Supporting information for "Dynamical symmetries and selection rules in high-harmonic generation spectroscopy of nonlinear molecules"

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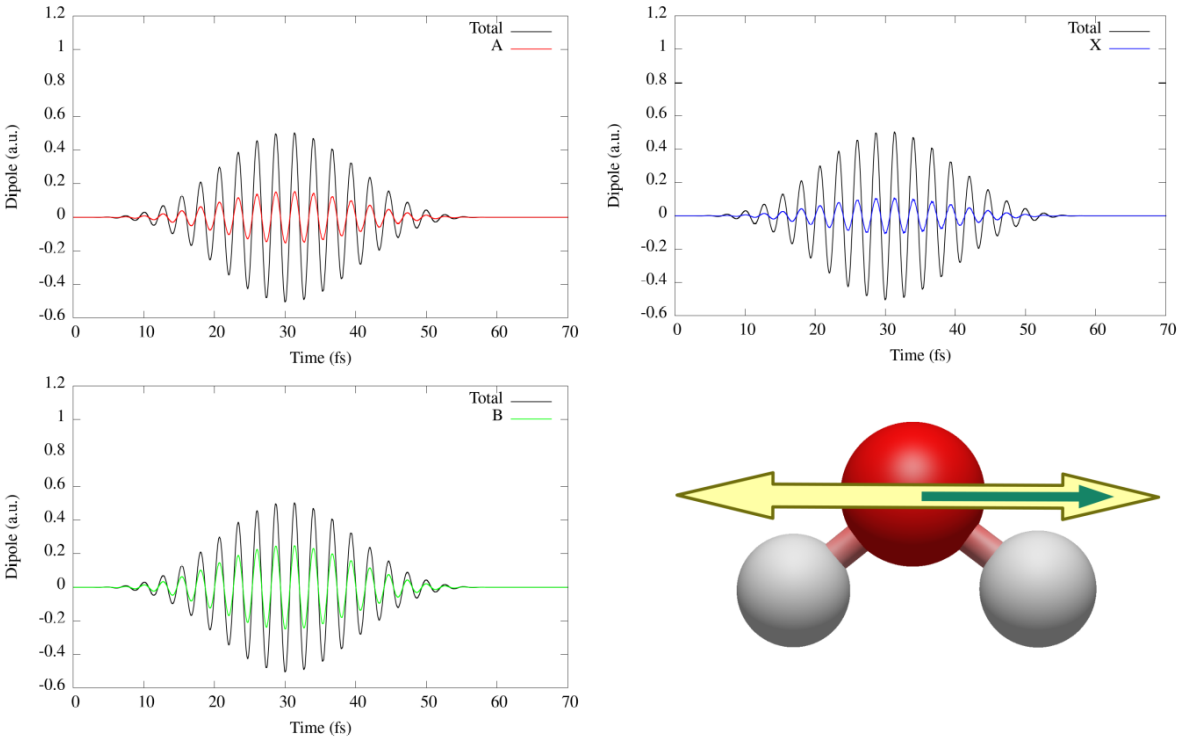

Figure S1: MO decomposition of the time-dependent dipole moment of H_2O, with laser pulse polarised along the x direction and detection along the same direction, at the RT-TD-CIS level of theory.

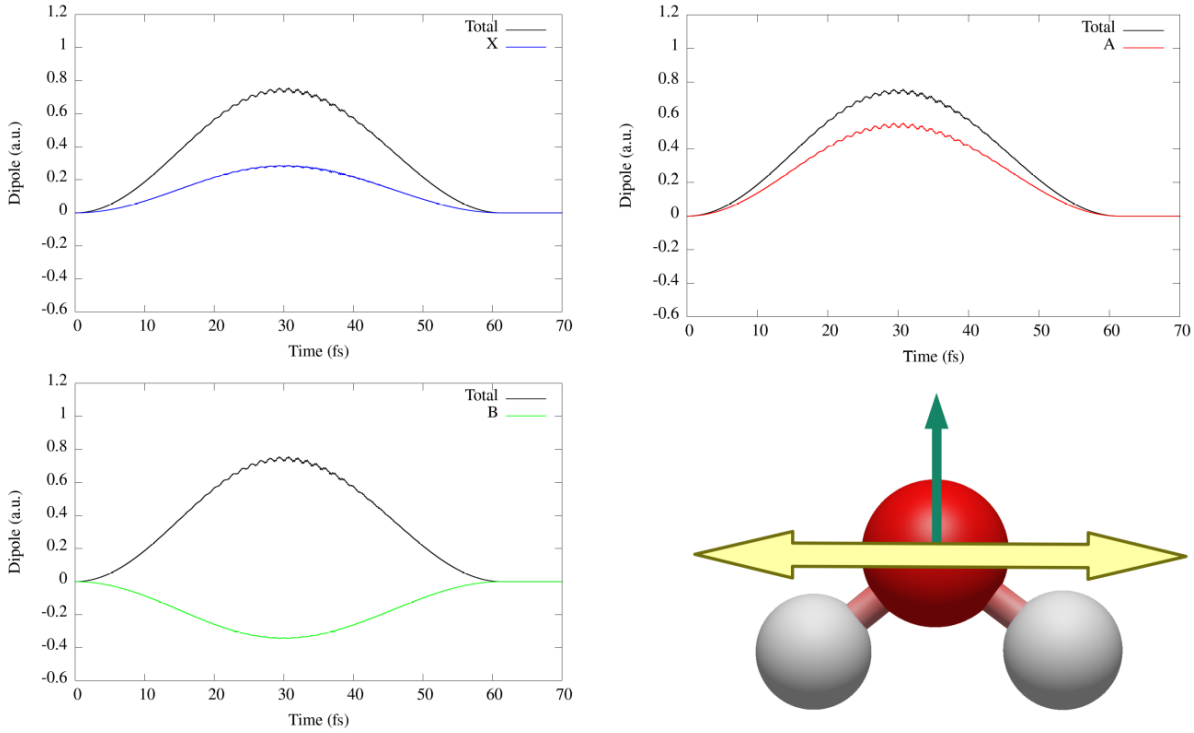

Figure S2: MO decomposition of the time-dependent dipole moment of H_2O, with laser pulse polarised along the x direction and detection along the z direction, at the RT-TD-CIS level of theory.

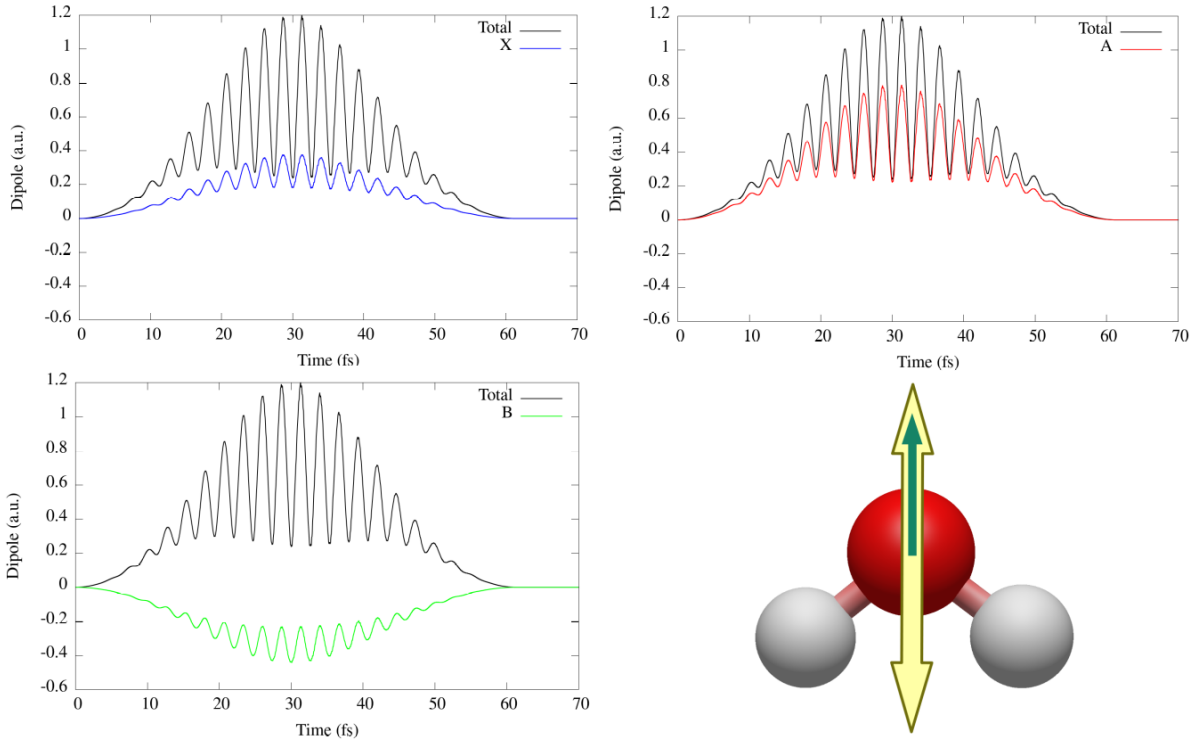

Figure S3: MO decomposition of the time-dependent dipole moment of H_2O, with laser pulse polarised along the z direction and detection along the same direction, at the RT-TD-CIS level of theory.

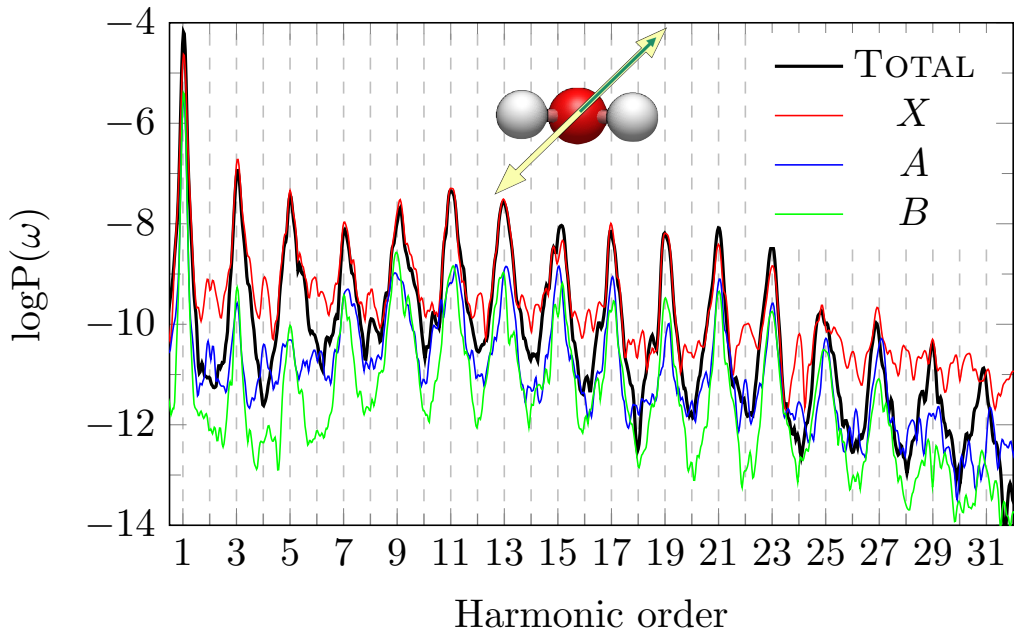

Figure S4: Channel-decomposition of the HHG spectrum, with pulse polarisation and detection in the xy plane, along a direction at 45° with respect to the molecular plane. The pulse polarisation is represented by the yellow double arrow, while a green arrow represents the direction of detection of HHG spectra.

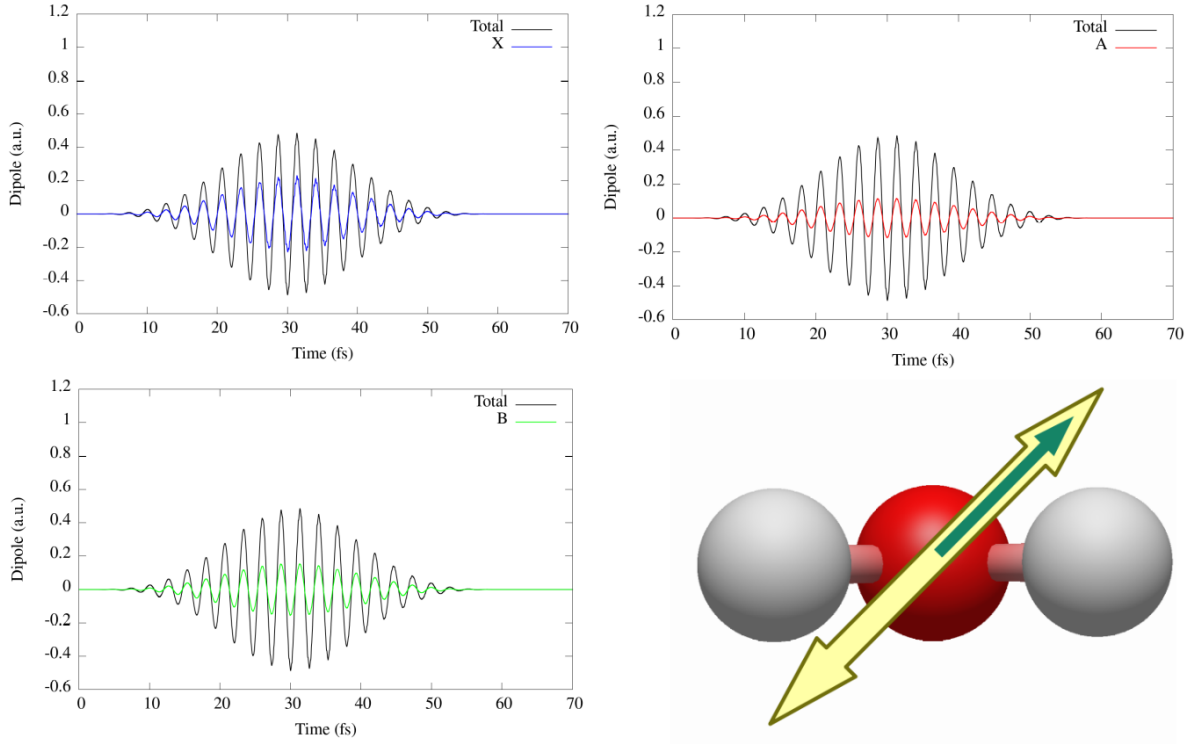

Figure S5: MO decomposition of the time-dependent dipole moment of H_2O, with laser pulse polarised with an angle of 45° in the xy plane and detection along the same direction, at the RT-TD-CIS level of theory.

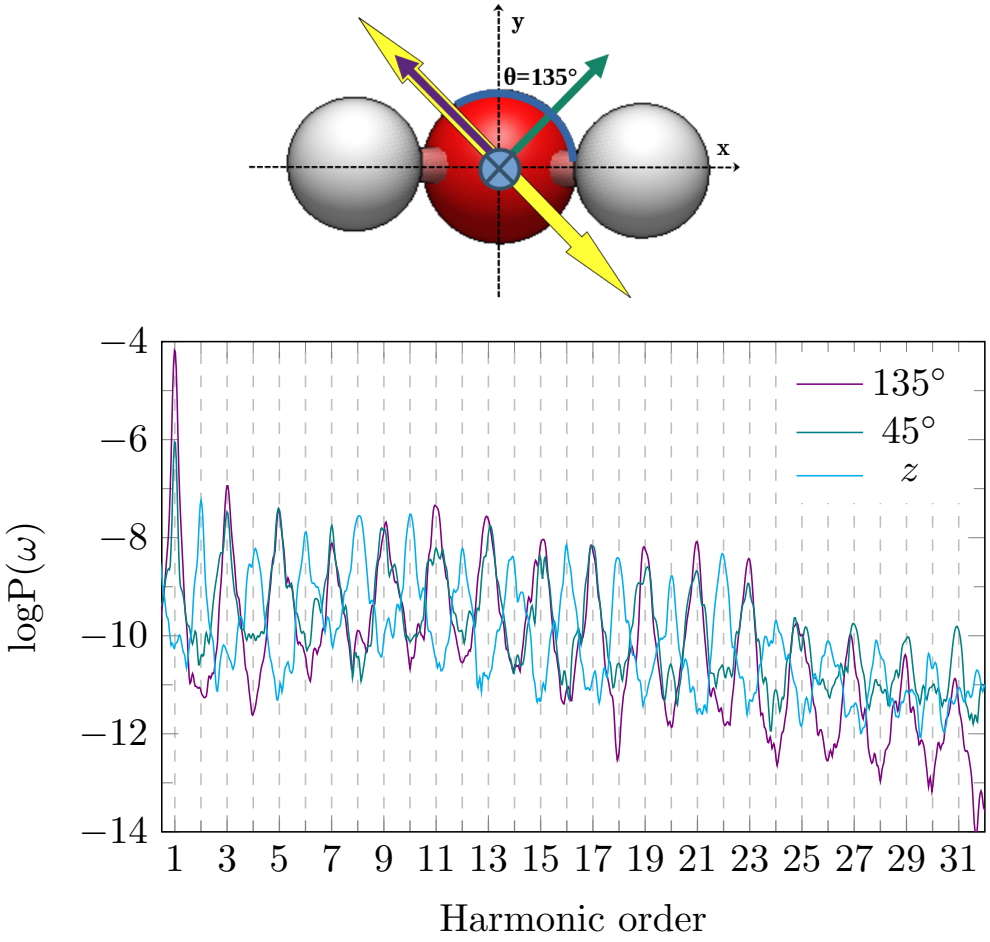

Figure S6: HHG spectra of H_2O with laser pulse polarized with an angle of 135° in the xy plane. The HHG spectra are detected along the pulse polarization (135° in the xy plane), with an angle of 45° in the xy plane, and along the z direction. For the detection in the xy plane, only odd harmonics are present, while in the z direction, only even harmonics are allowed.

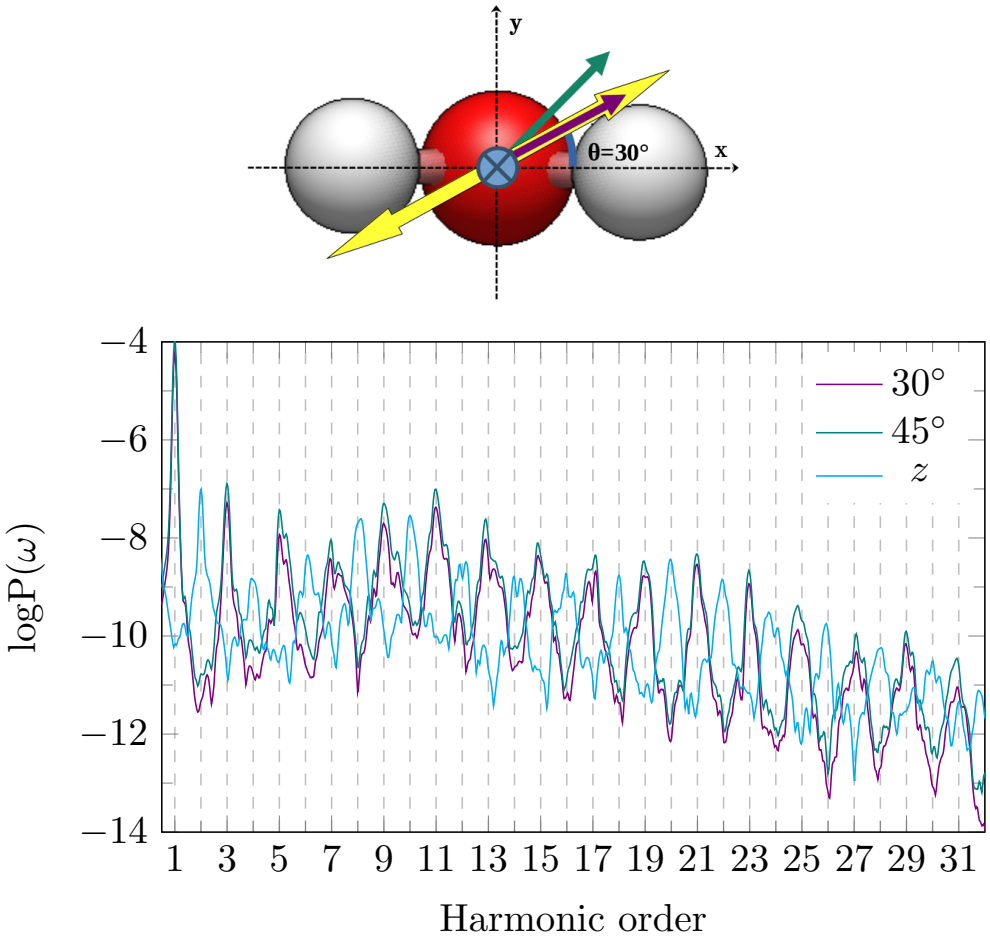

Figure S7: HHG spectra of H_2O with laser pulse polarized with an angle of 30° in the xy plane. The HHG spectra are detected along the pulse polarization (30° in the xy plane), with an angle of 45° in the xy plane, and along the z direction. Only odd harmonics are present for detection in the xy plane, while only even harmonics are allowed in the z direction.

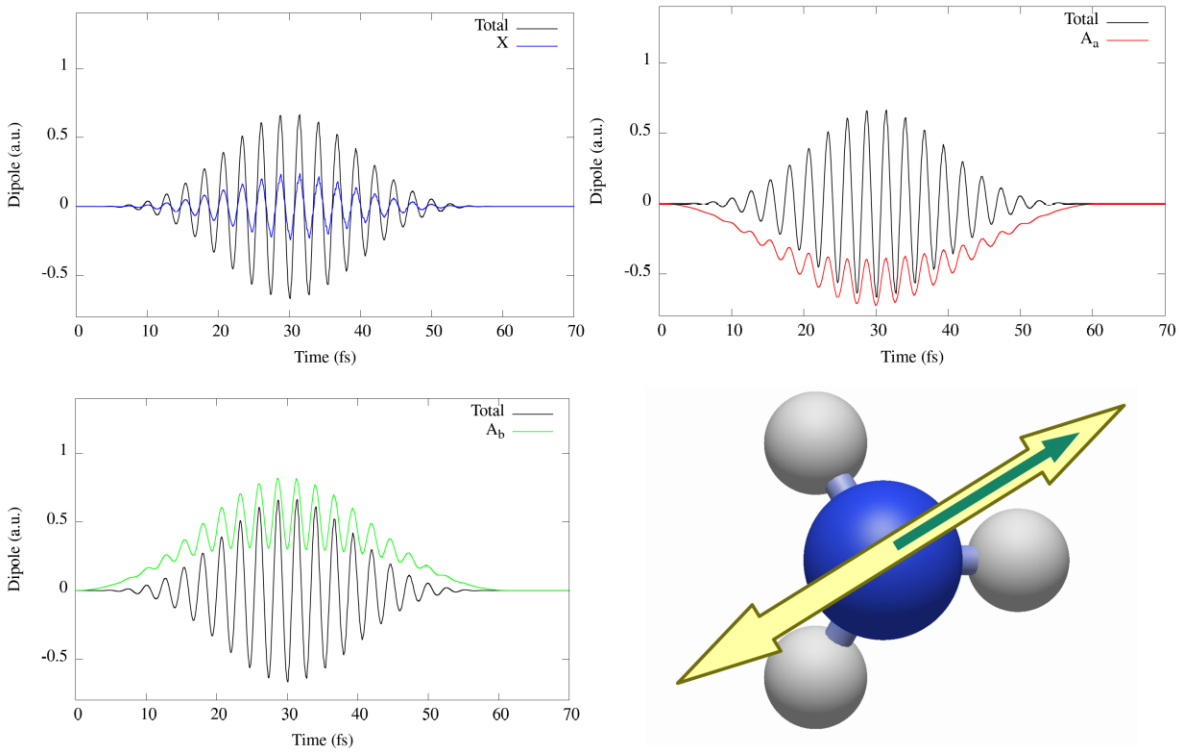

Figure S8: MO decomposition of the time-dependent dipole moment of NH_3, with laser pulse polarised perpendicular to the σ_v' reflection plane of the NH_3 molecule and detection along the same direction, at the RT-TD-CIS level of theory.

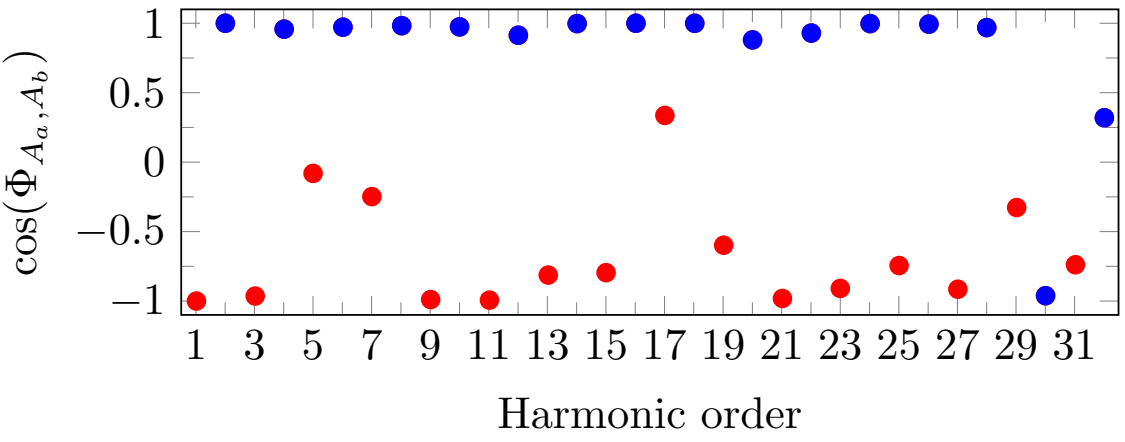

Figure S9: Phase of the interference between A_a and A_b channels of NH_3, with laser pulse polarised perpendicular to the σ_v' reflection plane of the NH_3 molecule and detection along the z direction, at the RT-TD-CIS level of theory.

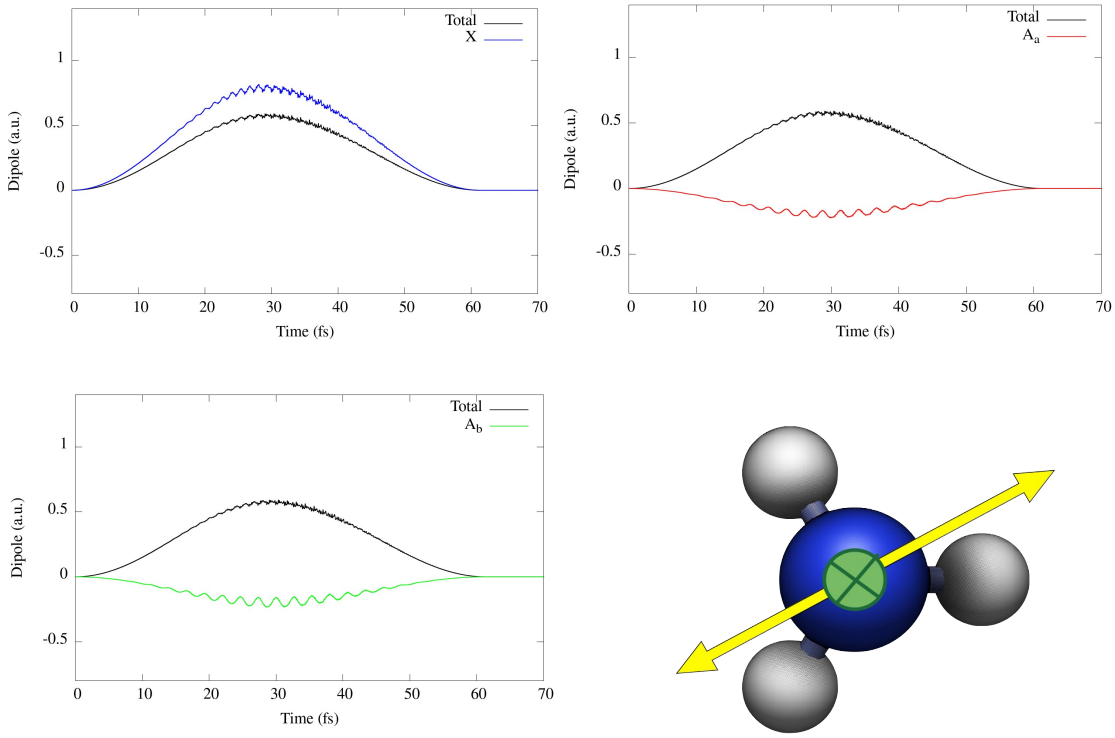

Figure S10: MO decomposition of the time-dependent dipole moment of NH_3, with laser pulse polarised perpendicular to the σ_v' reflection plane of the NH_3 molecule and detection along the z direction, at the RT-TD-CIS level of theory.

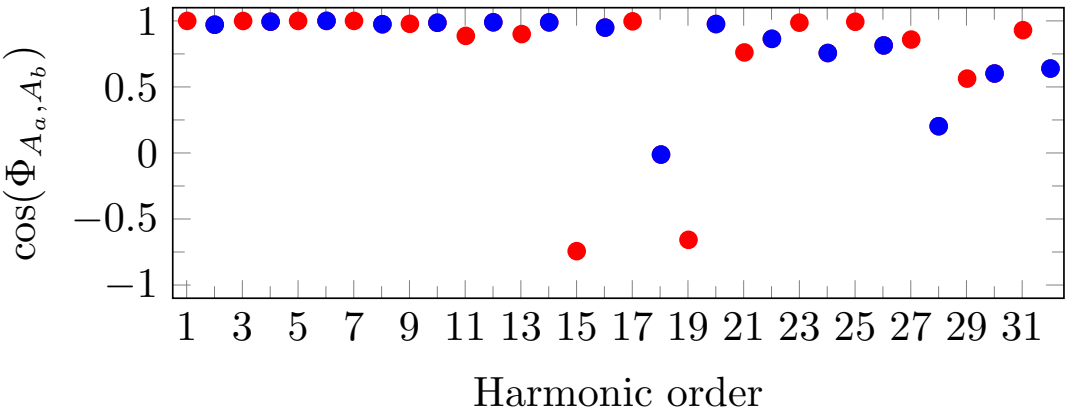

Figure S11: Phase of the interference between A_a and A_b channels of NH_3, with laser pulse along the z axis and detection along the same direction, at the RT-TD-CIS level of theory.

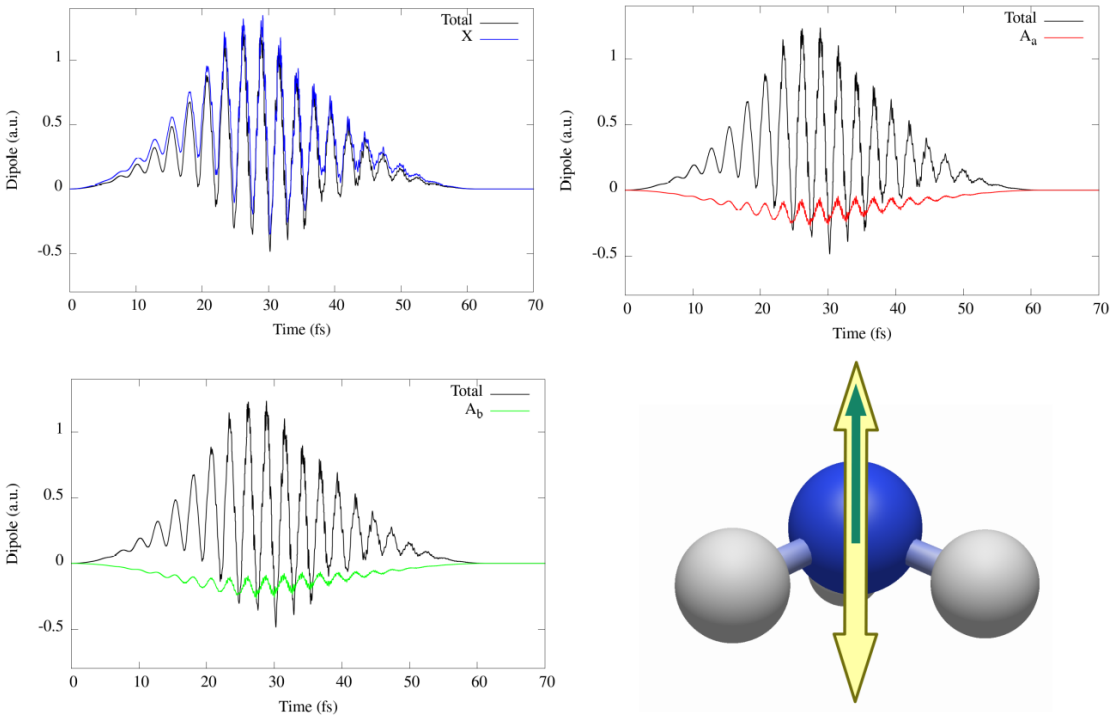

Figure S12: MO decomposition of the time-dependent dipole moment of NH_3, with laser pulse along the z axis and detection along the same direction, at the RT-TD-CIS level of theory.

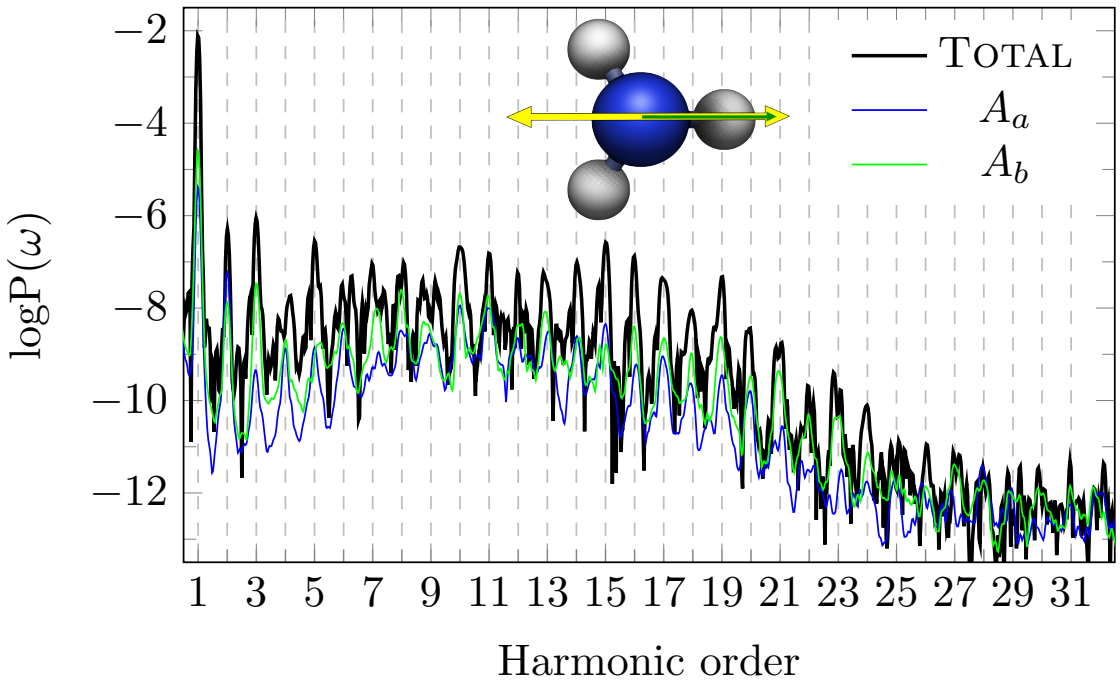

Figure S13: Comparison between A_a and A_b channels of NH_3, with laser pulse along the x axis and detection along the same direction, at the RT-TD-CIS level of theory.