

Supp. Table 1. Comparison of experimental values and calculated frequencies for GTP bound to the Ras protein.

Normal Modes	Exp.	Pre. Cal.	Aver.	S1	S2	S3	S4	S5	S6
$u_a(\text{PO}_2)_\alpha$	1263	1259	1268	1266	1260	1281	1268	1266	1268
$u_a(\text{PO}_2)_\beta$	1219	1192	1222	1215	1230	1212	1221	1233	1223
$u_a(\text{PO}_3)_\gamma$	1157	1182	1210	1209	1203	1200	1216	1217	1215
$u_a(\text{PO}_3)_\nu$	1143	1106	1138	1133	1143	1143	1134	1132	1146
$u_s(\text{PO}_2)_\beta$	1124	1063	1107	1111	1101	1107	1109	1110	1107
$u_s(\text{PO}_2)_\alpha$	1090	1048	1070	1070	1064	1072	1073	1075	1072
$u_s(\text{PO}_3)_\nu$	953	973	980	977	978	985	977	974	990
$u_s(\text{OP}_\beta\text{O})$	895	886	942	936	942	954	938	927	955
$u_a(\text{OP}_\beta\text{O})$	878	840	877	878	875	880	879	856	895
$u_s(\text{PO})_\alpha$			789	787	791	767	785	799	805
$u_s(\text{P}_\beta\text{OP}_\alpha)$			707	706	706	700	710	707	713
u_{b1}			672	671	670	673	671	675	672
u_{b2}			578	580	580	578	577	583	570
u_{b3}			564	570	568	568	568	563	551
u_{b4}			550	557	552	546	548	553	545
Aver.Devi.		28.1	20.9	18.5	19.3	21.7	19.4	21.3	25.4

The first column lists all the possible normal vibration modes. The first nine vibrations are beyond 800 cm^{-1} and the last six are below 800 cm^{-1} , obtained from calculations. The second column shows experimental values (Exp.) obtained from previous studies.^{30,32,33} The third column displays previously calculated results (Pre. Cal.).⁴¹ The fourth column presents our calculated average results (Aver.) based on six different snapshots (S1~S6) at 2.0, 2.1, 2.5, 3.0, 10.0 and 100 ps timepoints. The average absolute deviations (Aver. Devi.) relative to available experimental data have been estimated, as shown in the last row. The units of all values are cm^{-1} .