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DFT Study of the Molecular Structure, Conformational Preference, Spectroscopic and Vibrational Analysis of Cinnamic Acid and Cinnamaldehyde

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Supplementary Information

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Table S1. Calculated optimized geometrical parameters of cis/trans cinnamic acid and cinnamaldehyde.

Cinnamic acid			**Cinnamaldehyde**		
Bond length[1]	***s-cis***	***s-trans***	**Bond length[1]**	***s-cis***	***s-trans***
C1-C2	1.39	1.39	C1-C2	1.39	1.39
C1-C6	1.41	1.41	C1-C6	1.40	1.40
C1-H7	1.08	1.08	C1-H7	1.08	1.08
C2-C3	1.40	1.40	C2-C3	1.39	1.39
C2-H8	1.08	1.08	C2-H8	1.08	1.08
C3-C4	1.39	1.39	C3-C4	1.41	1.41
C3-H9	1.08	1.08	C3-H9	1.08	1.09
C4-C5	1.39	1.39	C4-C5	1.41	1.41
C4-H10	1.08	1.08	C4-C12	1.46	1.46
C5-C6	1.40	1.40	C5-C6	1.39	1.39
C5-H11	1.08	1.08	C5-H10	1.08	1.08
C6-C12	1.46	1.46	C6-H11	1.08	1.08
C12-C13	1.34	1.34	C12-C13	1.35	1.35
C12-H17	1.09	1.09	C12-H18	1.09	1.09
C13-C14	1.47	1.47	C13-C14	1.47	1.46
C13-H18	1.08	1.08	C13-H17	1.09	1.08
C14-O15	1.21	1.21	C14-O15	1.22	1.21
C14-O16	1.36	1.36	C14-H16	1.11	1.11
O16-H19	0.97	0.97			
Bond Angle[1] (°)					
C2-C1-C6	120.7	120.7	C2-C1-C6	119.8	119.7
C2-C1-H7	119.3	119.3	C2-C1-H7	120.2	120.2
C6-C1-H7	120.0	120.0	C6-C1-C2	119.8	120.1
C1-C2-C3	120.3	120.3	C1-C2-C3	119.9	119.9
C1-C2-H8	119.7	119.7	C1-C2-H8	120.2	120.2
C3-C2-H8	120.0	120.0	C3-C2-H8	119.9	119.9
C2-C3-C4	119.7	119.7	C2-C3-C4	121.1	121.1
C2-C3-H9	120.1	120.1	C2-C3-H9	119.8	119.8
C4-C3-H9	120.2	120.2	C4-C3-H9	119.1	119.2
C3-C4-C5	120.0	120.0	C3-C4-C5	118.2	118.3
C3-C4-H10	120.2	120.2	C3-C4-C12	118.6	118.8
C5-C4-H10	119.9	119.9	C5-C4-C12	123.3	122.9
C4-C5-C6	121.1	121.1	C4-C5-C6	120.7	120.7
C4-C5-H11	119.8	119.8	C4-C5-H10	120.0	120.0
C6-C5-H11	119.1	119.2	C6-C5-H10	119.3	119.3
C1-C6-C5	118.2	118.2	C1-C6-C5	120.3	120.3
C1-C6-C12	123.2	123.2	C1-C6-H11	120.0	120.0
C5-C6-C12	118.6	118.6	C5-C6-H11	119.8	119.7
C6-C12-C13	127.7	127.3	C4-C12-C13	128.2	128.2
C6-C12-H17	115.9	115.4	C4-C12-H18	115.8	114.8
C13-C12-H17	116.4	117.4	C13-C12-H18	116.1	116.97
C12-C13-C14	120.3	124	C12-C13-C14	121.5	120.6
C12-C13-H18	123.2	123	C12-C13-H17	122.2	123.1
C14-C13-H18	116.5	113.2	C14-C13-H17	116.3	116.2
C13-C14-O15	126.8	124.1	C13-C14-O15	125.3	124.6
C13-C14-O16	111.2	114.1	C13-C14-H16	114.8	114.9
O15-C14-O16	122.0	121.8			
C14-O16-H19	106.8	106.5			

[1]The numbering of atoms is provided in Fig. 1.

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Table S2. Experimental and calculated vibrational parameters of *s-cis* cinnamic acid.

No	Expt.[a]	Freq.[b]	IR Intensity[c]	Raman[d]	Assignment (PED > 10%)[e]
ν_1	-	3599	110.39	170.98	νOH(100)
ν_2	3067	3054	9.84	111.50	νCH(92)
ν_3	-	3050	8.12	245.51	νCH(79)
ν_4	-	3043	18.70	36.21	νCH(78)
ν_5	-	3035	9.79	91.07	νCH(84)
ν_6	3027	3027	0.04	111.39	νCH(94)
ν_7	-	3022	2.73	14.51	νCH(97)
ν_8	2977	3006	0.52	34.51	νCH(96)
ν_9	1688	1739	352.82	82.37	νOC(79)
ν_{10}	1631	1640	310.57	1065.47	νCC(61)
ν_{11}	-	1601	17.90	752.69	νCC(61) + δHCC(11)
ν_{12}	1578	1577	13.77	24.67	νCC(54) + δCCC(11)
ν_{13}	1496	1492	8.55	28.21	δHCC(63)
ν_{14}	1450	1446	18.63	16.92	δHCC(32)
ν_{15}	1341	1345	154.83	9.30	νOC(11) + CC(11) + δHCC(27) + δHOC(15)
ν_{16}	1335	1331	4.18	33.28	δHCC(72)
ν_{17}	1312	1318	2.62	30.89	δHCC(34)
ν_{18}	1288	1289	5.88	4.54	δHCC(18) + δHOC(38)
ν_{19}	1224	1246	8.52	102.61	δHCC(15) + νCC(13)
ν_{20}	1204	1200	16.88	81.88	νCC(26) + δHCC(29)
ν_{21}	-	1177	9.98	84.24	νCC(16) + δHCC(59)
ν_{22}	-	1158	0.94	11.29	νOC(12) + δHCC(71)
ν_{23}	-	1108	565.99	111.28	νOC(48) + δHOC(23)
ν_{24}	-	1079	26.22	1.82	νCC(30) + δHCC(40)
ν_{25}	-	1025	1.24	25.01	νCC(32)10 + δHCC(34) + δCCC(15)
ν_{26}	-	1003	30.91	1.66	τHCCC(81)
ν_{27}	984	992	2.68	80.04	νCC(17) + δCCC(55)
ν_{28}	982	981	1.53	0.15	τHCCC(67) + τCCCC(16)
ν_{29}	-	963	0.00	0.08	τHCCC(74) + τCCCC(11)
ν_{30}	945	943	13.29	10.18	νOC(11) + νCC(42)
ν_{31}	917	913	0.02	0.39	τHCCC(58) + τCCCC(5)
ν_{32}	-	872	14.69	8.40	τHCCC(60) + τOCOC(12)
ν_{33}	-	830	0.77	0.14	νCC(13) + δCCC(30) + τHCCC(84)
ν_{34}	-	830	3.30	6.45	τCCCC(18)
ν_{35}	769	770	60.20	1.07	τHCCC(40) + τCCCC(13) + τOCOC(26)
ν_{36}	712	715	0.50	0.87	τHCCC(31) + τOCOC(43)
ν_{37}	684	683	49.62	0.33	τHCCC(43) + τCCCC(25)
ν_{38}	-	652	10.77	12.01	νOC(14) + δCCC(66)
ν_{39}	-	618	0.02	9.04	δCCC(67)
ν_{40}	-	571	107.23	1.78	τHOCC(87)
ν_{41}	-	561	58.85	0.11	δCCC(60)
ν_{42}	-	508	8.00	0.31	δCCC(75)
ν_{43}	-	480	0.39	0.08	τCCCC(57)
ν_{44}	-	402	0.00	0.01	τCCCC(85)
ν_{45}	-	320	1.31	2.14	νCC(10) + δCCC(25)
ν_{46}	-	272	0.14	1.13	τHCCC(10) + τCCCC(62)
ν_{47}	-	233	1.16	3.78	νCC(11) + δCCC(61)
ν_{48}	-	132	0.92	0.65	τCCCC(11)
ν_{49}	-	99	0.22	0.14	δCCC(78) + τOCCC(65)
ν_{50}	-	83	0.02	1.49	τCCCC(83)
ν_{51}	-	34	0.95	0.19	τCCCC(76) + τOCCC(18)

[a]Experimental values taken from [42]
[b]Calculated IR vibrational wavenumbers, cm^{-1} (scaled with 0.955 above 1800 cm^{-1} and 0.977 below 1800 cm^{-1}).
[c]Calculated infrared intensities in km mol^{-1}.
[d]Calculated Raman intensities in Å4 amu^{-1}.
[e]ν is stretching, δ is bending, and τ is torsion.

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Table S3. Experimental and calculated vibrational parameters of *s-trans*-cinnamaldehyde acid.

No	Expt.[a]	Freq.[b]	IR Intensity[c]	Raman[d]	Assignment (PED > 10%)[e]
ν_1	3062	3051	10.70	300.95	νCH(83)
ν_2	3047	3045	19.16	64.50	νCH(83)
ν_3	3027	3037	5.77	105.47	νCH(83)
ν_4	-	3032	7.29	17.95	νCH(85)
ν_5	-	3026	0.04	103.14	νCH(94)
ν_6	3029	3020	4.92	30.10	νCH(78)
ν_7	2997	2979	11.09	46.28	νCH(99)
ν_8	2743	2744	113.57	141.19	νCH(99)
ν_9	1727	1709	517.77	386.86	νOC(89)
ν_{10}	1627	1633	143.43	848.34	νCC(58) + δHCC(12)
ν_{11}	1605	1601	22.13	811.22	νCC(58) + δHCC(18)
ν_{12}	1576	1577	10.86	42.66	νCC(56)
ν_{13}	1496	1491	2.79	34.92	δHCC(64) + δCCC(10)
ν_{14}	1450	1447	13.27	16.16	νCC(19) + δHCC(45)
ν_{15}	1393	1385	0.85	40.61	δHCO(77)
ν_{16}	1328	1331	5.77	36.66	δHCC(76)
ν_{17}	1306	1318	5.37	42.86	νCC(49) + δHCC(26)
ν_{18}	1294	1295	9.99	2.27	νCC(31) + δHCC(40)
ν_{19}	1252	1242	13.73	291.73	νCC(25) + δHCC(37)
ν_{20}	1204	1202	0.89	28.09	νCC(28) + δHCC(36)
ν_{21}	1178	1177	3.77	71.80	δHCC(63)
ν_{22}	1160	1158	1.17	12.54	νCC(15) + δHCC(77)
ν_{23}	1124	1113	208.97	120.80	νCC(58) + δCCC(11)
ν_{24}	1073	1077	14.71	4.91	νCC(40) + δHCC(36)
ν_{25}	1029	1025	1.67	24.49	νCC(39) + δHCC(19)+ δCCC(28)
ν_{26}	1007	1007	14.48	5.28	τHCCC(83)
ν_{27}	-	992	1.63	82.04	νCC(13)25 + δCCC(49)
ν_{28}	-	987	5.83	0.56	τHCCC(76) + τCCCC(13)
ν_{29}	973	978	24.84	0.93	τHCCC(77)
ν_{30}	-	966	0.01	0.06	τHCCC(75)
ν_{31}	-	918	0.01	0.80	τHCCC(68) + τCCCC(11) + τCCCC(11)
ν_{32}	-	854	0.44	8.90	τHCCC(67) + τCCCC(17)
ν_{33}	-	834	0.12	8.72	νCC(19) + δCCC(47)
ν_{34}	-	830	0.02	0.76	τHCCC(90)
ν_{35}	748	750	49.74	0.03	τHCCC(69) + τCCCC(12)
ν_{36}	689	685	34.72	0.02	τHCCC(56) + τCCCC(33)
ν_{37}	-	619	0.42	6.84	δCCC(78)
ν_{38}	606	606	8.65	8.97	δCCC(67)
ν_{39}	-	576	13.58	1.02	δCCC(66)
ν_{40}	500	502	5.07	0.10	τCCCC(76)
ν_{41}	493	404	0.00	0.01	τHCCC(23) + τCCCC(69)
ν_{42}	-	341	2.11	3.75	νCC(10)10 + δCCC(53)
ν_{43}	-	320	1.92	1.62	τHCCC(13) + τCCCC(55)
ν_{44}	-	296	7.85	5.34	νCC(36) + δCCC(64)
ν_{45}	-	168	8.09	0.71	τCCCC(62) + τCCCC(11)
ν_{46}	-	120	0.27	2.56	τCCCC(78)
ν_{47}	-	109	4.51	0.82	δCCC(89)
ν_{48}	-	55	2.91	0.69	τCCCC(85)

[a]Experimental values taken from [42]
[b]Calculated IR vibrational wavenumbers, cm^{-1} (scaled with 0.955 above 1800 cm^{-1} and 0.977 below 1800 cm^{-1}).
[c]Calculated infrared intensities in km mol^{-1}. [d] Calculated Raman intensities in Å4 amu^{-1}.
[e]ν is stretching, δ is bending, and τ is torsion.