

Reduced Two-Electron Interactions in Anharmonic Molecular Vibrational Calculations Involving Localized Normal Coordinates

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Vibrational Self-Consistent Field Convergence Notes

- L-VSCF RI-MP2/cc-pVDZ with cubic and quartic terms removed when between modes centered more than $3.2 \text{ } a_0$ apart: The VSCF calculation became divergent after cycle 701 and the convergence of ca. 0.0002 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF HF/cc-pVDZ with cubic and quartic terms calculated using Coulomb attenuated HF ($\omega = 0.20 \text{ } a_0^{-1}$) when between modes centered more than $1.8 \text{ } a_0$ apart: The VSCF calculation became divergent after cycle 1803 and the convergence of ca. 0.0010 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF HF/cc-pVDZ with cubic and quartic terms calculated using Coulomb attenuated HF ($\omega = 0.20 \text{ } a_0^{-1}$) when between modes centered more than $2.6 \text{ } a_0$ apart: The VSCF calculation became divergent after cycle 1512 and the convergence of ca. 0.0002 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF HF/cc-pVDZ with cubic and quartic terms calculated using Coulomb attenuated HF ($\omega = 0.20 \text{ } a_0^{-1}$) when between modes centered more than $3.2 \text{ } a_0$ apart: The VSCF calculation became divergent after cycle 1436 and the convergence of ca. 0.0001 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF HF/cc-pVDZ with cubic and quartic terms calculated using Coulomb attenuated HF ($\omega = 0.25 \text{ } a_0^{-1}$) when between modes centered more than $1.6 \text{ } a_0$ apart: The VSCF calculation became divergent after cycle 1686 and the convergence of ca. 0.0041 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF HF/cc-pVDZ with cubic and quartic terms calculated using Coulomb attenuated HF ($\omega = 0.35 \text{ } a_0^{-1}$) when between modes centered more than $0.2 \text{ } a_0$ apart: The mixing parameter “ b ” in Equation 5 of the main text set to 0.99. The VSCF calculation became divergent after cycle 1726 and the convergence of ca. 0.0002 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF HF/cc-pVDZ with cubic and quartic terms calculated using Coulomb attenuated HF ($\omega = 0.30 \text{ } a_0^{-1}$) when between modes centered more than $1.6 \text{ } a_0$ apart: The VSCF calculation became divergent after cycle 1915 and the convergence of ca. 0.0001 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF HF/cc-pVDZ with cubic and quartic terms calculated using Coulomb attenuated HF ($\omega = 0.30 \text{ } a_0^{-1}$) when between modes centered more than $2.6 \text{ } a_0$ apart: The VSCF calculation became divergent after cycle 1511 and the convergence of ca. 0.0001 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF HF/cc-pVDZ with cubic and quartic terms calculated using Coulomb attenuated HF ($\omega = 0.35 \text{ } a_0^{-1}$) when between modes centered more than $0.6 \text{ } a_0$ apart: The mixing parameter “ b ” in Equation 5 of the main text set to 0.80. The VSCF calculation became divergent after cycle 709 and the convergence of ca. 0.0001 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF RI-MP2/cc-pVDZ with cubic and quartic terms calculated using HF when between modes centered more than $5.8 \text{ } a_0$ apart: The VSCF calculation became divergent after cycle 235 and the convergence of ca. 0.0001 cm^{-1} at this cycle was taken to be sufficient.
- L-VSCF RI-MP2/cc-pVDZ with cubic and quartic terms calculated using HF when between modes centered more than $7.6 \text{ } a_0$ apart: The VSCF calculation became divergent after cycle 228 and the convergence of ca. 0.0001 cm^{-1} at this cycle was taken to be sufficient.
- Several other calculations achieved convergence with the mixing parameter “ b ” in Equation 5 of the main text set to 0.95 or 0.80, but failed to converge with the mixing parameter of 0.90.

Table S1. Calculated HF/cc-pVDZ 1MR VSCF frequencies (in cm^{-1}) for octatetraene calculated using Coulomb attenuated cubic and quartic terms.

ω (a_0^{-1})	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50
Mode 1	80.10	80.10	80.10	80.12	80.14	80.14	80.07	79.90	79.61	79.18	78.53
Mode 2	103.12	103.12	103.13	103.15	103.19	103.22	103.23	103.21	103.13	102.96	102.67
Mode 3	164.96	164.96	164.95	164.97	164.98	164.97	164.90	164.76	164.55	164.27	164.12
Mode 4	234.59	234.58	234.58	234.61	234.71	234.84	234.96	235.06	235.18	235.37	235.74
Mode 5	245.99	245.99	245.99	246.00	246.03	246.07	246.11	246.11	246.01	245.76	245.39
Mode 6	259.58	259.57	259.54	259.52	259.53	259.50	259.38	259.17	258.92	258.80	260.05
Mode 7	359.07	359.07	359.07	359.07	359.07	359.08	359.08	359.09	359.09	359.05	358.96
Mode 8	383.03	383.03	383.00	382.97	382.94	382.88	382.77	382.60	382.39	382.16	382.24
Mode 9	423.00	423.00	423.00	423.00	423.00	423.02	423.02	422.93	422.67	422.24	421.73
Mode 10	579.08	579.08	579.08	579.07	579.06	579.05	579.02	578.90	578.62	578.21	577.76
Mode 11	606.48	606.48	606.48	606.47	606.46	606.45	606.41	606.32	606.12	605.82	605.45
Mode 12	713.04	713.04	713.05	713.09	713.14	713.21	713.30	713.41	713.61	713.99	715.07
Mode 13	754.48	754.48	754.50	754.54	754.59	754.63	754.65	754.63	754.58	754.48	754.31
Mode 14	963.20	963.19	963.14	963.03	962.84	962.56	962.13	961.48	960.54	959.16	957.21
Mode 15	1016.07	1016.07	1016.08	1016.09	1016.13	1016.21	1016.33	1016.51	1016.74	1017.04	1017.43
Mode 16	1017.33	1017.32	1017.25	1017.09	1016.77	1016.17	1015.15	1013.54	1011.17	1007.89	1003.54
Mode 17	1039.29	1039.29	1039.30	1039.32	1039.38	1039.48	1039.66	1039.89	1040.17	1040.51	1040.92
Mode 18	1057.60	1057.60	1057.64	1057.73	1057.84	1057.95	1058.04	1058.15	1058.31	1058.46	1058.30
Mode 19	1063.76	1063.77	1063.81	1063.89	1063.95	1063.94	1063.81	1063.54	1063.13	1062.55	1061.68
Mode 20	1071.35	1071.35	1071.37	1071.42	1071.53	1071.71	1072.00	1072.49	1073.37	1074.78	1076.83
Mode 21	1100.82	1100.82	1100.81	1100.80	1100.80	1100.80	1100.80	1100.83	1100.95	1101.32	1102.42
Mode 22	1139.60	1139.59	1139.57	1139.52	1139.49	1139.47	1139.42	1139.29	1139.01	1138.50	1137.68
Mode 23	1149.87	1149.87	1149.85	1149.80	1149.74	1149.67	1149.55	1149.38	1149.12	1148.76	1148.29
Mode 24	1214.12	1214.12	1214.13	1214.14	1214.14	1214.12	1214.05	1213.95	1213.89	1214.00	1214.34
Mode 25	1230.90	1230.90	1230.90	1230.90	1230.91	1230.95	1231.01	1231.10	1231.25	1231.53	1232.02
Mode 26	1290.57	1290.57	1290.58	1290.59	1290.63	1290.68	1290.78	1290.92	1291.12	1291.35	1291.56
Mode 27	1343.49	1343.49	1343.49	1343.50	1343.55	1343.68	1343.92	1344.30	1344.85	1345.68	1346.98

Mode 28	1402.13	1402.13	1402.13	1402.13	1402.16	1402.25	1402.43	1402.70	1403.07	1403.56	1404.20
Mode 29	1414.88	1414.88	1414.88	1414.87	1414.88	1414.91	1414.98	1415.11	1415.34	1415.75	1416.43
Mode 30	1421.01	1421.01	1421.02	1421.05	1421.12	1421.22	1421.40	1421.65	1422.02	1422.60	1423.49
Mode 31	1432.68	1432.68	1432.68	1432.67	1432.70	1432.78	1432.97	1433.24	1433.59	1434.12	1434.96
Mode 32	1437.77	1437.77	1437.77	1437.79	1437.86	1437.99	1438.21	1438.51	1438.92	1439.58	1440.73
Mode 33	1545.45	1545.45	1545.45	1545.48	1545.56	1545.70	1545.93	1546.27	1546.73	1547.32	1548.05
Mode 34	1563.26	1563.27	1563.27	1563.30	1563.38	1563.52	1563.77	1564.12	1564.60	1565.23	1566.03
Mode 35	1781.51	1781.51	1781.51	1781.50	1781.50	1781.51	1781.54	1781.58	1781.67	1781.80	1781.99
Mode 36	1828.26	1828.26	1828.26	1828.27	1828.28	1828.28	1828.26	1828.21	1828.18	1828.24	1828.49
Mode 37	1875.88	1875.88	1875.88	1875.87	1875.87	1875.88	1875.91	1875.97	1876.10	1876.37	1876.88
Mode 38	1881.32	1881.28	1881.15	1881.07	1881.18	1881.46	1881.81	1882.15	1882.49	1882.93	1883.64
Mode 39	3303.32	3303.32	3303.32	3303.33	3303.35	3303.38	3303.43	3303.51	3303.58	3303.58	3303.46
Mode 40	3318.91	3318.91	3318.91	3318.92	3318.93	3318.97	3319.05	3319.16	3319.27	3319.33	3319.33
Mode 41	3305.56	3305.56	3305.53	3305.44	3305.28	3305.09	3305.01	3305.16	3305.50	3305.67	3305.40
Mode 42	3340.76	3340.76	3340.76	3340.78	3340.83	3340.93	3341.10	3341.31	3341.45	3341.43	3341.35
Mode 43	3284.13	3284.13	3284.08	3283.96	3283.76	3283.51	3283.37	3283.50	3283.77	3283.70	3282.94
Mode 44	3333.61	3333.61	3333.61	3333.62	3333.65	3333.71	3333.82	3333.96	3334.09	3334.15	3334.17
Mode 45	3299.39	3299.39	3299.36	3299.26	3299.08	3298.83	3298.63	3298.68	3299.04	3299.38	3299.24
Mode 46	3342.53	3342.53	3342.54	3342.55	3342.60	3342.68	3342.82	3343.02	3343.20	3343.27	3343.24
Mode 47	3421.07	3421.07	3421.08	3421.10	3421.15	3421.25	3421.41	3421.66	3422.00	3422.30	3422.38
Mode 48	3429.52	3429.52	3429.53	3429.57	3429.63	3429.75	3429.95	3430.23	3430.55	3430.77	3430.74
ZPE	35698.0	35697.9	35697.9	35697.9	35698.0	35698.2	35698.6	35699.0	35699.5	35699.9	35700.8

Table S2. Calculated HF/cc-pVDZ 1MR L-VSCF frequencies (in cm^{-1}) for octatetraene calculated using Coulomb attenuated cubic and quartic terms.

$\omega (\text{a}_0^{-1})$	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50
Mode 1	442.98	442.98	442.98	442.98	442.99	443.02	443.07	443.10	442.97	442.65	442.21
Mode 2	442.99	442.99	442.99	442.99	443.00	443.03	443.08	443.10	442.98	442.65	442.21
Mode 3	515.40	515.40	515.36	515.30	515.19	515.04	514.83	514.55	514.19	513.79	513.73
Mode 4	519.41	519.40	519.38	519.33	519.24	519.11	518.92	518.65	518.29	517.87	517.77
Mode 5	535.89	535.89	535.88	535.88	535.89	535.92	535.95	535.91	535.65	535.17	534.60
Mode 6	535.90	535.89	535.89	535.89	535.90	535.93	535.96	535.91	535.66	535.17	534.60
Mode 7	580.93	580.92	580.89	580.83	580.72	580.55	580.28	579.86	579.24	578.38	577.39
Mode 8	625.94	625.94	625.91	625.85	625.75	625.57	625.24	624.68	623.80	622.57	621.09
Mode 9	625.37	625.37	625.36	625.36	625.35	625.37	625.45	625.57	625.63	625.56	625.40
Mode 10	625.35	625.35	625.34	625.34	625.33	625.35	625.43	625.55	625.62	625.56	625.40
Mode 11	646.60	646.59	646.57	646.54	646.47	646.30	645.92	645.21	644.02	642.23	640.03
Mode 12	904.14	904.15	904.29	904.64	905.18	905.86	906.57	907.26	907.95	908.77	910.07
Mode 13	904.66	904.67	904.81	905.16	905.70	906.38	907.10	907.78	908.48	909.31	910.61
Mode 14	894.63	894.64	894.80	895.17	895.76	896.52	897.40	898.45	899.72	901.23	902.82
Mode 15	897.82	897.84	897.99	898.36	898.95	899.70	900.58	901.62	902.88	904.38	905.98
Mode 16	876.18	876.18	876.19	876.25	876.43	876.77	877.33	878.11	879.09	880.25	881.48
Mode 17	876.17	876.17	876.18	876.25	876.42	876.76	877.32	878.11	879.09	880.25	881.48
Mode 18	938.54	938.54	938.57	938.63	938.65	938.51	938.11	937.50	936.91	936.65	937.32
Mode 19	960.22	960.22	960.24	960.28	960.27	960.07	959.56	958.77	957.89	957.21	957.17
Mode 20	975.69	975.69	975.66	975.66	975.76	975.91	976.08	976.36	976.93	977.82	978.59
Mode 21	989.04	989.03	989.00	989.00	989.09	989.23	989.39	989.64	990.17	990.97	991.57
Mode 22	1151.16	1151.15	1151.11	1151.03	1150.96	1150.88	1150.76	1150.50	1150.05	1149.34	1148.28
Mode 23	1151.16	1151.15	1151.11	1151.03	1150.96	1150.88	1150.76	1150.50	1150.05	1149.34	1148.28
Mode 24	1374.48	1374.49	1374.51	1374.55	1374.56	1374.46	1374.21	1373.78	1373.25	1372.79	1372.66
Mode 25	1374.48	1374.49	1374.51	1374.55	1374.56	1374.46	1374.21	1373.78	1373.25	1372.79	1372.66
Mode 26	1425.11	1425.12	1425.19	1425.43	1425.98	1426.99	1428.59	1430.88	1433.97	1438.15	1443.58
Mode 27	1425.11	1425.12	1425.19	1425.43	1425.98	1426.99	1428.59	1430.88	1433.97	1438.15	1443.58

Mode 28	1435.23	1435.23	1435.31	1435.60	1436.24	1437.40	1439.21	1441.82	1445.52	1450.97	1459.18
Mode 29	1435.23	1435.23	1435.31	1435.60	1436.24	1437.40	1439.21	1441.82	1445.52	1450.97	1459.18
Mode 30	1444.39	1444.40	1444.47	1444.76	1445.42	1446.63	1448.56	1451.36	1455.28	1461.03	1469.62
Mode 31	1444.39	1444.40	1444.47	1444.76	1445.42	1446.63	1448.56	1451.36	1455.28	1461.03	1469.62
Mode 32	1427.92	1427.95	1428.09	1428.23	1428.17	1427.69	1426.62	1425.04	1423.39	1422.47	1423.06
Mode 33	1557.22	1557.23	1557.27	1557.41	1557.75	1558.38	1559.39	1560.85	1562.82	1565.30	1568.18
Mode 34	1557.22	1557.23	1557.27	1557.41	1557.75	1558.38	1559.39	1560.85	1562.82	1565.30	1568.18
Mode 35	1734.75	1734.75	1734.77	1734.81	1734.83	1734.69	1734.22	1733.36	1732.27	1731.38	1731.21
Mode 36	1734.75	1734.75	1734.77	1734.81	1734.83	1734.69	1734.22	1733.36	1732.27	1731.38	1731.21
Mode 37	1748.18	1748.18	1748.17	1748.16	1748.10	1747.90	1747.43	1746.64	1745.69	1745.01	1745.18
Mode 38	1748.18	1748.18	1748.17	1748.16	1748.10	1747.90	1747.43	1746.64	1745.69	1745.01	1745.18
Mode 39	3222.82	3222.81	3222.65	3222.08	3220.88	3219.04	3217.19	3216.51	3217.45	3218.74	3218.45
Mode 40	3222.82	3222.81	3222.64	3222.08	3220.88	3219.04	3217.19	3216.51	3217.45	3218.74	3218.45
Mode 41	3223.01	3223.00	3222.86	3222.34	3221.17	3219.32	3217.51	3216.96	3218.08	3219.49	3219.08
Mode 42	3223.01	3223.00	3222.86	3222.34	3221.17	3219.32	3217.51	3216.96	3218.08	3219.49	3219.08
Mode 43	3228.22	3228.21	3228.05	3227.55	3226.48	3224.82	3223.12	3222.48	3223.51	3225.15	3225.38
Mode 44	3228.22	3228.21	3228.05	3227.55	3226.48	3224.82	3223.12	3222.48	3223.51	3225.15	3225.38
Mode 45	3244.97	3244.95	3244.87	3244.59	3243.94	3242.78	3241.25	3239.79	3238.78	3237.95	3236.63
Mode 46	3244.97	3244.95	3244.87	3244.59	3243.94	3242.78	3241.25	3239.79	3238.78	3237.95	3236.63
Mode 47	3268.32	3268.31	3268.21	3267.97	3267.45	3266.56	3265.37	3264.37	3264.16	3264.62	3264.22
Mode 48	3268.32	3268.31	3268.21	3267.97	3267.45	3266.56	3265.37	3264.37	3264.16	3264.62	3264.22
ZPE	36603.0	36603.0	36603.0	36603.2	36603.2	36603.1	36603.6	36606.3	36612.7	36622.9	36636.1

Table S3. Calculated HF/cc-pVDZ 2MR VSCF frequencies (in cm^{-1}) for octatetraene calculated using Coulomb attenuated cubic and quartic terms.

ω (a_0^{-1})	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50
Mode 1	101.70	101.70	101.73	101.82	101.89	101.88	101.73	101.45	101.08	100.47	99.15
Mode 2	121.49	121.49	121.51	121.60	121.77	121.98	122.16	122.10	121.51	120.11	117.75
Mode 3	190.92	190.92	190.91	190.89	190.80	190.53	190.05	189.42	188.67	187.76	187.37
Mode 4	287.17	287.17	287.14	287.14	287.19	287.22	287.09	286.71	286.01	284.84	282.97
Mode 5	265.61	265.62	265.62	265.69	265.86	266.13	266.43	266.34	265.14	262.40	258.29
Mode 6	283.20	283.18	283.06	282.86	282.54	281.97	281.17	280.30	279.49	279.02	281.99
Mode 7	358.25	358.25	358.26	358.27	358.28	358.30	358.31	358.21	357.65	356.28	353.53
Mode 8	421.37	421.35	421.24	421.04	420.75	420.24	419.44	418.29	416.72	414.59	412.42
Mode 9	442.12	442.11	442.11	442.13	442.26	442.56	442.94	442.77	441.04	437.13	430.97
Mode 10	592.18	592.16	592.13	592.10	592.15	592.36	592.66	592.45	590.79	587.33	582.62
Mode 11	609.22	609.22	609.21	609.21	609.26	609.41	609.63	609.51	608.27	605.43	601.06
Mode 12	756.32	756.31	756.24	756.11	755.92	755.59	755.07	754.38	753.70	753.46	755.92
Mode 13	784.40	784.40	784.36	784.27	784.12	783.84	783.34	782.59	781.51	779.70	775.20
Mode 14	977.55	977.52	977.34	976.94	976.26	975.07	973.08	969.99	965.45	958.78	948.93
Mode 15	1023.94	1023.94	1023.95	1024.01	1024.22	1024.71	1025.64	1026.98	1028.48	1029.95	1031.48
Mode 16	1029.08	1029.05	1028.88	1028.45	1027.61	1026.05	1023.30	1018.85	1012.19	1002.63	989.36
Mode 17	1048.17	1048.17	1048.18	1048.26	1048.53	1049.15	1050.27	1051.81	1053.39	1054.77	1056.09
Mode 18	1081.74	1081.74	1081.84	1082.18	1082.70	1083.27	1083.63	1083.51	1082.73	1080.94	1077.63
Mode 19	1085.47	1085.48	1085.58	1085.89	1086.32	1086.67	1086.55	1085.48	1083.05	1079.05	1073.86
Mode 20	1087.92	1087.91	1087.91	1088.00	1088.21	1088.42	1088.46	1088.36	1088.25	1088.08	1087.69
Mode 21	1116.15	1116.14	1116.07	1115.96	1115.88	1115.71	1115.23	1114.33	1113.07	1111.77	1111.73
Mode 22	1149.07	1149.05	1148.91	1148.67	1148.42	1148.11	1147.48	1146.24	1144.05	1140.42	1134.65
Mode 23	1161.13	1161.11	1160.96	1160.67	1160.27	1159.61	1158.40	1156.31	1153.01	1148.12	1141.21
Mode 24	1202.54	1202.54	1202.58	1202.67	1202.82	1203.09	1203.69	1204.82	1206.36	1208.33	1211.38
Mode 25	1227.22	1227.22	1227.25	1227.41	1227.82	1228.69	1230.25	1232.55	1235.44	1238.98	1243.64
Mode 26	1280.38	1280.38	1280.42	1280.58	1280.99	1281.83	1283.34	1285.66	1288.63	1291.91	1295.09
Mode 27	1333.68	1333.68	1333.73	1333.99	1334.75	1336.36	1339.14	1343.01	1347.41	1351.99	1357.10

Mode 28	1392.12	1392.12	1392.15	1392.40	1393.13	1394.69	1397.43	1401.23	1405.47	1409.52	1413.01
Mode 29	1402.17	1402.17	1402.18	1402.34	1402.88	1404.02	1406.01	1408.81	1412.14	1415.70	1419.15
Mode 30	1406.86	1406.86	1406.88	1407.08	1407.65	1408.86	1411.07	1414.47	1419.00	1424.55	1430.96
Mode 31	1419.83	1419.82	1419.86	1420.12	1420.92	1422.76	1426.12	1430.81	1435.91	1440.64	1444.99
Mode 32	1425.31	1425.31	1425.35	1425.59	1426.33	1427.96	1430.80	1434.69	1439.04	1443.62	1448.95
Mode 33	1530.81	1530.81	1530.82	1530.99	1531.54	1532.76	1534.86	1537.75	1540.96	1543.75	1544.31
Mode 34	1548.03	1548.03	1548.06	1548.26	1548.88	1550.22	1552.55	1555.85	1559.66	1563.28	1565.09
Mode 35	1762.97	1762.96	1762.93	1763.00	1763.31	1763.94	1764.96	1766.37	1767.86	1768.98	1769.34
Mode 36	1808.35	1808.35	1808.35	1808.49	1808.87	1809.58	1810.68	1812.22	1814.14	1816.30	1818.26
Mode 37	1853.78	1853.78	1853.80	1853.99	1854.50	1855.41	1856.76	1858.65	1861.26	1864.94	1870.22
Mode 38	1860.94	1860.92	1860.94	1861.20	1861.92	1863.17	1864.94	1867.38	1870.83	1875.87	1882.81
Mode 39	3204.67	3204.66	3204.66	3204.80	3205.31	3206.43	3208.62	3212.29	3217.13	3221.65	3224.06
Mode 40	3210.93	3210.92	3210.93	3211.08	3211.59	3212.72	3214.84	3218.30	3222.75	3226.72	3228.57
Mode 41	3205.06	3205.05	3204.99	3205.06	3205.57	3206.98	3210.17	3215.96	3223.79	3231.02	3234.53
Mode 42	3224.05	3224.04	3224.01	3224.16	3224.83	3226.54	3230.24	3236.78	3245.51	3253.86	3259.23
Mode 43	3195.90	3195.88	3195.84	3195.94	3196.48	3197.95	3201.22	3206.97	3214.29	3220.41	3221.70
Mode 44	3227.94	3227.92	3227.87	3227.96	3228.47	3229.83	3232.83	3238.25	3245.70	3252.95	3256.58
Mode 45	3205.06	3205.04	3204.95	3204.92	3205.25	3206.35	3209.02	3214.13	3221.49	3229.11	3234.08
Mode 46	3234.36	3234.34	3234.26	3234.25	3234.56	3235.63	3238.35	3243.71	3251.63	3260.14	3265.85
Mode 47	3294.98	3294.97	3294.98	3295.11	3295.54	3296.45	3298.23	3301.33	3305.76	3310.40	3312.92
Mode 48	3298.85	3298.85	3298.85	3298.99	3299.42	3300.36	3302.15	3305.25	3309.67	3314.25	3316.70
ZPE	35503.5	35503.4	35503.2	35503.9	35506.9	35513.5	35525.4	35543.1	35563.1	35578.5	35582.9

Table S4. Calculated HF/cc-pVDZ 2MR L-VSCF frequencies (in cm⁻¹) for octatetraene calculated using Coulomb attenuated cubic and quartic terms.

ω (a ₀ ⁻¹)	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50
Mode 1	445.50	445.49	445.49	445.51	445.58	445.73	445.93	445.85	444.93	442.87	439.74
Mode 2	445.50	445.50	445.50	445.52	445.59	445.75	445.94	445.87	444.95	442.90	439.81
Mode 3	516.58	516.56	516.51	516.43	516.27	515.90	515.08	513.48	510.82	507.03	503.07
Mode 4	520.52	520.51	520.46	520.38	520.23	519.85	519.00	517.33	514.53	510.56	506.32
Mode 5	538.68	538.68	538.67	538.69	538.81	539.07	539.38	539.26	537.96	535.19	531.23
Mode 6	538.71	538.71	538.70	538.72	538.84	539.09	539.40	539.27	537.95	535.16	531.16
Mode 7	578.74	578.72	578.58	578.24	577.64	576.62	574.90	572.17	568.11	562.44	554.86
Mode 8	622.21	622.19	622.05	621.70	621.07	619.95	618.02	614.88	610.14	603.50	594.78
Mode 9	622.61	622.60	622.61	622.65	622.73	622.88	623.16	623.42	623.38	622.86	621.93
Mode 10	622.62	622.64	622.65	622.69	622.77	622.93	623.20	623.48	623.45	622.94	622.03
Mode 11	641.01	641.00	640.88	640.58	639.99	638.85	636.77	633.26	627.76	619.57	608.36
Mode 12	857.79	857.79	857.80	857.91	858.09	858.22	858.04	857.22	855.55	853.14	850.92
Mode 13	858.57	858.57	858.58	858.69	858.88	859.02	858.84	858.03	856.36	853.97	851.81
Mode 14	853.53	853.53	853.60	853.79	854.05	854.25	854.16	853.64	852.56	850.71	847.48
Mode 15	856.51	856.50	856.56	856.75	857.01	857.20	857.12	856.59	855.52	853.67	850.46
Mode 16	861.07	861.09	861.12	861.25	861.59	862.27	863.38	864.74	865.95	866.71	867.06
Mode 17	861.11	861.08	861.11	861.24	861.58	862.26	863.37	864.73	865.93	866.69	867.03
Mode 18	911.29	911.28	911.23	911.12	910.85	910.20	908.95	907.01	904.36	900.96	897.31
Mode 19	931.38	931.36	931.30	931.17	930.88	930.19	928.90	926.87	924.07	920.42	916.20
Mode 20	947.56	947.52	947.37	947.12	946.84	946.50	945.98	945.29	944.33	942.47	938.13
Mode 21	959.16	959.15	959.00	958.74	958.49	958.17	957.68	957.04	956.15	954.37	950.11
Mode 22	1142.57	1142.13	1142.00	1141.74	1141.44	1141.00	1140.16	1138.61	1135.95	1131.66	1125.13
Mode 23	1142.15	1142.54	1142.40	1142.14	1141.83	1141.38	1140.52	1138.93	1136.21	1131.84	1125.19
Mode 24	1358.69	1358.66	1358.71	1358.82	1359.03	1359.38	1360.00	1361.07	1362.66	1364.68	1366.99
Mode 25	1358.75	1358.78	1358.83	1358.94	1359.15	1359.50	1360.12	1361.20	1362.79	1364.80	1367.11
Mode 26	1394.02	1394.04	1394.09	1394.37	1395.14	1396.71	1399.38	1403.11	1407.54	1412.33	1417.24
Mode 27	1394.04	1394.03	1394.08	1394.36	1395.12	1396.69	1399.35	1403.08	1407.51	1412.30	1417.23

Mode 28	1402.87	1402.90	1402.99	1403.38	1404.41	1406.49	1410.00	1414.86	1420.70	1427.56	1436.25
Mode 29	1402.88	1402.86	1402.95	1403.34	1404.37	1406.45	1409.97	1414.84	1420.69	1427.56	1436.26
Mode 30	1409.19	1409.15	1409.23	1409.64	1410.70	1412.88	1416.59	1421.77	1427.93	1435.01	1443.83
Mode 31	1409.07	1409.12	1409.21	1409.61	1410.67	1412.84	1416.55	1421.73	1427.89	1434.97	1443.78
Mode 32	1414.68	1414.70	1414.79	1414.99	1415.26	1415.51	1415.77	1416.31	1417.58	1420.23	1425.29
Mode 33	1532.74	1532.72	1532.71	1532.83	1533.34	1534.56	1536.75	1539.84	1543.41	1546.65	1547.20
Mode 34	1532.72	1532.73	1532.72	1532.84	1533.34	1534.56	1536.75	1539.84	1543.40	1546.64	1547.12
Mode 35	1720.01	1720.01	1719.95	1719.99	1720.26	1720.75	1721.42	1722.26	1723.17	1723.85	1723.70
Mode 36	1720.24	1720.21	1720.14	1720.17	1720.43	1720.92	1721.58	1722.43	1723.35	1724.06	1723.99
Mode 37	1729.71	1729.68	1729.62	1729.62	1729.78	1730.14	1730.72	1731.55	1732.64	1734.01	1735.95
Mode 38	1729.56	1729.55	1729.50	1729.51	1729.67	1730.05	1730.64	1731.49	1732.57	1733.94	1735.86
Mode 39	3128.00	3126.76	3126.61	3126.38	3126.28	3126.80	3129.08	3134.46	3142.53	3150.16	3153.15
Mode 40	3126.78	3127.96	3127.82	3127.59	3127.49	3128.01	3130.30	3135.68	3143.74	3151.37	3154.37
Mode 41	3125.61	3124.28	3124.16	3124.00	3123.94	3124.47	3126.90	3132.66	3141.38	3149.80	3153.08
Mode 42	3124.30	3125.59	3125.48	3125.31	3125.25	3125.78	3128.22	3133.98	3142.68	3151.08	3154.36
Mode 43	3131.74	3131.42	3131.23	3130.88	3130.57	3130.74	3132.44	3137.03	3144.51	3152.43	3156.84
Mode 44	3131.45	3131.70	3131.51	3131.16	3130.85	3131.02	3132.72	3137.29	3144.76	3152.66	3157.06
Mode 45	3142.76	3142.55	3142.49	3142.44	3142.52	3142.93	3144.07	3146.34	3149.32	3151.00	3148.12
Mode 46	3142.58	3142.75	3142.69	3142.63	3142.71	3143.11	3144.24	3146.50	3149.47	3151.15	3148.30
Mode 47	3164.48	3164.46	3164.42	3164.43	3164.53	3164.76	3165.30	3166.58	3168.84	3171.36	3172.33
Mode 48	3164.46	3164.47	3164.43	3164.44	3164.53	3164.75	3165.28	3166.53	3168.75	3171.22	3172.13
ZPE	36233.0	36232.9	36232.6	36233.1	36235.5	36241.3	36251.9	36267.8	36285.6	36298.3	36298.1

Table S5. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0.2 and 2.4 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.20 \text{ a}_0^{-1}$.

Cutoff (a_0)	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20	2.40
Mode 1	445.34	447.61	448.94	447.77	445.35	445.44	445.91	445.95	445.75	446.16	445.47	447.78
Mode 2	445.56	445.44	445.35	451.25	447.80	445.50	448.84	445.59	445.47	447.40	445.85	447.43
Mode 3	516.28	516.64	516.48	518.50	516.44	516.51	517.60	516.69	516.52	516.03	516.52	516.95
Mode 4	520.42	520.34	520.22	522.04	520.64	520.56	521.34	521.47	520.47	521.16	520.32	520.94
Mode 5	538.84	541.86	538.72	543.48	538.56	540.65	540.51	538.95	538.73	538.33	539.76	538.82
Mode 6	539.14	538.52	540.26	541.90	544.12	538.99	539.37	539.91	539.74	540.20	539.01	539.94
Mode 7	577.95	577.93	577.61	572.25	579.03	578.71	578.70	579.21	578.54	580.98	578.31	578.48
Mode 8	620.71	618.59	622.62	620.30	619.55	622.62	623.31	621.69	622.21	616.46	622.29	622.97
Mode 9	621.12	623.01	618.15	622.71	620.57	619.09	622.70	622.80	622.64	623.52	620.90	622.18
Mode 10	622.73	622.63	620.70	622.75	621.25	622.68	622.64	620.89	621.25	621.04	622.72	623.80
Mode 11	635.97	640.39	640.49	641.29	637.33	637.31	640.91	641.41	641.05	642.51	641.68	641.33
Mode 12	856.86	856.46	855.73	870.22	856.86	857.74	867.12	858.31	856.83	853.56	857.70	856.70
Mode 13	858.05	858.20	851.80	866.56	856.88	857.72	863.90	869.58	858.07	866.10	859.38	856.91
Mode 14	852.49	851.48	848.42	855.49	849.56	850.78	851.43	853.88	853.21	852.58	853.28	855.32
Mode 15	855.26	854.59	854.35	860.58	855.56	855.72	856.74	855.80	854.30	855.80	855.99	860.17
Mode 16	860.73	860.65	860.93	870.30	859.92	861.23	867.05	859.59	860.90	862.01	861.21	862.21
Mode 17	859.44	861.00	858.32	868.46	860.59	859.61	865.22	866.40	861.25	860.32	859.41	861.97
Mode 18	913.06	909.74	902.68	897.38	922.36	912.87	900.87	911.48	915.89	912.30	911.27	918.20
Mode 19	929.00	925.75	942.46	935.62	927.96	944.00	935.82	931.19	931.64	936.52	931.77	933.68
Mode 20	947.66	947.63	925.13	832.90	947.53	947.18	935.73	953.83	947.69	946.59	947.87	929.08
Mode 21	958.83	867.68	957.14	865.32	867.36	959.46	965.30	959.15	965.53	941.63	965.47	947.02
Mode 22	1142.08	1129.47	1156.23	1115.41	1129.22	1141.23	1130.49	1141.38	1140.96	1147.86	1142.83	1140.48
Mode 23	1142.53	1140.26	1135.38	1135.96	1133.44	1136.11	1135.49	1133.42	1136.67	1143.10	1135.11	1146.94
Mode 24	1359.10	1358.80	1358.79	1356.60	1358.76	1359.16	1356.32	1356.59	1358.77	1359.73	1359.47	1359.89
Mode 25	1354.01	1359.59	1357.30	1354.70	1354.53	1353.68	1354.65	1352.96	1358.91	1359.03	1353.36	1359.36
Mode 26	1394.37	1394.29	1409.82	1394.42	1394.27	1394.47	1394.23	1393.98	1393.99	1402.68	1394.21	1402.81

Mode 27	1394.37	1394.03	1394.58	1409.40	1394.32	1394.04	1407.12	1393.76	1394.23	1391.76	1394.25	1403.29
Mode 28	1402.55	1403.09	1409.97	1402.66	1411.51	1402.62	1402.22	1402.71	1405.44	1407.52	1402.91	1405.51
Mode 29	1403.84	1403.51	1403.14	1412.25	1404.46	1412.09	1409.87	1402.45	1402.90	1400.97	1403.18	1402.76
Mode 30	1409.44	1410.42	1410.08	1436.43	1409.99	1409.45	1415.23	1409.02	1413.58	1410.06	1413.29	1413.57
Mode 31	1409.49	1435.95	1410.28	1437.56	1436.35	1409.63	1414.71	1413.29	1409.63	1408.66	1409.38	1409.52
Mode 32	1414.20	1410.52	1414.86	1404.85	1410.19	1414.11	1415.96	1413.83	1415.57	1407.86	1413.61	1415.13
Mode 33	1532.21	1532.48	1532.90	1536.32	1532.75	1532.63	1534.86	1532.37	1532.56	1534.47	1532.37	1533.95
Mode 34	1532.47	1532.49	1532.89	1536.12	1532.93	1532.76	1534.66	1533.89	1532.64	1534.20	1532.56	1533.88
Mode 35	1720.40	1720.38	1715.28	1717.41	1714.57	1719.67	1719.90	1720.16	1719.81	1724.62	1720.10	1720.04
Mode 36	1712.69	1722.23	1719.91	1723.16	1718.83	1710.58	1722.18	1711.24	1720.33	1704.29	1712.14	1720.38
Mode 37	1731.57	1729.66	1724.35	1719.42	1730.78	1730.98	1726.98	1730.84	1729.97	1732.75	1731.36	1732.17
Mode 38	1729.68	1730.01	1730.29	1724.47	1730.35	1730.14	1728.71	1726.97	1729.83	1729.35	1730.46	1731.85
Mode 39	3126.68	3127.81	3128.56	2965.04	3126.88	3130.04	3099.10	3127.88	3127.62	3127.01	3126.54	3106.60
Mode 40	3128.83	2972.26	3126.92	2971.86	2972.85	3126.08	3100.73	3106.01	3107.26	3127.38	3107.17	3127.06
Mode 41	3123.78	3119.33	3085.60	3124.69	3075.46	3078.46	3124.60	3125.44	3110.20	3104.03	3124.20	3126.04
Mode 42	3129.97	3131.66	3124.40	3084.89	3128.87	3128.15	3096.64	3124.93	3126.17	3122.87	3126.28	3109.43
Mode 43	3130.38	3131.33	3131.72	3040.14	3131.49	3130.20	3055.63	3130.34	3132.06	3129.79	3130.52	3080.73
Mode 44	3131.99	3130.92	3037.16	3130.53	3129.60	3132.08	3131.76	3131.99	3131.81	3077.85	3132.53	3079.68
Mode 45	3143.49	3143.41	3142.56	3120.62	3142.49	3142.72	3136.10	3142.59	3142.49	3141.99	3142.85	3135.17
Mode 46	3143.10	3143.09	3142.60	3119.31	3142.55	3142.63	3135.93	3142.71	3142.79	3142.06	3143.06	3134.86
Mode 47	3165.25	3164.88	3165.58	3125.24	3164.69	3164.84	3135.31	3135.84	3164.77	3148.88	3164.92	3155.17
Mode 48	3165.51	3164.91	3164.78	3126.20	3164.64	3164.72	3136.00	3164.68	3164.76	3161.71	3165.01	3155.08
ZPE	36228.9	36177.0	36197.3	36071.1	36165.2	36221.5	36186.5	36221.1	36227.6	36208.9	36226.6	36199.2

Table S6. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.6 and 4.8 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.20 \text{ a}_0^{-1}$.

Cutoff (a_0)	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60	4.80
Mode 1	446.26	446.38	446.33	446.04	446.00	445.56	445.66	445.68	445.58	445.76	445.92	445.62
Mode 2	445.44	446.10	445.51	445.51	445.49	445.63	445.66	445.50	445.54	445.56	445.64	445.53
Mode 3	516.07	516.91	516.66	517.05	516.67	516.70	516.68	516.64	516.51	516.66	516.87	516.71
Mode 4	521.54	520.95	520.65	521.30	520.64	520.96	520.70	520.43	520.47	520.84	520.55	520.38
Mode 5	537.35	539.82	539.25	540.35	538.43	538.89	539.41	539.33	538.84	539.43	538.84	538.77
Mode 6	540.46	540.01	539.66	538.80	540.36	539.83	539.29	539.00	538.93	538.62	540.26	539.19
Mode 7	582.40	579.51	579.02	574.91	576.95	575.88	579.04	578.67	579.12	578.83	579.79	578.99
Mode 8	617.30	622.68	622.58	622.74	621.86	622.08	622.31	621.95	622.42	622.55	622.53	622.15
Mode 9	620.86	619.54	621.13	624.89	624.44	620.67	620.92	620.84	622.86	623.95	624.07	622.43
Mode 10	624.58	622.82	622.56	619.91	619.83	622.73	622.73	622.65	622.55	622.29	622.58	623.46
Mode 11	642.86	642.10	641.77	642.11	641.86	642.04	641.85	641.86	641.05	642.05	642.63	641.69
Mode 12	857.83	857.90	854.86	860.74	857.00	856.87	857.11	858.43	856.25	857.58	856.68	857.85
Mode 13	862.75	859.21	862.84	861.69	858.39	859.02	857.51	858.81	857.77	857.75	857.34	858.91
Mode 14	853.26	852.57	853.12	850.52	852.95	853.42	852.78	853.12	852.64	852.86	852.01	853.34
Mode 15	855.97	854.00	856.30	853.65	854.39	854.61	855.32	856.52	855.57	855.96	855.66	856.23
Mode 16	863.51	862.99	861.04	861.44	859.82	861.01	860.83	861.26	860.77	859.79	859.34	859.66
Mode 17	859.16	861.16	861.46	862.51	860.32	859.32	859.20	859.49	860.73	860.54	858.87	860.93
Mode 18	910.07	916.81	911.65	913.35	913.71	914.13	912.62	910.94	912.53	911.56	911.73	910.97
Mode 19	931.62	931.98	931.80	934.74	931.49	931.27	931.16	931.45	931.46	931.77	932.59	931.45
Mode 20	947.91	954.95	954.62	948.48	947.68	947.40	948.83	947.39	948.81	948.78	948.87	947.55
Mode 21	958.66	966.37	959.38	960.91	960.27	959.28	960.32	959.14	960.49	959.17	960.24	959.16
Mode 22	1141.04	1135.35	1136.09	1140.65	1142.17	1142.07	1142.84	1142.41	1142.30	1142.49	1142.30	1142.63
Mode 23	1141.50	1135.91	1141.95	1141.24	1143.11	1142.67	1142.25	1142.11	1142.88	1142.63	1143.03	1142.08
Mode 24	1354.44	1359.63	1358.99	1357.66	1361.75	1353.12	1361.07	1357.46	1358.94	1356.69	1356.33	1355.01
Mode 25	1363.76	1353.34	1353.75	1358.63	1352.20	1359.21	1351.54	1354.98	1358.93	1358.24	1353.01	1358.89
Mode 26	1390.69	1396.00	1396.31	1394.06	1394.28	1394.18	1394.29	1394.04	1394.13	1394.20	1394.25	1394.20

Mode 27	1394.46	1395.72	1393.98	1396.82	1396.67	1393.85	1394.06	1394.24	1394.00	1396.19	1396.28	1395.23
Mode 28	1404.93	1405.99	1403.11	1402.99	1401.15	1404.87	1403.46	1403.18	1403.01	1401.07	1400.84	1402.27
Mode 29	1397.45	1402.15	1402.33	1405.64	1403.58	1402.74	1402.48	1402.45	1403.50	1403.36	1403.62	1402.84
Mode 30	1413.54	1413.25	1408.88	1412.82	1412.05	1409.60	1409.82	1409.07	1410.08	1409.44	1410.02	1409.23
Mode 31	1405.98	1413.37	1413.37	1407.41	1407.21	1408.69	1409.67	1408.94	1410.41	1409.77	1409.19	1409.35
Mode 32	1411.83	1413.36	1413.40	1412.01	1412.98	1411.86	1413.04	1412.95	1414.61	1412.08	1410.71	1411.63
Mode 33	1533.89	1532.96	1532.98	1533.93	1533.08	1532.84	1532.42	1532.46	1532.55	1533.10	1532.82	1532.78
Mode 34	1533.52	1533.09	1532.65	1533.40	1533.08	1532.46	1532.56	1532.66	1532.68	1532.65	1532.61	1532.43
Mode 35	1713.99	1721.70	1719.97	1720.46	1713.65	1713.65	1719.62	1720.32	1719.49	1712.37	1712.11	1713.77
Mode 36	1712.15	1711.15	1711.06	1709.45	1713.71	1720.51	1712.18	1711.31	1720.36	1721.04	1715.14	1721.16
Mode 37	1730.90	1731.77	1731.60	1731.24	1729.68	1729.95	1730.36	1730.73	1729.46	1729.89	1730.28	1729.92
Mode 38	1727.58	1731.33	1730.47	1726.41	1731.54	1727.94	1730.01	1729.90	1729.89	1729.61	1729.43	1730.02
Mode 39	3129.47	3105.78	3129.06	3121.86	3127.80	3126.61	3123.51	3126.47	3124.34	3128.01	3121.48	3126.42
Mode 40	3125.78	3105.79	3104.78	3123.71	3123.58	3128.10	3123.24	3128.84	3123.08	3122.33	3123.96	3128.30
Mode 41	3128.34	3125.46	3126.31	3111.53	3113.56	3113.74	3125.25	3123.81	3126.09	3120.99	3119.72	3124.04
Mode 42	3120.15	3109.41	3124.05	3116.14	3125.40	3125.80	3120.82	3126.20	3120.44	3124.42	3121.22	3126.05
Mode 43	3127.74	3122.73	3132.24	3128.58	3131.20	3131.87	3132.06	3131.85	3131.81	3131.47	3131.22	3131.56
Mode 44	3130.95	3120.27	3119.91	3132.16	3130.27	3132.00	3131.45	3131.75	3131.50	3131.55	3132.14	3131.75
Mode 45	3141.54	3143.60	3143.11	3141.72	3142.31	3142.58	3143.38	3142.64	3143.59	3142.94	3143.48	3143.06
Mode 46	3141.58	3142.62	3142.50	3142.91	3142.26	3142.87	3142.77	3143.36	3143.50	3142.19	3142.64	3142.73
Mode 47	3154.36	3154.17	3154.44	3154.00	3164.48	3164.85	3165.05	3164.58	3164.80	3164.51	3165.02	3164.83
Mode 48	3161.88	3154.13	3164.77	3152.77	3163.16	3164.44	3165.05	3164.60	3165.11	3163.82	3164.23	3164.79
ZPE	36224.1	36213.9	36223.1	36220.0	36225.1	36226.8	36227.7	36229.6	36232.0	36228.8	36224.1	36230.9

Table S7. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 5.0 and 7.2 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.20 \text{ a}_0^{-1}$.

Cutoff (a_0)	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00	7.20
Mode 1	445.49	445.57	445.55	445.50	445.55	445.49	445.49	445.53	445.54	445.50	445.49	445.50
Mode 2	445.51	445.47	445.53	445.57	445.53	445.54	445.48	445.54	445.53	445.50	445.50	445.50
Mode 3	516.58	516.56	516.60	516.66	516.59	516.58	516.59	516.59	516.59	516.60	516.57	516.58
Mode 4	520.53	520.55	520.57	520.61	520.51	520.53	520.54	520.53	520.53	520.54	520.52	520.52
Mode 5	538.72	538.55	538.80	538.83	538.81	538.78	538.64	538.77	538.74	538.70	538.68	538.68
Mode 6	538.70	538.93	538.82	538.89	538.72	538.69	538.66	538.75	538.78	538.68	538.71	538.71
Mode 7	578.63	578.50	578.78	578.99	578.96	578.72	578.76	578.78	578.78	578.73	578.74	578.74
Mode 8	622.16	622.16	622.13	622.13	622.22	622.23	622.20	622.23	622.23	622.21	622.21	622.22
Mode 9	622.62	622.78	622.60	622.49	622.68	622.62	622.52	622.61	622.61	622.62	622.60	622.61
Mode 10	622.66	622.49	622.74	622.71	622.59	622.66	622.61	622.65	622.65	622.61	622.64	622.62
Mode 11	640.94	640.85	641.01	641.26	640.97	640.96	640.81	640.97	641.00	640.93	640.99	641.01
Mode 12	857.98	857.83	857.37	858.09	857.20	857.25	857.65	857.19	857.18	857.64	857.78	857.82
Mode 13	858.67	858.14	858.83	858.03	857.50	858.40	858.72	857.88	857.85	858.37	858.57	858.59
Mode 14	853.49	853.50	853.48	853.54	853.61	853.53	853.44	853.60	853.61	853.54	853.53	853.53
Mode 15	856.50	856.46	856.49	856.52	856.57	856.49	856.40	856.58	856.58	856.52	856.50	856.51
Mode 16	861.09	861.72	859.70	859.74	861.03	861.12	860.79	861.13	861.09	860.99	861.08	861.11
Mode 17	861.06	860.33	861.30	859.75	860.88	860.99	861.13	861.10	861.12	860.96	861.07	861.07
Mode 18	911.29	911.28	911.32	911.29	911.34	911.30	911.33	911.33	911.33	911.29	911.29	911.29
Mode 19	931.36	931.33	931.34	931.35	931.41	931.38	931.39	931.41	931.41	931.37	931.37	931.37
Mode 20	947.57	947.54	948.24	948.20	948.19	947.50	948.14	948.10	948.11	947.54	947.55	947.55
Mode 21	959.18	959.93	959.18	959.18	959.81	959.82	959.14	959.72	959.72	959.15	959.17	959.15
Mode 22	1142.53	1142.53	1142.63	1142.13	1142.27	1142.25	1142.17	1142.66	1142.66	1142.56	1142.56	1142.57
Mode 23	1142.12	1142.26	1142.14	1142.55	1142.64	1142.57	1142.64	1142.25	1142.25	1142.14	1142.15	1142.15
Mode 24	1358.87	1358.45	1358.66	1358.23	1358.62	1358.83	1358.44	1358.70	1358.82	1358.72	1358.78	1358.75
Mode 25	1358.76	1359.10	1359.09	1358.99	1358.91	1358.73	1358.70	1358.82	1358.69	1358.69	1358.66	1358.70
Mode 26	1394.05	1394.22	1394.10	1394.08	1394.11	1394.06	1394.07	1394.04	1394.03	1394.07	1394.03	1394.04

Mode 27	1394.06	1393.89	1394.01	1393.81	1394.00	1394.05	1393.96	1394.03	1394.04	1394.02	1394.04	1394.02
Mode 28	1402.86	1403.02	1402.87	1402.75	1402.88	1402.83	1402.93	1402.86	1402.83	1402.85	1402.85	1402.88
Mode 29	1402.91	1402.77	1402.81	1402.79	1402.81	1402.86	1402.86	1402.83	1402.87	1402.85	1402.89	1402.87
Mode 30	1409.22	1409.84	1409.60	1409.10	1409.60	1409.62	1409.69	1409.54	1409.50	1409.10	1409.14	1409.06
Mode 31	1409.18	1409.01	1409.08	1409.47	1409.64	1409.19	1409.30	1409.51	1409.52	1409.19	1409.11	1409.18
Mode 32	1414.55	1414.63	1414.43	1413.46	1414.55	1414.66	1415.06	1414.51	1414.48	1414.41	1414.61	1414.55
Mode 33	1532.69	1532.42	1532.50	1532.66	1532.66	1532.73	1532.74	1532.74	1532.74	1532.74	1532.73	1532.72
Mode 34	1532.72	1533.01	1532.75	1532.57	1532.73	1532.71	1532.76	1532.73	1532.74	1532.76	1532.72	1532.74
Mode 35	1719.86	1719.82	1719.76	1719.04	1719.87	1720.03	1720.42	1719.87	1720.07	1720.20	1720.23	1720.25
Mode 36	1719.70	1719.96	1718.95	1718.58	1720.03	1719.77	1720.55	1720.08	1719.89	1719.98	1720.03	1720.01
Mode 37	1729.53	1729.60	1729.69	1729.57	1729.71	1729.58	1729.58	1729.71	1729.58	1729.51	1729.57	1729.56
Mode 38	1729.65	1729.56	1729.50	1729.33	1729.55	1729.70	1729.46	1729.59	1729.71	1729.64	1729.70	1729.71
Mode 39	3127.23	3127.12	3128.17	3124.57	3124.59	3127.04	3128.26	3124.90	3126.09	3126.84	3127.99	3126.78
Mode 40	3128.43	3125.83	3124.73	3128.20	3125.84	3125.84	3124.89	3126.03	3124.86	3128.05	3126.79	3128.00
Mode 41	3124.51	3124.44	3125.57	3124.18	3124.29	3124.29	3125.65	3124.30	3125.61	3124.32	3124.30	3124.30
Mode 42	3125.82	3125.89	3124.34	3125.53	3125.61	3125.59	3124.31	3125.61	3124.30	3125.62	3125.61	3125.61
Mode 43	3131.46	3131.49	3131.78	3131.50	3131.47	3131.46	3131.69	3131.47	3131.76	3131.44	3131.73	3131.45
Mode 44	3131.73	3131.70	3131.47	3131.76	3131.74	3131.76	3131.45	3131.76	3131.48	3131.73	3131.45	3131.74
Mode 45	3142.61	3142.56	3142.64	3142.55	3142.37	3142.58	3142.96	3142.38	3142.58	3142.55	3142.77	3142.58
Mode 46	3142.84	3142.84	3142.64	3142.68	3142.60	3142.78	3142.73	3142.58	3142.38	3142.72	3142.57	3142.75
Mode 47	3164.45	3164.44	3164.32	3164.56	3164.18	3164.36	3164.71	3164.26	3164.41	3164.69	3164.42	3164.33
Mode 48	3164.59	3164.42	3164.58	3165.55	3165.36	3164.34	3164.52	3164.36	3164.29	3164.65	3164.45	3164.34
ZPE	36233.2	36232.7	36232.1	36231.2	36232.2	36232.5	36233.1	36232.2	36232.2	36232.8	36233.0	36232.9

Table S8. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.4 and 8.0 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.20 \text{ a}_0^{-1}$, and the unattenuated 2MR result.

Cutoff (a_0)	7.40	7.60	7.80	8.00	2MR
Mode 1	445.49	445.49	445.49	445.49	445.50
Mode 2	445.50	445.50	445.50	445.50	445.51
Mode 3	516.58	516.58	516.57	516.58	516.57
Mode 4	520.52	520.52	520.52	520.52	520.52
Mode 5	538.71	538.71	538.71	538.71	538.71
Mode 6	538.68	538.68	538.68	538.68	538.68
Mode 7	578.74	578.74	578.74	578.74	578.74
Mode 8	622.21	622.21	622.21	622.21	622.21
Mode 9	622.60	622.60	622.60	622.60	622.60
Mode 10	622.64	622.64	622.64	622.64	622.64
Mode 11	641.01	641.01	641.01	641.01	641.02
Mode 12	857.82	857.82	857.77	857.83	857.80
Mode 13	858.60	858.60	858.60	858.61	858.58
Mode 14	853.53	853.53	853.53	853.53	853.54
Mode 15	856.50	856.50	856.50	856.50	856.51
Mode 16	861.11	861.11	861.09	861.11	861.09
Mode 17	861.10	861.10	861.09	861.10	861.08
Mode 18	911.29	911.30	911.29	911.29	911.30
Mode 19	931.37	931.37	931.37	931.37	931.37
Mode 20	947.55	947.55	947.55	947.55	947.55
Mode 21	959.17	959.17	959.17	959.16	959.17
Mode 22	1142.56	1142.57	1142.15	1142.56	1142.57
Mode 23	1142.15	1142.16	1142.56	1142.15	1142.15
Mode 24	1358.78	1358.78	1358.66	1358.78	1358.78
Mode 25	1358.67	1358.67	1358.78	1358.67	1358.66
Mode 26	1394.03	1394.03	1394.04	1394.03	1394.03

Mode 27	1394.04	1394.04	1394.03	1394.04	1394.04
Mode 28	1402.86	1402.86	1402.89	1402.85	1402.86
Mode 29	1402.89	1402.89	1402.86	1402.89	1402.89
Mode 30	1409.14	1409.14	1409.14	1409.11	1409.12
Mode 31	1409.11	1409.11	1409.11	1409.14	1409.15
Mode 32	1414.59	1414.59	1414.61	1414.60	1414.68
Mode 33	1532.74	1532.74	1532.73	1532.74	1532.73
Mode 34	1532.73	1532.73	1532.73	1532.73	1532.73
Mode 35	1720.23	1720.23	1720.03	1720.23	1720.23
Mode 36	1720.03	1720.03	1720.23	1720.03	1720.03
Mode 37	1729.58	1729.58	1729.69	1729.58	1729.57
Mode 38	1729.70	1729.70	1729.57	1729.70	1729.69
Mode 39	3126.79	3127.99	3126.79	3126.79	3126.79
Mode 40	3127.99	3126.79	3127.99	3127.99	3127.99
Mode 41	3124.30	3125.61	3124.30	3124.30	3124.30
Mode 42	3125.61	3124.30	3125.61	3125.61	3125.61
Mode 43	3131.45	3131.73	3131.45	3131.45	3131.45
Mode 44	3131.73	3131.45	3131.73	3131.73	3131.73
Mode 45	3142.57	3142.77	3142.57	3142.57	3142.57
Mode 46	3142.76	3142.57	3142.77	3142.76	3142.77
Mode 47	3164.33	3164.34	3164.46	3164.33	3164.47
Mode 48	3164.34	3164.33	3164.34	3164.34	3164.48
ZPE	36233.0	36233.0	36233.0	36233.0	36233.0

Table S9. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0.2 and 2.4 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.25 \text{ a}_0^{-1}$.

Cutoff (a_0)	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20	2.40
Mode 1	446.00	447.66	448.05	448.24	451.65	448.77	445.39	445.39	448.63	445.58	446.38	445.76
Mode 2	445.37	445.28	451.66	450.42	450.53	445.26	445.31	445.82	448.32	447.83	445.35	445.36
Mode 3	515.72	516.37	520.54	516.37	516.50	516.22	516.23	516.34	517.53	515.22	516.15	516.44
Mode 4	519.49	520.10	524.99	522.00	521.75	520.00	520.21	520.34	521.39	519.46	521.28	520.62
Mode 5	539.32	538.09	543.37	543.32	544.02	539.12	538.65	539.26	539.97	539.60	538.76	538.60
Mode 6	539.42	542.11	541.85	543.82	544.02	538.77	538.50	538.61	541.11	539.20	540.66	539.22
Mode 7	575.72	571.57	572.43	569.09	578.18	577.93	578.12	578.14	574.49	574.86	582.28	579.21
Mode 8	617.45	621.31	619.20	617.92	618.33	620.76	620.98	621.78	620.84	619.66	616.52	621.96
Mode 9	620.97	623.07	618.44	619.15	620.63	624.40	622.87	622.82	622.29	624.98	618.94	622.89
Mode 10	620.69	622.87	621.02	623.63	621.60	622.83	622.90	622.84	621.56	626.03	622.54	622.74
Mode 11	633.02	639.50	640.26	641.63	637.48	639.68	639.57	639.90	642.48	638.15	643.35	640.64
Mode 12	856.48	857.33	904.23	869.06	864.20	857.23	857.84	857.40	864.57	856.99	857.89	857.96
Mode 13	857.29	857.05	901.13	865.64	865.13	852.11	858.56	858.74	866.04	853.15	869.27	862.63
Mode 14	851.11	850.67	859.40	852.54	851.74	848.11	853.04	852.90	856.72	853.37	853.44	853.35
Mode 15	854.55	853.23	864.98	860.55	855.38	855.25	856.05	855.82	857.74	857.23	853.98	856.22
Mode 16	860.03	860.50	823.62	871.55	867.02	861.21	861.40	861.28	864.72	862.43	864.17	860.99
Mode 17	858.62	860.75	821.31	866.56	865.90	858.95	861.39	861.36	864.67	860.60	858.95	863.09
Mode 18	909.89	907.24	910.04	911.13	909.64	902.04	911.01	911.08	903.99	912.38	910.13	911.80
Mode 19	930.58	927.77	922.11	936.86	929.83	929.04	931.44	931.69	929.05	934.09	936.30	931.89
Mode 20	947.42	855.81	830.21	831.28	831.13	935.75	947.94	948.01	933.54	930.58	948.23	954.55
Mode 21	958.70	959.63	864.64	864.80	840.80	957.73	959.76	966.16	945.04	964.28	958.53	959.80
Mode 22	1142.81	1128.86	1125.39	1129.52	1130.23	1136.19	1141.79	1141.16	1142.36	1140.33	1140.58	1134.15
Mode 23	1142.71	1140.08	1117.29	1114.14	1129.60	1153.03	1142.12	1135.12	1141.75	1145.29	1142.17	1141.16
Mode 24	1354.48	1359.35	1351.63	1356.92	1356.21	1359.09	1359.03	1359.08	1353.72	1364.26	1354.61	1359.13
Mode 25	1354.53	1359.95	1350.13	1356.07	1348.72	1357.99	1358.83	1358.91	1351.20	1364.82	1357.55	1359.57
Mode 26	1394.49	1394.57	1394.44	1394.61	1409.79	1407.34	1394.22	1394.02	1406.70	1404.02	1391.34	1394.53

Mode 27	1398.11	1394.45	1410.65	1412.60	1412.23	1394.21	1394.22	1394.01	1406.28	1394.93	1395.01	1394.58
Mode 28	1405.22	1403.02	1403.22	1416.26	1416.39	1403.95	1403.75	1403.25	1406.27	1405.94	1405.87	1403.37
Mode 29	1405.62	1404.35	1412.48	1412.78	1413.92	1404.35	1403.18	1403.38	1406.44	1406.37	1401.50	1403.22
Mode 30	1413.40	1410.54	1438.50	1441.36	1440.00	1415.55	1409.92	1409.94	1412.22	1415.36	1412.72	1414.53
Mode 31	1412.74	1438.50	1438.22	1441.04	1441.89	1409.84	1410.04	1414.41	1413.62	1411.35	1405.71	1410.01
Mode 32	1397.91	1411.00	1405.25	1388.40	1385.28	1415.68	1415.28	1415.97	1407.20	1425.79	1406.92	1415.87
Mode 33	1531.14	1532.59	1521.07	1536.10	1536.11	1533.06	1532.80	1532.58	1534.64	1532.41	1533.66	1533.09
Mode 34	1532.99	1532.68	1520.96	1537.33	1537.15	1532.91	1532.78	1532.45	1534.67	1532.29	1534.47	1532.56
Mode 35	1696.40	1720.64	1718.41	1696.85	1695.15	1721.31	1721.59	1720.48	1716.10	1731.14	1714.42	1719.71
Mode 36	1694.80	1723.23	1723.08	1704.57	1694.90	1720.88	1720.11	1719.81	1711.79	1732.25	1703.09	1719.95
Mode 37	1734.48	1730.26	1715.00	1726.33	1722.77	1732.48	1730.61	1730.22	1730.91	1735.14	1729.71	1730.96
Mode 38	1732.86	1730.37	1720.83	1732.25	1732.32	1731.19	1731.09	1730.54	1731.01	1733.78	1732.65	1730.68
Mode 39	3127.83	3129.44	2963.46	2961.63	2960.20	3130.23	3128.96	3128.69	3103.00	3128.22	3129.25	3129.81
Mode 40	3128.18	2968.47	2969.77	2969.04	2972.26	3098.75	3130.16	3106.76	3104.87	3107.32	3127.00	3105.55
Mode 41	3126.74	3127.53	3122.87	3072.50	3086.54	3127.47	3126.16	3125.66	3122.01	3127.76	3109.90	3126.76
Mode 42	3126.83	3125.73	3087.13	3081.57	3070.96	3125.47	3127.51	3126.86	3107.01	3128.94	3119.11	3125.40
Mode 43	3131.43	3132.67	3030.32	3040.44	3038.60	3132.74	3132.63	3132.66	3063.51	3134.20	3128.52	3132.94
Mode 44	3133.32	3131.19	3131.75	3131.46	3040.44	3055.26	3133.04	3132.79	3064.47	3081.66	3130.55	3132.48
Mode 45	3145.24	3144.52	3107.54	3121.58	3121.22	3143.66	3143.06	3143.01	3136.55	3144.34	3142.00	3143.34
Mode 46	3146.51	3144.35	3107.69	3121.45	3121.82	3143.31	3143.49	3143.48	3136.66	3144.83	3142.22	3143.08
Mode 47	3171.64	3165.76	3032.27	3126.03	3131.68	3165.75	3165.14	3165.05	3133.34	3164.96	3143.01	3154.91
Mode 48	3167.73	3165.85	3032.89	3131.93	3126.95	3165.50	3165.14	3165.06	3140.84	3164.30	3166.52	3165.61
ZPE	36219.8	36178.4	36004.9	36054.7	36026.9	36209.6	36237.1	36231.7	36171.6	36236.4	36218.7	36232.2

Table S10. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm⁻¹) for octatetraene with couplings between modes centered beyond cutoff distance between 2.6 and 4.8 a₀ calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of ω = 0.25 a₀⁻¹.

Cutoff (a ₀)	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60	4.80
Mode 1	446.01	446.28	445.94	445.82	445.57	445.88	445.69	445.59	445.62	445.53	445.49	445.49
Mode 2	446.34	445.84	445.38	445.39	445.63	445.55	445.73	445.53	445.55	445.51	445.50	445.50
Mode 3	516.66	516.57	516.48	516.78	516.50	516.68	516.79	516.49	516.61	516.65	516.56	516.60
Mode 4	520.62	520.63	520.56	520.16	520.80	520.19	520.85	520.46	520.44	520.64	520.50	520.50
Mode 5	539.77	540.43	539.28	538.17	539.64	538.64	539.81	538.85	539.28	539.08	538.70	538.75
Mode 6	539.34	540.09	539.47	539.56	539.31	539.57	539.83	538.96	539.03	538.89	538.68	538.67
Mode 7	578.51	579.54	578.41	577.10	578.26	579.19	579.08	578.91	578.55	578.68	578.53	578.50
Mode 8	623.32	623.23	622.04	622.20	621.36	621.89	622.43	622.41	621.95	622.09	621.94	621.98
Mode 9	621.43	619.25	620.90	624.44	620.24	621.74	620.91	622.67	620.89	622.45	622.67	622.57
Mode 10	621.61	621.38	622.68	621.75	623.42	622.36	620.82	622.80	622.66	623.12	622.68	622.75
Mode 11	641.02	641.87	641.34	640.73	641.63	642.14	642.66	640.96	641.80	641.47	640.90	640.87
Mode 12	857.74	853.11	858.14	862.09	856.94	857.53	856.94	857.16	858.16	858.05	858.04	858.05
Mode 13	858.00	862.13	858.87	857.45	858.74	859.06	857.66	857.03	859.48	859.44	858.79	858.83
Mode 14	851.53	851.11	853.08	851.24	853.38	853.23	852.47	852.66	853.56	853.56	853.52	853.54
Mode 15	854.46	853.59	856.38	856.34	854.38	856.29	855.41	855.68	856.30	856.32	856.56	856.58
Mode 16	861.39	860.86	860.99	863.23	860.65	861.28	859.24	860.95	861.23	861.20	861.09	861.04
Mode 17	861.34	861.32	859.43	860.42	859.59	859.03	859.21	860.78	859.56	859.71	861.11	861.11
Mode 18	917.17	916.88	911.84	913.95	914.76	910.60	912.56	911.32	911.02	911.09	911.31	911.29
Mode 19	937.26	936.99	931.71	931.92	931.51	931.83	932.58	932.81	931.41	931.37	931.38	931.38
Mode 20	949.34	955.31	948.05	947.80	947.74	947.89	949.01	949.02	947.49	947.59	947.64	947.62
Mode 21	967.52	966.15	965.92	961.76	960.86	960.85	960.54	960.67	959.18	959.23	959.24	959.22
Mode 22	1142.38	1136.63	1136.22	1140.75	1142.21	1142.23	1142.36	1142.77	1142.08	1142.04	1142.54	1142.11
Mode 23	1137.34	1135.73	1141.86	1142.64	1142.76	1142.65	1142.77	1142.52	1142.43	1142.43	1142.10	1142.50
Mode 24	1359.33	1359.27	1359.56	1358.75	1359.63	1359.02	1356.13	1359.28	1359.43	1354.16	1359.00	1358.54
Mode 25	1359.56	1353.52	1353.37	1361.70	1352.92	1355.14	1351.58	1359.05	1353.29	1359.28	1359.03	1359.35
Mode 26	1397.04	1396.29	1394.48	1396.75	1394.14	1396.08	1394.31	1394.13	1394.23	1394.18	1394.20	1394.00

Mode 27	1396.82	1394.28	1394.32	1394.19	1394.64	1394.39	1394.35	1394.12	1394.20	1394.34	1394.25	1394.16
Mode 28	1405.79	1405.74	1403.71	1404.70	1404.95	1403.54	1403.75	1403.84	1403.05	1402.98	1402.94	1402.87
Mode 29	1406.25	1405.74	1402.81	1401.56	1403.15	1400.03	1403.42	1402.85	1402.65	1403.06	1402.94	1402.93
Mode 30	1410.07	1413.79	1413.92	1408.74	1409.87	1409.77	1410.05	1410.69	1409.28	1409.42	1409.37	1409.31
Mode 31	1413.89	1413.85	1409.68	1412.68	1409.92	1410.09	1409.70	1410.64	1409.28	1408.97	1409.49	1409.37
Mode 32	1415.12	1413.98	1413.38	1414.56	1413.04	1412.92	1410.22	1414.73	1413.15	1412.19	1414.51	1414.35
Mode 33	1533.20	1533.05	1532.48	1533.01	1532.61	1532.59	1532.58	1532.65	1532.50	1532.85	1532.71	1532.72
Mode 34	1533.29	1532.70	1532.68	1533.92	1532.60	1532.91	1532.60	1532.62	1532.69	1532.69	1532.69	1532.62
Mode 35	1719.79	1720.24	1720.54	1722.78	1719.60	1721.08	1714.20	1720.22	1719.76	1716.14	1719.45	1719.79
Mode 36	1721.26	1712.43	1711.53	1713.90	1711.63	1706.71	1712.89	1719.49	1711.82	1720.09	1719.68	1719.44
Mode 37	1731.36	1732.17	1731.59	1729.98	1729.66	1731.03	1730.69	1729.66	1730.63	1730.09	1729.92	1729.81
Mode 38	1731.64	1731.04	1731.16	1731.79	1731.81	1730.63	1730.15	1729.97	1730.20	1729.72	1729.73	1729.43
Mode 39	3106.84	3104.32	3128.72	3123.20	3128.58	3127.18	3121.26	3123.02	3129.49	3128.40	3129.09	3128.89
Mode 40	3128.56	3106.96	3105.64	3129.04	3123.20	3124.84	3123.64	3124.26	3127.19	3127.24	3127.86	3127.68
Mode 41	3110.16	3108.07	3125.80	3126.99	3114.15	3124.31	3119.39	3124.94	3126.46	3126.00	3126.20	3126.08
Mode 42	3108.89	3110.15	3125.83	3113.55	3125.78	3126.97	3120.86	3121.92	3124.29	3124.02	3124.86	3124.63
Mode 43	3115.73	3122.09	3132.84	3131.82	3132.39	3131.24	3131.86	3131.47	3131.85	3131.86	3131.80	3131.72
Mode 44	3119.76	3130.79	3131.11	3131.22	3130.65	3131.71	3132.16	3131.92	3131.87	3131.75	3131.39	3131.49
Mode 45	3143.14	3142.94	3143.48	3142.83	3142.99	3142.97	3143.26	3143.43	3143.30	3142.95	3142.97	3142.84
Mode 46	3142.83	3142.78	3143.24	3142.99	3143.11	3143.16	3143.27	3143.30	3142.84	3142.72	3142.76	3142.69
Mode 47	3154.63	3164.99	3165.38	3163.72	3165.38	3164.70	3165.38	3165.03	3164.82	3164.95	3164.72	3164.71
Mode 48	3154.61	3153.97	3165.40	3153.57	3165.04	3164.13	3165.10	3164.82	3164.76	3164.78	3164.71	3164.68
ZPE	36219.9	36215.2	36228.5	36231.4	36228.4	36229.9	36223.9	36232.6	36230.8	36231.6	36234.2	36233.7

Table S11. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm⁻¹) for octatetraene with couplings between modes centered beyond cutoff distance between 5.0 and 7.2 a₀ calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of ω = 0.25 a₀⁻¹.

Cutoff (a ₀)	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00	7.20
Mode 1	445.53	445.50	445.64	445.65	445.73	445.54	445.49	445.49	445.55	445.49	445.49	445.50
Mode 2	445.49	445.51	445.50	445.47	445.47	445.51	445.51	445.46	445.54	445.50	445.49	445.48
Mode 3	516.56	516.58	516.73	516.51	516.72	516.58	516.57	516.59	516.59	516.60	516.61	516.61
Mode 4	520.56	520.51	520.49	520.66	520.48	520.53	520.53	520.54	520.53	520.54	520.54	520.53
Mode 5	538.78	538.72	538.23	538.16	538.38	538.72	538.77	538.62	538.75	538.68	538.70	538.65
Mode 6	538.90	538.70	539.14	539.19	539.20	538.78	538.68	538.65	538.79	538.70	538.68	538.72
Mode 7	578.43	578.75	578.59	578.70	578.89	578.73	578.74	578.74	578.78	578.73	578.73	578.73
Mode 8	622.12	622.11	622.18	621.98	622.24	622.20	622.20	622.19	622.23	622.21	622.21	622.21
Mode 9	622.91	622.61	623.05	623.25	623.08	622.63	622.59	622.53	622.67	622.62	622.60	622.59
Mode 10	622.49	622.65	622.19	622.26	622.43	622.66	622.69	622.56	622.62	622.61	622.61	622.64
Mode 11	640.90	640.88	641.23	641.25	641.38	640.95	640.92	640.85	640.98	640.91	640.97	641.01
Mode 12	858.08	858.04	858.26	858.16	857.45	857.66	857.80	858.14	857.13	857.62	857.69	857.68
Mode 13	858.48	858.50	858.39	858.64	858.10	857.99	858.48	858.42	857.77	858.31	858.40	858.44
Mode 14	853.67	853.44	853.17	853.45	853.33	853.53	853.54	853.54	853.61	853.54	853.54	853.53
Mode 15	856.45	856.46	856.40	856.21	856.52	856.51	856.49	856.51	856.57	856.52	856.52	856.52
Mode 16	861.86	861.09	860.80	860.98	859.86	861.02	860.91	860.98	861.08	860.99	860.96	861.03
Mode 17	859.22	860.92	859.71	859.60	859.42	861.12	861.27	860.97	861.12	860.95	861.03	860.96
Mode 18	911.32	911.19	911.23	911.32	911.15	911.31	911.29	911.33	911.33	911.29	911.29	911.28
Mode 19	932.43	931.26	931.37	931.19	931.47	931.38	931.35	931.40	931.40	931.38	931.37	931.38
Mode 20	947.61	947.56	947.77	947.51	948.40	948.24	947.45	948.18	948.14	947.54	947.56	947.56
Mode 21	959.18	959.22	959.11	959.41	959.78	959.06	959.07	959.12	959.76	959.23	959.16	959.15
Mode 22	1142.27	1142.51	1142.70	1142.29	1142.20	1142.15	1142.53	1142.66	1142.66	1142.15	1142.14	1142.14
Mode 23	1142.48	1142.11	1142.04	1142.46	1142.77	1142.67	1142.14	1142.16	1142.26	1142.56	1142.56	1142.57
Mode 24	1359.15	1358.86	1358.11	1357.88	1359.56	1358.86	1358.91	1358.47	1358.71	1358.71	1358.65	1358.72
Mode 25	1358.78	1358.73	1359.98	1360.16	1358.47	1358.76	1358.64	1358.59	1358.89	1358.69	1358.71	1358.68
Mode 26	1394.27	1394.05	1395.22	1395.28	1394.06	1394.06	1393.98	1394.02	1394.09	1394.07	1394.01	1394.01

Mode 27	1393.88	1394.06	1394.00	1393.94	1394.96	1394.06	1394.09	1394.01	1394.04	1394.02	1394.02	1394.08
Mode 28	1403.00	1402.86	1402.70	1402.77	1402.14	1402.83	1402.82	1402.93	1402.84	1402.85	1402.86	1402.82
Mode 29	1403.42	1402.83	1402.32	1402.21	1402.84	1402.85	1402.91	1402.91	1402.80	1402.85	1402.87	1402.87
Mode 30	1409.32	1409.20	1409.73	1409.80	1409.27	1409.75	1409.09	1409.85	1409.56	1409.16	1409.09	1409.25
Mode 31	1409.01	1409.16	1408.72	1408.82	1410.21	1409.16	1409.13	1409.35	1409.58	1409.20	1409.20	1409.07
Mode 32	1414.19	1414.38	1412.73	1413.67	1413.67	1414.51	1414.40	1415.48	1414.45	1414.47	1414.43	1414.48
Mode 33	1532.28	1532.65	1532.69	1532.69	1532.72	1532.71	1532.82	1532.70	1532.72	1532.74	1532.77	1532.77
Mode 34	1532.96	1532.72	1532.76	1532.85	1532.55	1532.72	1532.69	1532.81	1532.73	1532.76	1532.75	1532.74
Mode 35	1719.54	1719.82	1719.93	1719.91	1716.06	1719.86	1719.90	1720.45	1719.80	1720.22	1720.00	1719.99
Mode 36	1719.09	1719.69	1716.89	1716.70	1720.39	1719.71	1719.76	1720.59	1719.98	1719.98	1720.23	1720.24
Mode 37	1729.66	1729.52	1729.46	1729.55	1729.73	1729.59	1729.59	1729.56	1729.73	1729.50	1729.64	1729.65
Mode 38	1729.62	1729.65	1729.68	1729.51	1729.46	1729.72	1729.71	1729.43	1729.59	1729.63	1729.49	1729.49
Mode 39	3128.69	3128.54	3127.36	3127.36	3124.47	3128.47	3128.40	3128.46	3125.99	3127.81	3126.79	3126.79
Mode 40	3127.65	3127.36	3128.51	3128.57	3125.66	3124.46	3127.24	3124.85	3124.75	3126.89	3128.00	3128.01
Mode 41	3122.37	3126.01	3124.12	3124.22	3124.29	3125.60	3125.60	3125.63	3125.61	3125.62	3124.31	3124.31
Mode 42	3124.64	3124.74	3125.67	3125.69	3125.58	3124.28	3124.27	3124.30	3124.29	3124.32	3125.62	3125.62
Mode 43	3131.73	3131.73	3131.10	3131.47	3131.20	3131.74	3131.73	3131.70	3131.75	3131.74	3131.45	3131.44
Mode 44	3131.50	3131.46	3131.76	3131.36	3131.80	3131.48	3131.48	3131.43	3131.48	3131.44	3131.74	3131.74
Mode 45	3142.68	3142.88	3142.83	3142.67	3142.86	3142.78	3142.79	3142.94	3142.60	3142.72	3142.53	3142.56
Mode 46	3142.73	3142.64	3142.99	3143.14	3142.65	3142.59	3142.56	3142.74	3142.38	3142.55	3142.71	3142.71
Mode 47	3164.69	3165.23	3164.71	3164.15	3165.07	3164.17	3164.49	3164.57	3164.39	3164.76	3164.52	3164.63
Mode 48	3164.54	3164.52	3164.26	3164.38	3164.41	3164.41	3164.32	3164.68	3164.25	3164.69	3164.73	3164.63
ZPE	36232.6	36233.3	36231.9	36232.1	36231.0	36232.5	36232.9	36233.4	36232.1	36232.8	36232.8	36232.9

Table S12. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.4 and 8.0 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.25 a_0^{-1}$, and the unattenuated 2MR result.

Cutoff (a_0)	7.40	7.60	7.80	8.00	2MR
Mode 1	445.48	445.49	445.50	445.48	445.50
Mode 2	445.49	445.49	445.51	445.48	445.51
Mode 3	516.58	516.58	516.58	516.59	516.57
Mode 4	520.53	520.52	520.52	520.53	520.52
Mode 5	538.71	538.68	538.71	538.70	538.71
Mode 6	538.68	538.71	538.69	538.68	538.68
Mode 7	578.73	578.73	578.74	578.71	578.74
Mode 8	622.20	622.20	622.21	622.18	622.21
Mode 9	622.59	622.61	622.60	622.60	622.60
Mode 10	622.63	622.61	622.64	622.60	622.64
Mode 11	641.03	641.03	641.01	641.04	641.02
Mode 12	857.64	857.62	857.82	857.80	857.80
Mode 13	858.42	858.42	858.60	858.57	858.58
Mode 14	853.53	853.53	853.54	853.52	853.54
Mode 15	856.50	856.51	856.51	856.50	856.51
Mode 16	861.10	861.07	861.11	861.06	861.09
Mode 17	861.09	861.10	861.10	861.09	861.08
Mode 18	911.29	911.29	911.30	911.29	911.30
Mode 19	931.37	931.37	931.37	931.37	931.37
Mode 20	947.55	947.56	947.55	947.57	947.55
Mode 21	959.17	959.16	959.17	959.17	959.17
Mode 22	1142.16	1142.57	1142.57	1142.15	1142.57
Mode 23	1142.57	1142.15	1142.16	1142.57	1142.15
Mode 24	1358.65	1358.73	1358.78	1358.71	1358.78
Mode 25	1358.76	1358.68	1358.67	1358.65	1358.66
Mode 26	1394.03	1394.04	1394.03	1394.04	1394.03

Mode 27	1394.03	1394.02	1394.04	1394.02	1394.04
Mode 28	1402.90	1402.89	1402.86	1402.91	1402.86
Mode 29	1402.87	1402.88	1402.89	1402.90	1402.89
Mode 30	1409.19	1409.11	1409.14	1409.19	1409.12
Mode 31	1409.16	1409.23	1409.11	1409.30	1409.15
Mode 32	1414.93	1414.93	1414.57	1415.52	1414.68
Mode 33	1532.73	1532.72	1532.74	1532.72	1532.73
Mode 34	1532.73	1532.74	1532.73	1532.73	1532.73
Mode 35	1719.98	1720.20	1720.23	1720.13	1720.23
Mode 36	1720.18	1719.96	1720.03	1719.89	1720.03
Mode 37	1729.68	1729.54	1729.58	1729.51	1729.57
Mode 38	1729.55	1729.69	1729.70	1729.66	1729.69
Mode 39	3128.00	3128.01	3126.79	3126.80	3126.79
Mode 40	3126.80	3126.79	3127.99	3128.02	3127.99
Mode 41	3125.59	3125.59	3124.30	3124.25	3124.30
Mode 42	3124.28	3124.28	3125.61	3125.56	3125.61
Mode 43	3131.73	3131.73	3131.46	3131.44	3131.45
Mode 44	3131.45	3131.44	3131.74	3131.73	3131.73
Mode 45	3142.76	3142.76	3142.57	3142.58	3142.57
Mode 46	3142.57	3142.58	3142.77	3142.76	3142.77
Mode 47	3164.69	3164.69	3164.33	3164.70	3164.47
Mode 48	3164.68	3164.71	3164.34	3164.71	3164.48
ZPE	36233.1	36233.1	36233.0	36233.3	36233.0

Table S13. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0.2 and 2.4 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.30 \text{ } a_0^{-1}$.

Cutoff (a_0)	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20	2.40
Mode 1	445.05	449.42	448.66	451.19	445.01	446.07	448.24	446.73	445.27	446.12	448.68	445.39
Mode 2	445.24	444.58	445.28	445.39	445.32	448.18	445.22	445.02	445.33	447.36	447.74	445.77
Mode 3	515.54	515.03	516.04	518.36	516.04	517.92	516.21	515.58	516.23	516.03	517.47	516.54
Mode 4	519.72	518.12	519.64	521.58	520.05	521.63	519.84	520.38	520.16	520.41	520.86	520.46
Mode 5	538.73	538.52	538.95	544.04	540.38	541.27	538.89	536.07	538.76	537.98	539.49	540.23
Mode 6	538.87	540.74	537.96	538.83	538.84	541.15	540.03	542.29	539.30	540.30	541.93	539.06
Mode 7	576.22	572.39	576.24	577.84	577.37	578.36	577.60	584.11	577.67	581.05	577.21	578.54
Mode 8	618.34	617.93	620.08	618.50	621.39	620.29	620.84	617.36	620.99	619.03	620.42	621.71
Mode 9	621.38	617.66	617.44	621.37	621.46	620.94	624.61	610.96	622.94	622.88	621.92	621.20
Mode 10	623.35	620.12	624.06	623.21	620.76	622.71	621.08	620.63	621.48	623.29	620.34	621.28
Mode 11	633.08	639.00	637.09	635.13	634.48	635.70	635.35	640.52	640.46	642.01	643.22	641.38
Mode 12	855.16	851.36	850.23	866.50	857.97	871.04	852.06	856.32	857.47	853.61	861.69	863.13
Mode 13	856.64	855.70	856.07	872.90	856.73	865.37	856.67	860.33	859.18	860.55	863.59	857.95
Mode 14	850.36	846.60	853.51	859.41	850.28	851.87	850.22	853.33	853.75	855.44	854.76	851.10
Mode 15	852.99	847.68	852.76	860.22	856.19	859.44	850.93	852.99	854.93	856.24	858.30	856.30
Mode 16	860.19	861.55	862.66	870.32	860.54	870.87	861.45	861.18	861.62	859.44	863.60	861.92
Mode 17	858.62	856.26	857.31	870.87	861.37	868.91	859.09	870.84	861.86	859.42	862.42	860.99
Mode 18	911.60	924.70	910.58	908.06	925.73	915.08	911.29	920.31	917.07	913.23	918.18	917.54
Mode 19	927.89	922.97	922.26	934.23	931.57	940.29	935.69	930.19	931.80	931.85	940.42	931.93
Mode 20	947.67	946.23	946.41	946.18	948.09	936.17	946.39	948.98	948.24	947.20	936.14	948.44
Mode 21	959.10	935.58	936.68	841.37	959.69	967.50	938.59	959.47	960.01	942.13	947.56	967.07
Mode 22	1141.62	1148.73	1141.96	1141.69	1141.10	1133.62	1135.60	1138.83	1141.58	1141.47	1139.95	1134.59
Mode 23	1141.83	1141.84	1156.64	1122.51	1134.59	1120.70	1153.66	1135.09	1142.02	1150.65	1141.18	1141.54
Mode 24	1361.23	1357.50	1364.03	1356.41	1360.05	1356.17	1359.19	1366.21	1359.68	1359.44	1355.34	1359.68
Mode 25	1354.94	1362.47	1354.98	1352.28	1355.05	1357.86	1357.99	1357.78	1359.56	1357.59	1358.75	1354.36
Mode 26	1395.72	1411.46	1411.83	1410.69	1395.07	1409.78	1408.25	1397.29	1394.68	1390.17	1401.54	1394.81

Mode 27	1395.95	1397.62	1395.13	1395.69	1395.60	1395.37	1395.17	1386.83	1394.99	1405.37	1404.76	1395.28
Mode 28	1403.92	1415.34	1404.94	1414.15	1414.41	1413.87	1411.86	1395.98	1407.13	1405.34	1407.57	1407.35
Mode 29	1404.87	1405.89	1404.02	1404.59	1404.51	1414.50	1404.27	1413.47	1404.12	1398.47	1406.47	1404.17
Mode 30	1412.29	1414.57	1412.81	1413.01	1412.94	1416.91	1411.15	1415.02	1410.38	1407.51	1416.01	1410.31
Mode 31	1412.11	1414.86	1412.24	1439.95	1411.78	1417.85	1410.42	1409.69	1410.84	1413.85	1413.02	1415.13
Mode 32	1415.46	1399.20	1416.94	1410.98	1416.02	1415.10	1416.21	1415.20	1416.43	1413.97	1407.24	1414.29
Mode 33	1532.90	1531.99	1534.12	1537.68	1534.29	1536.67	1533.15	1534.86	1532.66	1533.59	1535.39	1533.03
Mode 34	1533.03	1532.92	1533.58	1537.82	1534.24	1536.68	1532.97	1537.37	1532.66	1533.44	1535.26	1532.54
Mode 35	1722.10	1698.98	1724.14	1721.78	1716.47	1716.60	1722.57	1702.53	1720.44	1722.83	1699.77	1720.26
Mode 36	1711.90	1702.27	1718.46	1713.34	1716.14	1712.05	1720.75	1727.43	1720.46	1700.73	1723.51	1713.07
Mode 37	1732.92	1732.47	1726.18	1726.83	1732.59	1731.01	1733.39	1732.32	1731.06	1731.91	1732.11	1733.13
Mode 38	1731.21	1736.42	1731.27	1721.08	1732.59	1728.64	1731.65	1730.40	1730.92	1733.09	1732.07	1731.58
Mode 39	3129.76	3129.53	3131.75	2963.05	3130.58	3096.88	3131.37	3130.15	3129.91	3129.64	3102.31	3129.79
Mode 40	3132.26	3130.48	3130.43	3130.76	3131.42	3094.70	3130.74	3130.94	3131.27	3130.27	3104.18	3105.25
Mode 41	3127.36	3065.75	3126.18	3130.76	3073.72	3073.19	3083.39	3098.68	3109.31	3126.42	3098.86	3108.52
Mode 42	3133.81	3128.94	3130.71	3075.40	3132.35	3087.59	3131.59	3122.56	3128.30	3127.44	3109.33	3127.03
Mode 43	3133.11	3134.46	3135.08	3039.79	3134.29	3054.05	3133.89	3133.86	3134.55	3130.76	3074.95	3133.70
Mode 44	3134.97	3036.02	3034.83	3132.20	3133.44	3132.09	3055.25	3129.24	3134.50	3079.15	3073.49	3132.51
Mode 45	3146.85	3147.52	3145.28	3119.47	3144.07	3122.56	3143.72	3141.61	3143.71	3142.92	3134.12	3143.60
Mode 46	3146.54	3147.66	3143.06	3118.14	3144.09	3122.05	3143.72	3139.61	3144.04	3143.26	3133.88	3143.95
Mode 47	3168.04	3171.78	3168.19	3124.81	3166.53	3126.09	3166.28	3158.59	3166.06	3165.69	3139.93	3154.85
Mode 48	3168.44	3168.51	3167.25	3125.01	3166.36	3125.11	3165.29	3162.49	3166.04	3163.79	3148.56	3166.11
ZPE	36236.4	36192.2	36214.8	36129.5	36230.5	36169.5	36211.2	36226.6	36239.3	36220.9	36179.5	36229.0

Table S14. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.6 and 4.8 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.30 \text{ } a_0^{-1}$.

Cutoff (a_0)	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60	4.80
Mode 1	447.28	445.36	445.82	445.57	446.05	445.56	445.80	445.50	445.61	445.52	445.64	445.78
Mode 2	445.91	445.40	445.52	445.44	445.35	445.58	445.39	445.48	445.54	445.48	445.50	445.53
Mode 3	517.03	516.59	517.48	516.38	517.50	516.77	516.57	516.51	516.57	516.53	516.82	516.55
Mode 4	521.35	520.21	520.29	520.64	520.53	520.68	520.27	520.40	520.40	520.47	520.71	520.54
Mode 5	539.09	538.70	538.85	538.64	540.46	539.28	539.29	538.92	539.25	538.62	539.07	538.46
Mode 6	542.22	538.52	540.07	539.28	539.12	539.27	538.03	538.70	539.02	538.71	539.39	539.83
Mode 7	573.33	578.03	576.04	578.71	573.99	579.06	578.82	578.03	578.29	578.61	579.09	578.36
Mode 8	626.09	622.13	621.33	622.29	621.55	622.20	621.50	621.69	621.73	621.73	622.12	622.37
Mode 9	618.45	622.70	621.32	622.66	622.28	622.81	623.47	622.72	620.92	622.54	622.59	623.26
Mode 10	622.31	622.98	621.05	622.93	620.30	622.86	622.41	622.68	622.67	622.82	623.24	622.75
Mode 11	642.86	640.15	642.41	640.39	642.56	641.22	641.04	640.86	641.63	640.84	641.62	641.60
Mode 12	861.64	863.33	859.23	857.34	863.99	860.37	858.25	857.33	858.42	858.33	857.57	858.18
Mode 13	858.91	859.04	859.72	862.60	858.49	861.14	858.05	858.97	859.90	858.82	857.19	858.13
Mode 14	850.61	854.01	853.60	851.92	851.58	851.35	852.69	853.41	853.54	853.58	852.70	853.22
Mode 15	853.94	857.03	856.78	856.66	856.73	854.29	855.90	856.43	856.33	856.66	856.40	856.46
Mode 16	860.43	861.10	860.36	861.12	862.61	862.79	861.30	861.23	861.34	861.36	860.97	859.92
Mode 17	861.34	863.55	859.11	863.12	858.69	862.75	860.81	861.06	859.67	861.08	859.24	860.79
Mode 18	918.43	911.81	911.18	911.72	914.35	915.29	911.00	913.05	911.07	911.32	912.92	912.46
Mode 19	936.84	931.94	931.73	935.44	931.92	935.39	931.77	931.52	931.47	931.47	932.76	931.33
Mode 20	955.73	948.21	947.61	950.57	947.34	949.85	949.67	947.72	947.61	947.65	949.35	947.51
Mode 21	967.14	959.79	959.44	960.10	959.23	961.47	959.56	959.31	959.29	959.32	959.16	960.86
Mode 22	1136.63	1140.24	1143.28	1142.58	1142.55	1140.64	1142.95	1142.13	1142.07	1142.47	1142.86	1142.56
Mode 23	1134.44	1142.63	1142.71	1140.49	1139.42	1141.08	1142.09	1142.69	1142.42	1142.06	1142.23	1142.42
Mode 24	1360.60	1359.54	1354.44	1359.57	1355.02	1359.81	1358.97	1361.16	1359.70	1359.29	1354.45	1359.89
Mode 25	1352.12	1359.82	1355.23	1359.67	1355.43	1359.70	1361.18	1357.54	1353.35	1359.20	1359.37	1353.69
Mode 26	1394.50	1394.58	1396.35	1394.78	1396.68	1394.19	1395.65	1394.27	1394.26	1394.34	1394.21	1394.01

Mode 27	1394.34	1394.91	1394.75	1394.56	1394.56	1394.18	1394.26	1394.01	1394.22	1394.25	1394.51	1395.04
Mode 28	1407.50	1404.30	1405.49	1405.63	1406.63	1405.30	1403.81	1404.31	1403.21	1403.06	1403.66	1402.38
Mode 29	1403.10	1403.80	1401.05	1403.53	1401.93	1405.31	1400.99	1403.24	1402.78	1402.83	1403.96	1403.37
Mode 30	1416.75	1410.27	1408.59	1410.24	1412.33	1411.14	1409.05	1410.16	1409.79	1409.61	1410.61	1408.78
Mode 31	1413.40	1410.89	1411.29	1411.57	1407.31	1411.10	1412.84	1410.12	1409.66	1409.48	1408.97	1410.60
Mode 32	1411.04	1414.86	1410.43	1414.89	1409.74	1414.76	1414.67	1414.71	1413.32	1414.33	1412.30	1412.86
Mode 33	1534.01	1533.50	1532.80	1533.42	1533.07	1533.27	1532.63	1532.71	1532.62	1532.71	1532.82	1532.71
Mode 34	1534.69	1532.78	1532.78	1532.76	1533.94	1533.25	1532.96	1532.77	1532.75	1532.80	1532.81	1532.49
Mode 35	1727.16	1721.11	1706.06	1720.45	1716.40	1720.25	1720.96	1719.79	1719.75	1719.66	1716.17	1718.32
Mode 36	1692.29	1718.89	1716.08	1719.92	1704.07	1720.02	1716.30	1719.86	1712.02	1719.31	1720.08	1714.21
Mode 37	1733.97	1731.83	1732.48	1731.33	1733.12	1730.85	1729.84	1729.84	1730.78	1729.73	1729.73	1730.21
Mode 38	1727.87	1731.06	1727.28	1730.82	1727.58	1730.74	1730.39	1730.32	1730.41	1730.11	1729.26	1729.52
Mode 39	3104.42	3129.89	3128.19	3122.41	3128.22	3122.96	3130.08	3128.77	3127.92	3129.67	3122.78	3123.96
Mode 40	3104.04	3131.01	3130.41	3130.47	3129.30	3124.13	3122.79	3129.97	3130.19	3128.43	3128.07	3127.47
Mode 41	3111.00	3126.71	3123.99	3126.35	3112.41	3114.03	3127.08	3120.02	3124.84	3126.66	3120.19	3126.48
Mode 42	3100.78	3127.50	3127.19	3115.01	3127.23	3115.03	3125.38	3126.93	3126.98	3125.32	3120.78	3120.34
Mode 43	3110.90	3133.14	3131.22	3131.38	3130.19	3131.77	3131.96	3131.68	3131.94	3131.87	3131.48	3131.52
Mode 44	3131.30	3133.53	3131.61	3132.02	3131.30	3132.12	3131.22	3131.90	3131.94	3131.51	3132.04	3131.80
Mode 45	3140.69	3143.83	3144.01	3142.77	3143.45	3142.62	3143.91	3143.84	3143.26	3143.14	3143.86	3142.24
Mode 46	3142.06	3143.91	3142.94	3143.11	3142.79	3142.89	3143.82	3143.91	3143.72	3142.90	3142.55	3142.21
Mode 47	3154.58	3154.00	3165.83	3165.64	3153.82	3154.71	3164.53	3164.71	3164.81	3165.25	3165.39	3164.44
Mode 48	3150.74	3166.04	3165.90	3153.68	3164.62	3154.70	3164.47	3164.49	3164.95	3164.60	3165.21	3164.86
ZPE	36205.4	36240.0	36229.5	36234.6	36223.9	36229.4	36235.3	36235.6	36232.4	36235.2	36230.0	36229.5

Table S15. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 5.0 and 7.2 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.30 \text{ } a_0^{-1}$.

Cutoff (a_0)	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00	7.20
Mode 1	445.52	445.51	445.50	445.51	445.56	445.72	445.48	445.55	445.48	445.52	445.50	445.50
Mode 2	445.60	445.52	445.53	445.57	445.51	445.50	445.54	445.55	445.50	445.50	445.50	445.51
Mode 3	516.61	516.58	516.58	516.57	516.59	516.67	516.57	516.60	516.57	516.57	516.58	516.57
Mode 4	520.56	520.52	520.53	520.51	520.53	520.39	520.51	520.54	520.53	520.52	520.51	520.52
Mode 5	539.06	538.77	538.74	538.86	538.77	538.28	538.81	538.78	538.65	538.66	538.71	538.71
Mode 6	538.91	538.72	538.82	538.74	538.82	539.14	538.59	538.81	538.68	538.74	538.69	538.69
Mode 7	578.57	578.38	578.58	578.81	578.63	578.86	578.74	578.79	578.73	578.75	578.74	578.74
Mode 8	622.31	621.96	622.01	622.39	622.21	622.27	622.25	622.24	622.20	622.20	622.22	622.22
Mode 9	622.68	622.63	622.61	622.67	622.66	623.24	622.58	622.64	622.57	622.59	622.62	622.60
Mode 10	622.75	622.66	622.69	622.68	622.68	622.46	622.63	622.65	622.65	622.68	622.62	622.64
Mode 11	640.96	640.85	640.84	641.01	640.97	641.21	640.80	640.97	640.77	640.84	640.95	641.01
Mode 12	857.33	858.25	858.54	857.50	857.71	857.11	857.33	857.07	857.94	857.82	857.84	857.83
Mode 13	857.80	859.59	858.69	858.27	858.57	857.06	859.04	857.75	859.17	858.44	858.57	858.61
Mode 14	853.27	853.40	853.40	853.68	853.55	853.44	853.61	853.61	853.53	853.54	853.53	853.54
Mode 15	856.62	856.46	856.47	856.64	856.52	856.62	856.57	856.59	856.49	856.49	856.51	856.51
Mode 16	861.00	861.14	860.96	860.92	861.04	860.94	860.88	861.11	861.08	861.06	861.04	861.09
Mode 17	860.14	859.92	860.18	859.87	860.03	860.68	861.32	861.07	861.04	861.08	861.10	861.08
Mode 18	912.64	911.13	911.23	911.29	911.30	911.17	911.29	911.33	911.32	911.30	911.29	911.30
Mode 19	932.65	931.21	931.49	931.38	931.37	931.47	931.41	931.42	931.34	931.36	931.37	931.37
Mode 20	949.32	947.64	947.64	947.57	948.40	948.48	947.38	948.19	947.43	947.61	947.55	947.55
Mode 21	959.18	959.27	959.25	960.12	959.09	959.84	959.86	959.79	959.03	959.14	959.15	959.17
Mode 22	1142.89	1142.08	1142.50	1142.22	1142.13	1142.83	1142.54	1142.25	1142.13	1142.57	1142.56	1142.56
Mode 23	1142.28	1142.48	1142.13	1142.51	1142.66	1142.26	1142.27	1142.66	1142.55	1142.16	1142.15	1142.15
Mode 24	1358.86	1358.92	1358.97	1358.88	1358.89	1358.54	1358.63	1358.82	1358.82	1358.66	1358.75	1358.79
Mode 25	1359.11	1358.85	1358.78	1358.83	1358.85	1360.06	1358.74	1358.77	1358.56	1358.90	1358.69	1358.67
Mode 26	1394.08	1394.04	1394.00	1394.06	1394.05	1395.25	1394.07	1394.03	1394.03	1394.12	1394.04	1394.03

Mode 27	1394.05	1394.06	1394.12	1394.05	1394.06	1394.18	1393.96	1394.01	1394.03	1394.03	1394.02	1394.03
Mode 28	1403.64	1402.90	1402.87	1402.80	1402.82	1402.78	1402.90	1402.85	1402.84	1402.88	1402.87	1402.85
Mode 29	1403.51	1402.91	1402.90	1402.82	1402.82	1402.19	1402.86	1402.84	1402.92	1402.80	1402.87	1402.89
Mode 30	1410.32	1409.18	1409.16	1409.72	1409.16	1410.36	1409.76	1409.55	1409.16	1409.14	1409.05	1409.09
Mode 31	1409.13	1409.16	1409.13	1409.12	1409.82	1409.50	1409.12	1409.68	1409.23	1409.16	1409.16	1409.12
Mode 32	1413.97	1414.04	1414.06	1414.06	1414.30	1414.22	1414.49	1414.26	1414.51	1414.54	1414.46	1414.44
Mode 33	1532.62	1532.58	1532.70	1532.58	1532.62	1532.54	1532.70	1532.74	1532.72	1532.69	1532.71	1532.72
Mode 34	1532.61	1532.69	1532.64	1532.66	1532.69	1532.75	1532.81	1532.75	1532.72	1532.72	1532.73	1532.72
Mode 35	1719.68	1719.73	1719.61	1719.82	1719.70	1720.36	1719.66	1719.93	1719.82	1719.97	1720.26	1720.25
Mode 36	1719.21	1719.06	1719.08	1719.21	1719.23	1717.43	1720.92	1719.70	1720.69	1720.14	1720.03	1720.05
Mode 37	1729.76	1729.58	1729.58	1729.55	1729.62	1729.56	1729.68	1729.58	1729.56	1729.71	1729.57	1729.58
Mode 38	1729.58	1729.70	1729.65	1729.67	1729.72	1729.91	1729.59	1729.74	1729.71	1729.59	1729.72	1729.71
Mode 39	3122.17	3128.82	3128.82	3125.53	3128.73	3125.59	3125.90	3125.80	3128.52	3128.11	3127.99	3127.99
Mode 40	3129.16	3127.55	3127.59	3127.56	3124.24	3124.30	3127.39	3124.63	3127.48	3126.55	3126.78	3126.78
Mode 41	3120.70	3126.25	3125.26	3125.59	3125.59	3125.65	3125.69	3125.60	3125.57	3125.62	3125.62	3125.62
Mode 42	3122.19	3124.88	3124.39	3124.26	3124.24	3124.39	3124.26	3124.29	3124.38	3124.31	3124.30	3124.31
Mode 43	3131.51	3131.75	3131.72	3131.76	3131.76	3131.77	3131.70	3131.78	3131.75	3131.72	3131.74	3131.74
Mode 44	3131.78	3131.50	3131.51	3131.48	3131.51	3131.13	3131.49	3131.49	3131.42	3131.46	3131.45	3131.46
Mode 45	3141.99	3142.99	3142.92	3142.48	3142.81	3142.46	3142.57	3142.56	3142.78	3142.80	3142.75	3142.76
Mode 46	3142.54	3142.47	3142.53	3142.20	3142.53	3142.58	3142.35	3142.38	3142.56	3142.56	3142.57	3142.57
Mode 47	3164.47	3164.84	3164.67	3165.39	3164.37	3165.08	3164.44	3164.31	3164.47	3164.40	3164.40	3164.34
Mode 48	3164.94	3164.72	3164.42	3165.50	3164.64	3164.18	3164.26	3164.28	3164.43	3164.21	3164.26	3164.32
ZPE	36231.5	36233.2	36232.8	36232.6	36232.4	36232.0	36232.9	36232.0	36233.3	36232.8	36232.9	36232.9

Table S16. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.4 and 8.0 a_0 calculated using Coulomb attenuated HF/cc-pVDZ with an attenuation parameter of $\omega = 0.30 \text{ } a_0^{-1}$, and the unattenuated 2MR result.

Cutoff (a_0)	7.40	7.60	7.80	8.00	2MR
Mode 1	445.50	445.50	445.50	445.48	445.50
Mode 2	445.50	445.50	445.50	445.48	445.51
Mode 3	516.58	516.58	516.58	516.59	516.57
Mode 4	520.52	520.52	520.52	520.53	520.52
Mode 5	538.71	538.71	538.68	538.70	538.71
Mode 6	538.68	538.68	538.71	538.68	538.68
Mode 7	578.74	578.74	578.74	578.71	578.74
Mode 8	622.21	622.21	622.22	622.18	622.21
Mode 9	622.62	622.62	622.61	622.60	622.60
Mode 10	622.62	622.62	622.62	622.60	622.64
Mode 11	641.01	641.01	641.01	641.04	641.02
Mode 12	857.79	857.79	857.83	857.80	857.80
Mode 13	858.56	858.56	858.60	858.57	858.58
Mode 14	853.53	853.53	853.53	853.52	853.54
Mode 15	856.51	856.51	856.51	856.50	856.51
Mode 16	861.06	861.06	861.12	861.06	861.09
Mode 17	861.10	861.10	861.08	861.10	861.08
Mode 18	911.29	911.29	911.29	911.29	911.30
Mode 19	931.37	931.37	931.38	931.38	931.37
Mode 20	947.55	947.55	947.56	947.57	947.55
Mode 21	959.16	959.16	959.16	959.18	959.17
Mode 22	1142.15	1142.57	1142.15	1142.57	1142.57
Mode 23	1142.56	1142.15	1142.57	1142.16	1142.15
Mode 24	1358.69	1358.75	1358.75	1358.71	1358.78
Mode 25	1358.75	1358.69	1358.69	1358.65	1358.66
Mode 26	1394.02	1394.04	1394.04	1394.04	1394.03

Mode 27	1394.04	1394.02	1394.02	1394.02	1394.04
Mode 28	1402.87	1402.87	1402.88	1402.91	1402.86
Mode 29	1402.87	1402.87	1402.87	1402.91	1402.89
Mode 30	1409.18	1409.07	1409.18	1409.19	1409.12
Mode 31	1409.07	1409.18	1409.06	1409.30	1409.15
Mode 32	1414.62	1414.62	1414.57	1415.53	1414.68
Mode 33	1532.73	1532.72	1532.73	1532.72	1532.73
Mode 34	1532.72	1532.74	1532.74	1532.73	1532.73
Mode 35	1720.01	1720.24	1720.25	1720.12	1720.23
Mode 36	1720.24	1720.01	1720.01	1719.89	1720.03
Mode 37	1729.71	1729.56	1729.56	1729.51	1729.57
Mode 38	1729.56	1729.71	1729.71	1729.65	1729.69
Mode 39	3126.78	3128.00	3126.78	3128.02	3126.79
Mode 40	3128.00	3126.78	3128.00	3126.81	3127.99
Mode 41	3124.30	3125.61	3124.30	3125.56	3124.30
Mode 42	3125.61	3124.30	3125.61	3124.25	3125.61
Mode 43	3131.45	3131.74	3131.45	3131.73	3131.45
Mode 44	3131.74	3131.45	3131.74	3131.44	3131.73
Mode 45	3142.58	3142.76	3142.58	3142.76	3142.57
Mode 46	3142.76	3142.58	3142.75	3142.58	3142.77
Mode 47	3164.44	3164.45	3164.32	3164.71	3164.47
Mode 48	3164.45	3164.44	3164.34	3164.70	3164.48
ZPE	36233.0	36233.0	36233.0	36233.3	36233.0

Table S17. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0 and 2.2 a_0 truncated.

Cutoff (a_0)	0.00	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20
Mode 1	442.99	449.37	448.13	447.95	447.93	447.90	447.23	447.15	447.05	446.93	446.66	446.66
Mode 2	442.99	449.33	448.09	447.93	447.90	447.90	447.23	447.14	447.03	446.91	446.65	446.65
Mode 3	515.42	521.11	519.74	516.42	515.84	515.70	516.37	516.44	516.41	516.48	516.58	516.43
Mode 4	519.42	525.33	523.89	520.52	519.84	519.71	520.41	520.47	520.45	520.51	520.60	520.45
Mode 5	535.89	541.99	541.33	541.37	540.76	540.81	539.95	540.21	540.41	540.01	539.92	539.91
Mode 6	535.89	541.80	541.19	541.27	540.66	540.64	539.81	540.11	540.29	540.02	539.93	539.93
Mode 7	580.93	585.92	586.18	582.48	586.74	582.55	582.40	582.56	582.63	582.38	582.46	581.26
Mode 8	625.95	622.16	629.88	629.88	629.78	629.78	628.93	626.61	626.70	626.43	627.80	627.78
Mode 9	625.36	626.67	624.66	624.97	623.59	623.55	624.27	624.32	624.53	624.44	624.60	624.55
Mode 10	625.36	626.66	624.66	624.97	623.63	623.57	624.28	624.32	624.52	624.43	624.57	624.52
Mode 11	646.61	647.93	641.06	641.10	641.10	639.18	639.77	642.17	642.29	641.01	641.12	641.11
Mode 12	904.90	912.43	853.32	867.84	853.42	853.41	852.53	851.53	854.22	856.38	854.81	855.61
Mode 13	905.41	913.15	854.12	868.61	854.22	854.21	853.34	852.34	855.02	857.17	855.60	856.41
Mode 14	895.28	905.20	905.69	834.27	832.44	844.30	848.51	847.30	850.02	845.90	845.82	854.04
Mode 15	898.47	908.17	908.65	837.33	835.52	847.35	851.55	850.35	853.07	848.98	848.90	857.07
Mode 16	876.32	898.26	898.92	882.12	849.30	861.50	861.15	863.91	865.60	865.84	863.66	863.69
Mode 17	876.32	898.37	899.04	882.19	849.43	861.64	861.29	864.01	865.66	865.91	863.65	863.68
Mode 18	938.94	900.10	900.60	905.60	908.66	908.69	908.95	907.63	903.92	917.02	910.57	910.42
Mode 19	960.64	920.31	925.19	930.83	931.74	931.76	932.04	930.71	926.44	936.87	930.77	930.60
Mode 20	976.01	982.96	983.12	987.43	987.49	986.85	945.46	946.61	945.83	945.82	945.86	962.12
Mode 21	989.37	993.36	994.80	999.66	999.74	999.06	958.21	958.22	957.42	957.40	957.44	973.78
Mode 22	1151.25	1155.18	1131.40	1131.42	1130.80	1130.80	1130.93	1130.96	1130.39	1132.68	1131.91	1156.83
Mode 23	1151.25	1155.12	1131.33	1131.35	1130.73	1130.74	1130.86	1130.89	1130.32	1132.56	1132.77	1157.66
Mode 24	1374.50	1374.04	1376.09	1376.18	1364.97	1365.10	1365.48	1375.45	1373.23	1374.90	1364.94	1364.85
Mode 25	1374.50	1373.89	1375.92	1376.00	1365.12	1365.25	1365.61	1375.39	1373.18	1374.87	1364.91	1364.82
Mode 26	1425.45	1393.52	1393.94	1394.01	1396.63	1396.62	1395.92	1395.66	1394.82	1394.55	1394.46	1393.35

Mode 27	1425.45	1393.51	1393.93	1393.99	1396.62	1396.61	1395.91	1395.65	1394.83	1394.56	1394.48	1393.37
Mode 28	1435.58	1407.03	1406.65	1406.07	1404.79	1404.81	1404.79	1405.81	1405.73	1405.68	1405.84	1405.34
Mode 29	1435.58	1407.07	1406.83	1406.35	1405.08	1405.10	1405.08	1406.07	1406.00	1405.65	1405.81	1405.31
Mode 30	1444.79	1409.16	1409.88	1409.64	1411.11	1410.80	1411.62	1410.69	1409.43	1409.47	1409.62	1409.64
Mode 31	1444.79	1409.26	1409.97	1409.73	1411.22	1411.28	1411.95	1410.87	1409.56	1409.61	1409.75	1409.78
Mode 32	1428.12	1424.10	1424.11	1423.74	1424.37	1422.59	1426.14	1424.01	1423.33	1423.27	1422.71	1422.18
Mode 33	1557.29	1577.36	1577.13	1549.87	1527.75	1527.60	1532.53	1534.14	1533.73	1533.78	1533.91	1533.97
Mode 34	1557.29	1577.39	1577.17	1549.88	1527.78	1527.62	1532.56	1534.15	1533.74	1533.79	1533.93	1533.99
Mode 35	1735.00	1731.60	1728.43	1728.40	1728.30	1726.43	1730.05	1727.65	1727.07	1726.75	1726.49	1726.48
Mode 36	1735.00	1731.03	1728.78	1728.67	1728.54	1727.47	1730.49	1728.02	1727.20	1726.99	1726.73	1726.72
Mode 37	1748.38	1745.03	1744.64	1744.05	1740.65	1740.83	1737.47	1738.36	1740.19	1740.06	1739.25	1740.31
Mode 38	1748.38	1744.94	1744.41	1743.87	1740.42	1740.61	1737.22	1738.14	1740.04	1739.91	1739.09	1740.14
Mode 39	3224.83	3179.53	3178.09	3178.06	3177.62	3177.40	3139.51	3137.40	3133.50	3133.48	3133.23	3133.88
Mode 40	3224.83	3179.47	3177.29	3177.27	3176.83	3173.33	3136.30	3135.94	3132.20	3132.19	3131.94	3132.58
Mode 41	3225.03	3136.55	3135.96	3135.57	3135.97	3135.96	3135.87	3135.20	3133.97	3125.96	3125.63	3125.29
Mode 42	3225.03	3141.08	3141.34	3137.80	3138.32	3138.30	3138.21	3137.55	3136.31	3124.63	3124.27	3123.94
Mode 43	3230.23	3185.32	3159.73	3159.73	3155.98	3156.01	3156.51	3156.90	3156.07	3153.23	3147.36	3147.20
Mode 44	3230.23	3185.38	3159.79	3159.80	3155.97	3156.00	3156.51	3156.90	3156.08	3153.22	3147.11	3146.95
Mode 45	3247.02	3237.49	3239.01	3145.58	3143.75	3144.59	3143.45	3145.62	3145.75	3145.56	3145.33	3144.48
Mode 46	3247.02	3237.23	3238.74	3145.34	3143.52	3144.36	3143.24	3145.34	3145.48	3145.28	3145.05	3144.21
Mode 47	3270.34	3262.00	3209.64	3212.79	3170.38	3170.66	3170.70	3175.79	3176.21	3174.33	3167.10	3167.16
Mode 48	3270.34	3262.08	3209.62	3212.77	3170.42	3170.69	3170.73	3175.80	3176.21	3174.31	3167.09	3167.15
ZPE	36608.5	36504.3	36430.6	36344.1	36283.3	36292.0	36261.1	36268.5	36265.5	36265.4	36249.2	36273.4

Table S18. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.4 and 4.6 a_0 truncated.

Cutoff (a_0)	2.40	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60
Mode 1	446.75	446.09	445.95	445.95	445.71	445.68	445.73	445.70	445.70	445.67	445.67	445.67
Mode 2	446.74	446.08	445.95	445.95	445.64	445.57	445.71	445.66	445.66	445.67	445.67	445.68
Mode 3	516.70	516.61	516.67	516.80	516.91	516.68	516.57	516.43	516.42	516.40	516.70	516.68
Mode 4	520.72	520.63	520.69	520.81	520.90	520.78	520.68	520.41	520.41	520.40	520.64	520.61
Mode 5	539.95	539.89	540.05	539.83	539.59	539.59	539.81	539.69	539.69	539.67	539.16	539.24
Mode 6	539.96	539.89	540.08	539.85	539.90	539.89	539.79	539.67	539.67	539.67	539.14	539.20
Mode 7	582.67	582.70	580.69	580.67	580.43	580.43	581.02	579.28	579.28	578.14	579.27	579.21
Mode 8	624.82	624.78	624.86	624.82	625.00	623.14	623.22	621.79	622.44	622.43	622.91	622.68
Mode 9	624.54	624.20	623.64	623.39	623.39	623.58	622.89	622.83	622.82	622.90	623.49	623.32
Mode 10	624.50	624.16	623.59	623.37	622.83	622.98	622.79	622.86	622.85	622.86	623.46	623.41
Mode 11	641.12	641.17	641.24	641.25	641.27	641.28	641.88	641.62	641.62	641.61	641.50	642.58
Mode 12	853.12	853.18	853.37	853.34	850.46	850.44	859.00	857.17	857.17	857.17	857.09	857.09
Mode 13	853.93	853.98	854.16	854.14	851.18	851.17	859.78	857.95	857.95	857.94	857.87	857.87
Mode 14	853.96	852.20	852.22	852.19	852.13	852.15	852.09	853.36	853.53	855.54	855.80	855.81
Mode 15	857.00	855.25	855.28	855.25	855.24	855.28	855.16	856.43	856.86	858.91	858.96	859.12
Mode 16	862.80	862.18	862.70	864.13	864.24	864.16	863.82	863.04	863.04	863.03	862.22	862.34
Mode 17	862.79	862.17	862.67	864.10	863.98	863.94	863.86	862.98	862.98	863.02	862.22	862.29
Mode 18	910.41	909.87	909.88	909.16	908.56	908.62	908.17	910.85	910.85	910.90	910.71	910.73
Mode 19	930.60	930.11	930.11	929.39	928.93	929.00	928.31	930.87	930.87	930.92	930.71	930.71
Mode 20	962.11	947.02	946.78	946.77	944.22	944.51	944.37	944.52	944.30	946.40	946.48	946.46
Mode 21	973.79	958.62	958.41	958.40	955.84	956.07	955.99	956.13	955.89	957.96	958.04	958.03
Mode 22	1157.87	1149.21	1148.90	1150.42	1140.18	1140.21	1149.90	1143.25	1143.25	1143.23	1143.39	1143.36
Mode 23	1157.81	1149.16	1148.93	1150.44	1140.22	1140.28	1149.53	1142.86	1142.85	1142.81	1142.97	1142.97
Mode 24	1364.79	1364.59	1364.11	1363.62	1363.76	1363.74	1361.92	1361.71	1361.52	1360.16	1359.09	1359.18
Mode 25	1364.74	1364.54	1364.06	1363.57	1363.56	1363.50	1361.82	1360.00	1359.79	1359.76	1358.70	1358.80
Mode 26	1393.08	1393.39	1394.15	1394.50	1394.59	1394.67	1393.44	1393.54	1393.53	1393.53	1394.70	1394.61

Mode 27	1393.23	1393.55	1394.29	1394.63	1394.93	1394.97	1393.52	1393.43	1393.42	1393.50	1394.67	1394.54
Mode 28	1405.35	1404.82	1405.42	1405.39	1404.90	1404.94	1404.15	1404.03	1404.02	1404.08	1402.36	1402.51
Mode 29	1405.30	1404.78	1405.40	1405.42	1405.60	1405.66	1404.12	1404.05	1404.05	1404.05	1402.31	1402.38
Mode 30	1409.76	1409.89	1409.44	1409.71	1409.11	1409.09	1409.47	1409.46	1409.47	1409.46	1409.00	1408.95
Mode 31	1409.88	1410.02	1409.60	1409.87	1409.81	1409.79	1409.56	1409.55	1409.56	1409.55	1409.08	1409.00
Mode 32	1421.65	1422.07	1419.99	1419.91	1419.50	1419.39	1419.73	1419.66	1419.67	1419.66	1419.90	1419.79
Mode 33	1533.52	1533.19	1533.46	1533.35	1533.70	1533.78	1533.64	1533.41	1533.41	1533.41	1533.17	1533.22
Mode 34	1533.54	1533.21	1533.47	1533.35	1533.56	1533.60	1533.63	1533.42	1533.42	1533.44	1533.20	1533.22
Mode 35	1726.46	1726.36	1726.18	1725.86	1725.82	1725.81	1725.46	1725.31	1725.31	1725.33	1719.58	1719.54
Mode 36	1726.72	1726.62	1726.39	1726.08	1725.29	1725.26	1725.74	1725.65	1725.66	1725.64	1719.86	1719.65
Mode 37	1735.19	1734.64	1734.38	1733.93	1733.26	1731.97	1731.84	1731.69	1731.69	1731.70	1730.55	1730.24
Mode 38	1735.01	1734.47	1734.20	1733.75	1732.83	1733.45	1733.62	1731.76	1731.76	1731.75	1730.61	1730.33
Mode 39	3133.91	3133.30	3133.24	3133.12	3125.77	3125.77	3126.04	3126.00	3125.99	3126.07	3125.81	3125.81
Mode 40	3132.62	3132.01	3131.95	3131.83	3124.56	3124.56	3124.76	3124.72	3124.71	3124.78	3124.53	3124.54
Mode 41	3125.30	3125.94	3125.68	3124.28	3124.22	3124.75	3124.09	3123.11	3123.11	3123.12	3123.00	3122.99
Mode 42	3123.96	3124.60	3124.36	3122.90	3122.73	3123.28	3122.77	3121.66	3121.66	3121.68	3121.56	3121.59
Mode 43	3144.88	3132.69	3131.15	3130.94	3128.74	3128.91	3129.70	3129.60	3129.60	3129.63	3128.93	3129.00
Mode 44	3146.47	3134.26	3131.04	3130.84	3128.52	3128.62	3129.54	3129.31	3129.30	3129.34	3128.64	3128.73
Mode 45	3144.18	3139.85	3139.58	3139.60	3139.42	3139.59	3139.84	3139.84	3139.86	3140.08	3139.58	3139.16
Mode 46	3143.91	3139.58	3139.32	3139.34	3139.27	3139.37	3139.48	3139.63	3139.65	3139.79	3139.31	3139.28
Mode 47	3166.02	3165.88	3164.84	3164.85	3164.57	3164.71	3164.60	3160.84	3160.83	3160.87	3160.66	3160.71
Mode 48	3166.00	3165.86	3164.82	3164.82	3164.48	3164.72	3164.69	3160.85	3160.85	3160.85	3160.64	3160.67
ZPE	36267.6	36246.6	36244.0	36243.8	36230.7	36230.7	36237.9	36231.1	36231.2	36232.8	36227.5	36227.6

Table S19. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 4.8 and 7.0 a_0 truncated.

Cutoff (a_0)	4.80	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00
Mode 1	445.63	445.65	445.61	445.63	445.62	445.62	445.62	445.55	445.55	445.55	445.55	445.55
Mode 2	445.64	445.67	445.65	445.64	445.64	445.64	445.64	445.56	445.56	445.56	445.56	445.56
Mode 3	516.65	516.60	516.60	516.62	516.72	516.70	516.70	516.69	516.69	516.69	516.70	516.70
Mode 4	520.60	520.58	520.58	520.59	520.67	520.64	520.63	520.64	520.64	520.64	520.64	520.64
Mode 5	539.32	539.12	539.08	538.98	538.80	538.80	538.80	538.79	538.77	538.77	538.77	538.77
Mode 6	539.27	538.98	538.94	538.93	538.74	538.74	538.74	538.74	538.74	538.74	538.75	538.74
Mode 7	579.03	579.09	579.05	578.39	578.49	578.48	578.72	578.70	578.69	578.69	578.69	578.69
Mode 8	622.63	621.97	621.95	621.93	622.19	622.14	622.14	622.15	622.15	622.15	622.15	622.15
Mode 9	623.21	622.77	622.79	622.83	622.75	622.75	622.75	622.59	622.62	622.62	622.64	622.64
Mode 10	623.30	622.94	622.93	622.89	622.81	622.81	622.81	622.65	622.65	622.65	622.67	622.67
Mode 11	642.52	641.56	640.77	640.76	641.35	641.35	641.41	641.16	640.99	640.89	640.91	640.91
Mode 12	857.10	857.11	859.07	858.09	858.15	860.52	860.52	860.57	860.57	860.57	859.50	859.55
Mode 13	857.88	857.90	859.81	858.87	858.84	861.00	861.18	861.42	861.42	861.42	860.32	860.30
Mode 14	856.07	856.06	854.89	854.86	855.04	855.01	855.01	855.07	854.98	854.98	854.96	854.96
Mode 15	859.22	859.19	857.90	857.88	857.98	857.95	857.95	858.02	857.93	857.94	857.91	857.91
Mode 16	862.37	861.58	861.71	861.72	861.41	861.48	861.47	862.32	862.26	862.26	862.26	862.26
Mode 17	862.41	862.27	862.42	861.88	861.57	861.55	861.54	862.49	862.24	862.24	862.24	862.24
Mode 18	910.53	910.59	912.53	912.09	912.00	911.99	911.99	912.04	912.04	912.04	912.02	912.02
Mode 19	930.53	930.58	932.56	932.17	932.04	932.02	932.02	932.09	932.09	932.09	932.07	932.06
Mode 20	946.39	946.48	946.15	946.17	946.22	948.44	948.45	948.38	948.39	948.39	948.16	948.13
Mode 21	957.95	958.06	957.76	957.75	957.80	960.03	960.03	959.98	959.97	959.97	959.75	959.72
Mode 22	1143.33	1143.33	1143.26	1143.23	1143.29	1143.25	1143.24	1143.20	1143.21	1143.21	1143.18	1143.18
Mode 23	1142.92	1142.94	1142.87	1142.82	1142.87	1142.85	1142.85	1142.79	1142.80	1142.79	1142.76	1142.76
Mode 24	1358.91	1360.30	1359.45	1359.58	1359.17	1359.17	1359.17	1358.66	1358.73	1358.72	1358.78	1358.78
Mode 25	1358.53	1360.08	1359.81	1359.76	1359.35	1359.37	1359.37	1358.84	1358.84	1358.84	1358.90	1358.89
Mode 26	1394.30	1394.15	1394.13	1394.13	1394.57	1394.57	1394.57	1394.07	1394.10	1394.10	1394.10	1394.10

Mode 27	1394.23	1393.96	1393.97	1394.09	1394.52	1394.52	1394.52	1394.02	1394.10	1394.10	1394.10	1394.10
Mode 28	1403.18	1403.11	1403.17	1403.19	1402.71	1402.71	1402.71	1403.14	1403.10	1403.10	1403.08	1403.08
Mode 29	1403.12	1402.98	1403.02	1403.12	1402.64	1402.64	1402.64	1403.06	1403.05	1403.05	1403.03	1403.03
Mode 30	1409.10	1409.14	1409.09	1409.06	1409.22	1409.24	1409.24	1409.30	1409.32	1409.32	1409.26	1409.24
Mode 31	1409.15	1409.10	1409.06	1409.12	1409.28	1409.29	1409.29	1409.33	1409.38	1409.38	1409.32	1409.30
Mode 32	1419.39	1420.51	1420.49	1420.57	1414.76	1414.76	1414.76	1415.50	1415.37	1415.37	1414.87	1414.89
Mode 33	1533.23	1532.94	1532.84	1532.83	1532.76	1532.79	1532.79	1533.03	1533.04	1533.03	1533.02	1533.02
Mode 34	1533.27	1533.20	1533.12	1532.89	1532.81	1532.82	1532.81	1533.10	1533.09	1533.03	1533.02	1533.02
Mode 35	1719.86	1721.09	1720.87	1720.57	1719.53	1719.54	1719.54	1720.48	1720.44	1720.44	1720.12	1720.09
Mode 36	1719.97	1720.85	1720.55	1720.61	1719.56	1719.57	1719.57	1720.67	1720.64	1720.64	1720.33	1720.31
Mode 37	1730.55	1730.30	1730.27	1730.28	1729.88	1729.93	1729.93	1729.84	1729.84	1729.83	1729.86	1729.86
Mode 38	1730.64	1730.22	1730.19	1730.15	1729.76	1729.79	1729.79	1729.71	1729.71	1729.71	1729.73	1729.73
Mode 39	3125.85	3126.02	3125.32	3125.34	3125.21	3125.27	3125.27	3125.20	3125.24	3125.24	3124.59	3124.70
Mode 40	3124.58	3124.76	3124.07	3124.08	3123.96	3124.02	3124.02	3123.95	3123.99	3123.99	3123.33	3123.43
Mode 41	3122.43	3122.58	3122.66	3122.01	3122.02	3122.03	3122.03	3122.01	3122.00	3122.01	3122.01	3122.01
Mode 42	3121.00	3121.14	3121.22	3120.64	3120.65	3120.66	3120.66	3120.64	3120.64	3120.64	3120.64	3120.64
Mode 43	3129.07	3128.87	3128.88	3128.88	3128.63	3128.69	3128.69	3128.77	3128.76	3128.76	3128.77	3128.77
Mode 44	3128.80	3128.62	3128.63	3128.59	3128.35	3128.40	3128.40	3128.49	3128.47	3128.47	3128.47	3128.47
Mode 45	3138.86	3138.97	3138.88	3138.85	3138.85	3138.95	3138.95	3138.99	3138.82	3138.82	3138.75	3138.75
Mode 46	3138.66	3138.73	3138.62	3138.63	3138.64	3138.73	3138.78	3138.59	3138.61	3138.61	3138.54	3138.54
Mode 47	3160.86	3160.64	3160.75	3160.61	3160.56	3160.67	3160.73	3160.49	3160.47	3160.47	3160.42	3160.40
Mode 48	3160.83	3160.58	3160.68	3160.65	3160.53	3160.19	3160.24	3160.39	3160.39	3160.38	3160.34	3160.31
ZPE	36227.5	36227.8	36228.1	36226.7	36224.2	36226.5	36226.7	36227.5	36227.4	36227.3	36226.0	36226.1

Table S20. Calculated HF/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.2 and 8.0 a_0 truncated, and finally the untruncated 2MR result.

Cutoff (a_0)	7.20	7.40	7.60	7.80	8.00	2MR
Mode 1	445.55	445.55	445.55	445.55	445.54	445.55
Mode 2	445.56	445.56	445.56	445.56	445.55	445.56
Mode 3	516.70	516.69	516.69	516.69	516.69	516.69
Mode 4	520.65	520.64	520.64	520.64	520.64	520.64
Mode 5	538.77	538.78	538.78	538.78	538.78	538.78
Mode 6	538.74	538.75	538.75	538.75	538.75	538.75
Mode 7	578.69	578.68	578.68	578.68	578.68	578.69
Mode 8	622.15	622.15	622.15	622.15	622.14	622.15
Mode 9	622.64	622.63	622.63	622.63	622.63	622.63
Mode 10	622.67	622.66	622.66	622.66	622.66	622.67
Mode 11	640.91	640.91	640.91	640.91	640.92	640.91
Mode 12	859.55	859.54	859.54	859.54	859.52	859.50
Mode 13	860.33	860.31	860.31	860.31	860.29	860.28
Mode 14	854.96	854.95	854.95	854.95	854.95	854.95
Mode 15	857.91	857.91	857.91	857.91	857.91	857.91
Mode 16	862.26	862.30	862.30	862.30	862.30	862.30
Mode 17	862.25	862.30	862.30	862.30	862.29	862.29
Mode 18	912.02	912.02	912.02	912.02	912.02	912.02
Mode 19	932.06	932.07	932.07	932.07	932.07	932.07
Mode 20	948.13	948.13	948.13	948.13	948.14	948.13
Mode 21	959.72	959.72	959.72	959.72	959.73	959.72
Mode 22	1143.18	1143.18	1143.18	1143.18	1143.18	1143.18
Mode 23	1142.76	1142.76	1142.76	1142.76	1142.76	1142.76
Mode 24	1358.78	1358.76	1358.76	1358.76	1358.75	1358.77
Mode 25	1358.89	1358.88	1358.88	1358.88	1358.87	1358.89
Mode 26	1394.10	1394.08	1394.08	1394.08	1394.08	1394.08

Mode 27	1394.10	1394.07	1394.07	1394.07	1394.07	1394.08
Mode 28	1403.08	1403.12	1403.12	1403.12	1403.12	1403.11
Mode 29	1403.03	1403.06	1403.06	1403.06	1403.07	1403.05
Mode 30	1409.24	1409.25	1409.25	1409.25	1409.28	1409.22
Mode 31	1409.30	1409.30	1409.30	1409.30	1409.34	1409.28
Mode 32	1414.89	1415.07	1415.07	1415.07	1415.11	1414.73
Mode 33	1533.02	1533.03	1533.03	1533.03	1533.03	1533.03
Mode 34	1533.03	1533.03	1533.03	1533.03	1533.03	1533.03
Mode 35	1720.09	1720.08	1720.08	1720.08	1720.04	1720.10
Mode 36	1720.31	1720.29	1720.29	1720.29	1720.26	1720.31
Mode 37	1729.86	1729.88	1729.88	1729.88	1729.87	1729.89
Mode 38	1729.74	1729.75	1729.75	1729.75	1729.74	1729.76
Mode 39	3124.70	3124.70	3124.70	3124.70	3124.70	3124.69
Mode 40	3123.43	3123.44	3123.44	3123.44	3123.44	3123.43
Mode 41	3122.01	3121.99	3121.99	3121.99	3121.98	3122.00
Mode 42	3120.64	3120.62	3120.62	3120.62	3120.61	3120.63
Mode 43	3128.77	3128.77	3128.77	3128.77	3128.77	3128.77
Mode 44	3128.47	3128.48	3128.48	3128.48	3128.48	3128.48
Mode 45	3138.75	3138.76	3138.76	3138.76	3138.76	3138.76
Mode 46	3138.54	3138.55	3138.55	3138.55	3138.55	3138.55
Mode 47	3160.34	3160.37	3160.37	3160.37	3160.37	3160.28
Mode 48	3160.33	3160.36	3160.36	3160.36	3160.35	3160.27
ZPE	36226.1	36226.1	36226.1	36226.1	36226.1	36226.0

Table S21. Calculated RI-MP2/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0 and 2.2 a_0 truncated.

Cutoff (a_0)	0.00	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20
Mode 1	411.54	416.87	416.86	415.81	415.66	415.59	414.95	414.77	414.43	414.32	413.92	413.94
Mode 2	411.53	416.88	416.88	415.83	415.67	415.60	414.95	414.79	414.43	414.33	413.92	413.95
Mode 3	448.78	457.28	457.37	455.75	451.81	452.01	452.54	452.28	452.28	452.58	452.69	452.68
Mode 4	449.01	457.76	457.86	456.21	452.23	452.41	452.93	452.65	452.67	452.98	453.07	453.06
Mode 5	493.61	497.66	497.13	497.18	497.05	496.89	495.96	495.78	496.05	495.92	495.77	495.78
Mode 6	493.60	497.63	497.05	497.10	496.98	496.98	495.86	495.73	495.97	496.00	495.75	495.77
Mode 7	542.57	547.77	541.94	549.22	549.10	547.80	545.64	545.53	546.34	546.24	548.83	547.84
Mode 8	553.61	555.15	555.25	551.31	544.76	544.96	544.28	545.31	549.57	550.13	544.32	549.83
Mode 9	561.79	564.18	567.58	567.66	567.55	567.51	566.28	564.49	564.47	564.82	567.44	567.38
Mode 10	588.33	588.60	586.62	586.81	589.35	585.72	585.84	585.65	585.93	586.72	586.62	586.59
Mode 11	588.30	588.58	586.61	586.80	589.34	585.72	585.83	585.64	585.91	586.68	586.62	586.59
Mode 12	794.17	806.65	806.67	806.22	731.60	731.57	743.86	745.83	741.16	741.33	757.23	757.27
Mode 13	795.31	807.66	807.67	807.22	732.65	732.62	744.89	746.88	742.22	742.39	758.28	758.33
Mode 14	841.87	787.04	787.07	789.39	784.47	784.55	783.58	782.22	782.19	782.15	786.53	786.52
Mode 15	842.04	787.36	787.40	789.71	784.79	784.87	783.92	782.56	782.52	782.48	786.85	786.84
Mode 16	832.51	794.74	794.33	799.99	807.41	807.38	807.77	806.18	821.40	814.45	804.64	808.18
Mode 17	840.75	802.79	806.98	808.74	816.43	816.39	816.79	815.20	830.37	823.12	814.09	815.64
Mode 18	833.71	858.09	858.77	837.39	801.90	802.45	815.60	814.29	816.11	818.47	817.76	817.82
Mode 19	833.70	858.05	858.82	837.36	801.90	802.43	815.62	814.40	816.11	818.44	817.76	817.82
Mode 20	898.39	904.85	905.28	903.89	911.30	910.43	866.96	867.00	869.03	867.92	868.04	885.12
Mode 21	903.75	908.37	910.11	908.73	916.25	915.39	872.20	872.01	873.46	872.33	872.44	889.56
Mode 22	1056.27	1060.45	1060.40	1037.83	1037.85	1036.88	1036.31	1036.99	1051.48	1039.61	1054.69	1072.03
Mode 23	1056.27	1060.40	1060.35	1037.78	1037.79	1036.82	1036.26	1036.94	1051.35	1039.42	1054.72	1072.12
Mode 24	1323.03	1292.71	1291.96	1291.53	1291.37	1291.00	1290.97	1290.13	1289.76	1290.54	1290.42	1289.84
Mode 25	1323.03	1292.70	1292.02	1291.59	1291.42	1291.06	1291.02	1290.20	1289.81	1290.57	1290.42	1289.84
Mode 26	1324.66	1293.10	1292.74	1292.65	1296.54	1295.12	1293.99	1294.22	1293.91	1293.27	1293.00	1291.51

Mode 27	1324.66	1293.07	1292.72	1292.63	1296.51	1295.11	1293.97	1294.24	1293.88	1293.22	1292.95	1291.45
Mode 28	1331.66	1295.73	1296.36	1296.01	1296.15	1296.51	1294.91	1295.64	1294.20	1292.91	1293.11	1293.16
Mode 29	1331.66	1295.70	1296.32	1295.98	1296.11	1296.50	1294.88	1295.55	1294.19	1292.91	1293.11	1293.16
Mode 30	1307.09	1304.41	1301.79	1302.76	1303.01	1299.52	1299.48	1295.08	1296.37	1301.36	1301.49	1301.39
Mode 31	1307.09	1304.43	1301.79	1302.78	1303.03	1299.50	1299.49	1294.92	1296.41	1301.37	1301.50	1301.39
Mode 32	1364.20	1358.96	1358.70	1358.50	1357.71	1357.66	1353.99	1359.89	1358.95	1357.42	1357.07	1356.95
Mode 33	1455.57	1476.81	1476.83	1455.53	1424.74	1424.82	1424.71	1428.60	1428.37	1427.50	1429.17	1429.20
Mode 34	1455.57	1476.79	1476.81	1455.52	1424.73	1424.81	1424.70	1428.57	1428.37	1427.49	1429.16	1429.19
Mode 35	1554.86	1549.82	1549.52	1549.46	1546.98	1544.86	1543.74	1545.39	1544.69	1543.96	1543.64	1543.70
Mode 36	1554.86	1549.57	1549.26	1549.22	1547.21	1546.14	1543.99	1545.51	1544.79	1544.08	1543.83	1543.88
Mode 37	1573.91	1573.27	1568.06	1567.53	1567.41	1566.55	1562.65	1561.40	1565.24	1563.89	1563.00	1563.10
Mode 38	1573.91	1573.29	1568.11	1567.55	1567.45	1566.57	1562.70	1561.56	1565.28	1563.93	1563.05	1563.15
Mode 39	3086.32	3039.46	3039.13	3036.52	3036.77	3036.49	2998.39	2998.18	2997.55	2993.65	2993.99	2994.13
Mode 40	3086.32	3039.38	3039.05	3037.24	3037.48	3037.26	3000.04	2998.90	2996.85	2994.24	2993.40	2994.72
Mode 41	3088.08	3006.92	3002.81	3000.80	3001.23	3001.38	3001.34	3000.88	3001.00	2990.07	2987.37	2987.62
Mode 42	3088.08	3006.62	3001.94	3001.87	3002.29	3002.43	3002.39	3001.98	2999.92	2991.12	2988.10	2986.98
Mode 43	3101.78	3057.26	3057.51	3034.01	3033.84	3028.43	3028.54	3028.20	3024.72	3025.18	3018.10	3017.40
Mode 44	3101.78	3057.26	3057.53	3034.00	3033.83	3028.44	3028.54	3028.23	3024.70	3025.19	3017.95	3017.53
Mode 45	3136.87	3129.26	3129.30	3083.83	3039.38	3039.78	3037.86	3037.87	3037.81	3037.11	3037.81	3036.03
Mode 46	3136.87	3129.14	3129.18	3083.95	3039.50	3039.90	3037.98	3038.02	3037.69	3037.24	3037.68	3036.16
Mode 47	3160.44	3098.29	3098.35	3099.42	3059.29	3058.87	3058.98	3062.92	3063.50	3064.26	3061.77	3061.77
Mode 48	3160.44	3098.30	3098.36	3099.41	3059.28	3058.85	3058.97	3062.87	3063.51	3064.25	3061.77	3061.77
ZPE	34338.0	34189.2	34183.1	34123.8	34022.6	34014.0	33982.3	33984.0	33998.4	33985.5	33993.1	34011.2

Table S22. Calculated RI-MP2/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.4 and 4.6 a_0 truncated.

Cutoff (a_0)	2.40	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60
Mode 1	413.96	413.18	413.00	413.10	413.01	412.76	412.80	412.79	412.81	412.82	412.87	412.87
Mode 2	414.02	413.17	413.00	413.09	412.94	412.78	412.80	412.79	412.81	412.82	412.86	412.87
Mode 3	452.95	453.03	452.71	452.92	452.87	452.75	452.63	452.64	452.54	452.80	452.87	452.90
Mode 4	453.31	453.41	453.09	453.30	453.23	453.22	452.99	453.01	452.90	453.14	453.21	453.23
Mode 5	495.79	495.71	495.89	495.77	495.44	495.60	495.58	495.40	495.41	494.89	494.52	494.58
Mode 6	495.82	495.69	495.90	495.76	495.85	495.55	495.58	495.37	495.38	494.86	494.50	494.56
Mode 7	547.82	543.97	544.07	544.03	543.82	542.75	540.94	540.78	542.43	542.93	543.28	543.00
Mode 8	549.85	549.98	550.04	550.20	550.08	549.99	551.01	550.94	550.63	550.53	549.86	549.96
Mode 9	562.93	562.71	562.82	562.76	563.09	559.53	559.51	559.34	561.06	561.53	561.92	561.62
Mode 10	586.75	585.86	585.17	584.52	584.54	584.43	584.41	584.34	584.34	585.12	584.69	584.70
Mode 11	586.70	585.86	585.14	584.52	583.93	584.40	584.40	584.34	584.35	585.13	584.70	584.70
Mode 12	757.16	756.48	753.59	753.54	753.63	753.58	760.32	755.26	756.85	759.86	759.84	760.02
Mode 13	758.17	757.53	754.65	754.60	754.73	754.67	761.31	756.34	758.02	761.08	761.05	761.22
Mode 14	784.98	783.27	783.39	783.38	783.47	781.79	781.45	786.93	785.72	785.62	785.65	785.64
Mode 15	785.29	783.60	783.71	783.70	783.75	782.11	781.77	787.24	786.04	785.94	785.97	785.96
Mode 16	808.20	807.19	807.19	805.39	805.14	805.17	811.37	809.88	809.92	809.70	809.73	809.73
Mode 17	815.59	814.70	814.71	812.85	812.83	812.64	818.75	817.26	817.30	817.07	817.12	817.12
Mode 18	816.73	816.13	814.91	814.52	816.70	816.67	816.53	816.52	815.99	815.28	815.02	815.10
Mode 19	816.71	816.13	814.89	814.50	816.44	816.69	816.51	816.52	815.99	815.28	815.02	815.11
Mode 20	885.15	868.28	868.16	868.16	865.54	865.54	865.20	865.00	865.07	868.32	868.42	868.48
Mode 21	889.61	872.72	872.59	872.59	869.98	869.97	869.62	869.42	869.48	872.73	872.83	872.90
Mode 22	1071.90	1068.93	1057.93	1057.15	1049.23	1048.83	1049.50	1055.05	1051.07	1051.10	1051.18	1051.19
Mode 23	1071.70	1069.03	1058.03	1057.25	1049.34	1049.01	1049.24	1054.81	1050.81	1050.84	1050.92	1050.93
Mode 24	1289.87	1289.40	1289.95	1288.51	1287.77	1288.47	1289.23	1288.28	1288.28	1286.96	1286.12	1286.16
Mode 25	1289.84	1289.39	1289.97	1288.52	1288.66	1288.45	1289.22	1288.24	1288.25	1286.94	1286.10	1286.13
Mode 26	1291.33	1290.85	1292.46	1292.73	1292.61	1292.31	1291.01	1291.00	1290.79	1291.92	1292.03	1291.98

Mode 27	1291.02	1290.75	1292.39	1292.66	1292.34	1292.30	1290.94	1290.94	1290.82	1291.94	1292.06	1292.00
Mode 28	1293.25	1293.47	1293.14	1293.34	1293.07	1292.65	1292.47	1292.47	1292.47	1293.41	1292.35	1291.89
Mode 29	1293.27	1293.48	1293.09	1293.33	1292.35	1292.68	1292.45	1292.50	1292.50	1293.44	1292.36	1291.91
Mode 30	1302.22	1295.91	1295.47	1293.30	1292.54	1290.60	1290.29	1290.29	1290.25	1289.22	1291.41	1291.25
Mode 31	1302.29	1295.91	1295.51	1293.33	1292.92	1290.78	1290.50	1290.46	1290.42	1289.39	1291.59	1291.43
Mode 32	1356.54	1357.31	1355.06	1355.02	1354.54	1354.67	1354.51	1354.52	1354.52	1354.81	1356.20	1355.98
Mode 33	1428.61	1428.39	1428.07	1427.90	1428.25	1428.40	1428.40	1428.41	1428.23	1427.99	1427.93	1427.97
Mode 34	1428.59	1428.38	1428.07	1427.89	1428.49	1428.42	1428.39	1428.38	1428.20	1427.97	1427.93	1427.96
Mode 35	1543.63	1543.39	1543.20	1542.22	1542.66	1542.13	1542.22	1542.02	1542.02	1535.39	1536.14	1535.54
Mode 36	1543.84	1543.58	1543.30	1542.37	1541.59	1542.35	1542.37	1542.25	1542.25	1535.47	1536.24	1535.63
Mode 37	1557.45	1556.75	1556.32	1555.55	1555.49	1555.58	1553.49	1553.37	1553.28	1552.22	1551.74	1551.06
Mode 38	1557.51	1556.81	1556.39	1555.61	1555.83	1553.53	1553.53	1553.39	1553.29	1552.24	1551.75	1551.07
Mode 39	2994.18	2994.07	2993.50	2993.96	2986.45	2986.53	2986.27	2985.71	2986.27	2986.08	2985.87	2985.87
Mode 40	2994.76	2993.48	2994.08	2993.37	2985.88	2985.95	2985.69	2986.29	2985.69	2985.50	2985.30	2985.31
Mode 41	2987.60	2987.48	2987.70	2985.32	2985.13	2985.30	2985.56	2983.62	2982.95	2982.72	2982.80	2982.77
Mode 42	2986.98	2988.12	2987.11	2985.93	2985.91	2985.88	2986.16	2982.97	2983.61	2983.38	2983.46	2983.43
Mode 43	3016.98	3001.81	2999.52	2999.19	2999.19	2998.93	2998.59	2998.57	2998.57	2997.76	2997.33	2997.37
Mode 44	3013.96	3001.70	2999.64	2999.08	2998.90	2998.76	2998.49	2998.67	2998.38	2997.57	2997.14	2997.18
Mode 45	3035.73	3035.92	3029.15	3029.40	3029.25	3029.39	3029.75	3029.40	3029.62	3029.84	3029.11	3028.43
Mode 46	3035.86	3035.79	3029.26	3029.28	3029.39	3029.19	3029.65	3029.53	3029.49	3029.71	3028.98	3028.31
Mode 47	3059.94	3055.02	3053.86	3053.68	3053.76	3053.67	3053.07	3053.35	3051.03	3050.86	3050.62	3050.64
Mode 48	3059.94	3055.03	3053.85	3053.69	3053.63	3053.80	3053.08	3053.34	3051.05	3050.85	3050.62	3050.63
ZPE	34004.3	33979.5	33966.9	33961.7	33953.5	33950.0	33954.8	33955.3	33952.9	33951.4	33951.0	33949.9

Table S23. Calculated RI-MP2/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 4.8 and 7.0 a_0 truncated.

Cutoff (a_0)	4.80	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00
Mode 1	412.82	412.84	412.82	412.80	412.80	412.80	412.80	412.73	412.72	412.72	412.74	412.73
Mode 2	412.82	412.81	412.81	412.81	412.78	412.78	412.78	412.71	412.71	412.71	412.72	412.71
Mode 3	452.86	452.83	452.89	452.88	453.02	453.02	453.01	453.01	453.01	453.01	453.02	453.02
Mode 4	453.20	453.19	453.24	453.22	453.36	453.34	453.35	453.35	453.35	453.35	453.36	453.36
Mode 5	494.73	494.77	494.68	494.64	494.31	494.37	494.37	494.44	494.48	494.48	494.48	494.48
Mode 6	494.66	494.59	494.61	494.65	494.37	494.31	494.31	494.38	494.41	494.41	494.45	494.44
Mode 7	542.87	542.84	541.89	541.88	541.89	542.14	542.11	542.18	542.19	542.19	542.18	542.17
Mode 8	551.29	550.32	549.83	549.83	551.05	551.05	551.05	550.83	550.80	550.80	550.51	550.53
Mode 9	561.52	560.86	560.46	560.47	560.44	560.65	560.64	560.72	560.73	560.73	560.72	560.72
Mode 10	584.35	584.36	584.42	584.45	584.45	584.45	584.45	584.20	584.17	584.17	584.22	584.22
Mode 11	584.43	584.55	584.50	584.45	584.53	584.52	584.52	584.27	584.24	584.24	584.27	584.27
Mode 12	760.17	759.79	758.33	758.30	758.71	758.69	758.68	758.62	758.63	758.63	758.60	758.59
Mode 13	761.37	760.96	759.45	759.44	759.68	759.66	759.65	759.59	759.60	759.60	759.57	759.57
Mode 14	785.67	785.62	785.65	787.64	786.26	786.80	788.05	788.06	788.05	788.05	787.47	786.96
Mode 15	785.99	785.95	785.97	787.93	786.58	786.82	788.38	788.39	788.38	788.38	787.79	787.27
Mode 16	809.50	809.56	809.55	811.24	810.79	810.79	810.78	810.83	810.84	810.84	810.83	810.80
Mode 17	816.88	816.92	816.92	818.66	818.18	818.19	818.18	818.23	818.24	818.24	818.23	818.21
Mode 18	815.00	814.35	814.50	814.50	814.24	814.23	814.28	815.27	815.17	815.17	815.03	815.03
Mode 19	815.04	815.13	814.58	814.54	814.15	814.27	814.36	815.18	815.25	815.26	815.03	815.02
Mode 20	868.40	868.40	868.15	867.98	868.07	868.08	869.34	869.32	869.28	869.27	869.27	869.09
Mode 21	872.82	872.82	872.58	872.38	872.48	872.50	873.76	873.74	873.70	873.70	873.69	873.51
Mode 22	1051.14	1051.18	1051.13	1051.10	1051.12	1051.13	1051.12	1051.06	1051.05	1051.05	1051.05	1051.01
Mode 23	1050.88	1050.94	1050.87	1050.84	1050.86	1050.88	1050.86	1050.80	1050.79	1050.80	1050.79	1050.76
Mode 24	1286.97	1287.00	1286.96	1287.24	1286.42	1286.42	1286.42	1286.89	1286.96	1286.97	1286.88	1286.87
Mode 25	1286.95	1286.89	1286.93	1287.25	1286.40	1286.40	1286.40	1286.86	1286.94	1286.94	1286.87	1286.86
Mode 26	1291.49	1291.57	1291.62	1291.64	1292.27	1292.28	1292.28	1291.63	1291.54	1291.53	1291.62	1291.61

Mode 27	1291.55	1291.75	1291.67	1291.65	1292.33	1292.34	1292.33	1291.68	1291.58	1291.58	1291.64	1291.63
Mode 28	1292.04	1292.02	1291.88	1291.91	1292.09	1292.12	1292.12	1292.10	1292.05	1292.05	1292.03	1291.97
Mode 29	1292.10	1292.16	1291.93	1291.88	1292.14	1292.17	1292.16	1292.15	1292.13	1292.13	1292.07	1292.01
Mode 30	1291.09	1290.87	1290.73	1290.67	1290.33	1290.35	1290.35	1289.67	1289.58	1289.58	1289.69	1289.72
Mode 31	1291.23	1290.43	1290.55	1290.59	1290.15	1290.16	1290.17	1289.48	1289.40	1289.40	1289.57	1289.59
Mode 32	1355.73	1355.80	1355.78	1355.80	1348.64	1348.65	1348.65	1349.08	1349.10	1349.10	1348.63	1348.55
Mode 33	1427.91	1427.74	1427.41	1427.29	1427.22	1427.22	1427.27	1427.45	1427.48	1427.48	1427.38	1427.37
Mode 34	1427.88	1427.68	1427.38	1427.27	1427.20	1427.25	1427.26	1427.41	1427.44	1427.44	1427.38	1427.37
Mode 35	1536.49	1536.26	1535.97	1535.77	1534.12	1534.11	1534.11	1535.29	1535.34	1535.34	1534.69	1534.47
Mode 36	1536.36	1535.56	1535.81	1535.92	1533.96	1533.97	1533.97	1535.37	1535.41	1535.41	1534.79	1534.56
Mode 37	1551.32	1551.38	1551.07	1551.03	1550.48	1550.48	1550.51	1550.41	1550.42	1550.42	1550.44	1550.44
Mode 38	1551.29	1551.35	1551.13	1551.12	1550.54	1550.57	1550.58	1550.47	1550.48	1550.48	1550.51	1550.51
Mode 39	2985.38	2985.38	2984.84	2984.30	2984.06	2984.56	2984.61	2984.72	2984.13	2984.66	2984.62	2984.29
Mode 40	2985.92	2985.89	2984.31	2984.87	2984.59	2984.03	2984.08	2984.19	2984.65	2984.13	2984.08	2983.74
Mode 41	2982.73	2982.69	2982.00	2982.74	2982.11	2981.47	2981.47	2981.29	2981.91	2981.26	2981.27	2981.26
Mode 42	2982.05	2981.97	2982.67	2982.08	2981.47	2982.11	2982.11	2981.94	2981.25	2981.91	2981.91	2981.90
Mode 43	2997.40	2997.40	2997.50	2997.32	2996.91	2997.09	2997.11	2997.32	2997.19	2997.36	2997.36	2997.35
Mode 44	2997.57	2997.49	2997.33	2997.51	2997.06	2996.92	2996.95	2997.16	2997.36	2997.19	2997.18	2997.18
Mode 45	3027.89	3027.88	3027.94	3027.78	3027.68	3027.87	3027.87	3027.71	3027.55	3027.68	3027.65	3027.65
Mode 46	3028.03	3028.09	3027.79	3027.90	3027.80	3027.76	3027.75	3027.58	3027.68	3027.55	3027.54	3027.53
Mode 47	3050.79	3050.79	3050.76	3050.77	3050.52	3050.56	3050.01	3050.21	3050.24	3050.25	3050.20	3049.95
Mode 48	3050.80	3050.86	3050.76	3050.77	3050.55	3049.93	3049.98	3050.20	3050.25	3050.24	3050.20	3049.94
ZPE	33950.2	33949.0	33946.7	33948.5	33944.0	33944.3	33945.6	33946.3	33946.2	33946.3	33945.3	33944.6

Table S24. Calculated RI-MP2/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.2 and 8.0 a_0 truncated, and finally the untruncated 2MR result.

Cutoff (a_0)	7.20	7.40	7.60	7.80	8.00	2MR
Mode 1	412.73	412.71	412.71	412.71	412.69	412.70
Mode 2	412.71	412.71	412.70	412.70	412.70	412.71
Mode 3	453.02	453.02	453.02	453.02	453.02	453.02
Mode 4	453.36	453.35	453.35	453.36	453.36	453.35
Mode 5	494.48	494.49	494.53	494.53	494.48	494.49
Mode 6	494.44	494.53	494.50	494.49	494.52	494.53
Mode 7	542.17	542.18	542.18	542.18	542.16	542.17
Mode 8	550.53	550.59	550.62	550.62	550.63	550.62
Mode 9	560.72	560.73	560.73	560.73	560.71	560.73
Mode 10	584.23	584.18	584.17	584.17	584.17	584.18
Mode 11	584.27	584.20	584.21	584.21	584.19	584.20
Mode 12	758.59	758.60	758.60	758.62	758.59	758.61
Mode 13	759.57	759.58	759.58	759.58	759.58	759.60
Mode 14	786.97	786.99	787.00	787.01	786.93	786.93
Mode 15	787.28	787.29	787.31	787.32	787.24	787.24
Mode 16	810.81	810.80	810.82	810.82	810.80	810.82
Mode 17	818.21	818.22	818.22	818.22	818.22	818.23
Mode 18	815.03	815.15	815.14	815.14	815.12	815.16
Mode 19	815.02	815.11	815.14	815.15	815.15	815.12
Mode 20	869.09	869.09	869.08	869.08	869.11	869.10
Mode 21	873.52	873.50	873.51	873.51	873.51	873.51
Mode 22	1051.01	1051.01	1051.00	1051.00	1051.01	1051.01
Mode 23	1050.76	1050.74	1050.74	1050.74	1050.74	1050.74
Mode 24	1286.87	1286.99	1287.01	1287.01	1287.00	1287.00
Mode 25	1286.86	1287.02	1287.00	1287.01	1287.03	1287.03
Mode 26	1291.62	1291.45	1291.43	1291.43	1291.45	1291.45

Mode 27	1291.64	1291.44	1291.45	1291.45	1291.44	1291.44
Mode 28	1291.98	1291.97	1291.92	1291.92	1292.02	1291.99
Mode 29	1292.02	1291.91	1291.96	1291.96	1291.96	1291.93
Mode 30	1289.72	1289.52	1289.56	1289.56	1289.50	1289.51
Mode 31	1289.59	1289.49	1289.44	1289.44	1289.47	1289.48
Mode 32	1348.55	1348.54	1348.54	1348.54	1348.65	1348.28
Mode 33	1427.37	1427.39	1427.41	1427.41	1427.39	1427.40
Mode 34	1427.37	1427.41	1427.40	1427.41	1427.41	1427.42
Mode 35	1534.47	1534.48	1534.50	1534.50	1534.40	1534.45
Mode 36	1534.56	1534.61	1534.59	1534.59	1534.54	1534.59
Mode 37	1550.44	1550.42	1550.44	1550.44	1550.39	1550.41
Mode 38	1550.51	1550.52	1550.50	1550.50	1550.49	1550.51
Mode 39	2984.29	2984.33	2983.76	2983.76	2983.76	2983.75
Mode 40	2983.75	2983.75	2984.31	2984.31	2984.34	2984.33
Mode 41	2981.26	2981.18	2981.81	2981.82	2981.78	2981.80
Mode 42	2981.90	2981.81	2981.17	2981.18	2981.15	2981.18
Mode 43	2997.36	2997.44	2997.24	2997.24	2997.22	2997.24
Mode 44	2997.17	2997.23	2997.43	2997.43	2997.43	2997.43
Mode 45	3027.65	3027.57	3027.47	3027.47	3027.48	3027.49
Mode 46	3027.54	3027.49	3027.59	3027.59	3027.56	3027.57
Mode 47	3049.95	3050.01	3049.99	3050.00	3049.98	3049.91
Mode 48	3049.95	3050.01	3049.97	3049.97	3049.97	3049.89
ZPE	33944.6	33944.5	33944.6	33944.6	33944.5	33944.4

Table S25. Calculated RI-MP2/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0 and 2.2 a_0 calculated using HF/cc-pVDZ.

Cutoff (a_0)	0.00	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20
Mode 1	414.47	412.91	412.91	412.82	412.80	412.78	412.72	412.73	412.73	412.74	412.70	412.71
Mode 2	414.47	413.10	413.11	413.02	412.99	412.98	412.92	412.93	412.93	412.94	412.91	412.91
Mode 3	448.90	453.94	453.94	453.76	453.41	453.41	453.47	453.46	453.50	453.50	453.48	453.48
Mode 4	449.16	453.74	453.74	453.56	453.20	453.20	453.26	453.25	453.30	453.29	453.28	453.27
Mode 5	496.77	494.59	494.61	494.60	494.54	494.55	494.50	494.50	494.50	494.44	494.43	494.44
Mode 6	496.80	494.71	494.75	494.74	494.66	494.67	494.64	494.62	494.62	494.57	494.56	494.57
Mode 7	538.33	540.07	540.17	540.90	540.94	540.85	540.89	540.87	541.40	541.36	541.67	541.73
Mode 8	544.86	546.81	546.80	546.56	547.15	547.16	547.14	547.19	548.07	548.53	548.53	549.81
Mode 9	556.64	558.08	559.34	559.32	559.38	559.35	559.29	559.30	559.31	559.75	560.07	560.08
Mode 10	585.18	584.76	584.73	584.70	584.67	584.69	584.69	584.70	584.71	584.73	584.45	584.46
Mode 11	585.19	584.83	584.78	584.75	584.72	584.75	584.74	584.76	584.77	584.79	584.50	584.51
Mode 12	754.16	759.33	759.33	758.27	756.71	756.71	757.05	757.35	757.41	757.39	758.30	758.31
Mode 13	755.13	760.28	760.28	759.22	757.67	757.68	757.98	758.26	758.34	758.31	759.22	759.24
Mode 14	785.30	788.31	788.30	788.48	787.10	787.10	787.08	787.15	787.14	787.13	787.68	787.68
Mode 15	785.62	788.73	788.73	788.94	787.65	787.64	787.63	787.70	787.69	787.68	788.28	788.27
Mode 16	806.11	808.26	808.24	808.73	809.25	809.23	809.13	809.08	810.39	809.97	810.05	810.83
Mode 17	813.42	815.58	816.13	816.19	816.62	816.61	816.53	816.45	817.72	817.25	817.37	817.87
Mode 18	818.25	818.07	818.08	817.36	815.90	815.93	816.19	816.27	816.01	816.03	816.04	816.05
Mode 19	818.22	818.04	818.05	817.37	815.86	815.89	816.19	816.26	816.01	816.03	816.04	816.05
Mode 20	865.94	868.22	868.28	868.09	868.58	868.58	868.83	868.81	869.03	869.05	868.97	869.92
Mode 21	870.34	872.29	872.53	872.27	872.74	872.74	872.94	872.91	873.14	873.17	873.08	873.95
Mode 22	1048.96	1048.83	1048.81	1048.96	1048.73	1048.70	1048.49	1048.44	1049.15	1049.29	1050.03	1050.92
Mode 23	1048.71	1048.62	1048.58	1048.78	1048.54	1048.51	1048.31	1048.25	1048.97	1049.13	1049.92	1050.83
Mode 24	1288.74	1287.47	1287.42	1287.46	1287.48	1287.50	1287.55	1287.50	1287.17	1287.14	1287.01	1286.98
Mode 25	1288.75	1287.43	1287.35	1287.39	1287.40	1287.43	1287.48	1287.42	1287.11	1287.08	1287.02	1286.98
Mode 26	1292.07	1292.43	1292.39	1292.43	1292.03	1292.27	1292.29	1292.30	1292.37	1292.45	1292.44	1292.43

Mode 27	1292.05	1292.30	1292.31	1292.29	1291.80	1292.04	1292.10	1292.05	1292.06	1292.14	1292.06	1291.98
Mode 28	1293.77	1292.70	1292.74	1292.63	1292.60	1292.60	1292.48	1292.37	1292.12	1291.96	1291.97	1291.96
Mode 29	1293.67	1292.90	1292.85	1292.76	1292.81	1292.80	1292.74	1292.68	1292.47	1292.36	1292.36	1292.35
Mode 30	1289.33	1289.83	1289.83	1289.81	1289.56	1289.67	1289.65	1289.69	1289.67	1289.79	1289.88	1289.90
Mode 31	1289.29	1289.63	1289.63	1289.60	1289.34	1289.43	1289.42	1289.44	1289.43	1289.55	1289.64	1289.66
Mode 32	1347.20	1348.43	1348.45	1348.42	1348.35	1348.32	1348.56	1348.03	1348.15	1348.13	1348.08	1348.20
Mode 33	1430.56	1429.23	1429.24	1428.99	1428.02	1428.03	1428.05	1428.33	1428.30	1428.30	1428.15	1428.15
Mode 34	1430.57	1429.14	1429.15	1428.86	1427.88	1427.89	1427.91	1428.16	1428.14	1428.13	1427.96	1427.97
Mode 35	1536.14	1535.37	1535.34	1535.36	1535.66	1535.72	1535.57	1535.27	1535.65	1535.63	1535.63	1535.66
Mode 36	1536.31	1535.43	1535.40	1535.41	1535.59	1535.61	1535.48	1535.13	1535.49	1535.47	1535.47	1535.50
Mode 37	1552.75	1551.52	1551.57	1551.82	1551.54	1551.54	1551.23	1551.31	1550.95	1550.95	1550.99	1551.00
Mode 38	1552.87	1551.65	1551.73	1552.02	1551.72	1551.73	1551.46	1551.53	1551.21	1551.22	1551.27	1551.27
Mode 39	2982.17	2980.73	2980.73	2980.74	2980.78	2980.78	2984.57	2984.56	2984.20	2984.13	2984.12	2984.17
Mode 40	2981.53	2981.26	2981.31	2981.28	2981.27	2981.26	2984.99	2985.03	2984.67	2984.60	2984.59	2984.63
Mode 41	2979.11	2982.08	2982.69	2982.61	2982.58	2982.58	2982.57	2982.47	2982.17	2982.79	2982.86	2982.81
Mode 42	2978.42	2981.36	2981.79	2981.72	2981.72	2981.73	2981.70	2981.62	2981.32	2981.95	2982.23	2982.20
Mode 43	2995.17	2994.32	2994.34	2996.17	2996.09	2996.26	2996.11	2996.13	2996.28	2996.26	2996.99	2996.95
Mode 44	2995.40	2994.52	2994.53	2996.34	2996.28	2996.45	2996.27	2996.32	2996.46	2996.44	2997.16	2997.10
Mode 45	3024.46	3021.40	3021.39	3023.99	3028.50	3028.48	3027.85	3027.84	3027.82	3027.85	3027.92	3027.87
Mode 46	3024.55	3021.53	3021.51	3024.09	3028.59	3028.57	3027.94	3027.93	3027.91	3027.93	3028.00	3027.94
Mode 47	3046.38	3048.64	3048.64	3048.70	3051.07	3051.09	3051.05	3050.81	3050.74	3050.74	3050.47	3050.47
Mode 48	3046.36	3048.60	3048.60	3048.66	3051.01	3051.03	3050.99	3050.75	3050.68	3050.68	3050.40	3050.41
ZPE	33929.5	33939.3	33940.1	33941.5	33942.0	33942.3	33943.8	33943.6	33944.6	33944.9	33946.3	33947.8

Table S26. Calculated RI-MP2/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.4 and 4.6 a_0 calculated using HF/cc-pVDZ.

Cutoff (a_0)	2.40	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60
Mode 1	412.71	412.64	412.65	412.63	412.63	412.64	412.64	412.65	412.65	412.65	412.66	412.65
Mode 2	412.90	412.84	412.85	412.84	412.83	412.83	412.85	412.85	412.86	412.85	412.85	412.85
Mode 3	453.52	453.52	453.49	453.49	453.50	453.47	453.47	453.48	453.48	453.48	453.49	453.49
Mode 4	453.31	453.31	453.29	453.29	453.30	453.30	453.27	453.28	453.28	453.28	453.29	453.30
Mode 5	494.44	494.48	494.41	494.40	494.39	494.40	494.40	494.40	494.40	494.40	494.41	494.42
Mode 6	494.56	494.60	494.54	494.54	494.53	494.53	494.54	494.54	494.54	494.54	494.58	494.58
Mode 7	541.73	541.75	541.72	541.70	541.70	541.82	542.13	542.14	542.42	542.42	542.42	542.39
Mode 8	549.80	549.82	549.83	549.84	549.83	549.85	550.09	550.09	549.96	549.97	550.02	550.02
Mode 9	560.13	560.11	560.10	560.07	560.14	560.53	560.52	560.53	560.85	560.85	560.84	560.81
Mode 10	584.50	584.40	584.35	584.19	584.19	584.22	584.23	584.24	584.24	584.20	584.20	584.21
Mode 11	584.53	584.42	584.39	584.25	584.27	584.26	584.28	584.29	584.29	584.25	584.14	584.15
Mode 12	758.30	758.27	758.03	758.03	758.03	758.03	758.34	758.22	758.48	758.62	758.66	758.72
Mode 13	759.22	759.19	758.97	758.97	758.96	758.97	759.21	759.10	759.43	759.53	759.59	759.64
Mode 14	787.54	787.31	787.29	787.28	787.28	787.12	787.13	787.20	787.14	787.13	787.13	787.12
Mode 15	788.17	787.95	787.93	787.91	787.92	787.78	787.80	787.89	787.83	787.83	787.82	787.81
Mode 16	810.83	810.77	810.79	810.73	810.76	810.77	811.02	811.00	811.00	810.97	810.98	810.93
Mode 17	817.85	817.84	817.83	817.78	817.80	817.81	818.02	818.00	818.00	817.96	817.98	817.88
Mode 18	816.04	815.97	815.64	815.67	815.72	815.70	815.71	815.72	815.69	815.71	815.75	815.70
Mode 19	816.05	815.98	815.67	815.70	815.74	815.73	815.74	815.74	815.71	815.73	815.74	815.74
Mode 20	869.92	870.14	870.16	870.15	869.94	869.86	869.94	869.77	869.77	869.88	869.89	869.91
Mode 21	873.93	874.08	874.12	874.11	873.91	873.79	873.87	873.69	873.70	873.77	873.76	873.79
Mode 22	1050.90	1050.68	1050.54	1050.39	1050.68	1050.71	1050.91	1050.99	1050.91	1050.88	1050.89	1050.89
Mode 23	1050.77	1050.59	1050.46	1050.31	1050.57	1050.61	1050.76	1050.84	1050.76	1050.73	1050.74	1050.75
Mode 24	1286.99	1287.09	1287.03	1287.11	1287.14	1287.13	1287.20	1287.18	1287.19	1287.19	1287.14	1287.16
Mode 25	1286.98	1287.09	1287.03	1287.11	1287.14	1287.13	1287.19	1287.18	1287.18	1287.18	1287.15	1287.17
Mode 26	1292.42	1292.31	1292.45	1292.47	1292.47	1292.52	1292.19	1292.18	1292.10	1292.09	1292.12	1292.11

Mode 27	1291.81	1291.86	1291.83	1291.85	1291.85	1291.84	1291.45	1291.44	1291.38	1291.37	1291.37	1291.36
Mode 28	1291.98	1292.06	1292.06	1292.06	1292.02	1292.02	1291.67	1291.67	1291.67	1291.67	1291.66	1291.74
Mode 29	1292.36	1292.36	1292.45	1292.44	1292.43	1292.42	1292.12	1292.12	1292.13	1292.12	1292.09	1292.20
Mode 30	1289.95	1289.89	1289.93	1289.97	1289.95	1290.06	1290.06	1290.06	1290.06	1290.06	1289.81	1289.79
Mode 31	1289.71	1289.64	1289.66	1289.70	1289.67	1289.76	1289.76	1289.76	1289.75	1289.76	1289.52	1289.46
Mode 32	1348.30	1348.44	1348.45	1348.39	1348.38	1348.33	1348.28	1348.30	1348.30	1348.25	1348.12	1348.13
Mode 33	1428.13	1428.12	1428.03	1428.04	1428.16	1428.15	1428.17	1428.16	1428.15	1428.16	1428.16	1428.18
Mode 34	1427.94	1427.93	1427.82	1427.83	1427.94	1427.95	1427.95	1427.94	1427.93	1427.94	1427.96	1427.97
Mode 35	1535.70	1535.64	1535.59	1535.50	1535.49	1535.43	1535.47	1535.47	1535.47	1535.50	1535.18	1535.15
Mode 36	1535.54	1535.49	1535.43	1535.31	1535.30	1535.20	1535.24	1535.23	1535.23	1535.25	1534.99	1534.94
Mode 37	1550.67	1550.59	1550.59	1550.53	1550.45	1550.42	1550.72	1550.55	1550.55	1550.55	1550.52	1550.45
Mode 38	1550.99	1550.93	1550.91	1550.88	1550.83	1551.15	1551.15	1550.99	1550.99	1550.99	1551.01	1550.94
Mode 39	2984.16	2984.16	2984.19	2984.16	2984.63	2984.62	2984.32	2984.31	2984.31	2984.31	2984.11	2983.95
Mode 40	2984.64	2984.66	2984.65	2984.63	2985.09	2985.08	2984.77	2984.77	2984.77	2984.77	2984.58	2984.41
Mode 41	2982.83	2982.66	2982.67	2982.66	2982.40	2982.39	2982.41	2982.32	2982.32	2982.31	2982.17	2982.16
Mode 42	2982.21	2982.03	2982.05	2982.04	2981.78	2981.78	2981.80	2981.72	2981.72	2981.71	2981.57	2981.57
Mode 43	2996.93	2998.13	2997.94	2997.94	2997.94	2997.62	2997.28	2997.26	2997.27	2997.27	2997.26	2997.27
Mode 44	2997.43	2998.28	2998.09	2998.10	2998.09	2997.78	2997.40	2997.39	2997.36	2997.36	2997.38	2997.39
Mode 45	3027.82	3027.82	3028.14	3028.12	3028.12	3028.13	3028.17	3028.15	3028.17	3028.07	3027.88	3027.73
Mode 46	3027.90	3027.88	3028.21	3028.18	3028.19	3028.22	3028.23	3028.22	3028.23	3028.13	3027.92	3027.78
Mode 47	3050.34	3050.67	3050.47	3050.48	3050.47	3050.49	3050.38	3050.37	3050.39	3050.39	3050.39	3050.40
Mode 48	3050.27	3050.62	3050.41	3050.42	3050.41	3050.40	3050.34	3050.32	3050.35	3050.34	3050.34	3050.35
ZPE	33947.6	33948.0	33947.5	33947.3	33947.5	33947.4	33947.4	33947.2	33947.4	33947.4	33946.9	33946.7

Table S27. Calculated RI-MP2/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 4.8 and 7.0 a_0 calculated using HF/cc-pVDZ.

Cutoff (a_0)	4.80	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00
Mode 1	412.65	412.65	412.65	412.65	412.65	412.65	412.65	412.65	412.65	412.64	412.65	412.65
Mode 2	412.85	412.85	412.86	412.86	412.86	412.86	412.86	412.85	412.86	412.86	412.86	412.86
Mode 3	453.51	453.50	453.51	453.50	453.51	453.52	453.52	453.52	453.52	453.52	453.53	453.53
Mode 4	453.31	453.31	453.31	453.30	453.30	453.31	453.32	453.32	453.32	453.32	453.32	453.32
Mode 5	494.45	494.46	494.47	494.47	494.48	494.48	494.48	494.48	494.48	494.48	494.49	494.49
Mode 6	494.59	494.60	494.60	494.60	494.61	494.61	494.61	494.62	494.61	494.61	494.63	494.63
Mode 7	542.39	542.40	542.27	542.27	542.26	542.22	542.19	542.18	542.18	542.18	542.18	542.18
Mode 8	550.16	550.20	550.24	550.24	550.59	550.59	550.59	550.63	550.63	550.63	550.52	550.52
Mode 9	560.82	560.71	560.66	560.65	560.65	560.56	560.57	560.55	560.55	560.55	560.55	560.55
Mode 10	584.11	584.12	584.13	584.13	584.13	584.13	584.13	584.13	584.14	584.13	584.14	584.14
Mode 11	584.16	584.17	584.18	584.18	584.18	584.18	584.18	584.18	584.19	584.18	584.19	584.19
Mode 12	758.74	758.59	758.51	758.50	758.72	758.72	758.73	758.72	758.73	758.72	758.74	758.73
Mode 13	759.66	759.50	759.36	759.36	759.50	759.51	759.52	759.51	759.51	759.51	759.52	759.52
Mode 14	787.12	787.11	787.11	787.03	786.98	787.00	786.93	786.92	786.93	786.92	786.73	786.58
Mode 15	787.82	787.80	787.80	787.83	787.78	787.73	787.78	787.77	787.77	787.76	787.59	787.52
Mode 16	810.95	810.96	810.97	810.97	810.99	810.99	811.00	810.99	811.00	810.98	810.99	810.99
Mode 17	817.85	817.87	817.87	817.84	817.86	817.86	817.87	817.85	817.85	817.85	817.86	817.85
Mode 18	815.49	815.42	815.42	815.43	815.45	815.48	815.49	815.39	815.35	815.34	815.33	815.33
Mode 19	815.56	815.56	815.52	815.52	815.54	815.55	815.58	815.49	815.44	815.43	815.40	815.40
Mode 20	869.91	869.90	869.92	870.00	869.99	869.99	869.96	869.96	869.96	869.96	869.96	869.96
Mode 21	873.77	873.76	873.74	873.73	873.73	873.74	873.61	873.60	873.61	873.60	873.61	873.62
Mode 22	1050.90	1050.89	1050.90	1050.90	1050.90	1050.90	1050.91	1050.90	1050.91	1050.90	1050.90	1050.90
Mode 23	1050.75	1050.75	1050.75	1050.75	1050.76	1050.75	1050.76	1050.76	1050.76	1050.76	1050.76	1050.76
Mode 24	1287.00	1286.87	1286.88	1286.80	1286.80	1286.80	1286.81	1286.80	1286.79	1286.79	1286.79	1286.79
Mode 25	1287.00	1286.89	1286.89	1286.82	1286.82	1286.82	1286.83	1286.81	1286.81	1286.81	1286.81	1286.80
Mode 26	1292.03	1292.04	1292.05	1292.05	1292.03	1292.03	1292.04	1292.03	1292.05	1292.04	1292.04	1292.04

Mode 27	1291.31	1291.32	1291.32	1291.33	1291.31	1291.31	1291.31	1291.31	1291.32	1291.32	1291.32	1291.32	1291.32
Mode 28	1291.61	1291.59	1291.50	1291.51	1291.51	1291.49	1291.49	1291.50	1291.44	1291.44	1291.43	1291.43	1291.31
Mode 29	1292.10	1292.08	1292.03	1292.03	1292.04	1292.03	1292.03	1292.04	1292.08	1292.08	1292.07	1292.02	
Mode 30	1289.75	1289.78	1289.78	1289.79	1289.78	1289.78	1289.78	1289.79	1289.81	1289.80	1289.83	1289.83	
Mode 31	1289.43	1289.46	1289.47	1289.48	1289.47	1289.47	1289.47	1289.48	1289.50	1289.49	1289.51	1289.51	
Mode 32	1348.09	1348.04	1348.03	1348.05	1348.27	1348.13	1348.14	1348.18	1348.20	1348.18	1348.14	1348.13	
Mode 33	1428.20	1428.01	1427.95	1427.99	1427.99	1427.99	1428.00	1427.95	1427.97	1427.96	1427.94	1427.94	
Mode 34	1427.96	1427.76	1427.69	1427.71	1427.72	1427.72	1427.73	1427.66	1427.65	1427.65	1427.63	1427.63	
Mode 35	1535.18	1535.03	1535.03	1535.05	1535.00	1535.00	1535.00	1534.87	1534.88	1534.87	1534.69	1534.66	
Mode 36	1534.92	1534.71	1534.72	1534.73	1534.67	1534.67	1534.67	1534.46	1534.47	1534.46	1534.23	1534.18	
Mode 37	1550.30	1550.31	1550.35	1550.37	1550.37	1550.30	1550.31	1550.30	1550.31	1550.30	1550.30	1550.31	
Mode 38	1550.77	1550.78	1550.79	1550.80	1550.80	1550.74	1550.74	1550.73	1550.74	1550.73	1550.74	1550.74	
Mode 39	2983.88	2983.87	2983.86	2983.87	2983.87	2983.86	2983.86	2983.86	2983.83	2983.82	2983.82	2983.70	
Mode 40	2984.32	2984.31	2984.29	2984.29	2984.30	2984.28	2984.28	2984.27	2984.24	2984.24	2984.22	2984.09	
Mode 41	2982.08	2981.99	2981.99	2981.99	2981.85	2981.85	2981.86	2981.84	2981.85	2981.84	2981.83	2981.83	
Mode 42	2981.47	2981.40	2981.40	2981.40	2981.25	2981.25	2981.25	2981.24	2981.24	2981.24	2981.23	2981.23	
Mode 43	2997.24	2997.24	2997.24	2997.24	2997.25	2997.25	2997.25	2997.25	2997.25	2997.24	2997.25	2997.25	
Mode 44	2997.33	2997.33	2997.33	2997.33	2997.34	2997.33	2997.34	2997.33	2997.33	2997.33	2997.34	2997.33	
Mode 45	3027.65	3027.64	3027.64	3027.64	3027.57	3027.53	3027.53	3027.53	3027.54	3027.53	3027.51	3027.51	
Mode 46	3027.70	3027.69	3027.69	3027.69	3027.61	3027.56	3027.57	3027.56	3027.56	3027.56	3027.54	3027.53	
Mode 47	3050.39	3050.39	3050.40	3050.33	3050.26	3050.12	3050.07	3050.06	3050.06	3050.06	3050.05	3049.93	
Mode 48	3050.34	3050.35	3050.35	3050.28	3050.22	3050.21	3050.00	3050.00	3050.00	3049.99	3049.99	3049.86	
ZPE	33946.3	33945.9	33945.8	33945.7	33945.8	33945.6	33945.6	33945.4	33945.4	33945.3	33945.1	33944.9	

Table S28. Calculated RI-MP2/cc-pVDZ L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.2 and 8.0 a_0 calculated using HF/cc-pVDZ, and finally the full 2MR result.

Cutoff (a_0)	7.20	7.40	7.60	7.80	8.00	2MR
Mode 1	412.65	412.65	412.66	412.65	412.65	412.70
Mode 2	412.86	412.86	412.87	412.86	412.86	412.71
Mode 3	453.53	453.53	453.54	453.53	453.53	453.02
Mode 4	453.32	453.33	453.32	453.32	453.33	453.35
Mode 5	494.50	494.50	494.49	494.49	494.49	494.49
Mode 6	494.63	494.63	494.66	494.63	494.62	494.53
Mode 7	542.18	542.17	542.17	542.17	542.16	542.17
Mode 8	550.52	550.59	550.60	550.60	550.61	550.62
Mode 9	560.55	560.54	560.55	560.54	560.54	560.73
Mode 10	584.14	584.14	584.44	584.14	584.14	584.18
Mode 11	584.19	584.19	584.17	584.19	584.19	584.20
Mode 12	758.73	758.73	758.82	758.74	758.74	758.61
Mode 13	759.52	759.52	759.55	759.52	759.52	759.60
Mode 14	786.57	786.58	786.62	786.60	786.58	786.93
Mode 15	787.53	787.58	787.61	787.59	787.57	787.24
Mode 16	810.99	810.99	810.99	810.99	810.99	810.82
Mode 17	817.85	817.85	817.88	817.85	817.85	818.23
Mode 18	815.33	815.34	815.38	815.33	815.33	815.16
Mode 19	815.41	815.41	815.41	815.41	815.41	815.12
Mode 20	869.96	869.97	870.01	869.96	869.97	869.10
Mode 21	873.62	873.62	873.61	873.62	873.63	873.51
Mode 22	1050.90	1050.91	1050.91	1050.90	1050.91	1051.01
Mode 23	1050.77	1050.77	1050.78	1050.76	1050.77	1050.74
Mode 24	1286.79	1286.79	1286.79	1286.79	1286.80	1287.00
Mode 25	1286.80	1286.81	1286.83	1286.80	1286.82	1287.03
Mode 26	1292.04	1292.05	1292.05	1292.05	1292.05	1291.45

Mode 27	1291.32	1291.32	1291.32	1291.32	1291.32	1291.44
Mode 28	1291.31	1291.33	1291.37	1291.32	1291.35	1291.99
Mode 29	1292.02	1292.04	1292.00	1292.03	1292.06	1291.93
Mode 30	1289.83	1289.83	1289.79	1289.84	1289.82	1289.51
Mode 31	1289.52	1289.52	1289.57	1289.53	1289.51	1289.48
Mode 32	1348.13	1348.19	1348.20	1348.21	1348.27	1348.28
Mode 33	1427.94	1427.95	1427.94	1427.94	1427.94	1427.40
Mode 34	1427.63	1427.63	1427.64	1427.63	1427.63	1427.42
Mode 35	1534.66	1534.64	1534.65	1534.66	1534.61	1534.45
Mode 36	1534.18	1534.16	1534.18	1534.18	1534.13	1534.59
Mode 37	1550.31	1550.30	1550.31	1550.31	1550.29	1550.41
Mode 38	1550.74	1550.73	1550.73	1550.74	1550.72	1550.51
Mode 39	2983.70	2983.70	2983.70	2983.71	2983.71	2983.75
Mode 40	2984.09	2984.10	2984.11	2984.10	2984.10	2984.33
Mode 41	2981.83	2981.83	2981.82	2981.83	2981.81	2981.80
Mode 42	2981.23	2981.22	2981.24	2981.23	2981.21	2981.18
Mode 43	2997.25	2997.25	2997.26	2997.25	2997.25	2997.24
Mode 44	2997.33	2997.33	2997.35	2997.33	2997.33	2997.43
Mode 45	3027.51	3027.51	3027.53	3027.51	3027.51	3027.49
Mode 46	3027.53	3027.54	3027.53	3027.53	3027.53	3027.57
Mode 47	3049.93	3049.93	3049.92	3049.91	3049.91	3049.91
Mode 48	3049.86	3049.86	3049.86	3049.86	3049.86	3049.89
ZPE	33944.9	33944.9	33945.1	33944.9	33944.9	33944.4

Table S29. Calculated B3LYP/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0 and 2.2 a_0 truncated.

Cutoff (a_0)	0.00	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20
Mode 1	417.97	427.95	428.04	427.01	427.04	426.93	426.33	426.23	425.88	425.82	425.50	425.54
Mode 2	417.97	427.98	428.07	427.03	427.07	426.96	426.35	426.26	425.90	425.84	425.51	425.54
Mode 3	460.44	468.05	468.56	465.10	463.79	463.85	464.00	463.97	463.84	464.10	464.34	464.22
Mode 4	461.83	469.76	470.22	466.69	465.34	465.40	465.55	465.50	465.38	465.65	465.87	465.75
Mode 5	501.05	508.03	507.40	507.23	507.16	507.14	506.19	506.12	506.26	506.31	506.22	506.22
Mode 6	501.05	508.22	507.62	507.32	507.25	507.23	506.31	506.21	506.36	506.28	506.19	506.19
Mode 7	549.74	554.38	554.68	555.53	555.46	554.41	551.43	551.88	551.82	551.77	554.03	552.89
Mode 8	585.56	581.80	589.88	589.82	589.77	589.77	588.70	586.76	586.67	588.89	588.89	588.90
Mode 9	588.12	589.25	585.90	581.53	579.41	579.51	578.97	582.82	583.16	576.63	581.97	581.97
Mode 10	592.08	593.44	590.85	591.02	590.61	590.51	590.44	589.89	591.04	591.05	591.56	591.58
Mode 11	592.08	593.46	590.86	591.00	590.57	590.46	590.41	589.86	591.02	591.04	591.61	591.63
Mode 12	813.74	825.88	825.93	750.39	749.95	749.96	765.88	764.07	765.02	764.99	764.13	774.26
Mode 13	815.96	827.87	827.92	752.47	752.02	752.03	767.95	766.16	767.10	767.11	766.26	776.34
Mode 14	840.30	786.28	786.37	788.31	786.41	786.44	785.35	784.08	784.05	788.07	788.83	790.16
Mode 15	840.62	786.87	786.96	788.90	787.02	787.04	785.96	784.69	784.65	788.66	789.43	790.75
Mode 16	834.57	855.67	857.09	823.26	800.39	800.53	813.66	812.67	817.30	817.34	816.36	816.45
Mode 17	834.57	855.59	856.97	823.13	800.24	800.37	813.52	812.52	817.20	817.24	816.39	816.48
Mode 18	850.25	810.48	811.35	821.69	821.63	821.62	821.95	820.41	828.36	827.42	823.17	823.23
Mode 19	867.51	826.20	831.98	840.32	840.27	840.25	840.59	839.05	846.28	846.21	839.05	839.10
Mode 20	908.70	915.91	915.49	921.51	921.56	920.76	877.19	878.89	877.78	877.82	895.70	895.64
Mode 21	918.30	924.60	924.16	930.39	930.43	929.62	886.45	887.02	885.87	885.87	903.91	903.84
Mode 22	1068.35	1072.42	1072.30	1047.86	1047.86	1047.27	1046.48	1047.20	1051.07	1049.87	1068.87	1079.36
Mode 23	1068.35	1072.35	1072.23	1047.79	1047.80	1047.22	1046.41	1047.13	1050.74	1051.36	1069.07	1079.48
Mode 24	1301.48	1303.01	1296.50	1297.50	1296.65	1296.11	1291.05	1289.85	1300.04	1299.91	1298.85	1300.21
Mode 25	1301.48	1303.11	1296.43	1297.35	1296.40	1295.84	1290.84	1289.63	1300.11	1299.97	1298.92	1300.27
Mode 26	1349.42	1319.12	1318.20	1318.18	1318.16	1321.79	1320.77	1320.88	1320.18	1319.76	1319.66	1318.33

Mode 27	1349.42	1319.11	1318.21	1318.23	1318.25	1321.82	1320.81	1320.92	1320.22	1319.79	1319.69	1318.36
Mode 28	1353.08	1323.20	1322.53	1321.67	1321.20	1321.09	1320.89	1320.26	1321.11	1321.06	1321.22	1320.69
Mode 29	1353.08	1322.46	1322.48	1321.83	1321.38	1321.27	1321.06	1320.41	1321.26	1321.09	1321.25	1320.73
Mode 30	1364.46	1329.67	1331.09	1331.12	1331.35	1331.43	1330.12	1330.99	1328.40	1328.42	1328.59	1328.61
Mode 31	1364.46	1329.58	1331.01	1331.00	1331.21	1331.29	1329.93	1330.86	1328.31	1328.32	1328.49	1328.50
Mode 32	1353.86	1349.58	1349.17	1349.41	1348.41	1348.35	1345.97	1353.26	1350.41	1350.54	1350.13	1349.30
Mode 33	1470.43	1489.07	1488.76	1459.82	1435.57	1435.57	1440.65	1440.20	1441.91	1441.06	1441.61	1441.69
Mode 34	1470.43	1489.04	1488.73	1459.82	1435.56	1435.55	1440.63	1440.18	1441.92	1441.07	1441.61	1441.68
Mode 35	1565.18	1560.67	1559.97	1557.97	1557.96	1557.07	1555.26	1557.47	1555.95	1555.92	1555.74	1555.78
Mode 36	1565.18	1561.18	1560.41	1557.68	1557.72	1555.94	1554.92	1557.21	1555.92	1555.76	1555.61	1555.65
Mode 37	1594.90	1593.75	1588.85	1587.96	1587.27	1587.11	1584.02	1582.56	1587.64	1585.89	1585.16	1585.29
Mode 38	1594.90	1593.79	1589.03	1588.14	1587.52	1587.35	1584.26	1582.81	1587.74	1586.00	1585.28	1585.41
Mode 39	3049.74	3001.05	2998.84	2998.87	2998.86	2998.79	2958.35	2956.87	2951.64	2951.63	2952.21	2952.23
Mode 40	3049.74	3000.93	2997.64	2997.71	2997.70	2997.60	2955.68	2955.50	2950.52	2950.49	2951.10	2951.11
Mode 41	3052.15	2963.07	2962.36	2959.17	2959.40	2959.45	2959.49	2959.29	2947.47	2942.75	2942.73	2942.02
Mode 42	3052.15	2957.93	2957.53	2957.02	2957.23	2957.28	2957.33	2957.12	2945.29	2944.16	2943.96	2943.24
Mode 43	3056.10	3009.55	3010.18	2983.91	2983.65	2979.42	2978.96	2978.59	2980.17	2976.32	2969.44	2968.66
Mode 44	3056.10	3009.58	3010.22	2983.99	2983.76	2979.38	2978.93	2978.56	2980.16	2976.25	2969.11	2968.34
Mode 45	3096.66	3087.80	3087.92	2986.11	2986.20	2986.30	2983.46	2984.62	2984.86	2984.69	2984.37	2983.22
Mode 46	3096.66	3087.57	3087.69	2985.92	2986.03	2986.12	2983.29	2984.33	2984.63	2984.45	2984.13	2982.98
Mode 47	3125.53	3059.54	3059.73	3062.28	3016.19	3016.03	3016.18	3019.62	3021.73	3021.88	3019.68	3019.78
Mode 48	3125.53	3059.54	3059.71	3062.25	3016.27	3016.11	3016.25	3019.70	3021.74	3021.90	3019.69	3019.79
ZPE	34389.5	34234.9	34229.3	34101.1	34055.8	34053.7	34022.6	34024.4	34033.6	34030.0	34042.6	34052.0

Table S30. Calculated B3LYP/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.4 and 4.6 a_0 truncated.

Cutoff (a_0)	2.40	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60
Mode 1	425.59	424.91	424.75	424.77	424.61	424.55	424.53	424.54	424.54	424.54	424.58	424.60
Mode 2	425.63	424.91	424.75	424.77	424.65	424.58	424.57	424.54	424.54	424.55	424.59	424.61
Mode 3	464.31	464.41	464.24	464.37	464.31	464.25	464.18	464.22	464.05	464.01	464.39	464.37
Mode 4	465.82	465.93	465.76	465.88	465.82	465.86	465.67	465.72	465.55	465.51	465.84	465.80
Mode 5	506.28	506.22	506.37	506.19	506.20	506.12	506.10	505.96	505.96	505.96	505.48	505.26
Mode 6	506.26	506.19	506.33	506.17	505.93	506.12	506.11	505.94	505.94	505.94	505.46	505.24
Mode 7	552.87	549.59	549.68	549.62	549.43	550.12	548.27	546.58	546.58	547.59	548.23	548.33
Mode 8	584.82	584.68	584.76	584.68	584.99	583.18	581.37	581.25	582.29	582.28	582.87	582.66
Mode 9	581.99	582.06	582.14	582.21	582.13	583.10	583.10	583.02	582.68	582.67	582.57	582.02
Mode 10	591.54	589.60	589.98	590.13	589.59	589.62	589.74	589.68	589.68	589.69	590.37	589.99
Mode 11	591.63	589.65	590.04	590.17	590.22	589.72	589.72	589.74	589.74	589.74	590.44	590.05
Mode 12	774.15	773.71	771.94	771.85	771.89	771.91	776.45	773.31	773.51	776.46	776.12	776.09
Mode 13	776.22	775.81	774.05	773.95	774.15	774.04	778.45	775.42	776.11	778.69	778.35	778.48
Mode 14	786.79	786.35	786.43	786.40	786.44	784.30	784.06	784.08	788.84	788.83	788.73	788.79
Mode 15	787.39	786.94	787.01	786.98	786.96	784.87	784.65	784.65	789.41	789.40	789.31	789.36
Mode 16	814.75	814.77	814.63	814.34	815.95	815.94	815.82	815.88	815.29	815.29	814.35	814.21
Mode 17	814.78	814.80	814.67	814.38	816.29	815.92	815.91	815.91	815.31	815.31	814.38	814.31
Mode 18	823.24	822.39	822.37	821.68	820.59	820.50	825.22	824.11	824.10	824.06	823.83	823.87
Mode 19	839.07	838.34	838.31	837.61	836.66	836.35	840.92	839.84	839.81	839.79	839.54	839.59
Mode 20	895.67	878.27	878.13	878.16	875.80	875.62	875.61	875.37	875.37	877.71	877.80	877.89
Mode 21	903.88	886.35	886.20	886.24	883.85	883.70	883.69	883.42	883.40	885.74	885.83	885.92
Mode 22	1079.24	1076.46	1068.35	1067.76	1058.69	1059.19	1059.18	1059.03	1061.04	1060.92	1061.07	1061.08
Mode 23	1079.17	1076.60	1068.50	1067.92	1058.90	1058.76	1058.76	1058.59	1060.58	1060.47	1060.62	1060.64
Mode 24	1292.61	1292.41	1291.96	1291.59	1290.84	1289.55	1287.50	1287.19	1287.13	1287.13	1285.83	1288.26
Mode 25	1292.72	1292.48	1292.03	1291.67	1291.11	1289.68	1289.66	1287.60	1287.52	1287.53	1286.24	1288.67
Mode 26	1318.09	1317.59	1319.71	1320.16	1320.08	1319.18	1318.29	1318.37	1318.22	1318.22	1319.66	1319.43

Mode 27	1317.93	1317.57	1319.61	1320.05	1319.78	1319.13	1318.29	1318.29	1318.24	1318.24	1319.67	1319.44
Mode 28	1320.72	1320.16	1320.70	1320.92	1320.46	1319.67	1319.72	1319.48	1319.48	1319.48	1317.28	1317.28
Mode 29	1320.74	1320.20	1320.73	1321.02	1321.25	1319.74	1319.86	1319.54	1319.55	1319.55	1317.35	1317.35
Mode 30	1328.69	1328.79	1328.51	1328.75	1328.37	1328.04	1328.53	1328.55	1328.55	1328.54	1327.79	1328.15
Mode 31	1328.60	1328.68	1328.40	1328.64	1327.78	1327.97	1328.45	1328.47	1328.47	1328.46	1327.73	1328.09
Mode 32	1348.76	1348.88	1346.72	1346.64	1346.17	1346.40	1346.20	1346.18	1346.18	1346.04	1346.53	1347.62
Mode 33	1440.96	1440.96	1440.74	1440.67	1440.63	1441.02	1441.03	1441.05	1440.88	1440.88	1440.72	1440.68
Mode 34	1440.96	1440.95	1440.76	1440.67	1440.79	1441.06	1441.05	1441.04	1440.87	1440.87	1440.71	1440.70
Mode 35	1555.72	1555.61	1555.37	1554.73	1554.09	1554.53	1554.60	1554.45	1554.45	1554.47	1547.10	1548.51
Mode 36	1555.57	1555.48	1555.26	1554.60	1554.90	1554.36	1554.38	1554.26	1554.27	1554.29	1546.71	1548.10
Mode 37	1580.47	1579.98	1579.57	1579.19	1578.92	1578.98	1576.96	1576.91	1576.83	1576.85	1575.50	1574.96
Mode 38	1580.60	1580.12	1579.71	1579.33	1579.32	1577.06	1576.96	1576.96	1576.87	1576.88	1575.54	1575.00
Mode 39	2952.24	2951.43	2951.45	2951.31	2942.85	2942.95	2942.34	2942.32	2942.34	2942.44	2941.87	2942.04
Mode 40	2951.13	2950.32	2950.34	2950.20	2941.74	2941.86	2941.25	2941.23	2941.25	2941.35	2940.77	2940.94
Mode 41	2942.01	2942.55	2942.22	2940.72	2941.08	2940.63	2940.83	2939.02	2939.03	2939.05	2938.94	2939.05
Mode 42	2943.22	2943.77	2943.43	2941.98	2942.40	2941.84	2942.05	2940.35	2940.38	2940.39	2940.28	2940.39
Mode 43	2965.48	2951.78	2949.92	2949.59	2949.54	2948.76	2948.61	2948.60	2948.64	2948.68	2947.63	2947.52
Mode 44	2967.97	2951.58	2949.73	2949.40	2949.15	2948.55	2948.49	2948.45	2948.27	2948.32	2947.26	2947.15
Mode 45	2983.08	2983.13	2977.58	2977.61	2977.51	2977.72	2977.91	2977.75	2977.82	2977.98	2977.02	2976.51
Mode 46	2982.85	2982.89	2977.36	2977.39	2977.39	2977.44	2977.77	2977.54	2977.58	2977.74	2976.77	2976.84
Mode 47	3012.48	3011.14	3011.24	3011.16	3011.24	3010.93	3010.32	3010.36	3008.06	3008.07	3007.60	3007.44
Mode 48	3012.48	3011.14	3011.23	3011.16	3011.23	3011.02	3010.36	3010.34	3008.05	3008.05	3007.61	3007.45
ZPE	34037.9	34017.7	34009.8	34007.8	33998.2	33994.4	33996.4	33992.1	33994.5	33997.4	33990.0	33991.5

Table S31. Calculated B3LYP/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 4.8 and 7.0 a_0 truncated.

Cutoff (a_0)	4.80	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00
Mode 1	424.56	424.59	424.56	424.56	424.58	424.55	424.55	424.48	424.47	424.47	424.48	424.47
Mode 2	424.56	424.56	424.56	424.56	424.58	424.54	424.54	424.48	424.46	424.47	424.48	424.47
Mode 3	464.33	464.29	464.34	464.34	464.46	464.45	464.45	464.45	464.45	464.45	464.45	464.46
Mode 4	465.79	465.79	465.79	465.80	465.92	465.88	465.90	465.90	465.90	465.90	465.90	465.91
Mode 5	505.38	505.32	505.35	505.31	505.09	505.07	505.07	505.11	505.13	505.13	505.18	505.15
Mode 6	505.39	505.44	505.36	505.31	505.10	505.08	505.08	505.11	505.14	505.11	505.16	505.13
Mode 7	547.88	547.86	547.32	547.02	547.12	547.37	547.27	547.31	547.31	547.30	547.31	547.31
Mode 8	582.59	581.92	581.67	581.62	581.99	581.81	581.81	581.87	581.87	581.87	581.88	581.87
Mode 9	583.10	581.78	581.79	581.76	582.47	582.46	582.46	582.24	582.23	581.94	582.01	581.98
Mode 10	589.71	589.86	589.78	589.76	589.74	589.81	589.81	589.57	589.52	589.52	589.56	589.55
Mode 11	589.65	589.68	589.76	589.73	589.71	589.78	589.78	589.54	589.50	589.53	589.56	589.55
Mode 12	776.49	776.49	774.90	774.87	775.03	775.01	775.01	775.19	775.13	775.11	775.08	775.08
Mode 13	778.69	778.60	777.00	776.96	777.00	776.98	776.98	777.17	777.11	777.10	777.07	777.07
Mode 14	788.84	788.75	788.80	789.57	789.68	791.35	791.34	791.36	791.36	791.36	790.77	790.29
Mode 15	789.42	789.35	789.35	790.15	790.09	791.73	791.94	791.96	791.96	791.96	791.36	790.86
Mode 16	813.80	813.95	813.47	813.44	813.05	813.08	813.17	814.12	814.17	813.94	813.94	813.95
Mode 17	813.77	813.18	813.33	813.33	812.94	813.07	813.06	814.01	814.06	813.99	813.99	814.00
Mode 18	823.65	823.76	823.71	825.06	824.95	824.94	824.94	825.01	825.02	825.01	825.01	825.00
Mode 19	839.35	839.40	839.41	840.79	840.68	840.67	840.67	840.75	840.76	840.76	840.76	840.74
Mode 20	877.79	877.78	877.50	877.50	877.58	879.06	879.05	879.00	878.96	878.97	878.95	878.77
Mode 21	885.83	885.85	885.54	885.54	885.62	887.10	887.09	887.05	887.02	887.02	886.99	886.82
Mode 22	1061.06	1061.11	1061.07	1060.97	1061.02	1061.02	1061.02	1061.00	1060.98	1060.99	1060.97	1060.95
Mode 23	1060.60	1060.65	1060.61	1060.51	1060.56	1060.56	1060.56	1060.54	1060.52	1060.53	1060.51	1060.49
Mode 24	1287.73	1287.72	1287.57	1287.56	1287.02	1287.25	1287.25	1286.59	1286.49	1286.50	1286.61	1286.59
Mode 25	1288.13	1287.27	1287.44	1287.42	1286.87	1287.09	1287.10	1286.45	1286.34	1286.41	1286.53	1286.51
Mode 26	1318.94	1319.01	1319.11	1319.11	1319.69	1319.77	1319.77	1319.17	1319.05	1319.12	1319.12	1319.12

Mode 27	1319.00	1319.22	1319.13	1319.14	1319.72	1319.80	1319.80	1319.20	1319.08	1319.11	1319.11	1319.11
Mode 28	1317.96	1318.02	1317.98	1318.05	1317.53	1317.60	1317.60	1318.00	1318.09	1318.05	1318.01	1318.02
Mode 29	1317.97	1317.96	1317.98	1318.06	1317.54	1317.61	1317.61	1318.00	1318.10	1318.07	1318.03	1318.04
Mode 30	1327.88	1327.85	1327.76	1327.76	1327.93	1328.01	1328.01	1328.04	1328.20	1328.23	1328.14	1328.12
Mode 31	1327.85	1327.91	1327.72	1327.72	1327.90	1327.97	1327.97	1328.00	1328.17	1328.17	1328.07	1328.05
Mode 32	1347.45	1347.51	1347.47	1347.49	1339.75	1340.74	1340.73	1341.20	1341.16	1341.15	1340.53	1340.55
Mode 33	1440.59	1440.19	1440.05	1439.90	1439.86	1439.89	1439.91	1440.08	1440.11	1440.08	1440.07	1440.07
Mode 34	1440.57	1440.13	1439.88	1439.88	1439.84	1439.89	1439.89	1440.05	1440.08	1440.09	1440.08	1440.08
Mode 35	1549.08	1548.67	1548.47	1548.39	1546.94	1546.96	1546.96	1548.66	1548.66	1548.65	1548.04	1548.06
Mode 36	1548.88	1549.15	1548.32	1548.24	1546.81	1546.83	1546.83	1548.47	1548.47	1548.45	1547.83	1547.84
Mode 37	1575.38	1575.21	1575.18	1575.13	1574.62	1574.61	1574.63	1574.57	1574.55	1574.55	1574.58	1574.58
Mode 38	1575.37	1575.33	1575.29	1575.28	1574.77	1574.77	1574.77	1574.71	1574.69	1574.70	1574.73	1574.73
Mode 39	2942.21	2942.17	2941.34	2941.36	2941.15	2941.18	2941.18	2941.26	2941.17	2941.17	2941.14	2940.83
Mode 40	2941.13	2941.13	2940.27	2940.29	2940.09	2940.11	2940.11	2940.19	2940.10	2940.09	2940.06	2939.74
Mode 41	2938.11	2937.82	2937.84	2937.33	2937.39	2937.39	2937.39	2937.25	2937.19	2937.21	2937.21	2937.21
Mode 42	2939.45	2939.21	2939.19	2938.63	2938.68	2938.68	2938.68	2938.54	2938.48	2938.49	2938.49	2938.49
Mode 43	2947.77	2947.67	2947.71	2947.71	2947.29	2947.33	2947.32	2947.54	2947.59	2947.58	2947.60	2947.59
Mode 44	2947.45	2947.44	2947.37	2947.37	2946.95	2946.99	2946.99	2947.20	2947.25	2947.21	2947.24	2947.23
Mode 45	2976.07	2976.15	2976.01	2975.99	2976.02	2976.05	2976.05	2975.97	2975.94	2975.94	2975.90	2975.90
Mode 46	2975.89	2975.92	2975.85	2975.80	2975.84	2975.87	2975.86	2975.77	2975.74	2975.75	2975.71	2975.70
Mode 47	3007.65	3007.75	3007.68	3007.63	3007.44	3007.58	3007.08	3007.36	3007.41	3007.37	3007.35	3007.28
Mode 48	3007.63	3007.62	3007.62	3007.60	3007.42	3007.00	3007.00	3007.29	3007.35	3007.33	3007.31	3007.25
ZPE	33991.0	33990.0	33987.9	33988.5	33985.2	33987.3	33987.3	33988.5	33988.4	33988.3	33987.5	33987.0

Table S32. Calculated B3LYP/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.2 and 8.0 a_0 truncated, and finally the untruncated 2MR result.

Cutoff (a_0)	7.20	7.40	7.60	7.80	8.00	2MR
Mode 1	424.47	424.45	424.45	424.45	424.44	424.46
Mode 2	424.47	424.46	424.46	424.46	424.45	424.46
Mode 3	464.46	464.45	464.45	464.45	464.46	464.45
Mode 4	465.91	465.91	465.91	465.91	465.91	465.90
Mode 5	505.15	505.19	505.19	505.19	505.18	505.18
Mode 6	505.13	505.17	505.17	505.17	505.16	505.17
Mode 7	547.31	547.31	547.31	547.31	547.29	547.31
Mode 8	581.87	581.88	581.88	581.88	581.86	581.87
Mode 9	582.03	581.99	581.99	581.99	582.01	582.00
Mode 10	589.55	589.50	589.50	589.50	589.49	589.51
Mode 11	589.55	589.50	589.50	589.50	589.49	589.49
Mode 12	775.08	775.12	775.12	775.12	775.12	775.12
Mode 13	777.07	777.12	777.12	777.12	777.11	777.11
Mode 14	790.33	790.32	790.32	790.32	790.30	790.28
Mode 15	790.86	790.88	790.88	790.88	790.86	790.84
Mode 16	813.95	814.08	814.08	814.08	814.08	814.07
Mode 17	814.00	814.12	814.12	814.12	814.12	814.09
Mode 18	825.00	825.01	825.01	825.01	825.00	825.01
Mode 19	840.74	840.76	840.76	840.76	840.75	840.75
Mode 20	878.77	878.75	878.75	878.75	878.77	878.75
Mode 21	886.82	886.80	886.80	886.80	886.82	886.81
Mode 22	1060.95	1060.94	1060.94	1060.94	1060.95	1060.94
Mode 23	1060.49	1060.48	1060.48	1060.48	1060.49	1060.48
Mode 24	1286.59	1286.46	1286.46	1286.46	1286.44	1286.48
Mode 25	1286.51	1286.38	1286.38	1286.38	1286.36	1286.37
Mode 26	1319.12	1318.96	1318.96	1318.96	1318.95	1318.96

Mode 27	1319.11	1318.95	1318.95	1318.95	1318.95	1318.97
Mode 28	1318.02	1318.14	1318.14	1318.14	1318.16	1318.14
Mode 29	1318.04	1318.16	1318.16	1318.16	1318.18	1318.15
Mode 30	1328.12	1328.09	1328.09	1328.09	1328.15	1328.08
Mode 31	1328.05	1328.02	1328.02	1328.02	1328.08	1328.05
Mode 32	1340.55	1340.83	1340.83	1340.83	1341.07	1340.54
Mode 33	1440.07	1440.09	1440.09	1440.09	1440.09	1440.09
Mode 34	1440.08	1440.10	1440.10	1440.10	1440.10	1440.09
Mode 35	1548.06	1548.07	1548.07	1548.07	1547.98	1548.05
Mode 36	1547.84	1547.86	1547.86	1547.86	1547.77	1547.85
Mode 37	1574.58	1574.58	1574.58	1574.58	1574.55	1574.58
Mode 38	1574.73	1574.73	1574.73	1574.73	1574.69	1574.72
Mode 39	2940.83	2940.84	2940.84	2940.84	2940.85	2940.84
Mode 40	2939.74	2939.76	2939.76	2939.76	2939.76	2939.76
Mode 41	2937.21	2937.14	2937.14	2937.14	2937.11	2937.14
Mode 42	2938.49	2938.42	2938.42	2938.42	2938.39	2938.42
Mode 43	2947.59	2947.66	2947.66	2947.66	2947.65	2947.64
Mode 44	2947.23	2947.30	2947.30	2947.30	2947.29	2947.30
Mode 45	2975.90	2975.87	2975.87	2975.87	2975.87	2975.87
Mode 46	2975.70	2975.68	2975.68	2975.68	2975.68	2975.68
Mode 47	3007.28	3007.29	3007.29	3007.29	3007.29	3007.21
Mode 48	3007.25	3007.32	3007.32	3007.32	3007.31	3007.22
ZPE	33987.0	33987.1	33987.1	33987.1	33987.1	33986.9

Table S33. Calculated B3LYP-D2/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0 and 2.2 a_0 truncated.

Cutoff (a_0)	0.00	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20
Mode 1	418.94	430.68	432.64	431.64	431.71	431.59	431.08	430.95	430.47	430.36	430.02	430.05
Mode 2	418.92	430.65	432.66	431.64	431.74	431.61	431.09	430.97	430.48	430.38	430.02	430.06
Mode 3	460.25	466.63	468.13	464.67	463.38	463.43	463.64	463.57	463.67	463.72	463.96	463.86
Mode 4	461.91	468.58	470.05	466.65	465.19	465.24	465.46	465.35	465.47	465.53	465.76	465.65
Mode 5	501.93	511.64	512.48	512.24	512.16	512.12	511.23	511.12	511.53	511.44	511.31	511.30
Mode 6	501.92	511.80	512.26	512.14	512.07	512.03	511.12	511.03	511.42	511.44	511.32	511.30
Mode 7	547.18	551.29	552.20	553.04	552.98	551.92	548.83	549.30	549.26	549.20	551.41	550.26
Mode 8	583.86	579.91	588.19	588.13	588.09	588.09	587.00	584.99	584.92	587.07	587.07	587.08
Mode 9	587.29	587.92	585.12	580.81	578.70	578.79	578.25	582.09	582.43	575.85	581.21	581.22
Mode 10	589.22	591.45	588.03	588.21	587.72	587.68	587.56	587.05	588.55	588.49	589.13	589.13
Mode 11	589.18	591.45	588.01	588.20	587.74	587.69	587.56	587.05	588.53	588.48	589.11	589.12
Mode 12	815.48	825.22	827.52	751.78	751.25	751.26	767.05	764.99	766.01	766.05	765.36	775.22
Mode 13	817.75	827.28	829.57	753.93	753.38	753.38	769.17	767.12	768.13	768.21	767.52	777.35
Mode 14	839.29	782.17	785.72	787.70	785.76	785.78	784.86	783.30	783.35	787.30	788.09	790.11
Mode 15	839.61	782.78	786.32	785.27	786.36	786.38	785.47	783.91	783.96	787.90	788.69	790.71
Mode 16	831.45	850.82	855.72	822.44	799.46	799.57	812.19	810.97	815.70	815.69	814.76	814.83
Mode 17	831.46	850.94	855.64	822.58	799.37	799.48	812.11	810.88	815.66	815.65	814.76	814.84
Mode 18	853.69	811.39	814.60	824.65	824.60	824.59	824.91	823.37	831.42	830.46	826.20	826.26
Mode 19	870.95	827.61	835.23	843.31	843.26	843.25	843.58	842.03	849.37	849.31	842.07	842.11
Mode 20	911.03	916.43	917.65	923.45	923.50	922.69	879.06	880.75	879.64	879.67	897.40	897.34
Mode 21	920.81	925.30	926.46	932.46	932.51	931.69	888.47	889.02	887.88	887.88	905.77	905.70
Mode 22	1068.10	1070.77	1071.88	1047.23	1047.24	1046.63	1045.80	1046.53	1050.13	1050.70	1068.24	1078.39
Mode 23	1068.10	1070.84	1071.96	1047.31	1047.31	1046.70	1045.87	1046.61	1050.47	1049.26	1068.05	1078.28
Mode 24	1302.82	1305.29	1297.35	1298.10	1297.34	1296.89	1292.49	1291.33	1301.28	1301.13	1300.04	1301.38
Mode 25	1302.82	1305.45	1297.37	1298.07	1297.23	1296.77	1292.42	1291.25	1301.32	1301.17	1300.08	1301.41
Mode 26	1343.00	1314.80	1313.35	1313.25	1313.33	1317.51	1316.58	1316.77	1315.39	1315.06	1314.90	1313.53

Mode 27	1343.00	1314.83	1313.32	1313.24	1313.35	1317.50	1316.57	1316.76	1315.36	1315.05	1314.88	1313.50
Mode 28	1350.38	1322.47	1322.01	1321.21	1320.75	1320.65	1320.42	1319.89	1321.46	1321.42	1321.58	1321.05
Mode 29	1350.38	1321.77	1321.97	1321.37	1320.92	1320.82	1320.59	1320.04	1321.61	1321.43	1321.59	1321.06
Mode 30	1362.69	1329.91	1331.74	1331.75	1332.03	1332.09	1330.79	1331.68	1329.14	1329.14	1329.26	1329.29
Mode 31	1362.69	1329.76	1331.68	1331.64	1331.90	1331.97	1330.63	1331.57	1329.08	1329.08	1329.20	1329.23
Mode 32	1355.69	1353.80	1350.31	1350.59	1349.47	1349.43	1347.18	1354.39	1351.64	1351.62	1351.20	1350.37
Mode 33	1465.01	1485.49	1484.55	1454.43	1436.08	1436.07	1441.38	1440.75	1442.20	1442.17	1442.87	1442.93
Mode 34	1465.01	1485.46	1484.51	1457.28	1436.08	1436.06	1441.37	1440.73	1442.19	1442.16	1442.86	1442.92
Mode 35	1566.76	1564.00	1561.25	1559.28	1559.24	1558.37	1556.53	1558.90	1557.41	1557.35	1557.18	1557.23
Mode 36	1566.76	1563.42	1561.66	1558.94	1558.94	1557.17	1556.12	1558.58	1557.28	1557.11	1556.95	1557.00
Mode 37	1592.09	1593.05	1585.72	1584.61	1584.13	1584.05	1581.13	1579.67	1584.00	1583.41	1582.66	1583.57
Mode 38	1592.09	1593.04	1585.87	1584.94	1584.30	1584.21	1581.30	1579.84	1584.10	1583.51	1582.78	1583.68
Mode 39	3044.82	3000.55	2992.24	2992.33	2992.32	2992.23	2949.93	2949.79	2944.94	2944.91	2945.52	2945.53
Mode 40	3044.82	3000.43	2993.42	2993.47	2993.46	2993.41	2952.65	2951.18	2946.09	2946.07	2946.65	2946.67
Mode 41	3047.00	2957.07	2956.59	2953.42	2953.61	2953.64	2953.68	2953.39	2941.66	2936.86	2936.84	2936.15
Mode 42	3047.00	2962.26	2951.74	2951.24	2951.41	2951.45	2951.51	2951.19	2939.47	2938.32	2938.12	2937.43
Mode 43	3050.15	3008.10	3004.38	2977.86	2977.61	2972.99	2972.50	2972.11	2973.65	2969.92	2963.00	2962.25
Mode 44	3050.15	3008.16	3004.40	2977.90	2977.67	2972.97	2972.49	2972.10	2973.66	2969.86	2962.69	2961.94
Mode 45	3086.68	3087.33	3078.13	2978.86	2979.03	2979.11	2977.15	2980.41	2980.28	2980.27	2979.95	2978.75
Mode 46	3086.68	3087.57	3077.89	2978.37	2978.82	2978.90	2976.94	2980.15	2980.04	2980.02	2979.70	2978.50
Mode 47	3115.76	3058.14	3049.93	3052.50	3010.10	3009.99	3010.13	3015.76	3017.47	3017.68	3015.59	3015.75
Mode 48	3115.76	3058.16	3049.93	3052.69	3010.13	3010.02	3010.15	3015.79	3017.48	3017.68	3015.59	3015.74
ZPE	34329.9	34201.6	34176.9	34048.8	34008.0	34006.2	33975.6	33978.9	33987.8	33985.0	33997.6	34007.4

Table S34. Calculated B3LYP-D2/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.4 and 4.6 a_0 truncated.

Cutoff (a_0)	2.40	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60
Mode 1	430.09	429.42	429.23	429.26	429.08	429.04	429.03	429.03	429.03	429.03	429.10	429.11
Mode 2	430.13	429.42	429.23	429.26	429.16	429.06	429.08	429.03	429.03	429.03	429.11	429.11
Mode 3	463.93	464.04	463.88	464.04	463.99	463.92	463.86	463.88	463.71	463.68	464.07	464.04
Mode 4	465.70	465.82	465.67	465.81	465.76	465.80	465.72	465.64	465.48	465.44	465.78	465.74
Mode 5	511.37	511.28	511.49	511.19	510.97	511.22	511.22	511.05	511.05	511.05	510.32	510.11
Mode 6	511.36	511.28	511.50	511.21	511.27	511.19	511.16	511.03	511.04	511.04	510.31	510.10
Mode 7	550.24	546.99	547.07	547.01	546.83	547.61	547.60	544.13	544.13	545.10	545.75	545.85
Mode 8	583.02	582.89	582.96	582.88	583.34	581.57	579.76	579.63	580.63	580.62	581.22	581.01
Mode 9	581.24	581.30	581.38	581.45	581.38	582.34	582.33	582.12	581.89	581.88	581.79	581.23
Mode 10	589.15	587.17	587.03	588.43	588.47	588.02	588.06	588.06	588.05	588.06	588.64	588.26
Mode 11	589.10	587.16	587.01	588.41	587.95	587.95	588.09	588.03	588.03	588.03	588.61	588.23
Mode 12	775.13	774.69	773.00	772.86	772.91	772.94	777.30	774.35	774.55	777.41	777.05	777.01
Mode 13	777.23	776.82	775.14	775.01	775.20	775.09	779.36	776.49	777.15	779.67	779.30	779.43
Mode 14	786.02	785.58	785.66	785.63	785.67	783.55	783.26	783.29	788.11	788.10	788.01	788.06
Mode 15	786.61	786.18	786.26	786.22	786.21	784.14	783.88	783.88	788.70	788.69	788.60	788.65
Mode 16	813.06	813.04	813.44	813.04	814.66	814.62	814.52	814.54	813.95	813.95	812.95	812.82
Mode 17	813.06	813.04	813.42	813.06	814.92	814.58	814.54	814.54	813.94	813.94	812.95	812.89
Mode 18	826.27	825.43	824.82	824.70	823.65	823.53	828.08	827.03	827.00	826.98	826.73	826.77
Mode 19	842.09	841.36	840.75	840.60	839.67	839.35	843.76	842.71	842.68	842.67	842.40	842.45
Mode 20	897.37	880.20	880.03	880.08	877.74	877.57	877.57	877.37	877.35	879.64	879.76	879.85
Mode 21	905.73	888.44	888.27	888.32	885.93	885.81	885.82	885.57	885.55	887.83	887.95	888.05
Mode 22	1078.17	1075.42	1067.45	1067.00	1058.01	1057.85	1057.86	1057.69	1059.72	1059.60	1059.76	1059.78
Mode 23	1078.10	1075.55	1067.59	1066.86	1057.81	1058.29	1058.26	1058.17	1060.18	1060.06	1060.22	1060.23
Mode 24	1293.78	1293.48	1293.03	1292.51	1291.81	1290.69	1288.62	1288.31	1288.25	1288.25	1286.89	1289.42
Mode 25	1293.71	1293.44	1292.99	1292.55	1292.01	1290.77	1290.78	1288.69	1288.61	1288.62	1287.27	1289.80
Mode 26	1313.05	1312.71	1315.35	1316.02	1315.94	1315.05	1314.62	1314.78	1314.59	1314.59	1316.21	1315.97

Mode 27	1313.31	1312.79	1315.44	1315.92	1315.63	1315.01	1314.69	1314.68	1314.63	1314.63	1316.25	1316.01
Mode 28	1321.07	1320.46	1321.07	1321.28	1320.78	1320.19	1320.24	1320.05	1320.05	1320.05	1317.37	1317.38
Mode 29	1321.08	1320.46	1321.07	1321.33	1321.55	1320.16	1320.29	1320.02	1320.02	1320.02	1317.36	1317.37
Mode 30	1329.33	1329.44	1329.06	1329.49	1329.12	1328.71	1329.84	1329.86	1329.86	1329.85	1328.84	1329.24
Mode 31	1329.37	1329.49	1329.13	1329.42	1328.48	1328.72	1329.85	1329.86	1329.86	1329.85	1328.82	1329.22
Mode 32	1349.80	1349.84	1347.67	1347.59	1347.14	1347.36	1347.20	1347.13	1347.13	1346.99	1347.49	1348.61
Mode 33	1442.16	1442.15	1442.17	1442.03	1442.01	1442.42	1442.38	1442.45	1442.27	1442.28	1442.01	1441.95
Mode 34	1442.18	1442.16	1442.18	1442.03	1442.14	1442.44	1442.43	1442.42	1442.25	1442.25	1442.00	1441.97
Mode 35	1556.92	1556.84	1556.61	1556.18	1555.62	1556.01	1556.09	1555.94	1555.94	1555.96	1547.70	1549.06
Mode 36	1557.17	1557.07	1556.83	1555.97	1556.21	1555.70	1555.72	1555.62	1555.62	1555.65	1547.46	1548.80
Mode 37	1578.13	1577.63	1577.17	1576.59	1576.25	1576.32	1576.26	1574.26	1574.17	1574.19	1572.82	1572.25
Mode 38	1578.00	1577.50	1577.04	1576.72	1576.62	1574.41	1574.28	1574.29	1574.19	1574.21	1572.84	1572.29
Mode 39	2945.55	2944.74	2944.75	2944.57	2936.13	2936.25	2935.64	2935.61	2935.63	2935.73	2935.00	2935.20
Mode 40	2946.69	2945.87	2945.89	2945.71	2937.24	2937.36	2936.76	2936.73	2936.75	2936.85	2936.11	2936.32
Mode 41	2936.14	2936.70	2936.36	2934.70	2935.05	2934.65	2934.88	2933.13	2933.14	2933.16	2932.96	2933.07
Mode 42	2937.40	2937.97	2937.62	2935.98	2936.42	2935.87	2936.09	2934.48	2934.50	2934.51	2934.31	2934.43
Mode 43	2959.09	2945.49	2943.51	2943.13	2943.06	2942.24	2942.17	2942.16	2942.20	2942.24	2941.18	2941.04
Mode 44	2961.55	2945.32	2943.34	2942.96	2942.71	2942.05	2942.01	2941.82	2941.85	2941.90	2940.83	2940.70
Mode 45	2978.56	2978.61	2973.11	2973.17	2973.07	2973.26	2973.45	2973.29	2973.36	2973.52	2972.54	2972.02
Mode 46	2978.32	2978.37	2972.88	2972.93	2972.94	2972.95	2973.21	2973.05	2973.09	2973.26	2972.29	2972.35
Mode 47	3008.55	3007.05	3007.09	3006.99	3007.07	3006.76	3006.02	3006.16	3003.85	3003.86	3003.36	3003.22
Mode 48	3008.54	3007.05	3007.09	3006.99	3007.08	3006.85	3006.15	3006.15	3003.84	3003.85	3003.34	3003.20
ZPE	33992.5	33972.3	33964.5	33963.2	33953.6	33950.1	33953.4	33948.3	33950.8	33953.6	33945.0	33946.6

Table S35. Calculated B3LYP-D2/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 4.8 and 7.0 a_0 truncated.

Cutoff (a_0)	4.80	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00
Mode 1	429.04	429.07	429.04	429.04	429.07	429.04	429.04	428.92	428.91	428.92	428.93	428.92
Mode 2	429.03	429.02	429.02	429.02	429.05	429.02	429.02	428.90	428.89	428.91	428.93	428.91
Mode 3	463.95	463.97	464.00	464.00	464.12	464.10	464.10	464.11	464.11	464.11	464.11	464.12
Mode 4	465.67	465.70	465.73	465.72	465.83	465.80	465.81	465.82	465.82	465.82	465.82	465.83
Mode 5	510.33	510.34	510.27	510.23	509.94	509.92	509.92	510.01	510.01	509.97	510.02	510.00
Mode 6	510.26	510.20	510.22	510.18	509.89	509.87	509.87	509.95	509.95	509.95	510.00	509.97
Mode 7	545.39	545.38	544.55	544.51	544.61	544.62	544.76	544.81	544.80	544.79	544.80	544.80
Mode 8	580.94	579.96	579.96	579.92	580.27	580.10	580.10	580.17	580.16	580.16	580.17	580.16
Mode 9	582.46	581.13	581.13	581.11	581.80	581.78	581.80	581.52	581.53	581.22	581.30	581.27
Mode 10	587.92	587.95	587.99	587.98	587.89	587.96	587.96	587.73	587.73	587.76	587.79	587.78
Mode 11	588.01	588.09	588.05	588.04	587.95	588.02	588.02	587.80	587.79	587.79	587.83	587.82
Mode 12	777.42	777.43	775.87	775.83	775.98	775.96	775.95	776.20	776.09	776.06	776.03	776.03
Mode 13	779.65	779.60	777.98	777.94	777.98	777.96	777.96	778.20	778.10	778.09	778.06	778.06
Mode 14	788.04	788.04	788.07	788.85	788.93	790.62	790.61	790.63	790.62	790.62	790.02	789.54
Mode 15	788.63	788.63	788.66	789.44	789.36	790.79	791.22	791.25	791.24	791.24	790.63	790.12
Mode 16	812.96	812.99	812.53	812.53	812.12	812.16	812.25	813.39	813.41	813.17	813.18	813.19
Mode 17	812.90	812.20	812.38	812.38	811.98	812.11	812.10	813.24	813.26	813.18	813.19	813.20
Mode 18	826.68	826.70	826.66	828.01	827.89	827.88	827.88	827.98	827.98	827.96	827.96	827.95
Mode 19	842.36	842.34	842.33	843.71	843.60	843.59	843.59	843.69	843.69	843.69	843.68	843.67
Mode 20	879.75	879.75	879.48	879.48	879.56	881.06	881.04	880.95	880.95	880.97	880.94	880.76
Mode 21	887.96	887.97	887.70	887.69	887.77	889.27	889.26	889.18	889.18	889.18	889.16	888.98
Mode 22	1059.79	1059.80	1059.76	1059.66	1059.71	1059.72	1059.72	1059.67	1059.68	1059.68	1059.67	1059.65
Mode 23	1060.25	1060.26	1060.22	1060.13	1060.18	1060.18	1060.18	1060.14	1060.14	1060.15	1060.13	1060.11
Mode 24	1288.99	1288.86	1288.77	1288.77	1288.22	1288.45	1288.45	1287.66	1287.66	1287.67	1287.79	1287.77
Mode 25	1289.35	1288.44	1288.56	1288.56	1288.01	1288.23	1288.24	1287.45	1287.45	1287.53	1287.65	1287.63
Mode 26	1315.59	1315.65	1315.73	1315.74	1316.35	1316.43	1316.43	1315.65	1315.65	1315.74	1315.75	1315.75

Mode 27	1315.68	1315.85	1315.80	1315.81	1316.42	1316.50	1316.50	1315.71	1315.71	1315.76	1315.77	1315.77
Mode 28	1318.79	1318.78	1318.73	1318.80	1318.19	1318.25	1318.25	1318.84	1318.85	1318.79	1318.75	1318.76
Mode 29	1318.76	1318.69	1318.70	1318.77	1318.16	1318.23	1318.23	1318.81	1318.83	1318.79	1318.75	1318.76
Mode 30	1329.27	1329.28	1329.18	1329.17	1329.34	1329.41	1329.41	1329.54	1329.66	1329.70	1329.60	1329.58
Mode 31	1329.31	1329.35	1329.19	1329.19	1329.35	1329.42	1329.42	1329.59	1329.70	1329.70	1329.60	1329.58
Mode 32	1348.76	1348.85	1348.82	1348.84	1340.56	1341.59	1341.59	1342.07	1342.01	1341.99	1341.37	1341.38
Mode 33	1441.81	1441.81	1441.50	1441.50	1441.42	1441.45	1441.48	1441.83	1441.85	1441.80	1441.79	1441.80
Mode 34	1441.77	1441.58	1441.46	1441.46	1441.40	1441.46	1441.46	1441.79	1441.80	1441.80	1441.79	1441.80
Mode 35	1549.60	1549.34	1548.96	1548.88	1547.50	1547.53	1547.53	1549.51	1549.46	1549.44	1548.83	1548.84
Mode 36	1549.58	1549.71	1549.00	1548.92	1547.53	1547.55	1547.55	1549.34	1549.29	1549.26	1548.64	1548.65
Mode 37	1572.98	1572.69	1572.65	1572.63	1572.14	1572.12	1572.15	1572.03	1572.03	1572.03	1572.07	1572.07
Mode 38	1572.96	1572.79	1572.78	1572.76	1572.27	1572.27	1572.27	1572.16	1572.16	1572.17	1572.20	1572.20
Mode 39	2935.35	2935.35	2934.51	2934.53	2934.32	2934.35	2934.35	2934.32	2934.36	2934.34	2934.31	2933.98
Mode 40	2936.45	2936.42	2935.59	2935.61	2935.40	2935.43	2935.43	2935.40	2935.43	2935.43	2935.39	2935.08
Mode 41	2932.08	2932.08	2932.11	2931.58	2931.63	2931.63	2931.63	2931.49	2931.47	2931.49	2931.49	2931.49
Mode 42	2933.45	2933.49	2933.48	2932.91	2932.95	2932.94	2932.94	2932.81	2932.79	2932.80	2932.79	2932.80
Mode 43	2941.29	2941.22	2941.22	2941.23	2940.83	2940.87	2940.87	2941.08	2941.08	2941.06	2941.09	2941.08
Mode 44	2940.98	2940.96	2940.91	2940.92	2940.51	2940.55	2940.56	2940.77	2940.76	2940.73	2940.75	2940.74
Mode 45	2971.70	2971.67	2971.55	2971.53	2971.57	2971.59	2971.62	2971.47	2971.48	2971.48	2971.44	2971.43
Mode 46	2971.50	2971.46	2971.35	2971.33	2971.38	2971.41	2971.42	2971.25	2971.26	2971.28	2971.23	2971.23
Mode 47	3003.58	3003.58	3003.47	3003.45	3003.36	3003.48	3002.98	3003.27	3003.29	3003.25	3003.23	3003.15
Mode 48	3003.54	3003.41	3003.43	3003.40	3003.30	3002.87	3002.86	3003.18	3003.21	3003.19	3003.17	3003.09
ZPE	33947.4	33946.3	33944.2	33945.0	33941.4	33943.4	33943.5	33944.9	33944.7	33944.0	33943.4	

Table S36. Calculated B3LYP-D2/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.2 and 8.0 a_0 truncated, and finally the untruncated 2MR result.

Cutoff (a_0)	7.20	7.40	7.60	7.80	8.00	2MR
Mode 1	428.92	428.90	428.90	428.90	428.89	428.90
Mode 2	428.91	428.89	428.89	428.89	428.88	428.89
Mode 3	464.12	464.11	464.11	464.11	464.12	464.11
Mode 4	465.83	465.82	465.82	465.82	465.83	465.82
Mode 5	510.00	510.04	510.04	510.04	510.04	510.04
Mode 6	509.97	510.01	510.01	510.01	510.01	510.01
Mode 7	544.80	544.80	544.80	544.80	544.78	544.80
Mode 8	580.16	580.17	580.17	580.17	580.15	580.17
Mode 9	581.31	581.28	581.28	581.28	581.30	581.28
Mode 10	587.78	587.75	587.75	587.75	587.74	587.75
Mode 11	587.82	587.78	587.78	587.78	587.77	587.78
Mode 12	776.03	776.08	776.08	776.08	776.07	776.08
Mode 13	778.05	778.10	778.10	778.10	778.10	778.10
Mode 14	789.57	789.56	789.56	789.56	789.55	789.53
Mode 15	790.13	790.14	790.14	790.14	790.13	790.10
Mode 16	813.19	813.32	813.32	813.32	813.31	813.31
Mode 17	813.20	813.32	813.32	813.32	813.32	813.31
Mode 18	827.95	827.97	827.97	827.97	827.96	827.97
Mode 19	843.67	843.69	843.69	843.69	843.68	843.69
Mode 20	880.76	880.74	880.74	880.74	880.76	880.74
Mode 21	888.98	888.96	888.96	888.96	888.98	888.96
Mode 22	1059.64	1059.64	1059.64	1059.64	1059.64	1059.64
Mode 23	1060.11	1060.10	1060.10	1060.10	1060.11	1060.10
Mode 24	1287.77	1287.64	1287.64	1287.64	1287.62	1287.64
Mode 25	1287.63	1287.50	1287.50	1287.50	1287.48	1287.50
Mode 26	1315.75	1315.58	1315.58	1315.58	1315.57	1315.58

Mode 27	1315.77	1315.59	1315.59	1315.59	1315.59	1315.59
Mode 28	1318.76	1318.90	1318.90	1318.90	1318.92	1318.90
Mode 29	1318.76	1318.89	1318.89	1318.89	1318.91	1318.89
Mode 30	1329.58	1329.54	1329.54	1329.54	1329.60	1329.54
Mode 31	1329.58	1329.54	1329.54	1329.54	1329.60	1329.54
Mode 32	1341.38	1341.70	1341.70	1341.70	1341.94	1341.42
Mode 33	1441.80	1441.84	1441.84	1441.84	1441.83	1441.83
Mode 34	1441.80	1441.83	1441.83	1441.83	1441.83	1441.83
Mode 35	1548.84	1548.86	1548.86	1548.86	1548.77	1548.85
Mode 36	1548.65	1548.67	1548.67	1548.67	1548.58	1548.66
Mode 37	1572.07	1572.07	1572.07	1572.07	1572.03	1572.06
Mode 38	1572.20	1572.20	1572.20	1572.20	1572.16	1572.19
Mode 39	2933.98	2934.00	2934.00	2934.00	2934.01	2934.00
Mode 40	2935.08	2935.09	2935.09	2935.09	2935.10	2935.09
Mode 41	2931.49	2931.43	2931.43	2931.43	2931.40	2931.42
Mode 42	2932.80	2932.73	2932.73	2932.73	2932.71	2932.73
Mode 43	2941.08	2941.13	2941.13	2941.13	2941.13	2941.13
Mode 44	2940.74	2940.80	2940.80	2940.80	2940.79	2940.79
Mode 45	2971.43	2971.41	2971.41	2971.41	2971.41	2971.41
Mode 46	2971.23	2971.21	2971.21	2971.21	2971.21	2971.21
Mode 47	3003.15	3003.16	3003.16	3003.16	3003.15	3003.07
Mode 48	3003.09	3003.17	3003.17	3003.17	3003.16	3003.08
ZPE	33943.5	33943.6	33943.6	33943.6	33943.5	33943.4

Table S37. Calculated B3LYP-D3(CSO)/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0 and 2.2 a_0 truncated.

Cutoff (a_0)	0.00	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20
Mode 1	418.88	429.40	429.25	428.21	428.24	428.14	427.54	427.44	427.07	427.01	426.69	426.73
Mode 2	418.86	429.43	429.27	428.23	428.27	428.16	427.55	427.46	427.09	427.03	426.69	426.73
Mode 3	459.95	467.25	468.07	464.60	463.29	463.35	463.50	463.48	463.35	463.61	463.84	463.72
Mode 4	461.41	469.07	469.80	466.26	464.91	464.96	465.13	465.07	464.96	465.23	465.45	465.33
Mode 5	501.92	509.35	508.58	508.41	508.34	508.31	507.37	507.29	507.45	507.49	507.41	507.40
Mode 6	501.94	509.54	508.80	508.51	508.43	508.42	507.49	507.39	507.57	507.49	507.40	507.40
Mode 7	548.75	552.75	553.73	554.59	554.51	553.45	550.45	550.91	550.86	550.80	553.06	551.91
Mode 8	584.74	580.21	589.08	589.02	588.97	588.97	587.89	585.94	585.85	588.06	588.05	588.06
Mode 9	587.40	588.25	585.19	580.81	578.68	578.78	578.24	582.11	582.45	575.90	581.25	581.26
Mode 10	593.05	594.58	591.81	591.97	591.54	591.43	591.37	590.82	591.96	591.97	592.51	592.53
Mode 11	593.01	594.55	591.79	591.96	591.55	591.44	591.37	590.82	591.94	591.95	592.49	592.51
Mode 12	813.68	825.46	825.89	750.20	749.75	749.76	765.63	763.82	764.78	764.74	763.88	774.03
Mode 13	815.90	827.46	827.88	752.28	751.83	751.84	767.71	765.90	766.85	766.85	766.00	776.11
Mode 14	839.97	785.44	785.93	787.86	785.93	785.95	784.87	783.59	783.55	787.59	788.35	789.63
Mode 15	840.29	786.04	786.52	788.45	786.53	786.55	785.47	784.20	784.16	788.18	788.95	790.22
Mode 16	835.77	857.36	858.33	824.47	801.42	801.55	814.67	813.66	818.27	818.30	817.45	817.54
Mode 17	835.75	857.43	858.41	824.54	801.51	801.65	814.76	813.76	818.29	818.33	817.45	817.53
Mode 18	850.82	810.72	811.80	822.08	822.02	822.01	822.34	820.80	828.82	827.87	823.60	823.65
Mode 19	867.96	826.28	832.31	840.59	840.54	840.52	840.86	839.32	846.62	846.55	839.34	839.39
Mode 20	908.88	915.48	915.67	921.63	921.68	920.88	877.14	878.84	877.75	877.78	895.65	895.58
Mode 21	918.52	924.51	924.36	930.54	930.58	929.77	886.42	887.00	885.86	885.87	903.89	903.81
Mode 22	1068.25	1071.91	1072.20	1047.69	1047.68	1047.09	1046.29	1047.03	1050.92	1049.71	1068.67	1079.19
Mode 23	1068.25	1071.99	1072.12	1047.61	1047.61	1047.03	1046.22	1046.95	1050.58	1051.18	1068.85	1079.30
Mode 24	1305.02	1307.99	1300.07	1301.01	1300.06	1299.51	1294.60	1293.39	1303.56	1303.42	1302.37	1303.67
Mode 25	1305.02	1308.08	1300.06	1301.03	1300.19	1299.66	1294.70	1293.50	1303.53	1303.38	1302.34	1303.64
Mode 26	1349.65	1319.19	1318.46	1318.47	1318.49	1322.12	1321.11	1321.23	1320.46	1320.05	1319.94	1318.59

Mode 27	1349.65	1319.17	1318.48	1318.47	1318.45	1322.12	1321.10	1321.22	1320.48	1320.06	1319.96	1318.61
Mode 28	1353.55	1323.79	1323.13	1322.29	1321.81	1321.70	1321.50	1320.87	1321.77	1321.72	1321.87	1321.35
Mode 29	1353.55	1323.04	1323.07	1322.43	1321.98	1321.87	1321.66	1321.01	1321.90	1321.73	1321.88	1321.36
Mode 30	1364.76	1329.84	1331.36	1331.34	1331.55	1331.63	1330.29	1331.21	1328.68	1328.69	1328.86	1328.88
Mode 31	1364.76	1329.92	1331.41	1331.43	1331.66	1331.74	1330.45	1331.31	1328.72	1328.74	1328.91	1328.92
Mode 32	1359.54	1357.02	1354.85	1355.07	1354.05	1354.00	1351.65	1358.90	1356.06	1356.19	1355.80	1354.97
Mode 33	1470.43	1489.10	1488.89	1459.90	1435.61	1435.61	1440.67	1440.21	1441.89	1441.04	1441.60	1441.67
Mode 34	1470.43	1489.07	1488.86	1459.89	1435.60	1435.60	1440.65	1440.19	1441.88	1441.03	1441.59	1441.66
Mode 35	1569.29	1566.69	1564.12	1562.12	1562.11	1561.22	1559.40	1561.62	1560.13	1560.09	1559.93	1559.97
Mode 36	1569.29	1566.20	1564.53	1561.78	1561.82	1560.03	1559.00	1561.31	1560.00	1559.84	1559.69	1559.73
Mode 37	1596.61	1596.20	1590.78	1589.89	1589.27	1589.11	1586.03	1584.58	1589.49	1587.75	1587.03	1587.17
Mode 38	1596.61	1596.25	1590.63	1589.77	1589.09	1588.93	1585.85	1584.39	1589.39	1587.65	1586.92	1587.06
Mode 39	3049.64	3002.41	2997.42	2997.49	2997.47	2997.37	2955.24	2955.05	2950.14	2950.12	2950.73	2950.74
Mode 40	3049.64	3002.53	2998.61	2998.65	2998.63	2998.56	2957.92	2956.43	2951.27	2951.26	2951.85	2951.87
Mode 41	3052.03	2964.36	2957.14	2956.62	2956.83	2956.88	2956.94	2956.74	2944.89	2943.75	2943.55	2942.83
Mode 42	3052.03	2959.20	2961.98	2958.77	2959.00	2959.05	2959.09	2958.90	2947.05	2942.30	2942.28	2941.56
Mode 43	3056.23	3011.26	3010.30	2983.93	2983.68	2979.39	2978.95	2978.58	2980.16	2976.28	2969.35	2968.58
Mode 44	3056.23	3011.28	3010.32	2983.98	2983.75	2979.36	2978.94	2978.56	2980.17	2976.22	2969.05	2968.27
Mode 45	3096.47	3088.24	3087.70	2985.67	2985.78	2985.87	2983.10	2984.28	2984.47	2984.30	2983.99	2982.82
Mode 46	3096.47	3088.47	3087.47	2985.45	2985.58	2985.67	2982.90	2984.01	2984.23	2984.05	2983.74	2982.57
Mode 47	3125.93	3060.62	3059.92	3062.48	3016.29	3016.13	3016.27	3019.75	3021.84	3022.00	3019.79	3019.89
Mode 48	3125.93	3060.62	3059.92	3062.47	3016.33	3016.18	3016.31	3019.80	3021.84	3022.00	3019.78	3019.89
ZPE	34408.7	34262.4	34249.0	34120.4	34074.9	34072.9	34041.7	34043.5	34052.5	34048.9	34061.5	34070.9

Table S38. Calculated B3LYP-D3(CSO)/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.4 and 4.6 a_0 truncated.

Cutoff (a_0)	2.40	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60
Mode 1	426.78	426.10	425.94	425.96	425.86	425.74	425.72	425.73	425.73	425.73	425.78	425.80
Mode 2	426.82	426.10	425.94	425.96	425.91	425.76	425.76	425.73	425.73	425.73	425.78	425.80
Mode 3	463.82	463.92	463.75	463.88	463.85	463.76	463.68	463.72	463.55	463.51	463.89	463.88
Mode 4	465.40	465.52	465.34	465.46	465.42	465.45	465.25	465.30	465.13	465.09	465.42	465.38
Mode 5	507.47	507.40	507.56	507.39	507.50	507.31	507.29	507.15	507.15	507.15	506.65	506.43
Mode 6	507.48	507.40	507.55	507.38	507.22	507.35	507.33	507.16	507.17	507.17	506.66	506.44
Mode 7	551.89	548.62	548.71	548.65	548.48	549.12	547.28	545.57	545.57	546.58	547.23	547.33
Mode 8	583.99	583.85	583.93	583.85	584.22	582.38	580.55	580.43	581.46	581.46	582.05	581.84
Mode 9	581.28	581.34	581.42	581.49	581.43	582.39	582.38	582.31	581.96	581.95	581.85	581.29
Mode 10	592.53	590.54	590.94	591.09	590.97	590.64	590.63	590.66	590.66	590.66	591.36	590.98
Mode 11	592.48	590.52	590.90	591.07	590.35	590.58	590.70	590.64	590.65	590.65	591.33	590.95
Mode 12	773.93	773.49	771.72	771.62	771.64	771.69	776.23	773.11	773.31	776.26	775.91	775.88
Mode 13	775.99	775.58	773.82	773.72	773.91	773.80	778.21	775.20	775.89	778.47	778.13	778.25
Mode 14	786.30	785.86	785.94	785.90	785.98	783.80	783.55	783.57	788.36	788.35	788.25	788.31
Mode 15	786.89	786.45	786.53	786.50	786.51	784.39	784.16	784.16	788.94	788.93	788.84	788.89
Mode 16	815.85	815.87	815.74	815.45	817.24	816.99	816.97	816.97	816.37	816.37	815.45	815.39
Mode 17	815.85	815.86	815.72	815.42	816.92	817.03	816.91	816.97	816.38	816.38	815.45	815.32
Mode 18	823.66	822.82	822.81	822.12	821.00	820.94	825.65	824.55	824.54	824.50	824.27	824.31
Mode 19	839.36	838.63	838.61	837.91	836.94	836.64	841.21	840.13	840.10	840.08	839.83	839.88
Mode 20	895.61	878.28	878.13	878.17	875.79	875.63	875.62	875.38	875.37	877.72	877.82	877.91
Mode 21	903.85	886.39	886.24	886.27	883.86	883.74	883.44	883.47	883.44	885.79	885.88	885.98
Mode 22	1079.06	1076.29	1068.16	1067.57	1058.45	1059.00	1058.98	1058.83	1060.86	1060.74	1060.90	1060.91
Mode 23	1078.98	1076.42	1068.30	1067.71	1058.66	1058.56	1058.56	1058.39	1060.40	1060.28	1060.44	1060.47
Mode 24	1296.27	1296.03	1295.59	1295.22	1293.79	1293.23	1293.20	1291.14	1291.06	1291.07	1289.79	1292.24
Mode 25	1296.20	1296.00	1295.55	1295.18	1293.50	1293.16	1290.84	1290.78	1290.72	1290.72	1289.43	1291.87
Mode 26	1318.15	1317.78	1319.86	1320.31	1319.87	1319.40	1318.56	1318.55	1318.51	1318.51	1319.97	1319.75

Mode 27	1318.38	1317.86	1319.95	1320.40	1320.18	1319.43	1318.53	1318.62	1318.47	1318.47	1319.93	1319.71
Mode 28	1321.38	1320.82	1321.37	1321.65	1319.94	1320.41	1320.46	1320.23	1320.23	1320.23	1317.97	1317.98
Mode 29	1321.37	1320.83	1321.38	1321.69	1320.73	1320.38	1320.50	1320.19	1320.20	1320.20	1317.96	1317.97
Mode 30	1328.97	1329.06	1328.75	1329.00	1328.05	1328.34	1328.88	1328.89	1328.89	1328.88	1328.16	1328.54
Mode 31	1329.01	1329.10	1328.81	1329.07	1328.66	1328.33	1328.87	1328.89	1328.89	1328.88	1328.18	1328.56
Mode 32	1354.42	1354.56	1352.39	1352.32	1351.94	1352.08	1351.88	1351.86	1351.86	1351.72	1352.26	1353.43
Mode 33	1440.95	1440.94	1440.73	1440.65	1440.57	1441.01	1441.02	1441.03	1440.86	1440.87	1440.70	1440.66
Mode 34	1440.93	1440.93	1440.73	1440.64	1440.73	1441.02	1441.01	1441.01	1440.83	1440.84	1440.68	1440.67
Mode 35	1559.92	1559.79	1559.55	1558.90	1558.06	1558.75	1558.83	1558.67	1558.67	1558.69	1551.19	1552.59
Mode 36	1559.65	1559.55	1559.35	1558.70	1558.88	1558.43	1558.44	1558.33	1558.34	1558.36	1550.97	1552.35
Mode 37	1582.34	1581.86	1581.46	1581.08	1581.06	1578.80	1578.70	1578.70	1578.61	1578.63	1577.28	1576.74
Mode 38	1582.22	1581.73	1581.32	1580.95	1580.66	1580.74	1578.72	1578.67	1578.59	1578.61	1577.26	1576.71
Mode 39	2950.76	2949.95	2949.99	2949.84	2941.44	2941.51	2940.89	2940.86	2940.88	2940.99	2940.40	2940.57
Mode 40	2951.87	2951.07	2951.10	2950.96	2942.56	2942.60	2941.97	2941.97	2941.98	2942.08	2941.49	2941.66
Mode 41	2942.80	2943.35	2943.00	2941.55	2941.90	2941.42	2941.64	2939.95	2939.97	2939.99	2939.90	2940.01
Mode 42	2941.55	2942.10	2941.76	2940.29	2940.59	2940.21	2940.41	2938.62	2938.63	2938.65	2938.56	2938.67
Mode 43	2965.39	2951.75	2949.86	2949.53	2949.46	2948.69	2948.58	2948.57	2948.61	2948.65	2947.58	2947.47
Mode 44	2967.90	2951.58	2949.69	2949.36	2949.07	2948.51	2948.48	2948.44	2948.26	2948.31	2947.24	2947.13
Mode 45	2982.68	2982.72	2977.15	2977.19	2977.16	2977.30	2977.50	2977.33	2977.40	2977.56	2976.59	2976.08
Mode 46	2982.44	2982.48	2976.91	2976.95	2977.06	2977.00	2977.33	2977.09	2977.14	2977.30	2976.34	2976.41
Mode 47	3012.67	3011.31	3011.41	3011.33	3011.29	3011.10	3010.47	3010.51	3008.21	3008.21	3007.77	3007.61
Mode 48	3012.65	3011.31	3011.40	3011.33	3011.28	3011.19	3010.52	3010.50	3008.20	3008.20	3007.74	3007.58
ZPE	34056.9	34036.7	34028.7	34026.9	34015.9	34013.5	34015.3	34011.2	34013.6	34016.5	34009.1	34010.7

Table S39. Calculated B3LYP-D3(CSO)/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 4.8 and 7.0 a_0 truncated.

Cutoff (a_0)	4.80	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00
Mode 1	425.77	425.78	425.75	425.76	425.78	425.75	425.74	425.66	425.65	425.66	425.67	425.66
Mode 2	425.76	425.75	425.74	425.74	425.76	425.73	425.73	425.65	425.65	425.65	425.67	425.66
Mode 3	463.80	463.81	463.85	463.84	463.97	463.95	463.95	463.96	463.96	463.96	463.97	463.97
Mode 4	465.33	465.36	465.38	465.39	465.50	465.47	465.48	465.49	465.48	465.48	465.48	465.49
Mode 5	506.57	506.50	506.52	506.48	506.26	506.24	506.24	506.31	506.32	506.29	506.34	506.31
Mode 6	506.61	506.63	506.57	506.53	506.30	506.28	506.28	506.36	506.32	506.32	506.37	506.34
Mode 7	546.88	546.86	546.33	546.03	546.14	546.39	546.29	546.34	546.32	546.32	546.32	546.32
Mode 8	581.77	580.83	580.84	580.80	581.16	580.99	580.99	581.06	581.05	581.05	581.06	581.05
Mode 9	582.38	581.05	581.06	581.03	581.74	581.73	581.75	581.48	581.50	581.21	581.29	581.26
Mode 10	590.60	590.62	590.68	590.65	590.63	590.70	590.70	590.41	590.48	590.47	590.50	590.50
Mode 11	590.70	590.80	590.75	590.73	590.71	590.78	590.78	590.49	590.45	590.49	590.52	590.51
Mode 12	776.27	776.27	774.70	774.67	774.82	774.80	774.80	775.04	774.91	774.88	774.85	774.85
Mode 13	778.45	778.39	776.78	776.74	776.77	776.76	776.75	776.99	776.89	776.89	776.86	776.86
Mode 14	788.29	788.30	788.32	789.10	789.21	790.89	790.88	790.90	790.90	790.90	790.31	789.83
Mode 15	788.88	788.88	788.88	789.69	789.63	791.28	791.48	791.51	791.50	791.50	790.90	790.39
Mode 16	815.01	814.30	814.47	814.47	814.08	814.21	814.20	815.34	815.31	815.08	815.08	815.10
Mode 17	815.07	815.10	814.65	814.62	814.23	814.26	814.35	815.49	815.21	815.14	815.15	815.16
Mode 18	824.17	824.19	824.16	825.50	825.39	825.38	825.38	825.47	825.45	825.44	825.44	825.43
Mode 19	839.73	839.71	839.71	841.09	840.99	840.98	840.98	841.07	841.08	841.08	841.07	841.06
Mode 20	877.80	877.81	877.52	877.51	877.59	879.08	879.07	879.00	878.99	879.00	878.98	878.80
Mode 21	885.88	885.89	885.59	885.59	885.67	887.16	887.15	887.09	887.07	887.07	887.05	886.87
Mode 22	1060.92	1060.93	1060.90	1060.80	1060.85	1060.84	1060.85	1060.81	1060.81	1060.81	1060.80	1060.77
Mode 23	1060.46	1060.46	1060.43	1060.33	1060.38	1060.39	1060.39	1060.34	1060.35	1060.36	1060.34	1060.32
Mode 24	1291.75	1290.85	1290.99	1290.97	1290.42	1290.64	1290.64	1289.87	1290.07	1290.07	1290.19	1290.17
Mode 25	1291.41	1291.29	1291.19	1291.18	1290.64	1290.86	1290.86	1290.08	1289.92	1290.00	1290.12	1290.10
Mode 26	1319.32	1319.49	1319.42	1319.43	1320.03	1320.11	1320.11	1319.34	1319.34	1319.42	1319.42	1319.42

Mode 27	1319.24	1319.29	1319.37	1319.37	1319.96	1320.04	1320.04	1319.28	1319.37	1319.40	1319.41	1319.41
Mode 28	1318.78	1318.77	1318.74	1318.82	1318.28	1318.34	1318.34	1318.85	1318.83	1318.80	1318.76	1318.78
Mode 29	1318.77	1318.70	1318.72	1318.80	1318.27	1318.33	1318.33	1318.83	1318.83	1318.78	1318.74	1318.75
Mode 30	1328.29	1328.34	1328.17	1328.16	1328.34	1328.42	1328.42	1328.55	1328.62	1328.67	1328.57	1328.55
Mode 31	1328.27	1328.27	1328.16	1328.15	1328.33	1328.41	1328.41	1328.51	1328.59	1328.58	1328.48	1328.47
Mode 32	1353.15	1353.25	1353.20	1353.22	1345.46	1346.45	1346.45	1346.97	1346.89	1346.87	1346.25	1346.27
Mode 33	1440.21	1440.21	1440.08	1439.93	1439.89	1439.91	1439.94	1440.14	1440.10	1440.11	1440.10	1440.11
Mode 34	1440.17	1440.00	1439.90	1439.89	1439.86	1439.92	1439.91	1440.10	1440.13	1440.10	1440.09	1440.09
Mode 35	1553.20	1552.87	1552.57	1552.49	1551.03	1551.05	1551.05	1552.89	1552.63	1552.61	1551.99	1552.00
Mode 36	1553.21	1553.36	1552.64	1552.56	1551.10	1551.12	1551.12	1552.73	1552.83	1552.82	1552.21	1552.22
Mode 37	1577.22	1577.05	1577.04	1577.02	1576.51	1576.52	1576.52	1576.44	1576.30	1576.30	1576.33	1576.33
Mode 38	1577.25	1576.97	1576.95	1576.90	1576.39	1576.38	1576.40	1576.32	1576.45	1576.45	1576.49	1576.49
Mode 39	2940.77	2940.76	2939.91	2939.93	2939.72	2939.75	2939.74	2939.84	2939.73	2939.71	2939.68	2939.36
Mode 40	2941.84	2941.81	2940.96	2940.98	2940.77	2940.80	2940.80	2940.90	2940.80	2940.81	2940.77	2940.47
Mode 41	2938.80	2938.86	2938.84	2938.27	2938.34	2938.33	2938.33	2938.14	2936.83	2936.86	2936.85	2936.86
Mode 42	2937.45	2937.45	2937.47	2936.96	2937.03	2937.02	2937.02	2936.83	2938.12	2938.13	2938.13	2938.13
Mode 43	2947.72	2947.63	2947.66	2947.67	2947.23	2947.27	2947.27	2947.55	2947.21	2947.17	2947.19	2947.18
Mode 44	2947.43	2947.40	2947.35	2947.36	2946.92	2946.96	2946.96	2947.24	2947.54	2947.54	2947.56	2947.55
Mode 45	2975.72	2975.69	2975.57	2975.56	2975.59	2975.61	2975.64	2975.49	2975.30	2975.31	2975.27	2975.27
Mode 46	2975.52	2975.48	2975.41	2975.36	2975.41	2975.44	2975.46	2975.28	2975.50	2975.50	2975.46	2975.46
Mode 47	3007.92	3007.91	3007.85	3007.80	3007.62	3007.75	3007.25	3007.58	3007.49	3007.48	3007.46	3007.39
Mode 48	3007.87	3007.74	3007.77	3007.74	3007.55	3007.13	3007.13	3007.49	3007.56	3007.52	3007.49	3007.42
ZPE	34010.3	34009.1	34007.2	34007.8	34004.5	34006.6	34006.6	34007.9	34007.7	34007.5	34006.8	34006.2

Table S40. Calculated B3LYP-D3(CSO)/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.2 and 8.0 a_0 truncated, and finally the untruncated 2MR result.

Cutoff (a_0)	7.20	7.40	7.60	7.80	8.00	2MR
Mode 1	425.66	425.65	425.65	425.65	425.64	425.65
Mode 2	425.66	425.64	425.64	425.64	425.63	425.64
Mode 3	463.97	463.97	463.97	463.97	463.97	463.97
Mode 4	465.49	465.49	465.49	465.49	465.49	465.48
Mode 5	506.31	506.35	506.35	506.35	506.35	506.35
Mode 6	506.34	506.38	506.38	506.38	506.38	506.38
Mode 7	546.32	546.32	546.32	546.32	546.30	546.32
Mode 8	581.05	581.06	581.06	581.06	581.04	581.06
Mode 9	581.30	581.27	581.27	581.27	581.29	581.27
Mode 10	590.50	590.44	590.44	590.44	590.43	590.44
Mode 11	590.51	590.46	590.46	590.46	590.45	590.46
Mode 12	774.85	774.90	774.90	774.90	774.89	774.90
Mode 13	776.86	776.91	776.91	776.91	776.90	776.91
Mode 14	789.86	789.85	789.85	789.85	789.84	789.81
Mode 15	790.40	790.41	790.41	790.41	790.40	790.38
Mode 16	815.10	815.23	815.23	815.23	815.22	815.21
Mode 17	815.16	815.28	815.28	815.28	815.27	815.26
Mode 18	825.43	825.44	825.44	825.44	825.44	825.44
Mode 19	841.06	841.08	841.08	841.08	841.07	841.08
Mode 20	878.80	878.78	878.78	878.78	878.80	878.78
Mode 21	886.87	886.85	886.85	886.85	886.87	886.86
Mode 22	1060.77	1060.77	1060.77	1060.77	1060.77	1060.76
Mode 23	1060.32	1060.31	1060.31	1060.31	1060.31	1060.31
Mode 24	1290.17	1290.03	1290.03	1290.03	1290.01	1290.03
Mode 25	1290.10	1289.96	1289.96	1289.96	1289.94	1289.96
Mode 26	1319.42	1319.25	1319.25	1319.25	1319.24	1319.25

Mode 27	1319.41	1319.24	1319.24	1319.24	1319.23	1319.24
Mode 28	1318.78	1318.90	1318.90	1318.90	1318.92	1318.90
Mode 29	1318.75	1318.88	1318.88	1318.88	1318.90	1318.88
Mode 30	1328.55	1328.52	1328.52	1328.52	1328.58	1328.52
Mode 31	1328.47	1328.44	1328.44	1328.44	1328.50	1328.44
Mode 32	1346.27	1346.54	1346.54	1346.54	1346.79	1346.26
Mode 33	1440.11	1440.13	1440.13	1440.13	1440.12	1440.12
Mode 34	1440.09	1440.11	1440.11	1440.11	1440.11	1440.11
Mode 35	1552.00	1552.02	1552.02	1552.02	1551.93	1552.01
Mode 36	1552.22	1552.24	1552.24	1552.24	1552.15	1552.23
Mode 37	1576.33	1576.33	1576.33	1576.33	1576.29	1576.33
Mode 38	1576.49	1576.49	1576.49	1576.49	1576.45	1576.48
Mode 39	2939.36	2939.38	2939.38	2939.38	2939.39	2939.38
Mode 40	2940.47	2940.48	2940.48	2940.48	2940.49	2940.48
Mode 41	2936.86	2936.78	2936.78	2936.78	2936.75	2936.78
Mode 42	2938.13	2938.06	2938.06	2938.06	2938.03	2938.05
Mode 43	2947.18	2947.25	2947.25	2947.25	2947.25	2947.25
Mode 44	2947.55	2947.62	2947.62	2947.62	2947.61	2947.62
Mode 45	2975.27	2975.24	2975.24	2975.24	2975.23	2975.24
Mode 46	2975.46	2975.42	2975.42	2975.42	2975.42	2975.42
Mode 47	3007.39	3007.47	3007.47	3007.47	3007.46	3007.38
Mode 48	3007.42	3007.44	3007.44	3007.44	3007.43	3007.35
ZPE	34006.3	34006.3	34006.3	34006.3	34006.3	34006.2

Table S41. Calculated B3LYP-D3(CSO)*/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0 and 2.2 a_0 truncated.

Cutoff (a_0)	0.00	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20
Mode 1	418.87	429.40	429.24	428.20	428.23	428.13	427.53	427.43	427.06	427.00	426.68	426.72
Mode 2	418.85	429.42	429.26	428.22	428.26	428.15	427.54	427.45	427.08	427.02	426.69	426.72
Mode 3	459.97	467.26	468.08	464.61	463.30	463.36	463.51	463.49	463.36	463.62	463.86	463.73
Mode 4	461.42	469.08	469.81	466.28	464.92	464.97	465.14	465.08	464.97	465.24	465.46	465.34
Mode 5	501.92	509.35	508.79	508.50	508.42	508.41	507.48	507.38	507.56	507.48	507.39	507.39
Mode 6	501.93	509.54	508.57	508.39	508.33	508.30	507.36	507.28	507.44	507.48	507.39	507.39
Mode 7	548.76	552.77	553.74	554.59	554.52	553.46	550.45	550.92	550.87	550.81	553.07	551.92
Mode 8	584.75	580.24	589.08	589.02	588.98	588.97	587.89	585.94	585.86	588.06	588.06	588.07
Mode 9	587.41	588.26	585.20	580.82	578.69	578.78	578.25	582.12	582.46	575.90	581.26	581.26
Mode 10	593.05	594.56	591.82	591.98	591.55	591.43	591.38	590.83	591.97	591.98	592.52	592.54
Mode 11	593.01	594.59	591.80	591.97	591.56	591.45	591.38	590.83	591.95	591.96	592.50	592.51
Mode 12	813.69	825.48	825.90	750.22	749.77	749.78	765.65	763.84	764.79	764.76	763.90	774.05
Mode 13	815.92	827.49	827.90	752.30	751.84	751.86	767.72	765.92	766.87	766.87	766.01	776.13
Mode 14	840.00	785.47	785.96	787.89	785.96	785.98	784.90	783.62	783.59	787.62	788.39	789.66
Mode 15	840.32	786.07	786.55	788.48	786.56	786.58	785.51	784.23	784.19	788.21	788.98	790.25
Mode 16	835.75	857.43	858.31	824.45	801.40	801.53	814.65	813.65	818.25	818.28	817.44	817.52
Mode 17	835.74	857.34	858.40	824.52	801.49	801.63	814.74	813.74	818.27	818.31	817.43	817.52
Mode 18	850.84	810.74	811.82	822.10	822.05	822.03	822.36	820.82	828.85	827.89	823.62	823.68
Mode 19	867.98	826.31	832.33	840.61	840.56	840.54	840.88	839.34	846.64	846.57	839.36	839.41
Mode 20	908.91	915.52	915.70	921.66	921.70	920.90	877.16	878.87	877.77	877.81	895.67	895.61
Mode 21	918.55	924.54	924.39	930.56	930.60	929.79	886.45	887.02	885.89	885.89	903.91	903.84
Mode 22	1068.26	1072.01	1072.21	1047.70	1047.69	1047.11	1046.30	1047.04	1050.93	1049.72	1068.68	1079.19
Mode 23	1068.26	1071.93	1072.14	1047.62	1047.62	1047.04	1046.23	1046.96	1050.59	1051.19	1068.86	1079.30
Mode 24	1305.01	1308.07	1300.06	1301.01	1300.06	1299.51	1294.60	1293.39	1303.56	1303.41	1302.37	1303.66
Mode 25	1305.01	1307.97	1300.06	1301.03	1300.19	1299.66	1294.69	1293.49	1303.52	1303.38	1302.34	1303.63
Mode 26	1349.64	1319.16	1318.45	1318.46	1318.48	1322.11	1321.10	1321.22	1320.45	1320.04	1319.93	1318.58

Mode 27	1349.64	1319.17	1318.47	1318.46	1318.44	1322.11	1321.09	1321.21	1320.47	1320.05	1319.95	1318.60
Mode 28	1353.53	1323.03	1323.12	1322.27	1321.80	1321.69	1321.48	1320.85	1321.75	1321.70	1321.86	1321.33
Mode 29	1353.53	1323.78	1323.05	1322.42	1321.96	1321.85	1321.64	1321.00	1321.88	1321.71	1321.87	1321.34
Mode 30	1364.75	1329.92	1331.35	1331.33	1331.54	1331.63	1330.29	1331.20	1328.67	1328.68	1328.85	1328.87
Mode 31	1364.75	1329.83	1331.40	1331.42	1331.66	1331.73	1330.44	1331.30	1328.71	1328.73	1328.90	1328.91
Mode 32	1359.55	1357.02	1354.86	1355.08	1354.06	1354.01	1351.66	1358.91	1356.07	1356.20	1355.81	1354.97
Mode 33	1470.44	1489.07	1488.90	1459.91	1435.62	1435.62	1440.68	1440.22	1441.90	1441.05	1441.61	1441.68
Mode 34	1470.44	1489.10	1488.87	1459.91	1435.61	1435.61	1440.66	1440.20	1441.89	1441.04	1441.59	1441.66
Mode 35	1569.30	1566.19	1564.13	1562.13	1562.12	1561.22	1559.40	1561.62	1560.14	1560.10	1559.94	1559.98
Mode 36	1569.30	1566.70	1564.53	1561.79	1561.82	1560.03	1559.01	1561.31	1560.01	1559.85	1559.70	1559.74
Mode 37	1596.62	1596.24	1590.79	1589.90	1589.28	1589.12	1586.03	1584.59	1589.50	1587.76	1587.04	1587.18
Mode 38	1596.62	1596.21	1590.64	1589.78	1589.10	1588.94	1585.86	1584.40	1589.40	1587.66	1586.93	1587.07
Mode 39	3049.68	3002.40	2998.65	2998.69	2998.67	2998.60	2957.96	2956.47	2951.31	2951.30	2951.89	2951.91
Mode 40	3049.68	3002.52	2997.46	2997.53	2997.51	2997.41	2955.28	2955.09	2950.18	2950.16	2950.77	2950.78
Mode 41	3052.07	2964.36	2962.03	2958.82	2959.05	2959.09	2959.13	2958.95	2947.10	2942.34	2942.33	2941.60
Mode 42	3052.07	2959.19	2957.18	2956.67	2956.88	2956.93	2956.99	2956.78	2944.93	2943.79	2943.59	2942.87
Mode 43	3056.25	3011.25	3010.32	2983.95	2983.69	2979.41	2978.97	2978.60	2980.18	2976.30	2969.37	2968.60
Mode 44	3056.25	3011.27	3010.34	2984.00	2983.77	2979.38	2978.96	2978.58	2980.19	2976.24	2969.07	2968.29
Mode 45	3096.47	3088.24	3087.70	2985.67	2985.78	2985.87	2983.09	2984.28	2984.47	2984.30	2983.98	2982.81
Mode 46	3096.47	3088.47	3087.47	2985.44	2985.58	2985.67	2982.90	2984.00	2984.23	2984.05	2983.74	2982.57
Mode 47	3125.93	3060.61	3059.93	3062.49	3016.29	3016.13	3016.28	3019.76	3021.84	3022.00	3019.79	3019.89
Mode 48	3125.93	3060.62	3059.92	3062.47	3016.33	3016.18	3016.31	3019.81	3021.84	3022.01	3019.79	3019.89
ZPE	34408.9	34262.6	34249.2	34120.6	34075.1	34073.1	34041.9	34043.7	34052.7	34049.1	34061.7	34071.1

Table S42. Calculated B3LYP-D3(CSO)*/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.4 and 4.6 a_0 truncated.

Cutoff (a_0)	2.40	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60
Mode 1	426.77	426.09	425.93	425.95	425.85	425.74	425.71	425.72	425.72	425.72	425.77	425.79
Mode 2	426.81	426.09	425.93	425.95	425.90	425.76	425.75	425.72	425.72	425.72	425.77	425.79
Mode 3	463.83	463.93	463.76	463.89	463.86	463.77	463.70	463.73	463.56	463.53	463.91	463.89
Mode 4	465.41	465.53	465.35	465.48	465.43	465.46	465.26	465.31	465.14	465.10	465.44	465.40
Mode 5	507.47	507.39	507.54	507.37	507.21	507.33	507.32	507.14	507.14	507.14	506.64	506.42
Mode 6	507.46	507.39	507.55	507.38	507.49	507.30	507.28	507.15	507.15	507.16	506.65	506.43
Mode 7	551.90	548.63	548.71	548.65	548.49	549.13	547.29	545.58	545.58	546.59	547.24	547.34
Mode 8	583.99	583.86	583.94	583.86	584.22	582.38	580.56	580.43	581.47	581.46	582.06	581.85
Mode 9	581.28	581.35	581.43	581.50	581.44	582.39	582.39	582.32	581.97	581.96	581.86	581.30
Mode 10	592.54	590.55	590.95	591.09	590.98	590.65	590.64	590.67	590.67	590.67	591.36	590.99
Mode 11	592.49	590.53	590.91	591.07	590.35	590.59	590.71	590.65	590.65	590.65	591.34	590.96
Mode 12	773.94	773.50	771.73	771.64	771.65	771.71	776.24	773.12	773.33	776.28	775.93	775.89
Mode 13	776.00	775.59	773.83	773.74	773.92	773.81	778.23	775.21	775.90	778.49	778.14	778.27
Mode 14	786.33	785.89	785.97	785.94	786.02	783.84	783.59	783.61	788.39	788.38	788.29	788.34
Mode 15	786.92	786.48	786.56	786.53	786.54	784.42	784.19	784.19	788.98	788.96	788.87	788.93
Mode 16	815.83	815.85	815.73	815.43	817.23	816.97	816.95	816.95	816.36	816.35	815.43	815.37
Mode 17	815.83	815.85	815.70	815.41	816.90	817.02	816.89	816.95	816.36	816.36	815.44	815.30
Mode 18	823.69	822.84	822.83	822.14	821.02	820.96	825.68	824.57	824.56	824.52	824.29	824.33
Mode 19	839.38	838.65	838.63	837.93	836.96	836.66	841.23	840.15	840.12	840.10	839.85	839.90
Mode 20	895.63	878.31	878.16	878.20	875.82	875.65	875.65	875.40	875.40	877.75	877.84	877.93
Mode 21	903.87	886.41	886.27	886.30	883.89	883.77	883.47	883.49	883.47	885.81	885.90	886.00
Mode 22	1079.07	1076.30	1068.17	1067.58	1058.47	1059.01	1058.99	1058.40	1060.41	1060.29	1060.45	1060.48
Mode 23	1078.99	1076.43	1068.31	1067.72	1058.68	1058.57	1058.57	1058.85	1060.87	1060.75	1060.91	1060.93
Mode 24	1296.26	1296.03	1295.59	1295.22	1293.78	1293.23	1293.20	1291.14	1291.06	1291.07	1289.79	1292.23
Mode 25	1296.20	1296.00	1295.55	1295.17	1293.49	1293.16	1290.84	1290.77	1290.71	1290.72	1289.43	1291.87
Mode 26	1318.14	1317.77	1319.85	1320.30	1319.86	1319.39	1318.55	1318.54	1318.50	1318.50	1319.96	1319.74

Mode 27	1318.37	1317.85	1319.94	1320.39	1320.17	1319.42	1318.52	1318.61	1318.46	1318.46	1319.92	1319.70
Mode 28	1321.36	1320.80	1321.35	1321.63	1319.92	1320.39	1320.44	1320.21	1320.21	1320.21	1317.95	1317.96
Mode 29	1321.35	1320.81	1321.37	1321.68	1320.71	1320.37	1320.48	1320.18	1320.18	1320.18	1317.94	1317.95
Mode 30	1328.96	1329.05	1328.74	1328.99	1328.04	1328.33	1328.87	1328.88	1328.88	1328.87	1328.15	1328.53
Mode 31	1329.00	1329.09	1328.81	1329.06	1328.65	1328.33	1328.86	1328.88	1328.88	1328.87	1328.17	1328.55
Mode 32	1354.43	1354.57	1352.40	1352.33	1351.94	1352.09	1351.89	1351.87	1351.87	1351.73	1352.27	1353.44
Mode 33	1440.96	1440.95	1440.74	1440.66	1440.58	1441.02	1441.03	1441.04	1440.87	1440.87	1440.71	1440.66
Mode 34	1440.94	1440.94	1440.74	1440.65	1440.74	1441.03	1441.02	1441.01	1440.84	1440.84	1440.69	1440.68
Mode 35	1559.92	1559.80	1559.55	1558.91	1558.07	1558.75	1558.83	1558.67	1558.67	1558.70	1551.20	1552.59
Mode 36	1559.66	1559.56	1559.35	1558.71	1558.89	1558.44	1558.45	1558.34	1558.34	1558.37	1550.97	1552.35
Mode 37	1582.35	1581.87	1581.46	1581.09	1581.07	1578.81	1578.71	1578.71	1578.62	1578.63	1577.29	1576.75
Mode 38	1582.23	1581.74	1581.33	1580.95	1580.67	1580.74	1578.73	1578.68	1578.59	1578.62	1577.27	1576.72
Mode 39	2951.91	2951.11	2951.14	2951.00	2942.60	2942.64	2942.02	2942.01	2942.02	2942.12	2941.53	2941.70
Mode 40	2950.80	2949.99	2950.03	2949.88	2941.48	2941.55	2940.93	2940.90	2940.92	2941.03	2940.44	2940.61
Mode 41	2941.59	2942.14	2941.81	2940.33	2940.63	2940.25	2940.45	2939.99	2940.02	2940.03	2939.94	2940.05
Mode 42	2942.84	2943.40	2943.05	2941.59	2941.95	2941.46	2941.68	2938.66	2938.67	2938.69	2938.61	2938.71
Mode 43	2965.41	2951.77	2949.88	2949.55	2949.48	2948.71	2948.60	2948.46	2948.28	2948.33	2947.26	2947.15
Mode 44	2967.92	2951.60	2949.71	2949.38	2949.09	2948.52	2948.50	2948.59	2948.63	2948.67	2947.60	2947.49
Mode 45	2982.68	2982.72	2977.15	2977.19	2977.16	2977.30	2977.49	2977.09	2977.13	2977.30	2976.34	2976.41
Mode 46	2982.44	2982.48	2976.91	2976.95	2977.05	2976.99	2977.33	2977.33	2977.40	2977.56	2976.59	2976.07
Mode 47	3012.67	3011.32	3011.42	3011.34	3011.30	3011.11	3010.48	3010.51	3008.20	3008.21	3007.75	3007.59
Mode 48	3012.66	3011.31	3011.41	3011.34	3011.28	3011.20	3010.52	3010.52	3008.21	3008.22	3007.77	3007.62
ZPE	34057.1	34036.9	34028.9	34027.1	34016.1	34013.7	34015.5	34011.4	34013.8	34016.7	34009.3	34010.9

Table S43. Calculated B3LYP-D3(CSO)*/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 4.8 and 7.0 a_0 truncated.

Cutoff (a_0)	4.80	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00
Mode 1	425.76	425.77	425.74	425.75	425.77	425.74	425.74	425.65	425.65	425.65	425.67	425.66
Mode 2	425.75	425.74	425.74	425.74	425.75	425.72	425.72	425.64	425.64	425.64	425.66	425.65
Mode 3	463.81	463.82	463.86	463.85	463.98	463.97	463.96	463.97	463.97	463.97	463.97	463.98
Mode 4	465.34	465.38	465.39	465.40	465.51	465.48	465.49	465.50	465.49	465.49	465.50	465.50
Mode 5	506.55	506.49	506.51	506.47	506.25	506.22	506.22	506.34	506.33	506.31	506.35	506.33
Mode 6	506.60	506.62	506.56	506.52	506.29	506.27	506.27	506.30	506.29	506.29	506.33	506.31
Mode 7	546.88	546.87	546.34	546.04	546.15	546.40	546.29	546.35	546.34	546.33	546.34	546.33
Mode 8	581.78	580.84	580.84	580.80	581.17	580.99	580.99	581.06	581.05	581.05	581.05	581.05
Mode 9	582.39	581.06	581.06	581.03	581.75	581.74	581.76	581.49	581.50	581.22	581.30	581.27
Mode 10	590.61	590.63	590.68	590.66	590.64	590.71	590.71	590.42	590.43	590.46	590.50	590.49
Mode 11	590.71	590.80	590.75	590.74	590.72	590.78	590.78	590.50	590.50	590.51	590.54	590.53
Mode 12	776.29	776.29	774.71	774.68	774.84	774.82	774.81	775.05	774.94	774.91	774.88	774.88
Mode 13	778.47	778.41	776.79	776.75	776.79	776.77	776.77	777.01	776.90	776.89	776.86	776.86
Mode 14	788.32	788.33	788.36	789.14	789.24	790.92	790.91	790.94	790.93	790.93	790.34	789.86
Mode 15	788.92	788.91	788.92	789.72	789.67	791.31	791.52	791.54	791.53	791.53	790.94	790.43
Mode 16	814.99	814.29	814.46	814.46	814.07	814.19	814.19	815.33	815.18	815.10	815.10	815.12
Mode 17	815.05	815.09	814.63	814.60	814.21	814.24	814.33	815.48	815.33	815.09	815.09	815.11
Mode 18	824.19	824.21	824.18	825.53	825.42	825.41	825.41	825.50	825.49	825.48	825.48	825.46
Mode 19	839.75	839.73	839.73	841.11	841.00	841.00	841.00	841.10	841.09	841.09	841.08	841.07
Mode 20	877.83	877.83	877.54	877.53	877.62	879.10	879.09	879.02	879.01	879.02	879.00	878.82
Mode 21	885.90	885.92	885.62	885.61	885.70	887.19	887.18	887.12	887.10	887.11	887.08	886.90
Mode 22	1060.47	1060.47	1060.44	1060.34	1060.39	1060.40	1060.40	1060.82	1060.82	1060.83	1060.81	1060.79
Mode 23	1060.93	1060.95	1060.91	1060.81	1060.86	1060.86	1060.86	1060.35	1060.36	1060.36	1060.35	1060.32
Mode 24	1291.75	1290.85	1290.99	1290.97	1290.41	1290.63	1290.64	1289.86	1289.88	1289.96	1290.08	1290.06
Mode 25	1291.41	1291.29	1291.19	1291.18	1290.63	1290.86	1290.86	1290.08	1290.10	1290.11	1290.23	1290.21
Mode 26	1319.31	1319.48	1319.41	1319.42	1320.02	1320.10	1320.10	1319.33	1319.36	1319.41	1319.41	1319.41

Mode 27	1319.23	1319.28	1319.36	1319.36	1319.95	1320.03	1320.03	1319.27	1319.31	1319.39	1319.39	1319.39
Mode 28	1318.76	1318.75	1318.73	1318.80	1318.26	1318.32	1318.33	1318.83	1318.83	1318.78	1318.74	1318.75
Mode 29	1318.75	1318.68	1318.70	1318.78	1318.25	1318.31	1318.31	1318.81	1318.81	1318.78	1318.73	1318.75
Mode 30	1328.28	1328.33	1328.16	1328.15	1328.33	1328.41	1328.41	1328.54	1328.61	1328.62	1328.52	1328.51
Mode 31	1328.26	1328.26	1328.15	1328.14	1328.32	1328.40	1328.40	1328.50	1328.57	1328.61	1328.51	1328.50
Mode 32	1353.16	1353.26	1353.21	1353.23	1345.47	1346.46	1346.46	1346.98	1346.90	1346.88	1346.26	1346.28
Mode 33	1440.21	1440.21	1440.08	1439.94	1439.89	1439.92	1439.94	1440.15	1440.15	1440.12	1440.11	1440.11
Mode 34	1440.18	1440.01	1439.91	1439.90	1439.87	1439.93	1439.92	1440.10	1440.11	1440.11	1440.10	1440.10
Mode 35	1553.20	1552.88	1552.58	1552.50	1551.04	1551.06	1551.06	1552.89	1552.83	1552.81	1552.20	1552.21
Mode 36	1553.22	1553.37	1552.65	1552.57	1551.10	1551.12	1551.12	1552.73	1552.67	1552.63	1552.01	1552.02
Mode 37	1577.23	1577.05	1577.04	1577.03	1576.52	1576.53	1576.53	1576.45	1576.44	1576.45	1576.48	1576.48
Mode 38	1577.26	1576.97	1576.96	1576.91	1576.39	1576.39	1576.41	1576.33	1576.32	1576.32	1576.35	1576.35
Mode 39	2941.88	2941.85	2941.00	2941.02	2940.81	2940.84	2940.84	2940.94	2940.83	2940.83	2940.80	2940.49
Mode 40	2940.81	2940.80	2939.95	2939.97	2939.76	2939.78	2939.78	2939.88	2939.78	2939.77	2939.74	2939.42
Mode 41	2938.85	2938.90	2938.88	2938.31	2938.38	2938.37	2938.37	2936.87	2936.86	2936.89	2936.89	2936.89
Mode 42	2937.49	2937.49	2937.51	2937.00	2937.07	2937.07	2937.07	2938.18	2938.17	2938.19	2938.18	2938.19
Mode 43	2947.45	2947.42	2947.37	2947.38	2946.94	2946.98	2946.98	2947.57	2947.55	2947.54	2947.56	2947.55
Mode 44	2947.74	2947.65	2947.68	2947.68	2947.25	2947.29	2947.29	2947.26	2947.24	2947.20	2947.23	2947.22
Mode 45	2975.52	2975.48	2975.40	2975.35	2975.41	2975.44	2975.45	2975.49	2975.50	2975.51	2975.46	2975.46
Mode 46	2975.72	2975.69	2975.57	2975.55	2975.58	2975.61	2975.64	2975.28	2975.29	2975.31	2975.26	2975.26
Mode 47	3007.87	3007.74	3007.77	3007.75	3007.56	3007.14	3007.13	3007.58	3007.58	3007.54	3007.51	3007.44
Mode 48	3007.92	3007.92	3007.86	3007.80	3007.62	3007.76	3007.25	3007.49	3007.49	3007.47	3007.45	3007.38
ZPE	34010.5	34009.3	34007.4	34008.0	34004.7	34006.8	34006.8	34008.1	34007.9	34007.7	34007.0	34006.4

Table S44. Calculated B3LYP-D3(CSO)*/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.2 and 8.0 a_0 truncated, and finally the untruncated 2MR result.

Cutoff (a_0)	7.20	7.40	7.60	7.80	8.00	2MR
Mode 1	425.66	425.64	425.64	425.64	425.63	425.64
Mode 2	425.65	425.63	425.63	425.63	425.62	425.63
Mode 3	463.98	463.97	463.97	463.97	463.98	463.97
Mode 4	465.50	465.50	465.50	465.50	465.51	465.50
Mode 5	506.33	506.37	506.34	506.34	506.34	506.34
Mode 6	506.31	506.34	506.37	506.37	506.36	506.37
Mode 7	546.33	546.34	546.34	546.34	546.32	546.33
Mode 8	581.05	581.06	581.06	581.06	581.04	581.06
Mode 9	581.31	581.28	581.28	581.28	581.30	581.28
Mode 10	590.49	590.43	590.44	590.44	590.43	590.43
Mode 11	590.53	590.48	590.48	590.48	590.47	590.48
Mode 12	774.88	774.93	774.93	774.93	774.92	774.93
Mode 13	776.86	776.91	776.90	776.90	776.90	776.90
Mode 14	789.89	789.88	789.88	789.88	789.86	789.84
Mode 15	790.44	790.45	790.45	790.45	790.44	790.41
Mode 16	815.12	815.24	815.24	815.24	815.23	815.22
Mode 17	815.11	815.24	815.24	815.24	815.23	815.22
Mode 18	825.46	825.48	825.48	825.48	825.47	825.48
Mode 19	841.07	841.08	841.08	841.08	841.08	841.08
Mode 20	878.82	878.80	878.80	878.80	878.81	878.80
Mode 21	886.90	886.89	886.89	886.89	886.90	886.89
Mode 22	1060.79	1060.78	1060.31	1060.31	1060.32	1060.31
Mode 23	1060.32	1060.32	1060.78	1060.78	1060.78	1060.78
Mode 24	1290.06	1289.92	1289.92	1289.92	1289.90	1289.92
Mode 25	1290.21	1290.07	1290.07	1290.07	1290.05	1290.07
Mode 26	1319.41	1319.24	1319.24	1319.24	1319.24	1319.24

Mode 27	1319.39	1319.22	1319.22	1319.22	1319.22	1319.22
Mode 28	1318.75	1318.87	1318.87	1318.87	1318.89	1318.87
Mode 29	1318.75	1318.87	1318.87	1318.87	1318.89	1318.87
Mode 30	1328.51	1328.47	1328.47	1328.47	1328.53	1328.48
Mode 31	1328.50	1328.47	1328.47	1328.47	1328.53	1328.47
Mode 32	1346.28	1346.55	1346.55	1346.55	1346.79	1346.27
Mode 33	1440.11	1440.13	1440.13	1440.13	1440.13	1440.13
Mode 34	1440.10	1440.12	1440.12	1440.12	1440.12	1440.12
Mode 35	1552.21	1552.23	1552.23	1552.23	1552.13	1552.22
Mode 36	1552.02	1552.05	1552.04	1552.04	1551.95	1552.04
Mode 37	1576.48	1576.48	1576.48	1576.48	1576.44	1576.47
Mode 38	1576.35	1576.35	1576.35	1576.35	1576.32	1576.35
Mode 39	2940.49	2940.51	2940.51	2940.51	2940.51	2940.51
Mode 40	2939.42	2939.44	2939.44	2939.44	2939.44	2939.44
Mode 41	2936.89	2936.81	2938.11	2938.11	2938.08	2938.11
Mode 42	2938.19	2938.11	2936.81	2936.81	2936.79	2936.81
Mode 43	2947.55	2947.62	2947.29	2947.29	2947.28	2947.29
Mode 44	2947.22	2947.29	2947.62	2947.62	2947.62	2947.62
Mode 45	2975.46	2975.43	2975.22	2975.22	2975.22	2975.22
Mode 46	2975.26	2975.22	2975.43	2975.43	2975.43	2975.43
Mode 47	3007.44	3007.45	3007.46	3007.46	3007.45	3007.37
Mode 48	3007.38	3007.46	3007.45	3007.45	3007.44	3007.36
ZPE	34006.5	34006.5	34006.5	34006.5	34006.5	34006.4

Table S45. Calculated B3LYP-D2/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 0.2 and 2.4 a_0 calculated using B3LYP/6-31G(d,p).

Cutoff (a_0)	0.20	0.40	0.60	0.80	1.00	1.20	1.40	1.60	1.80	2.00	2.20	2.40
Mode 1	428.90	428.90	428.90	428.89	428.88	428.89	428.89	428.89	428.89	428.89	428.89	428.89
Mode 2	428.91	428.91	428.91	428.89	428.89	428.90	428.90	428.90	428.90	428.90	428.90	428.89
Mode 3	464.11	464.11	464.13	464.14	464.13	464.12	464.08	464.09	464.09	464.09	464.10	464.08
Mode 4	465.82	465.83	465.85	465.85	465.84	465.84	465.80	465.80	465.80	465.81	465.81	465.79
Mode 5	510.11	510.10	510.10	510.11	510.13	510.13	510.13	510.13	510.13	510.12	510.12	510.11
Mode 6	510.13	510.12	510.12	510.13	510.15	510.15	510.15	510.15	510.15	510.14	510.14	510.13
Mode 7	544.87	544.87	544.85	544.85	544.83	544.81	544.82	544.82	544.82	544.83	544.82	544.82
Mode 8	580.23	580.22	580.22	580.23	580.22	580.22	580.19	580.20	580.20	580.20	580.20	580.18
Mode 9	581.33	581.30	581.30	581.29	581.28	581.28	581.27	581.27	581.26	581.27	581.26	581.26
Mode 10	586.70	586.69	586.68	586.66	586.78	586.78	586.78	586.76	586.76	587.01	587.01	587.01
Mode 11	586.73	586.73	586.72	586.69	586.82	586.82	586.81	586.80	586.80	587.04	587.04	587.05
Mode 12	776.19	776.18	776.20	776.19	776.21	776.30	776.08	776.08	776.01	776.17	776.14	776.14
Mode 13	778.22	778.21	778.23	778.22	778.24	778.33	778.10	778.11	778.04	778.20	778.16	778.17
Mode 14	789.82	789.81	790.14	789.83	789.84	790.01	789.75	789.76	789.71	789.73	789.74	789.72
Mode 15	790.39	790.39	790.43	790.41	790.41	790.58	790.32	790.33	790.28	790.30	790.32	790.29
Mode 16	812.52	812.51	812.71	812.83	812.86	812.74	812.52	812.55	812.55	812.64	812.64	812.63
Mode 17	812.53	812.52	812.72	812.83	812.87	812.74	812.52	812.56	812.56	812.64	812.64	812.63
Mode 18	828.17	828.16	828.12	828.13	828.13	828.13	828.14	828.10	828.10	828.05	828.05	828.05
Mode 19	843.88	843.88	843.84	843.84	843.85	843.85	843.86	843.82	843.82	843.77	843.77	843.77
Mode 20	881.13	881.14	881.11	881.10	881.08	880.79	880.79	880.80	880.81	880.78	880.76	880.77
Mode 21	889.34	889.34	889.31	889.31	889.28	889.01	889.01	889.02	889.02	888.99	888.98	888.98
Mode 22	1060.40	1060.40	1060.27	1060.25	1060.24	1060.25	1060.18	1060.09	1060.06	1060.04	1060.00	1060.01
Mode 23	1059.93	1059.93	1059.80	1059.78	1059.78	1059.79	1059.72	1059.63	1059.60	1059.57	1059.54	1059.54
Mode 24	1287.13	1287.12	1287.07	1286.99	1287.03	1287.22	1287.20	1287.46	1287.45	1287.42	1287.42	1287.52
Mode 25	1286.99	1286.98	1286.93	1286.85	1286.89	1287.09	1287.06	1287.32	1287.31	1287.28	1287.28	1287.39
Mode 26	1313.88	1313.89	1313.81	1313.75	1314.07	1314.11	1314.12	1314.11	1314.10	1314.07	1314.12	1314.13

Mode 27	1313.90	1313.90	1313.82	1313.76	1314.08	1314.12	1314.13	1314.12	1314.11	1314.08	1314.13	1314.13
Mode 28	1318.15	1318.14	1318.12	1318.13	1318.17	1318.14	1318.25	1318.57	1318.56	1318.56	1318.58	1318.59
Mode 29	1318.16	1318.14	1318.12	1318.14	1318.17	1318.15	1318.26	1318.57	1318.57	1318.56	1318.59	1318.59
Mode 30	1328.73	1328.73	1328.75	1328.73	1328.71	1328.49	1328.48	1328.88	1328.88	1328.88	1328.88	1328.88
Mode 31	1328.73	1328.72	1328.73	1328.72	1328.70	1328.50	1328.48	1328.88	1328.88	1328.88	1328.88	1328.88
Mode 32	1341.25	1341.24	1341.28	1341.28	1341.38	1341.53	1341.51	1341.53	1341.54	1341.49	1341.45	1341.43
Mode 33	1436.00	1436.00	1438.24	1440.71	1440.73	1440.93	1440.86	1441.45	1441.45	1441.44	1441.44	1441.44
Mode 34	1436.00	1436.00	1438.54	1440.71	1440.72	1440.93	1440.85	1441.45	1441.45	1441.43	1441.43	1441.44
Mode 35	1548.97	1548.94	1548.93	1548.94	1549.02	1549.02	1549.12	1549.09	1549.09	1549.05	1549.06	1549.07
Mode 36	1548.78	1548.75	1548.74	1548.75	1548.83	1548.83	1548.93	1548.90	1548.90	1548.86	1548.87	1548.87
Mode 37	1571.26	1571.19	1571.11	1571.02	1571.07	1571.41	1571.36	1571.78	1571.76	1571.75	1571.76	1572.06
Mode 38	1571.39	1571.32	1571.25	1571.15	1571.20	1571.54	1571.49	1571.91	1571.89	1571.88	1571.89	1572.19
Mode 39	2935.40	2935.40	2935.40	2935.40	2935.42	2935.34	2935.33	2935.32	2935.32	2935.31	2935.31	2935.31
Mode 40	2934.31	2934.30	2934.30	2934.30	2934.32	2934.24	2934.24	2934.22	2934.22	2934.21	2934.21	2934.21
Mode 41	2932.81	2932.81	2932.83	2932.83	2932.84	2932.84	2932.84	2932.83	2932.82	2932.81	2932.84	2932.84
Mode 42	2931.50	2931.50	2931.51	2931.52	2931.52	2931.53	2931.53	2931.51	2931.51	2931.50	2931.53	2931.53
Mode 43	2940.88	2940.87	2940.78	2940.79	2940.89	2940.93	2940.92	2940.92	2940.91	2940.88	2940.91	2940.92
Mode 44	2941.21	2941.20	2941.12	2941.12	2941.23	2941.27	2941.25	2941.26	2941.25	2941.22	2941.25	2941.25
Mode 45	2965.40	2965.40	2968.37	2968.35	2968.35	2969.07	2971.09	2971.10	2971.10	2971.11	2971.14	2971.14
Mode 46	2965.61	2965.61	2968.58	2968.56	2968.56	2969.28	2971.30	2971.31	2971.31	2971.32	2971.34	2971.35
Mode 47	2996.91	2996.90	2996.89	3000.11	3000.12	3000.13	3002.23	3002.21	3002.21	3002.36	3002.36	3002.95
Mode 48	2996.90	2996.89	2996.86	3000.10	3000.11	3000.12	3002.21	3002.20	3002.19	3002.35	3002.34	3002.93
ZPE	33933.2	33933.1	33935.6	33938.0	33938.4	33938.9	33940.3	33941.2	33941.1	33941.3	33941.3	33941.7

Table S46. Calculated B3LYP-D2/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 2.6 and 4.8 a_0 calculated using B3LYP/6-31G(d,p).

Cutoff (a_0)	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.20	4.40	4.60	4.80
Mode 1	428.89	428.90	428.90	428.90	428.90	428.90	428.90	428.90	428.90	428.90	428.91	428.89
Mode 2	428.90	428.90	428.91	428.91	428.91	428.91	428.91	428.91	428.91	428.91	428.91	428.90
Mode 3	464.08	464.08	464.11	464.12	464.12	464.12	464.12	464.12	464.12	464.14	464.14	464.12
Mode 4	465.80	465.80	465.82	465.83	465.83	465.83	465.83	465.83	465.83	465.84	465.84	465.82
Mode 5	510.10	510.09	510.05	510.05	510.06	510.06	510.05	510.05	510.05	510.03	510.03	510.03
Mode 6	510.12	510.11	510.07	510.07	510.07	510.07	510.07	510.07	510.07	510.05	510.05	510.05
Mode 7	544.81	544.81	544.83	544.84	544.82	544.83	544.82	544.82	544.81	544.83	544.83	544.81
Mode 8	580.19	580.19	580.20	580.20	580.19	580.19	580.19	580.19	580.19	580.20	580.20	580.18
Mode 9	581.27	581.27	581.31	581.31	581.31	581.31	581.30	581.29	581.29	581.32	581.32	581.32
Mode 10	587.05	587.06	587.72	587.71	587.70	587.70	587.70	587.70	587.70	587.76	587.76	587.74
Mode 11	587.08	587.09	587.75	587.74	587.73	587.74	587.73	587.73	587.73	587.79	587.79	587.78
Mode 12	776.14	776.14	776.11	776.12	776.12	776.08	776.10	776.10	776.09	776.09	776.09	776.10
Mode 13	778.17	778.16	778.14	778.15	778.15	778.11	778.13	778.13	778.12	778.12	778.12	778.13
Mode 14	789.62	789.62	789.61	789.61	789.61	789.61	789.61	789.59	789.59	789.58	789.59	789.58
Mode 15	790.19	790.19	790.19	790.19	790.18	790.18	790.18	790.16	790.16	790.16	790.16	790.15
Mode 16	812.61	813.06	812.99	812.99	812.98	812.98	812.98	812.99	812.99	812.95	812.95	813.19
Mode 17	812.61	813.07	813.00	812.99	812.99	812.99	812.99	812.99	813.00	812.96	812.96	813.19
Mode 18	828.05	828.04	828.00	827.97	827.97	827.94	827.95	827.95	827.94	827.94	827.94	827.97
Mode 19	843.77	843.76	843.72	843.70	843.70	843.67	843.67	843.67	843.67	843.66	843.66	843.69
Mode 20	880.70	880.71	880.73	880.73	880.74	880.74	880.72	880.72	880.71	880.73	880.73	880.75
Mode 21	888.92	888.93	888.94	888.94	888.95	888.95	888.94	888.94	888.93	888.94	888.94	888.96
Mode 22	1060.01	1060.07	1060.08	1059.98	1060.06	1060.07	1060.07	1060.08	1060.07	1060.08	1060.08	1060.10
Mode 23	1059.55	1059.60	1059.61	1059.51	1059.59	1059.60	1059.60	1059.62	1059.61	1059.61	1059.62	1059.63
Mode 24	1287.50	1287.53	1287.44	1287.42	1287.64	1287.65	1287.64	1287.64	1287.64	1287.59	1287.61	1287.65
Mode 25	1287.37	1287.40	1287.31	1287.29	1287.51	1287.52	1287.51	1287.51	1287.51	1287.46	1287.47	1287.52
Mode 26	1314.11	1314.70	1314.80	1314.78	1314.79	1315.37	1315.37	1315.36	1315.36	1315.42	1315.43	1315.56

Mode 27	1314.12	1314.71	1314.82	1314.80	1314.81	1315.38	1315.38	1315.38	1315.38	1315.44	1315.44	1315.58
Mode 28	1318.55	1318.53	1318.44	1318.41	1318.54	1318.54	1318.57	1318.57	1318.57	1318.52	1318.52	1318.89
Mode 29	1318.55	1318.53	1318.43	1318.40	1318.53	1318.54	1318.56	1318.56	1318.56	1318.51	1318.51	1318.88
Mode 30	1328.87	1328.89	1328.94	1328.87	1328.87	1329.40	1329.40	1329.40	1329.40	1329.14	1329.14	1329.48
Mode 31	1328.87	1328.89	1328.94	1328.87	1328.86	1329.39	1329.39	1329.39	1329.39	1329.13	1329.13	1329.47
Mode 32	1341.28	1341.28	1341.07	1341.08	1341.08	1341.08	1341.07	1341.07	1341.05	1340.94	1340.95	1341.35
Mode 33	1441.44	1441.58	1441.56	1441.56	1441.64	1441.63	1441.63	1441.63	1441.63	1441.62	1441.62	1441.76
Mode 34	1441.43	1441.57	1441.55	1441.55	1441.63	1441.63	1441.63	1441.63	1441.63	1441.62	1441.62	1441.75
Mode 35	1549.04	1549.03	1548.84	1548.85	1548.85	1548.85	1548.86	1548.86	1548.86	1548.72	1548.72	1548.67
Mode 36	1548.85	1548.84	1548.65	1548.65	1548.66	1548.66	1548.67	1548.67	1548.67	1548.52	1548.53	1548.48
Mode 37	1572.05	1572.06	1571.98	1571.92	1571.92	1571.90	1571.90	1571.90	1571.90	1571.85	1571.85	1572.06
Mode 38	1572.18	1572.19	1572.11	1572.06	1572.05	1572.03	1572.03	1572.03	1572.03	1571.98	1571.98	1572.19
Mode 39	2935.30	2935.30	2935.25	2935.22	2935.22	2935.19	2935.19	2935.19	2935.19	2935.10	2935.10	2935.10
Mode 40	2934.20	2934.20	2934.15	2934.13	2934.13	2934.10	2934.09	2934.09	2934.09	2934.01	2934.01	2934.00
Mode 41	2932.83	2932.84	2932.68	2932.66	2932.77	2932.77	2932.75	2932.75	2932.75	2932.74	2932.74	2932.73
Mode 42	2931.52	2931.53	2931.37	2931.35	2931.46	2931.46	2931.44	2931.44	2931.44	2931.43	2931.43	2931.42
Mode 43	2940.84	2940.95	2940.88	2940.88	2940.85	2940.83	2940.83	2940.83	2940.83	2940.79	2940.78	2940.80
Mode 44	2941.18	2941.28	2941.22	2941.21	2941.19	2941.17	2941.17	2941.17	2941.17	2941.13	2941.12	2941.14
Mode 45	2971.14	2971.21	2971.22	2971.21	2971.21	2971.21	2971.22	2971.22	2971.21	2971.20	2971.20	2971.22
Mode 46	2971.35	2971.41	2971.42	2971.41	2971.41	2971.41	2971.42	2971.42	2971.42	2971.41	2971.40	2971.42
Mode 47	3002.94	3002.95	3002.92	3002.91	3002.91	3002.98	3002.98	3003.00	3003.00	3002.98	3002.98	3003.03
Mode 48	3002.93	3002.94	3002.91	3002.90	3002.90	3002.97	3002.96	3002.99	3002.99	3002.97	3002.97	3003.01
ZPE	33941.5	33942.2	33942.1	33941.9	33942.2	33942.7	33942.7	33942.7	33942.7	33942.4	33942.4	33943.2

Table S47. Calculated B3LYP-D2/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 5.0 and 7.2 a_0 calculated using B3LYP/6-31G(d,p).

Cutoff (a_0)	5.00	5.20	5.40	5.60	5.80	6.00	6.20	6.40	6.60	6.80	7.00	7.20
Mode 1	428.89	428.89	428.89	428.89	428.89	428.89	428.89	428.89	428.89	428.89	428.89	428.89
Mode 2	428.90	428.89	428.90	428.89	428.89	428.89	428.89	428.89	428.89	428.89	428.89	428.89
Mode 3	464.12	464.12	464.12	464.11	464.12	464.12	464.11	464.11	464.11	464.11	464.11	464.11
Mode 4	465.82	465.83	465.83	465.82	465.82	465.82	465.82	465.82	465.82	465.82	465.82	465.82
Mode 5	510.03	510.03	510.03	510.03	510.03	510.03	510.02	510.02	510.02	510.02	510.02	510.02
Mode 6	510.05	510.05	510.05	510.05	510.05	510.05	510.04	510.04	510.04	510.04	510.04	510.04
Mode 7	544.81	544.80	544.80	544.80	544.80	544.80	544.80	544.80	544.80	544.80	544.80	544.80
Mode 8	580.17	580.17	580.17	580.17	580.17	580.17	580.17	580.17	580.17	580.17	580.17	580.17
Mode 9	581.32	581.32	581.32	581.32	581.32	581.32	581.30	581.30	581.28	581.28	581.28	581.28
Mode 10	587.74	587.74	587.74	587.75	587.75	587.75	587.74	587.75	587.74	587.74	587.75	587.75
Mode 11	587.78	587.78	587.78	587.78	587.78	587.78	587.78	587.78	587.78	587.78	587.78	587.78
Mode 12	776.10	776.07	776.07	776.08	776.08	776.08	776.08	776.08	776.08	776.08	776.08	776.08
Mode 13	778.13	778.10	778.10	778.11	778.11	778.11	778.11	778.11	778.11	778.11	778.11	778.11
Mode 14	789.58	789.58	789.57	789.53	789.53	789.53	789.53	789.53	789.53	789.53	789.53	789.53
Mode 15	790.15	790.15	790.14	790.11	790.10	790.10	790.11	790.10	790.10	790.10	790.10	790.10
Mode 16	813.19	813.19	813.19	813.18	813.18	813.18	813.31	813.31	813.31	813.31	813.31	813.31
Mode 17	813.19	813.19	813.19	813.18	813.18	813.18	813.31	813.32	813.32	813.32	813.32	813.32
Mode 18	827.97	827.97	827.96	827.96	827.96	827.96	827.96	827.97	827.97	827.97	827.97	827.97
Mode 19	843.69	843.69	843.69	843.69	843.69	843.69	843.69	843.69	843.69	843.69	843.69	843.69
Mode 20	880.75	880.75	880.75	880.75	880.74	880.74	880.74	880.74	880.74	880.74	880.74	880.74
Mode 21	888.96	888.96	888.96	888.96	888.95	888.95	888.96	888.96	888.96	888.96	888.96	888.96
Mode 22	1060.10	1060.09	1060.10	1060.09	1060.09	1060.09	1060.10	1060.10	1060.10	1060.10	1060.10	1060.10
Mode 23	1059.63	1059.63	1059.63	1059.63	1059.63	1059.63	1059.63	1059.64	1059.64	1059.64	1059.64	1059.64
Mode 24	1287.65	1287.65	1287.65	1287.65	1287.65	1287.65	1287.63	1287.63	1287.63	1287.63	1287.63	1287.63
Mode 25	1287.52	1287.52	1287.52	1287.52	1287.52	1287.52	1287.49	1287.50	1287.50	1287.50	1287.50	1287.50
Mode 26	1315.56	1315.56	1315.56	1315.56	1315.56	1315.56	1315.56	1315.56	1315.56	1315.56	1315.56	1315.56

Mode 27	1315.58	1315.58	1315.58	1315.57	1315.57	1315.57	1315.58	1315.58	1315.58	1315.58	1315.58	1315.58	1315.58
Mode 28	1318.89	1318.89	1318.88	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91
Mode 29	1318.89	1318.89	1318.88	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91	1318.91
Mode 30	1329.48	1329.47	1329.47	1329.47	1329.47	1329.47	1329.53	1329.55	1329.55	1329.55	1329.54	1329.54	1329.54
Mode 31	1329.47	1329.46	1329.46	1329.46	1329.46	1329.46	1329.52	1329.54	1329.54	1329.54	1329.53	1329.53	1329.53
Mode 32	1341.35	1341.34	1341.34	1341.42	1341.41	1341.41	1341.45	1341.44	1341.44	1341.44	1341.44	1341.44	1341.44
Mode 33	1441.76	1441.76	1441.76	1441.76	1441.76	1441.76	1441.84	1441.84	1441.84	1441.84	1441.84	1441.84	1441.84
Mode 34	1441.75	1441.75	1441.75	1441.75	1441.75	1441.75	1441.83	1441.83	1441.83	1441.83	1441.83	1441.83	1441.83
Mode 35	1548.67	1548.66	1548.65	1548.66	1548.67	1548.67	1548.86	1548.86	1548.86	1548.87	1548.86	1548.86	1548.86
Mode 36	1548.48	1548.46	1548.46	1548.47	1548.47	1548.47	1548.67	1548.67	1548.67	1548.67	1548.67	1548.67	1548.67
Mode 37	1572.06	1572.06	1572.06	1572.06	1572.06	1572.06	1572.05	1572.06	1572.06	1572.06	1572.06	1572.06	1572.06
Mode 38	1572.19	1572.19	1572.19	1572.19	1572.19	1572.19	1572.18	1572.19	1572.19	1572.19	1572.19	1572.19	1572.19
Mode 39	2935.10	2935.09	2935.10	2935.10	2934.00	2934.00	2934.00	2934.00	2934.00	2934.00	2934.00	2934.00	2934.00
Mode 40	2934.00	2934.00	2934.00	2934.00	2935.10	2935.10	2935.10	2935.10	2935.10	2935.10	2935.10	2935.10	2935.10
Mode 41	2932.73	2932.73	2932.72	2932.72	2931.41	2931.41	2931.42	2931.42	2931.42	2931.42	2931.42	2931.42	2931.42
Mode 42	2931.42	2931.42	2931.41	2931.41	2932.72	2932.72	2932.73	2932.73	2932.73	2932.73	2932.73	2932.73	2932.73
Mode 43	2940.80	2940.80	2940.80	2940.81	2941.14	2941.14	2941.14	2941.14	2941.14	2941.14	2941.14	2941.14	2941.14
Mode 44	2941.14	2941.14	2941.14	2941.14	2940.80	2940.80	2940.80	2940.80	2940.80	2940.80	2940.80	2940.80	2940.80
Mode 45	2971.22	2971.21	2971.21	2971.20	2971.40	2971.40	2971.40	2971.41	2971.41	2971.41	2971.41	2971.41	2971.41
Mode 46	2971.42	2971.42	2971.42	2971.41	2971.20	2971.20	2971.20	2971.21	2971.21	2971.21	2971.21	2971.21	2971.21
Mode 47	3003.02	3003.02	3003.02	3003.10	3003.09	3003.08	3003.08	3003.09	3003.09	3003.09	3003.09	3003.07	3003.07
Mode 48	3003.01	3003.01	3003.01	3003.09	3003.10	3003.09	3003.09	3003.10	3003.10	3003.10	3003.08	3003.08	3003.08
ZPE	33943.2	33943.2	33943.2	33943.2	33943.2	33943.2	33943.4	33943.4	33943.4	33943.4	33943.4	33943.4	33943.4

Table S48. Calculated B3LYP-D2/6-31G(d,p) L-VSCF frequencies (in cm^{-1}) for octatetraene with couplings between modes centered beyond cutoff distance between 7.4 and 8.0 a_0 calculated using B3LYP/6-31G(d,p), and finally the full 2MR result.

Cutoff (a_0)	7.40	7.60	7.80	8.00	2MR
Mode 1	428.89	428.89	428.89	428.89	428.90
Mode 2	428.90	428.90	428.90	428.90	428.89
Mode 3	464.11	464.11	464.11	464.11	464.11
Mode 4	465.82	465.82	465.82	465.82	465.82
Mode 5	510.02	510.02	510.02	510.02	510.04
Mode 6	510.04	510.04	510.04	510.04	510.01
Mode 7	544.80	544.80	544.80	544.80	544.80
Mode 8	580.17	580.17	580.17	580.17	580.17
Mode 9	581.28	581.28	581.28	581.28	581.28
Mode 10	587.75	587.75	587.75	587.75	587.75
Mode 11	587.78	587.78	587.78	587.78	587.78
Mode 12	776.08	776.08	776.08	776.08	776.08
Mode 13	778.11	778.11	778.11	778.11	778.10
Mode 14	789.53	789.53	789.53	789.53	789.53
Mode 15	790.10	790.10	790.10	790.10	790.10
Mode 16	813.31	813.31	813.31	813.31	813.31
Mode 17	813.32	813.32	813.32	813.32	813.31
Mode 18	827.97	827.97	827.97	827.97	827.97
Mode 19	843.69	843.69	843.69	843.69	843.69
Mode 20	880.74	880.74	880.74	880.74	880.74
Mode 21	888.96	888.96	888.96	888.96	888.96
Mode 22	1060.10	1060.10	1060.10	1060.10	1059.64
Mode 23	1059.64	1059.64	1059.64	1059.64	1060.10
Mode 24	1287.64	1287.64	1287.64	1287.64	1287.64
Mode 25	1287.50	1287.50	1287.50	1287.50	1287.50
Mode 26	1315.57	1315.57	1315.57	1315.57	1315.58

Mode 27	1315.58	1315.58	1315.58	1315.58	1315.59
Mode 28	1318.91	1318.91	1318.91	1318.91	1318.90
Mode 29	1318.90	1318.90	1318.90	1318.90	1318.89
Mode 30	1329.54	1329.54	1329.54	1329.54	1329.54
Mode 31	1329.53	1329.53	1329.53	1329.53	1329.54
Mode 32	1341.42	1341.42	1341.42	1341.42	1341.42
Mode 33	1441.83	1441.83	1441.83	1441.83	1441.83
Mode 34	1441.83	1441.83	1441.83	1441.83	1441.83
Mode 35	1548.86	1548.86	1548.86	1548.86	1548.85
Mode 36	1548.67	1548.67	1548.67	1548.67	1548.66
Mode 37	1572.06	1572.06	1572.06	1572.06	1572.06
Mode 38	1572.19	1572.19	1572.19	1572.19	1572.19
Mode 39	2934.00	2934.00	2934.00	2934.00	2934.00
Mode 40	2935.10	2935.10	2935.10	2935.10	2935.09
Mode 41	2931.42	2931.42	2931.42	2931.42	2931.42
Mode 42	2932.73	2932.73	2932.73	2932.73	2932.73
Mode 43	2941.14	2941.14	2941.14	2941.14	2941.13
Mode 44	2940.80	2940.80	2940.80	2940.80	2940.79
Mode 45	2971.41	2971.41	2971.41	2971.41	2971.41
Mode 46	2971.21	2971.21	2971.21	2971.21	2971.21
Mode 47	3003.07	3003.07	3003.07	3003.07	3003.07
Mode 48	3003.08	3003.08	3003.08	3003.08	3003.08
ZPE	33943.4	33943.4	33943.4	33943.4	33943.4

Table S49. The numbers of localized mode pairs that have centres located beyond the given cutoff distances for a representative subset of the theories tested.

Cutoff (a_0)	HF	RI-MP2	B3LYP-D2
0.20	1048	1039	1040
0.40	1007	1023	1019
0.60	957	969	957
0.80	919	926	930
1.00	896	900	908
1.20	835	842	834
1.40	797	792	793
1.60	740	745	736
1.80	694	720	702
2.00	664	672	670
2.20	597	619	607
2.40	580	590	584
2.60	550	550	550
2.80	512	512	516
3.00	500	488	500
3.20	466	458	470
3.40	440	410	412
3.60	372	358	366
3.80	338	342	346
4.00	332	328	330
4.20	314	306	310
4.40	284	282	286
4.60	276	256	268
4.80	226	222	214
5.00	208	206	206
5.20	182	186	182
5.40	156	162	154

5.60	130	132	130
5.80	102	104	99
6.00	90	90	86
6.20	66	76	70
6.40	58	60	60
6.60	56	60	56
6.80	32	44	44
7.00	14	16	16
7.20	10	16	12
7.40	6	8	6
7.60	6	6	6
7.80	6	6	6
8.00	2	2	2