Supporting Information to "Fermi Resonance Effects in the Vibrational Spectroscopy of Methyl and Methoxy Groups"

Edwin L. Sibert III,[†] Daniel P. Tabor,[†] Nathanael M. Kidwell,[‡] Jacob C. Dean,[‡] and Timothy S. Zwier*,[‡]

Department of Chemistry and Theoretical Chemistry Institute University of Wisconsin-Madison, Madison, Wisconsin 53706 U.S.A., and Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084 U.S.A.

E-mail: sibert@chem.wisc.edu

*To whom correspondence should be addressed

[†]Department of Chemistry and Theoretical Chemistry Institute University of Wisconsin-Madison, Madison, Wisconsin 53706 U.S.A.

[‡]Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084 U.S.A.

Table 1: B3LYP/6-311+G(d,p) optimized geometry for DPE in angstroms

Atom	x	y	z
C	-0.82654	0.86930	-0.83458
C	-0.82654	0.86930	0.69424
C	0.36686	0.86930	1.42559
C	0.35141	0.92113	2.81741
C	-0.86027	0.96966	3.50641
C	-2.05514	0.96575	2.79068
C	-2.03463	0.91614	1.39700
H	-2.97138	0.91258	0.84772
H	-3.00408	0.99780	3.31489
H	-0.87183	1.00531	4.58996
H	1.28726	0.91741	3.36564
H	1.31600	0.81503	0.90342
C	0.11134	-0.18909	-1.41275
C	-0.25180	-1.53970	-1.31608
C	0.56870	-2.54522	-1.81637
C	1.78079	-2.22073	-2.42734
C	2.15454	-0.88474	-2.53269
C	1.32547	0.12143	-2.03140
H	1.63544	1.15436	-2.13421
H	3.09181	-0.61848	-3.00918
H	2.42256	-3.00179	-2.81916
H	0.26303	-3.58234	-1.73160
H	-1.18998	-1.80332	-0.83767
C	-0.58049	2.29252	-1.36957
H	-1.83830	0.58417	-1.14465
H	-1.35095	2.96878	-0.99245
H	0.38506	2.68644	-1.04219
H	-0.60990	2.31372	-2.46247

Table 2: B3LYP/6-311+G(d,p) Unscaled CH stretch frequencies and intensities for DPE

Frequency (cm^{-1})	Intensity (km/mol)
3017.07	11.77
3027.87	23.05
3094.47	30.08
3098.45	26.63

Table 3: B3LYP/6-311+G(d,p) optimized geometry for DPP in angstroms

Atom	x	y	z
C	-0.17467	-1.13336	-0.70662
C	-0.17467	-1.13336	0.82218
C	1.05147	-1.13336	1.50058
C	1.10824	-1.11454	2.89080
C	-0.06894	-1.09315	3.63901
C	-1.29499	-1.09470	2.98029
C	-1.34647	-1.11637	1.58533
H	-2.31419	-1.12729	1.09814
H	-2.21785	-1.08307	3.55017
H	-0.02906	-1.07939	4.72239
H	2.07065	-1.11853	3.39089
H	1.97389	-1.14553	0.92829
C	0.12219	0.25970	-1.26232
C	1.20304	0.46672	-2.12447
C	1.47203	1.72957	-2.65334
C	0.65840	2.81088	-2.32622
C	-0.42253	2.61889	-1.46522
C	-0.68488	1.35729	-0.93819
H	-1.51862	1.22897	-0.25630
H	-1.05905	3.45572	-1.19892
H	0.86460	3.79418	-2.73375
H	2.31710	1.86566	-3.31945
H	1.84249	-0.37005	-2.38759
C	-1.45209	-1.74223	-1.33017
H	-1.66907	-2.68563	-0.81773
H	-2.30538	-1.08207	-1.14278
C	-1.33550	-1.99614	-2.83546
H	-2.25344	-2.44530	-3.22399
H	-1.15654	-1.07032	-3.38756
H	-0.51169	-2.68198	-3.05805
H	0.66007	-1.77469	-1.01322

Table 4: B3LYP/6-311+G(d,p) Unscaled CH stretch frequencies and intensities for DPP

Frequency (cm^{-1})	Intensity (km/mol)
3011.32	6.96
3020.85	17.05
3022.34	43.22
3053.43	17.29
3082.65	38.95
3095.87	39.00

Table 5: B3LYP/6-311+G(d,p) optimized geometry for guaiacol in angstroms

Atom	x	y	z
C	-1.44932	0.00022	-2.49275
O	-1.44932	0.00022	-1.07057
C	-0.24220	0.00022	-0.41312
C	1.01333	0.00061	-1.01010
C	2.16046	0.00046	-0.20885
C	2.04478	-0.00007	1.17640
C	0.78376	-0.00044	1.77649
C	-0.35889	-0.00031	0.98923
O	-1.59051	-0.00075	1.57390
H	-2.25181	-0.00087	0.86883
H	1.10994	0.00101	-2.08802
H	3.13697	0.00075	-0.67813
H	2.93239	-0.00021	1.79792
H	0.67042	-0.00088	2.85401
H	-0.95605	-0.89422	-2.88687
H	-2.49559	-0.00024	-2.79360
H	-0.95685	0.89509	-2.88689

Table 6: B3LYP/6-311+G(d,p) Unscaled CH stretch frequencies and intensities for guaiacol

Frequency (cm^{-1})	Intensity (km/mol)
3010.26	51.01
3071.03	33.67
3135.94	19.02

Table 7: B3LYP/6-311+G(d,p) optimized geometry for syringol in angstroms

Atom	x	y	z
C	-1.90925	0.00068	-3.07900
O	-1.90925	0.00068	-1.65708
C	-0.70145	0.00068	-0.99884
C	0.55416	0.00143	-1.60533
C	1.68834	0.00121	-0.79667
C	1.57994	0.00021	0.59228
C	0.31873	-0.00059	1.19796
C	-0.83092	-0.00027	0.39530
O	-2.06054	-0.00100	0.97942
H	-2.71443	-0.00075	0.26740
H	0.65255	0.00215	-2.68217
H	2.67028	0.00179	-1.25437
H	2.47561	0.00006	1.19767
O	0.09622	-0.00173	2.54120
C	1.21862	-0.00316	3.41027
H	-1.41676	-0.89386	-3.47366
H	-2.95580	0.00056	-3.37922
H	-1.41700	0.89532	-3.47373
H	1.83598	0.89117	3.27024
H	0.81013	-0.00436	4.41959
H	1.83549	-0.89744	3.26787

Table 8: B3LYP/6-311+G(d,p) Unscaled CH stretch frequencies and intensities for syringol

Frequency (cm^{-1})	Intensity (km/mol)
3000.98	61.71
3010.68	53.63
3058.26	40.30
3071.44	33.87
3131.78	22.16
3134.72	20.01