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Supplementary Table 1: Approximate Center Frequencies of the Rotational Transitions of $^{15}N^{1}$-Alaninamide-Water.

transition	obs. frequency / MHz	obs. - calc. / MHz
$3_{13} - 2_{12}$	6825.000	0.054
$3_{03} - 2_{02}$	7046.700	-0.003
$3_{12} - 2_{11}$	7304.722	-0.048
$4_{14} - 3_{13}$	9093.895	-0.002
$4_{04} - 3_{03}$	9370.785	0.031
$4_{13} - 3_{12}$	9733.184	0.051
$5_{15} - 4_{14}$	11357.971	-0.039
$5_{05} - 4_{04}$	11674.345	-0.008
$5_{14} - 4_{13}$	12155.507	-0.019

Supplementary Table 2: Approximate Center Frequencies of the Rotational Transitions of $^{15}N^2$-Alaninamide-Water.

transition	obs. frequency / MHz	obs. - calc. / MHz
$3_{13} - 2_{12}$	6888.250	0.009
$3_{03} - 2_{02}$	7113.410	0.029
$3_{12} - 2_{11}$	7376.250	0.012
$4_{14} - 3_{13}$	9178.058	-0.004
$4_{04} - 3_{03}$	9458.730	0.026
$4_{13} - 3_{12}$	9828.200	0.037
$5_{15} - 4_{14}$	11462.849	-0.018
$5_{05} - 4_{04}$	11782.820	-0.007
$5_{14} - 4_{13}$	12273.820	-0.052

Supplementary Table 3: Frequencies of the Rotational Transitions of $^{15}N^1$, $^{15}N^2$-Alaninamide-Water.

transition	obs. frequency / MHz	obs. - calc. / MHz
$3_{13} - 2_{12}$	6807.830	0.002
$3_{03} - 2_{02}$	7031.995	0.007
$3_{12} - 2_{11}$	7294.000	0.001
$4_{14} - 3_{13}$	9070.798	-0.001
$4_{04} - 3_{03}$	9350.068	-0.002
$4_{13} - 3_{12}$	9718.448	-0.011
$5_{15} - 4_{14}$	11328.720	-0.002
$5_{05} - 4_{04}$	11646.873	-0.001
$5_{14} - 4_{13}$	12136.663	0.007