Supporting Information for "Frozen Virtual Natural Orbitals for Coupled Cluster Linear-Response Theory"

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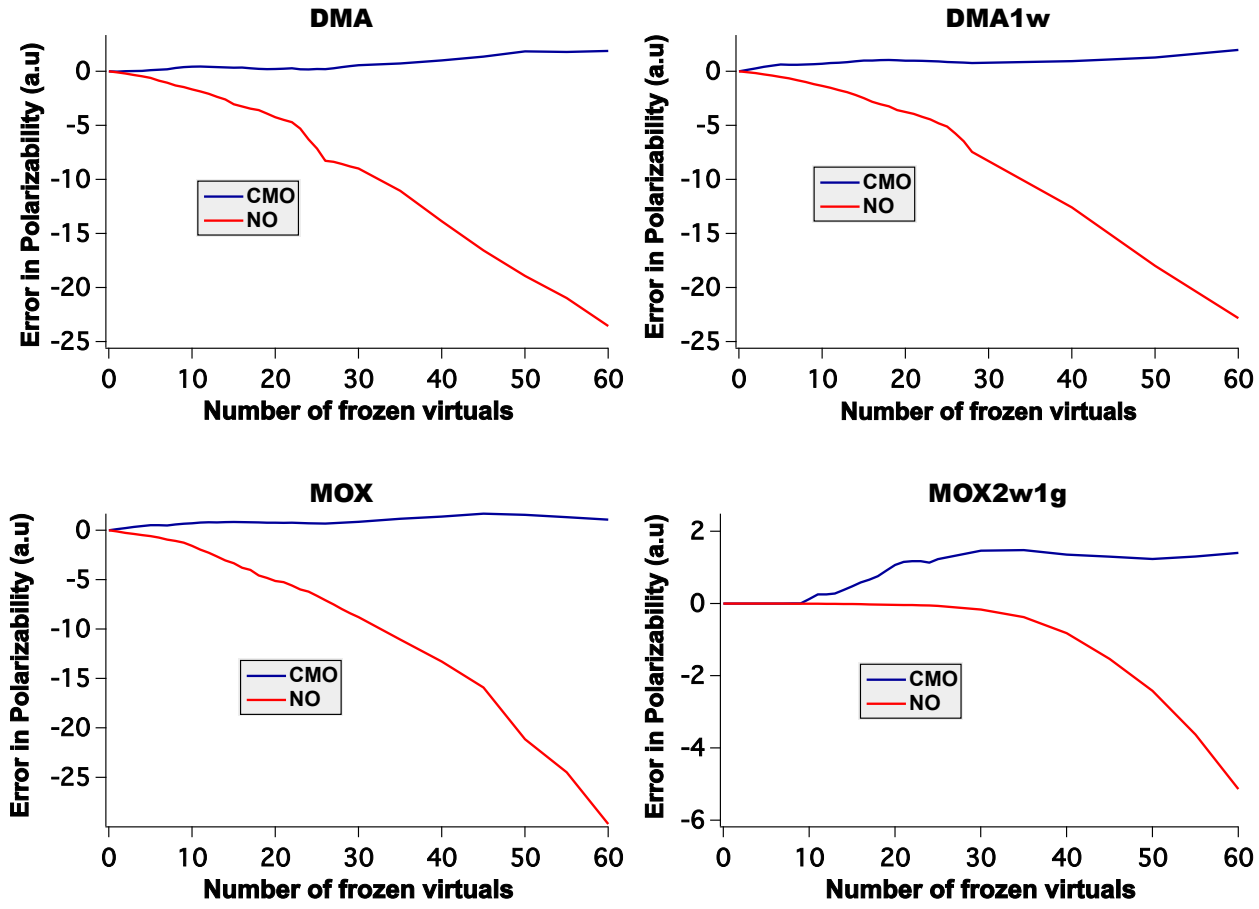

Figure S1: Errors in the CCSD/aDZ dynamic polarizability (589 nm) in both CMO and NO bases as a function of number of virtual orbitals removed for four additional test cases: (*P*)-dimethylallene (DMA), (*P*)-dimethylallene and one water molecule (DMA1w), (*S*)-Methyloxirane (MOX), and (*S*)-Methyloxirane and two water molecules with one of the water molecules removed leaving only its basis functions.

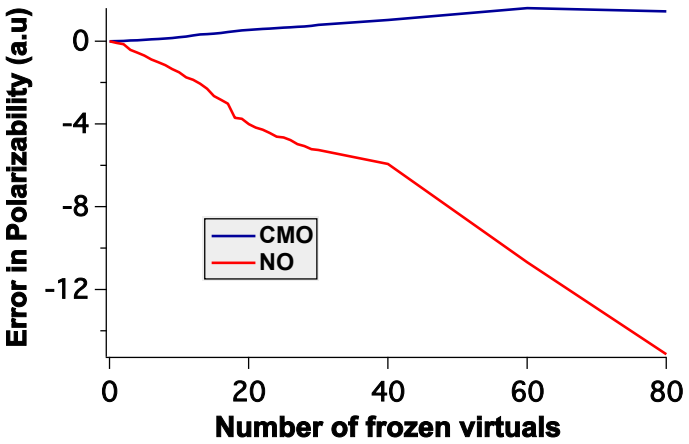

Figure S2: Errors in the CCSD/aTZ dynamic polarizability (589 nm) of H_2O_2 in in both CMO and NO bases as a function of number of virtual orbitals removed.

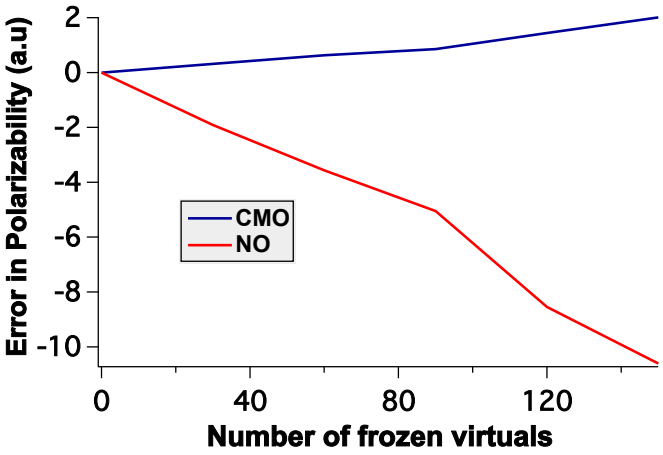

Figure S3: Errors in the CCSD/aQZ dynamic polarizability (589 nm) of H_2O_2 in in both CMO and NO bases as a function of number of virtual orbitals removed.

Table S1: B3LYP/aug-cc-pVDZ optimized geometry (Å) of hydrogen peroxide.

Atomic symbol	X	Y	Z
O	-0.028962160801	-0.694396279686	-0.049338350190
O	0.028962160801	0.694396279686	-0.049338350190
H	0.350498145881	-0.910645626300	0.783035421467
H	-0.350498145881	0.910645626300	0.783035421467

Table S2: B3LYP/aug-cc-pVDZ optimized geometry (Å) of (*P*)-dimethylallene.

Atomic symbol	X	Y	Z
C	0.00000000	0.00000000	0.00000000
C	-0.87382800	0.87178900	0.87038800
C	-0.87382800	2.18536200	0.87080500
C	-0.87382800	3.49893500	0.87038800
H	-0.19165900	4.01714100	1.55371200
C	-1.74765600	4.37072400	0.00000000
H	-2.39264800	3.76601200	-0.64911100
H	-2.38616500	5.02111900	0.61760600
H	-1.13340200	5.02895100	-0.63367100
H	-1.55599700	0.35358300	1.55371200
H	0.64499200	0.60471200	-0.64911100
H	0.63850900	-0.65039500	0.61760600
H	-0.61425400	-0.65822700	-0.63367100

Table S3: B3LYP/aug-cc-pVDZ optimized geometry (Å) of (*P*)-dimethylallene and one water molecule.

Atomic symbol	X	Y	Z
C	0.00000000	0.00000000	0.00000000
C	-1.46444400	-0.36643000	0.02694600
C	-2.44105800	0.44524100	0.36174100
C	-3.41923100	1.26314500	0.68806000
H	-3.71780300	1.32103000	1.74107500
C	-4.16801100	2.15536700	-0.27447800
H	-3.80129000	2.02991300	-1.30007100
H	-5.24434000	1.92768500	-0.25838400
H	-4.05435400	3.21167600	0.01259000
H	-1.72145400	-1.39204600	-0.25890200
H	0.15629600	1.04448300	0.29557800
H	0.57342800	-0.64609200	0.68212100
H	0.41596400	-0.14458000	-1.00872300
O	-5.05428200	-1.67323100	-0.06746500
H	-4.46520000	-0.94134100	0.17201000
H	-5.19373900	-2.15473700	0.75630300

Table S4: B3LYP/aug-cc-pVDZ optimized geometry (Å) of (*S*)-methyloxirane.

Atomic symbol	X	Y	Z
C	14.60000000	14.52999999	15.13000000
O	14.60000000	14.52999999	16.53000000
C	15.85999999	14.52999999	15.84999999
C	14.51999999	15.70999999	14.30000000
H	13.57999999	15.70999999	13.75000000
H	14.58000000	16.60000000	14.91999999
H	15.35000000	15.70999999	13.58999999
H	14.08999999	13.64000000	14.76999999
H	16.43000000	13.64000000	15.59000000
H	16.43000000	15.41999999	15.59000000

Table S5: B3LYP/aug-cc-pVDZ optimized geometry (Å) of (*S*)-methyloxirane and two water molecules. The water molecule that has been removed leaving only its basis functions is indicated by the "Gh" notation.

Atomic symbol	X	Y	Z
C	14.60000000	14.52999999	15.13000000
O	14.60000000	14.52999999	16.53000000
C	15.85999999	14.52999999	15.84999999
C	14.51999999	15.70999999	14.30000000
H	13.57999999	15.70999999	13.75000000
H	14.58000000	16.60000000	14.91999999
H	15.35000000	15.70999999	13.58999999
H	14.08999999	13.64000000	14.76999999
H	16.43000000	13.64000000	15.59000000
H	16.43000000	15.41999999	15.59000000
O	11.04999999	14.87999999	13.42000000
H	11.06999999	14.67000000	14.34999999
H	11.77999999	15.49000000	13.28999999
Gh(O)	18.57999999	15.27999999	15.68999999
Gh(H)	18.51000000	14.46000000	15.22000000
Gh(H)	19.39000000	15.19999999	16.19999999