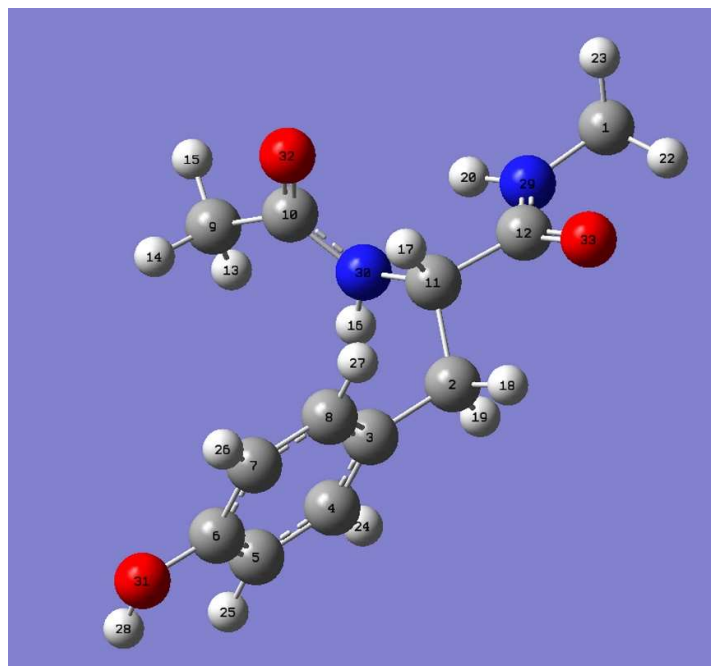


Supplementary Table S2. Comparison of observed bands of polycrystalline powder of N-acetyl-tyrosine-methyl-amide and vibrations calculated using Gaussian1, scaled by factor 0.9497 (see text).



Raman	infrared	calculated scaled	mode description
3353 m	3309 m	3635	v(OH)
3337 m			
3229 vw	3219 m,br	3457	v(N29-H20)
3209 vw	3182 m	3434	v(N30-H16)
	3114 m,sh		
3067 ms	3065 m	3050	v(CH) benzene
3049 ms			
3035 m		3021	v(CH) benzene
3015 s	3018 m	3017,3001,2999	v(CH) benzene
2974 s		2987,2968	v(CH ₃), v(CH ₃)
2943 s	2938 mw	2951, 2950.9	v(CH ₂), v(CH ₃)
2928 s		2931	v(CH)
2906 m,sh	2904 mw		
	2898 w	2900	v(CH ₃) symmetric
2870 m		2885,2880	v(CH ₃) symm., v(CH ₂) symmetric
2802 w			
1664 w	1649 s,br	1672	v(C10=O32)
1655 w		1655	v(C12=O33)

Table S2. continued.

Raman	infrared	calculated scaled	mode description
1615 m	1614 ms		
1600 m	1599 ms	1580	benzene ring stretching
1556 vw	1549 m,sh	1555	benzene ring stretching
1532 vw	1533 s,br	1485	$\nu(\text{C12-N29})$
1514 vw	1512 s,br	1474	$\varphi(\text{CH})$ benzene
1462 w,sh		1445	$\delta(\text{N30-H16})$
1450 w	1457 ms, 1446 ms	1434,1419,1415	$\delta(\text{CH}_3)$, $\delta(\text{CH}_3)$, $\delta(\text{CH}_2)$
1411 w	1410 ms	1414,1400,1396	$\delta(\text{CH}_3)$, $\delta(\text{CH}_3)$, $\delta(\text{C-OH})$
1379 vw,br	1371 ms	1375	$\delta(\text{CH}_3)$ symmetric bending
1336 m	1337 m	1333	$\delta(\text{CH}_3)$ symmetric bending
1306 m	1307 m	1307	$\delta(\text{C11-H17})$
1283 mw	1282 m	1301,1296	$\varphi(\text{CH})$ benzene
1257 mw	1268 m	1266	$\delta(\text{CH}_2)$ bending
1249 w	1247s	1230	$\delta(\text{C11-H17}) + \delta(\text{CH}_2)$
1237 1211 m	1235	1223,1206	$\varphi(\text{CH})$ benzene, $\nu(\text{C10-N30})$
1186 w	1183 ms	1197	$\nu(\text{C12-N29})$
1176 w	1174 ms	1165	benzene ring + $\delta(\text{CH}_2)$
1158 w	1155 ms	1150,1138	$\delta(\text{CH}_2)$ twisting, $\varphi(\text{CH})$ benzene
1121 w	1120 m	1124,1120	$\delta(\text{COH})$, $\delta(\text{CH}_3)$ rocking
1108 w	1107 m	1088	$\delta(\text{CH}_3)$ twisting
1078 vw	1078 m	1075,1065	$\varphi(\text{CH})$ benzene
1033 m	1034 m,br	1043	$\nu(\text{C11-N30}) + \nu(\text{C11-C12})$
	1012 m	1002,994	$\delta(\text{CH}_3)$, $\delta(\text{CH}_2) + \delta(\text{CH})$
	1004 m	976	benzene ring str.
956 m	955 m	958	$\delta(\text{CH}_3)$ rocking
943 w	943 m	925	$\gamma(\text{CH})$ benzene
912 m	914 w	905	$\delta(\text{O32=C10-N30}) + \gamma(\text{CH})$
871 w	872 mw	892	$\gamma(\text{CH})$ benzene
854 m	854 m	863	$\nu(\text{C11-C12})$
844 m	839 ms		
834 m		835	$\gamma(\text{CH})$ benzene+ $\delta(\text{CH}_2)$ rock.
825 m	826 ms	814	$\nu(\text{C-C})$ benzene
809 m	806 s	799	$\gamma(\text{CH})$ benzene
733 w	751 m,br	777	$\gamma(\text{CH})$ benzene
722 w	727 m	769	$\gamma(\text{C12=O33})$
	719 ms	702	$\nu(\text{C2-C3})$
669 w,br	671 w	685	$\delta(\text{CCCC})$ benzene
644 m			
637 w,sh	625 ms, br	633, 622	$\tau(\text{C10-N30})$, benzene ring

580 w	581 ms	605, 593	$\delta(\text{O32}=\text{C10-N30}), \gamma(\text{N-H})$
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Table S2. continued

Raman	infrared	calculated scaled	mode description
541 w	561 m,sh	551	$\gamma(\text{N30-C11})$
533 w	530 s,br	511,501	$\delta(\text{C-C-C})$ benzene
494 mw	491 s	472	torsion benzene
453 w		450	$\gamma(\text{NH})$
438 w		413,403	$\delta(\text{C2-C3-C4})$
384 mw		399	$\tau(\text{C2-C3})$
347 m		353	$\delta(\text{N30-C10-C9})$
338 mw		324	$\tau(\text{C11-N30})$
316 m		308	$\gamma(\text{OH})$
297 vw		302, 298	$\tau(\text{C2-C11})$, skeletal
264 w		240	$\delta(\text{C12-N29-C1})$
216 mw,sh			
203 mw,sh			
196 m		185, 177	skeletal
153 m		148	skeletal
137 ms		118	skeletal
103 vs			
83 s		86	$\tau(\text{CH}_3)$
63 vs		66,61	skeletal, $\tau(\text{CH}_3)$
55 vs			
48 s,sh		48	$\tau(\text{C10-N30})$
41 vs		41	$\tau(\text{CH}_3)$
30 vs		32	skeletal
20 vs		22	$\tau(\text{C2-C3})$
		17	skeletal

abbreviations: v – stretching, δ – bending, γ – out of plane bending, τ – torsion, ϕ – in plane bending, vs -very strong, s – strong, ms – medium strong, m – medium, w – weak, sh - shoulder