 -> 22        -0.01094
#states=29 #states>0=15 #states<0=14

9    Singlet-A1   13.6624         90.75    0.4377    0.000
max(1)=        7 -> 11         0.58606
max(2)=        8 -> 13         0.33292
max(3)=        7 -> 16         0.07521
max(4)=        6 -> 13         0.02747
max(5)=        8 -> 26         0.01669
min(1)=        9 -> 14        -0.11802
min(2)=        8 -> 15        -0.09211
min(3)=        7 -> 12        -0.08284
min(4)=        8 -> 10        -0.07602
min(5)=        9 -> 20        -0.04588
#states=34 #states>0=15 #states<0=19

10   Singlet-B2   13.8864         89.28    0.0418    0.000
max(1)=        8 -> 12         0.65398
max(2)=        8 -> 11         0.10921
max(3)=        7 -> 15         0.03021
max(4)=        8 -> 22         0.02657
max(5)=        6 -> 11         0.02025
min(1)=        7 -> 10        -0.22128
min(2)=        8 -> 16        -0.08366
min(3)=        7 -> 13        -0.03516
min(4)=        9 -> 19        -0.01324
min(5)=        6 -> 16        -0.01071
#states=26 #states>0=15 #states<0=11

11   Singlet-B1   14.6024         84.91    0.1917    0.000
max(1)=        8 -> 14         0.57188
max(2)=        6 -> 14         0.02306
max(3)=        8 -> 27         0.01721
max(4)=        9 -> 18         0.01592
max(5)=        9 -> 17         0.00826
min(1)=        9 -> 15        -0.40764
min(2)=        9 -> 13        -0.05529
min(3)=        9 -> 10        -0.03066
min(4)=        8 -> 20        -0.02703
min(5)=        7 -> 19        -0.01888
#states=22 #states>0=11 #states<0=11

12   Singlet-A1   15.0230         82.53    0.0624    0.000
max(1)=        8 -> 13         0.55913
max(2)=        9 -> 14         0.20483
max(3)=        8 -> 15         0.11323
max(4)=        8 -> 10         0.07694
max(5)=        9 -> 20         0.02621
min(1)=        7 -> 11        -0.27715
min(2)=        7 -> 12        -0.21317
min(3)=        7 -> 22        -0.02652
min(4)=        6 -> 17        -0.02498
min(5)=        8 -> 17        -0.02454
#states=36 #states>0=17 #states<0=19
```

13 Singlet-B1 15.0892 82.17 0.3497 0.000

max(1)= 9 -> 15 0.55687

max(2)= 8 -> 14 0.41379

max(3)= 9 -> 13 0.07593

max(4)= 9 -> 10 0.06299

max(5)= 8 -> 20 0.05776

min(1)= 6 -> 14 -0.03077

min(2)= 9 -> 18 -0.02858

min(3)= 8 -> 25 -0.01303

min(4)= 9 -> 30 -0.01140

min(5)= 6 -> 20 -0.01103

#states=22 #states>0=10 #states<0=12

14 Singlet-A2 16.1920 76.57 0.0000 0.000

max(1)= 9 -> 16 0.68481

max(2)= 9 -> 12 0.07979

max(3)= 9 -> 22 0.03659

max(4)= 7 -> 14 0.02087

max(5)= 7 -> 20 0.00394

min(1)= 9 -> 11 -0.14917

min(2)= 9 -> 28 -0.02258

min(3)= 9 -> 23 -0.00754

min(4)= 9 -> 31 -0.00508

min(5)= 6 -> 24 -0.00448

#states=15 #states>0=9 #states<0=6

15 Singlet-A1 17.0097 72.89 0.0006 0.000

max(1)= 7 -> 12 0.52676

max(2)= 8 -> 15 0.42837

max(3)= 8 -> 13 0.12368

max(4)= 7 -> 11 0.08776

max(5)= 9 -> 14 0.08552

min(1)= 8 -> 18 -0.04567

min(2)= 9 -> 20 -0.04442

min(3)= 8 -> 17 -0.03462

min(4)= 6 -> 15 -0.02922

min(5)= 6 -> 17 -0.01887

#states=36 #states>0=22 #states<0=14

16 Singlet-B2 17.1768 72.18 0.0381 0.000

max(1)= 7 -> 13 0.68943

max(2)= 8 -> 11 0.03639

max(3)= 6 -> 11 0.02536

max(4)= 7 -> 21 0.02406

max(5)= 7 -> 18 0.01921

min(1)= 7 -> 10 -0.13665

min(2)= 9 -> 19 -0.03357

min(3)= 7 -> 15 -0.02057

min(4)= 8 -> 12 -0.01820

min(5)= 8 -> 16 -0.01751

#states=27 #states>0=14 #states<0=13

17 Singlet-A2 17.5608 70.60 0.0000 0.000

max(1)= 7 -> 14 0.70593

max(2)= 7 -> 27 0.01561

max(3)= 7 -> 20 0.01196

max(4)= 8 -> 19 0.01105

max(5)= 6 -> 24 0.00488

min(1)= 7 -> 25 -0.02345

min(2)= 9 -> 16 -0.02107

min(3)= 6 -> 19 -0.00897

min(4)= 9 -> 12 -0.00511

min(5)= 8 -> 24 -0.00412

#states=16 #states>0=6 #states<0=10

18 Singlet-A1 18.4442 67.22 0.0525 0.000

max(1)= 8 -> 15 0.52475

max(2)= 7 -> 11 0.09097

max(3)= 8 -> 21 0.04737

max(4)= 6 -> 17 0.04519

max(5)= 8 -> 10 0.03741

min(1)= 7 -> 12 -0.39045

min(2)= 9 -> 14 -0.15935

min(3)= 8 -> 13 -0.15024

min(4)= 7 -> 16 -0.07807

min(5)= 8 -> 18 -0.03334

#states=37 #states>0=18 #states<0=19

19 Singlet-B2 19.4648 63.70 0.0170 0.000

max(1)= 8 -> 16 0.61072

max(2)= 8 -> 12 0.08582

max(3)= 7 -> 18 0.04182

max(4)= 7 -> 17 0.02978

max(5)= 8 -> 22 0.02737

min(1)= 7 -> 15 -0.31294

min(2)= 8 -> 11 -0.10696

min(3)= 7 -> 10 -0.06738

min(4)= 9 -> 19 -0.03711

min(5)= 7 -> 21 -0.01860

#states=29 #states>0=17 #states<0=12

20 Singlet-B2 20.6228 60.12 0.1434 0.000

max(1)= 7 -> 15 0.60606

max(2)= 8 -> 16 0.30223

max(3)= 7 -> 10 0.04738

max(4)= 7 -> 18 0.03086

max(5)= 7 -> 13 0.02800

min(1)= 9 -> 19 -0.17337

min(2)= 6 -> 11 -0.06650

min(3)= 7 -> 17 -0.02562

min(4)= 6 -> 16 -0.01600

min(5)= 7 -> 26 -0.01249

#states=31 #states>0=19 #states<0=12

21 Singlet-A1 22.4841 55.14 0.0044 0.000

max(1)= 7 -> 16 0.66850

max(2)= 8 -> 15 0.05812

max(3)= 8 -> 17 0.03117

max(4)= 7 -> 22 0.02442

max(5)= 6 -> 21 0.01377

min(1)= 9 -> 20 -0.14210

min(2)= 6 -> 10 -0.10299

min(3)= 7 -> 11 -0.07685

min(4)= 8 -> 18 -0.06477

min(5)= 6 -> 13 -0.04927

#states=36 #states>0=17 #states<0=19

22 Singlet-B1 22.9087 54.12 0.2891 0.000

max(1)= 9 -> 17 0.67671

max(2)= 9 -> 18 0.18405

max(3)= 9 -> 10 0.06453

max(4)= 6 -> 14 0.04007

max(5)= 6 -> 27 0.01071

min(1)= 8 -> 20 -0.03162

min(2)= 7 -> 19 -0.02276

min(3)= 8 -> 14 -0.01301

min(4)= 9 -> 30 -0.01280

min(5)= 9 -> 21 -0.01019

#states=23 #states>0=13 #states<0=10

23 Singlet-B2 23.2098 53.42 0.0020 0.000

max(1)= 6 -> 11 0.67826

max(2)= 6 -> 16 0.13457

max(3)= 7 -> 15 0.04326

max(4)= 7 -> 17 0.01610

max(5)= 8 -> 16 0.01539

min(1)= 9 -> 19 -0.10357

min(2)= 6 -> 12 -0.08538

min(3)= 7 -> 13 -0.02411

min(4)= 8 -> 12 -0.02148

min(5)= 6 -> 28 -0.00878

#states=31 #states>0=14 #states<0=17

24 Singlet-B1 23.2490 53.33 0.0912 0.000

max(1)= 9 -> 18 0.67944

max(2)= 8 -> 20 0.04431

max(3)= 7 -> 19 0.03545

max(4)= 9 -> 15 0.02539

max(5)= 9 -> 26 0.02399

min(1)= 9 -> 17 -0.17843

min(2)= 6 -> 14 -0.03089

min(3)= 9 -> 29 -0.02282

min(4)= 9 -> 10 -0.01832

min(5)= 9 -> 21 -0.00711

#states=22 #states>0=12 #states<0=10

25 Singlet-A1 23.9737 51.72 0.0267 0.000

max(1)= 6 -> 10 0.68376

max(2)= 7 -> 16 0.10727

max(3)= 6 -> 13 0.04879

max(4)= 8 -> 15 0.03537

max(5)= 9 -> 20 0.03218

min(1)= 6 -> 15 -0.10323

min(2)= 9 -> 14 -0.04660

```
        min(3)=      6 -> 17      -0.02330
        min(4)=      9 -> 25      -0.02039
        min(5)=      8 -> 13      -0.01979
        #states=38 #states>0=22 #states<0=16

26   Singlet-A1   25.7829   48.09   0.0246   0.000
        max(1)=      9 -> 20       0.53598
        max(2)=      8 -> 17       0.06690
        max(3)=      7 -> 16       0.06441
        max(4)=      6 -> 13       0.03817
        max(5)=      8 -> 29       0.01684
        min(1)=      8 -> 18      -0.44563
        min(2)=      6 -> 10      -0.04562
        min(3)=      9 -> 25      -0.02035
        min(4)=      8 -> 26      -0.01530
        min(5)=      6 -> 15      -0.01423
        #states=32 #states>0=18 #states<0=14

27   Singlet-A1   25.9826   47.72   0.0525   0.000
        max(1)=      8 -> 17       0.69735
        max(2)=      8 -> 10       0.06052
        max(3)=      8 -> 18       0.05459
        max(4)=      6 -> 13       0.03048
        max(5)=      8 -> 15       0.02624
        min(1)=      9 -> 20      -0.04304
        min(2)=      7 -> 16      -0.03203
        min(3)=      7 -> 22      -0.01743
        min(4)=      6 -> 15      -0.01633
        min(5)=      8 -> 21      -0.01496
        #states=36 #states>0=21 #states<0=15

28   Singlet-B2   26.2831   47.17   0.4513   0.000
        max(1)=      9 -> 19       0.54843
        max(2)=      6 -> 12       0.32973
        max(3)=      7 -> 18       0.22509
        max(4)=      6 -> 11       0.12144
        max(5)=      7 -> 15       0.11253
        min(1)=      8 -> 22      -0.04148
        min(2)=      9 -> 24      -0.02500
        min(3)=      7 -> 21      -0.02163
        min(4)=      6 -> 16      -0.01091
        min(5)=      7 -> 29      -0.00514
        #states=30 #states>0=20 #states<0=10

29   Singlet-B2   27.3836   45.28   0.0244   0.000
        max(1)=      6 -> 12       0.60364
        max(2)=      6 -> 11       0.04340
        max(3)=      7 -> 10       0.04293
        max(4)=      8 -> 22       0.02612
        max(5)=      6 -> 23       0.01654
        min(1)=      9 -> 19      -0.25686
        min(2)=      7 -> 18      -0.24109
        min(3)=      7 -> 15      -0.05294
        min(4)=      8 -> 11      -0.03880
        min(5)=      7 -> 17      -0.02469
        #states=30 #states>0=16 #states<0=14

30   Singlet-A1   27.4499   45.17   0.0862   0.000
        max(1)=      6 -> 13       0.68473
        max(2)=      8 -> 18       0.12654
        max(3)=      7 -> 16       0.06091
        max(4)=      9 -> 20       0.04956
        max(5)=      6 -> 15       0.03752
        min(1)=      6 -> 10      -0.05575
        min(2)=      8 -> 17      -0.03697
        min(3)=      7 -> 11      -0.01656
        min(4)=      8 -> 13      -0.01134
        min(5)=      9 -> 14      -0.00505
        #states=33 #states>0=19 #states<0=14

31   Singlet-A2   27.8593   44.50   0.0000   0.000
        max(1)=      8 -> 19       0.70440
        max(2)=      7 -> 20       0.04287
        max(3)=      7 -> 25       0.00611
        max(4)=      9 -> 12       0.00475
        max(5)=      7 -> 27       0.00348
        min(1)=      8 -> 24      -0.03651
        min(2)=      6 -> 24      -0.01568
        min(3)=      9 -> 22      -0.01320
        min(4)=      7 -> 14      -0.01187
        min(5)=      9 -> 16      -0.00359
        #states=17 #states>0=9 #states<0=8
```

32 Singlet-B1 28.0712 44.17 0.0259 0.000

max(1)= 6 -> 14 0.68642

max(2)= 8 -> 20 0.15865

max(3)= 9 -> 15 0.02140

max(4)= 7 -> 19 0.02128

max(5)= 9 -> 21 0.01638

min(1)= 9 -> 17 -0.03629

min(2)= 6 -> 25 -0.02477

min(3)= 9 -> 29 -0.00325

min(4)= 9 -> 32 -0.00303

min(5)= 8 -> 14 -0.00287

#states=23 #states>0=13 #states<0=10

33 Singlet-B2 28.5619 43.41 0.0609 0.000

max(1)= 7 -> 17 0.69996

max(2)= 7 -> 10 0.05014

max(3)= 7 -> 15 0.02719

max(4)= 6 -> 22 0.02123

max(5)= 7 -> 13 0.01600

min(1)= 6 -> 16 -0.04718

min(2)= 7 -> 18 -0.04293

min(3)= 7 -> 21 -0.02361

min(4)= 7 -> 26 -0.01829

min(5)= 7 -> 30 -0.01100

#states=32 #states>0=13 #states<0=19

34 Singlet-B1 29.4276 42.13 0.1699 0.000

max(1)= 8 -> 20 0.61419

max(2)= 9 -> 21 0.18257

max(3)= 9 -> 17 0.03571

max(4)= 6 -> 20 0.01659

max(5)= 7 -> 24 0.01149

min(1)= 7 -> 19 -0.25679

min(2)= 6 -> 14 -0.13514

min(3)= 9 -> 15 -0.04316

min(4)= 8 -> 25 -0.02617

min(5)= 9 -> 18 -0.01927

#states=22 #states>0=9 #states<0=13

35 Singlet-A1 29.9642 41.38 0.4855 0.000

max(1)= 6 -> 15 0.58105

max(2)= 6 -> 10 0.09990

max(3)= 7 -> 22 0.06465

max(4)= 6 -> 13 0.05422

max(5)= 8 -> 21 0.04070

min(1)= 8 -> 18 -0.29450

min(2)= 9 -> 20 -0.21756

min(3)= 7 -> 16 -0.05893

min(4)= 6 -> 17 -0.03765

min(5)= 8 -> 15 -0.03296

#states=34 #states>0=14 #states<0=20

36 Singlet-A1 30.9514 40.06 1.3451 0.000

max(1)= 8 -> 18 0.41756

max(2)= 6 -> 15 0.38131

max(3)= 9 -> 20 0.35079

max(4)= 7 -> 16 0.11347

max(5)= 8 -> 15 0.06554

min(1)= 6 -> 13 -0.13218

min(2)= 8 -> 21 -0.08333

min(3)= 7 -> 22 -0.07424

min(4)= 8 -> 10 -0.02169

min(5)= 9 -> 25 -0.01317

#states=37 #states>0=22 #states<0=15

37 Singlet-B2 31.3201 39.59 1.2738 0.000

max(1)= 7 -> 18 0.60533

max(2)= 8 -> 22 0.13722

max(3)= 6 -> 12 0.10996

max(4)= 7 -> 21 0.10270

max(5)= 7 -> 17 0.03935

min(1)= 9 -> 19 -0.26592

min(2)= 8 -> 16 -0.10003

min(3)= 8 -> 11 -0.06017

min(4)= 7 -> 15 -0.05849

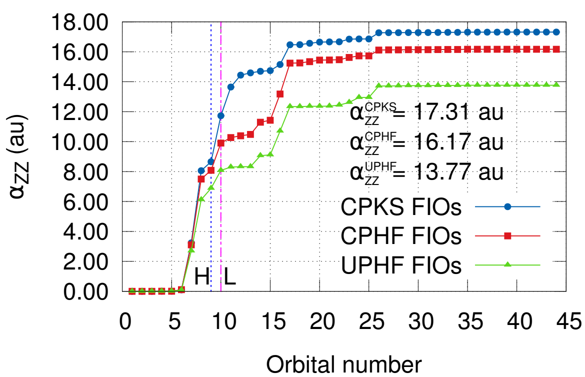
min(5)= 7 -> 13 -0.03313

#states=32 #states>0=15 #states<0=17

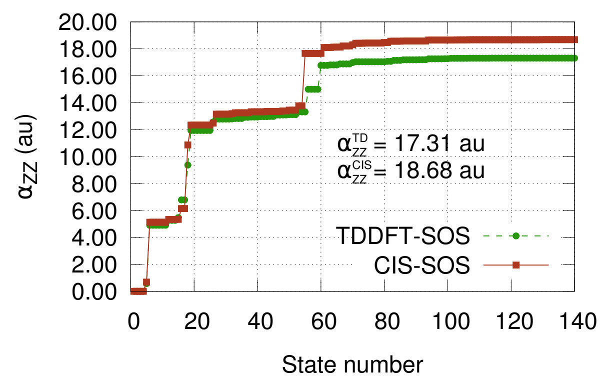
8.2 6-311++G(d,p)

8.2.1 Plots

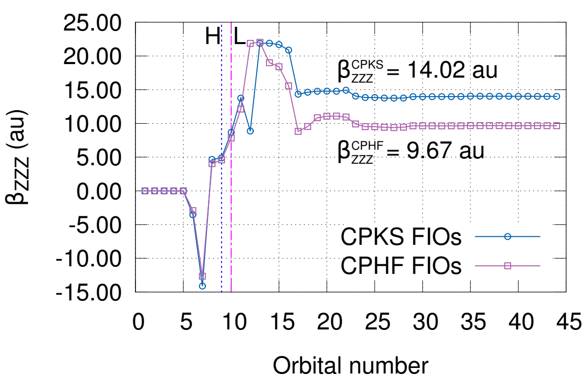
Figure S12: For H_2S molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S12a and S12c) or states (SOS approaches, in Plots S12b and S12d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.02 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



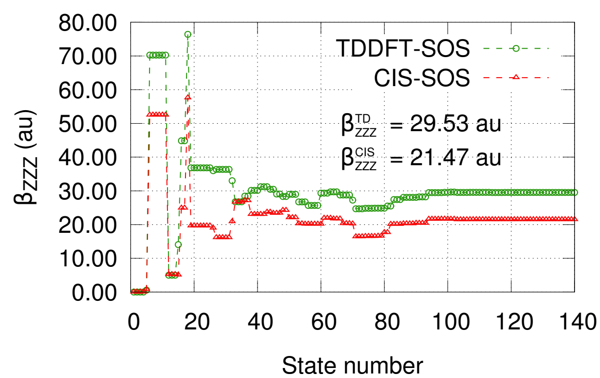
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

8.2.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1       Singlet-B1    5.8982        210.21    0.0486    0.000
        max(1)=        9 -> 10         0.68903
        max(2)=        9 -> 19         0.01598
        max(3)=        9 -> 27         0.00650
        max(4)=        6 -> 26         0.00364
        max(5)=        6 -> 20         0.00262
        min(1)=        9 -> 17        -0.15758
        min(2)=        9 -> 24        -0.01260
        min(3)=        9 -> 13        -0.01112
        min(4)=        9 -> 15        -0.00952
        min(5)=        7 -> 25        -0.00731
        #CIs=30 #CIs>0=16 #CIs<0=13

2       Singlet-A2    6.0526        204.84    0.0000    0.000
        max(1)=        9 -> 11         0.57869
        max(2)=        9 -> 22         0.03410
        max(3)=        6 -> 25         0.00671
        max(4)=        8 -> 25         0.00469
        max(5)=        9 -> 34         0.00412
        min(1)=        9 -> 12        -0.35211
        min(2)=        9 -> 16        -0.20026
        min(3)=        9 -> 28        -0.00594
        min(4)=        7 -> 14        -0.00450
        min(5)=        7 -> 20        -0.00368
        #CIs=21 #CIs>0=7 #CIs<0=13

3       Singlet-A2    7.6518        162.03    0.0000    0.000
        max(1)=        9 -> 12         0.60616
        max(2)=        9 -> 11         0.35473
        max(3)=        9 -> 18         0.07047
        max(4)=        7 -> 14         0.00394
        max(5)=        9 -> 28         0.00377
        min(1)=        9 -> 16        -0.04178
        min(2)=        8 -> 25        -0.00083
        min(3)=        7 -> 26        -0.00060
        min(4)=        7 -> 20        -0.00059
        min(5)=        9 -> 29        -0.00059
        #CIs=21 #CIs>0=8 #CIs<0=12

4       Singlet-B1    7.9539        155.88    0.0256    0.000
        max(1)=        9 -> 13         0.70336
        max(2)=        9 -> 19         0.06468
        max(3)=        9 -> 15         0.01784
        max(4)=        8 -> 14         0.01081
        max(5)=        9 -> 10         0.00506
        min(1)=        9 -> 17        -0.02254
        min(2)=        9 -> 21        -0.01111
        min(3)=        8 -> 33        -0.00125
        min(4)=        7 -> 30        -0.00120
        min(5)=        8 -> 20        -0.00110
        #CIs=30 #CIs>0=16 #CIs<0=13

5       Singlet-A1    8.2969        149.44    0.0178    0.000
        max(1)=        9 -> 14         0.68625
        max(2)=        8 -> 17         0.03457
        max(3)=        9 -> 20         0.02136
        max(4)=        7 -> 16         0.01664
        max(5)=        8 -> 15         0.01396
        min(1)=        8 -> 10        -0.15111
        min(2)=        8 -> 13        -0.03731
        min(3)=        7 -> 11        -0.03663
        min(4)=        8 -> 19        -0.02913
        min(5)=        7 -> 18        -0.02161
        #CIs=49 #CIs>0=19 #CIs<0=26

6       Singlet-A1    8.8803        139.62    0.1538    0.000
        max(1)=        8 -> 10         0.67052
        max(2)=        9 -> 14         0.14764
        max(3)=        7 -> 12         0.04488
        max(4)=        7 -> 16         0.03557
        max(5)=        8 -> 23         0.00473
        min(1)=        8 -> 17        -0.13181
        min(2)=        8 -> 13        -0.06874
        min(3)=        7 -> 11        -0.05081
        min(4)=        8 -> 15        -0.01756
        min(5)=        6 -> 13        -0.01121
        #CIs=49 #CIs>0=21 #CIs<0=25

7       Singlet-B1    9.2056        134.68    0.2307    0.000
        max(1)=        9 -> 15         0.52238
```

```
        max(2)=       8 -> 14        0.04840
        max(3)=       6 -> 14        0.02020
        max(4)=       9 -> 27        0.01406
        max(5)=       9 -> 19        0.01366
        min(1)=       9 -> 17       -0.46048
        min(2)=       9 -> 10       -0.09871
        min(3)=       9 -> 13       -0.02946
        min(4)=       9 -> 24       -0.02694
        min(5)=       7 -> 25       -0.02588
        #CIs=30 #CIs>0=18 #CIs<0=11

8       Singlet-A2    9.6474        128.52    0.0000    0.000
        max(1)=       9 -> 16        0.67365
        max(2)=       9 -> 11        0.19582
        max(3)=       7 -> 14        0.00404
        max(4)=       9 -> 28        0.00257
        max(5)=       7 -> 20        0.00191
        min(1)=       9 -> 12       -0.06665
        min(2)=       9 -> 22       -0.05697
        min(3)=       9 -> 18       -0.01235
        min(4)=       6 -> 25       -0.00306
        min(5)=       8 -> 25       -0.00197
        #CIs=21 #CIs>0=12 #CIs<0=9

9       Singlet-B1    9.7084        127.71    0.1949    0.000
        max(1)=       9 -> 17        0.50990
        max(2)=       9 -> 15        0.47159
        max(3)=       9 -> 10        0.12419
        max(4)=       8 -> 14        0.03115
        max(5)=       9 -> 24        0.01831
        min(1)=       9 -> 19       -0.02227
        min(2)=       8 -> 26       -0.00575
        min(3)=       7 -> 25       -0.00415
        min(4)=       6 -> 33       -0.00191
        min(5)=       7 -> 30       -0.00183
        #CIs=30 #CIs>0=18 #CIs<0=11

10      Singlet-B2    9.8143        126.33    0.1778    0.000
        max(1)=       8 -> 11        0.63905
        max(2)=       7 -> 17        0.08951
        max(3)=       9 -> 25        0.04407
```

```
        max(4)=       7 -> 21        0.03816
        max(5)=       8 -> 18        0.02081
        min(1)=       8 -> 12       -0.22991
        min(2)=       8 -> 16       -0.11479
        min(3)=       7 -> 10       -0.10629
        min(4)=       7 -> 15       -0.05686
        min(5)=       7 -> 23       -0.02450
        #CIs=40 #CIs>0=13 #CIs<0=26

11      Singlet-B2    10.5179       117.88    0.0059    0.000
        max(1)=       8 -> 12        0.60674
        max(2)=       8 -> 11        0.25824
        max(3)=       7 -> 10        0.23335
        max(4)=       8 -> 18        0.06229
        max(5)=       7 -> 15        0.01864
        min(1)=       7 -> 17       -0.06214
        min(2)=       8 -> 16       -0.04493
        min(3)=       9 -> 25       -0.01410
        min(4)=       7 -> 21       -0.00973
        min(5)=       6 -> 11       -0.00838
        #CIs=40 #CIs>0=26 #CIs<0=13

12      Singlet-A1    10.9492       113.24    0.0197    0.000
        max(1)=       8 -> 13        0.69040
        max(2)=       7 -> 16        0.04826
        max(3)=       8 -> 10        0.04678
        max(4)=       9 -> 14        0.04365
        max(5)=       8 -> 19        0.03299
        min(1)=       7 -> 11       -0.11307
        min(2)=       9 -> 20       -0.04585
        min(3)=       7 -> 18       -0.02607
        min(4)=       8 -> 17       -0.01265
        min(5)=       6 -> 17       -0.00987
        #CIs=49 #CIs>0=22 #CIs<0=25

13      Singlet-B1    11.0167       112.54    0.0021    0.000
        max(1)=       8 -> 14        0.70172
        max(2)=       8 -> 20        0.06167
        max(3)=       8 -> 26        0.01052
        max(4)=       9 -> 17        0.00758
        max(5)=       7 -> 25        0.00750
```

```
        min(1)=     9 -> 15     -0.05793
        min(2)=     9 -> 19     -0.01041
        min(3)=     9 -> 13     -0.00811
        min(4)=     9 -> 27     -0.00702
        min(5)=     6 -> 20     -0.00316
        #CIs=29 #CIs>0=12 #CIs<0=17

14  Singlet-B2  11.0882   111.82   0.3185   0.000
        max(1)=     7 -> 10      0.64118
        max(2)=     8 -> 16      0.06923
        max(3)=     7 -> 13      0.04248
        max(4)=     8 -> 11      0.03188
        max(5)=     7 -> 19      0.02242
        min(1)=     8 -> 12     -0.26208
        min(2)=     7 -> 17     -0.09176
        min(3)=     7 -> 15     -0.05217
        min(4)=     6 -> 12     -0.01974
        min(5)=     8 -> 22     -0.01522
        #CIs=40 #CIs>0=17 #CIs<0=21

15  Singlet-A1  11.5622   107.23   0.0120   0.000
        max(1)=     8 -> 15      0.48634
        max(2)=     7 -> 12      0.16657
        max(3)=     7 -> 16      0.08374
        max(4)=     9 -> 20      0.03104
        max(5)=     6 -> 23      0.00855
        min(1)=     7 -> 11     -0.33339
        min(2)=     8 -> 17     -0.31842
        min(3)=     8 -> 10     -0.08846
        min(4)=     8 -> 13     -0.05918
        min(5)=     8 -> 21     -0.04967
        #CIs=49 #CIs>0=26 #CIs<0=19

16  Singlet-A1  12.2341   101.34   0.0886   0.000
        max(1)=     8 -> 15      0.49266
        max(2)=     7 -> 11      0.42887
        max(3)=     8 -> 17      0.22323
        max(4)=     8 -> 10      0.09374
        max(5)=     8 -> 13      0.06661
        min(1)=     9 -> 20     -0.05449
        min(2)=     7 -> 12     -0.04808
        min(3)=     8 -> 19     -0.04425
        min(4)=     7 -> 16     -0.02658
        min(5)=     7 -> 22     -0.01615
        #CIs=49 #CIs>0=21 #CIs<0=24

17  Singlet-B2  12.6563    97.96   0.0166   0.000
        max(1)=     8 -> 16      0.67087
        max(2)=     8 -> 11      0.13550
        max(3)=     7 -> 15      0.12728
        max(4)=     7 -> 13      0.04392
        max(5)=     7 -> 23      0.01539
        min(1)=     7 -> 10     -0.07585
        min(2)=     7 -> 17     -0.05973
        min(3)=     8 -> 22     -0.04188
        min(4)=     7 -> 21     -0.03211
        min(5)=     9 -> 25     -0.02836
        #CIs=40 #CIs>0=24 #CIs<0=14

18  Singlet-A1  12.7242    97.44   0.1884   0.000
        max(1)=     8 -> 17      0.51398
        max(2)=     8 -> 15      0.11440
        max(3)=     9 -> 20      0.10137
        max(4)=     8 -> 10      0.08893
        max(5)=     8 -> 19      0.02376
        min(1)=     7 -> 11     -0.41039
        min(2)=     7 -> 12     -0.17228
        min(3)=     8 -> 13     -0.05511
        min(4)=     9 -> 14     -0.03861
        min(5)=     7 -> 18     -0.02366
        #CIs=49 #CIs>0=30 #CIs<0=17

19  Singlet-A1  13.0752    94.82   0.1975   0.000
        max(1)=     7 -> 12      0.65892
        max(2)=     8 -> 17      0.24161
        max(3)=     7 -> 18      0.02474
        max(4)=     7 -> 22      0.02070
        max(5)=     6 -> 13      0.01790
        min(1)=     8 -> 15     -0.05552
        min(2)=     9 -> 26     -0.04094
        min(3)=     8 -> 23     -0.03548
        min(4)=     7 -> 16     -0.02258
```

```
        min(5)=       6 -> 10        -0.01628
        #CIs=49 #CIs>0=24 #CIs<0=23

20      Singlet-B2   13.1913        93.99    0.0003    0.000
        max(1)=       7 -> 13         0.69749
        max(2)=       7 -> 15         0.06639
        max(3)=       7 -> 19         0.05696
        max(4)=       6 -> 12         0.01613
        max(5)=       7 -> 24         0.00914
        min(1)=       8 -> 16        -0.05932
        min(2)=       7 -> 10        -0.03602
        min(3)=       8 -> 11        -0.01658
        min(4)=       6 -> 11        -0.01500
        min(5)=       7 -> 21        -0.01194
        #CIs=40 #CIs>0=20 #CIs<0=18

21      Singlet-A2   13.2692        93.44    0.0000    0.000
        max(1)=       7 -> 14         0.70381
        max(2)=       7 -> 20         0.06498
        max(3)=       8 -> 25         0.00308
        max(4)=       9 -> 11         0.00167
        max(5)=       6 -> 25         0.00143
        min(1)=       9 -> 18        -0.01854
        min(2)=       9 -> 16        -0.00596
        min(3)=       9 -> 22        -0.00457
        min(4)=       9 -> 12        -0.00373
        min(5)=       7 -> 31        -0.00189
        #CIs=21 #CIs>0=10 #CIs<0=11

22      Singlet-A2   14.0257        88.40    0.0000    0.000
        max(1)=       9 -> 18         0.70263
        max(2)=       9 -> 28         0.02116
        max(3)=       7 -> 14         0.01835
        max(4)=       9 -> 22         0.01648
        max(5)=       9 -> 16         0.01646
        min(1)=       9 -> 12        -0.06344
        min(2)=       9 -> 11        -0.02973
        min(3)=       9 -> 29        -0.00574
        min(4)=       8 -> 25        -0.00106
        min(5)=       7 -> 26        -0.00058
        #CIs=21 #CIs>0=13 #CIs<0=7

23      Singlet-B2   14.3271        86.54    0.1762    0.000
        max(1)=       7 -> 15         0.67788
        max(2)=       9 -> 25         0.04252
        max(3)=       8 -> 18         0.03449
        max(4)=       7 -> 10         0.03337
        max(5)=       8 -> 11         0.02817
        min(1)=       8 -> 16        -0.13150
        min(2)=       7 -> 17        -0.08719
        min(3)=       7 -> 13        -0.07336
        min(4)=       8 -> 12        -0.06517
        min(5)=       8 -> 22        -0.02567
        #CIs=40 #CIs>0=16 #CIs<0=23

24      Singlet-B1   14.7434        84.09    0.0012    0.000
        max(1)=       9 -> 19         0.70081
        max(2)=       9 -> 17         0.03232
        max(3)=       8 -> 26         0.01141
        max(4)=       8 -> 14         0.01006
        max(5)=       9 -> 32         0.00952
        min(1)=       9 -> 13        -0.06448
        min(2)=       9 -> 21        -0.05497
        min(3)=       9 -> 10        -0.00980
        min(4)=       8 -> 20        -0.00731
        min(5)=       9 -> 23        -0.00542
        #CIs=30 #CIs>0=13 #CIs<0=16

25      Singlet-B2   14.8207        83.66    0.2415    0.000
        max(1)=       7 -> 17         0.68011
        max(2)=       7 -> 10         0.11999
        max(3)=       7 -> 15         0.10272
        max(4)=       8 -> 16         0.06026
        max(5)=       8 -> 12         0.04516
        min(1)=       8 -> 18        -0.04790
        min(2)=       7 -> 19        -0.04553
        min(3)=       8 -> 11        -0.03767
        min(4)=       9 -> 25        -0.02276
        min(5)=       6 -> 11        -0.01335
        #CIs=40 #CIs>0=24 #CIs<0=14

26      Singlet-A1   14.9766        82.79    0.0638    0.000
```

max(1)= 7 -> 16 0.65021
max(2)= 9 -> 20 0.24160
max(3)= 7 -> 11 0.10509
max(4)= 8 -> 17 0.03890
max(5)= 8 -> 19 0.01197
min(1)= 8 -> 15 -0.03894
min(2)= 7 -> 18 -0.03694
min(3)= 9 -> 26 -0.02848
min(4)= 7 -> 22 -0.02824
min(5)= 8 -> 21 -0.02399
#CIs=49 #CIs>0=25 #CIs<0=22

27 Singlet-A1 15.9097 77.93 0.0247 0.000
max(1)= 9 -> 20 0.60937
max(2)= 8 -> 13 0.07183
max(3)= 6 -> 10 0.06076
max(4)= 7 -> 11 0.05139
max(5)= 8 -> 21 0.04047
min(1)= 7 -> 16 -0.22814
min(2)= 8 -> 19 -0.22674
min(3)= 7 -> 18 -0.06616
min(4)= 8 -> 17 -0.05976
min(5)= 6 -> 17 -0.05210
#CIs=49 #CIs>0=24 #CIs<0=23

28 Singlet-B2 16.9734 73.05 0.0039 0.000
max(1)= 8 -> 18 0.69812
max(2)= 8 -> 22 0.04963
max(3)= 7 -> 17 0.04650
max(4)= 8 -> 16 0.03778
max(5)= 6 -> 12 0.01871
min(1)= 8 -> 12 -0.04793
min(2)= 8 -> 11 -0.03995
min(3)= 9 -> 25 -0.02765
min(4)= 7 -> 15 -0.02096
min(5)= 7 -> 21 -0.01447
#CIs=40 #CIs>0=25 #CIs<0=14

29 Singlet-B1 17.5688 70.57 0.0355 0.000
max(1)= 9 -> 21 0.68589
max(2)= 9 -> 19 0.05225
max(3)= 8 -> 26 0.03964
max(4)= 7 -> 25 0.03951
max(5)= 9 -> 24 0.01438
min(1)= 8 -> 20 -0.14525
min(2)= 9 -> 23 -0.03525
min(3)= 9 -> 17 -0.02302
min(4)= 6 -> 20 -0.02017
min(5)= 6 -> 14 -0.01276
#CIs=30 #CIs>0=11 #CIs<0=18

30 Singlet-A2 17.8273 69.55 0.0000 0.000
max(1)= 9 -> 22 0.70340
max(2)= 9 -> 16 0.06399
max(3)= 9 -> 12 0.01214
max(4)= 9 -> 34 0.01176
max(5)= 7 -> 14 0.00567
min(1)= 9 -> 18 -0.01720
min(2)= 9 -> 28 -0.01491
min(3)= 9 -> 11 -0.01220
min(4)= 7 -> 20 -0.01049
min(5)= 7 -> 26 -0.00272
#CIs=21 #CIs>0=9 #CIs<0=12

31 Singlet-B1 18.0813 68.57 0.0000 0.000
max(1)= 8 -> 20 0.68834
max(2)= 9 -> 21 0.14149
max(3)= 8 -> 26 0.02785
max(4)= 7 -> 25 0.02197
max(5)= 9 -> 19 0.01889
min(1)= 8 -> 14 -0.06142
min(2)= 9 -> 27 -0.01308
min(3)= 6 -> 14 -0.01257
min(4)= 9 -> 23 -0.01196
min(5)= 6 -> 20 -0.00896
#CIs=30 #CIs>0=11 #CIs<0=17

32 Singlet-A1 18.2286 68.02 0.0018 0.000
max(1)= 8 -> 19 0.61500
max(2)= 9 -> 20 0.14251
max(3)= 6 -> 10 0.12815
max(4)= 7 -> 11 0.05560

```
max(5)=   9 -> 26    0.04037
min(1)=   7 -> 18   -0.25068
min(2)=   7 -> 16   -0.08313
min(3)=   6 -> 17   -0.06013
min(4)=   7 -> 22   -0.04421
min(5)=   8 -> 24   -0.02106
#CIs=49 #CIs>0=24 #CIs<0=23

33   Singlet-A1   19.4951   63.60   0.0055   0.000
max(1)=   6 -> 10    0.53889
max(2)=   7 -> 18    0.43630
max(3)=   8 -> 19    0.05832
max(4)=   6 -> 19    0.01720
max(5)=   9 -> 20    0.01635
min(1)=   6 -> 17   -0.10752
min(2)=   8 -> 21   -0.04274
min(3)=   6 -> 15   -0.01735
min(4)=   8 -> 24   -0.01223
min(5)=   6 -> 24   -0.01051
#CIs=49 #CIs>0=25 #CIs<0=22

34   Singlet-B2   19.9154   62.26   0.0003   0.000
max(1)=   7 -> 19    0.58715
max(2)=   6 -> 12    0.19697
max(3)=   6 -> 16    0.09757
max(4)=   8 -> 22    0.03689
max(5)=   7 -> 17    0.02564
min(1)=   6 -> 11   -0.31257
min(2)=   7 -> 13   -0.05920
min(3)=   9 -> 25   -0.05005
min(4)=   8 -> 28   -0.01000
min(5)=   7 -> 10   -0.00931
#CIs=40 #CIs>0=25 #CIs<0=14

35   Singlet-B2   20.1768   61.45   0.0024   0.000
max(1)=   6 -> 11    0.52639
max(2)=   7 -> 19    0.37951
max(3)=   9 -> 25    0.04692
max(4)=   7 -> 17    0.04440
max(5)=   8 -> 18    0.02637
min(1)=   6 -> 12   -0.21867
min(2)=   6 -> 16   -0.12975
min(3)=   7 -> 21   -0.07301
min(4)=   8 -> 22   -0.04728
min(5)=   7 -> 13   -0.01771
#CIs=40 #CIs>0=22 #CIs<0=17

36   Singlet-A1   20.2517   61.22   0.0156   0.000
max(1)=   8 -> 21    0.54533
max(2)=   7 -> 18    0.32908
max(3)=   8 -> 19    0.13990
max(4)=   9 -> 20    0.08104
max(5)=   8 -> 15    0.02891
min(1)=   6 -> 10   -0.23773
min(2)=   8 -> 23   -0.06646
min(3)=   9 -> 26   -0.06539
min(4)=   8 -> 17   -0.02542
min(5)=   8 -> 24   -0.02512
#CIs=49 #CIs>0=23 #CIs<0=24

37   Singlet-A2   20.3124   61.04   0.0000   0.000
max(1)=   7 -> 20    0.70381
max(2)=   9 -> 22    0.01113
max(3)=   7 -> 33    0.01006
max(4)=   8 -> 25    0.00891
max(5)=   7 -> 26    0.00337
min(1)=   7 -> 14   -0.06501
min(2)=   7 -> 31   -0.00971
min(3)=   8 -> 30   -0.00232
min(4)=   9 -> 16   -0.00139
min(5)=   9 -> 28   -0.00134
#CIs=21 #CIs>0=11 #CIs<0=10

38   Singlet-A1   20.7269   59.82   0.0042   0.000
max(1)=   8 -> 21    0.42217
max(2)=   6 -> 10    0.34541
max(3)=   7 -> 22    0.12348
max(4)=   7 -> 16    0.05906
max(5)=   6 -> 17    0.05689
min(1)=   7 -> 18   -0.34743
min(2)=   8 -> 19   -0.18501
min(3)=   9 -> 20   -0.13622
```

```
        min(4)=        9 -> 14        -0.02604
        min(5)=        7 -> 11        -0.02602
        #CIs=49 #CIs>0=20 #CIs<0=27

39      Singlet-B2   20.9056        59.31    0.0121    0.000
        max(1)=        8 -> 22         0.68155
        max(2)=        7 -> 21         0.12328
        max(3)=        9 -> 25         0.10096
        max(4)=        6 -> 11         0.05097
        max(5)=        8 -> 16         0.04340
        min(1)=        8 -> 18        -0.03953
        min(2)=        7 -> 23        -0.03637
        min(3)=        6 -> 12        -0.03596
        min(4)=        7 -> 17        -0.02271
        min(5)=        6 -> 16        -0.00929
        #CIs=40 #CIs>0=14 #CIs<0=25

40      Singlet-B2   21.4084        57.91    0.0128    0.000
        max(1)=        6 -> 12         0.63167
        max(2)=        6 -> 11         0.29795
        max(3)=        7 -> 21         0.06648
        max(4)=        6 -> 18         0.05626
        max(5)=        9 -> 25         0.03342
        min(1)=        7 -> 19        -0.04818
        min(2)=        6 -> 16        -0.01384
        min(3)=        7 -> 17        -0.00918
        min(4)=        8 -> 18        -0.00881
        min(5)=        7 -> 23        -0.00781
        #CIs=40 #CIs>0=17 #CIs<0=22
```

8.2.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1       Singlet-A2    6.5227       190.08    0.0000    0.000
        max(1)=        9 -> 16         0.49044
        max(2)=        9 -> 14         0.42062
        max(3)=        9 -> 28         0.01715
        max(4)=        9 -> 18         0.00637
        max(5)=        7 -> 13         0.00368
        min(1)=        9 -> 11        -0.26651
        min(2)=        9 -> 22        -0.10463
        min(3)=        9 -> 34        -0.01290
        min(4)=        6 -> 30        -0.00472
        min(5)=        7 -> 31        -0.00163
        #CIs=21 #CIs>0=14 #CIs<0=7

2       Singlet-B1    6.5983       187.90    0.0563    0.000
        max(1)=        9 -> 10         0.64239
        max(2)=        9 -> 19         0.03151
        max(3)=        9 -> 35         0.00433
        max(4)=        9 -> 36         0.00367
        max(5)=        9 -> 27         0.00300
        min(1)=        9 -> 17        -0.25373
        min(2)=        9 -> 15        -0.13769
        min(3)=        9 -> 23        -0.03448
        min(4)=        9 -> 21        -0.02287
        min(5)=        9 -> 12        -0.02260
        #CIs=29 #CIs>0=12 #CIs<0=17

3       Singlet-A2    8.3178       149.06    0.0000    0.000
        max(1)=        9 -> 11         0.58575
        max(2)=        9 -> 14         0.37733
        max(3)=        9 -> 18         0.11920
        max(4)=        9 -> 28         0.01130
        max(5)=        9 -> 22         0.01018
        min(1)=        9 -> 16        -0.00501
        min(2)=        9 -> 29        -0.00210
        min(3)=        6 -> 25        -0.00208
        min(4)=        8 -> 25        -0.00197
        min(5)=        9 -> 37        -0.00070
        #CIs=21 #CIs>0=11 #CIs<0=10

4       Singlet-B1    8.5688       144.69    0.0265    0.000
        max(1)=        9 -> 12         0.69437
        max(2)=        9 -> 19         0.11305
```

```
max(3)=    9 -> 15    0.04461
max(4)=    8 -> 13    0.01975
max(5)=    9 -> 10    0.01443
min(1)=    9 -> 17    -0.03483
min(2)=    9 -> 21    -0.03267
min(3)=    8 -> 26    -0.00181
min(4)=    6 -> 26    -0.00178
min(5)=    6 -> 31    -0.00132
#CIs=29 #CIs>0=17 #CIs<0=12

5    Singlet-A1    8.8869    139.51    0.0244    0.000
max(1)=    9 -> 13    0.67763
max(2)=    9 -> 20    0.07299
max(3)=    8 -> 17    0.06454
max(4)=    8 -> 15    0.04310
max(5)=    7 -> 16    0.03246
min(1)=    8 -> 10    -0.15225
min(2)=    7 -> 11    -0.03594
min(3)=    8 -> 19    -0.03526
min(4)=    7 -> 18    -0.02893
min(5)=    8 -> 12    -0.02525
#CIs=47 #CIs>0=26 #CIs<0=21

6    Singlet-A1    9.8106    126.38    0.1925    0.000
max(1)=    8 -> 10    0.62489
max(2)=    9 -> 13    0.16583
max(3)=    7 -> 16    0.03883
max(4)=    7 -> 14    0.03184
max(5)=    7 -> 11    0.00980
min(1)=    8 -> 17    -0.22837
min(2)=    8 -> 15    -0.12285
min(3)=    8 -> 12    -0.09917
min(4)=    8 -> 23    -0.02744
min(5)=    6 -> 12    -0.01853
#CIs=47 #CIs>0=19 #CIs<0=28

7    Singlet-B1    9.9124    125.08    0.3483    0.000
max(1)=    9 -> 17    0.53366
max(2)=    9 -> 10    0.12544
max(3)=    9 -> 21    0.07785
max(4)=    9 -> 12    0.05906
max(5)=    8 -> 26    0.03578
min(1)=    9 -> 15    -0.42620
min(2)=    8 -> 13    -0.06070
min(3)=    6 -> 13    -0.02250
min(4)=    8 -> 20    -0.02142
min(5)=    6 -> 20    -0.01703
#CIs=30 #CIs>0=13 #CIs<0=16

8    Singlet-A2    10.3408    119.90    0.0000    0.000
max(1)=    9 -> 14    0.41724
max(2)=    9 -> 22    0.10332
max(3)=    9 -> 18    0.01948
max(4)=    9 -> 34    0.00695
max(5)=    6 -> 30    0.00228
min(1)=    9 -> 16    -0.48695
min(2)=    9 -> 11    -0.27861
min(3)=    9 -> 28    -0.00698
min(4)=    9 -> 29    -0.00195
min(5)=    7 -> 26    -0.00131
#CIs=21 #CIs>0=8 #CIs<0=13

9    Singlet-B1    10.3860    119.38    0.1375    0.000
max(1)=    9 -> 15    0.53651
max(2)=    9 -> 17    0.36504
max(3)=    9 -> 10    0.26624
max(4)=    9 -> 23    0.05257
max(5)=    8 -> 13    0.03795
min(1)=    9 -> 19    -0.03860
min(2)=    9 -> 12    -0.01574
min(3)=    9 -> 35    -0.00415
min(4)=    9 -> 32    -0.00260
min(5)=    9 -> 36    -0.00256
#CIs=30 #CIs>0=20 #CIs<0=9

10    Singlet-B2    10.6813    116.08    0.3373    0.000
max(1)=    8 -> 16    0.40596
max(2)=    8 -> 14    0.40382
max(3)=    7 -> 15    0.03284
max(4)=    6 -> 11    0.01902
max(5)=    6 -> 18    0.01743
min(1)=    8 -> 11    -0.39084
```

```
min(2)=   7 -> 17   -0.07921
min(3)=   8 -> 22   -0.05494
min(4)=   7 -> 21   -0.05129
min(5)=   9 -> 25   -0.05098
#CIs=39 #CIs>0=25 #CIs<0=14

11   Singlet-B2   11.3469   109.27   0.0061   0.000
max(1)=   8 -> 11   0.49666
max(2)=   8 -> 14   0.42610
max(3)=   7 -> 10   0.20797
max(4)=   8 -> 18   0.11406
max(5)=   8 -> 16   0.03385
min(1)=   7 -> 17   -0.10755
min(2)=   7 -> 15   -0.02332
min(3)=   9 -> 25   -0.01713
min(4)=   7 -> 21   -0.01680
min(5)=   6 -> 11   -0.01480
#CIs=39 #CIs>0=22 #CIs<0=16

12   Singlet-A1   11.7640   105.39   0.0130   0.000
max(1)=   8 -> 12   0.68494
max(2)=   8 -> 10   0.09164
max(3)=   8 -> 19   0.08109
max(4)=   7 -> 16   0.07525
max(5)=   9 -> 13   0.04747
min(1)=   7 -> 11   -0.05168
min(2)=   9 -> 20   -0.05038
min(3)=   7 -> 18   -0.02623
min(4)=   7 -> 22   -0.02377
min(5)=   8 -> 21   -0.01438
#CIs=47 #CIs>0=21 #CIs<0=26

13   Singlet-B1   11.8629   104.51   0.0055   0.000
max(1)=   8 -> 13   0.69367
max(2)=   8 -> 20   0.11096
max(3)=   9 -> 17   0.02142
max(4)=   7 -> 25   0.01109
max(5)=   8 -> 26   0.00988
min(1)=   9 -> 15   -0.07336
min(2)=   9 -> 12   -0.01404
min(3)=   6 -> 26   -0.00436
min(4)=   9 -> 27   -0.00431
min(5)=   9 -> 19   -0.00324
#CIs=29 #CIs>0=12 #CIs<0=17

14   Singlet-B2   12.1946   101.67   0.3237   0.000
max(1)=   7 -> 10   0.60063
max(2)=   7 -> 12   0.06986
max(3)=   7 -> 19   0.06028
max(4)=   8 -> 16   0.02002
max(5)=   6 -> 16   0.01014
min(1)=   7 -> 17   -0.22526
min(2)=   8 -> 14   -0.20293
min(3)=   8 -> 11   -0.13718
min(4)=   7 -> 15   -0.12838
min(5)=   6 -> 11   -0.02808
#CIs=39 #CIs>0=18 #CIs<0=21

15   Singlet-A1   12.5694   98.64   0.0002   0.000
max(1)=   8 -> 17   0.46224
max(2)=   7 -> 11   0.11189
max(3)=   8 -> 21   0.10632
max(4)=   8 -> 10   0.09383
max(5)=   7 -> 22   0.03225
min(1)=   8 -> 15   -0.45146
min(2)=   7 -> 16   -0.16463
min(3)=   7 -> 14   -0.14176
min(4)=   8 -> 23   -0.00950
min(5)=   9 -> 20   -0.00835
#CIs=47 #CIs>0=22 #CIs<0=25

16   Singlet-A1   13.3328   92.99   0.0645   0.000
max(1)=   8 -> 15   0.46535
max(2)=   7 -> 11   0.32126
max(3)=   8 -> 17   0.18482
max(4)=   8 -> 10   0.17879
max(5)=   8 -> 23   0.04971
min(1)=   7 -> 16   -0.22566
min(2)=   7 -> 14   -0.22559
min(3)=   9 -> 20   -0.05126
min(4)=   8 -> 19   -0.04961
min(5)=   6 -> 12   -0.01471
```

```
        #CIs=48 #CIs>0=24 #CIs<0=23

17      Singlet-B2   13.5681         91.38    0.0366    0.000
        max(1)=        8 -> 14         0.32443
        max(2)=        8 -> 22         0.09473
        max(3)=        7 -> 10         0.06733
        max(4)=        7 -> 17         0.04674
        max(5)=        7 -> 21         0.03721
        min(1)=        8 -> 16        -0.54074
        min(2)=        8 -> 11        -0.26899
        min(3)=        7 -> 15        -0.09863
        min(4)=        7 -> 12        -0.02071
        min(5)=        7 -> 23        -0.01363
        #CIs=39 #CIs>0=15 #CIs<0=23

18      Singlet-A1   13.6718         90.69    0.3968    0.000
        max(1)=        8 -> 17         0.40246
        max(2)=        8 -> 15         0.23207
        max(3)=        7 -> 16         0.20686
        max(4)=        8 -> 10         0.19007
        max(5)=        9 -> 20         0.16130
        min(1)=        7 -> 11        -0.37018
        min(2)=        8 -> 12        -0.07097
        min(3)=        9 -> 13        -0.06362
        min(4)=        7 -> 18        -0.04802
        min(5)=        9 -> 26        -0.02918
        #CIs=48 #CIs>0=31 #CIs<0=16

19      Singlet-A1   14.2641         86.92    0.1355    0.000
        max(1)=        7 -> 14         0.51662
        max(2)=        7 -> 11         0.42603
        max(3)=        7 -> 16         0.16742
        max(4)=        8 -> 17         0.11107
        max(5)=        7 -> 18         0.08091
        min(1)=        9 -> 26        -0.04262
        min(2)=        6 -> 10        -0.02424
        min(3)=        6 -> 21        -0.01428
        min(4)=        7 -> 22        -0.01373
        min(5)=        8 -> 23        -0.00971
        #CIs=48 #CIs>0=21 #CIs<0=26

20      Singlet-A2   14.5870         85.00    0.0000    0.000
        max(1)=        7 -> 13         0.69796
        max(2)=        7 -> 20         0.11248
        max(3)=        7 -> 26         0.00596
        max(4)=        8 -> 25         0.00525
        max(5)=        7 -> 31         0.00521
        min(1)=        9 -> 16        -0.00456
        min(2)=        9 -> 14        -0.00449
        min(3)=        6 -> 25        -0.00423
        min(4)=        9 -> 11        -0.00319
        min(5)=        9 -> 22        -0.00304
        #CIs=21 #CIs>0=10 #CIs<0=11

21      Singlet-B2   14.6146         84.84    0.0010    0.000
        max(1)=        7 -> 12         0.68744
        max(2)=        7 -> 15         0.09721
        max(3)=        7 -> 19         0.09134
        max(4)=        6 -> 14         0.02397
        max(5)=        8 -> 14         0.02176
        min(1)=        7 -> 10        -0.07295
        min(2)=        8 -> 16        -0.03018
        min(3)=        7 -> 21        -0.02906
        min(4)=        8 -> 11        -0.02359
        min(5)=        7 -> 17        -0.02095
        #CIs=39 #CIs>0=22 #CIs<0=17

22      Singlet-A2   14.7664         83.96    0.0000    0.000
        max(1)=        9 -> 18         0.69305
        max(2)=        9 -> 22         0.04602
        max(3)=        9 -> 28         0.04395
        max(4)=        9 -> 16         0.01981
        max(5)=        9 -> 34         0.01715
        min(1)=        9 -> 11        -0.09065
        min(2)=        9 -> 14        -0.08078
        min(3)=        9 -> 29        -0.01071
        min(4)=        6 -> 25        -0.00489
        min(5)=        8 -> 25        -0.00470
        #CIs=21 #CIs>0=11 #CIs<0=9

23      Singlet-B1   15.4506         80.25    0.0006    0.000
        max(1)=        9 -> 19         0.68763
```

max(2)= 9 -> 17 0.05786
max(3)= 9 -> 35 0.02229
max(4)= 9 -> 32 0.02053
max(5)= 9 -> 15 0.01883
min(1)= 9 -> 12 -0.11482
min(2)= 9 -> 21 -0.09230
min(3)= 9 -> 10 -0.01394
min(4)= 6 -> 26 -0.00680
min(5)= 9 -> 39 -0.00208
#CIs=30 #CIs>0=14 #CIs<0=15

24 Singlet-B2 15.5161 79.91 0.3631 0.000
max(1)= 7 -> 17 0.45545
max(2)= 8 -> 16 0.13245
max(3)= 7 -> 12 0.10126
max(4)= 7 -> 21 0.07148
max(5)= 7 -> 10 0.06620
min(1)= 7 -> 15 -0.49512
min(2)= 8 -> 18 -0.05767
min(3)= 9 -> 25 -0.05562
min(4)= 7 -> 24 -0.02477
min(5)= 6 -> 16 -0.01968
#CIs=39 #CIs>0=22 #CIs<0=17

25 Singlet-B2 16.0080 77.45 0.1302 0.000
max(1)= 7 -> 15 0.45665
max(2)= 7 -> 17 0.43819
max(3)= 7 -> 10 0.28284
max(4)= 7 -> 23 0.04826
max(5)= 7 -> 21 0.03647
min(1)= 7 -> 19 -0.08412
min(2)= 8 -> 18 -0.07901
min(3)= 6 -> 16 -0.01208
min(4)= 7 -> 12 -0.01007
min(5)= 7 -> 32 -0.00693
#CIs=40 #CIs>0=19 #CIs<0=20

26 Singlet-A1 16.1480 76.78 0.0166 0.000
max(1)= 7 -> 14 0.30409
max(2)= 7 -> 22 0.07599
max(3)= 7 -> 18 0.06333
max(4)= 9 -> 13 0.05265
max(5)= 8 -> 19 0.05120
min(1)= 7 -> 16 -0.41110
min(2)= 9 -> 20 -0.40704
min(3)= 7 -> 11 -0.22906
min(4)= 8 -> 12 -0.01831
min(5)= 9 -> 33 -0.01294
#CIs=49 #CIs>0=25 #CIs<0=22

27 Singlet-A1 16.8777 73.46 0.0853 0.000
max(1)= 9 -> 20 0.48422
max(2)= 7 -> 14 0.18679
max(3)= 8 -> 12 0.09887
max(4)= 8 -> 21 0.06091
max(5)= 7 -> 22 0.03031
min(1)= 7 -> 16 -0.37106
min(2)= 8 -> 19 -0.24936
min(3)= 8 -> 17 -0.08455
min(4)= 9 -> 13 -0.03978
min(5)= 7 -> 18 -0.03846
#CIs=48 #CIs>0=23 #CIs<0=24

28 Singlet-B2 17.9748 68.98 0.0145 0.000
max(1)= 8 -> 18 0.68190
max(2)= 7 -> 17 0.09406
max(3)= 8 -> 22 0.07850
max(4)= 8 -> 16 0.05028
max(5)= 8 -> 28 0.03581
min(1)= 8 -> 11 -0.08703
min(2)= 8 -> 14 -0.07103
min(3)= 9 -> 25 -0.03976
min(4)= 8 -> 29 -0.00906
min(5)= 7 -> 19 -0.00605
#CIs=38 #CIs>0=23 #CIs<0=15

29 Singlet-B1 18.6697 66.41 0.0598 0.000
max(1)= 9 -> 21 0.64725
max(2)= 9 -> 19 0.09579
max(3)= 8 -> 26 0.05518
max(4)= 9 -> 24 0.04728
max(5)= 7 -> 25 0.04344

```
min(1)=   8 -> 20   -0.23127
min(2)=   9 -> 17   -0.07871
min(3)=   9 -> 23   -0.03743
min(4)=   6 -> 20   -0.01985
min(5)=   9 -> 36   -0.01244
#CIs=29 #CIs>0=12 #CIs<0=17

30   Singlet-A2   18.9977   65.26   0.0000   0.000
max(1)=   9 -> 22   0.68842
max(2)=   9 -> 16   0.14728
max(3)=   9 -> 34   0.02703
max(4)=   6 -> 30   0.00485
max(5)=   7 -> 13   0.00460
min(1)=   9 -> 18   -0.04861
min(2)=   9 -> 28   -0.03300
min(3)=   8 -> 25   -0.00660
min(4)=   9 -> 29   -0.00606
min(5)=   9 -> 37   -0.00514
#CIs=21 #CIs>0=8 #CIs<0=13

31   Singlet-B1   19.0207   65.18   0.0035   0.000
max(1)=   8 -> 20   0.65655
max(2)=   9 -> 21   0.22658
max(3)=   7 -> 25   0.03447
max(4)=   8 -> 26   0.03269
max(5)=   9 -> 24   0.02881
min(1)=   8 -> 13   -0.10860
min(2)=   9 -> 17   -0.03139
min(3)=   6 -> 26   -0.01069
min(4)=   9 -> 15   -0.00857
min(5)=   9 -> 36   -0.00517
#CIs=29 #CIs>0=13 #CIs<0=15

32   Singlet-A1   19.3606   64.04   0.0057   0.000
max(1)=   8 -> 19   0.60591
max(2)=   9 -> 20   0.17066
max(3)=   7 -> 11   0.06404
max(4)=   7 -> 14   0.05160
max(5)=   9 -> 26   0.03822
min(1)=   7 -> 18   -0.25028
min(2)=   7 -> 16   -0.13781
min(3)=   8 -> 12   -0.05243
min(4)=   7 -> 22   -0.05164
min(5)=   8 -> 17   -0.04092
#CIs=49 #CIs>0=24 #CIs<0=23

33   Singlet-A1   21.1122   58.73   0.0139   0.000
max(1)=   7 -> 18   0.54241
max(2)=   8 -> 21   0.36841
max(3)=   8 -> 19   0.19227
max(4)=   9 -> 20   0.09807
max(5)=   8 -> 15   0.04426
min(1)=   9 -> 26   -0.06394
min(2)=   8 -> 23   -0.05659
min(3)=   8 -> 17   -0.05002
min(4)=   7 -> 11   -0.04866
min(5)=   7 -> 14   -0.04314
#CIs=49 #CIs>0=25 #CIs<0=22

34   Singlet-B2   21.5193   57.62   0.0041   0.000
max(1)=   7 -> 19   0.68470
max(2)=   7 -> 17   0.08298
max(3)=   7 -> 15   0.05569
max(4)=   6 -> 16   0.05139
max(5)=   6 -> 14   0.04631
min(1)=   7 -> 12   -0.10098
min(2)=   9 -> 25   -0.04436
min(3)=   7 -> 21   -0.03604
min(4)=   7 -> 24   -0.02160
min(5)=   7 -> 10   -0.01446
#CIs=39 #CIs>0=23 #CIs<0=16

35   Singlet-A2   21.7805   56.92   0.0000   0.000
max(1)=   7 -> 20   0.69685
max(2)=   7 -> 33   0.02330
max(3)=   7 -> 31   0.02098
max(4)=   7 -> 26   0.01511
max(5)=   8 -> 25   0.01491
min(1)=   7 -> 13   -0.11293
min(2)=   6 -> 25   -0.01006
min(3)=   8 -> 30   -0.00474
min(4)=   9 -> 18   -0.00455
```

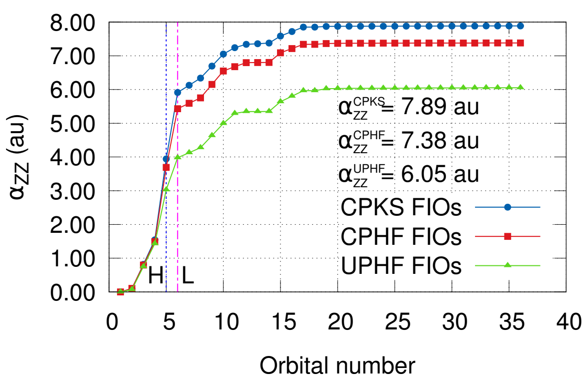
```
        min(5)=      9 -> 28       -0.00298
        #CIs=21 #CIs>0=11 #CIs<0=10

36   Singlet-A1  21.9704      56.43   0.0001   0.000
        max(1)=      8 -> 21        0.56708
        max(2)=      7 -> 22        0.06851
        max(3)=      6 -> 17        0.06815
        max(4)=      7 -> 16        0.06610
        max(5)=      8 -> 27        0.05054
        min(1)=      7 -> 18       -0.33552
        min(2)=      6 -> 10       -0.12972
        min(3)=      9 -> 20       -0.10719
        min(4)=      8 -> 19       -0.08926
        min(5)=      8 -> 17       -0.07249
        #CIs=49 #CIs>0=20 #CIs<0=27

37   Singlet-B2  22.2530      55.72   0.0070   0.000
        max(1)=      8 -> 22        0.67426
        max(2)=      8 -> 16        0.11639
        max(3)=      9 -> 25        0.11134
        max(4)=      7 -> 21        0.06162
        max(5)=      6 -> 14        0.04432
        min(1)=      8 -> 18       -0.07692
        min(2)=      7 -> 17       -0.03774
        min(3)=      7 -> 23       -0.03600
        min(4)=      8 -> 28       -0.02761
        min(5)=      6 -> 28       -0.01376
        #CIs=39 #CIs>0=20 #CIs<0=19

38   Singlet-A1  23.1118      53.65   0.0167   0.000
        max(1)=      6 -> 10        0.63434
        max(2)=      8 -> 21        0.10634
        max(3)=      7 -> 22        0.10216
        max(4)=      9 -> 26        0.05384
        max(5)=      6 -> 12        0.04296
        min(1)=      6 -> 17       -0.21465
        min(2)=      6 -> 15       -0.10396
        min(3)=      9 -> 20       -0.06308
        min(4)=      7 -> 18       -0.05537
        min(5)=      8 -> 19       -0.04711
        #CIs=49 #CIs>0=22 #CIs<0=25

39   Singlet-B2  23.1222      53.62   0.0003   0.000
        max(1)=      6 -> 16        0.46672
        max(2)=      6 -> 14        0.40758
        max(3)=      7 -> 23        0.01291
        max(4)=      7 -> 17        0.00920
        max(5)=      7 -> 27        0.00741
        min(1)=      6 -> 11       -0.30483
        min(2)=      6 -> 22       -0.08648
        min(3)=      9 -> 25       -0.08632
        min(4)=      7 -> 19       -0.07349
        min(5)=      8 -> 22       -0.03450
        #CIs=38 #CIs>0=16 #CIs<0=22

40   Singlet-B1  23.2765      53.27   0.0099   0.000
        max(1)=      9 -> 24        0.64169
        max(2)=      6 -> 13        0.01962
        max(3)=      9 -> 35        0.01888
        max(4)=      6 -> 20        0.01100
        max(5)=      9 -> 27        0.00959
        min(1)=      9 -> 23       -0.28361
        min(2)=      9 -> 21       -0.05587
        min(3)=      8 -> 26       -0.03849
        min(4)=      7 -> 25       -0.03128
        min(5)=      9 -> 32       -0.02920
        #CIs=30 #CIs>0=17 #CIs<0=12
```

9 NH_3

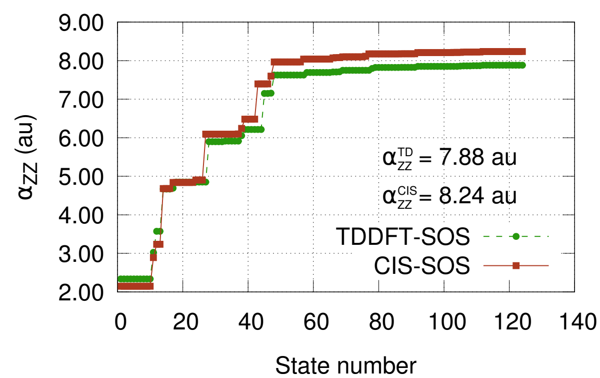
9.1 6-311G(d,p)

9.1.1 Plots

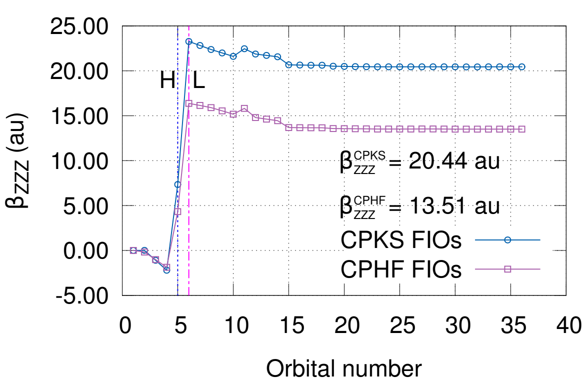
Figure S13: For NH_3 molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S13a and S13c) or states (SOS approaches, in Plots S13b and S13d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.02 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



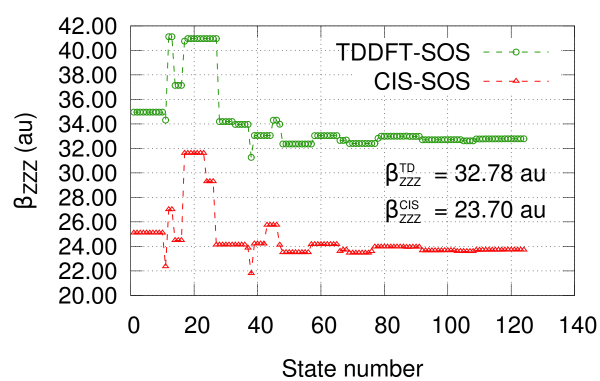
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

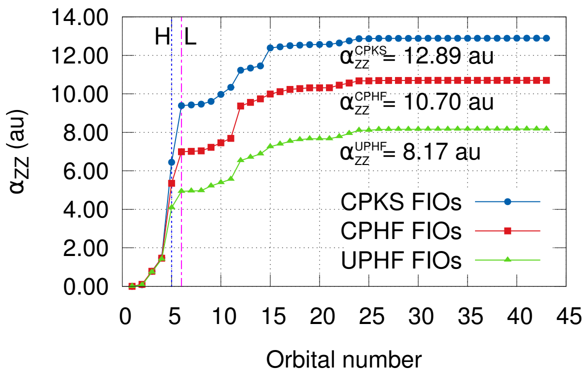


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

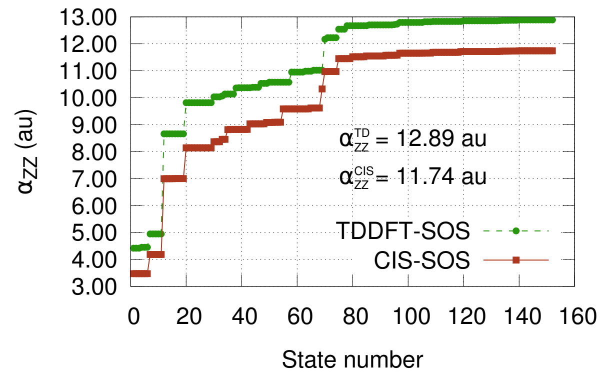
9.2 6-311++G(d,p)

9.2.1 Plots

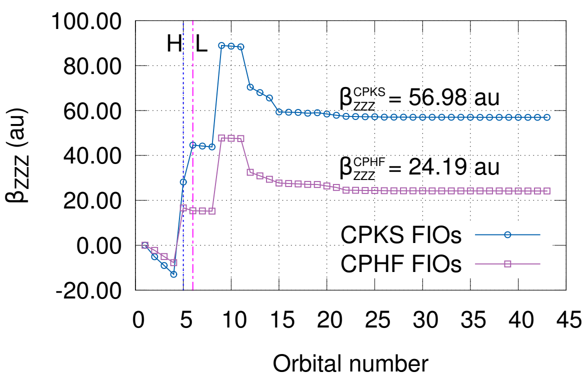
Figure S14: For NH_3 molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S14a and S14c) or states (SOS approaches, in Plots S14b and S14d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.12 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



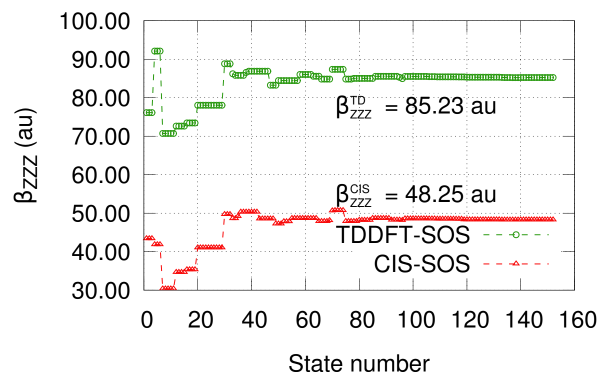
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



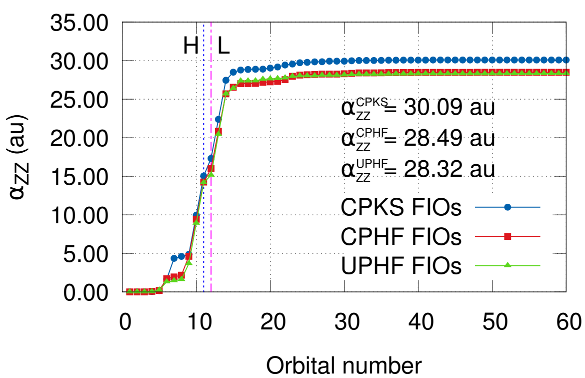
(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

10 F-CC-H

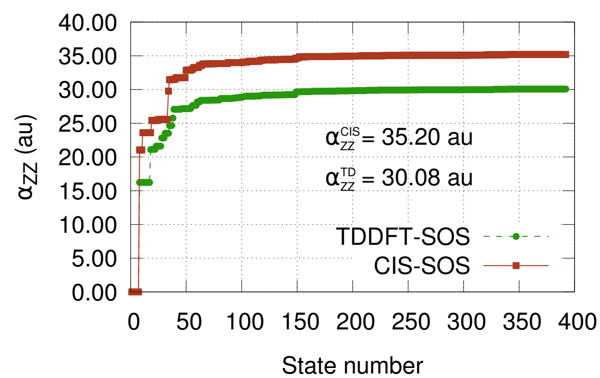
10.1 6-311G(d,p)

10.1.1 Plots

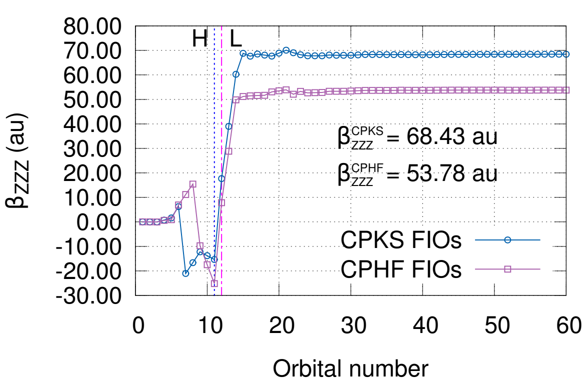
Figure S15: For F−C≡C−H molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S15a and S15c) or states (SOS approaches, in Plots S15b and S15d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.03 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



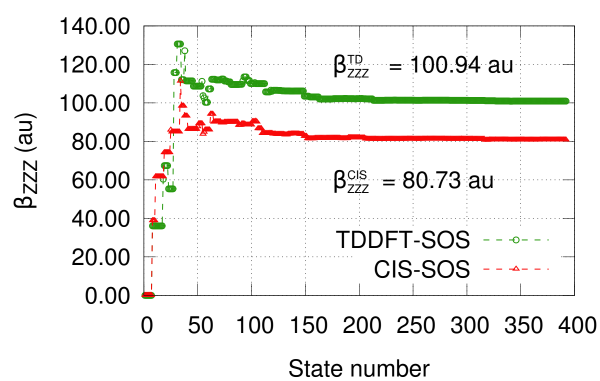
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

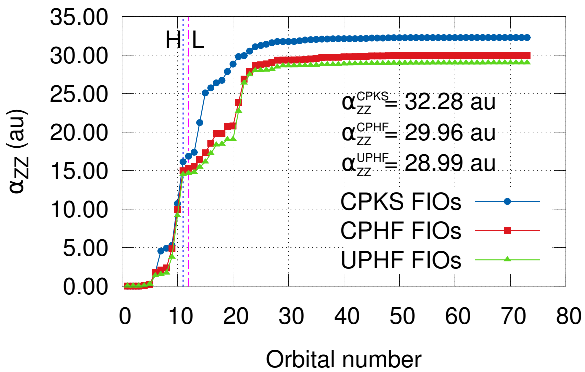


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

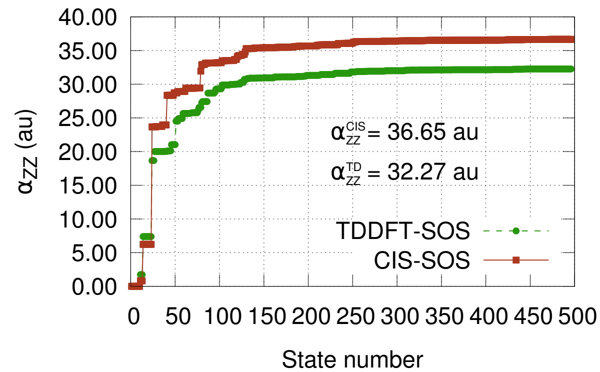
10.2 6-311++G(d,p)

10.2.1 Plots

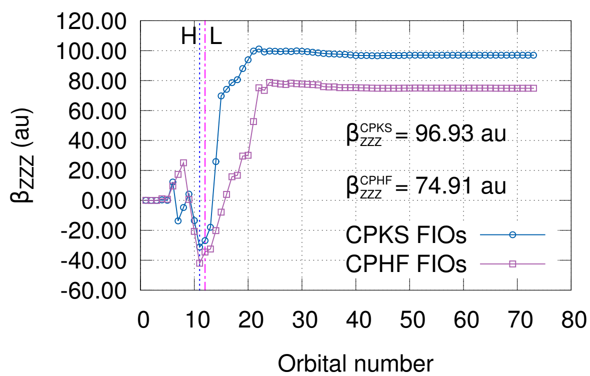
Figure S16: For F−C≡C−H molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (bottom) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S16a and S16c) or states (SOS approaches, in Plots S16b and S16d). For α FIOs, three approaches were considered: CPKS (CAM-B3LYP), CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. All elements of the β tensor were recomputed with an error less than 0.03 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



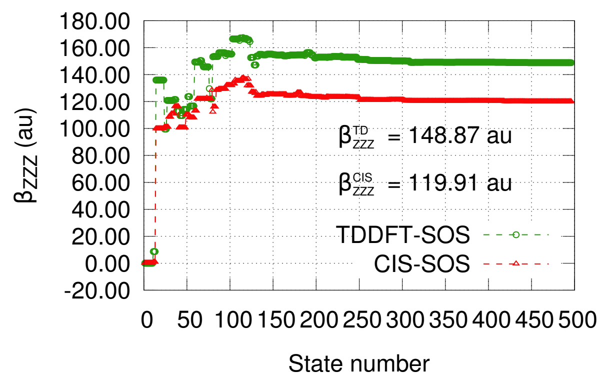
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.



(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.



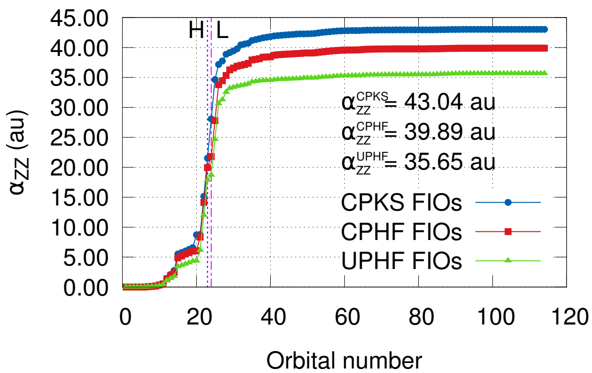
(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

11 $HCCCF_3$

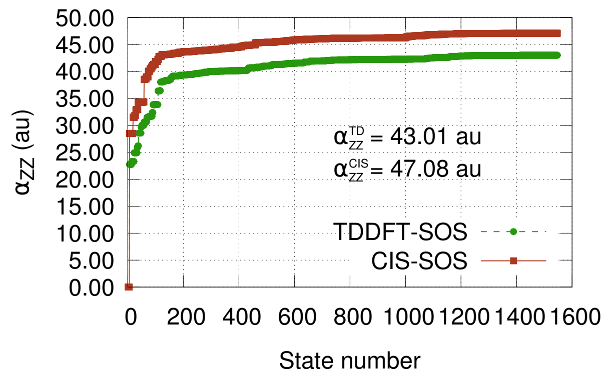
11.1 6-311G(d,p)

11.1.1 Plots

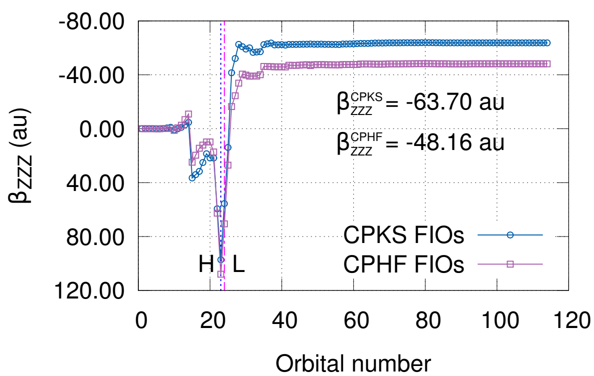
Figure S17: For H−C≡C−CF_3 molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S17a and S17b) or states (SOS approaches, in Plots S17c and S17d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S17e and S17f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.20 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



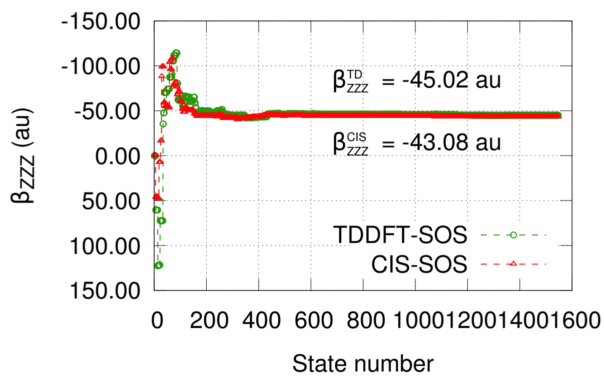
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

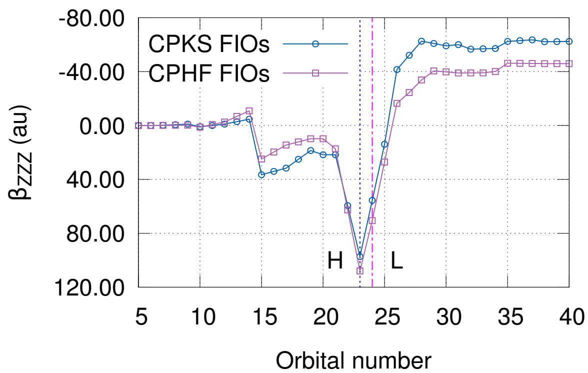


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

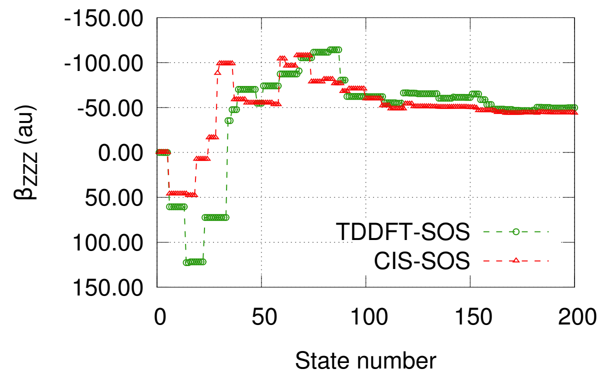


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S17: (continued) For H−C≡C−CF_3 molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S17a and S17b) or states (SOS approaches, in Plots S17c and S17d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S17e and S17f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.20 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 5 and 40.

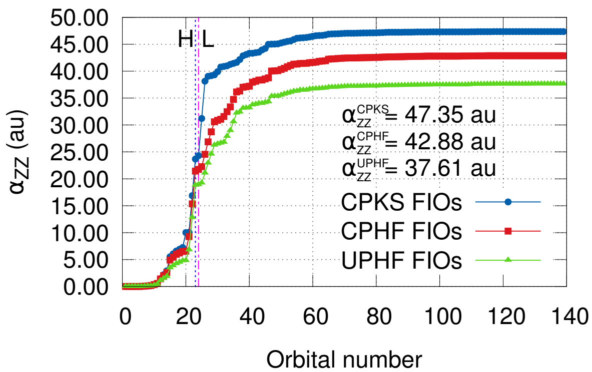


(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 200.

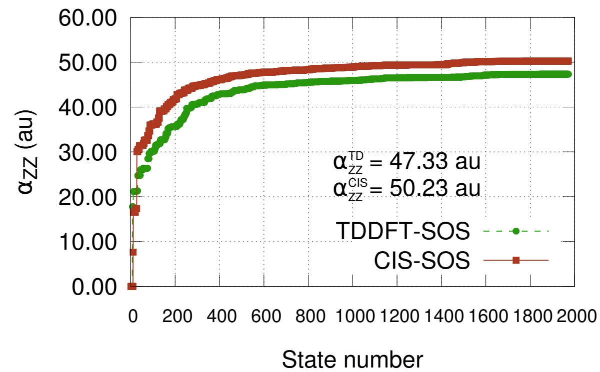
11.2 6-311++G(d,p)

11.2.1 Plots

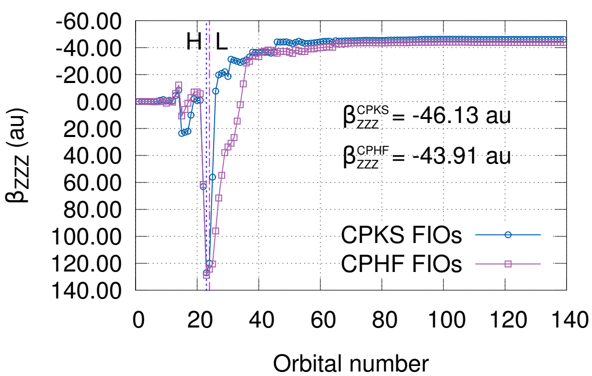
Figure S18: For H−C≡C−CF_3 molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S18a and S18b) or states (SOS approaches, in Plots S18c and S18d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S18e and S18f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.20 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



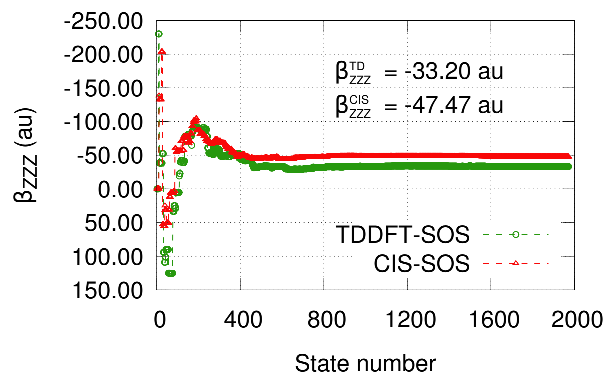
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

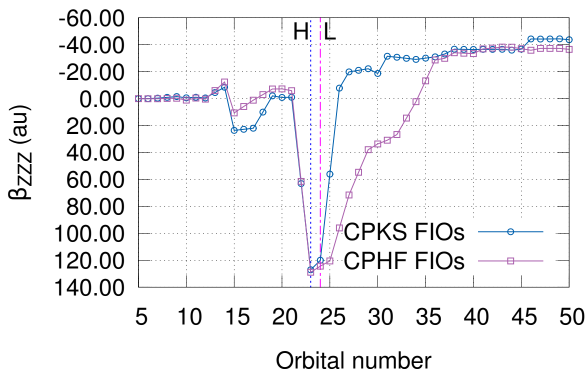


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

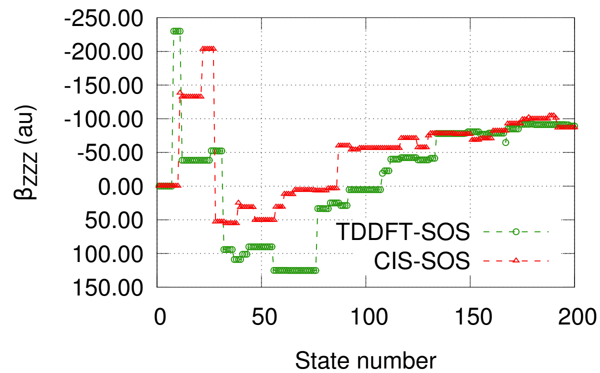


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S18: (continued) For H−C≡C−CF_3 molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S18a and S18b) or states (SOS approaches, in Plots S18c and S18d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S18e and S18f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.20 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 5 and 50.



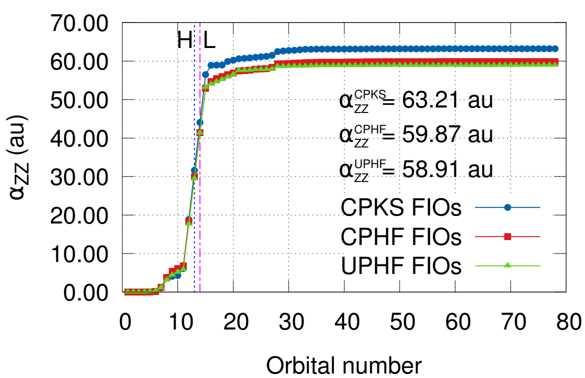
(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 200.

12 CN-CC-H

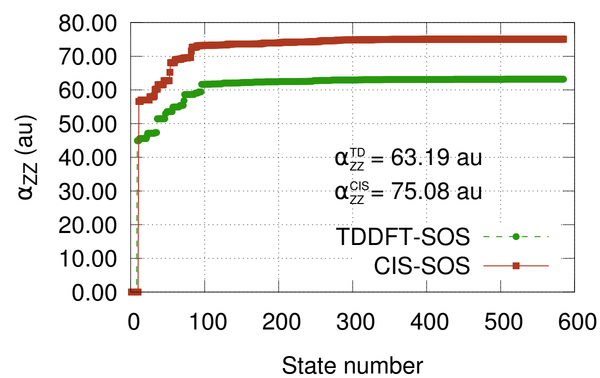
12.1 6-311G(d,p)

12.1.1 Plots

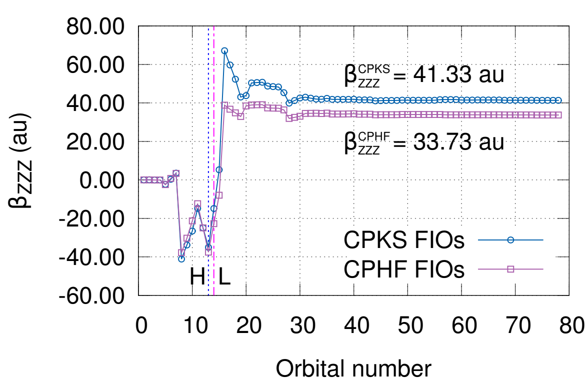
Figure S19: For CN−C≡C−H molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S19a and S19b) or states (SOS approaches, in Plots S19c and S19d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S19e and S19f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.13 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



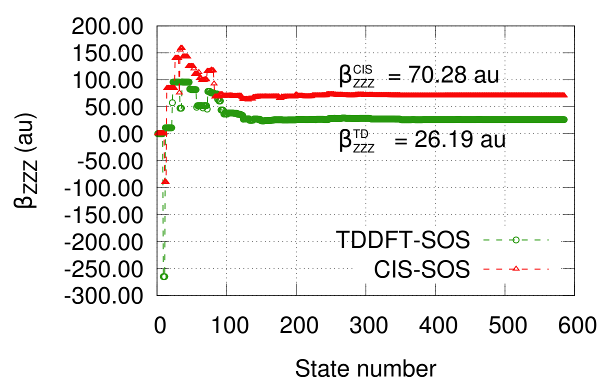
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

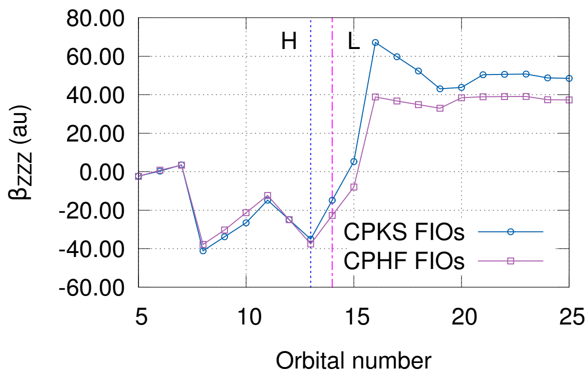


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

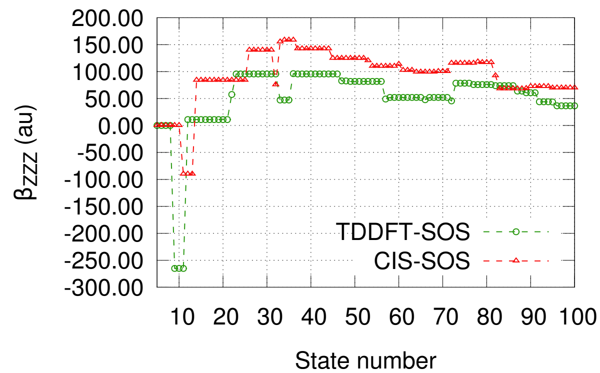


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S19: (continued) For CN−C≡C−H molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S19a and S19b) or states (SOS approaches, in Plots S19c and S19d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S19e and S19f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.13 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 5 and 25.

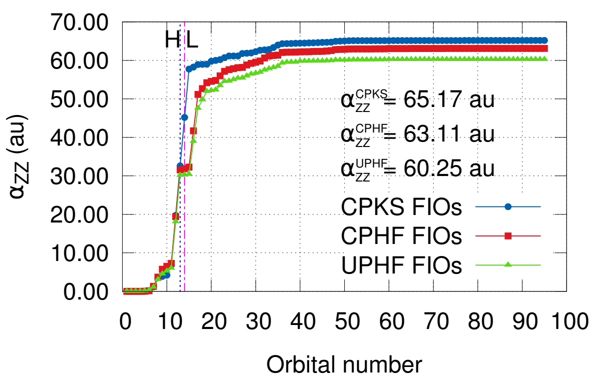


(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 5 and 100.

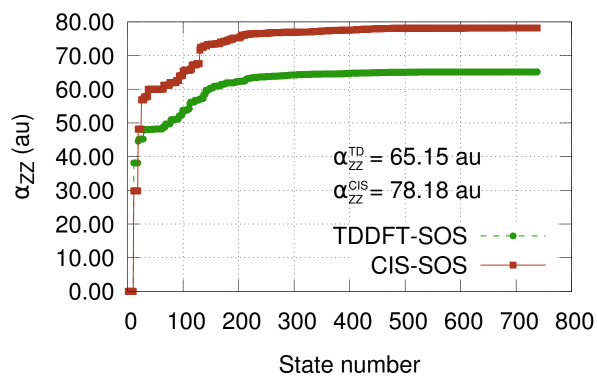
12.2 6-311++G(d,p)

12.2.1 Plots

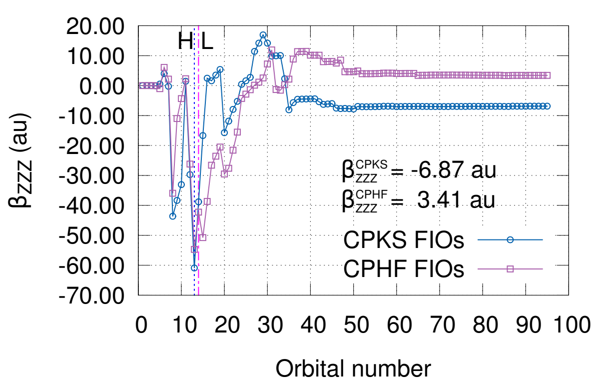
Figure S20: For CN−C≡C−H molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S20a and S20b) or states (SOS approaches, in Plots S20c and S20d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S20e and S20f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.13 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



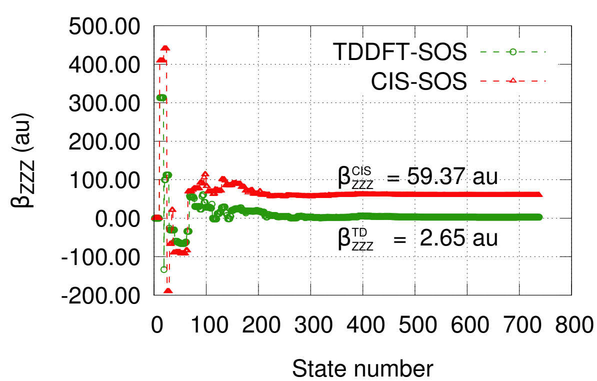
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

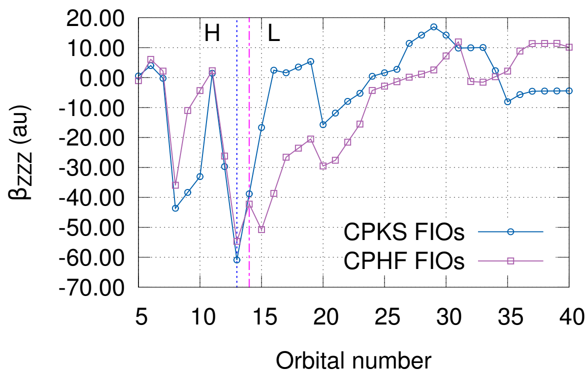


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

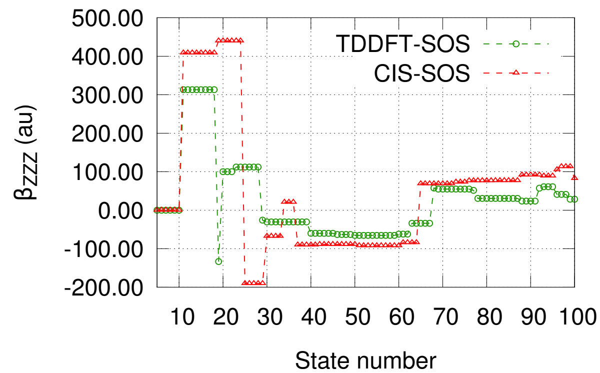


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S20: (continued) For CN−C≡C−H molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S20a and S20b) or states (SOS approaches, in Plots S20c and S20d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S20e and S20f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.13 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 5 and 40.



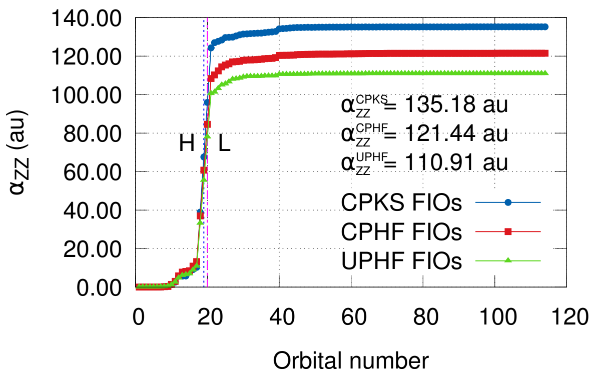
(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 5 and 100.

13 CN-CC-CC-H

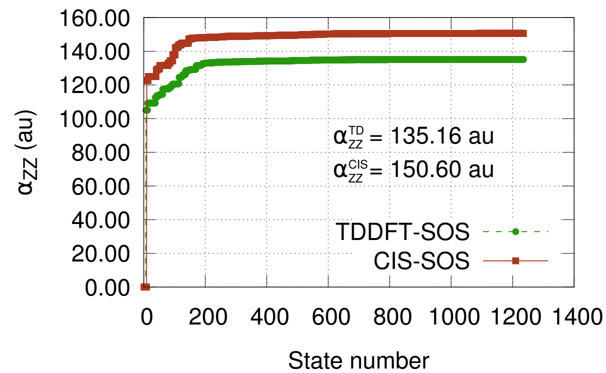
13.1 6-311G(d,p)

13.1.1 Plots

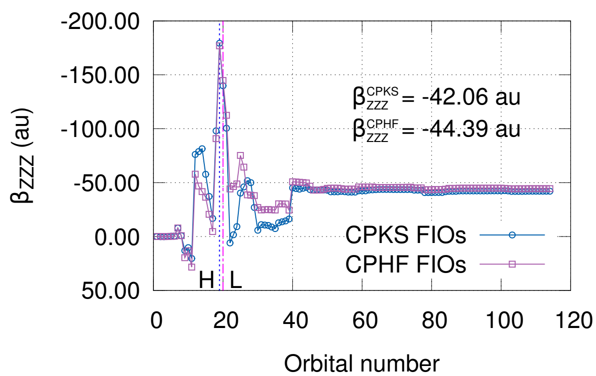
Figure S21: For CN−C≡C−C≡C−H molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S21a and S21b) or states (SOS approaches, in Plots S21c and S21d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S21e and S21f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.12 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



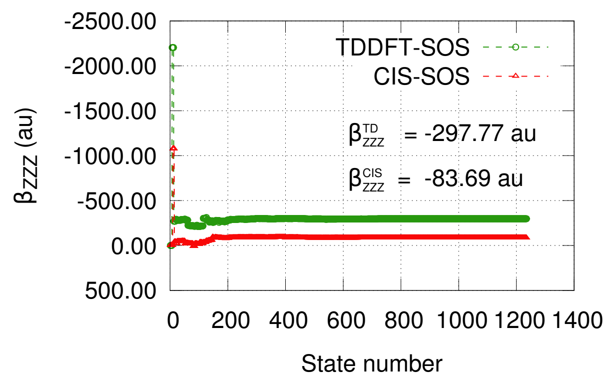
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

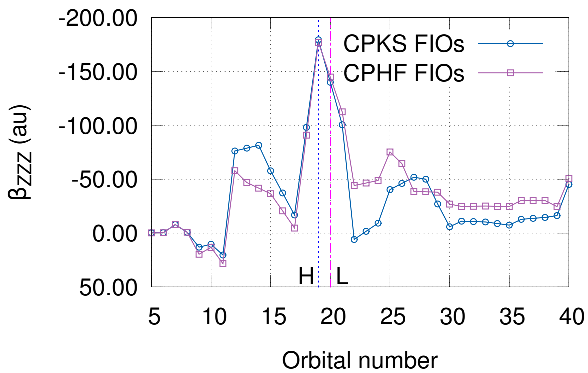


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

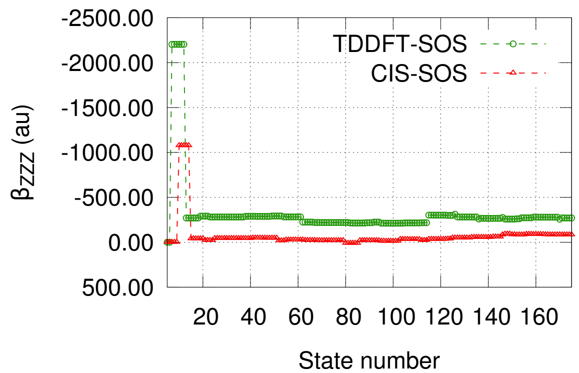


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S21: (continued) For CN−C≡C−C≡C−H molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S21a and S21b) or states (SOS approaches, in Plots S21c and S21d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S21e and S21f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.12 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 5 and 40.

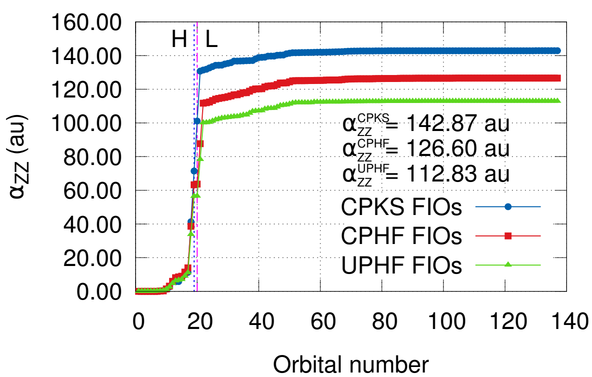


(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 5 and 175.

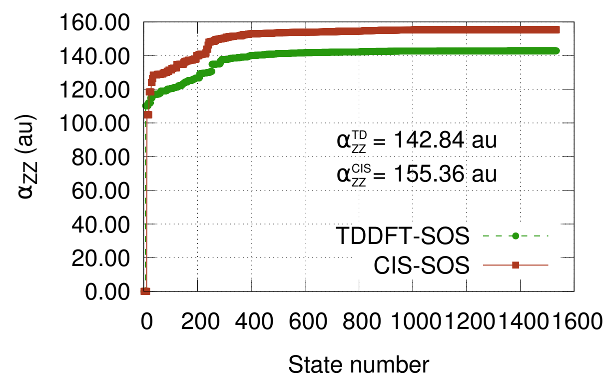
13.2 6-311++G(d,p)

13.2.1 Plots

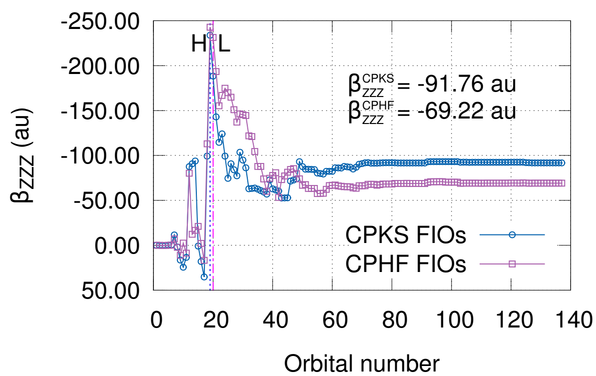
Figure S22: For CN−C≡C−C≡C−H molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S22a and S22b) or states (SOS approaches, in Plots S22c and S22d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S22e and S22f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.24 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



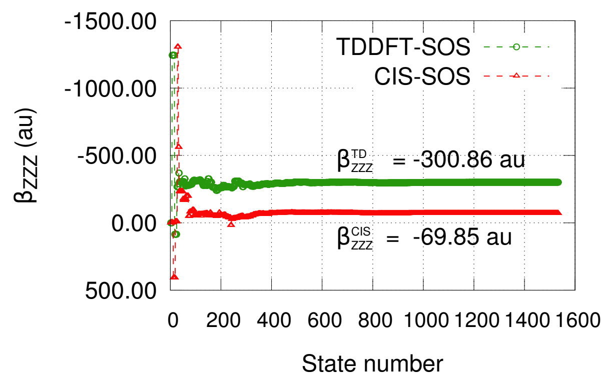
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

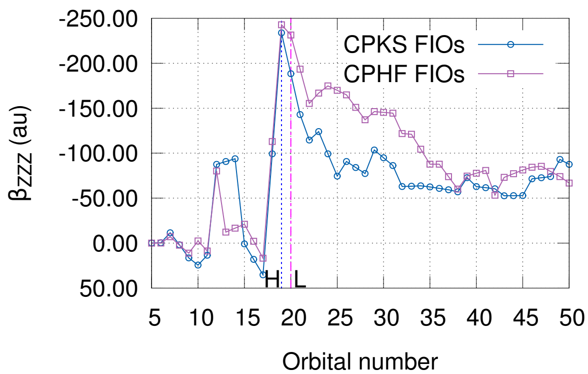


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

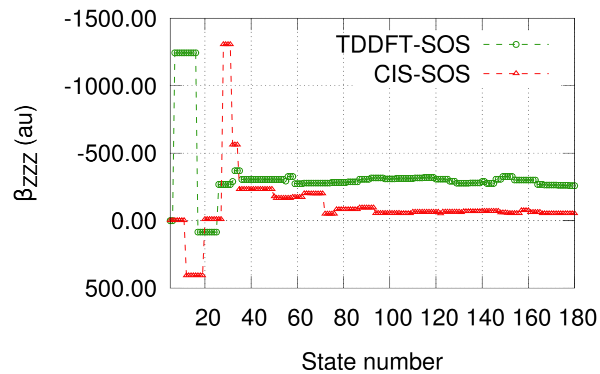


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S22: (continued) For CN−C≡C−C≡C−H molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S22a and S22b) or states (SOS approaches, in Plots S22c and S22d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S22e and S22f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.24 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 5 and 40.



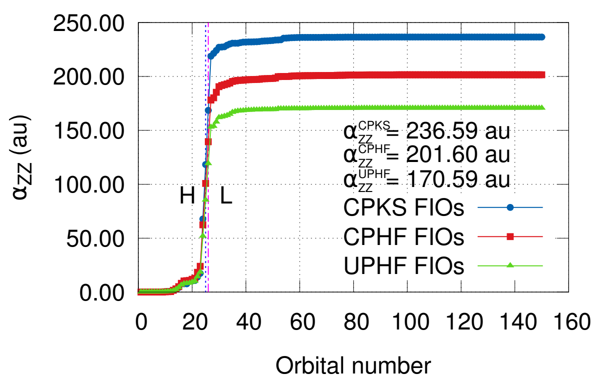
(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 5 and 175.

14 CN-CC-CC-CC-H

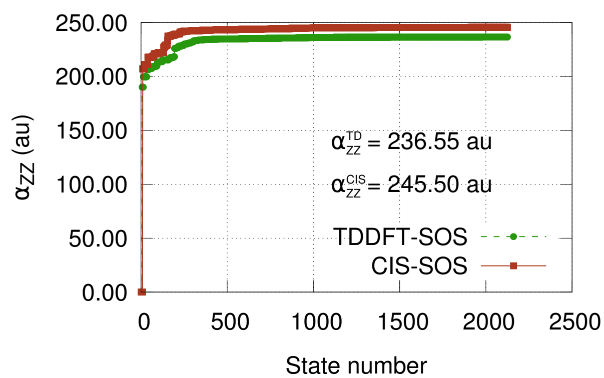
14.1 6-311G(d,p)

14.1.1 Plots

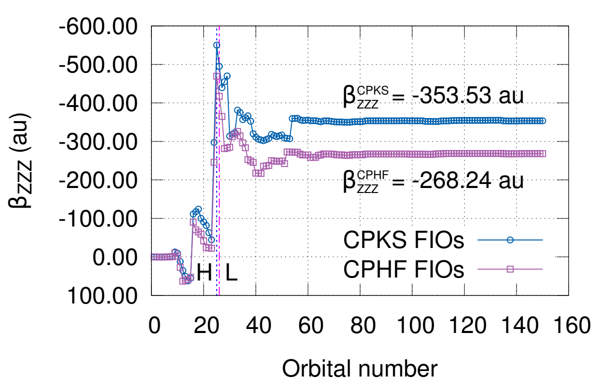
Figure S23: For CN−C≡C−C≡C−C≡C−H molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S23a and S23b) or states (SOS approaches, in Plots S23c and S23d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S23e and S23f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.41 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



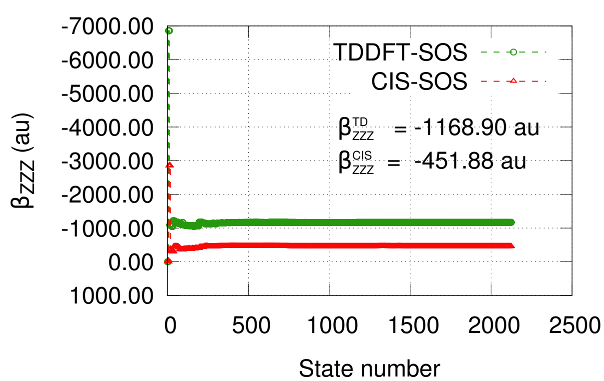
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

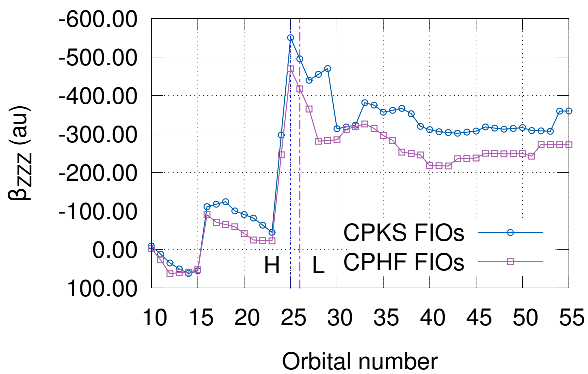


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

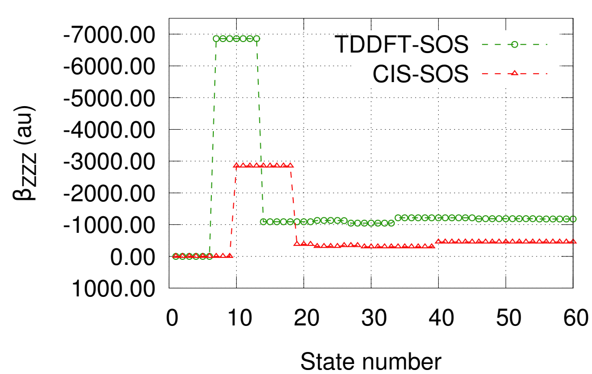


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S23: (continued) For CN−C≡C−C≡C−C≡C−H molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S23a and S23b) or states (SOS approaches, in Plots S23c and S23d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S23e and S23f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.41 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 10 and 55.

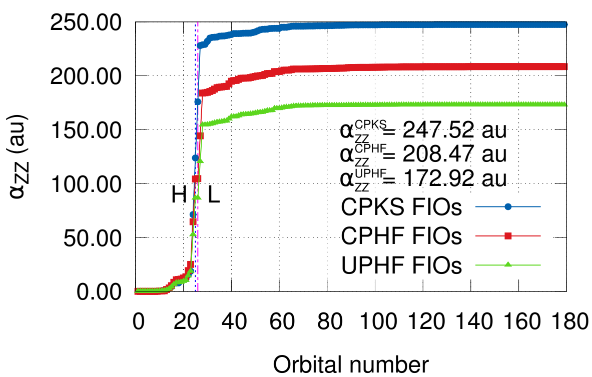


(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 60.

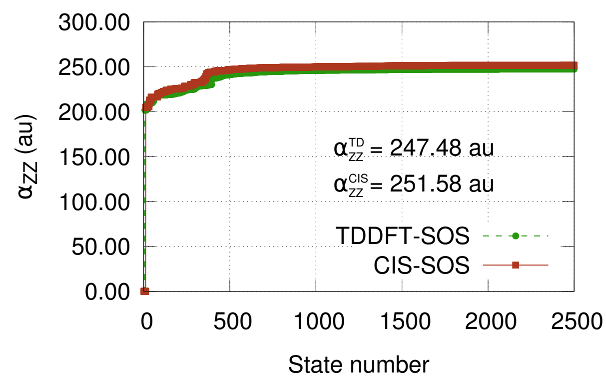
14.2 6-311++G(d,p)

14.2.1 Plots

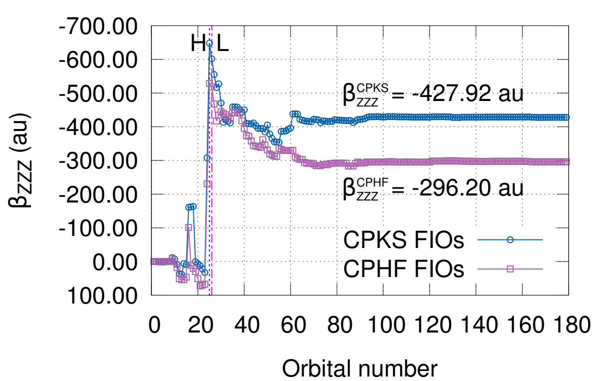
Figure S24: For CN−C≡C−C≡C−C≡C−H molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S24a and S24b) or states (SOS approaches, in Plots S24c and S24d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S24e and S24f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.21 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



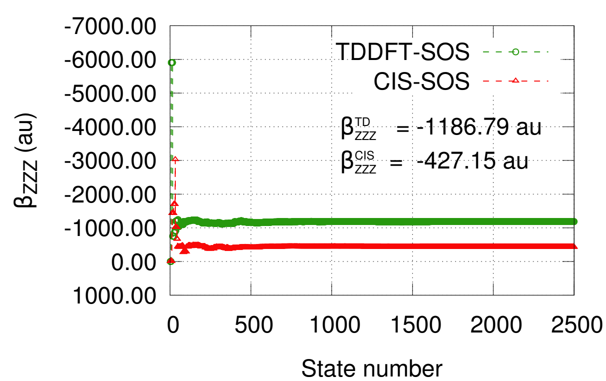
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

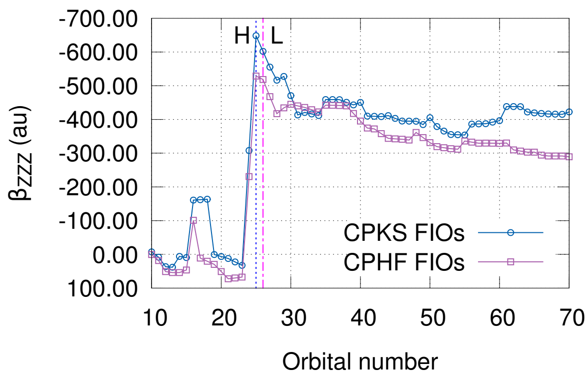


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

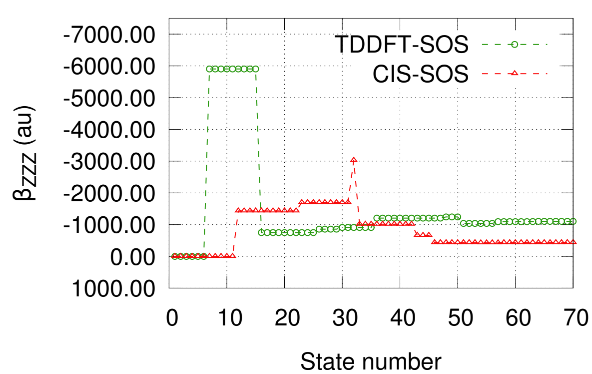


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S24: (continued) For CN−C≡C−C≡C−C≡C−H molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S24a and S24b) or states (SOS approaches, in Plots S24c and S24d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S24e and S24f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.21 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 10 and 70.



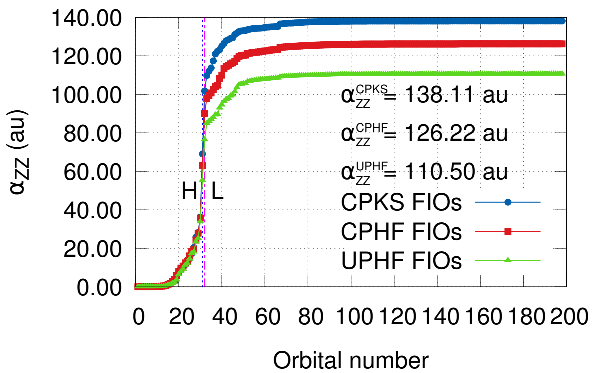
(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 70.

15 *p*-cyanoaniline

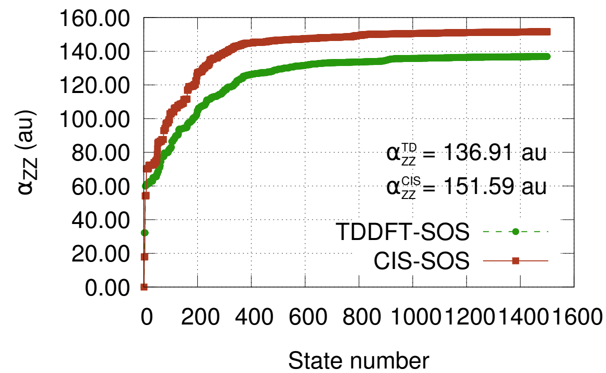
15.1 6-311G(d,p)

15.1.1 Plots

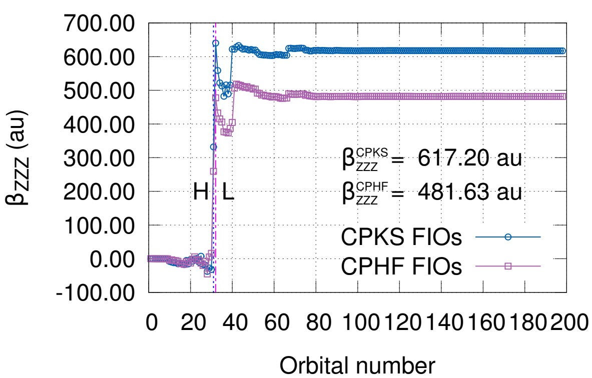
Figure S25: For *p*-cyanoaniline molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S25a and S25b) or states (SOS approaches, in Plots S25c and S25d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S25d and S25f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.11 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



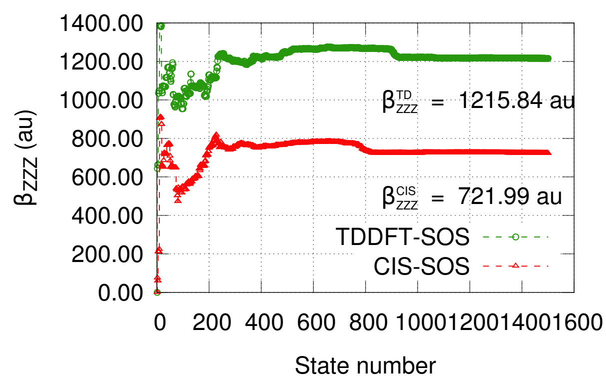
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

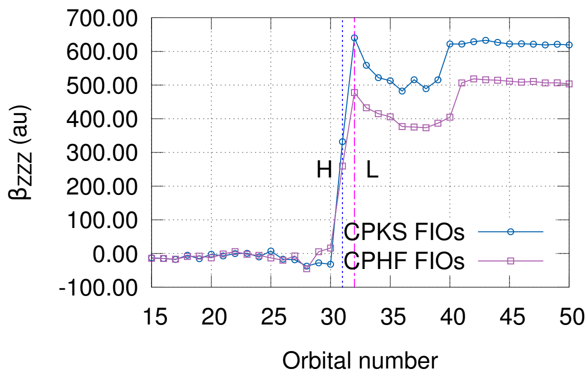


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

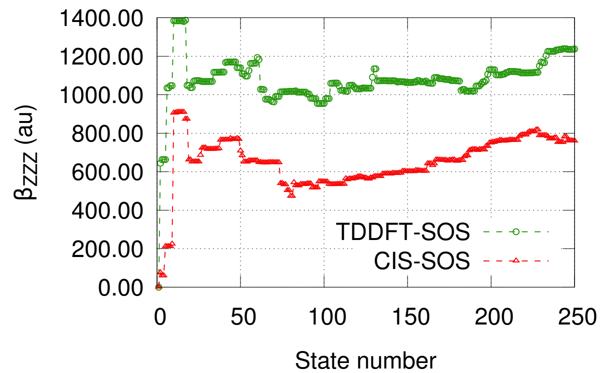


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S25: (continued) For p-cyanoaniline molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S25a and S25b) or states (SOS approaches, in Plots S25c and S25d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S25d and S25f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.11 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 15 and 50.

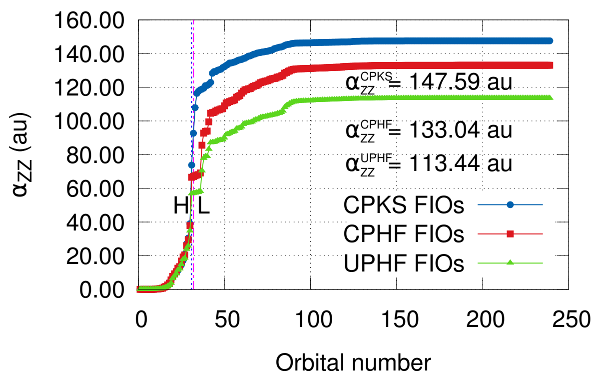


(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 250.

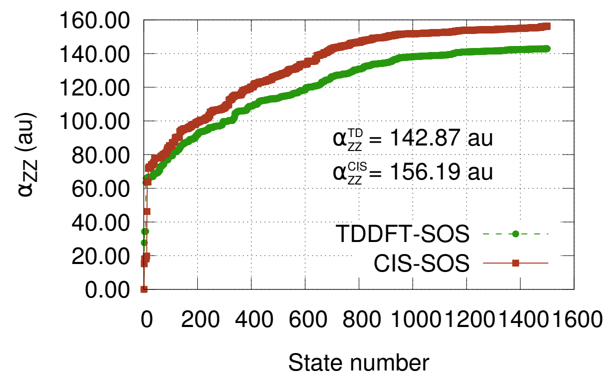
15.2 6-311++G(d,p)

15.2.1 Plots

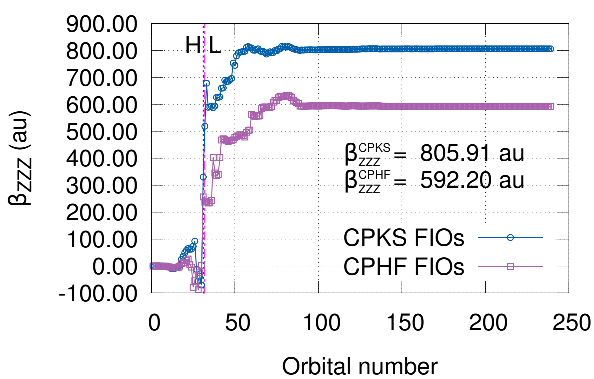
Figure S26: For p-cyanoaniline molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S26a and S26b) or states (SOS approaches, in Plots S26c and S26d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S26d and S26f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.11 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



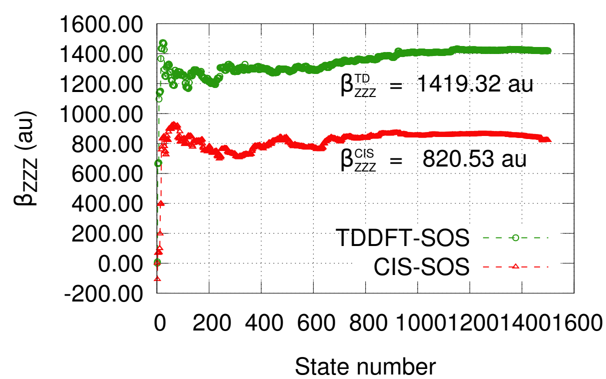
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

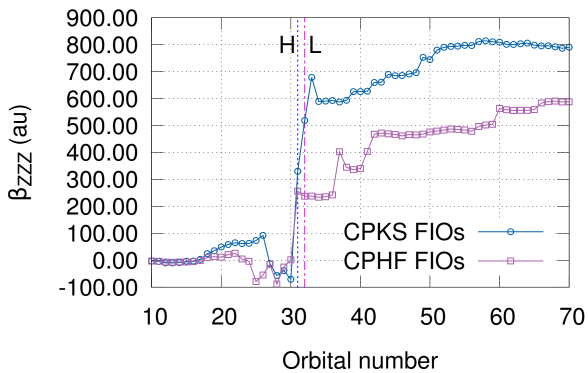


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

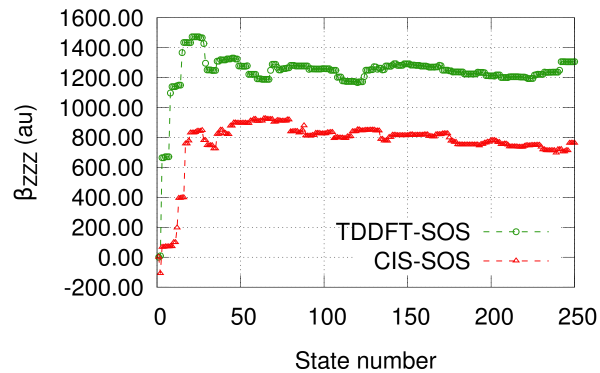


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S26: (continued) For p-cyanoaniline molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S26a and S26b) or states (SOS approaches, in Plots S26c and S26d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S26d and S26f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.11 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 15 and 50.



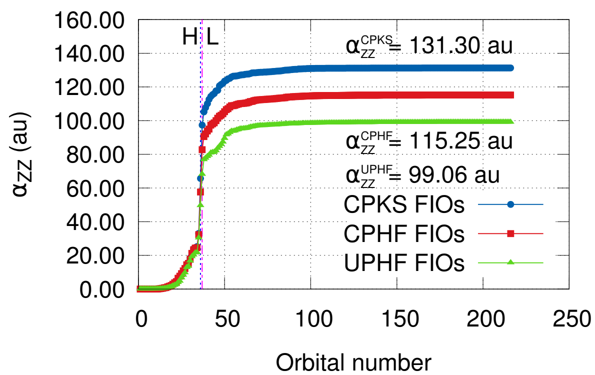
(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 250.

16 *p*-nitroaniline

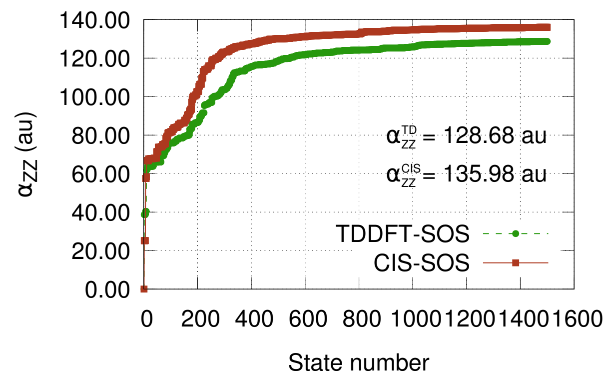
16.1 6-311G(d,p)

16.1.1 Plots

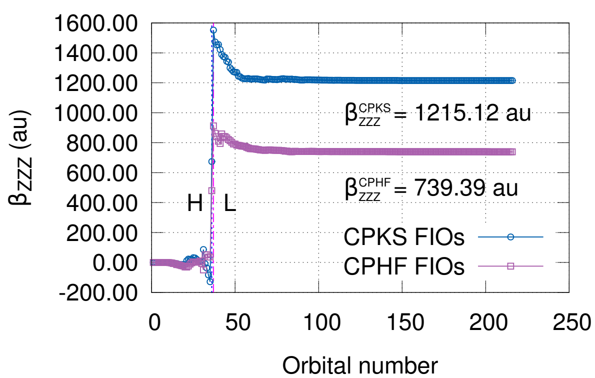
Figure S27: For *p*-nitroaniline molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S27a and S27b) or states (SOS approaches, in Plots S27c and S27d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S27e and S27f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.37 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



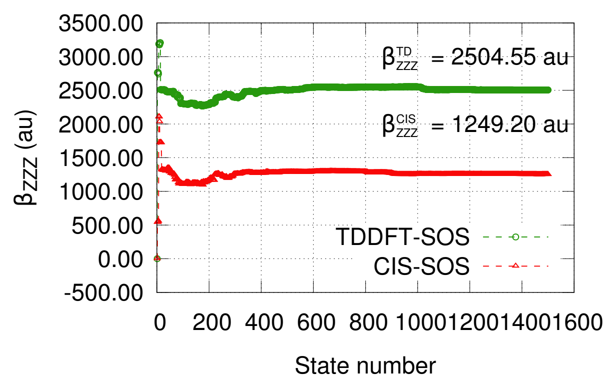
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

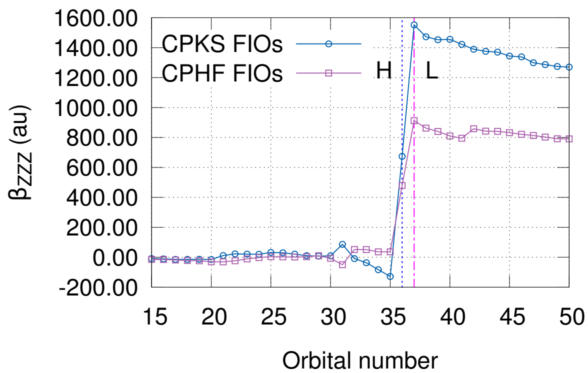


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

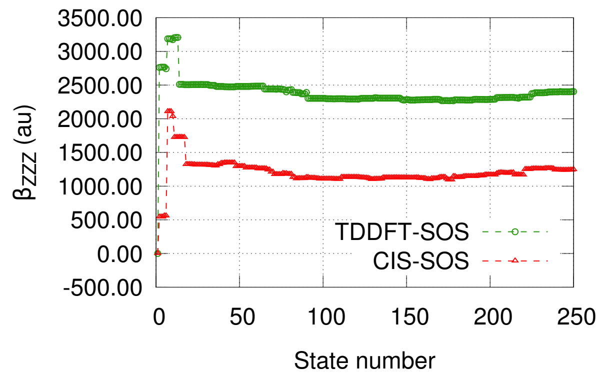


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S27: (continued) For *p*-nitroaniline molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S27a and S27b) or states (SOS approaches, in Plots S27c and S27d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S27e and S27f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.37 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 15 and 50.



(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 250.

16.1.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength    ___f___ _<S**2>_
                                                        2        Singlet-A'    4.5920         270.00     0.3670     0.000
1        Singlet-A"    4.1147         301.32     0.0000    0.000          max(1)=        36 -> 37          0.68965
               max(1)=        34 -> 37          0.67431                    max(2)=        35 -> 38          0.10043
               max(2)=        27 -> 40          0.01118                    max(3)=        31 -> 40          0.04187
               max(3)=        26 -> 37          0.01054                    max(4)=        31 -> 39          0.03005
               max(4)=        30 -> 37          0.00937                    max(5)=        29 -> 37          0.01343
               max(5)=        27 -> 39          0.00637                    min(1)=        31 -> 37         -0.09692
               min(1)=        34 -> 40         -0.17798                    min(2)=        30 -> 50         -0.02180
               min(2)=        34 -> 39         -0.10948                    min(3)=        32 -> 47         -0.01837
               min(3)=        34 -> 46         -0.02774                    min(4)=        32 -> 37         -0.01730
               min(4)=        27 -> 37         -0.01731                    min(5)=        34 -> 45         -0.01695
               min(5)=        34 -> 42         -0.01418                    #CIs=2384 #CIs>0=1051 #CIs<0=1061
               #CIs=2195 #CIs>0=781 #CIs<0=803
```

```
3        Singlet-A'    4.6429        267.04    0.0004    0.000
         max(1)=       32 -> 37         0.67546
         max(2)=       25 -> 37         0.02320
         max(3)=       28 -> 37         0.01979
         max(4)=       36 -> 37         0.01789
         max(5)=       29 -> 37         0.01470
         min(1)=       32 -> 40        -0.17158
         min(2)=       32 -> 39        -0.10632
         min(3)=       32 -> 46        -0.02523
         min(4)=       25 -> 40        -0.01736
         min(5)=       32 -> 42        -0.01392
         #CIs=2370 #CIs>0=920 #CIs<0=932

4        Singlet-A"    4.9397        251.00    0.0078    0.000
         max(1)=       36 -> 38         0.56495
         max(2)=       33 -> 37         0.06008
         max(3)=       22 -> 38         0.01137
         max(4)=       33 -> 40         0.01077
         max(5)=       35 -> 68         0.00757
         min(1)=       35 -> 37        -0.39877
         min(2)=       35 -> 40        -0.11204
         min(3)=       35 -> 39        -0.05993
         min(4)=       31 -> 38        -0.04252
         min(5)=       35 -> 42        -0.01043
         #CIs=2284 #CIs>0=938 #CIs<0=1006

5        Singlet-A"    5.8000        213.77    0.0805    0.000
         max(1)=       35 -> 37         0.57965
         max(2)=       36 -> 38         0.39505
         max(3)=       33 -> 37         0.06330
         max(4)=       31 -> 38         0.04339
         max(5)=       35 -> 56         0.01607
         min(1)=       35 -> 40        -0.04377
         min(2)=       35 -> 39        -0.02591
         min(3)=       36 -> 41        -0.01366
         min(4)=       26 -> 48        -0.01303
         min(5)=       27 -> 48        -0.01253
         #CIs=2288 #CIs>0=941 #CIs<0=1005

6        Singlet-A'    6.2642        197.92    0.0016    0.000
         max(1)=       36 -> 39         0.66406
         max(2)=       31 -> 39         0.11595
         max(3)=       35 -> 38         0.05525
         max(4)=       31 -> 37         0.03750
         max(5)=       29 -> 39         0.01269
         min(1)=       36 -> 40        -0.16744
         min(2)=       31 -> 40        -0.06675
         min(3)=       36 -> 42        -0.04391
         min(4)=       31 -> 42        -0.04329
         min(5)=       35 -> 41        -0.04238
         #CIs=2380 #CIs>0=1048 #CIs<0=994

7        Singlet-A'    6.6277        187.07    0.0327    0.000
         max(1)=       36 -> 40         0.53002
         max(2)=       35 -> 38         0.42128
         max(3)=       31 -> 37         0.11707
         max(4)=       36 -> 39         0.09771
         max(5)=       32 -> 47         0.03359
         min(1)=       31 -> 39        -0.05435
         min(2)=       33 -> 38        -0.05033
         min(3)=       36 -> 37        -0.04930
         min(4)=       29 -> 37        -0.04028
         min(5)=       31 -> 40        -0.02849
         #CIs=2386 #CIs>0=1091 #CIs<0=1029

8        Singlet-A"    6.7048        184.92    0.1439    0.000
         max(1)=       33 -> 37         0.69091
         max(2)=       32 -> 54         0.04678
         max(3)=       32 -> 50         0.04168
         max(4)=       34 -> 53         0.03616
         max(5)=       34 -> 55         0.03615
         min(1)=       36 -> 38        -0.08037
         min(2)=       31 -> 38        -0.06296
         min(3)=       34 -> 51        -0.05866
         min(4)=       33 -> 40        -0.02648
         min(5)=       33 -> 39        -0.02329
         #CIs=2286 #CIs>0=998 #CIs<0=977

9        Singlet-A"    7.1817        172.64    0.0007    0.000
         max(1)=       36 -> 41         0.66631
         max(2)=       31 -> 41         0.10009
         max(3)=       35 -> 40         0.02612
```

```
max(4)=       35 -> 44          0.02377
max(5)=       36 -> 52          0.01737
min(1)=       35 -> 39         -0.13953
min(2)=       36 -> 43         -0.10302
min(3)=       35 -> 42         -0.07181
min(4)=       31 -> 43         -0.06226
min(5)=       36 -> 45         -0.02544
#CIs=2279 #CIs>0=896 #CIs<0=941

10      Singlet-A'    7.1897        172.45    0.4941    0.000
max(1)=       35 -> 38          0.53271
max(2)=       36 -> 42          0.08728
max(3)=       36 -> 46          0.03948
max(4)=       28 -> 49          0.02864
max(5)=       30 -> 50          0.02776
min(1)=       36 -> 40         -0.36762
min(2)=       31 -> 37         -0.19607
min(3)=       36 -> 39         -0.12175
min(4)=       36 -> 37         -0.09733
min(5)=       31 -> 40         -0.04234
#CIs=2383 #CIs>0=1034 #CIs<0=1070

11      Singlet-A'    7.4228        167.03    0.0220    0.000
max(1)=       36 -> 42          0.66257
max(2)=       34 -> 38          0.15575
max(3)=       31 -> 37          0.06325
max(4)=       36 -> 39          0.05626
max(5)=       36 -> 49          0.04302
min(1)=       35 -> 38         -0.07269
min(2)=       35 -> 41         -0.06998
min(3)=       31 -> 39         -0.05663
min(4)=       36 -> 44         -0.05501
min(5)=       31 -> 44         -0.04814
#CIs=2382 #CIs>0=1044 #CIs<0=1007

12      Singlet-A'    7.4434        166.57    0.0007    0.000
max(1)=       34 -> 38          0.68458
max(2)=       27 -> 38          0.04068
max(3)=       35 -> 41          0.01889
max(4)=       36 -> 44          0.01465
max(5)=       31 -> 39          0.01255
min(1)=       36 -> 42         -0.15049
min(2)=       28 -> 37         -0.02735
min(3)=       31 -> 37         -0.02660
min(4)=       26 -> 38         -0.02507
min(5)=       30 -> 38         -0.02437
#CIs=2377 #CIs>0=924 #CIs<0=958

13      Singlet-A"    7.5448        164.33    0.0000    0.000
max(1)=       30 -> 37          0.66268
max(2)=       32 -> 38          0.16383
max(3)=       30 -> 40          0.11088
max(4)=       30 -> 39          0.05602
max(5)=       26 -> 40          0.03096
min(1)=       26 -> 37         -0.08087
min(2)=       27 -> 37         -0.05126
min(3)=       25 -> 38         -0.04847
min(4)=       26 -> 46         -0.02996
min(5)=       18 -> 37         -0.02679
#CIs=2246 #CIs>0=914 #CIs<0=880

14      Singlet-A'    7.6230        162.64    0.0391    0.000
max(1)=       31 -> 37          0.63006
max(2)=       35 -> 38          0.09946
max(3)=       28 -> 37          0.08293
max(4)=       36 -> 37          0.07994
max(5)=       31 -> 40          0.03923
min(1)=       36 -> 40         -0.20456
min(2)=       29 -> 37         -0.10439
min(3)=       36 -> 39         -0.10260
min(4)=       33 -> 38         -0.08697
min(5)=       36 -> 42         -0.04849
#CIs=2384 #CIs>0=984 #CIs<0=1104

15      Singlet-A"    7.7354        160.28    0.0001    0.000
max(1)=       32 -> 38          0.67753
max(2)=       19 -> 38          0.02657
max(3)=       27 -> 37          0.02113
max(4)=       27 -> 46          0.01497
max(5)=       17 -> 38          0.01420
min(1)=       30 -> 37         -0.16407
min(2)=       28 -> 38         -0.05006
```

```
        min(3)=       34 -> 40        -0.04518
        min(4)=       29 -> 38        -0.03759
        min(5)=       25 -> 38        -0.03612
        #CIs=2267 #CIs>0=826 #CIs<0=884

16   Singlet-A"   7.8651      157.64   0.0993   0.000
        max(1)=       35 -> 40         0.47058
        max(2)=       35 -> 39         0.40130
        max(3)=       31 -> 38         0.29149
        max(4)=       36 -> 38         0.12151
        max(5)=       36 -> 41         0.08271
        min(1)=       35 -> 37        -0.05165
        min(2)=       33 -> 40        -0.02993
        min(3)=       33 -> 39        -0.02822
        min(4)=       30 -> 49        -0.01664
        min(5)=       27 -> 48        -0.01563
        #CIs=2287 #CIs>0=979 #CIs<0=975

17   Singlet-A'   7.9323      156.30   0.0001   0.000
        max(1)=       33 -> 38         0.69822
        max(2)=       31 -> 37         0.09378
        max(3)=       35 -> 38         0.03286
        max(4)=       36 -> 40         0.01651
        max(5)=       32 -> 42         0.01537
        min(1)=       22 -> 37        -0.01804
        min(2)=       34 -> 43        -0.01095
        min(3)=       22 -> 46        -0.00934
        min(4)=       33 -> 43        -0.00677
        min(5)=       34 -> 41        -0.00641
        #CIs=2377 #CIs>0=976 #CIs<0=971

18   Singlet-A"   8.1246      152.60   0.0000   0.000
        max(1)=       35 -> 39         0.45817
        max(2)=       35 -> 42         0.30658
        max(3)=       36 -> 41         0.11483
        max(4)=       29 -> 41         0.05276
        max(5)=       35 -> 47         0.03375
        min(1)=       35 -> 40        -0.36951
        min(2)=       36 -> 43        -0.13542
        min(3)=       31 -> 38        -0.09207
        min(4)=       36 -> 45        -0.06702
        min(5)=       31 -> 43        -0.05483
        #CIs=2281 #CIs>0=932 #CIs<0=910

19   Singlet-A'   8.2584      150.13   0.0072   0.000
        max(1)=       30 -> 38         0.69695
        max(2)=       34 -> 38         0.02548
        max(3)=       29 -> 37         0.02274
        max(4)=       28 -> 37         0.02218
        max(5)=       30 -> 67         0.02019
        min(1)=       25 -> 37        -0.05918
        min(2)=       25 -> 46        -0.05514
        min(3)=       35 -> 41        -0.04625
        min(4)=       18 -> 38        -0.02335
        min(5)=       36 -> 44        -0.02257
        #CIs=2365 #CIs>0=883 #CIs<0=926

20   Singlet-A"   8.2595      150.11   0.0000   0.000
        max(1)=       34 -> 40         0.55705
        max(2)=       34 -> 39         0.34114
        max(3)=       34 -> 37         0.21020
        max(4)=       34 -> 46         0.11978
        max(5)=       32 -> 38         0.05640
        min(1)=       26 -> 37        -0.04796
        min(2)=       28 -> 38        -0.02493
        min(3)=       21 -> 37        -0.02372
        min(4)=       29 -> 38        -0.01843
        min(5)=       26 -> 40        -0.01467
        #CIs=2255 #CIs>0=846 #CIs<0=885
```

16.1.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___   Exc.E Osc._Strength   ___f___ _<S**2>_
1    Singlet-A"   5.5098      225.03   0.0000   0.000
        max(1)=       33 -> 37         0.58784
```

max(2)= 33 -> 41 0.05815
max(3)= 33 -> 47 0.05713
max(4)= 27 -> 42 0.03547
max(5)= 33 -> 44 0.02378
min(1)= 33 -> 42 -0.36190
min(2)= 33 -> 39 -0.05465
min(3)= 33 -> 46 -0.05187
min(4)= 33 -> 92 -0.04773
min(5)= 27 -> 37 -0.03918
#states=936 #states>0=500 #states<0=436

2 Singlet-A’ 5.7079 217.22 0.3688 0.000
max(1)= 36 -> 37 0.63296
max(2)= 36 -> 42 0.09732
max(3)= 32 -> 42 0.05243
max(4)= 32 -> 47 0.02898
max(5)= 32 -> 39 0.02407
min(1)= 35 -> 38 -0.24506
min(2)= 32 -> 37 -0.09776
min(3)= 31 -> 37 -0.03827
min(4)= 29 -> 42 -0.03238
min(5)= 32 -> 46 -0.03001
#states=1569 #states>0=810 #states<0=759

3 Singlet-A’ 5.8463 212.07 0.0001 0.000
max(1)= 31 -> 37 0.56145
max(2)= 32 -> 42 0.10947
max(3)= 31 -> 41 0.05369
max(4)= 31 -> 47 0.05100
max(5)= 28 -> 37 0.04833
min(1)= 31 -> 42 -0.33298
min(2)= 32 -> 37 -0.18679
min(3)= 31 -> 39 -0.05136
min(4)= 25 -> 42 -0.04556
min(5)= 31 -> 46 -0.04288
#states=1129 #states>0=554 #states<0=575

4 Singlet-A" 5.8607 211.55 0.0093 0.000
max(1)= 36 -> 38 0.55319
max(2)= 35 -> 37 0.40760
max(3)= 35 -> 42 0.13750
max(4)= 35 -> 46 0.01616
max(5)= 22 -> 38 0.01370
min(1)= 32 -> 38 -0.03869
min(2)= 29 -> 38 -0.03234
min(3)= 34 -> 37 -0.02463
min(4)= 36 -> 66 -0.01699
min(5)= 35 -> 47 -0.01625
#states=1243 #states>0=638 #states<0=605

5 Singlet-A’ 7.3223 169.33 0.0023 0.000
max(1)= 36 -> 39 0.64341
max(2)= 32 -> 39 0.19934
max(3)= 31 -> 39 0.06652
max(4)= 29 -> 39 0.05574
max(5)= 32 -> 37 0.04943
min(1)= 35 -> 40 -0.09036
min(2)= 36 -> 41 -0.08159
min(3)= 32 -> 41 -0.07216
min(4)= 29 -> 41 -0.04635
min(5)= 32 -> 42 -0.02954
#states=1237 #states>0=606 #states<0=631

6 Singlet-A" 7.4245 166.99 0.1003 0.000
max(1)= 35 -> 37 0.47927
max(2)= 34 -> 37 0.31672
max(3)= 33 -> 53 0.03411
max(4)= 34 -> 41 0.02654
max(5)= 35 -> 42 0.02202
min(1)= 36 -> 38 -0.34403
min(2)= 34 -> 42 -0.16032
min(3)= 36 -> 40 -0.03537
min(4)= 34 -> 39 -0.02745
min(5)= 30 -> 49 -0.01941
#states=1511 #states>0=734 #states<0=777

7 Singlet-A’ 7.6171 162.77 0.8431 0.000
max(1)= 35 -> 38 0.57447
max(2)= 36 -> 37 0.24933
max(3)= 32 -> 42 0.08185
max(4)= 36 -> 41 0.04127
max(5)= 29 -> 37 0.03859

```
        min(1)=    36 -> 42    -0.26216
        min(2)=    32 -> 37    -0.04104
        min(3)=    29 -> 46    -0.03809
        min(4)=    32 -> 47    -0.03222
        min(5)=    35 -> 40    -0.02944
        #states=1497 #states>0=746 #states<0=751

8    Singlet-A"   8.0297   154.41   0.5747   0.000
        max(1)=    34 -> 37     0.49417
        max(2)=    36 -> 40     0.21626
        max(3)=    36 -> 38     0.21187
        max(4)=    32 -> 38     0.05888
        max(5)=    32 -> 40     0.05388
        min(1)=    35 -> 37    -0.24062
        min(2)=    34 -> 42    -0.21080
        min(3)=    35 -> 39    -0.08995
        min(4)=    36 -> 43    -0.06050
        min(5)=    35 -> 41    -0.04964
        #states=1565 #states>0=837 #states<0=728

9    Singlet-A"   8.1873   151.43   0.1561   0.000
        max(1)=    36 -> 40     0.53804
        max(2)=    35 -> 37     0.13588
        max(3)=    32 -> 40     0.12651
        max(4)=    34 -> 42     0.07477
        max(5)=    35 -> 44     0.05043
        min(1)=    35 -> 39    -0.23817
        min(2)=    34 -> 37    -0.17936
        min(3)=    35 -> 41    -0.17678
        min(4)=    36 -> 43    -0.10495
        min(5)=    36 -> 38    -0.09972
        #states=1439 #states>0=694 #states<0=745

10   Singlet-A’   8.4423   146.86   0.0443   0.000
        max(1)=    36 -> 41     0.60649
        max(2)=    36 -> 39     0.09661
        max(3)=    36 -> 49     0.07681
        max(4)=    32 -> 41     0.04884
        max(5)=    36 -> 57     0.03479
        min(1)=    35 -> 40    -0.18959
        min(2)=    36 -> 42    -0.10571
        min(3)=    32 -> 37    -0.10099
        min(4)=    35 -> 38    -0.09470
        min(5)=    36 -> 44    -0.08983
        #states=1381 #states>0=695 #states<0=686

11   Singlet-A’   8.6676   143.04   0.2843   0.000
        max(1)=    36 -> 42     0.53589
        max(2)=    32 -> 37     0.28404
        max(3)=    35 -> 38     0.22981
        max(4)=    36 -> 41     0.14066
        max(5)=    31 -> 37     0.09234
        min(1)=    29 -> 37    -0.07116
        min(2)=    35 -> 40    -0.06031
        min(3)=    36 -> 46    -0.06008
        min(4)=    32 -> 39    -0.05625
        min(5)=    36 -> 44    -0.05621
        #states=1589 #states>0=808 #states<0=781

12   Singlet-A"   9.0484   137.02   0.0097   0.000
        max(1)=    35 -> 41     0.42280
        max(2)=    35 -> 39     0.37819
        max(3)=    36 -> 40     0.21023
        max(4)=    29 -> 40     0.10646
        max(5)=    32 -> 40     0.03901
        min(1)=    36 -> 43    -0.23315
        min(2)=    36 -> 45    -0.15818
        min(3)=    32 -> 43    -0.12828
        min(4)=    32 -> 45    -0.06225
        min(5)=    31 -> 43    -0.04259
        #states=1112 #states>0=559 #states<0=553

13   Singlet-A"   9.4584   131.08   0.0001   0.000
        max(1)=    30 -> 37     0.62707
        max(2)=    30 -> 42     0.20653
        max(3)=    25 -> 38     0.08646
        max(4)=    26 -> 47     0.07326
        max(5)=    26 -> 42     0.06247
        min(1)=    31 -> 38    -0.08043
        min(2)=    26 -> 37    -0.07234
        min(3)=    26 -> 46    -0.06514
        min(4)=    18 -> 37    -0.06292
```

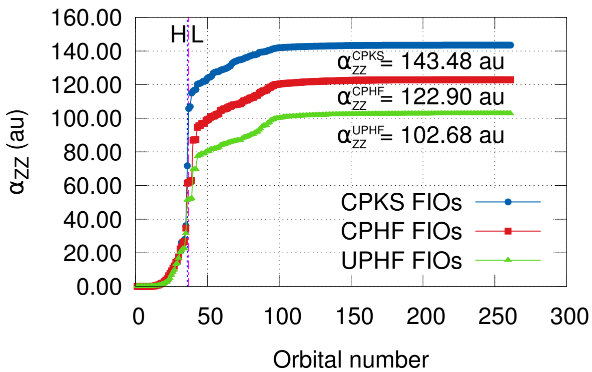
```
min(5)=       27 -> 37        -0.05227
#states=1177 #states>0=581 #states<0=596

14   Singlet-A'   9.5700   129.56   0.0321   0.000
max(1)=       35 -> 40         0.53968
max(2)=       36 -> 41         0.21176
max(3)=       36 -> 44         0.19202
max(4)=       30 -> 38         0.15759
max(5)=       35 -> 43         0.15757
min(1)=       32 -> 41        -0.13994
min(2)=       36 -> 47        -0.06309
min(3)=       36 -> 46        -0.06235
min(4)=       32 -> 39        -0.05651
min(5)=       31 -> 41        -0.04790
#states=1053 #states>0=529 #states<0=524

15   Singlet-A"   9.8449   125.94   0.0088   0.000
max(1)=       36 -> 43         0.35496
max(2)=       35 -> 42         0.31945
max(3)=       35 -> 39         0.31872
max(4)=       36 -> 40         0.23643
max(5)=       36 -> 45         0.09520
min(1)=       32 -> 38        -0.22183
min(2)=       35 -> 41        -0.11590
min(3)=       32 -> 40        -0.07422
min(4)=       35 -> 37        -0.07377
min(5)=       31 -> 38        -0.06564
#states=1277 #states>0=634 #states<0=643

16   Singlet-A'   9.8472   125.91   0.0037   0.000
max(1)=       30 -> 38         0.64910
max(2)=       25 -> 37         0.09071
max(3)=       25 -> 46         0.06155
max(4)=       32 -> 41         0.02758
max(5)=       19 -> 37         0.02354
min(1)=       35 -> 40        -0.15095
min(2)=       25 -> 47        -0.06939
min(3)=       33 -> 38        -0.06715
min(4)=       28 -> 37        -0.06247
min(5)=       27 -> 38        -0.05452
#states=1242 #states>0=622 #states<0=620

17   Singlet-A"   9.9934   124.07   0.0538   0.000
max(1)=       35 -> 42         0.31484
max(2)=       32 -> 40         0.12946
max(3)=       35 -> 39         0.07920
max(4)=       35 -> 47         0.07183
max(5)=       29 -> 38         0.04884
min(1)=       36 -> 43        -0.40473
min(2)=       35 -> 41        -0.28927
min(3)=       32 -> 38        -0.17211
min(4)=       36 -> 40        -0.16871
min(5)=       36 -> 45        -0.10903
#states=1321 #states>0=647 #states<0=674

18   Singlet-A'   10.0448   123.43   0.0418   0.000
max(1)=       32 -> 37         0.53182
max(2)=       32 -> 42         0.18720
max(3)=       31 -> 37         0.16067
max(4)=       28 -> 37         0.08075
max(5)=       36 -> 37         0.07715
min(1)=       36 -> 42        -0.28445
min(2)=       35 -> 38        -0.14260
min(3)=       29 -> 37        -0.06647
min(4)=       36 -> 46        -0.04413
min(5)=       22 -> 42        -0.04243
#states=1556 #states>0=769 #states<0=787

19   Singlet-A"   10.1433   122.23   0.0055   0.000
max(1)=       35 -> 41         0.37503
max(2)=       35 -> 42         0.33782
max(3)=       35 -> 44         0.11629
max(4)=       35 -> 48         0.06013
max(5)=       29 -> 43         0.05686
min(1)=       35 -> 39        -0.38699
min(2)=       32 -> 38        -0.20323
min(3)=       31 -> 38        -0.07251
min(4)=       35 -> 37        -0.06022
min(5)=       35 -> 46        -0.04214
#states=1218 #states>0=618 #states<0=600

20   Singlet-A"   10.4551   118.59   0.0429   0.000
```

```
max(1)=       28 -> 38         0.41404
max(2)=       32 -> 38         0.30771
max(3)=       35 -> 42         0.15807
max(4)=       27 -> 37         0.14279
max(5)=       29 -> 38         0.13131
min(1)=       31 -> 38        -0.30491
min(2)=       26 -> 37        -0.11425
min(3)=       27 -> 47        -0.07235
min(4)=       30 -> 37        -0.06792
min(5)=       21 -> 37        -0.04397
#states=1360 #states>0=681 #states<0=679
```

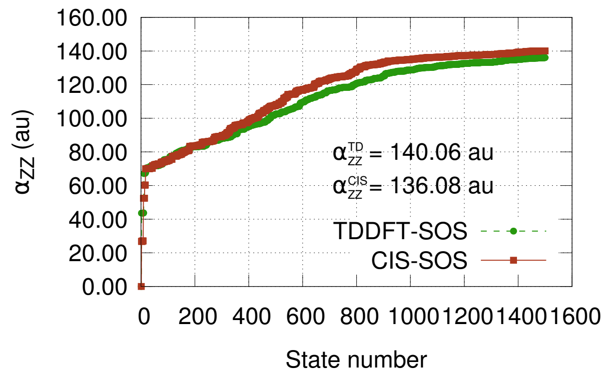
16.2 6-311++G(d,p)

16.2.1 Plots

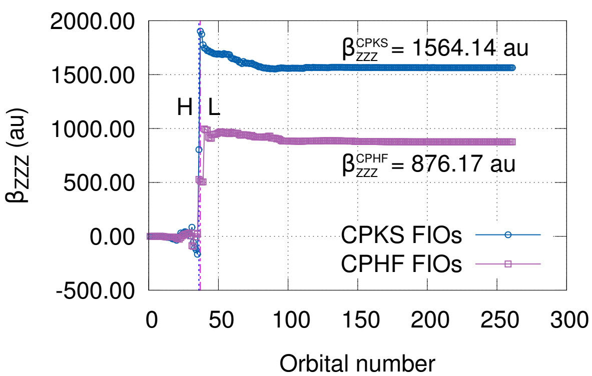
Figure S28: For *p*-nitroaniline molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S28a and S28b) or states (SOS approaches, in Plots S28c and S28d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S28e and S28f as well (bottom). All elements of the β tensor were recomputed with an error less than 1.00 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



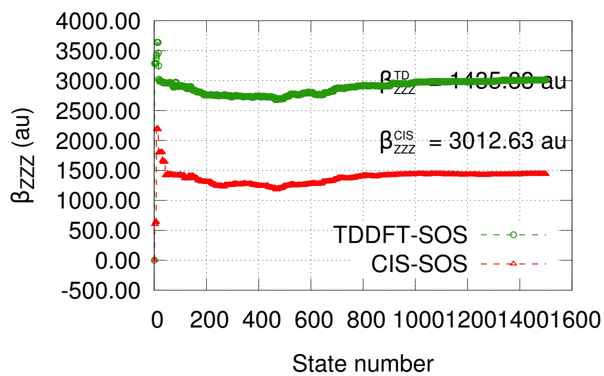
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

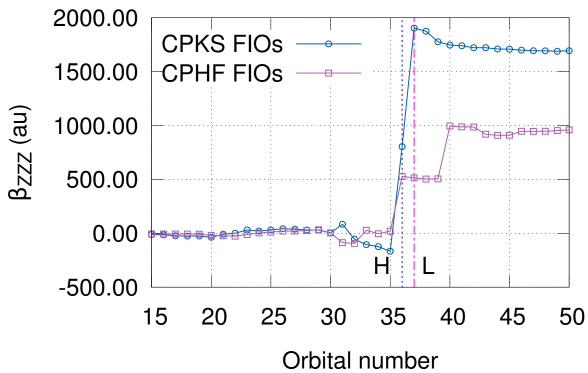


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

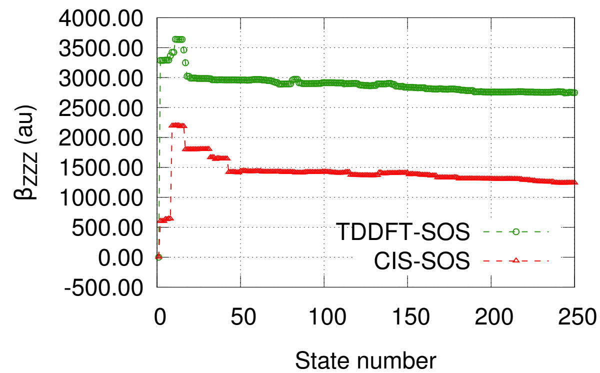


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S28: (continued) For p-nitroaniline molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S28a and S28b) or states (SOS approaches, in Plots S28c and S28d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S28e and S28f as well (bottom). All elements of the β tensor were recomputed with an error less than 1.00 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 15 and 50.



(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 250.

16.2.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___     Exc.E Osc._Strength    ___f___ _<S**2>_

1        Singlet-A"    4.0380         307.04     0.0000    0.000
              max(1)=        34 -> 37          0.67514
              max(2)=        34 -> 51          0.04697
              max(3)=        34 -> 47          0.03502
              max(4)=        34 -> 55          0.03023
              max(5)=        34 -> 38          0.02310
              min(1)=        34 -> 43         -0.19017
              min(2)=        34 -> 44         -0.02750
              min(3)=        34 -> 88         -0.01996
              min(4)=        34 -> 41         -0.01990
              min(5)=        34 -> 70         -0.01800
              #CIs=2762 #CIs>0=994 #CIs<0=1022

2        Singlet-A'    4.4033         281.57     0.3807    0.000
              max(1)=        36 -> 37          0.68961
              max(2)=        35 -> 39          0.09295
              max(3)=        31 -> 43          0.05405
              max(4)=        36 -> 43          0.02201
              max(5)=        29 -> 37          0.01632
              min(1)=        31 -> 37         -0.09702
              min(2)=        31 -> 55         -0.01284
              min(3)=        30 -> 64         -0.01111
              min(4)=        30 -> 90         -0.01042
              min(5)=        29 -> 43         -0.01023
              #CIs=2983 #CIs>0=1335 #CIs<0=1343
```

```
3        Singlet-A'    4.6012        269.46    0.0005    0.000
         max(1)=       32 -> 37         0.67632
         max(2)=       32 -> 51         0.04506
         max(3)=       32 -> 47         0.03300
         max(4)=       32 -> 55         0.02868
         max(5)=       25 -> 37         0.02423
         min(1)=       32 -> 43        -0.18398
         min(2)=       32 -> 44        -0.02653
         min(3)=       32 -> 88        -0.02030
         min(4)=       32 -> 41        -0.01939
         min(5)=       25 -> 43        -0.01768
         #CIs=2927 #CIs>0=1152 #CIs<0=1123

4        Singlet-A"    4.8452        255.89    0.0038    0.000
         max(1)=       36 -> 39         0.54751
         max(2)=       33 -> 37         0.05185
         max(3)=       35 -> 47         0.05100
         max(4)=       35 -> 55         0.02119
         max(5)=       35 -> 63         0.01279
         min(1)=       35 -> 37        -0.42106
         min(2)=       35 -> 43        -0.10818
         min(3)=       36 -> 40        -0.04074
         min(4)=       31 -> 39        -0.03949
         min(5)=       36 -> 58        -0.03053
         #CIs=2854 #CIs>0=1217 #CIs<0=1280

5        Singlet-A'    5.3620        231.23    0.0020    0.000
         max(1)=       36 -> 38         0.67834
         max(2)=       31 -> 38         0.09982
         max(3)=       36 -> 50         0.08541
         max(4)=       36 -> 45         0.08150
         max(5)=       31 -> 50         0.02506
         min(1)=       36 -> 48        -0.06907
         min(2)=       36 -> 41        -0.04091
         min(3)=       31 -> 41        -0.03789
         min(4)=       36 -> 52        -0.03591
         min(5)=       35 -> 40        -0.03430
         #CIs=2974 #CIs>0=1235 #CIs<0=1213

6        Singlet-A"    5.5921        221.71    0.0721    0.000
         max(1)=       35 -> 37         0.56127
         max(2)=       36 -> 39         0.41501
         max(3)=       33 -> 37         0.08803
         max(4)=       35 -> 47         0.04140
         max(5)=       31 -> 39         0.03590
         min(1)=       35 -> 43        -0.03629
         min(2)=       33 -> 43        -0.01788
         min(3)=       29 -> 49        -0.01043
         min(4)=       35 -> 63        -0.00994
         min(5)=       30 -> 76        -0.00968
         #CIs=2854 #CIs>0=1277 #CIs<0=1244

7        Singlet-A"    6.1467        201.71    0.0000    0.000
         max(1)=       36 -> 40         0.66365
         max(2)=       36 -> 53         0.12893
         max(3)=       31 -> 40         0.05851
         max(4)=       36 -> 46         0.05195
         max(5)=       36 -> 39         0.03825
         min(1)=       36 -> 42        -0.11042
         min(2)=       35 -> 38        -0.10476
         min(3)=       31 -> 42        -0.04446
         min(4)=       35 -> 41        -0.04142
         min(5)=       33 -> 37        -0.02922
         #CIs=2853 #CIs>0=1172 #CIs<0=1186

8        Singlet-A'    6.2617        198.00    0.0013    0.000
         max(1)=       36 -> 43         0.50496
         max(2)=       36 -> 41         0.38669
         max(3)=       35 -> 39         0.23111
         max(4)=       31 -> 37         0.12674
         max(5)=       36 -> 44         0.05491
         min(1)=       36 -> 52        -0.06324
         min(2)=       35 -> 40        -0.04274
         min(3)=       33 -> 39        -0.03313
         min(4)=       36 -> 37        -0.03080
         min(5)=       36 -> 55        -0.02845
         #CIs=2983 #CIs>0=1331 #CIs<0=1372

9        Singlet-A'    6.3706        194.62    0.0086    0.000
         max(1)=       36 -> 41         0.55650
         max(2)=       36 -> 45         0.08250
         max(3)=       36 -> 59         0.05380
```

```
        max(4)=       36 -> 38        0.02285
        max(5)=       33 -> 39        0.02265
        min(1)=       36 -> 43       -0.34025
        min(2)=       35 -> 39       -0.18111
        min(3)=       36 -> 52       -0.08849
        min(4)=       31 -> 37       -0.07197
        min(5)=       31 -> 38       -0.05881
        #CIs=2984 #CIs>0=1376 #CIs<0=1313

10      Singlet-A"    6.4572        192.01    0.1724    0.000
        max(1)=       33 -> 37        0.68122
        max(2)=       34 -> 96        0.05025
        max(3)=       34 -> 44        0.03938
        max(4)=       34 -> 48        0.03795
        max(5)=       32 -> 90        0.03702
        min(1)=       36 -> 39       -0.08917
        min(2)=       33 -> 43       -0.06393
        min(3)=       31 -> 39       -0.05969
        min(4)=       35 -> 37       -0.04034
        min(5)=       34 -> 54       -0.03209
        #CIs=2856 #CIs>0=1256 #CIs<0=1264

11      Singlet-A’    6.9434        178.56    0.5070    0.000
        max(1)=       35 -> 39        0.61556
        max(2)=       31 -> 55        0.02354
        max(3)=       36 -> 70        0.02034
        max(4)=       27 -> 86        0.01854
        max(5)=       36 -> 61        0.01844
        min(1)=       36 -> 43       -0.26399
        min(2)=       31 -> 37       -0.13989
        min(3)=       36 -> 37       -0.08901
        min(4)=       36 -> 51       -0.07876
        min(5)=       31 -> 43       -0.07366
        #CIs=2984 #CIs>0=1274 #CIs<0=1375

12      Singlet-A’    6.9779        177.68    0.0040    0.000
        max(1)=       36 -> 44        0.51090
        max(2)=       36 -> 45        0.42854
        max(3)=       35 -> 40        0.11198
        max(4)=       36 -> 65        0.05676
        max(5)=       35 -> 53        0.03004
        min(1)=       36 -> 50       -0.13576
        min(2)=       36 -> 38       -0.04860
        min(3)=       36 -> 41       -0.04205
        min(4)=       31 -> 48       -0.03759
        min(5)=       36 -> 48       -0.03572
        #CIs=2971 #CIs>0=1234 #CIs<0=1235

13      Singlet-A"    7.0142        176.76    0.0019    0.000
        max(1)=       35 -> 38        0.62903
        max(2)=       35 -> 41        0.22546
        max(3)=       36 -> 40        0.09845
        max(4)=       35 -> 45        0.09103
        max(5)=       36 -> 46        0.04799
        min(1)=       36 -> 42       -0.10323
        min(2)=       35 -> 52       -0.08787
        min(3)=       35 -> 48       -0.06013
        min(4)=       35 -> 43       -0.04093
        min(5)=       33 -> 38       -0.04007
        #CIs=2845 #CIs>0=1093 #CIs<0=1103

14      Singlet-A"    7.1298        173.89    0.0001    0.000
        max(1)=       36 -> 42        0.63959
        max(2)=       36 -> 40        0.14774
        max(3)=       35 -> 38        0.11679
        max(4)=       36 -> 56        0.08620
        max(5)=       35 -> 45        0.03191
        min(1)=       36 -> 46       -0.14068
        min(2)=       35 -> 41       -0.07388
        min(3)=       31 -> 40       -0.06385
        min(4)=       35 -> 43       -0.05714
        min(5)=       36 -> 67       -0.04713
        #CIs=2837 #CIs>0=1150 #CIs<0=1154

15      Singlet-A"    7.4100        167.32    0.0000    0.000
        max(1)=       30 -> 37        0.67688
        max(2)=       30 -> 43        0.10821
        max(3)=       32 -> 39        0.08552
        max(4)=       26 -> 37        0.08246
        max(5)=       27 -> 37        0.05401
        min(1)=       30 -> 47       -0.05384
        min(2)=       25 -> 39       -0.04243
```

```
        min(3)=       26 -> 43        -0.03745
        min(4)=       30 -> 63        -0.02272
        min(5)=       30 -> 55        -0.02160
        #CIs=2810 #CIs>0=1147 #CIs<0=1170

16      Singlet-A'    7.4219        167.05    0.0052    0.000
        max(1)=       34 -> 39         0.51139
        max(2)=       36 -> 43         0.13467
        max(3)=       36 -> 45         0.10919
        max(4)=       29 -> 37         0.05526
        max(5)=       33 -> 39         0.04262
        min(1)=       31 -> 37        -0.41041
        min(2)=       36 -> 44        -0.07501
        min(3)=       28 -> 37        -0.07433
        min(4)=       35 -> 40        -0.06690
        min(5)=       36 -> 37        -0.05811
        #CIs=2984 #CIs>0=1365 #CIs<0=1343

17      Singlet-A'    7.4309        166.85    0.0069    0.000
        max(1)=       34 -> 39         0.47294
        max(2)=       31 -> 37         0.46124
        max(3)=       36 -> 37         0.06585
        max(4)=       36 -> 44         0.05242
        max(5)=       35 -> 39         0.05097
        min(1)=       36 -> 43        -0.14697
        min(2)=       29 -> 37        -0.09327
        min(3)=       36 -> 45        -0.08373
        min(4)=       33 -> 39        -0.04826
        min(5)=       34 -> 40        -0.03174
        #CIs=2985 #CIs>0=1388 #CIs<0=1324

18      Singlet-A'    7.4595        166.21    0.0389    0.000
        max(1)=       36 -> 45         0.47267
        max(2)=       36 -> 47         0.19990
        max(3)=       31 -> 37         0.18109
        max(4)=       31 -> 41         0.08042
        max(5)=       36 -> 62         0.07406
        min(1)=       36 -> 44        -0.34822
        min(2)=       35 -> 40        -0.17109
        min(3)=       36 -> 48        -0.09933
        min(4)=       36 -> 41        -0.07089
        min(5)=       36 -> 38        -0.06655
        #CIs=2983 #CIs>0=1352 #CIs<0=1276

19      Singlet-A"    7.5125        165.04    0.1146    0.000
        max(1)=       35 -> 43         0.57148
        max(2)=       35 -> 41         0.27311
        max(3)=       31 -> 39         0.17692
        max(4)=       36 -> 49         0.12499
        max(5)=       36 -> 42         0.11060
        min(1)=       35 -> 38        -0.05084
        min(2)=       35 -> 37        -0.04955
        min(3)=       35 -> 52        -0.04762
        min(4)=       31 -> 40        -0.04005
        min(5)=       33 -> 43        -0.03767
        #CIs=2856 #CIs>0=1268 #CIs<0=1254

20      Singlet-A'    7.5199        164.87    0.0472    0.000
        max(1)=       36 -> 47         0.64074
        max(2)=       35 -> 40         0.21820
        max(3)=       36 -> 44         0.07051
        max(4)=       35 -> 39         0.05217
        max(5)=       36 -> 51         0.04827
        min(1)=       36 -> 45        -0.10077
        min(2)=       36 -> 50        -0.04312
        min(3)=       31 -> 41        -0.03790
        min(4)=       31 -> 37        -0.03734
        min(5)=       36 -> 52        -0.02799
        #CIs=2980 #CIs>0=1355 #CIs<0=1283
```

16.2.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_
1       Singlet-A"    5.4601        227.07    0.0000    0.000
        max(1)=       32 -> 40         0.56057
```

```
max(2)=   32 -> 46   0.21314
max(3)=   32 -> 59   0.20856
max(4)=   32 -> 51   0.16403
max(5)=   32 -> 49   0.10395
min(1)=   32 -> 50   -0.14314
min(2)=   32 -> 85   -0.08570
min(3)=   32 -> 39   -0.06996
min(4)=   32 -> 61   -0.03493
min(5)=   32 -> 52   -0.02717
#CIs=2523 #CIs>0=1143 #CIs<0=1128

2   Singlet-A’   5.5320   224.12   0.3691   0.000
max(1)=   36 -> 40   0.61814
max(2)=   36 -> 37   0.07568
max(3)=   35 -> 44   0.06593
max(4)=   35 -> 58   0.05880
max(5)=   33 -> 77   0.02798
min(1)=   35 -> 43   -0.21217
min(2)=   36 -> 39   -0.10936
min(3)=   36 -> 49   -0.09839
min(4)=   33 -> 40   -0.09761
min(5)=   36 -> 59   -0.07120
#CIs=2897 #CIs>0=1389 #CIs<0=1383

3   Singlet-A"   5.7395   216.02   0.0062   0.000
max(1)=   36 -> 43   0.52167
max(2)=   35 -> 40   0.38920
max(3)=   36 -> 38   0.03241
max(4)=   36 -> 57   0.03108
max(5)=   35 -> 65   0.02952
min(1)=   36 -> 44   -0.14860
min(2)=   36 -> 58   -0.11972
min(3)=   35 -> 49   -0.09802
min(4)=   35 -> 59   -0.08874
min(5)=   35 -> 39   -0.05974
#CIs=2735 #CIs>0=1259 #CIs<0=1311

4   Singlet-A’   5.8059   213.55   0.0005   0.000
max(1)=   31 -> 40   0.55976
max(2)=   31 -> 46   0.20766
max(3)=   31 -> 59   0.19698
max(4)=   31 -> 51   0.15770
max(5)=   31 -> 49   0.10335
min(1)=   31 -> 50   -0.13834
min(2)=   31 -> 85   -0.08107
min(3)=   33 -> 40   -0.07846
min(4)=   31 -> 39   -0.06999
min(5)=   31 -> 61   -0.03180
#CIs=2677 #CIs>0=1235 #CIs<0=1213

5   Singlet-A’   6.0323   205.53   0.0036   0.000
max(1)=   36 -> 37   0.62829
max(2)=   36 -> 45   0.15624
max(3)=   33 -> 37   0.11191
max(4)=   36 -> 64   0.03261
max(5)=   33 -> 50   0.02337
min(1)=   36 -> 52   -0.12608
min(2)=   36 -> 47   -0.12334
min(3)=   36 -> 40   -0.08206
min(4)=   35 -> 38   -0.06464
min(5)=   33 -> 39   -0.05356
#CIs=2840 #CIs>0=1304 #CIs<0=1317

6   Singlet-A"   6.7357   184.07   0.0030   0.000
max(1)=   36 -> 38   0.60907
max(2)=   36 -> 53   0.17128
max(3)=   33 -> 38   0.06875
max(4)=   35 -> 52   0.06733
max(5)=   36 -> 44   0.04821
min(1)=   35 -> 37   -0.20201
min(2)=   36 -> 41   -0.10169
min(3)=   35 -> 40   -0.08146
min(4)=   35 -> 39   -0.07873
min(5)=   33 -> 41   -0.04583
#CIs=2705 #CIs>0=1281 #CIs<0=1231

7   Singlet-A’   6.9208   179.15   0.0115   0.000
max(1)=   36 -> 39   0.62081
max(2)=   36 -> 45   0.16666
max(3)=   36 -> 40   0.11158
max(4)=   36 -> 61   0.08302
max(5)=   36 -> 60   0.06382
```

```
        min(1)=      36 -> 50       -0.14421
        min(2)=      36 -> 51       -0.08616
        min(3)=      33 -> 37       -0.07892
        min(4)=      35 -> 38       -0.06887
        min(5)=      29 -> 37       -0.03420
        #CIs=2844 #CIs>0=1325 #CIs<0=1322

8       Singlet-A"    7.0942       174.77    0.1002    0.000
        max(1)=      35 -> 40        0.47223
        max(2)=      34 -> 40        0.28945
        max(3)=      34 -> 46        0.09456
        max(4)=      36 -> 38        0.07751
        max(5)=      34 -> 59        0.07741
        min(1)=      36 -> 43       -0.33466
        min(2)=      35 -> 39       -0.10578
        min(3)=      34 -> 50       -0.05909
        min(4)=      35 -> 46       -0.04391
        min(5)=      34 -> 39       -0.03449
        #CIs=2764 #CIs>0=1334 #CIs<0=1311

9       Singlet-A'    7.3490       168.71    0.6163    0.000
        max(1)=      35 -> 43        0.46680
        max(2)=      36 -> 46        0.32288
        max(3)=      36 -> 40        0.18878
        max(4)=      36 -> 49        0.18059
        max(5)=      36 -> 59        0.13681
        min(1)=      35 -> 44       -0.13310
        min(2)=      35 -> 58       -0.09137
        min(3)=      33 -> 40       -0.08952
        min(4)=      36 -> 39       -0.05736
        min(5)=      36 -> 50       -0.05735
        #CIs=2892 #CIs>0=1373 #CIs<0=1399

10      Singlet-A"    7.4772       165.82    0.0000    0.000
        max(1)=      35 -> 37        0.50125
        max(2)=      35 -> 39        0.31202
        max(3)=      36 -> 38        0.20028
        max(4)=      35 -> 45        0.15582
        max(5)=      36 -> 44        0.08418
        min(1)=      36 -> 41       -0.13539
        min(2)=      35 -> 50       -0.11241
        min(3)=      35 -> 52       -0.09551
        min(4)=      35 -> 47       -0.08585
        min(5)=      35 -> 51       -0.07931
        #CIs=2664 #CIs>0=1220 #CIs<0=1235

11      Singlet-A'    7.5006       165.30    0.0092    0.000
        max(1)=      36 -> 45        0.45034
        max(2)=      35 -> 38        0.26614
        max(3)=      36 -> 52        0.12928
        max(4)=      35 -> 53        0.08970
        max(5)=      36 -> 64        0.08536
        min(1)=      36 -> 42       -0.34821
        min(2)=      36 -> 39       -0.10921
        min(3)=      36 -> 37       -0.09211
        min(4)=      36 -> 46       -0.09183
        min(5)=      36 -> 50       -0.07922
        #CIs=2824 #CIs>0=1295 #CIs<0=1307

12      Singlet-A"    7.6771       161.50    0.4758    0.000
        max(1)=      34 -> 40        0.44373
        max(2)=      36 -> 43        0.17733
        max(3)=      34 -> 46        0.12478
        max(4)=      34 -> 59        0.10269
        max(5)=      34 -> 49        0.09601
        min(1)=      36 -> 41       -0.29941
        min(2)=      35 -> 40       -0.18282
        min(3)=      36 -> 38       -0.11498
        min(4)=      35 -> 37       -0.10557
        min(5)=      34 -> 50       -0.08083
        #CIs=2771 #CIs>0=1351 #CIs<0=1304

13      Singlet-A"    7.7719       159.53    0.2152    0.000
        max(1)=      36 -> 41        0.52931
        max(2)=      34 -> 40        0.24608
        max(3)=      36 -> 38        0.14201
        max(4)=      36 -> 43        0.12393
        max(5)=      35 -> 37        0.10787
        min(1)=      35 -> 40       -0.16573
        min(2)=      36 -> 44       -0.14958
        min(3)=      33 -> 38       -0.06021
        min(4)=      33 -> 44       -0.05106
```

```
min(5)=      36 -> 68       -0.05081
#CIs=2772 #CIs>0=1318 #CIs<0=1328

14      Singlet-A'    7.7816       159.33    0.2110    0.000
max(1)=      36 -> 46        0.50483
max(2)=      36 -> 45        0.20155
max(3)=      36 -> 42        0.12923
max(4)=      35 -> 44        0.09358
max(5)=      35 -> 48        0.08210
min(1)=      35 -> 43       -0.29792
min(2)=      36 -> 40       -0.14992
min(3)=      33 -> 40       -0.13218
min(4)=      36 -> 51       -0.06724
min(5)=      36 -> 47       -0.05133
#CIs=2891 #CIs>0=1357 #CIs<0=1385

15      Singlet-A'    7.9885       155.20    0.0398    0.000
max(1)=      35 -> 38        0.53063
max(2)=      36 -> 37        0.16237
max(3)=      35 -> 53        0.15578
max(4)=      36 -> 39        0.14934
max(5)=      36 -> 46        0.11778
min(1)=      36 -> 45       -0.28426
min(2)=      33 -> 39       -0.06547
min(3)=      36 -> 42       -0.06364
min(4)=      36 -> 62       -0.05141
min(5)=      33 -> 37       -0.03875
#CIs=2783 #CIs>0=1290 #CIs<0=1260

16      Singlet-A'    8.1699       151.76    0.0072    0.000
max(1)=      36 -> 42        0.51288
max(2)=      35 -> 38        0.24333
max(3)=      36 -> 45        0.19098
max(4)=      35 -> 41        0.08936
max(5)=      36 -> 62        0.07853
min(1)=      36 -> 46       -0.20932
min(2)=      36 -> 47       -0.19989
min(3)=      36 -> 37       -0.05265
min(4)=      36 -> 67       -0.04304
min(5)=      36 -> 65       -0.03742
#CIs=2826 #CIs>0=1303 #CIs<0=1307

17      Singlet-A'    8.2644       150.02    0.2966    0.000
max(1)=      35 -> 43        0.20136
max(2)=      33 -> 40        0.19315
max(3)=      36 -> 46        0.16526
max(4)=      36 -> 50        0.10622
max(5)=      36 -> 45        0.05643
min(1)=      36 -> 49       -0.54999
min(2)=      36 -> 59       -0.16457
min(3)=      36 -> 51       -0.13190
min(4)=      35 -> 44       -0.05889
min(5)=      29 -> 40       -0.04521
#CIs=2885 #CIs>0=1381 #CIs<0=1352

18      Singlet-A"    8.2945       149.48    0.0011    0.000
max(1)=      35 -> 39        0.51715
max(2)=      35 -> 40        0.13513
max(3)=      36 -> 41        0.13071
max(4)=      35 -> 61        0.06443
max(5)=      35 -> 47        0.06388
min(1)=      35 -> 37       -0.34594
min(2)=      35 -> 42       -0.14199
min(3)=      35 -> 50       -0.13977
min(4)=      35 -> 51       -0.10355
min(5)=      33 -> 38       -0.03193
#CIs=2716 #CIs>0=1269 #CIs<0=1260

19      Singlet-A"    8.5058       145.76    0.0033    0.000
max(1)=      35 -> 45        0.49950
max(2)=      35 -> 52        0.14012
max(3)=      35 -> 56        0.10254
max(4)=      35 -> 64        0.07537
max(5)=      35 -> 65        0.06999
min(1)=      35 -> 42       -0.27621
min(2)=      36 -> 44       -0.19296
min(3)=      35 -> 46       -0.13266
min(4)=      35 -> 39       -0.12101
min(5)=      36 -> 41       -0.08612
#CIs=2733 #CIs>0=1252 #CIs<0=1299

20      Singlet-A"    8.7087       142.37    0.0164    0.000
```

max(1)=	36 -> 44	0.39478
max(2)=	36 -> 48	0.37400
max(3)=	35 -> 45	0.25623
max(4)=	35 -> 46	0.22651
max(5)=	36 -> 41	0.10705
min(1)=	35 -> 39	-0.10682
min(2)=	34 -> 40	-0.05794
min(3)=	36 -> 38	-0.05773
min(4)=	36 -> 75	-0.04844
min(5)=	35 -> 69	-0.03570

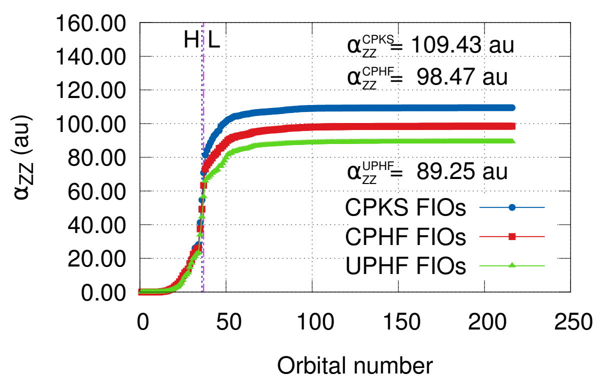
#CIs=2770 #CIs>0=1307 #CIs<0=1315

17 m-nitroaniline

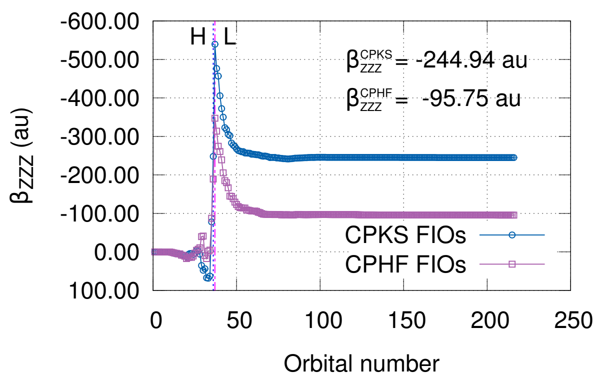
17.1 6-311G(d,p)

17.1.1 Plots

Figure S29: For m-nitroaniline molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S29a and **??**) or states (SOS approaches, in Plots S29b and **??**). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S29c and **??** as well (bottom). All elements of the β tensor were recomputed with an error less than 0.10 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.

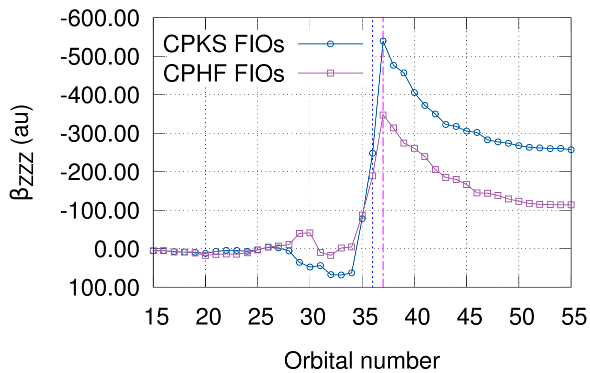


(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

Figure S29: (continued) For m-nitroaniline molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S29a and **??**) or states (SOS approaches, in Plots S29b and **??**). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S29c and **??** as well (bottom). All elements of the β tensor were recomputed with an error less than 0.37 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



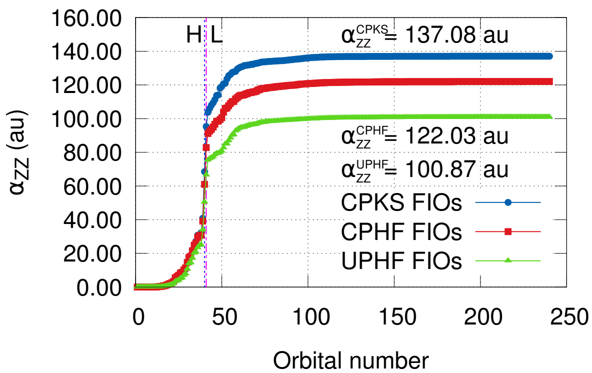
(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 15 and 55.

18 *p*-methoxy-nitrobenzene

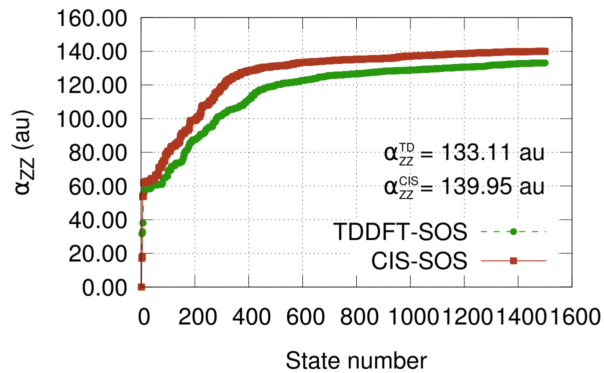
18.1 6-311G(d,p)

18.1.1 Plots

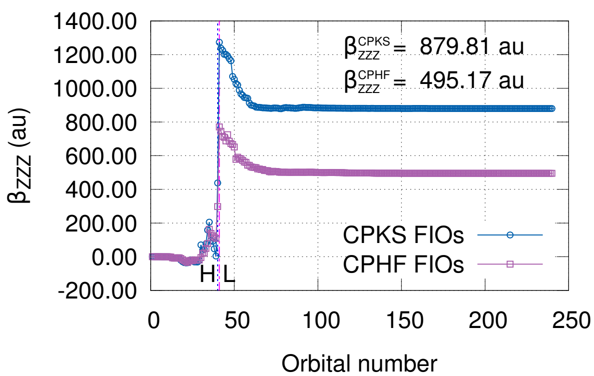
Figure S30: For *p*-methoxy-nitrobenzene molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S30a and S30b) or states (SOS approaches, in Plots S30c and S30d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S30e and S30f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.51 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



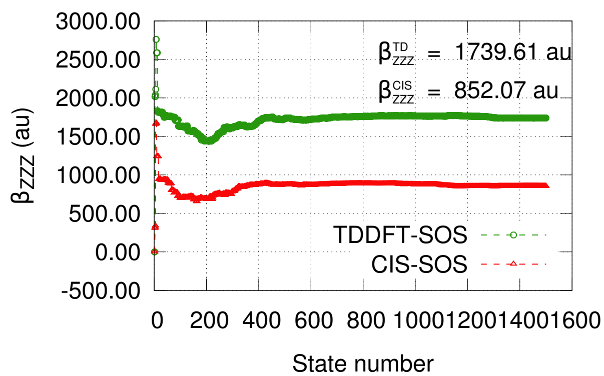
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

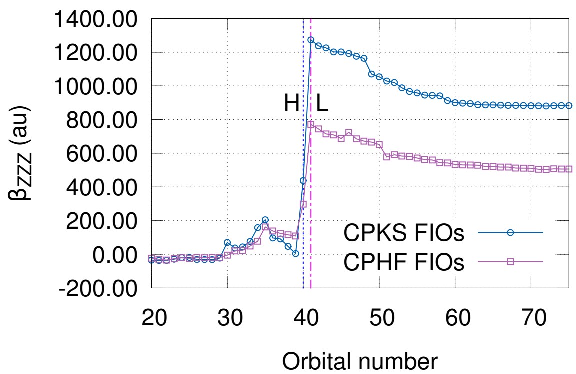


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

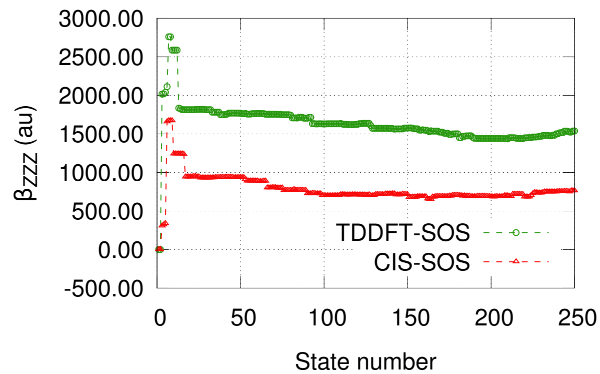


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S30: (continued) For *p*-methoxy-nitrobenzene molecule and 6-311G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S30a and S30b) or states (SOS approaches, in Plots S30c and S30d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S30e and S30f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.51 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 20 and 70.



(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 250.

18.1.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___      Exc.E Osc._Strength    ___f___ _<S**2>_          #CIs=2265 #CIs>0=849 #CIs<0=819

1        Singlet-A"    4.1023          302.23     0.0000     20.000   Singlet-A"    4.6149          268.66     0.0001     0.000
                max(1)=         38 -> 41          0.67368                       max(1)=         36 -> 41          0.67564
                max(2)=         38 -> 42          0.02078                       max(2)=         36 -> 42          0.01993
                max(3)=         30 -> 41          0.01671                       max(3)=         31 -> 43          0.01869
                max(4)=         35 -> 43          0.01198                       max(4)=         28 -> 43          0.01613
                max(5)=         29 -> 41          0.00843                       max(5)=         29 -> 41          0.01013
                min(1)=         38 -> 43         -0.20915                       min(1)=         36 -> 43         -0.20131
                min(2)=         38 -> 52         -0.02528                       min(2)=         31 -> 41         -0.02534
                min(3)=         35 -> 41         -0.02455                       min(3)=         36 -> 52         -0.02263
                min(4)=         30 -> 43         -0.01284                       min(4)=         28 -> 41         -0.01770
                min(5)=         38 ->101         -0.01049                       min(5)=         30 -> 41         -0.01316
```

```
#CIs=2276 #CIs>0=921 #CIs<0=901

3  Singlet-A'  4.8366  256.35  0.3324  0.000
   max(1)=  40 -> 41   0.68850
   max(2)=  34 -> 43   0.04889
   max(3)=  32 -> 41   0.02924
   max(4)=  36 -> 53   0.01721
   max(5)=  38 -> 51   0.01583
   min(1)=  39 -> 42  -0.10676
   min(2)=  34 -> 41  -0.09180
   min(3)=  32 -> 43  -0.02268
   min(4)=  36 -> 45  -0.01367
   min(5)=  35 -> 56  -0.01241
   #CIs=3510 #CIs>0=1483 #CIs<0=1566

4  Singlet-A'  5.0828  243.93  0.0011  0.000
   max(1)=  39 -> 41   0.52452
   max(2)=  40 -> 42   0.45028
   max(3)=  39 -> 43   0.12534
   max(4)=  37 -> 41   0.05425
   max(5)=  40 -> 43   0.01601
   min(1)=  34 -> 42  -0.04868
   min(2)=  39 -> 42  -0.01687
   min(3)=  39 -> 48  -0.01053
   min(4)=  40 -> 41  -0.00987
   min(5)=  39 -> 76  -0.00756
   #CIs=3497 #CIs>0=1444 #CIs<0=1530

5  Singlet-A'  5.9952  206.81  0.0892  0.000
   max(1)=  40 -> 42   0.49975
   max(2)=  37 -> 41   0.12410
   max(3)=  39 -> 43   0.11675
   max(4)=  32 -> 41   0.01387
   max(5)=  38 -> 45   0.01105
   min(1)=  39 -> 41  -0.46933
   min(2)=  39 -> 42  -0.02469
   min(3)=  34 -> 41  -0.01961
   min(4)=  39 -> 64  -0.01757
   min(5)=  38 -> 57  -0.01691
   #CIs=3508 #CIs>0=1542 #CIs<0=1489

6  Singlet-A'  6.7020  185.00  0.1597  0.000
   max(1)=  37 -> 41   0.63153
   max(2)=  40 -> 43   0.15679
   max(3)=  34 -> 41   0.05029
   max(4)=  39 -> 41   0.03565
   max(5)=  38 -> 62   0.02688
   min(1)=  39 -> 42  -0.20550
   min(2)=  40 -> 42  -0.11877
   min(3)=  39 -> 43  -0.05829
   min(4)=  38 -> 57  -0.05788
   min(5)=  34 -> 42  -0.04164
   #CIs=3513 #CIs>0=1592 #CIs<0=1538

7  Singlet-A'  6.7415  183.91  0.1247  0.000
   max(1)=  39 -> 42   0.50139
   max(2)=  37 -> 41   0.26366
   max(3)=  40 -> 41   0.06912
   max(4)=  32 -> 41   0.05114
   max(5)=  34 -> 43   0.04716
   min(1)=  40 -> 43  -0.38820
   min(2)=  34 -> 41  -0.09085
   min(3)=  39 -> 43  -0.03049
   min(4)=  38 -> 57  -0.02533
   min(5)=  40 -> 42  -0.01811
   #CIs=3515 #CIs>0=1561 #CIs<0=1594

8  Singlet-A"  7.2821  170.26  0.0000  0.000
   max(1)=  35 -> 41   0.61418
   max(2)=  35 -> 43   0.17491
   max(3)=  38 -> 43   0.04769
   max(4)=  38 -> 41   0.03530
   max(5)=  29 -> 43   0.03053
   min(1)=  33 -> 41  -0.26577
   min(2)=  29 -> 41  -0.05835
   min(3)=  36 -> 42  -0.05006
   min(4)=  31 -> 41  -0.04116
   min(5)=  38 -> 42  -0.03996
   #CIs=2281 #CIs>0=1004 #CIs<0=997

9  Singlet-A'  7.3195  169.39  0.4348  0.000
   max(1)=  40 -> 43   0.47634
```

max(2)= 39 -> 42 0.41656

max(3)= 34 -> 41 0.27191

max(4)= 40 -> 41 0.09293

max(5)= 34 -> 43 0.04124

min(1)= 32 -> 41 -0.04631

min(2)= 37 -> 42 -0.03911

min(3)= 40 -> 52 -0.03158

min(4)= 34 -> 52 -0.02720

min(5)= 36 -> 53 -0.02650

#CIs=3505 #CIs>0=1528 #CIs<0=1521

10 Singlet-A" 7.4686 166.01 0.0000 0.000

max(1)= 38 -> 42 0.69198

max(2)= 35 -> 42 0.07191

max(3)= 35 -> 41 0.03536

max(4)= 31 -> 41 0.02301

max(5)= 40 -> 45 0.02240

min(1)= 40 -> 44 -0.06014

min(2)= 30 -> 42 -0.04222

min(3)= 33 -> 41 -0.03507

min(4)= 38 -> 43 -0.03244

min(5)= 38 -> 41 -0.03056

#CIs=2278 #CIs>0=960 #CIs<0=902

11 Singlet-A" 7.5127 165.03 0.0155 0.000

max(1)= 40 -> 44 0.66539

max(2)= 34 -> 44 0.06977

max(3)= 38 -> 42 0.06432

max(4)= 34 -> 45 0.04359

max(5)= 40 -> 46 0.03712

min(1)= 40 -> 45 -0.16458

min(2)= 39 -> 44 -0.09140

min(3)= 39 -> 46 -0.05065

min(4)= 40 -> 66 -0.01977

min(5)= 40 -> 51 -0.01947

#CIs=2278 #CIs>0=953 #CIs<0=953

12 Singlet-A" 7.7384 160.22 0.0000 0.000

max(1)= 36 -> 42 0.69305

max(2)= 31 -> 42 0.06138

max(3)= 35 -> 41 0.05891

max(4)= 28 -> 42 0.03514

max(5)= 30 -> 42 0.02439

min(1)= 38 -> 43 -0.05242

min(2)= 36 -> 43 -0.03813

min(3)= 36 -> 41 -0.03198

min(4)= 21 -> 42 -0.02791

min(5)= 38 -> 52 -0.02717

#CIs=2272 #CIs>0=961 #CIs<0=902

13 Singlet-A’ 7.8309 158.33 0.0612 0.000

max(1)= 34 -> 41 0.58382

max(2)= 34 -> 43 0.07720

max(3)= 40 -> 41 0.07164

max(4)= 40 -> 42 0.02889

max(5)= 40 -> 52 0.01755

min(1)= 40 -> 43 -0.29090

min(2)= 32 -> 41 -0.16931

min(3)= 37 -> 42 -0.13082

min(4)= 39 -> 42 -0.10273

min(5)= 39 -> 43 -0.04538

#CIs=3510 #CIs>0=1517 #CIs<0=1498

14 Singlet-A’ 7.9597 155.77 0.1890 0.000

max(1)= 39 -> 43 0.63604

max(2)= 37 -> 42 0.08477

max(3)= 34 -> 41 0.05477

max(4)= 37 -> 43 0.03654

max(5)= 37 -> 41 0.01815

min(1)= 34 -> 42 -0.21352

min(2)= 40 -> 42 -0.17111

min(3)= 40 -> 43 -0.04024

min(4)= 39 -> 48 -0.02797

min(5)= 39 -> 41 -0.02716

#CIs=3509 #CIs>0=1525 #CIs<0=1477

15 Singlet-A’ 7.9704 155.56 0.0015 0.000

max(1)= 37 -> 42 0.68495

max(2)= 34 -> 41 0.13032

max(3)= 40 -> 42 0.02240

max(4)= 34 -> 43 0.02117

max(5)= 37 -> 48 0.01892

```
        min(1)=      39 -> 43        -0.08931
        min(2)=      39 -> 42        -0.03473
        min(3)=      37 -> 43        -0.02219
        min(4)=      32 -> 41        -0.02016
        min(5)=      24 -> 41        -0.01735
        #CIs=3512 #CIs>0=1454 #CIs<0=1436

16      Singlet-A"    8.0487        154.04    0.0029    0.000
        max(1)=      35 -> 42         0.63529
        max(2)=      38 -> 43         0.03758
        max(3)=      36 -> 42         0.02602
        max(4)=      35 -> 43         0.02493
        max(5)=      38 -> 41         0.01536
        min(1)=      33 -> 42        -0.28015
        min(2)=      38 -> 42        -0.07496
        min(3)=      28 -> 52        -0.04642
        min(4)=      28 -> 41        -0.04135
        min(5)=      33 -> 41        -0.02624
        #CIs=2277 #CIs>0=974 #CIs<0=940

17      Singlet-A"    8.1010        153.05    0.0049    0.000
        max(1)=      40 -> 45         0.60894
        max(2)=      40 -> 46         0.14342
        max(3)=      39 -> 45         0.14131
        max(4)=      40 -> 44         0.11644
        max(5)=      34 -> 44         0.09018
        min(1)=      39 -> 44        -0.20381
        min(2)=      40 -> 50        -0.06878
        min(3)=      40 -> 53        -0.04256
        min(4)=      34 -> 50        -0.04134
        min(5)=      32 -> 46        -0.03640
        #CIs=2282 #CIs>0=974 #CIs<0=1001

18      Singlet-A"    8.1969        151.26    0.0000    0.000
        max(1)=      38 -> 43         0.61220
        max(2)=      33 -> 41         0.21891
        max(3)=      38 -> 41         0.19536
        max(4)=      38 -> 52         0.10676
        max(5)=      38 -> 42         0.05201
        min(1)=      30 -> 41        -0.09128
        min(2)=      26 -> 41        -0.03753
        min(3)=      25 -> 41        -0.03567
        min(4)=      40 -> 45        -0.03295
        min(5)=      35 -> 52        -0.02818
        #CIs=2283 #CIs>0=989 #CIs<0=983

19      Singlet-A"    8.3200        149.02    0.0020    0.000
        max(1)=      39 -> 44         0.45209
        max(2)=      40 -> 45         0.23296
        max(3)=      40 -> 44         0.14028
        max(4)=      40 -> 49         0.12169
        max(5)=      39 -> 46         0.05302
        min(1)=      39 -> 45        -0.32054
        min(2)=      40 -> 46        -0.27199
        min(3)=      34 -> 46        -0.06695
        min(4)=      40 -> 50        -0.05688
        min(5)=      34 -> 50        -0.03130
        #CIs=2281 #CIs>0=995 #CIs<0=962

20      Singlet-A"    8.4095        147.43    0.0001    0.000
        max(1)=      33 -> 41         0.53185
        max(2)=      35 -> 41         0.20826
        max(3)=      35 -> 43         0.17436
        max(4)=      29 -> 41         0.12321
        max(5)=      33 -> 43         0.10802
        min(1)=      38 -> 43        -0.21945
        min(2)=      36 -> 43        -0.13569
        min(3)=      30 -> 41        -0.10369
        min(4)=      31 -> 41        -0.07894
        min(5)=      38 -> 41        -0.06440
        #CIs=2278 #CIs>0=1075 #CIs<0=1011
```

18.1.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-A"    5.4890        225.88    0.0000    0.000
         max(1)=       37 -> 41         0.58235
         max(2)=       37 -> 46         0.36535
         max(3)=       37 ->101         0.04189
         max(4)=       37 -> 42         0.03832
         max(5)=       30 -> 41         0.03673
         min(1)=       34 -> 41        -0.07416
         min(2)=       37 -> 53        -0.07198
         min(3)=       34 -> 46        -0.05147
         min(4)=       36 -> 41        -0.03624
         min(5)=       36 -> 98        -0.02687
         #states=840 #states>0=400 #states<0=440

2        Singlet-A"    5.8145        213.23    0.0001    0.000
         max(1)=       36 -> 41         0.59144
         max(2)=       36 -> 46         0.35599
         max(3)=       28 -> 46         0.03825
         max(4)=       36 ->101         0.03774
         max(5)=       36 -> 42         0.03751
         min(1)=       36 -> 53        -0.06488
         min(2)=       31 -> 41        -0.04925
         min(3)=       31 -> 46        -0.04465
         min(4)=       37 -> 98        -0.02842
         min(5)=       30 -> 41        -0.02690
         #states=1029 #states>0=512 #states<0=517

3        Singlet-A'    5.8919        210.43    0.2659    0.000
         max(1)=       40 -> 41         0.61052
         max(2)=       39 -> 46         0.03767
         max(3)=       40 -> 48         0.02787
         max(4)=       39 -> 48         0.01468
         max(5)=       32 -> 48         0.01378
         min(1)=       39 -> 42        -0.27165
         min(2)=       35 -> 41        -0.09381
         min(3)=       39 -> 41        -0.09099
         min(4)=       40 -> 42        -0.09079
         min(5)=       40 -> 46        -0.08810
         #states=2172 #states>0=1083 #states<0=1089

4        Singlet-A'    6.0167        206.07    0.0085    0.000
         max(1)=       40 -> 42         0.48970
         max(2)=       39 -> 41         0.46178
         max(3)=       40 -> 41         0.11220
         max(4)=       39 -> 48         0.03575
         max(5)=       32 -> 42         0.02833
         min(1)=       39 -> 46        -0.14255
         min(2)=       39 -> 42        -0.06232
         min(3)=       40 -> 46        -0.03830
         min(4)=       35 -> 42        -0.03114
         min(5)=       40 -> 48        -0.02249
         #states=1870 #states>0=949 #states<0=921

5        Singlet-A'    7.5232        164.80    0.0663    0.000
         max(1)=       38 -> 41         0.39897
         max(2)=       40 -> 42         0.35179
         max(3)=       38 -> 46         0.19531
         max(4)=       36 -> 58         0.02875
         max(5)=       37 -> 87         0.02740
         min(1)=       39 -> 41        -0.38865
         min(2)=       37 -> 59        -0.04054
         min(3)=       35 -> 42        -0.03109
         min(4)=       37 -> 73        -0.02368
         min(5)=       37 -> 66        -0.02301
         #states=2181 #states>0=1077 #states<0=1104

6        Singlet-A'    7.6657        161.74    0.9391    0.000
         max(1)=       39 -> 42         0.56871
         max(2)=       40 -> 41         0.27636
         max(3)=       40 -> 46         0.22247
         max(4)=       40 -> 42         0.06229
         max(5)=       32 -> 53         0.04479
         min(1)=       38 -> 41        -0.08592
         min(2)=       35 -> 46        -0.07240
         min(3)=       35 -> 41        -0.05075
         min(4)=       39 -> 41        -0.04565
         min(5)=       32 -> 41        -0.03974
         #states=2143 #states>0=1087 #states<0=1056

7        Singlet-A'    8.1377        152.36    0.8699    0.000
         max(1)=       38 -> 41         0.46251
```

max(2)= 39 -> 41 0.31719

max(3)= 38 -> 46 0.19474

max(4)= 39 -> 42 0.10510

max(5)= 40 -> 41 0.06137

min(1)= 40 -> 42 -0.31141

min(2)= 37 -> 59 -0.04261

min(3)= 37 -> 66 -0.02771

min(4)= 37 -> 65 -0.02510

min(5)= 37 -> 73 -0.02424

#states=2171 #states>0=1072 #states<0=1099

8 Singlet-A" 8.6473 143.38 0.0227 0.000

max(1)= 40 -> 43 0.54002

max(2)= 35 -> 43 0.08322

max(3)= 39 -> 50 0.07128

max(4)= 40 -> 52 0.06277

max(5)= 40 -> 45 0.04883

min(1)= 40 -> 44 -0.29367

min(2)= 39 -> 43 -0.22191

min(3)= 39 -> 45 -0.16523

min(4)= 40 -> 50 -0.06307

min(5)= 40 -> 55 -0.03921

#states=1095 #states>0=593 #states<0=502

9 Singlet-A" 8.9099 139.15 0.0001 0.000

max(1)= 39 -> 43 0.38454

max(2)= 39 -> 52 0.05471

max(3)= 39 -> 49 0.04791

max(4)= 40 -> 49 0.04709

max(5)= 40 -> 50 0.04512

min(1)= 39 -> 44 -0.40047

min(2)= 40 -> 44 -0.29040

min(3)= 40 -> 45 -0.24405

min(4)= 35 -> 45 -0.08245

min(5)= 32 -> 45 -0.07836

#states=1023 #states>0=505 #states<0=518

10 Singlet-A' 8.9479 138.56 0.2917 0.000

max(1)= 40 -> 46 0.56553

max(2)= 40 -> 53 0.05479

max(3)= 35 -> 53 0.03614

max(4)= 39 -> 41 0.02131

max(5)= 34 -> 43 0.02061

min(1)= 35 -> 41 -0.29035

min(2)= 39 -> 42 -0.21885

min(3)= 32 -> 41 -0.11058

min(4)= 40 -> 41 -0.05291

min(5)= 40 -> 48 -0.04139

#states=2135 #states>0=1117 #states<0=1018

11 Singlet-A" 9.2454 134.10 0.0001 0.000

max(1)= 34 -> 41 0.56076

max(2)= 37 -> 41 0.08002

max(3)= 33 -> 46 0.06566

max(4)= 28 -> 42 0.06094

max(5)= 34 -> 48 0.05118

min(1)= 33 -> 41 -0.26131

min(2)= 34 -> 46 -0.22610

min(3)= 29 -> 53 -0.08083

min(4)= 29 -> 41 -0.05940

min(5)= 36 -> 42 -0.05801

#states=1266 #states>0=644 #states<0=622

12 Singlet-A" 9.5991 129.16 0.0005 0.000

max(1)= 40 -> 43 0.36726

max(2)= 40 -> 44 0.30890

max(3)= 39 -> 45 0.26705

max(4)= 39 -> 43 0.22991

max(5)= 40 -> 45 0.21866

min(1)= 39 -> 44 -0.13174

min(2)= 39 -> 47 -0.10809

min(3)= 32 -> 43 -0.07972

min(4)= 33 -> 42 -0.06650

min(5)= 35 -> 45 -0.04637

#states=1162 #states>0=593 #states<0=569

13 Singlet-A" 9.6814 128.06 0.0502 0.000

max(1)= 34 -> 42 0.33701

max(2)= 39 -> 45 0.21689

max(3)= 39 -> 44 0.17619

max(4)= 40 -> 45 0.16607

max(5)= 40 -> 52 0.08363

min(1)= 40 -> 44 -0.34549
min(2)= 33 -> 42 -0.20276
min(3)= 40 -> 47 -0.14885
min(4)= 35 -> 43 -0.12033
min(5)= 40 -> 43 -0.10712
#states=1286 #states>0=615 #states<0=671

14 Singlet-A" 9.7815 126.75 0.0046 0.000
max(1)= 34 -> 42 0.44076
max(2)= 40 -> 44 0.17112
max(3)= 40 -> 47 0.11986
max(4)= 37 -> 42 0.09907
max(5)= 35 -> 43 0.08598
min(1)= 33 -> 42 -0.26005
min(2)= 40 -> 45 -0.24336
min(3)= 39 -> 45 -0.20851
min(4)= 39 -> 43 -0.13004
min(5)= 39 -> 44 -0.07889
#states=1345 #states>0=688 #states<0=657

15 Singlet-A" 10.0305 123.61 0.0001 0.000
max(1)= 40 -> 45 0.45114
max(2)= 34 -> 42 0.06004
max(3)= 32 -> 43 0.05436
max(4)= 39 -> 52 0.05320
max(5)= 40 -> 44 0.03495
min(1)= 39 -> 45 -0.29857
min(2)= 39 -> 44 -0.28953
min(3)= 40 -> 51 -0.15475
min(4)= 39 -> 49 -0.13526
min(5)= 40 -> 43 -0.12113
#states=1234 #states>0=603 #states<0=631

16 Singlet-A' 10.0659 123.17 0.1781 0.000
max(1)= 39 -> 46 0.62218
max(2)= 35 -> 42 0.21246
max(3)= 39 -> 41 0.10398
max(4)= 32 -> 42 0.09787
max(5)= 40 -> 42 0.09364
min(1)= 39 -> 48 -0.08816
min(2)= 34 -> 43 -0.02394
min(3)= 29 -> 54 -0.02023
min(4)= 35 -> 46 -0.02008
min(5)= 30 -> 43 -0.01738
#states=1891 #states>0=968 #states<0=923

17 Singlet-A' 10.3444 119.86 0.0320 0.000
max(1)= 35 -> 41 0.54493
max(2)= 40 -> 46 0.28334
max(3)= 32 -> 41 0.17849
max(4)= 40 -> 41 0.07830
max(5)= 24 -> 46 0.04531
min(1)= 35 -> 46 -0.19056
min(2)= 39 -> 42 -0.10950
min(3)= 40 -> 53 -0.08082
min(4)= 35 -> 42 -0.06437
min(5)= 39 -> 46 -0.04269
#states=2101 #states>0=1061 #states<0=1040

18 Singlet-A" 10.4528 118.61 0.0000 0.000
max(1)= 36 -> 42 0.34733
max(2)= 31 -> 42 0.23736
max(3)= 33 -> 41 0.23233
max(4)= 30 -> 42 0.16546
max(5)= 34 -> 41 0.10761
min(1)= 30 -> 41 -0.22885
min(2)= 40 -> 51 -0.17485
min(3)= 26 -> 41 -0.13565
min(4)= 34 -> 46 -0.09912
min(5)= 33 -> 42 -0.08241
#states=1546 #states>0=775 #states<0=771

19 Singlet-A" 10.5039 118.04 0.0000 0.000
max(1)= 40 -> 51 0.44010
max(2)= 35 -> 51 0.21498
max(3)= 36 -> 42 0.17584
max(4)= 40 -> 50 0.15036
max(5)= 31 -> 42 0.14499
min(1)= 40 -> 47 -0.13417
min(2)= 39 -> 43 -0.11072
min(3)= 39 -> 44 -0.10335
min(4)= 40 -> 44 -0.09769

min(5)= 35 -> 43 -0.07781

#states=1558 #states>0=761 #states<0=797

20 Singlet-A" 10.6873 116.01 0.0008 0.000

max(1)= 31 -> 42 0.28813

max(2)= 31 -> 41 0.25985

max(3)= 37 -> 42 0.25573

max(4)= 36 -> 42 0.16339

max(5)= 30 -> 41 0.14460

min(1)= 33 -> 41 -0.21356

min(2)= 29 -> 42 -0.17358

min(3)= 30 -> 42 -0.14985

min(4)= 26 -> 42 -0.13181

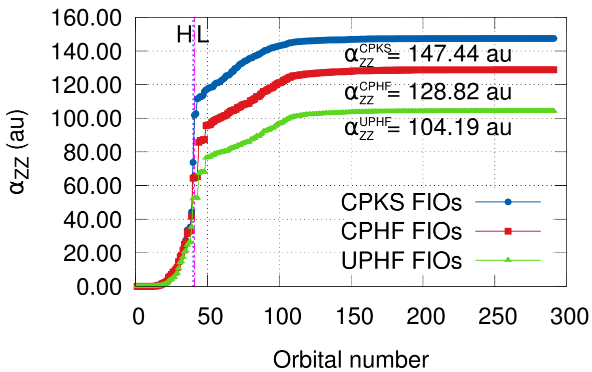
min(5)= 40 -> 51 -0.10522

#states=1429 #states>0=729 #states<0=700

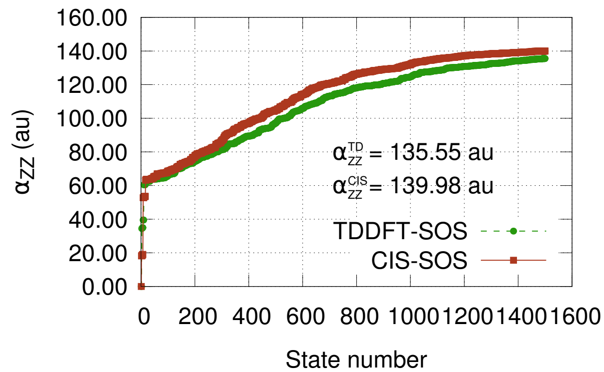
18.2 6-311++G(d,p)

18.2.1 Plots

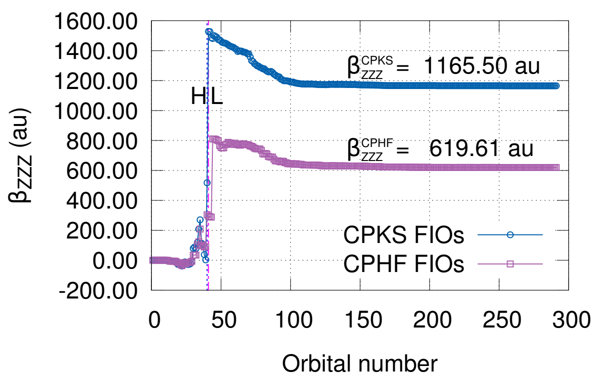
Figure S31: For p-methoxy-nitrobenzene molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S31a and S31b) or states (SOS approaches, in Plots S31c and S31d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S31e and S31f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.51 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



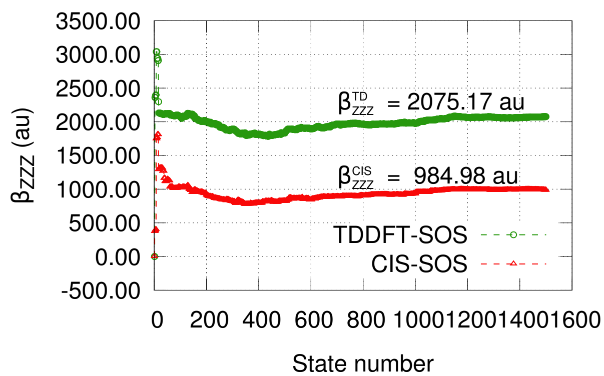
(a) CPKS-, CPHF- and UPHF-FIOs decomposition of α_{ZZ} into MOs.



(b) TDDFT- and CIS-SOS decomposition of α_{ZZ} into states.

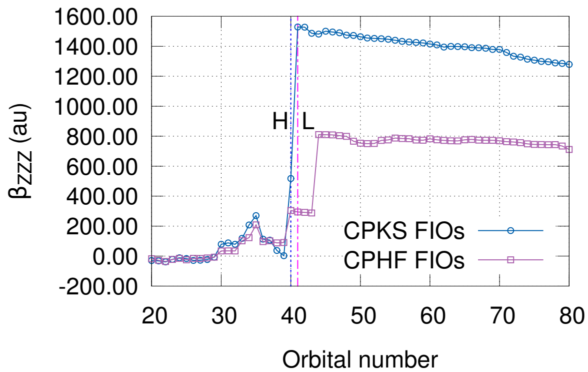


(c) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} into MOs.

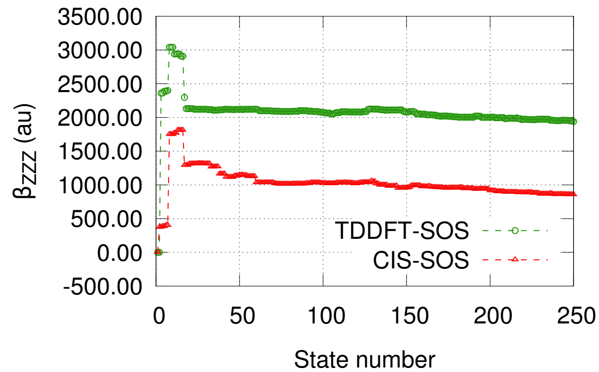


(d) TDDFT- and CIS-SOS decomposition of β_{ZZZ} into states.

Figure S31: (continued) For p-methoxy-nitrobenzene molecule and 6-311++G(d,p) basis set, variation of α_{ZZ} (top) and β_{ZZZ} (middle) with respect to the number of orbitals (FIOs decomposition presented in this work, in Plots S31a and S31b) or states (SOS approaches, in Plots S31c and S31d). For α FIOs, three approaches were considered: CPKS, CPHF and UPHF. For β FIOs, the results of CPKS and CPHF approaches are provided. Besides, a shorten range of number of orbitals/states can be seen in Plots S31e and S31f as well (bottom). All elements of the β tensor were recomputed with an error less than 0.51 au in the case of the FIOs. For SOS approach, TDDFT (CAM-B3LYP) and CIS methods were employed. Recomputed values of α_{ZZ} and β_{ZZZ} for the different approaches are included in each plot. HOMO (H) and LUMO (L) are represented by blue and pink dotted lines, respectively.



(e) CPKS- and CPHF-FIOs decomposition of β_{ZZZ} between MOs 20 and 70.



(f) TDDFT- and CIS-SOS decomposition of β_{ZZZ} between states 1 and 250.

18.2.2 Main contributions from different excited states at TDDFT (CAM-B3LYP) approach

```
#_exc.st ___symm___      Exc.E Osc._Strength    ___f___ _<S**2>_          #CIs=2799 #CIs>0=1065 #CIs<0=1120

1        Singlet-A"     4.0301         307.65      0.0000      20.000    Singlet-A"     4.5769         270.89      0.0004      0.000
                   max(1)=        38 -> 41            0.67612                       max(1)=        36 -> 41            0.67784
                   max(2)=        38 -> 46            0.07207                       max(2)=        36 -> 46            0.06939
                   max(3)=        38 -> 58            0.03313                       max(3)=        36 -> 58            0.03143
                   max(4)=        38 -> 43            0.02194                       max(4)=        36 -> 43            0.02109
                   max(5)=        38 -> 97            0.01694                       max(5)=        28 -> 41            0.01886
                   min(1)=        38 -> 48           -0.18123                       min(1)=        36 -> 48           -0.17439
                   min(2)=        35 -> 41           -0.02622                       min(2)=        31 -> 41           -0.02686
                   min(3)=        38 -> 57           -0.02058                       min(3)=        36 -> 57           -0.01969
                   min(4)=        30 -> 41           -0.01747                       min(4)=        28 -> 48           -0.01439
                   min(5)=        38 -> 54           -0.01287                       min(5)=        36 -> 54           -0.01247
```

```
      #CIs=2815 #CIs>0=1204 #CIs<0=1114

3      Singlet-A'   4.6655      265.75   0.3377   0.000
      max(1)=      40 -> 41        0.68869
      max(2)=      34 -> 48        0.04650
      max(3)=      32 -> 41        0.03304
      max(4)=      36 -> 75        0.01424
      max(5)=      37 -> 43        0.01117
      min(1)=      39 -> 43       -0.09737
      min(2)=      34 -> 41       -0.09645
      min(3)=      32 -> 48       -0.01966
      min(4)=      34 -> 43       -0.01226
      min(5)=      37 -> 86       -0.01198
      #CIs=4451 #CIs>0=2002 #CIs<0=1980

4      Singlet-A'   4.9848      248.72   0.0013   0.000
      max(1)=      39 -> 41        0.55676
      max(2)=      40 -> 43        0.41162
      max(3)=      39 -> 48        0.10910
      max(4)=      37 -> 41        0.04036
      max(5)=      40 -> 48        0.02276
      min(1)=      34 -> 43       -0.04580
      min(2)=      39 -> 46       -0.04157
      min(3)=      39 -> 65       -0.02292
      min(4)=      39 -> 53       -0.01856
      min(5)=      39 -> 43       -0.01781
      #CIs=4453 #CIs>0=1940 #CIs<0=1950

5      Singlet-A'   5.8296      212.68   0.0727   0.000
      max(1)=      40 -> 43        0.52325
      max(2)=      37 -> 41        0.16026
      max(3)=      39 -> 48        0.11622
      max(4)=      40 -> 46        0.02045
      max(5)=      32 -> 41        0.01426
      min(1)=      39 -> 41       -0.42632
      min(2)=      39 -> 53       -0.03907
      min(3)=      39 -> 43       -0.02866
      min(4)=      39 -> 46       -0.02284
      min(5)=      34 -> 41       -0.02225
      #CIs=4451 #CIs>0=1933 #CIs<0=2027

6      Singlet-A"   6.3456      195.39   0.0153   0.000
      max(1)=      40 -> 42        0.64733
      max(2)=      40 -> 45        0.13022
      max(3)=      40 -> 44        0.12554
      max(4)=      40 -> 56        0.10508
      max(5)=      40 -> 50        0.10036
      min(1)=      39 -> 42       -0.04343
      min(2)=      40 -> 51       -0.03984
      min(3)=      34 -> 45       -0.03592
      min(4)=      40 -> 60       -0.02224
      min(5)=      40 -> 52       -0.01912
      #CIs=2811 #CIs>0=1190 #CIs<0=1090

7      Singlet-A'   6.4800      191.33   0.1925   0.000
      max(1)=      37 -> 41        0.66115
      max(2)=      40 -> 48        0.06831
      max(3)=      39 -> 41        0.06545
      max(4)=      38 ->109        0.04083
      max(5)=      34 -> 41        0.03239
      min(1)=      40 -> 43       -0.14305
      min(2)=      39 -> 43       -0.08166
      min(3)=      39 -> 48       -0.05865
      min(4)=      37 -> 48       -0.05592
      min(5)=      34 -> 43       -0.04068
      #CIs=4451 #CIs>0=1950 #CIs<0=2013

8      Singlet-A'   6.5823      188.36   0.0921   0.000
      max(1)=      39 -> 43        0.49637
      max(2)=      40 -> 46        0.22150
      max(3)=      37 -> 41        0.11606
      max(4)=      40 -> 41        0.05619
      max(5)=      32 -> 41        0.05603
      min(1)=      40 -> 48       -0.39922
      min(2)=      34 -> 41       -0.11344
      min(3)=      39 -> 48       -0.01776
      min(4)=      40 -> 58       -0.01445
      min(5)=      34 -> 74       -0.01399
      #CIs=4454 #CIs>0=2010 #CIs<0=2032

9      Singlet-A"   6.8634      180.64   0.0001   0.000
      max(1)=      40 -> 44        0.60394
```

max(2)= 40 -> 50 0.17378
max(3)= 39 -> 42 0.15203
max(4)= 40 -> 47 0.12851
max(5)= 40 -> 49 0.08067
min(1)= 40 -> 42 -0.14861
min(2)= 40 -> 60 -0.09906
min(3)= 40 -> 45 -0.05847
min(4)= 40 -> 71 -0.03000
min(5)= 40 -> 56 -0.02663
#CIs=2819 #CIs>0=1195 #CIs<0=1172

10 Singlet-A" 7.0788 175.15 0.0021 0.000
max(1)= 40 -> 45 0.61872
max(2)= 40 -> 44 0.10334
max(3)= 39 -> 44 0.05688
max(4)= 40 -> 61 0.05206
max(5)= 40 -> 56 0.04704
min(1)= 40 -> 49 -0.14969
min(2)= 40 -> 50 -0.13099
min(3)= 40 -> 47 -0.11137
min(4)= 40 -> 42 -0.09398
min(5)= 40 -> 59 -0.09289
#CIs=2814 #CIs>0=1193 #CIs<0=1195

11 Singlet-A’ 7.1549 173.29 0.4820 0.000
max(1)= 39 -> 43 0.45938
max(2)= 40 -> 48 0.42136
max(3)= 34 -> 41 0.24928
max(4)= 40 -> 41 0.09324
max(5)= 34 -> 48 0.04544
min(1)= 40 -> 46 -0.13900
min(2)= 40 -> 54 -0.04478
min(3)= 32 -> 41 -0.04055
min(4)= 40 -> 53 -0.04017
min(5)= 34 -> 43 -0.02576
#CIs=4448 #CIs>0=1978 #CIs<0=1989

12 Singlet-A" 7.1634 173.08 0.0001 0.000
max(1)= 35 -> 41 0.61247
max(2)= 35 -> 48 0.15640
max(3)= 38 -> 48 0.03829
max(4)= 38 -> 41 0.03411
max(5)= 28 -> 43 0.02925
min(1)= 33 -> 41 -0.27420
min(2)= 29 -> 41 -0.06219
min(3)= 35 -> 46 -0.06137
min(4)= 31 -> 41 -0.04126
min(5)= 36 -> 43 -0.03636
#CIs=2818 #CIs>0=1239 #CIs<0=1272

13 Singlet-A" 7.2331 171.41 0.0004 0.000
max(1)= 39 -> 42 0.49158
max(2)= 39 -> 45 0.25476
max(3)= 39 -> 44 0.14370
max(4)= 40 -> 42 0.13192
max(5)= 39 -> 56 0.09789
min(1)= 40 -> 50 -0.25576
min(2)= 40 -> 47 -0.17130
min(3)= 40 -> 45 -0.12935
min(4)= 40 -> 49 -0.05762
min(5)= 40 -> 55 -0.04840
#CIs=2820 #CIs>0=1230 #CIs<0=1195

14 Singlet-A" 7.3079 169.66 0.0004 0.000
max(1)= 40 -> 50 0.41409
max(2)= 39 -> 42 0.30174
max(3)= 40 -> 47 0.25805
max(4)= 40 -> 45 0.16131
max(5)= 39 -> 45 0.13968
min(1)= 40 -> 44 -0.27780
min(2)= 40 -> 52 -0.06599
min(3)= 39 -> 44 -0.05174
min(4)= 40 -> 42 -0.05164
min(5)= 34 -> 42 -0.04168
#CIs=2818 #CIs>0=1275 #CIs<0=1211

15 Singlet-A’ 7.4243 167.00 0.0118 0.000
max(1)= 40 -> 46 0.61644
max(2)= 40 -> 48 0.25621
max(3)= 34 -> 46 0.05892
max(4)= 34 -> 54 0.02950
max(5)= 40 -> 65 0.02038

```
          min(1)=       40 -> 53        -0.15894
          min(2)=       40 -> 58        -0.09569
          min(3)=       39 -> 43        -0.06345
          min(4)=       39 -> 46        -0.05092
          min(5)=       40 -> 70        -0.03678
          #CIs=4431 #CIs>0=1770 #CIs<0=1825

16      Singlet-A"    7.4766        165.83    0.0000    0.000
          max(1)=       38 -> 43         0.69260
          max(2)=       35 -> 43         0.07815
          max(3)=       30 -> 43         0.04095
          max(4)=       38 -> 46         0.03919
          max(5)=       31 -> 41         0.02549
          min(1)=       33 -> 41        -0.03325
          min(2)=       38 -> 41        -0.03220
          min(3)=       38 -> 54        -0.02708
          min(4)=       36 -> 48        -0.02334
          min(5)=       33 -> 43        -0.02161
          #CIs=2812 #CIs>0=1204 #CIs<0=1163

17      Singlet-A’    7.6496        162.08    0.0893    0.000
          max(1)=       34 -> 41         0.53837
          max(2)=       39 -> 46         0.18040
          max(3)=       40 -> 46         0.10485
          max(4)=       40 -> 43         0.08529
          max(5)=       40 -> 41         0.07290
          min(1)=       39 -> 48        -0.23496
          min(2)=       40 -> 48        -0.20826
          min(3)=       32 -> 41        -0.16141
          min(4)=       39 -> 43        -0.08881
          min(5)=       37 -> 43        -0.06543
          #CIs=4451 #CIs>0=2034 #CIs<0=1954

18      Singlet-A’    7.6903        161.22    0.1834    0.000
          max(1)=       39 -> 48         0.48646
          max(2)=       34 -> 41         0.25947
          max(3)=       40 -> 53         0.09348
          max(4)=       39 -> 53         0.04460
          max(5)=       40 -> 41         0.03375
          min(1)=       39 -> 46        -0.32247
          min(2)=       40 -> 48        -0.15014
          min(3)=       40 -> 43        -0.13385
          min(4)=       34 -> 43        -0.13256
          min(5)=       32 -> 41        -0.07470
          #CIs=4443 #CIs>0=1926 #CIs<0=1995

19      Singlet-A"    7.7200        160.60    0.0130    0.000
          max(1)=       39 -> 44         0.45546
          max(2)=       40 -> 47         0.30224
          max(3)=       40 -> 49         0.28181
          max(4)=       39 -> 50         0.10045
          max(5)=       40 -> 52         0.09736
          min(1)=       40 -> 50        -0.19210
          min(2)=       40 -> 51        -0.08793
          min(3)=       39 -> 60        -0.07783
          min(4)=       40 -> 42        -0.07371
          min(5)=       40 -> 44        -0.07293
          #CIs=2815 #CIs>0=1227 #CIs<0=1255

20      Singlet-A"    7.7763        159.44    0.0171    0.000
          max(1)=       39 -> 44         0.39781
          max(2)=       40 -> 50         0.33177
          max(3)=       40 -> 51         0.08126
          max(4)=       39 -> 50         0.07246
          max(5)=       40 -> 55         0.07031
          min(1)=       40 -> 47        -0.38169
          min(2)=       40 -> 52        -0.12976
          min(3)=       39 -> 42        -0.11391
          min(4)=       39 -> 60        -0.06045
          min(5)=       40 -> 45        -0.05422
          #CIs=2818 #CIs>0=1243 #CIs<0=1216
```

18.2.3 Main contributions from different excited states at CIS approach

```
#_exc.st ___symm___     Exc.E Osc._Strength   ___f___ _<S**2>_

1        Singlet-A"    5.4417        227.84    0.0000    0.000
         max(1)=       37 -> 44         0.56394
         max(2)=       37 -> 55         0.21093
         max(3)=       37 -> 53         0.16581
         max(4)=       37 -> 77         0.08136
         max(5)=       37 -> 52         0.08087
         min(1)=       37 -> 60        -0.17457
         min(2)=       37 -> 65        -0.12725
         min(3)=       37 -> 45        -0.07900
         min(4)=       34 -> 44        -0.07854
         min(5)=       37 -> 95        -0.07442
         #CIs=2612 #CIs>0=1158 #CIs<0=1156

2        Singlet-A'    5.7590        215.29    0.2717    0.000
         max(1)=       40 -> 44         0.61076
         max(2)=       39 -> 49         0.24810
         max(3)=       40 -> 49         0.07286
         max(4)=       40 -> 65         0.07161
         max(5)=       39 -> 52         0.04367
         min(1)=       35 -> 44        -0.09621
         min(2)=       39 -> 44        -0.07625
         min(3)=       40 -> 55        -0.07272
         min(4)=       40 -> 45        -0.07159
         min(5)=       35 -> 55        -0.03788
         #CIs=4323 #CIs>0=2038 #CIs<0=2064

3        Singlet-A"    5.7760        214.66    0.0004    0.000
         max(1)=       36 -> 44         0.57446
         max(2)=       36 -> 55         0.20997
         max(3)=       36 -> 53         0.16263
         max(4)=       36 -> 52         0.07995
         max(5)=       36 -> 77         0.07250
         min(1)=       36 -> 60        -0.16891
         min(2)=       36 -> 65        -0.12044
         min(3)=       36 -> 45        -0.07973
         min(4)=       36 -> 95        -0.07176
         min(5)=       36 -> 49        -0.04839
         #CIs=2667 #CIs>0=1210 #CIs<0=1215

4        Singlet-A'    5.9273        209.18    0.0051    0.000
         max(1)=       40 -> 49         0.46402
         max(2)=       39 -> 55         0.11611
         max(3)=       40 -> 57         0.07390
         max(4)=       40 -> 52         0.06926
         max(5)=       40 -> 69         0.06310
         min(1)=       39 -> 44        -0.46429
         min(2)=       40 -> 44        -0.09742
         min(3)=       39 -> 65        -0.09139
         min(4)=       40 -> 68        -0.06034
         min(5)=       39 -> 49        -0.04954
         #CIs=4237 #CIs>0=1921 #CIs<0=2079

5        Singlet-A"    6.9182        179.21    0.0204    0.000
         max(1)=       40 -> 41         0.53951
         max(2)=       40 -> 43         0.29808
         max(3)=       40 -> 48         0.15344
         max(4)=       40 -> 54         0.12210
         max(5)=       40 -> 61         0.05593
         min(1)=       40 -> 50        -0.16048
         min(2)=       40 -> 56        -0.13192
         min(3)=       39 -> 42        -0.07691
         min(4)=       40 -> 42        -0.06092
         min(5)=       39 -> 41        -0.05089
         #CIs=2666 #CIs>0=1213 #CIs<0=1210

6        Singlet-A'    7.2310        171.46    0.0443    0.000
         max(1)=       38 -> 44         0.40097
         max(2)=       38 -> 55         0.15162
         max(3)=       38 -> 53         0.08027
         max(4)=       38 -> 68         0.04275
         max(5)=       38 -> 52         0.04169
         min(1)=       39 -> 44        -0.37360
         min(2)=       40 -> 49        -0.34379
         min(3)=       38 -> 60        -0.07751
         min(4)=       38 -> 65        -0.06061
         min(5)=       38 -> 45        -0.05084
         #CIs=4276 #CIs>0=2020 #CIs<0=2056

7        Singlet-A"    7.3532        168.61    0.0003    0.000
         max(1)=       39 -> 41         0.38704
```

```
        max(2)=      39 -> 43        0.28650
        max(3)=      40 -> 43        0.12592
        max(4)=      39 -> 54        0.09573
        max(5)=      40 -> 48        0.07344
        min(1)=      40 -> 42       -0.40149
        min(2)=      39 -> 56       -0.13192
        min(3)=      40 -> 59       -0.11795
        min(4)=      40 -> 41       -0.11630
        min(5)=      39 -> 50       -0.07058
        #CIs=2655 #CIs>0=1188 #CIs<0=1184

8       Singlet-A'   7.4607      166.18   0.8529   0.000
        max(1)=      39 -> 49        0.52800
        max(2)=      40 -> 45        0.12052
        max(3)=      40 -> 49        0.10690
        max(4)=      40 -> 65        0.10093
        max(5)=      38 -> 44        0.08678
        min(1)=      40 -> 44       -0.23406
        min(2)=      40 -> 55       -0.19049
        min(3)=      40 -> 53       -0.10875
        min(4)=      39 -> 45       -0.08302
        min(5)=      40 -> 52       -0.07993
        #CIs=4316 #CIs>0=2025 #CIs<0=2083

9       Singlet-A"   7.6934      161.16   0.0023   0.000
        max(1)=      40 -> 42        0.47577
        max(2)=      39 -> 41        0.31673
        max(3)=      39 -> 43        0.23904
        max(4)=      40 -> 41        0.14332
        max(5)=      39 -> 54        0.11718
        min(1)=      39 -> 50       -0.11336
        min(2)=      40 -> 48       -0.09826
        min(3)=      39 -> 56       -0.08577
        min(4)=      39 -> 51       -0.04678
        min(5)=      35 -> 46       -0.04517
        #CIs=2694 #CIs>0=1211 #CIs<0=1231

10      Singlet-A"   7.8093      158.77   0.0137   0.000
        max(1)=      40 -> 43        0.44909
        max(2)=      40 -> 47        0.24365
        max(3)=      40 -> 42        0.14855
        max(4)=      40 -> 54        0.12104
        max(5)=      40 -> 48        0.11890
        min(1)=      40 -> 41       -0.29797
        min(2)=      40 -> 51       -0.18154
        min(3)=      39 -> 43       -0.09425
        min(4)=      40 -> 58       -0.09237
        min(5)=      35 -> 41       -0.08849
        #CIs=2677 #CIs>0=1239 #CIs<0=1223

11      Singlet-A'   7.8317      158.31   0.8939   0.000
        max(1)=      38 -> 44        0.43510
        max(2)=      39 -> 44        0.31852
        max(3)=      40 -> 49        0.29890
        max(4)=      38 -> 55        0.14301
        max(5)=      38 -> 53        0.07932
        min(1)=      39 -> 49       -0.10908
        min(2)=      38 -> 60       -0.08179
        min(3)=      40 -> 45       -0.07872
        min(4)=      39 -> 52       -0.07098
        min(5)=      39 -> 53       -0.05942
        #CIs=4294 #CIs>0=2031 #CIs<0=2056

12      Singlet-A"   7.8498      157.94   0.0028   0.000
        max(1)=      39 -> 42        0.36451
        max(2)=      40 -> 48        0.35346
        max(3)=      39 -> 59        0.11836
        max(4)=      39 -> 41        0.11813
        max(5)=      40 -> 54        0.09701
        min(1)=      40 -> 43       -0.26168
        min(2)=      40 -> 50       -0.25083
        min(3)=      39 -> 43       -0.07811
        min(4)=      39 -> 48       -0.05394
        min(5)=      40 -> 82       -0.05046
        #CIs=2692 #CIs>0=1264 #CIs<0=1220

13      Singlet-A'   8.0037      154.91   0.0064   0.000
        max(1)=      40 -> 45        0.58291
        max(2)=      40 -> 44        0.14178
        max(3)=      40 -> 55        0.08463
        max(4)=      40 -> 49        0.07134
        max(5)=      35 -> 45        0.04660
```

```
        min(1)=       40 -> 52        -0.19725
        min(2)=       40 -> 53        -0.19655
        min(3)=       39 -> 49        -0.11713
        min(4)=       40 -> 60        -0.10028
        min(5)=       40 -> 57        -0.08786
        #CIs=4179 #CIs>0=1931 #CIs<0=1928

14      Singlet-A"    8.1909        151.37    0.0290    0.000
        max(1)=       39 -> 42         0.43307
        max(2)=       40 -> 50         0.21093
        max(3)=       40 -> 41         0.17001
        max(4)=       40 -> 43         0.13250
        max(5)=       39 -> 59         0.11765
        min(1)=       40 -> 48        -0.26679
        min(2)=       39 -> 43        -0.14822
        min(3)=       39 -> 48        -0.12208
        min(4)=       40 -> 42        -0.11948
        min(5)=       40 -> 54        -0.10381
        #CIs=2713 #CIs>0=1270 #CIs<0=1241

15      Singlet-A"    8.4294        147.09    0.0003    0.000
        max(1)=       40 -> 46         0.55741
        max(2)=       40 -> 51         0.13526
        max(3)=       40 -> 64         0.11410
        max(4)=       40 -> 43         0.11244
        max(5)=       39 -> 41         0.09334
        min(1)=       40 -> 47        -0.26919
        min(2)=       39 -> 43        -0.11028
        min(3)=       39 -> 47        -0.08316
        min(4)=       40 -> 41        -0.07283
        min(5)=       35 -> 50        -0.05311
        #CIs=2711 #CIs>0=1249 #CIs<0=1257

16      Singlet-A"    8.5288        145.37    0.0049    0.000
        max(1)=       39 -> 48         0.46032
        max(2)=       39 -> 54         0.14575
        max(3)=       39 -> 56         0.08654
        max(4)=       39 -> 75         0.08463
        max(5)=       39 -> 59         0.07813
        min(1)=       39 -> 50        -0.30107
        min(2)=       39 -> 43        -0.25453
        min(3)=       39 -> 51        -0.13080
        min(4)=       40 -> 42        -0.11140
        min(5)=       39 -> 62        -0.07575
        #CIs=2681 #CIs>0=1234 #CIs<0=1224

17      Singlet-A'    8.5830        144.45    0.3249    0.000
        max(1)=       40 -> 55         0.52281
        max(2)=       39 -> 49         0.22491
        max(3)=       40 -> 52         0.10998
        max(4)=       39 -> 52         0.09261
        max(5)=       40 -> 57         0.06617
        min(1)=       35 -> 44        -0.23292
        min(2)=       40 -> 65        -0.16409
        min(3)=       40 -> 60        -0.10900
        min(4)=       39 -> 45        -0.09423
        min(5)=       32 -> 44        -0.09161
        #CIs=4300 #CIs>0=2034 #CIs<0=2073

18      Singlet-A"    8.6446        143.42    0.0123    0.000
        max(1)=       40 -> 47         0.49541
        max(2)=       40 -> 46         0.32563
        max(3)=       40 -> 41         0.12348
        max(4)=       40 -> 62         0.09108
        max(5)=       40 -> 63         0.06750
        min(1)=       40 -> 43        -0.18706
        min(2)=       40 -> 51        -0.11391
        min(3)=       39 -> 42        -0.11307
        min(4)=       40 -> 42        -0.10609
        min(5)=       40 -> 54        -0.09694
        #CIs=2727 #CIs>0=1223 #CIs<0=1264

19      Singlet-A"    8.6824        142.80    0.0009    0.000
        max(1)=       39 -> 43         0.34062
        max(2)=       39 -> 47         0.30103
        max(3)=       39 -> 42         0.22707
        max(4)=       40 -> 46         0.16421
        max(5)=       39 -> 54         0.09044
        min(1)=       39 -> 41        -0.35398
        min(2)=       39 -> 51        -0.15009
        min(3)=       39 -> 58        -0.07170
        min(4)=       40 -> 42        -0.06026
```

```
        min(5)=       39 -> 50        -0.05533
        #CIs=2699 #CIs>0=1227 #CIs<0=1238

20      Singlet-A'    8.6992        142.52    0.0135    0.000
        max(1)=       39 -> 45         0.52645
        max(2)=       39 -> 49         0.13107
        max(3)=       40 -> 55         0.09209
        max(4)=       40 -> 57         0.04490
        max(5)=       39 -> 69         0.03783
        min(1)=       39 -> 53        -0.27774
        min(2)=       40 -> 52        -0.20099
        min(3)=       39 -> 52        -0.18626
        min(4)=       39 -> 57        -0.08587
        min(5)=       40 -> 49        -0.06516
        #CIs=4215 #CIs>0=1984 #CIs<0=1977
```