Supplementary Material: Electronic circular dichroism from real-time propagation in state space

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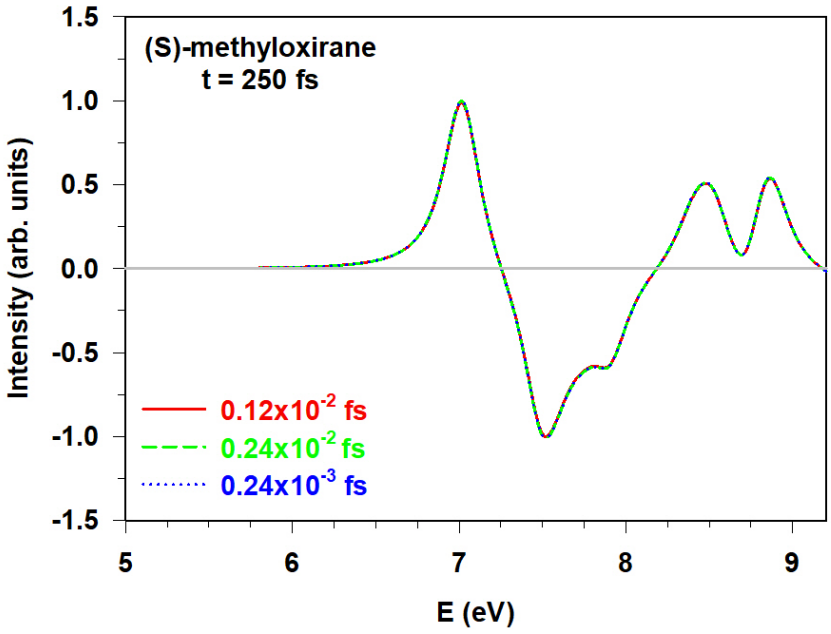

FIG. S1: Time-domain ECD spectra of (S)-methyloxirane calculated for 250 fs with a time step δt of 0.12×10^{-2} (solid red line), 0.24×10^{-2} (dashed green line), and 0.24×10^{-3} (dotted blue line) fs.

Conformation	ΔE (kJ/mol)	$P(i)_{norm}$ (T=300 K)
1	0.0	0.60
2	4.7	0.092
3	4.9	0.083
4	5.1	0.077
5	5.5	0.067
6	5.8	0.058
7	8.3	0.022

TABLE S1: Conformation, relative energy and normalized probability values ($\sum_{i=1}^{7} P(i)_{norm} = 1$) for the 7 stable structures investigated in the work by Meinert *et al.* [1].

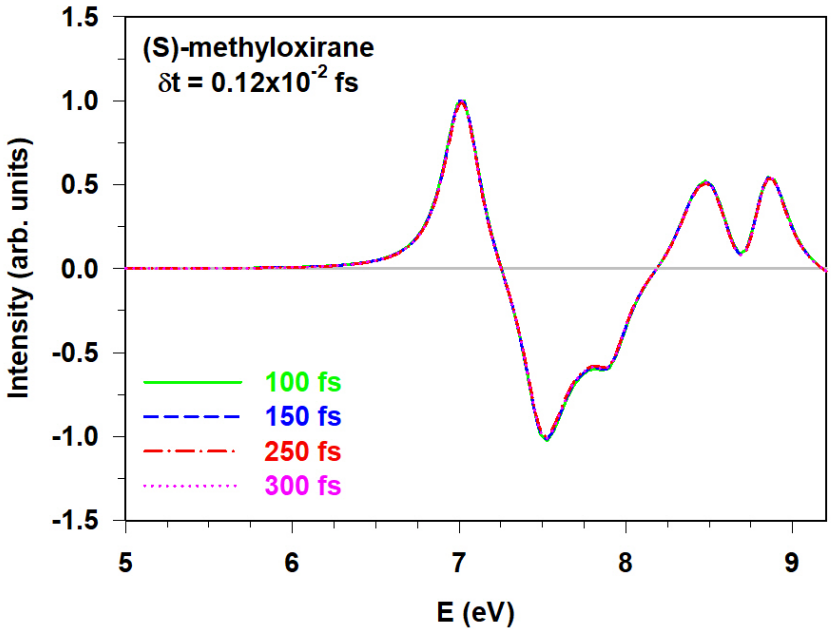

FIG. S2: Time-domain ECD spectra of (S)-methyloxirane calculated for 100 (solid green line), 150 (dashed blue line), 250 fs (dashed and dotted red line), and 300 (dotted pink line) fs with a time step δt of 0.12×10^{-2} fs.

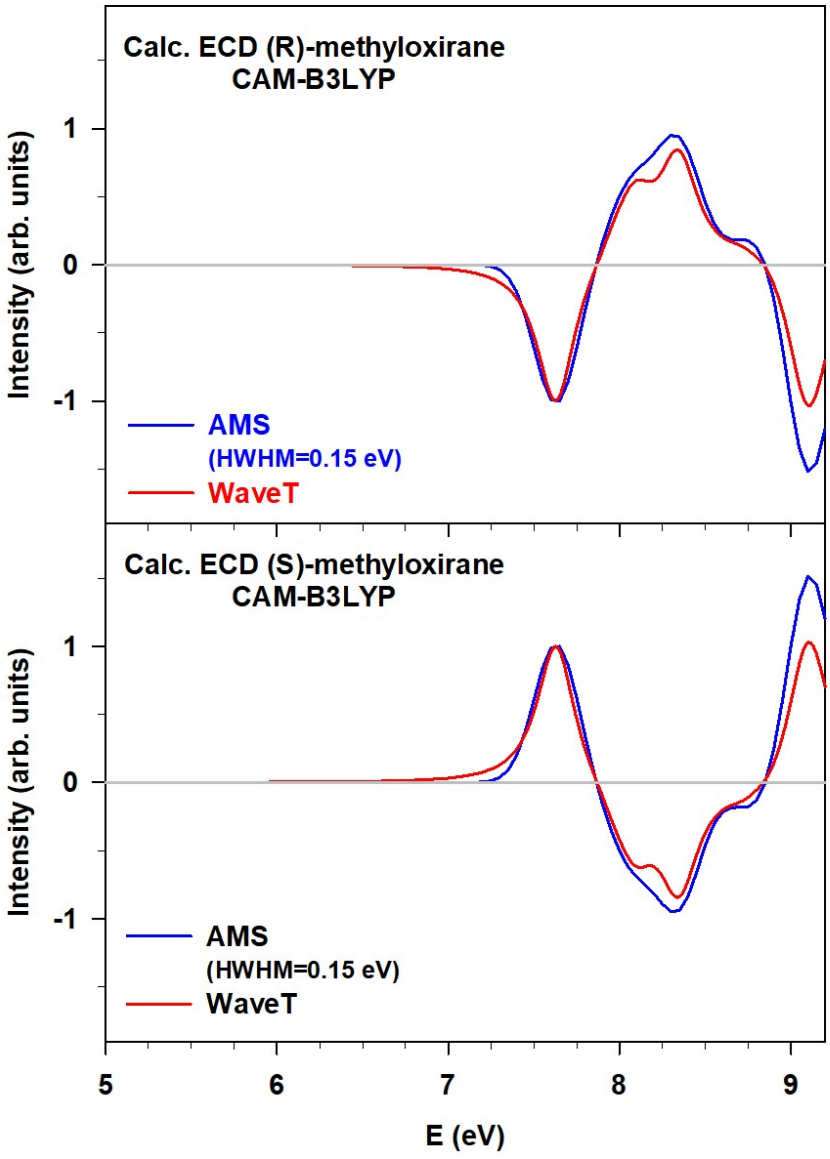

FIG. S3: Comparison of the ECD spectra calculated for the (R)-, (top panel) and (S)- (bottom panel) methyloxirane using the CAM-B3LYP functional and the AMS (frequency-domain, solid blue line) and WaveT (time-domain, solid red line) code. All the intensities have been normalized and reported in arbitrary units (arb. units).

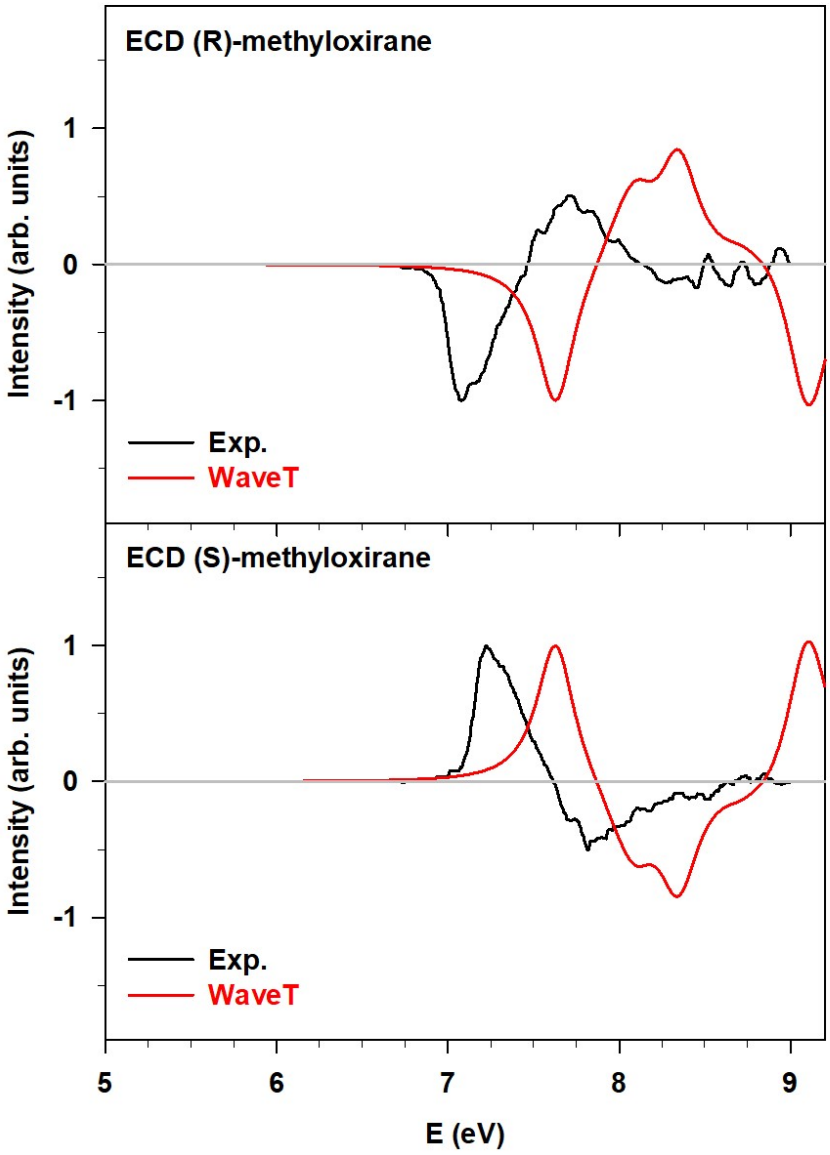

FIG. S4: Comparison between the experimental (solid black line) and calculated with WaveT (CAM-B3LYP) (solid red line) ECD spectra of the (R)-, (top panel) and (S)- (bottom panel) methyloxirane. All the intensities have been normalized and reported in arbitrary units (arb. units).

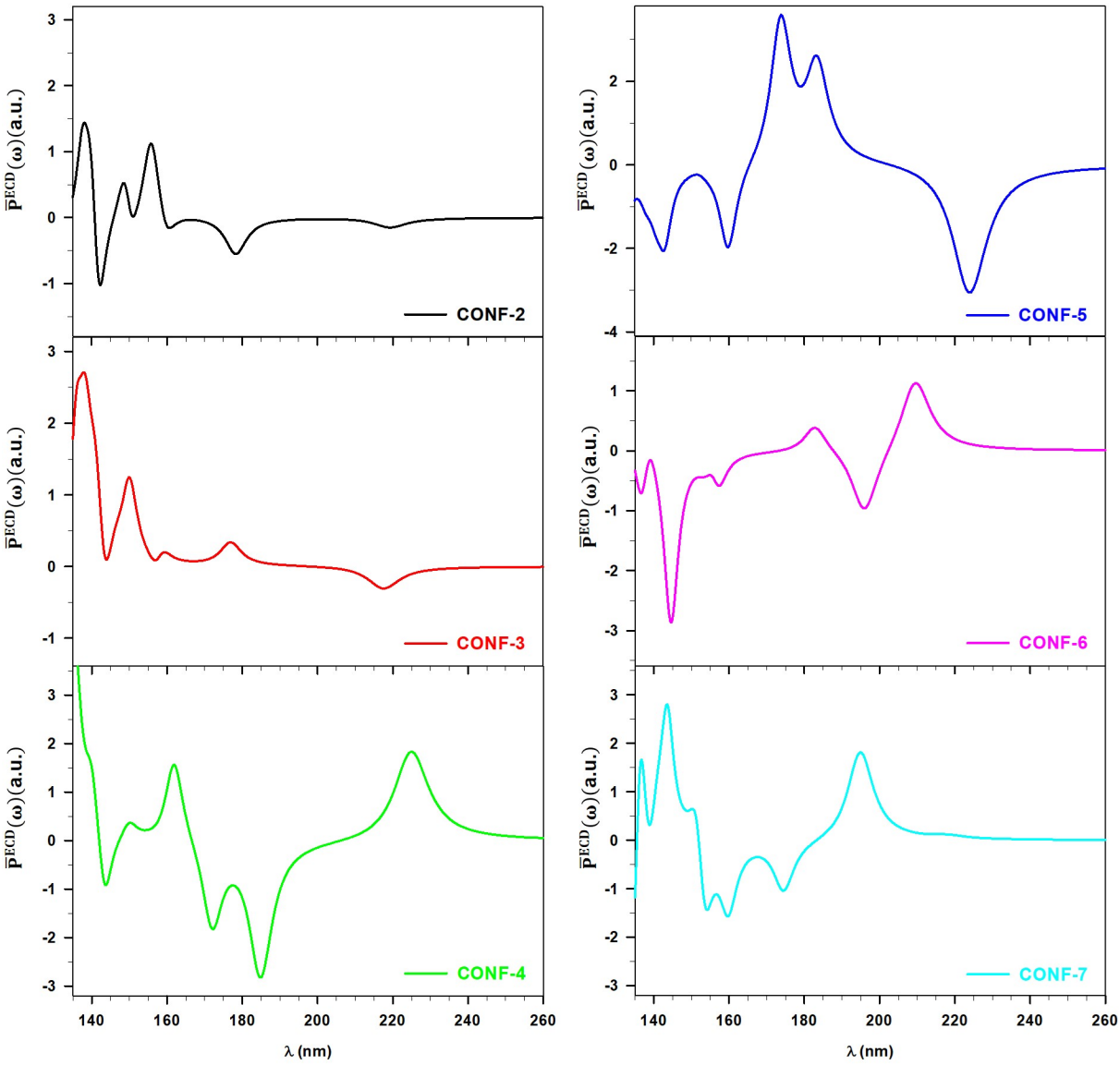

FIG. S5: Individual time-domain ECD spectra for the L-alanine higher-energy conformers (from 2 to 7). All the intensities have been reported in atomic units (a.u.)

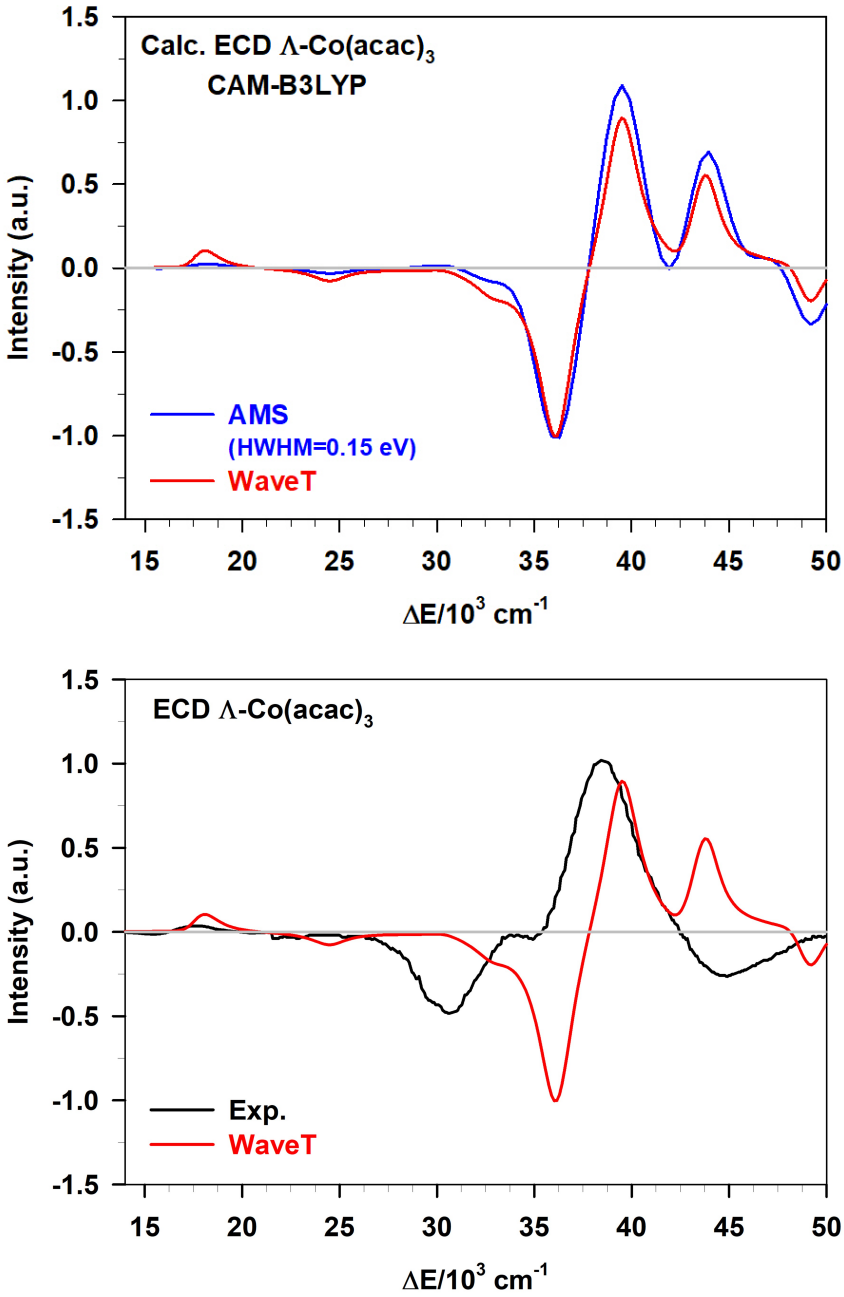

FIG. S6: Top panel: Comparison of the ECD spectra calculated for the Λ-Co(acac)$_3$ using the CAM-B3LYP functional and the AMS (frequency-domain, solid blue line) or WaveT (time-domain, solid red line) code. Bottom panel: Comparison between the experimental (solid black line) and calculated with WaveT (CAM-B3LYP) (solid red line) ECD spectra of Λ-Co(acac)$_3$. All the intensities have been normalized and reported in arbitrary units (arb. units).

[1] C. Meinert, A. D. Garcia, J. Topin, N. C. Jones, M. Diekmann, R. Berger, L. Nahon, S. V. Hoffman, and U. J. Meierhenrich, Nat. Commun. **13**, 502 (2022).