

Supplementary Information

Table: S1 Calculated vibrational wave numbers, measured infrared and Raman band positions (cm^{-1}) and assignments for S-Phenylsuccinic acid

B3LYP/6311G(d,p) ν_{cal}	ν_{IR}	ν_{Raman}	Assignments
3556			O ₁₇ -H ₁₈ stretch
3548			O ₂₃ -H ₂₄ stretch
3068		3067 s	2 arom. C-H stretch & O-H stretch
3053		3050 sh	7a arom. C-H stretch & O-H stretch
3031	3032 m	3026 vvw	20b arom. C-H stretch & O-H stretch
2947	2964 w	2956 s	CH ₂ asym. stretch
2910	2925 m	2929 s	CH ₂ sym. stretch
	2745 w		Fermiresonance
	2643 w		Combination/ Overtone
	1961 vw		Combination/ Overtone
1788	1697 vvsbr		C ₁₃ =O ₁₆ & C ₂₁ =O ₂₂ stretch
1785		1666 mbr	C ₁₃ =O ₁₆ & C ₂₁ =O ₂₂ stretch
1605	1600 m	1607 s	8a ring stretch

1584	1584 m	1590 vvw	8b ring stretch
1492	1497 m		19a ring stretch
1448	1456 vw	1465 w	19b ring stretch
1438		1442 m	CH ₂ scissoring
	1420 s	1425 w	C-O-H deformation i.p bend
	1403 sh	1410 m	C-O-H deformation i.p bend
1361		1370 vvw	14 C-H i.p bend
1311	1307 vs	1309 w	C-O stretch
1277	1274 m	1280 w	CH ₂ wagging
1264		1256 w	3 C-H i.p bend
1235	1245 w		C ₇ -H ₁₄ i.p bend + CH ₂ twisting
1201	1207 s	1207 vvw	C ₇ -H ₁₄ i.p bend + CH ₂ twisting
1180	1189 m	1184 s	9a C-H i.p bend
1176	1173 sh	1165 m	15 C-H i.p bend
1078	1071 w	1078 vw	18b C-H i.p bend
1024	1029 w	1030 m	1 ring breath
1008	1005 m	1012 vs	12 ring i.p bend
982		983 vvw	17a C-H o.p bend
959		957 m	CH ₂ rocking
926	916 sh	906 w	C-H o.p bend + O-H...O o.p wag

885	870 w		17b C-H o.p bend
868	856 m	857 m	10b C-H o.p bend
814	820 w	822 m	C-H o.p bend
779	762 s	766 m	10a C-H o.p bend
724	726 s	732 m	11 C-H o.p bend
689	701 sh	696 vvw	4 ring o.p bend
675	694 m		O-H o.p bend bend
639	647 sh		O-H o.p bend bend
616	618 m	620 vvw	6b ring o.p bend
609	606 w	596 vw	Ring puckering
514	511 w	519 vvw	6a ring o.p bend
508	496 s	500 vvw	16 b ring o.p bend
390		387 vvw	16a ring o.p bend
334		328 vvw	9b C-H i.p bend
274		267 vvw	Hydrogen bonded vibrations
184		171 vs	Hydrogen bonded vibrations
112		120 vvs	Hydrogen bonded vibrations
64		57 sh	Hydrogen bonded vibrations