Electronic Supplementary Information:

A complex-polarization-propagator protocol for magneto-chiral axial dichroism and birefringence dispersion

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We collect here the results of the basis set study of the electronic circular dichroism, magnetic circular dichroism, magneto-chiral dichroism, optical rotatory dispersion, magnetic optical rotation dispersion and magneto-chiral birefringence dispersion in the resonant frequency regions of R-methyloxirane and L-alanine at the Hartree-Fock, B3LYP and CAMB3LYP levels of theory. Tables collecting excitation energies, oscillator strangths and rotatory strenths for the first ten excitations for all three systems and methods, plus a plot illustrating the dependence on the choice of gauge-origin of the magneto-chiral dicroism of R-methyloxirane, are also included.

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I. R-METHYLOXIRANE

TABLE I. Excitation energies, oscillator strengths (f) and rotatory strengths (R) for the first 10 excitations of R-methyloxirane. Hartree–Fock and TD-DFT results in the t-aug-cc-pVDZ basis set.

	Hartree–Fock				CAMB3LYP				B3LYP			
No.	ω_i, eV	λ, nm	f	R	ω_i, eV	λ, nm	f	R	ω_i, eV	λ, nm	f	R
1	8.831	140.4	0.0026	−1.009	7.101	174.6	0.0075	−14.047	6.442	192.5	0.0092	−16.326
2	8.980	138.1	0.0068	4.706	7.365	168.3	0.0169	−8.042	6.836	181.4	0.0068	7.493
3	9.214	134.6	0.0457	−19.796	7.515	165.0	0.0134	8.717	6.866	180.6	0.0221	−2.007
4	9.265	133.8	0.0326	−10.746	7.671	161.6	0.0160	6.089	6.899	179.7	0.0040	5.471
5	9.366	132.4	0.0198	−4.041	7.851	157.9	0.0053	9.508	7.214	171.9	0.0005	−1.080
6	9.514	130.3	0.0130	−12.327	8.244	150.4	0.0090	−9.597	7.273	170.5	0.0007	0.616
7	9.648	128.5	0.0075	10.261	8.279	149.8	0.0147	9.733	7.280	170.3	0.0012	−0.250
8	9.870	125.6	0.0347	6.773	8.309	149.2	0.0260	−10.258	7.284	170.2	0.0009	0.911
9	9.997	124.0	0.0030	−2.728	8.349	148.5	0.0042	0.74	7.302	169.8	0.0056	6.634
10	10.160	122.0	0.0305	7.693	8.373	148.1	0.0103	−5.869	7.313	169.5	0.0001	0.243

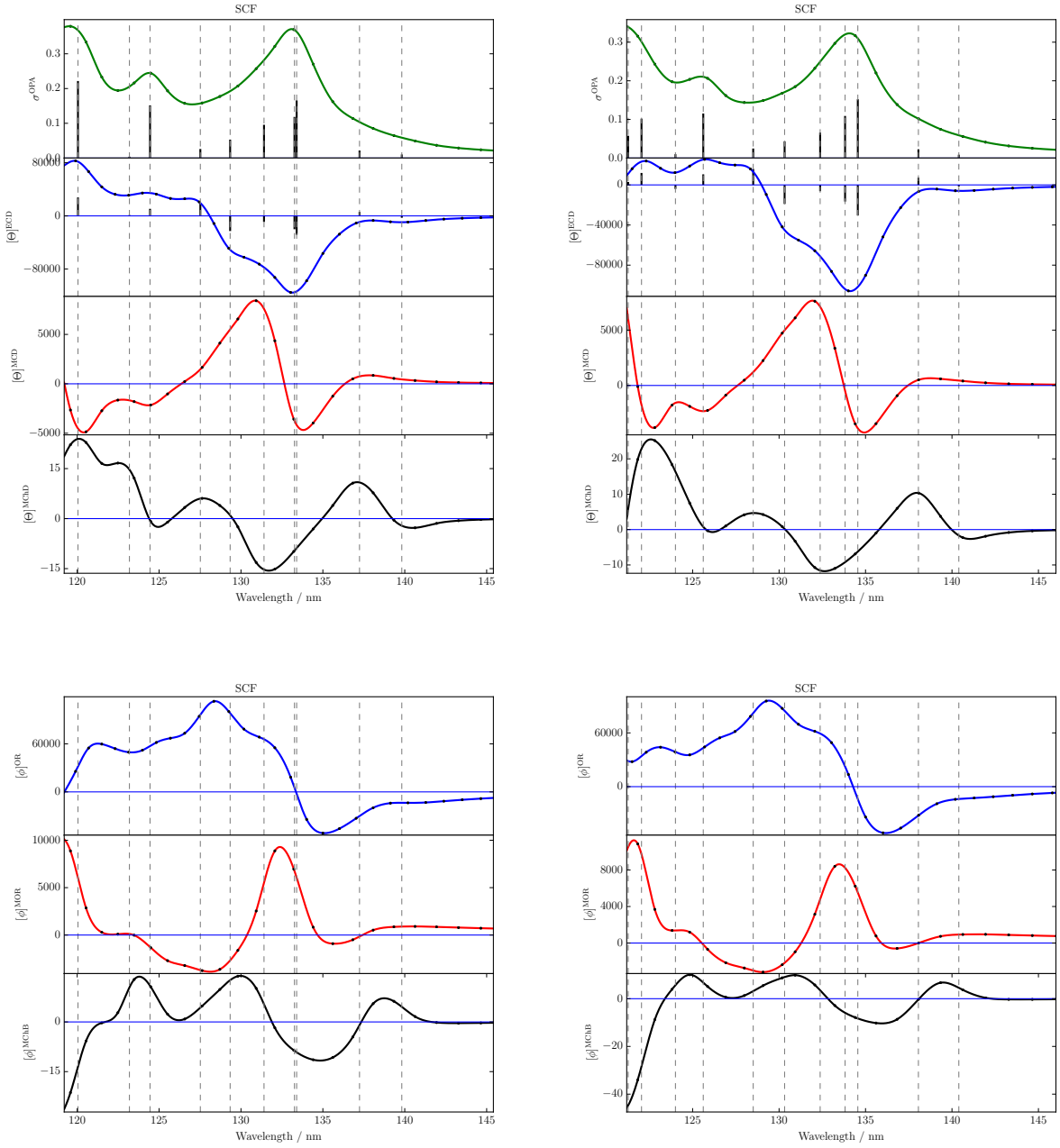

FIG. 1. R-Methyloxirane. Upper panels: One Photon Absorption (OPA) cross sections, Electronic Circular Dichroism (ECD), Magnetic Circular Dichroism (MCD) and Magneto-chiral Dichroism (MChD) calculated at the Hartree-Fock level for basis set aug-cc-pVDZ (left) and d-aug-cc-pVDZ (right). Lower panels: Natural Optical Rotatory (OR), Magnetic Optical Rotation (MOR) and Magneto-chiral Birefringence (MChB) dispersions calculated at the calculated acalculated at the Hartree-Fock level for basis set aug-cc-pVDZ (left) and d-aug-cc-pVDZ (right). Absorption cross sections are given in atomic units.

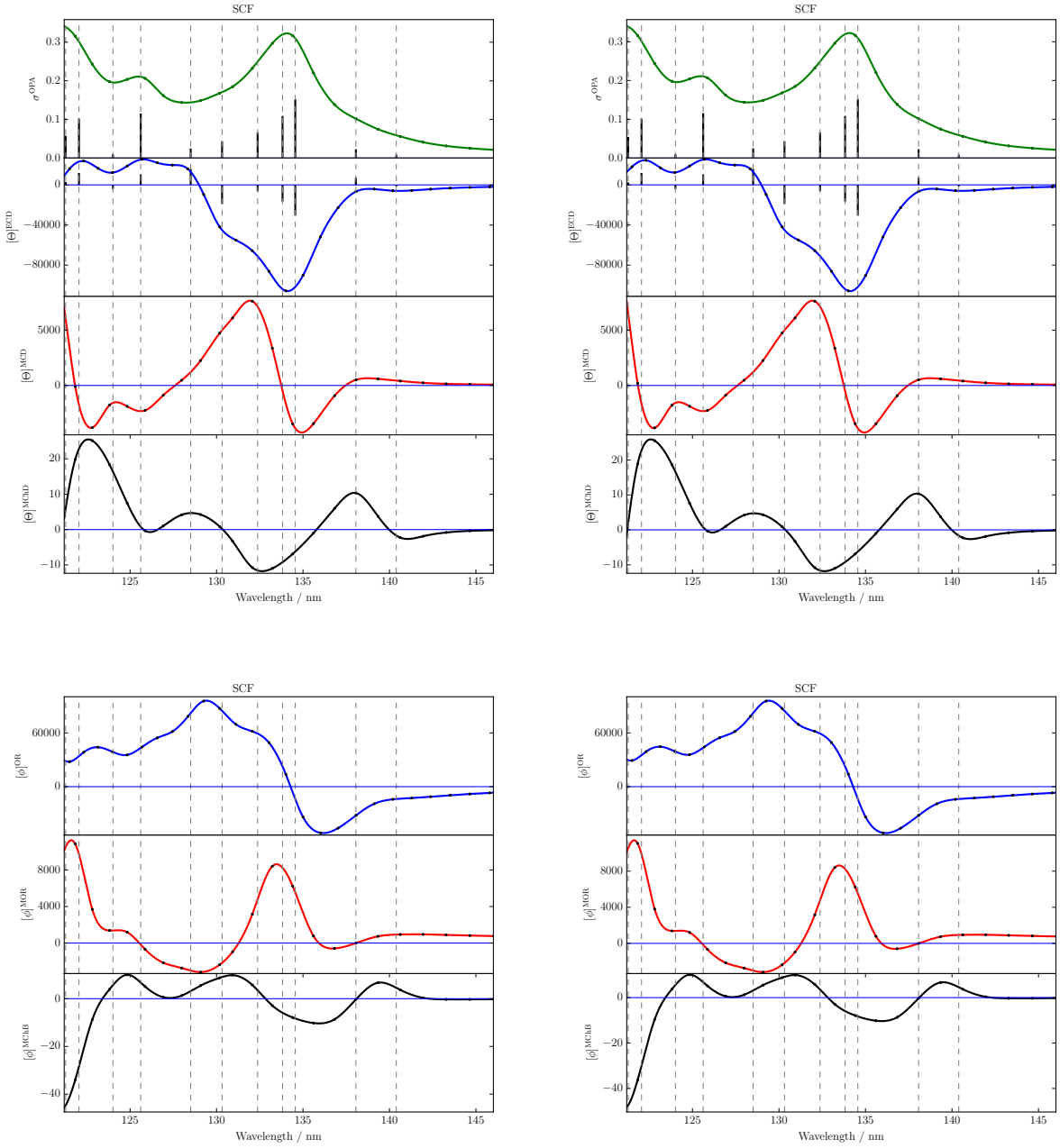

FIG. 2. R-Methyloxirane. Upper panels: One Photon Absorption (OPA) cross sections, Electronic Circular Dichroism (ECD), Magnetic Circular Dichroism (MCD) and Magneto-chiral Dichroism (MChD) calculated at the Hartree-Fock level for basis set d-aug-cc-pVDZ (left) and t-aug-cc-pVDZ (right). Lower panels: Natural Optical Rotatory (OR), Magnetic Optical Rotation (MOR) and Magneto-chiral Birefringence (MChB) dispersions calculated at the calculated at the Hartree-Fock level for basis set d-aug-cc-pVDZ (left) and t-aug-cc-pVDZ (right).

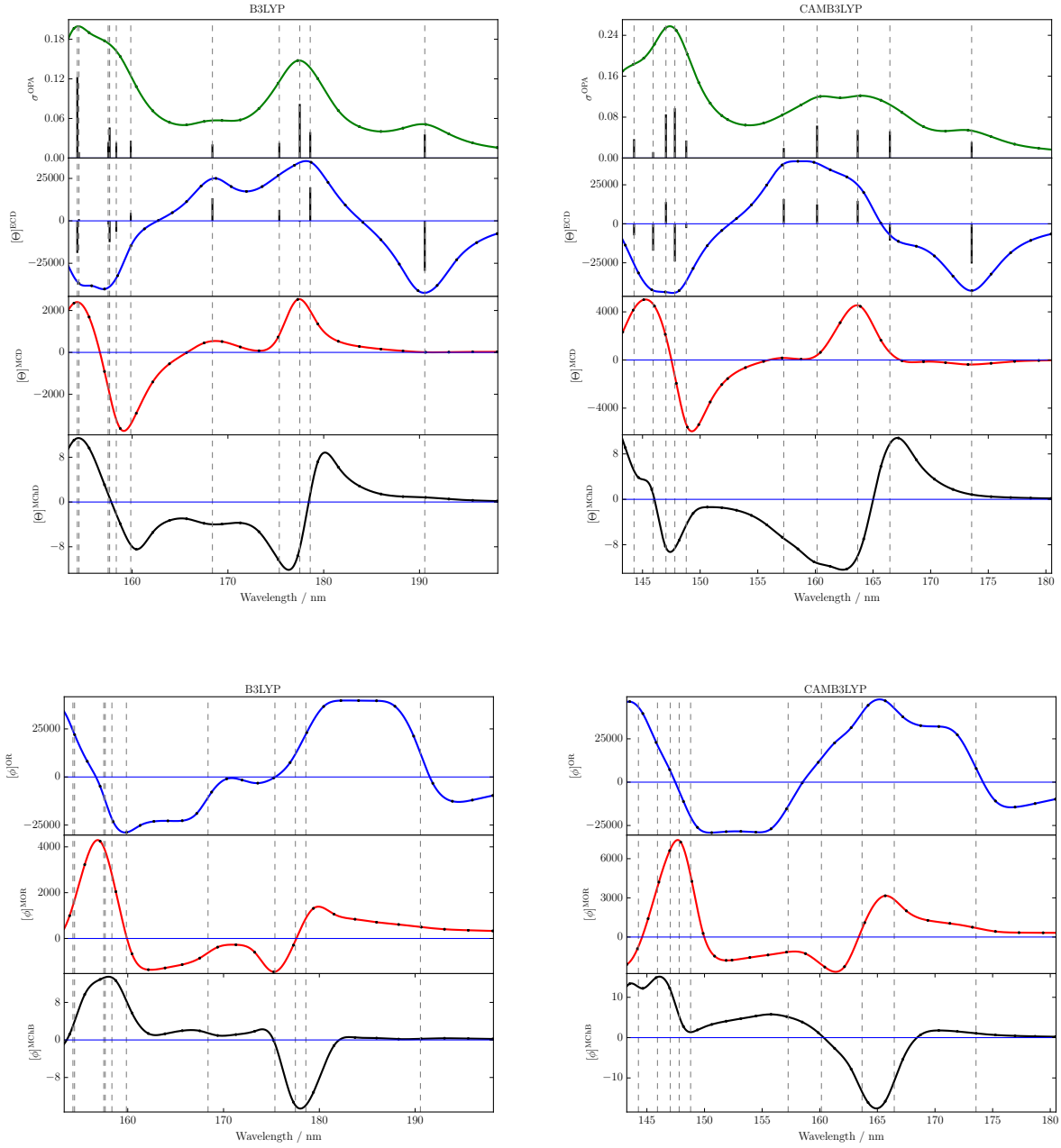

FIG. 3. R-Methyloxirane. Upper panels: One Photon Absorption (OPA) cross sections, Electronic Circular Dichroism (ECD), Magnetic Circular Dichroism (MCD) and Magneto-chiral Dichroism (MChD) calculated at the B3LYP/aug-cc-pVDZ (left) and CAMB3LYP/aug-cc-pVDZ (right) levels. Lower panels: Natural Optical Rotatory (OR), Magnetic Optical Rotation (MOR) and Magneto-chiral Birefringence (MChB) dispersions calculated at the B3LYP/aug-cc-pVDZ (left) and CAMB3LYP/aug-cc-pVDZ (right) levels.

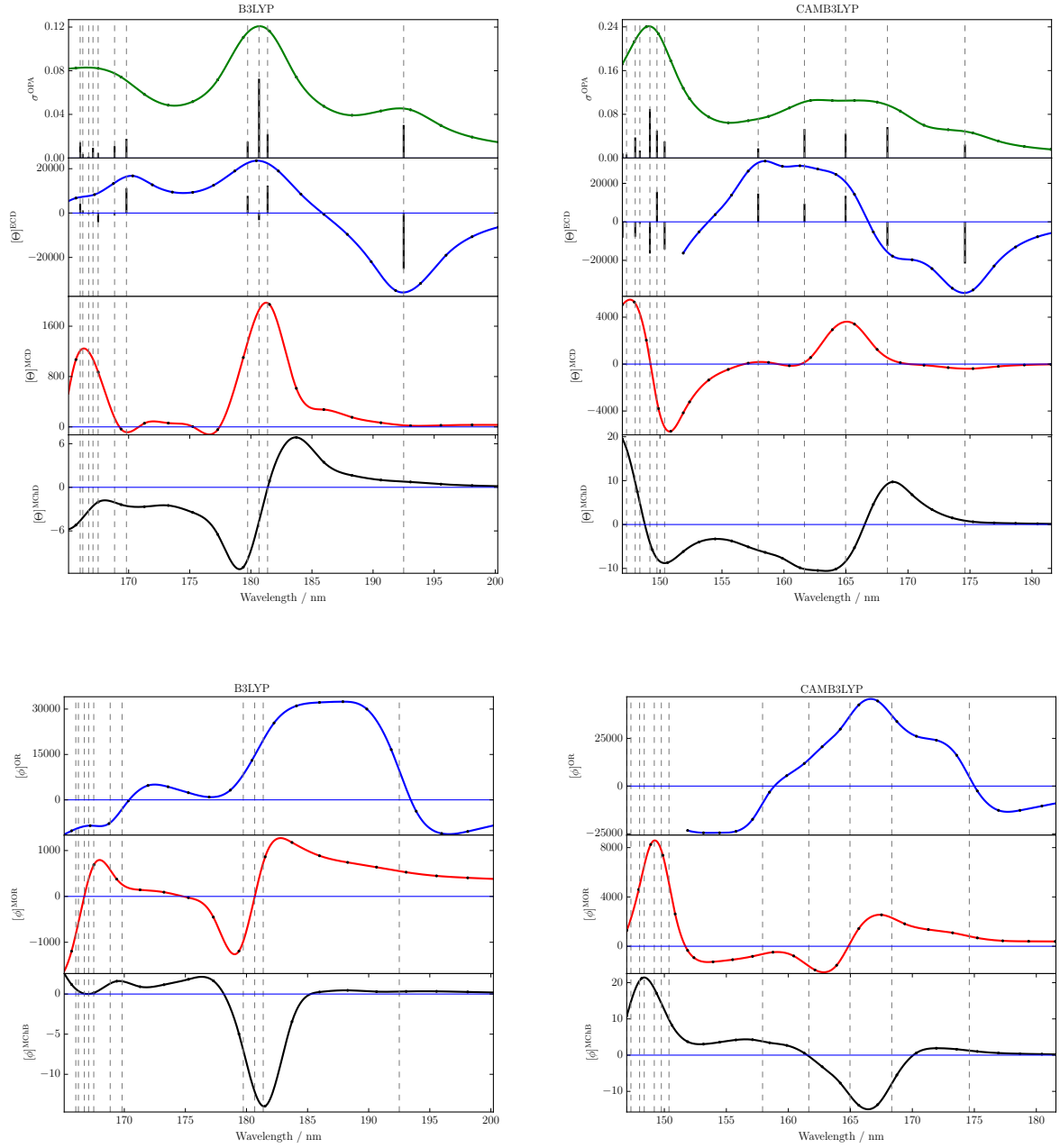

FIG. 4. R-Methyloxirane. Upper panels: One Photon Absorption (OPA) cross sections, Electronic Circular Dichroism (ECD), Magnetic Circular Dichroism (MCD) and Magneto-chiral Dichroism (MChD) calculated at the B3LYP/d-aug-cc-pVDZ (left) and CAMB3LYP/d-aug-cc-pVDZ (right) levels. Lower panels: Natural Optical Rotatory (OR), Magnetic Optical Rotation (MOR) and Magneto-chiral Birefringence (MChB) dispersions calculated at the B3LYP/d-aug-cc-pVDZ (left) and CAMB3LYP/d-aug-cc-pVDZ (right) levels.

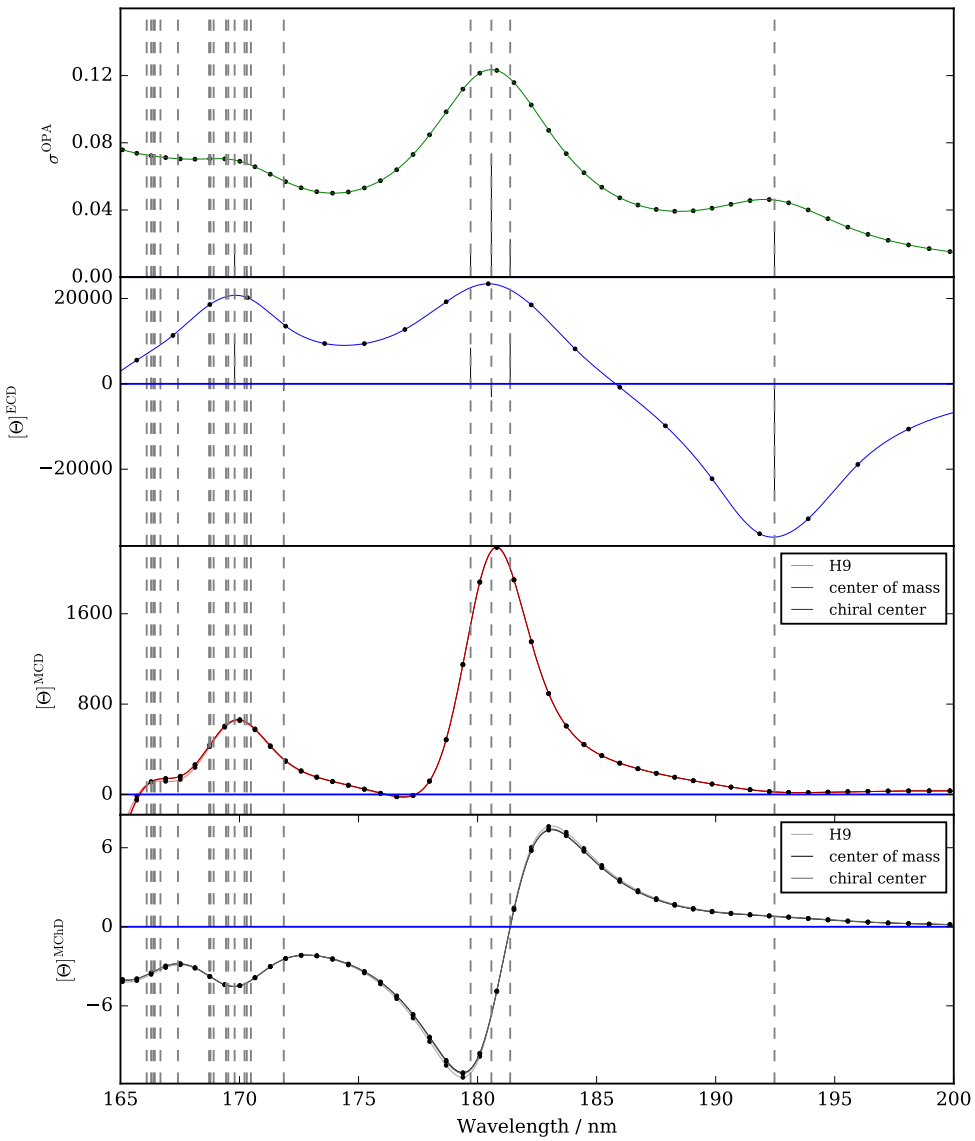

FIG. 5. R-Methyloxirane. One Photon Absorption (OPA) cross sections, Electronic Circular Dichroism (ECD), Magnetic Circular Dichroism (MCD) and Magneto-chiral Dichroism (MChD) calculated at the B3LYP/t-aug-cc-pVDZ level. Dependence of the MCD and MChD spectra on the choice of gauge-origin. H9 is the hydrogen atom positioned furthest away from the center of mass.

II. L-ALANINE

TABLE II. L-Alanine, conformer I. Excitation energies, oscillator strengths (f) and rotatory strengths (R) for the first 10 excitations. Hartree–Fock and TD-DFT results in the t-aug-cc-pVDZ basis set. Ionisation potentials according to Koopmans' theorem: B3LYP = 7.12 eV; CAMB3LYP=8.92 eV; SCF=11.24 eV

	Hartree–Fock				CAMB3LYP				B3LYP			
No.	ω_i, eV	λ, nm	f	R	ω_i, eV	λ, nm	f	R	ω_i, eV	λ, nm	f	R
1	6.625	187.1	0.0016	8.218	5.806	213.5	0.0012	7.65	5.591	221.8	0.0024	7.249
2	7.760	159.8	0.0214	−2.045	6.363	194.9	0.0123	−1.519	5.870	211.2	0.0046	−7.145
3	8.654	143.3	0.0105	1.091	6.664	186.1	0.0025	1.518	5.972	207.6	0.0012	7.463
4	8.875	139.7	0.0336	12.43	7.070	175.4	0.0763	−13.15	6.323	196.1	0.0605	−3.580
5	8.918	139.0	0.0622	−38.31	7.171	172.9	0.0076	−2.206	6.527	190.0	0.0018	−0.928
6	9.324	133.0	0.0273	2.183	7.394	167.7	0.0062	−0.637	6.644	186.6	0.0106	3.214
7	9.404	131.8	0.0353	9.016	7.524	164.8	0.0077	1.751	6.694	185.2	0.0162	−9.533
8	9.525	130.2	0.0766	−4.452	7.856	157.8	0.0073	−0.374	6.900	179.7	0.0003	−0.481
9	9.546	129.9	0.0004	−0.775	7.951	155.9	0.0053	5.397	6.956	178.2	0.0006	0.109
10	9.641	128.6	0.0053	−1.803	7.979	155.4	0.0016	0.294	6.976	177.7	0.0001	−0.045

TABLE III. L-Alanine, conformer IIA. Excitation energies, oscillator strengths (f) and rotatory strengths R for the first 10 excitations. Hartree–Fock and TD-DFT results in the t-aug-cc-pVDZ basis set. Ionisation potentials according to Koopmanns theorem: B3LYP = 7.27 eV; CAMB3LYP= 9.08 eV; SCF=11.54 eV

	Hartree–Fock				CAMB3LYP				B3LYP			
No.	ω_i, eV	λ, nm	f	R	ω_i, eV	λ, nm	f	R	ω_i, eV	λ, nm	f	R
1	6.4805	191.3	0.0015	1.759	5.664	218.9	0.0010	3.967	5.536	224.0	0.0014	11.68
2	7.8523	157.9	0.0166	1.634	6.420	193.1	0.0098	−4.790	5.759	215.3	0.0106	−12.91
3	8.8477	140.1	0.0412	−9.635	7.124	174.0	0.0402	4.835	6.559	189.0	0.0008	−2.827
4	9.0465	137.0	0.0055	12.44	7.374	168.1	0.0015	−1.924	6.602	187.8	0.0296	2.747
5	9.1889	134.9	0.0614	−16.92	7.505	165.2	0.0100	−11.31	6.704	184.9	0.0014	−2.127
6	9.2661	133.8	0.1258	8.618	7.593	163.3	0.0126	−9.311	6.772	183.1	0.0128	−9.692
7	9.5483	129.8	0.0096	2.867	7.817	158.6	0.0093	−5.362	7.010	176.9	0.0009	−0.422
8	9.6668	128.2	0.0202	−16.92	7.973	155.5	0.0040	−2.759	7.069	175.4	0.0074	−6.236
9	9.6709	128.2	0.0004	2.49	8.053	154.0	0.0003	−0.604	7.110	174.4	0.0003	−0.432
10	9.8265	126.2	0.0085	5.183	8.106	153.0	0.0006	0.964	7.124	174.0	0.0001	−0.069

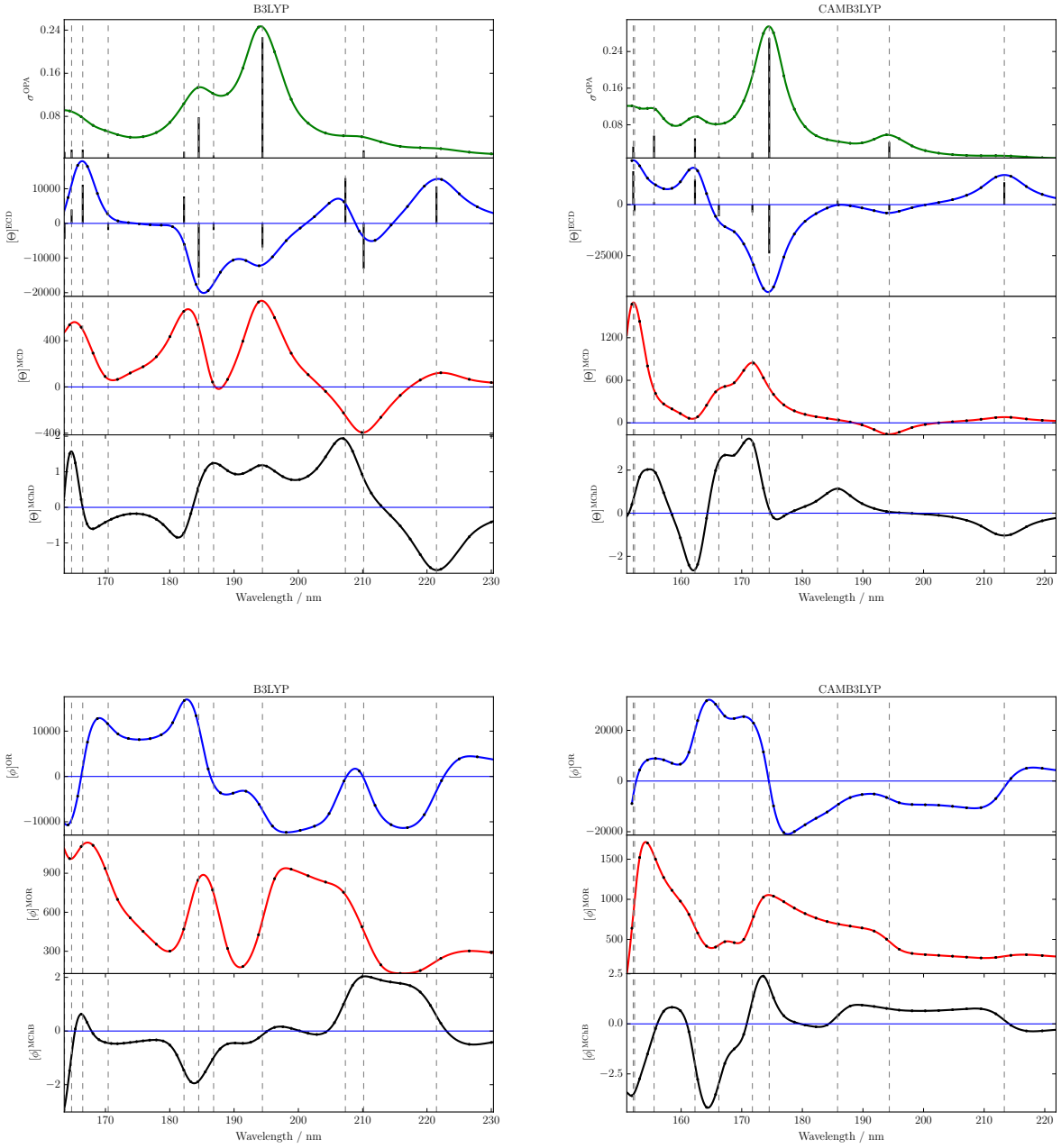

FIG. 6. L-Alanine, conformer I. Upper panels: One Photon Absorption (OPA) cross sections, Electronic Circular Dichroism (ECD), Magnetic Circular Dichroism (MCD) and Magneto-chiral Dichroism (MChD), calculated at the B3LYP/aug-cc-pVDZ (left) and CAMB3LYP/aug-cc-pVDZ (right) levels. Lower panels: Natural Optical Rotatory (OR), Magnetic Optical Rotation (MOR) and Magneto-chiral Birefringence (MChB) dispersions, calculated at B3LYP/aug-cc-pVDZ (left) and CAMB3LYP/aug-cc-pVDZ (right) levels.

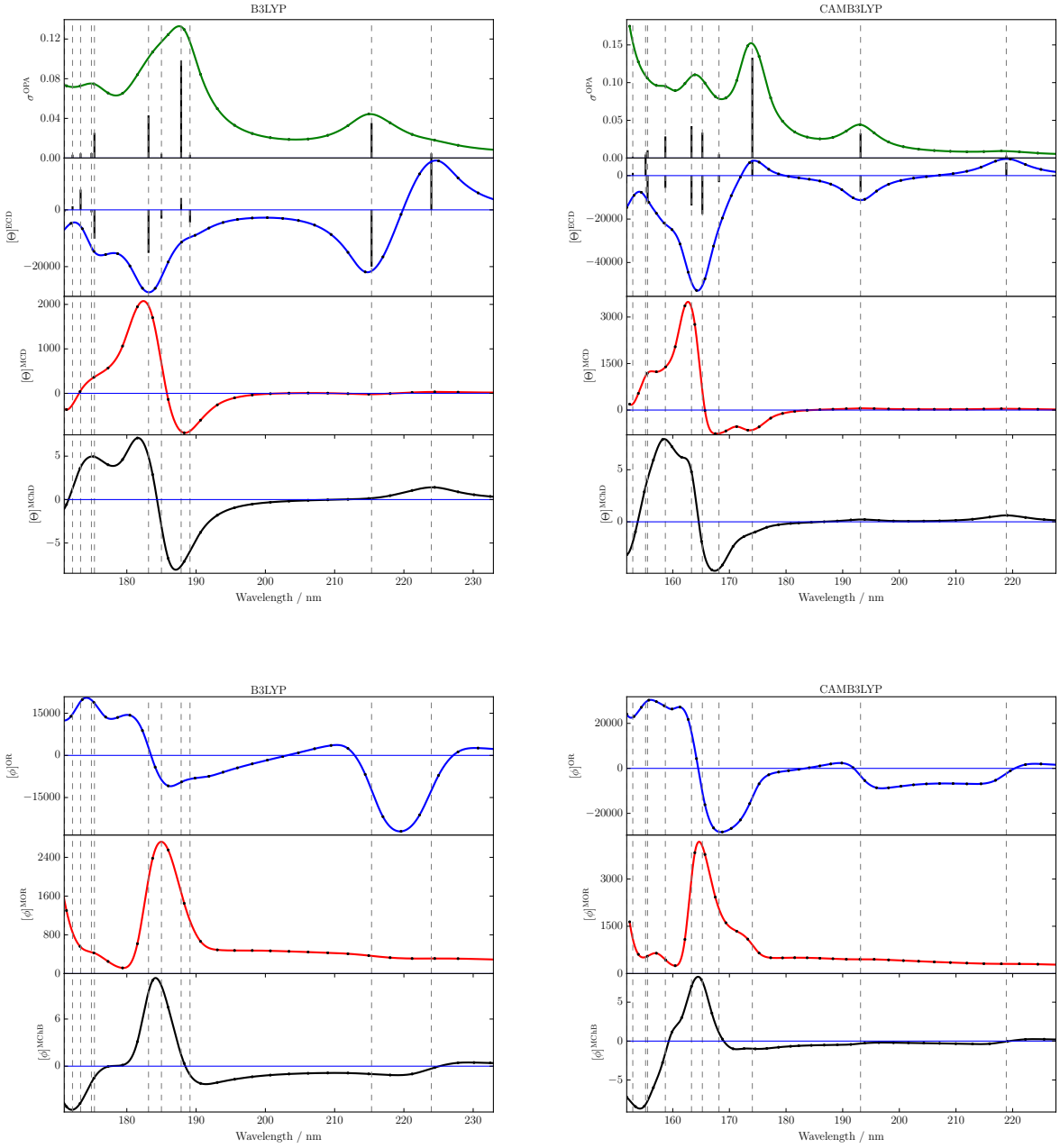

FIG. 7. L-Alanine, conformer IIA. Upper panels: One Photon Absorption (OPA) cross section, Electronic Circular Dichroism (ECD), Magnetic Circular Dichroism (MCD) and Magneto-chiral Dichroism (MChD), calculated at B3LYP/d-aug-cc-pVDZ (left) and CAMB3LYP/d-aug-cc-pVDZ (right) levels of theory. Lower panels: Natural Optical Rotatory (OR), Magnetic Optical Rotation (MOR) and Magneto-chiral Birefringence (MChB) dispersions, calculated at B3LYP/d-aug-cc-pVDZ (left) and CAMB3LYP/d-aug-cc-pVDZ (right) levels of theory.