

New Insights in the Vibrational and Optical Signatures of Trans-Stilbene from Integrated
Experimental and Quantum Mechanical Approaches
Supplementary Information

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Experimental		B3LYP/m-aug-cc-pvtz			B2PLYP/m-aug-cc-pvtz		Symmetry	Assignment ¹
Arenas et al. ²	Ünsalan et al. ³	v(harm) (cm ⁻¹)	v(anharm) (cm ⁻¹)	Δ(Harm- Anh) _{B3LYP} (cm ⁻¹)	v(harm) (cm ⁻¹)	v _{calc} (Anh)= v(harm)-Δ (cm ⁻¹)		st:stretching ipb: in-plane bending opb: out-of-plane bending
410	n.o.	413.4	410.5	2.9	409.9	407.0	A _u	antisym torsion
419	467.2	474.8	462.5	12.3	471.3	459.0	B _u	C-X ipb
528	528.3	544.3	536.6	7.7	540.5	532.8	A _u	C-X opb
541	541.4	552.6	546.6	6	550.1	544.1	B _u	anti sym def
620	n.o.	637.6	632.0	5.6	634.2	628.6	B _u	anti sym def
692	689.5	708.4	701.9	6.5	703.7	697.2	A _u	puckering
764	763.7	788.0	774.7	13.3	779.6	766.3	A _u	puckering, ring CH opb
824	812.9	835.0	814.1	20.9	835.4	814.5	B _u	ring C-C st
847	833.5	853.8	841.9	11.9	853.7	841.8	A _u	ring CH opb
909	904.6	933.1	918.8	14.3	925.6	911.3	A _u	ring CH opb
966	n.o.	993.7	979.4	14.3	986.5	972.2	A _u	ring CH opb
971	961.5	997.7	985.0	12.7	992.1	979.4	A _u	C-X torsion, CH wag
984	981.3	1016.8	1001.0	15.8	1006.7	990.9	A _u	ring CH opb, C-X torsion
1001	988.4	1018.6	1002.1	16.5	1018.6	1002.1	B _u	ring trigonal def
1028	1034.2	1051.9	1038.7	13.2	1052.8	1039.6	B _u	ring C-C st
1071	1072.6	1103.4	1082.2	21.2	1103.4	1082.2	B _u	ring C-C st, CH ipb
1155	1158.5	1181.8	1173.0	8.8	1183.7	1174.9	B _u	ring CH ipb, ring C-C st
1182	1181.2	1204.7	1186.7	18	1206.2	1188.2	B _u	ring CH ipb
1220	1222.7	1251.3	1227.8	23.5	1255.4	1231.9	B _u	CH rock, C-C st
1264	1265.1	1290.3	1264.7	25.6	1301.0	1275.4	B _u	C-X st, ring C-C st
1300	1327.5	1356.9	1318.4	38.5	1369.5	1331.0	B _u	C-H rock, ring C-C st, CdbdC st
1332	1340.5	1374.7	1351.2	23.5	1380.8	1357.3	B _u	ring C-C st, ring C-H ipb
1450	1455.6	1487.8	1464.0	23.8	1488.4	1464.6	B _u	CH ipb, ring C-C st
1494	1501.9	1534.4	1501.9	32.5	1536.4	1503.9	B _u	ring, CH ipb
1577	1584.3	1616.7	1577.7	39	1621.5	1582.5	B _u	ring C-C st
1597	1605.0	1643.5	1599.9	43.6	1646.4	1602.8	B _u	ring C-C st
3020	n.o.	3144.4	3042.6	101.8	3165.4	3063.6	B _u	C-H st
3031	3037.7	3156.5	3018.6	137.9	3178.6	3040.7	B _u	ring C-H st
3056	n.o.	3164.0	3034.1	129.9	3186.8	3056.9	B _u	ring C-H st
n.o.	3069.5	3173.3	3052.3	121	3196.4	3075.4	B _u	ring C-H st
3076	3089.5	3190.2	3060.6	129.6	3213.5	3083.9	B _u	ring C-H st
3095	3109.0	3183.0	3069.9	113.1	3205.4	3092.3	B _u	ring C-H st
MAE		36.9	11.3		40.4	7.7		
MAE		41.3	12.1		44.5	10.8		

Table 1. Observed and calculated Vibrational frequencies of Trans-Stilbene.

1 C. H. Choi and M. Kertesz, *J. Phys. Chem. A*, 1997, **101**, 3823–3831.

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