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Supporting Information for

Aggregation of lactic acid in cold rare gas matrices and the link to solution: a matrix isolation–vibrational circular dichroism study

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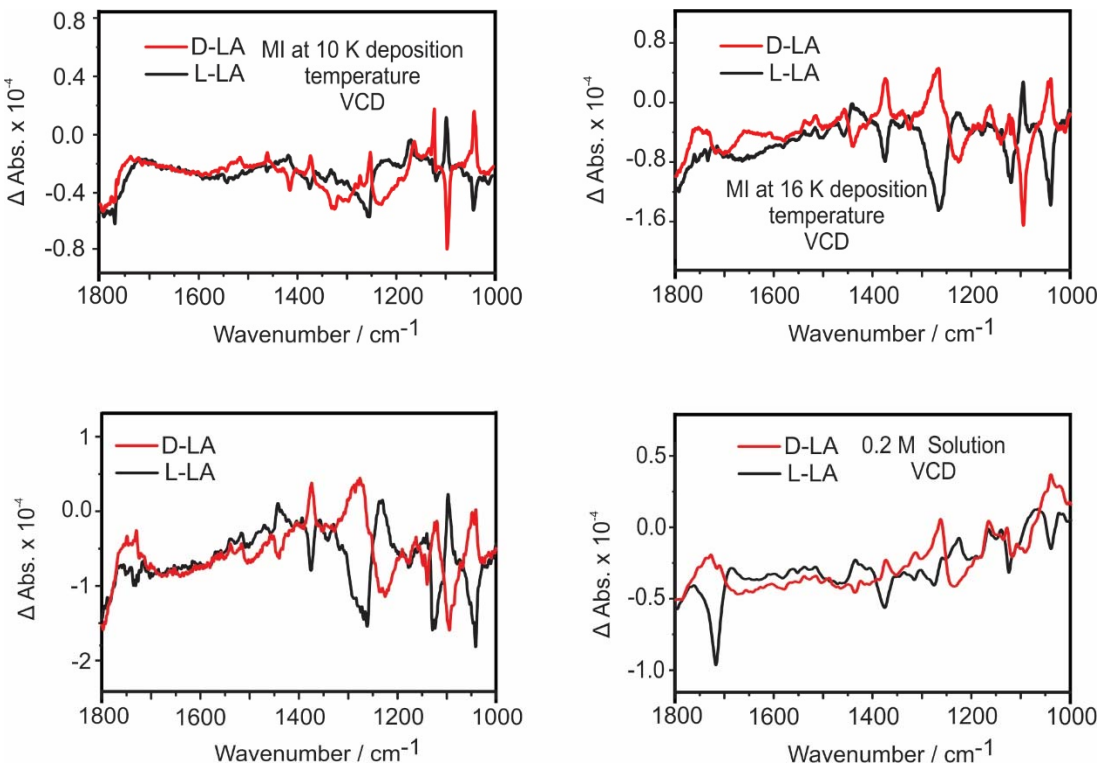

Figure S1. The raw, experimental VCD spectra of D-LA and L-LA in the cold Ar matrices at 10 K, 16 K and 24 K and in a 0.2 M solution in $CDCl_3$.

Table S1. Comparison of the relative energies (ΔE in kJ mol^{-1}) and Boltzmann factor (Bf in %) at 298 K of the LA monomer conformers computed at the B3LYP and B3LYP-D3BJ/6-311++G(2d,p) and the B3LYP-D3BJ/def2-TZVPD levels of theory.

Conf.	B3LYP/ 6-311++g(2d,p)		B3LYP-D3BJ/ 6-311++G(2d,p)		B3LYP-D3BJ/ def2-TZVPD	
	ΔE	Bf	ΔE	Bf	ΔE	Bf
M1	0.0 (0.0)[1]	95.0 (79.1)	0.0 (0.0)	94.9 (75.0)	0.0 (0.0)	95.1 (53.6)
M2	9.4 (8.0)	2.2 (3.2)	9.6 (8.2)	2.0 (2.7)	9.8 (6.3)	1.8 (1.9)
M3	9.9 (7.8)	1.8 (3.4)	9.8 (7.7)	1.9 (3.4)	10.0 (7.0)	1.7 (2.3)
M4	11.2 (4.2)	1.0 (14.4)	10.6 (3.4)	1.3 (18.9)	10.4 (7.0)	1.4 (39.5)

[1] The values in brackets are obtained with the PCM of $CDCl_3$ added to the calculations.

Table S2. Comparison of the relative energies (ΔE in kJ mol^{-1}) and Boltzmann factor (Bf in %) at 298 K[1] of the LA dimer conformers computed at the B3LYP and B3LYP-D3BJ/6-311++G(2d,p) and the B3LYP-D3BJ/def2-TZVPD levels of theory.

Dimer Conf.	B3LYP/ 6-311++g(2d,p)		B3LYP-D3BJ/ 6-311++G(2d,p)		B3LYP-D3BJ/ def2-TZVPD	
	ΔE	Bf	ΔE	Bf	ΔE	Bf
D1	0.0 (0.0)[2]	85.2 (79.5)	0.0 (0.0)	84.5 (78.8)	0.0 (0.0)	83.9 (78.4)
D2	6.2 (5.4)	7.0 (8.9)	6.2 (5.5)	6.8 (8.5)	6.1 (5.5)	7.1 (8.7)
D3	6.5 (5.5)	6.1 (8.5)	6.2 (5.3)	6.8 (9.4)	6.2 (5.2)	7.0 (9.6)
D4	12.1 (10.9)	0.6 (1.0)	12.2 (11.0)	0.6 (0.9)	11.9 (10.9)	0.6 (1.0)
D5	12.4 (10.7)	0.6 (1.1)	12.1 (10.5)	0.6 (1.1)	11.9 (10.4)	0.6 (1.2)
D6	12.9 (10.7)	0.5 (1.1)	12.3 (10.3)	0.6 (1.2)	12.2 (10.2)	0.5 (1.3)

[1] For the relevant cold matrix temperatures of 10, 16 and 24 K, only the most stable conformer D1 contributes dominantly to the experimental spectra. See text for discussion.
[2] The values in brackets are obtained with the PCM of $CDCl_3$ added to the calculations.

Table S3. Comparison of the relative free energies (ΔE in kJ mol^{-1}) and Boltzmann factor (Bf in %) at 298 K[1] of the LA trimers and tetramers computed at the B3LYP and B3LYP-D3BJ/6-311++G(2d,p) and the B3LYP-D3BJ/def2-TZVPD levels of theory.[2]

$(LA)_3$ &$(LA)_4$ Conf.	B3LYP/ 6-311++g(2d,p)		B3LYP-D3BJ/ 6-311++G(2d,p)		B3LYP-D3BJ/ def2-TZVPD	
	ΔE	Bf	ΔE	Bf	ΔE	Bf
T1	0.0 (0.0)[3]	52.4 (52.3)	0.0 (0.0)	62.2 (82.7)	0.0 (0.0)	63.4 (57.9)
T2	0.3 (0.2)	47.4 (47.6)	1.2 (3.9)	37.7 (17.2)	1.4 (1.2)	36.4 (35.2)
T3	14.3 (14.5)	0.2 (0.2)	18.1 (20.9)	0.0 (0.0)	18.1 (18.3)	0.0 (0.0)
Te1	0.0 (0.0)	38.2 (38.6)	0.0 (0.0)	49.6 (50.1)	0.0 (0.0)	51.5 (52.8)
Te2	0.5 (0.5)	31.7 (31.7)	1.1 (1.3)	31.2 (29.5)	1.3 (1.5)	30.5 (28.3)
Te3	0.6 (0.7)	30.4 (29.7)	2.4 (2.2)	19.2 (20.4)	2.6 (2.6)	18.0 (18.8)

[1] For the relevant cold matrix temperatures of 10, 16 and 24 K, only the most stable conformers T1 and Te1 contribute mostly to the experimental spectra at the B3LYP-D3BJ/def2-TZVPD level.
[2] Only the three conformers listed are included in the Boltzmann factor calculations for easy comparison among different levels of theory.
[3] The values in brackets are obtained with the PCM of $CDCl_3$ added to the calculations.

Table S4. The α[1] values of the C=O stretching modes of the most stable conformers of each LA species calculated.

Conf.	Vibrational Frequency (cm^{-1})	θ (°)
M1	1797.0	90.2
D1	1683.8	180.0
D1	1738.9	85
T1	1669.2	82.1
T1	1722.8	106.6
T1	1747.5	65.6
Te1	1662.8	0.0
Te1	1708.5	74.6
Te1	1737.1	180
Te1	1750.7	14.5

[1] α is defined as the angle between the electric and magnetic dipole transition moment vectors.

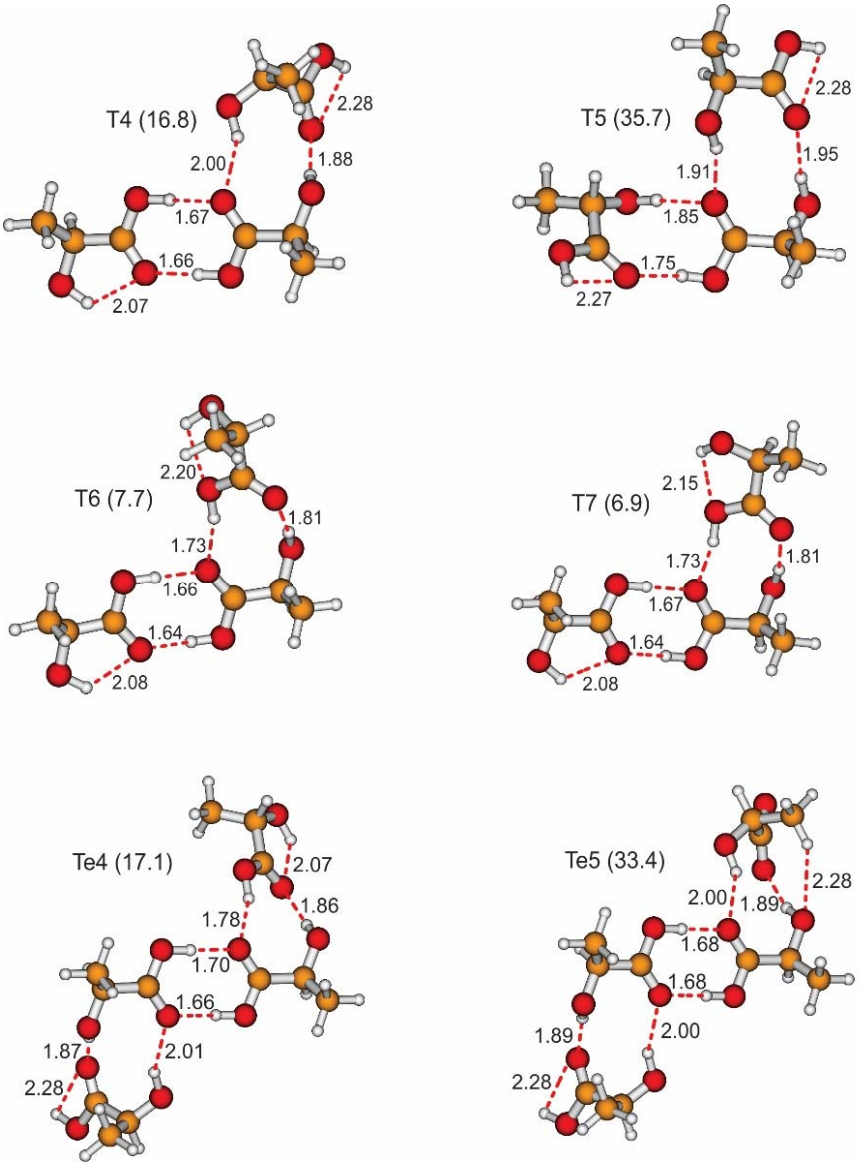

Figure S2. Geometries of the additional conformers of the LA trimer and tetramer in the gas phase. The relative free energy values in $kJmol^{-1}$ at the B3LYP-D3BJ/def2-TZPVD level of theory are indicated in brackets.

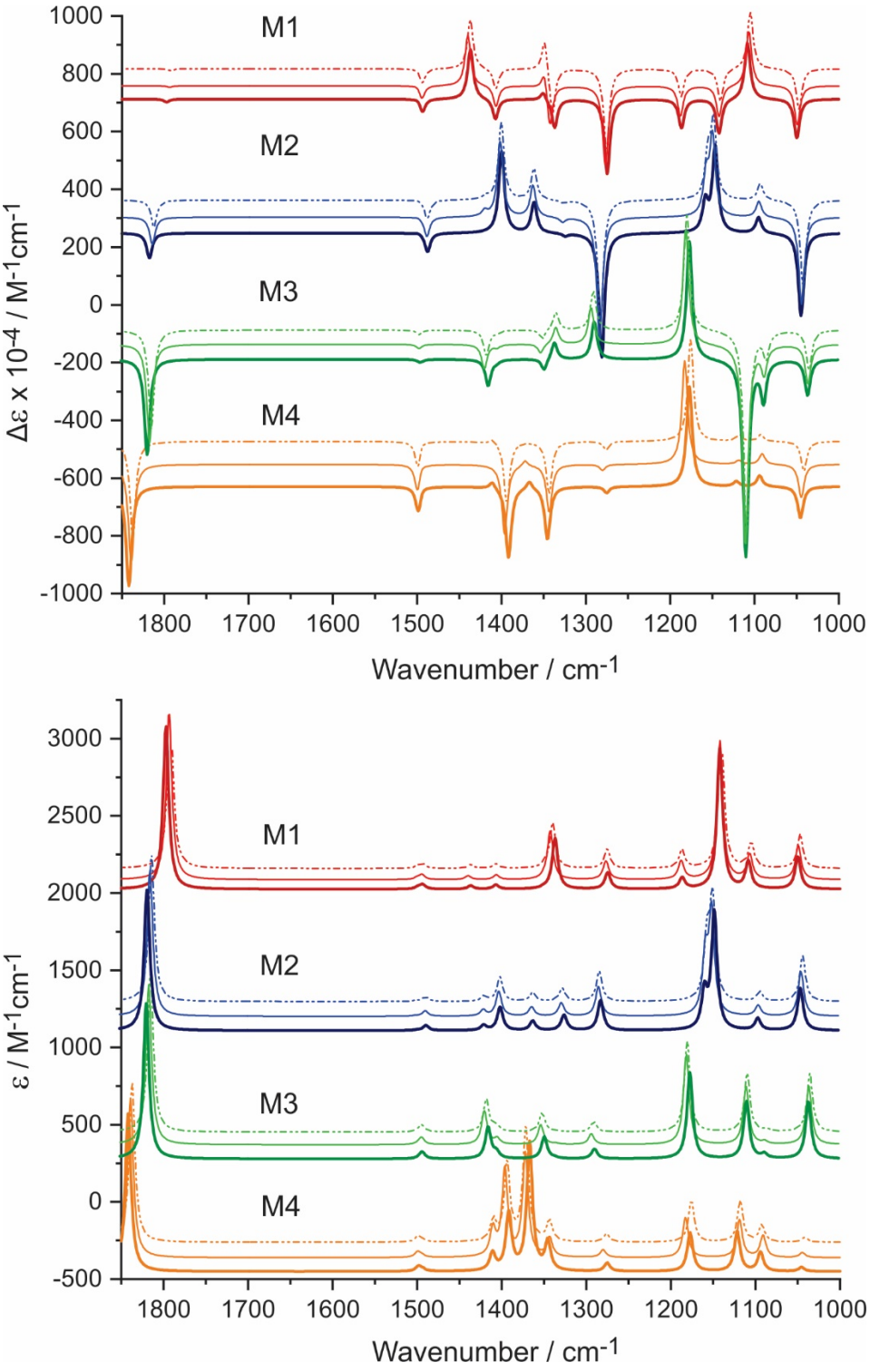

Figure S3. Predicted IR and VCD spectra of the four most stable conformers of the LA monomer in the gas phase at the B3LYP and B3LYP-D3BJ/6-311++G(2d,p) and the B3LYP-D3BJ/def2-TZVPD levels of theory from top to bottom.

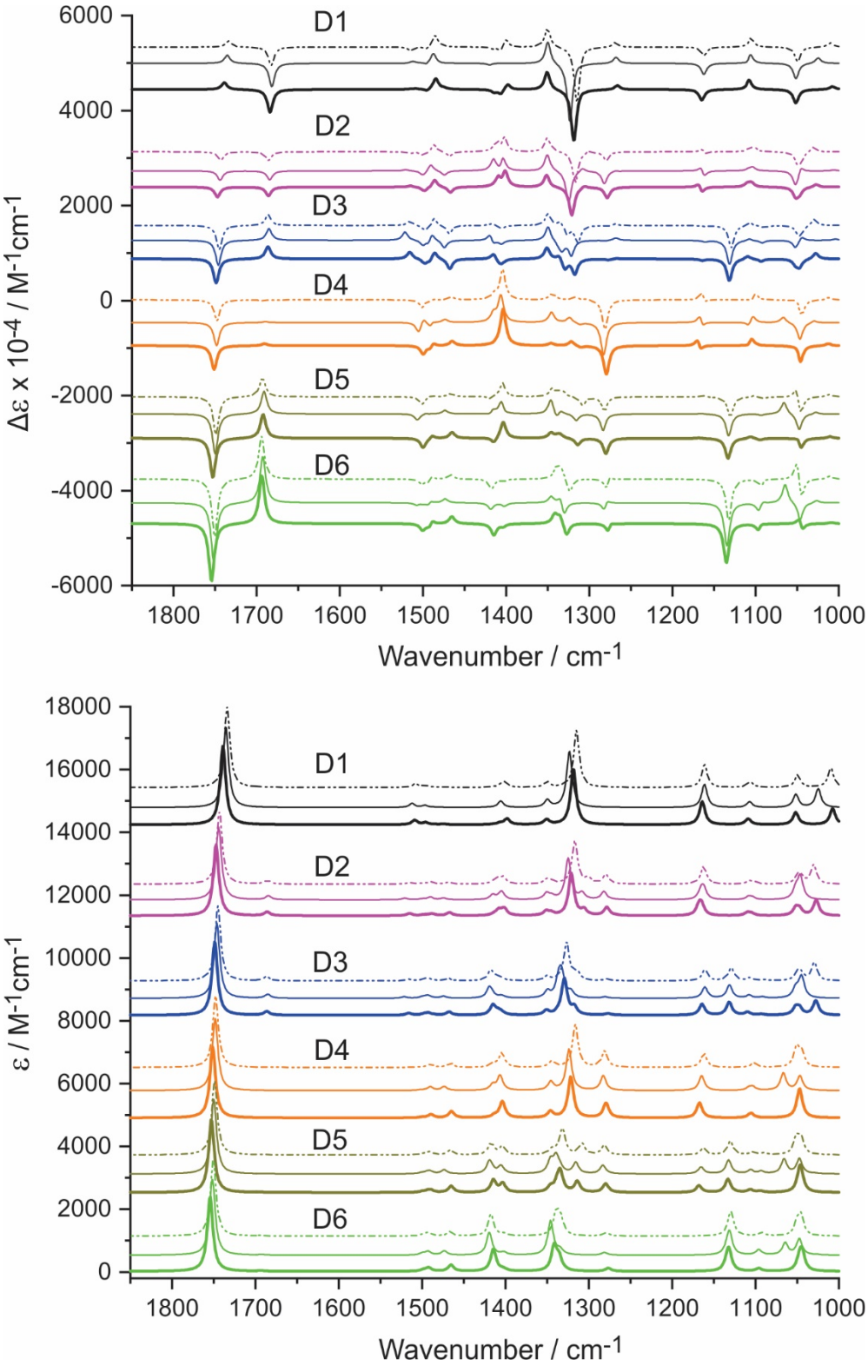

Figure S4. Predicted IR and VCD spectra of the six most stable conformers of the LA dimer in the gas phase at the B3LYP and B3LYP-D3BJ/6-311++G(2d,p) and the B3LYP-D3BJ/def2-TZVPD levels of theory from top to bottom.

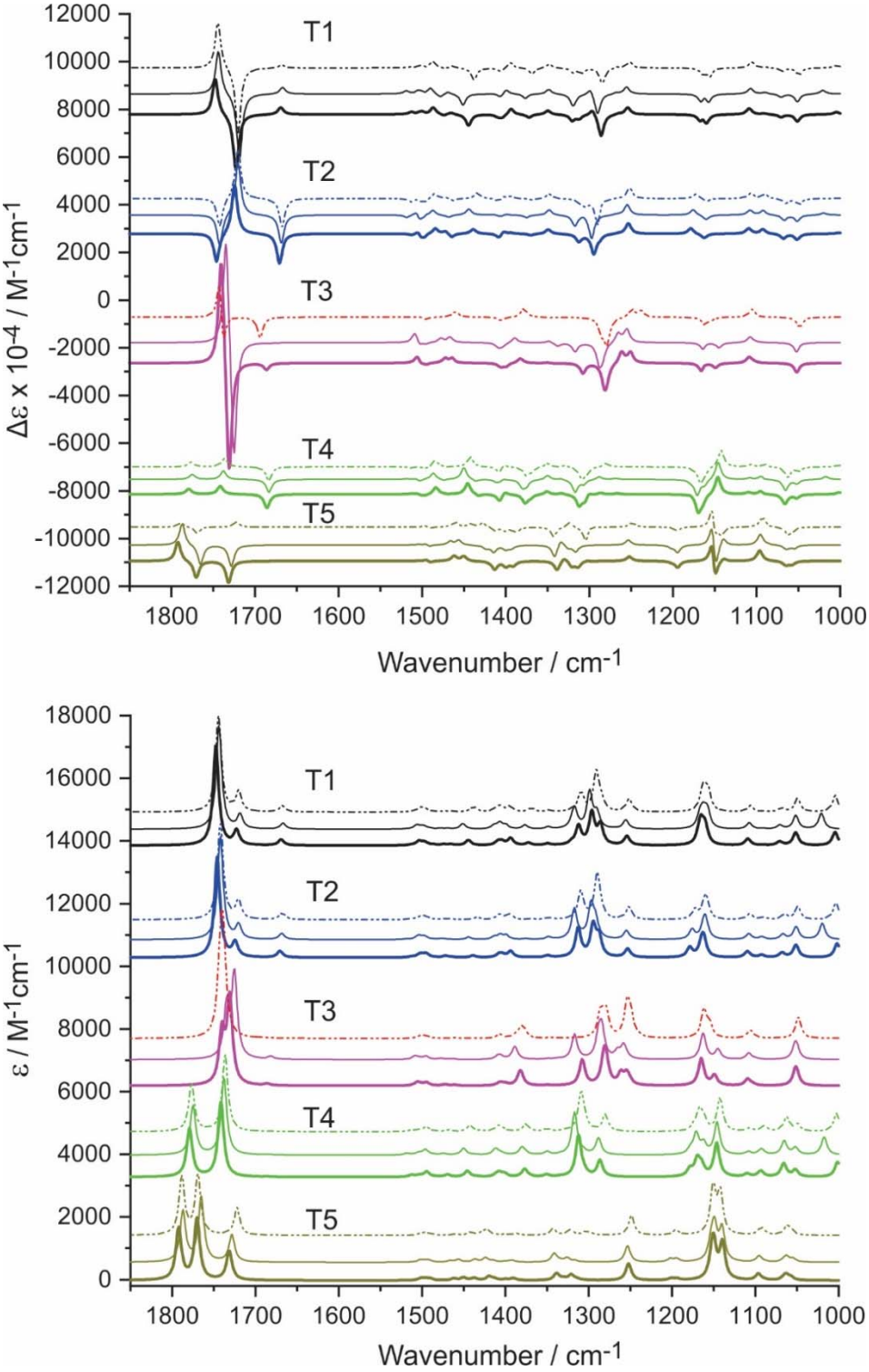

Figure S5. Predicted IR and VCD spectra of the five stable conformers of the LA trimer in the gas phase at the B3LYP and B3LYP-D3BJ/6-311++G(2d,p) and the B3LYP-D3BJ/def2-TZVPD levels of theory from top to bottom.

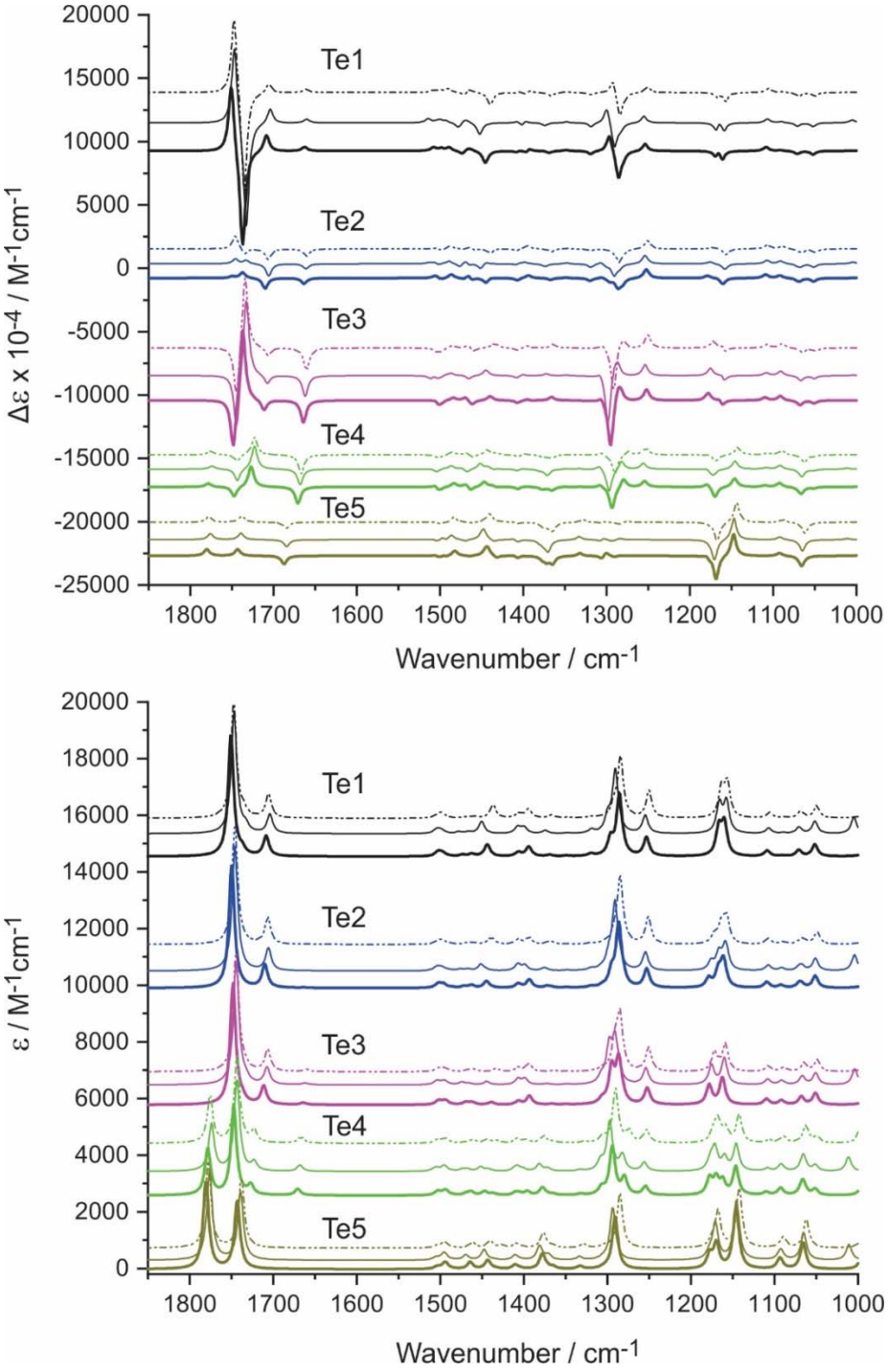

Figure S6. Predicted IR and VCD spectra of the five stable conformers of the LA tetramer in the gas phase at the B3LYP and B3LYP-D3BJ/6-311++G(2d,p) and the B3LYP-D3BJ/def2-TZVPD levels of theory from top to bottom.

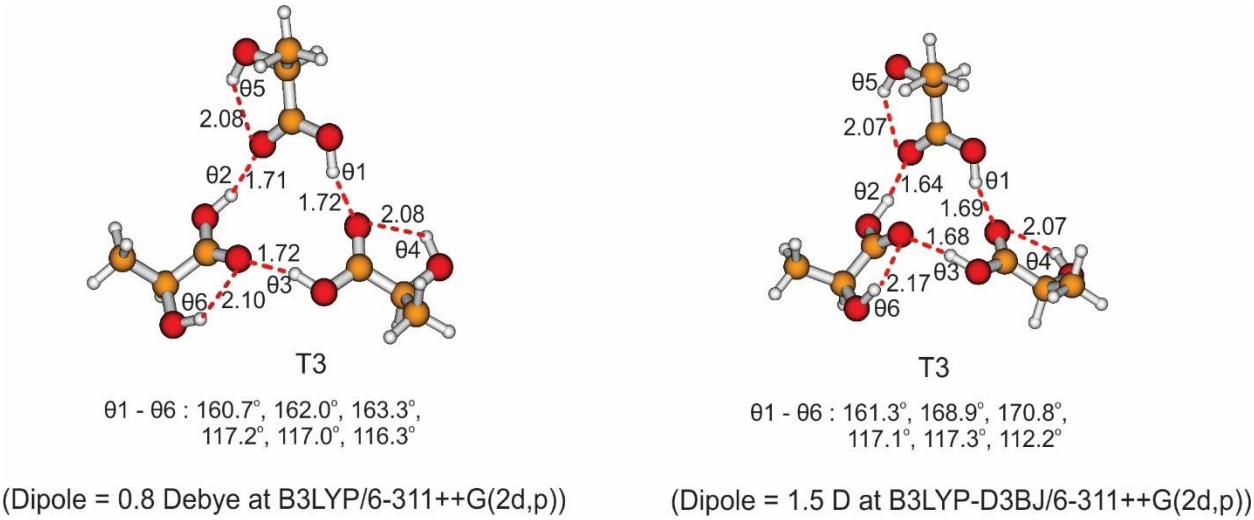

Figure S7. Optimized geometries of T3 in the gas phase obtained with and without the dispersion correction (D3BJ) with the basis set 6-311++G(2d,p). The optimized geometry obtained at the B3LYP-D3BJ/def2-TZVPD level is very similar to that at the B3LYP-D3BJ/6311++G(2d,p) and the dipole moment is 1.4 D.

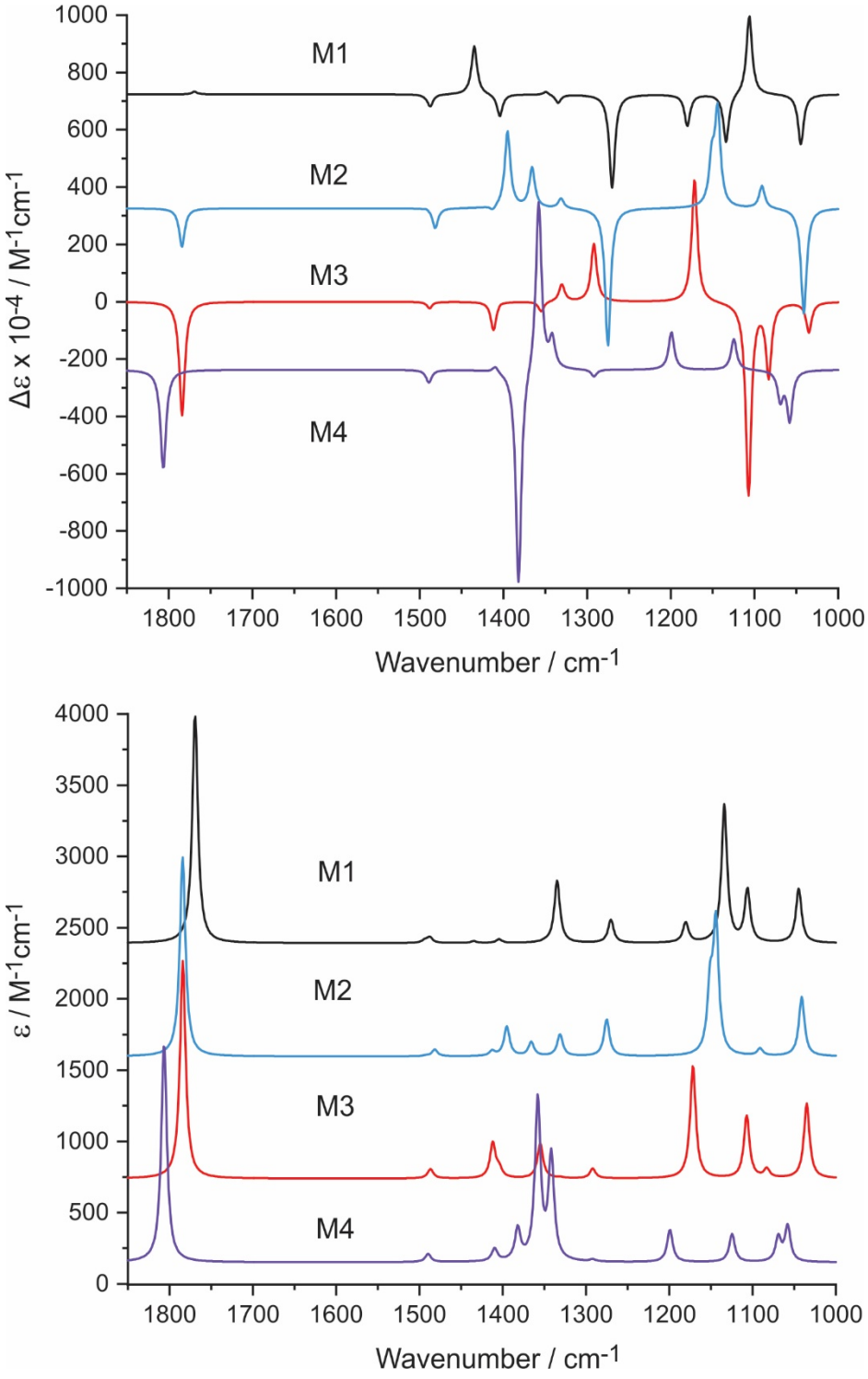

Figure S8. Predicted IR and VCD spectra of the four most stable conformers of the LA monomer in the PCM of $CDCl_3$ at the B3LYP-D3BJ/def2-TZVPD level of theory.

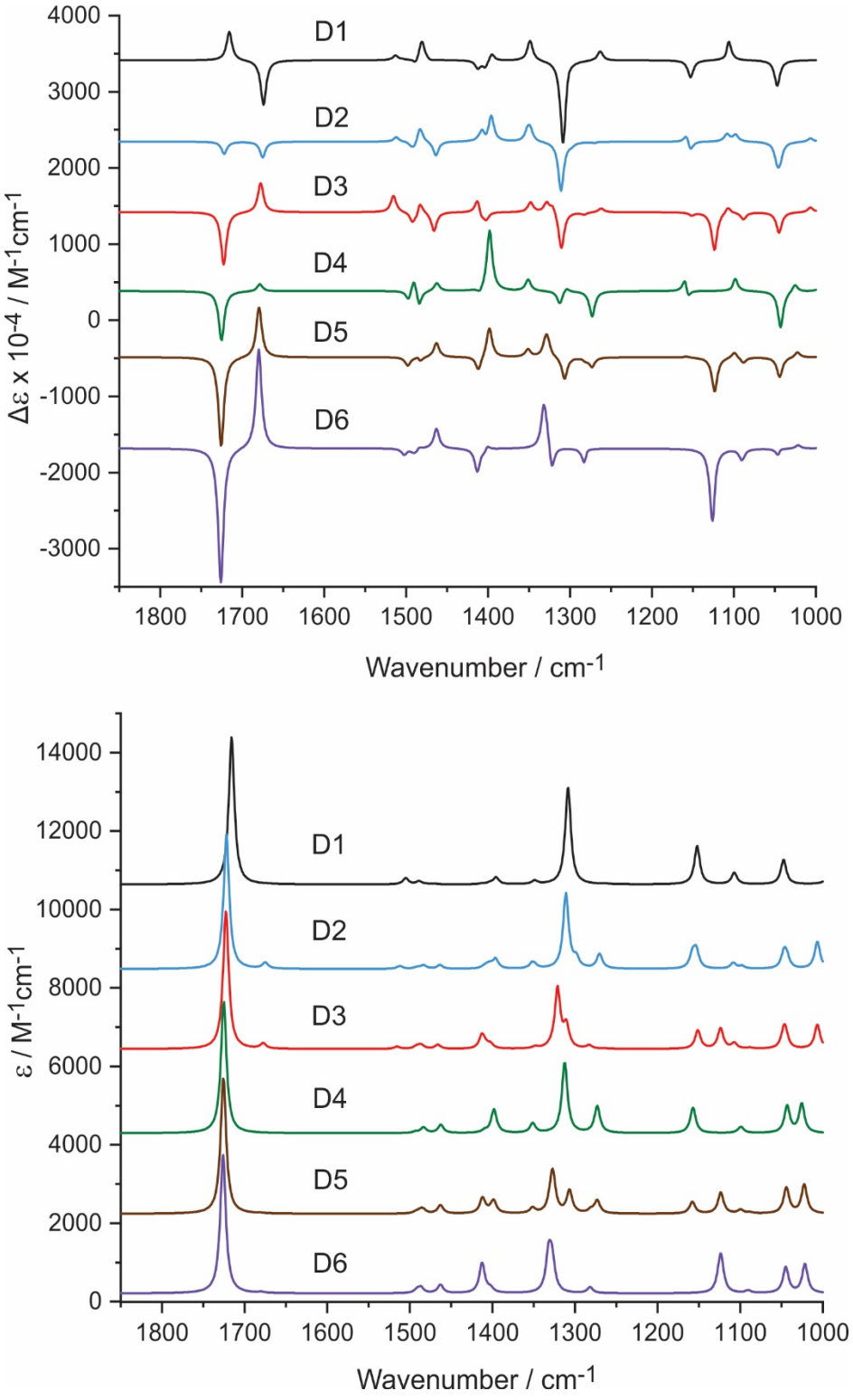

Figure S9. Predicted IR and VCD spectra of the six most stable conformers of the LA dimer in the PCM of $CDCl_3$ at the B3LYP-D3BJ/def2-TZVPD level of theory.

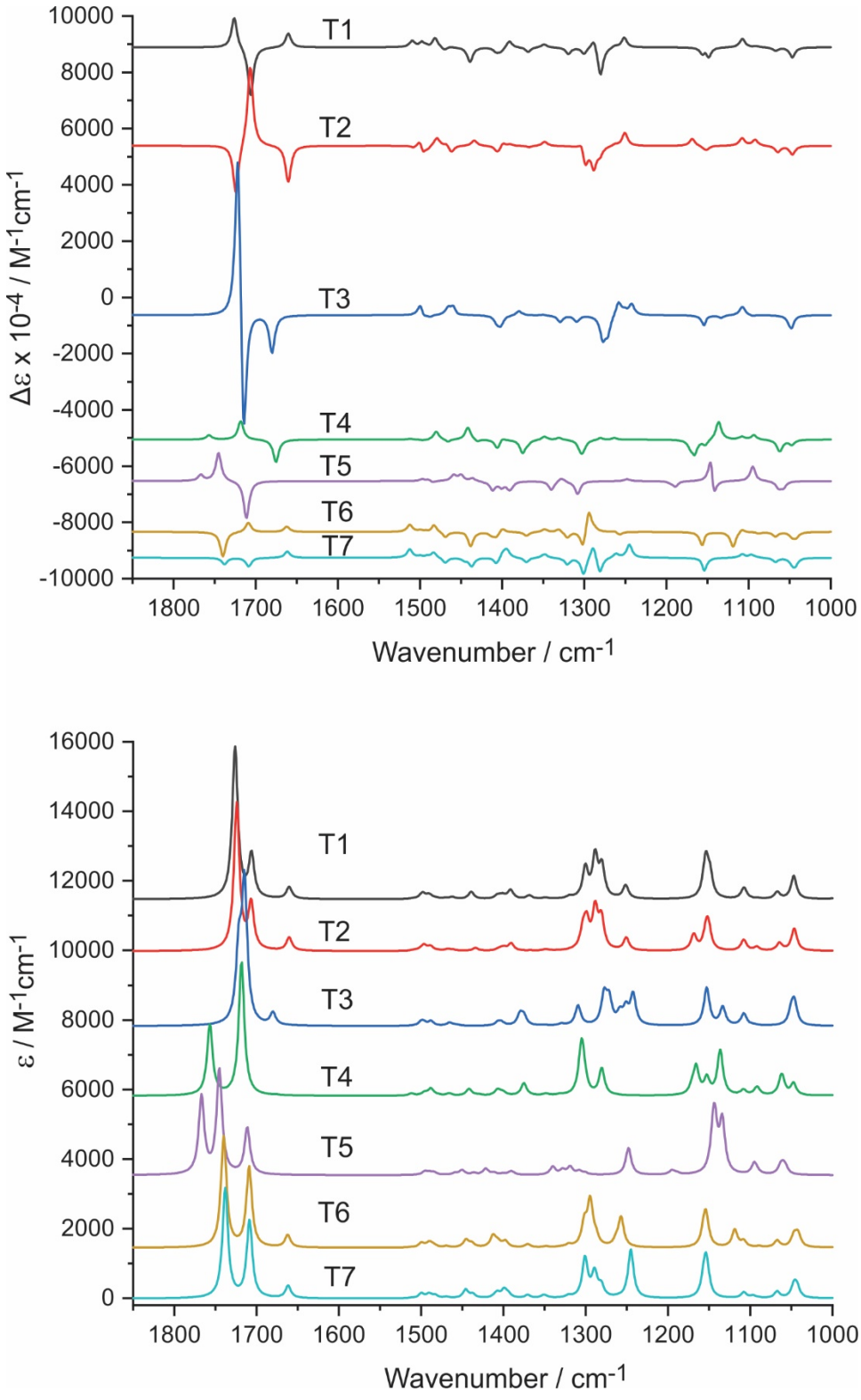

Figure S10. Predicted IR and VCD spectra of the seven $(LA)_3$ conformers in the PCM of $CDCl_3$ at the B3LYP-D3BJ/def2-TZVPD level of theory. The Boltzmann factors for T1-T7 (in %) at 298 K are: 60.9, 28.9, 0.2, 0.2, 0.0, 3.4, and 6.4.

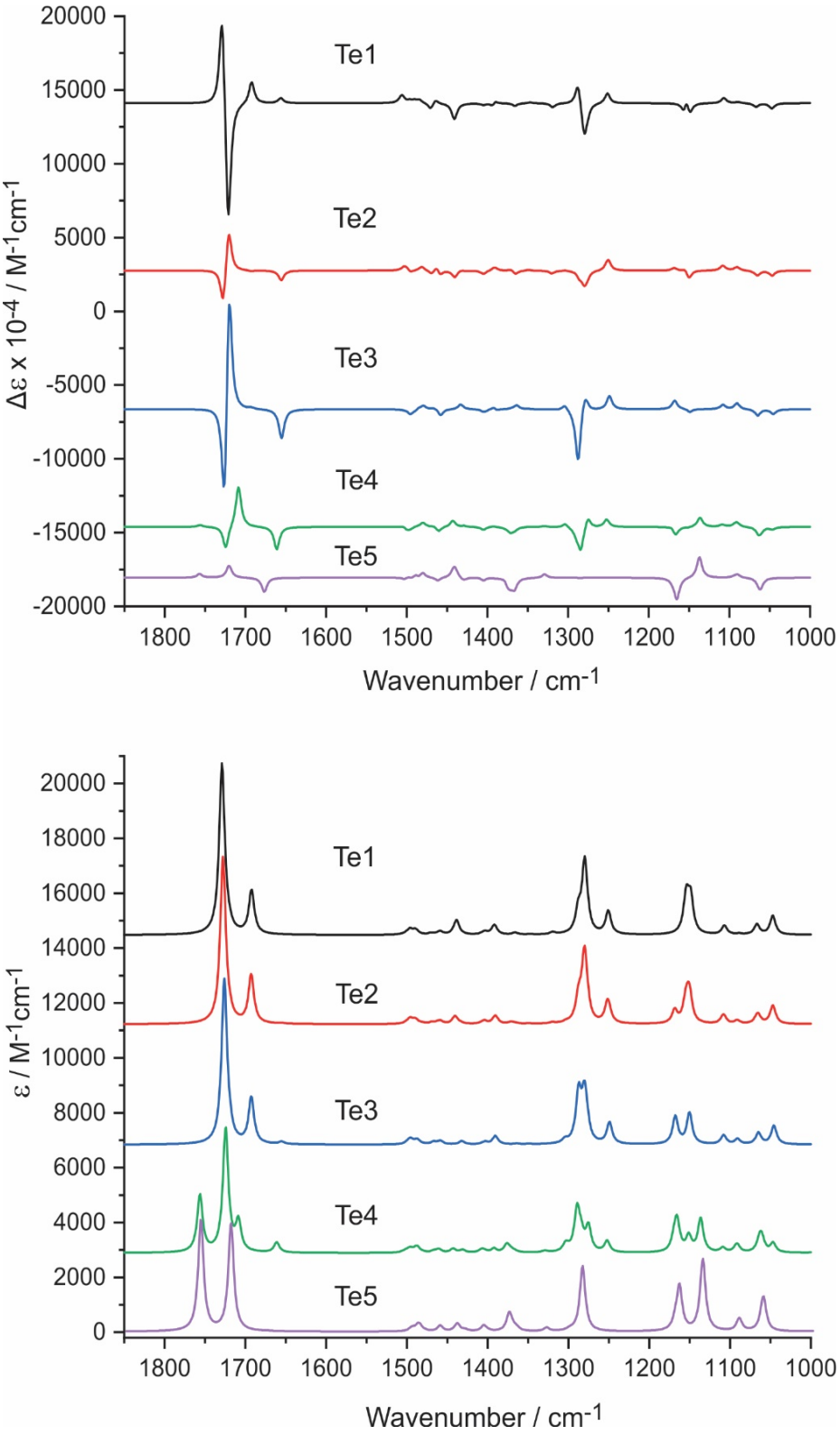

Figure S11. Predicted IR and VCD spectra of the five $(LA)_4$ conformers in the PCM of $CDCl_3$ at the B3LYP-D3BJ/def2-TZVPD level of theory. The Boltzmann factors for Te1-Te5 (in %) at 298 K are: 76.9, 5.1, 17.9, 0.1, and 0.0.

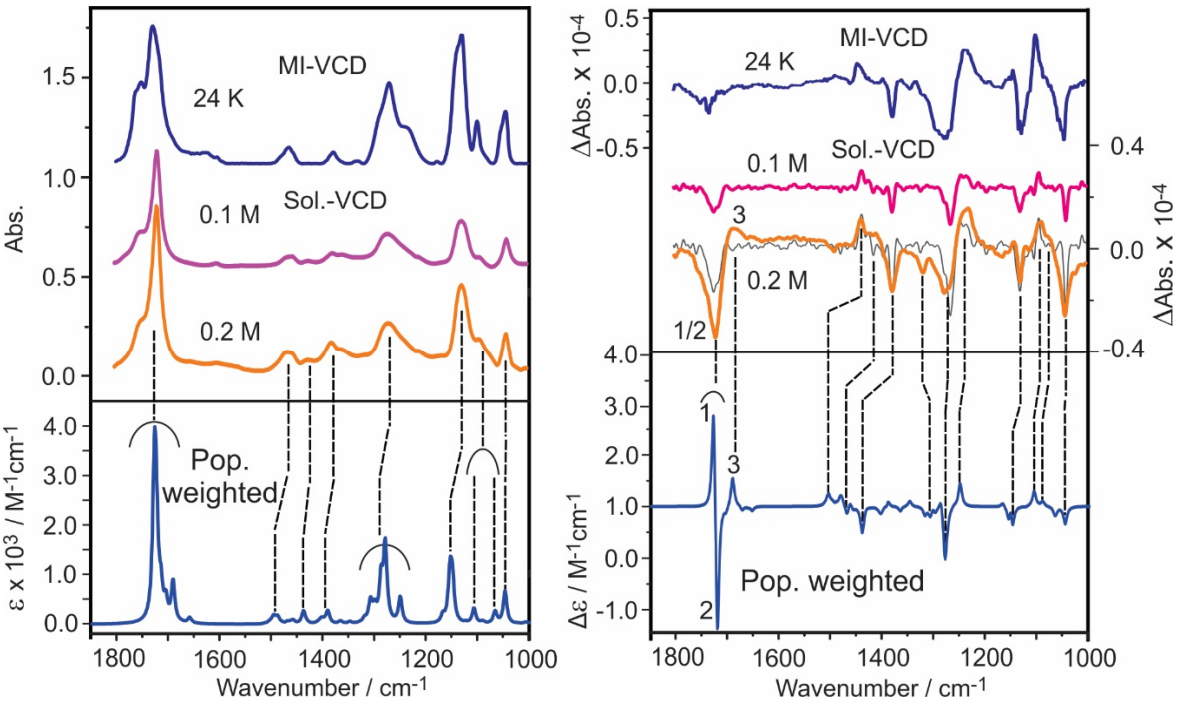

Figure S12. Comparison of the experimental IR and VCD spectra at 24 K, in 0.1 M and in 0.2M solution with the empirically population weighted IR and VCD spectra of the LA monomer, dimer, trimer and tetramer calculated at the B3LYP-D3BJ/def2-TZVPD level of theory. The population weighted spectra contain 20% LA dimer, 30% LA trimer and 50 % LA tetramer.

Completion of Ref. 31.

Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

Cartesian coordinates for M1 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	-0.6838390	0.0669900	-0.3994220
O	-1.3740950	-1.1481310	-0.2168140
C	0.7755140	-0.1176100	-0.0284510
O	1.2218370	-1.1360210	0.4380040
H	-0.7414130	-1.7899060	0.1396220
O	1.5215850	0.9726700	-0.2756180
H	2.4335270	0.7721350	-0.0109910
H	-0.7083480	0.3400240	-1.4617840
C	-1.3313400	1.1855700	0.4156880
H	-0.8520720	2.1435210	0.2155130
H	-2.3842330	1.2511440	0.1442460
H	-1.2640910	0.9652310	1.4819310

Cartesian coordinates for M2 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	-0.6806620	0.1018410	0.3719140
H	-0.7349600	0.0783480	1.4718380
C	-1.6276580	-0.9410580	-0.1913640
C	0.7733050	-0.2332520	0.0551000
H	-1.5819920	-0.9415400	-1.2806310
H	-1.3619790	-1.9313070	0.1730570
H	-2.6456920	-0.7042200	0.1148940
O	1.2360220	-1.3404670	0.0101380
O	1.5242610	0.8825050	-0.1123700
H	2.4385490	0.5973440	-0.2666670
O	-1.0768880	1.3737840	-0.1080480
H	-0.3709940	2.0096130	0.0558470

Cartesian coordinates for M3 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	0.6818700	-0.1437270	-0.4216020
O	1.2714090	1.1400640	-0.5069740
C	-0.8099720	-0.0966480	-0.1251640
O	-1.6086070	-0.9182450	-0.4855270
H	1.0325810	1.6475220	0.2781340
O	-1.1387820	0.9599340	0.6557700
H	-2.0909580	0.9063680	0.8334390
H	0.7825690	-0.5877950	-1.4115850
C	1.3698570	-1.0365990	0.6129320
H	0.9357770	-2.0370490	0.6101790
H	2.4299570	-1.1074420	0.3721920
H	1.2673860	-0.6137830	1.6144940

Cartesian coordinates for M4 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	0.6409090	-0.0960240	-0.4214040
H	0.7209100	-0.3795710	-1.4749030
C	1.3931200	-1.0968340	0.4430390
C	-0.8522530	-0.1166670	-0.0817940
H	1.3212250	-0.8259280	1.4979940
H	0.9690760	-2.0907220	0.3093080
H	2.4464470	-1.1305370	0.1558170
O	-1.5311360	-1.0886420	-0.2611490
O	-1.3357440	1.0183710	0.4414410
H	-0.6044050	1.6618660	0.4722290
O	1.1176950	1.2439230	-0.2536290
H	2.0495650	1.2328280	-0.0127960

Cartesian coordinates for D1 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	-1.9027630	0.0890560	-0.2195340
O	-1.3106280	-0.9858340	-0.2212460
C	-3.4175400	0.1466930	-0.2103440
H	-3.7100850	0.7330020	-1.0902400
C	-3.9335940	0.8476180	1.0458880
H	-5.0225090	0.8458220	1.0241080
H	-3.5790190	1.8766800	1.0917070
H	-3.6064740	0.3135830	1.9391120
O	-3.9599120	-1.1500090	-0.3169050
H	-3.2213750	-1.7760360	-0.3320270
O	-1.3171810	1.2597730	-0.2247770
H	-0.3174200	1.1629000	-0.2253160
C	1.9027640	-0.0890450	-0.2195400
O	1.3106330	0.9858470	-0.2212510
C	3.4175390	-0.1466890	-0.2103490
H	3.7100780	-0.7329730	-1.0902660
C	3.9335930	-0.8476580	1.0458570
H	5.0225080	-0.8458670	1.0240730
H	3.5790120	-1.8767190	1.0916430
H	3.6064800	-0.3136500	1.9391000
O	3.9599150	1.1500160	-0.3168630
H	3.2213780	1.7760430	-0.3320080
O	1.3171760	-1.2597610	-0.2247660
H	0.3174100	-1.1628870	-0.2252970

Cartesian coordinates for D2 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	-1.8785700	-0.0672570	0.1618160
O	-1.2490110	-1.1101920	0.0533910
C	-3.3855880	-0.0577570	0.3709840
H	-3.5176110	-0.3985300	1.4100470
C	-4.0865080	-1.0366400	-0.5574240
H	-5.1532360	-1.0330270	-0.3378660
H	-3.6942750	-2.0421690	-0.4184780
H	-3.9453700	-0.7374780	-1.5964230
O	-3.9607750	1.2215650	0.2028620
H	-3.3135940	1.8934400	0.4486780
O	-1.3324150	1.1296880	0.1619850
H	-0.3317640	1.0728850	0.0636610
C	1.9001950	-0.0863490	-0.2022330
O	1.2786750	0.9673850	-0.0893710
C	3.4094510	-0.0875890	-0.3470340
H	3.6282730	-0.6117910	-1.2857740
C	4.0732410	-0.8392230	0.8059700
H	5.1536450	-0.7961830	0.6749590
H	3.7569090	-1.8814820	0.8248890
H	3.8232100	-0.3693710	1.7582270
O	3.8979940	1.2322830	-0.4278200
H	3.1406280	1.8299260	-0.3454810
O	1.3540210	-1.2735530	-0.2109870
H	0.3519540	-1.2147440	-0.1093900

Cartesian coordinates for D3 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	1.8836530	-0.1953540	-0.1981710
O	1.2199680	-1.2214140	-0.1418040
C	3.3993050	-0.2270140	-0.2906880
H	3.6565260	-1.0653320	-0.9387310
C	3.9752690	-0.4689450	1.1078090
H	5.0608270	-0.5228680	1.0371830
H	3.5976890	-1.4021360	1.5269790
H	3.7107900	0.3514190	1.7779220
O	3.9341290	0.9301240	-0.9001720
H	3.4740940	1.7049290	-0.5538460
O	1.3830810	1.0188660	-0.1296540
H	0.3821980	0.9944160	-0.0254150
C	-1.8890510	-0.1002000	0.1984090
O	-1.2311120	0.9362300	0.1495340
C	-3.3974370	-0.0573480	0.3457660
H	-3.6372470	-0.6396240	1.2440130
C	-4.0854920	-0.6987610	-0.8587210
H	-5.1639170	-0.6268620	-0.7240090
H	-3.8063580	-1.7474900	-0.9540050
H	-3.8170170	-0.1699370	-1.7743250
O	-3.8373050	1.2701920	0.5242000
H	-3.0606810	1.8453590	0.4634310
O	-1.3853350	-1.3041230	0.1313360
H	-0.3817880	-1.2751390	0.0268520

Cartesian coordinates for D4 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	1.8896420	-0.0509930	-0.1881680
O	1.2271070	-1.0808180	-0.1934560
C	3.4095580	-0.0802920	-0.2452860
H	3.6370160	-0.3932120	-1.2764350
C	3.9865280	-1.1077300	0.7158610
H	5.0698990	-1.1279340	0.6060130
H	3.5852350	-2.0967920	0.5036160
H	3.7475170	-0.8371220	1.7447500
O	3.9982000	1.1761350	0.0206060
H	3.3841550	1.8728030	-0.2410950
O	1.3773750	1.1580550	-0.1829940
H	0.3653450	1.1299560	-0.1860710
C	-1.8896160	0.0509950	-0.1878890
O	-1.2270810	1.0808190	-0.1933250
C	-3.4095270	0.0802900	-0.2452450
H	-3.6368620	0.3932110	-1.2764230
C	-3.9866260	1.1077260	0.7158220
H	-5.0699820	1.1279180	0.6058310
H	-3.5853120	2.0967900	0.5036250
H	-3.7477450	0.8371220	1.7447430
O	-3.9982090	-1.1761340	0.0205770
H	-3.3841250	-1.8728090	-0.2410130
O	-1.3773410	-1.1580510	-0.1829130
H	-0.3653090	-1.1299570	-0.1860670

Cartesian coordinates for D5 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	1.8804960	-0.1840670	-0.2181720
O	1.1503040	-1.1671110	-0.2136110
C	3.3920750	-0.3156500	-0.1540260
H	3.6593890	-1.1703670	-0.7765060
C	3.8033820	-0.5938870	1.2950760
H	4.8847420	-0.7171480	1.3368270
H	3.3255840	-1.5008600	1.6667610
H	3.5242330	0.2423780	1.9389900
O	4.0624200	0.8045120	-0.6951130
H	3.5885510	1.6044490	-0.4352120
O	1.4557700	1.0580610	-0.2219610
H	0.4448140	1.1032190	-0.2222570
C	-1.8805000	0.1840670	-0.2182300
O	-1.1503090	1.1671110	-0.2136480
C	-3.3920790	0.3156500	-0.1540360
H	-3.6594080	1.1703720	-0.7765010
C	-3.8033470	0.5938790	1.2950800
H	-4.8847050	0.7171440	1.3368630
H	-3.3255360	1.5008470	1.6667590
H	-3.5241830	-0.2423920	1.9389810
O	-4.0624460	-0.8045010	-0.6951160
H	-3.5885720	-1.6044440	-0.4352400
O	-1.4557710	-1.0580610	-0.2219720
H	-0.4448120	-1.1032330	-0.2222350

Cartesian coordinates for D6 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	-1.8756390	0.0610930	-0.1885690
O	-1.1785120	1.0663750	-0.1370260
C	-3.3939810	0.1443930	-0.2407630
H	-3.6112570	0.5105610	-1.2565240
C	-3.9362670	1.1459260	0.7664080
H	-5.0182610	1.2081630	0.6587720
H	-3.5012870	2.1293020	0.5989490
H	-3.7071570	0.8209000	1.7817290
O	-4.0240440	-1.1024540	-0.0298600
H	-3.4390760	-1.8057940	-0.3365420
O	-1.4051650	-1.1631320	-0.2539040
H	-0.3925920	-1.1701440	-0.2610700
C	1.8970530	-0.1729710	-0.2233490
O	1.2005960	-1.1789480	-0.2764630
C	3.4122820	-0.2565190	-0.1652150
H	3.7078240	-1.0686650	-0.8303150
C	3.8341830	-0.5938440	1.2681620
H	4.9190740	-0.6831820	1.3043070
H	3.3870630	-1.5337150	1.5933610
H	3.5279120	0.1988870	1.9534860
O	4.0432990	0.9114690	-0.6494300
H	3.5535660	1.6815480	-0.3345650
O	1.4300650	1.0519640	-0.1557220
H	0.4184850	1.0614910	-0.1523900

Cartesian coordinates for T1 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	0.3163530	1.8576500	-0.2927140
O	0.1813010	0.6389660	-0.4202980
O	1.4779870	2.4338600	-0.1293860
H	2.2270830	1.7644150	-0.0994640
C	-0.8524860	2.8326010	-0.2782220
C	-1.1275280	3.2639900	1.1664130
H	-0.5295770	3.7014330	-0.8564930
H	-1.9303600	4.0001810	1.1643210
H	-1.4444960	2.4076230	1.7642170
H	-0.2413710	3.7060150	1.6212650
O	-1.9786120	2.3079360	-0.9198340
H	-2.4491220	1.6987790	-0.3197190
C	3.3307490	-0.5218900	-0.1965890
O	3.4564740	0.6888420	-0.0467020
O	2.1865140	-1.1262830	-0.4061310
H	1.4357620	-0.4662840	-0.4189420
C	4.5287200	-1.4481800	-0.1510810
C	4.3985290	-2.4622220	0.9848630
H	4.5387720	-1.9855930	-1.1077180
H	5.2888800	-3.0893160	0.9954930
H	4.3276930	-1.9489640	1.9447960
H	3.5201930	-3.0917120	0.8470600
O	5.7201020	-0.7064960	-0.0226200
H	5.4808550	0.2301100	0.0300080
C	-2.9694770	-0.8084330	0.1387210
O	-3.2176070	0.3019180	0.5794510
O	-1.8605940	-1.1260010	-0.4987190
H	-1.2342860	-0.3579590	-0.5320720
C	-3.9453790	-1.9608100	0.2817340
C	-4.4195730	-2.4502720	-1.0864960
H	-3.4058610	-2.7727990	0.7837510
H	-5.1413030	-3.2528880	-0.9401770
H	-4.9096720	-1.6407630	-1.6292140
H	-3.5844540	-2.8242210	-1.6780290
O	-5.0380000	-1.5708280	1.0833480
H	-4.9286940	-0.6279870	1.2782520

Cartesian coordinates for T2 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	3.0643520	-0.6223450	-0.1706790
O	3.1653880	0.4884750	-0.6806250
O	1.9862260	-1.0657860	0.4287650
H	1.2647200	-0.3733720	0.4153250
C	4.2169990	-1.6052450	-0.1934570
C	4.6699640	-1.9548540	1.2238100
H	3.8387990	-2.5131220	-0.6798140
H	5.5124090	-2.6421220	1.1604340
H	4.9972730	-1.0567890	1.7494200
H	3.8649980	-2.4276220	1.7853110
O	5.2898750	-1.0886190	-0.9471420
H	5.0414500	-0.2015490	-1.2449000
C	0.1678080	1.8975100	-0.1306080
O	0.0622670	0.7821870	0.3818280
O	1.2569960	2.3113870	-0.7233450
H	1.9794890	1.6131600	-0.7048480

C	-0.9580390	2.9239430	-0.1414010
C	-0.5341180	4.1773450	0.6205720
H	-1.1075130	3.1847040	-1.1982800
H	-1.3390330	4.9082310	0.5632470
H	-0.3643100	3.9340870	1.6702270
H	0.3728280	4.6058150	0.1986980
O	-2.1295070	2.4304060	0.4399120
H	-2.5073760	1.7133570	-0.1034340
C	-2.9977830	-0.7969900	0.1091790
O	-3.1568200	0.1091260	-0.6923520
O	-2.0122890	-0.8540090	0.9834030
H	-1.3817670	-0.1020470	0.8505660
C	-3.9475940	-1.9774500	0.1802940
C	-3.2271210	-3.2894990	-0.1255150
H	-4.3264010	-2.0106440	1.2095050
H	-3.9509030	-4.1029070	-0.0934430
H	-2.7900850	-3.2575630	-1.1246160
H	-2.4416100	-3.4819050	0.6045210
O	-5.0264100	-1.7834290	-0.7064760
H	-4.8756020	-0.9421050	-1.1628300

Cartesian coordinates for T3 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	0.5223400	2.1529460	-0.2219090
O	0.1564300	1.4048420	0.6772090
C	0.2304760	3.6418080	-0.1971240
H	-0.1704030	3.9149180	-1.1769360
C	1.5225630	4.4245350	0.0540590
H	1.2866690	5.4871280	0.0902390
H	2.2480250	4.2455720	-0.7392970
H	1.9621720	4.1356770	1.0103550
O	-0.7571460	3.9351650	0.7661050
H	-0.7330150	3.2361550	1.4344450
O	1.2191510	1.7670600	-1.2599070
H	1.4549790	0.7975640	-1.1960850
C	1.9624610	-1.6458350	-0.3148780
O	2.1401220	-0.6892720	-1.0564650
C	3.1287810	-2.4794260	0.1825640
H	2.9363970	-3.5091880	-0.1439160
C	3.2159980	-2.4502780	1.7076410
H	4.0838130	-3.0303370	2.0187300
H	2.3207420	-2.8776700	2.1575330
H	3.3416330	-1.4257670	2.0604920
O	4.3340510	-2.0257270	-0.3906380
H	4.1167080	-1.2862120	-0.9769240
O	0.7972890	-2.0578010	0.1177430
H	0.0344940	-1.5318340	-0.2445020
O	-1.5277080	-1.1010180	-0.7274970
C	-2.4373510	-0.6093910	-0.0746040
O	-2.2809040	0.3360580	0.8242470
H	-1.3439200	0.6630560	0.8343530
C	-3.8751540	-1.0546490	-0.2579640
H	-4.4361000	-0.1619800	-0.5638180
O	-3.9588600	-2.0302430	-1.2715410
C	-4.4646040	-1.5862260	1.0471530
H	-4.4779730	-0.8119010	1.8131380
H	-5.4843540	-1.9191730	0.8587450

H	-3.8851430	-2.4380680	1.4055190
H	-3.0671890	-2.1613610	-1.6257590

Cartesian coordinates for T4 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	3.2100640	-0.4278220	-0.2095180
O	3.2087750	0.7525590	-0.5460270
O	2.1563570	-1.0870190	0.1978170
H	1.3435380	-0.4997550	0.2047710
C	4.4852020	-1.2475160	-0.2423780
C	4.8459780	-1.7620240	1.1503680
H	4.2839010	-2.1047470	-0.8968670
H	5.7768340	-2.3238510	1.0852320
H	4.9954940	-0.9265790	1.8357840
H	4.0629230	-2.4113670	1.5400910
O	5.5430700	-0.4885160	-0.7836340
H	5.1966600	0.3940360	-0.9808990
C	0.0142920	1.6719180	-0.1291430
O	0.0263160	0.4970040	0.2202040
O	1.0748670	2.3161690	-0.5555950
H	1.8847530	1.7234570	-0.5514570
C	-1.2435560	2.5311400	-0.1154010
C	-1.0963370	3.6658700	0.8939250
H	-1.3250600	2.9596640	-1.1234590
H	-1.9928420	4.2833980	0.8624980
H	-0.9936390	3.2574980	1.9002520
H	-0.2279860	4.2810330	0.6657230
O	-2.3835950	1.7897300	0.2197300
H	-2.5512190	1.0988480	-0.4468580
C	-3.5731770	-1.3218620	-0.7810250
O	-3.1471040	-0.3610230	-1.3819380
O	-4.6130320	-2.0404710	-1.2319220
H	-4.9262820	-1.6276330	-2.0535300
C	-3.0463570	-1.8303550	0.5545990
C	-3.7461890	-1.0747140	1.6885840
H	-3.2908910	-2.8912300	0.6179000
H	-3.3969240	-1.4745960	2.6400570
H	-3.5042110	-0.0122440	1.6427940
H	-4.8295460	-1.1960370	1.6331420
O	-1.6479020	-1.7452510	0.6142120
H	-1.3470220	-0.8231450	0.5419780

Cartesian coordinates for T5 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	0.4165680	-2.0846630	-0.3954520
O	0.3331890	-0.8660820	-0.4144040
O	-0.6288080	-2.8825160	-0.4780540
H	-1.4632760	-2.3470720	-0.4506880
C	1.7391400	-2.8108070	-0.2157090
C	1.9029710	-3.1695690	1.2661020
H	1.6975620	-3.7258760	-0.8087040
H	2.8396360	-3.7103270	1.3952650
H	1.9408220	-2.2615810	1.8711990
H	1.0798420	-3.7941860	1.6152240
O	2.8128640	-2.0568510	-0.7124190
H	2.8475610	-1.1962320	-0.2623050
C	2.5539240	1.6412570	-0.0586710

O	3.0140710	0.6244870	0.3997150
O	3.2071250	2.3862320	-0.9691540
H	4.0482240	1.9423470	-1.1628600
C	1.1863980	2.2239470	0.2745480
C	1.2967320	3.6326120	0.8438280
H	0.6423290	2.2624010	-0.6801810
H	0.2956970	4.0055150	1.0577990
H	1.8652920	3.6189210	1.7743970
H	1.7815870	4.3021930	0.1359180
O	0.5074710	1.4197020	1.2054950
H	0.5394400	0.5063870	0.8800790
C	-3.2071740	-0.3368540	0.2827630
O	-2.8835590	-1.4742160	0.0162210
O	-4.1479950	-0.0776460	1.2026110
H	-4.4475120	-0.9259080	1.5677200
C	-2.6036180	0.9311470	-0.3099950
C	-3.6753540	1.9137950	-0.7668200
H	-2.0299730	1.3796290	0.5155250
H	-3.1845660	2.8043850	-1.1564890
H	-4.2732500	1.4743610	-1.5662030
H	-4.3293500	2.1966140	0.0553030
O	-1.7736530	0.6442970	-1.4001930
H	-1.0332150	0.0839870	-1.1031110

Cartesian coordinates for T6 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	0.2351500	1.9716760	-0.2232080
O	0.0867810	0.7709820	-0.4614130
O	1.3987130	2.5085610	0.0347950
H	2.1343850	1.8245940	0.0353350
C	-0.9181840	2.9635180	-0.1701780
C	-1.2467540	3.2709610	1.2952350
H	-0.5564200	3.8736760	-0.6545050
H	-2.0361930	4.0208700	1.3255480
H	-1.6047380	2.3719650	1.7998340
H	-0.3734170	3.6525760	1.8237590
O	-2.0231400	2.5192810	-0.9009110
H	-2.5308100	1.8702330	-0.3754620
C	3.2004000	-0.4710060	-0.2138390
O	3.3438410	0.7195310	0.0426660
O	2.0533870	-1.0290240	-0.5170640
H	1.3174320	-0.3515730	-0.5040450
C	4.3773030	-1.4251180	-0.2020510
C	4.1809320	-2.5309800	0.8342470
H	4.4165870	-1.8773550	-1.2011350
H	5.0581090	-3.1764020	0.8253280
H	4.0797590	-2.1017640	1.8319850
H	3.2975380	-3.1264020	0.6066160
O	5.5762930	-0.7250140	0.0387990
H	5.3538530	0.2097020	0.1575830
C	-3.1078630	-0.6428260	-0.0966200
O	-3.3498230	0.4425840	0.3930350
O	-1.9804110	-0.9394560	-0.7296620
H	-1.3415390	-0.1817140	-0.6992320
C	-4.0541550	-1.8265000	0.0174040
C	-3.9117540	-2.4408450	1.4129600
H	-5.0635340	-1.4313680	-0.1024940

H	-4.6129960	-3.2689350	1.5079520
H	-2.9001810	-2.8243480	1.5603990
H	-4.1251090	-1.7010980	2.1852150
O	-3.8703420	-2.7834400	-1.0077960
H	-2.9255720	-2.8679800	-1.1859730

Cartesian coordinates for T7 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	0.2736720	1.9475150	-0.2353270
O	0.1326210	0.7464290	-0.4757690
O	1.4317720	2.4887060	0.0369900
H	2.1700660	1.8071150	0.0479820
C	-0.8838700	2.9351160	-0.1966470
C	-1.2276030	3.2469130	1.2642930
H	-0.5213870	3.8447780	-0.6813670
H	-2.0202390	3.9938000	1.2843190
H	-1.5864830	2.3484380	1.7691810
H	-0.3607850	3.6340290	1.7994340
O	-1.9807240	2.4834320	-0.9357360
H	-2.4886850	1.8329880	-0.4119920
C	3.2491890	-0.4824160	-0.1854190
O	3.3825760	0.7089400	0.0733310
O	2.1101250	-1.0463260	-0.5065290
H	1.3699950	-0.3740150	-0.5015500
C	4.4301710	-1.4308260	-0.1539840
C	4.2259980	-2.5290350	0.8891990
H	4.4830160	-1.8908490	-1.1486930
H	5.1053560	-3.1715150	0.8950540
H	4.1124840	-2.0920420	1.8822200
H	3.3469540	-3.1291640	0.6571100
O	5.6234720	-0.7231320	0.0936150
H	5.3937360	0.2092690	0.2165170
C	-3.0611450	-0.6779920	-0.1459370
O	-3.3079840	0.4048720	0.3472260
O	-1.9251170	-0.9674180	-0.7667270
H	-1.2873110	-0.2089640	-0.7215980
C	-4.0621240	-1.8257230	-0.1672820
C	-4.8104100	-1.9411380	1.1495910
H	-4.7764360	-1.5489190	-0.9586690
H	-5.5530680	-2.7339240	1.0703720
H	-4.1193910	-2.1920240	1.9549650
H	-5.3087420	-1.0035090	1.3875910
O	-3.4703060	-3.0758850	-0.4639810
H	-2.7338420	-2.9369150	-1.0711480

Cartesian coordinates for Te1 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	1.2182460	-1.5045840	-0.7057630
O	1.6211740	-0.3408110	-0.6794160
O	-0.0523670	-1.8163030	-0.7466730
H	-0.6306020	-1.0002200	-0.7278280
C	2.1394420	-2.7148010	-0.6622650
C	2.1071390	-3.3187720	0.7460680
H	1.7258360	-3.4359680	-1.3711870
H	2.7284840	-4.2133270	0.7560930
H	2.5088670	-2.6098440	1.4721350
H	1.0919820	-3.5882580	1.0365380
O	3.4301510	-2.4030280	-1.0988140
H	3.9279490	-1.9683160	-0.3804110
C	-1.2182320	1.5046070	-0.7057590
O	-1.6211620	0.3408340	-0.6794580
O	0.0523830	1.8163220	-0.7466240
H	0.6306130	1.0002360	-0.7277800
C	-2.1394260	2.7148270	-0.6622520
C	-2.1071500	3.3187640	0.7460960
H	-1.7258010	3.4360090	-1.3711480
H	-2.7284900	4.2133230	0.7561290
H	-2.5088980	2.6098220	1.4721370
H	-1.0919980	3.5882380	1.0365940
O	-3.4301280	2.4030740	-1.0988360
H	-3.9279480	1.9683560	-0.3804510
C	4.8938840	0.3093380	0.4302030
O	4.8316720	-0.8630240	0.7621020
O	3.9849080	0.9255530	-0.2992940
H	3.2238760	0.3248520	-0.5025260
C	6.0593870	1.1930180	0.8312790
C	6.8270260	1.6779560	-0.3985330
H	5.6357650	2.0599820	1.3520960
H	7.6725620	2.2798540	-0.0680510
H	7.2095890	0.8281460	-0.9655360
H	6.1893660	2.2815400	-1.0437130
O	6.9104320	0.4977540	1.7147370
H	6.5786230	-0.4102820	1.7788570
C	-4.8939180	-0.3093350	0.4300120
O	-4.8316900	0.8630040	0.7619900
O	-3.9849110	-0.9255350	-0.2994590
H	-3.2238710	-0.3248280	-0.5026440
C	-6.0593870	-1.1930510	0.8311080
C	-6.8270480	-1.6779800	-0.3986930
H	-5.6357360	-2.0600170	1.3518990
H	-7.6725660	-2.2798970	-0.0681970
H	-7.2096390	-0.8281670	-0.9656710
H	-6.1893940	-2.2815430	-1.0438980
O	-6.9104250	-0.4978190	1.7145990
H	-6.5786380	0.4102250	1.7787190

Cartesian coordinates for Te2 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	-0.9992480	-1.4746090	-0.2091470
O	-1.4114380	-0.3654180	0.1333740
O	0.2306880	-1.6852210	-0.6041330
H	0.7640460	-0.8383900	-0.6088560

C	-1.8709860	-2.7211980	-0.2450730
C	-2.2568300	-3.0208770	-1.6978060
H	-1.2508680	-3.5357660	0.1365210
H	-2.8373060	-3.9422360	-1.7214140
H	-2.8710960	-2.2140530	-2.1012850
H	-1.3730900	-3.1417920	-2.3238760
O	-2.9737260	-2.6103570	0.6066770
H	-3.6731230	-2.0813030	0.1778690
C	1.2775710	1.6547930	-0.2491890
O	1.6795740	0.5509460	-0.6171090
O	0.0582740	1.8611100	0.1809540
H	-0.4813150	1.0191640	0.1646260
C	2.1452870	2.9063450	-0.2421190
C	1.5542690	3.9616980	-1.1741410
H	2.1081240	3.2830770	0.7894800
H	2.1704760	4.8575390	-1.1194090
H	1.5665740	3.5978720	-2.2023470
H	0.5329790	4.2088180	-0.8912400
O	3.4554020	2.6416290	-0.6496390
H	3.9132340	2.0823390	0.0062410
C	-4.8777170	0.2285820	0.1861870
O	-4.9002040	-0.8490170	-0.3853730
O	-3.8004730	0.7608530	0.7287560
H	-3.0040770	0.1933720	0.5703160
C	-6.1236980	1.0801090	0.3362840
C	-6.4896280	1.2605170	1.8094780
H	-5.8915460	2.0606570	-0.0962060
H	-7.4049370	1.8475350	1.8730450
H	-6.6687650	0.2911480	2.2766530
H	-5.6959050	1.7770110	2.3483650
O	-7.1917870	0.5032020	-0.3809710
H	-6.8800460	-0.3461390	-0.7276250
C	4.9547460	-0.2603410	0.1487090
O	4.8129820	0.7329290	0.8428700
O	4.1231240	-0.6248620	-0.8081860
H	3.3362870	-0.0257840	-0.8342390
C	6.1347510	-1.1969140	0.3228360
C	5.6761250	-2.5993110	0.7196590
H	6.6376140	-1.2488510	-0.6509180
H	6.5542080	-3.2276020	0.8634570
H	5.1208000	-2.5648430	1.6580700
H	5.0470540	-3.0372710	-0.0546010
O	7.0285450	-0.6754120	1.2802830
H	6.6451500	0.1496880	1.6132820

Cartesian coordinates for Te3 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	-1.2153820	-1.5038480	-1.1127700
O	-1.6176430	-0.3403450	-1.1046990
O	0.0556360	-1.8176310	-1.1218870
H	0.6329280	-1.0002520	-1.1193900
C	-2.1407220	-2.7134860	-1.1067340
C	-1.9395620	-3.5346310	-2.3783860
H	-1.8305290	-3.3164300	-0.2420700
H	-2.5818190	-4.4124010	-2.3302650
H	-2.2267380	-2.9454450	-3.2502270
H	-0.9036310	-3.8512090	-2.4824620

O	-3.4868400	-2.3472160	-1.0261590
H	-3.6814450	-1.9441850	-0.1588490
C	1.2153970	1.5042000	-1.1123080
O	1.6176560	0.3406940	-1.1046030
O	-0.0556210	1.8179880	-1.1213290
H	-0.6329150	1.0006120	-1.1190690
C	2.1407360	2.7138360	-1.1058870
C	1.9395830	3.5353860	-2.3772790
H	1.8305420	3.3165050	-0.2410330
H	2.5818370	4.4131420	-2.3288750
H	2.2267640	2.9464770	-3.2493060
H	0.9036510	3.8519950	-2.4812590
O	3.4868540	2.3475400	-1.0254230
H	3.6814530	1.9442370	-0.1582390
C	4.4317650	-0.3199060	0.7928790
O	4.1697890	0.8061840	1.1826590
O	3.8997080	-0.8803850	-0.2761550
H	3.2092400	-0.2925700	-0.6718660
C	5.4239950	-1.2077140	1.5190830
C	4.7558520	-2.4812450	2.0350230
H	6.1923200	-1.4810200	0.7849900
H	5.4957110	-3.0714390	2.5742380
H	3.9468610	-2.2323850	2.7233750
H	4.3581720	-3.0736730	1.2116800
O	6.0242240	-0.4963740	2.5778920
H	5.6290410	0.3881010	2.5915820
O	-3.8996930	0.8804740	-0.2758690
H	-3.2092250	0.2927800	-0.6717630
C	-4.4317460	0.3196660	0.7929940
O	-4.1697980	-0.8065580	1.1824080
C	-5.4240110	1.2072330	1.5194440
H	-6.1923120	1.4807730	0.7854130
C	-4.7558940	2.4805990	2.0358210
O	-6.0242740	0.4955460	2.5780010
H	-4.3581890	3.0732970	1.2126840
H	-5.4957750	3.0706130	2.5752020
H	-3.9469250	2.2315200	2.7241200
H	-5.6290730	-0.3889250	2.5914320

Cartesian coordinates for Te4 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	1.2811630	1.7894530	-0.4485110
O	1.6328590	0.6699180	-0.8248650
O	0.0333150	2.1165550	-0.2453170
H	-0.5882680	1.3507850	-0.4313640
C	2.2588520	2.9236270	-0.1668250
C	1.9808670	4.1018960	-1.0968990
H	2.0574570	3.2334730	0.8679360
H	2.6640380	4.9119410	-0.8467320
H	2.1598340	3.8080260	-2.1320310
H	0.9550350	4.4497140	-0.9934130
O	3.5898710	2.5309610	-0.3386340
H	3.8442620	1.8739640	0.3361870
C	-1.2747410	-1.0198950	-1.1045540
O	-1.6122930	0.1021660	-0.7471500
O	-0.0247250	-1.3717930	-1.3058290
H	0.5912430	-0.6048540	-1.1313010

C	-2.2642130	-2.1494490	-1.3564290
C	-2.2538190	-2.5386980	-2.8319110
H	-1.9065240	-3.0003500	-0.7610730
H	-2.9440440	-3.3676500	-2.9812720
H	-2.5876940	-1.6973980	-3.4406850
H	-1.2572180	-2.8392320	-3.1498210
O	-3.5707860	-1.7900450	-1.0043010
H	-3.6304280	-1.6135290	-0.0474180
C	-4.8906440	-0.1914500	1.7936750
O	-4.1069610	-1.1018140	1.6404640
O	-5.8024250	-0.1943330	2.7776900
H	-5.7113970	-1.0287950	3.2666520
C	-4.9932100	1.0408330	0.9043960
C	-5.9037740	0.7243860	-0.2858690
H	-5.4371660	1.8375060	1.5021210
H	-6.0072350	1.6231650	-0.8929980
H	-5.4678670	-0.0658400	-0.8983310
H	-6.8943160	0.4103700	0.0482070
O	-3.7231340	1.4976420	0.5225140
H	-3.2508710	0.8282810	-0.0011420
C	4.5883170	-0.5819730	0.4379890
O	4.4272090	0.3637470	1.1920420
O	3.9127360	-0.7697670	-0.6779800
H	3.2067210	-0.0817180	-0.7824510
C	5.6143310	-1.6630040	0.7211690
C	4.9497900	-3.0279570	0.8921120
H	6.2798120	-1.6973380	-0.1504340
H	5.7172160	-3.7657390	1.1231000
H	4.2382470	-3.0016450	1.7187090
H	4.4313300	-3.3253930	-0.0188000
O	6.3652350	-1.3274940	1.8665910
H	6.0131150	-0.4903030	2.2044950

Cartesian coordinates for Te5 calculated at the B3LYP-D3BJ/def2-TZVPD level of theory.

C	-1.3504500	-1.3648870	-0.5609900
O	-1.6358220	-0.1724960	-0.5781920
O	-0.1215580	-1.8209070	-0.5441530
H	0.5441650	-1.0720370	-0.5530730
C	-2.3976910	-2.4711470	-0.5496430
C	-2.3016280	-3.3037800	-1.8243520
H	-2.1504120	-3.1078980	0.3105330
H	-3.0370020	-4.1057650	-1.7775190
H	-2.5240080	-2.6817680	-2.6925380
H	-1.3076910	-3.7329190	-1.9353160
O	-3.6999360	-1.9633670	-0.4529260
H	-3.8181280	-1.4799800	0.3846540
C	1.3504640	1.3649400	-0.5607820
O	1.6358400	0.1725510	-0.5781060
O	0.1215720	1.8209560	-0.5439330
H	-0.5441510	1.0720880	-0.5529760
C	2.3977030	2.4712020	-0.5492770
C	2.3016710	3.3039860	-1.8238890
H	2.1503990	3.1078500	0.3109680
H	3.0370410	4.1059680	-1.7769410
H	2.5240760	2.6820790	-2.6921440
H	1.3077350	3.7331350	-1.9348290

O	3.6999460	1.9634150	-0.4525870
H	3.8181220	1.4799410	0.3849440
C	5.1667990	-0.5171300	1.4906870
O	4.4413510	0.4165650	1.7495990
O	6.1955060	-0.8609020	2.2821460
H	6.2296250	-0.2263410	3.0167840
C	5.0626970	-1.3978450	0.2523740
C	5.8469770	-0.7470530	-0.8914700
H	5.5110060	-2.3606860	0.5001310
H	5.8046970	-1.4042950	-1.7595130
H	5.4052460	0.2145300	-1.1554180
H	6.8923490	-0.5954870	-0.6162480
O	3.7245090	-1.6596030	-0.0737540
H	3.2462550	-0.8399860	-0.2886380
C	-5.1668380	0.5169720	1.4905700
O	-4.4414010	-0.4167520	1.7494050
O	-6.1955720	0.8606600	2.2820320
H	-6.2297160	0.2260200	3.0166000
C	-5.0626970	1.3978200	0.2523560
C	-5.8469490	0.7471550	-0.8915810
H	-5.5110080	2.3606360	0.5002040
H	-5.8046400	1.4044900	-1.7595530
H	-5.4052150	-0.2144020	-1.1556200
H	-6.8923290	0.5955660	-0.6164040
O	-3.7244990	1.6596070	-0.0737080
H	-3.2462420	0.8400110	-0.2886640