

Supporting Information

Table S1: Calculated harmonic frequencies^a (cm⁻¹) of the glycine conformers

	I	II	III	IV	V
1	54 ^b	79 ^b	50 ^b	96 ^b	75 ^b
2	239 ^b	274 ^b	268	220 ^b	251 ^b
3	260	321	293 ^b	288	292
4	470	509	469	464	451
5	495 ^b	549	536	521 ^b	550
6	625	655	608 ^b	624	594 ^b
7	641	848	686	668	707
8	844	865 ^b	828	858	845
9	927	910	918	869	867
10	951	960	936	1041	1035
11	1144	1098	1154	1126	1095
12	1188	1169	1165	1157	1151
13	1191	1239	1224	1229	1244
14	1317	1336	1355	1292	1312
15	1401	1380	1382	1338	1360
16	1419	1435	1406	1469	1448
17	1475	1484	1479	1513	1512
18	1679	1659	1673	1645	1653
19	1821	1844	1816	1827	1829
20	3100	3104	3095	3024	3021
21	3152	3164	3168	3146	3172
22	3554	3546	3556	3552	3552
23	3644	3572	3650	3654	3651
24	3804	3664	3803	3804	3807

^aFrequencies calculated at the MP2/6-311++G** level of theory.

^bTorsional vibrations determined by visualization of the normal modes.