

## Electronic Supplementary Information

for

# The shape of D-glucosamine

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**Table S1.** Measured rotational transitions (in MHz) assigned to conformer  $\alpha$ -G-g/cc/t using CP-FTMW spectroscopy.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$\nu_{\text{obs}}$	$\nu_{\text{obs}} - \nu_{\text{cal}}$
5	0	5	4	1	4	6088.345	0.004
5	1	5	4	1	4	6126.814	0.040
5	2	4	4	2	3	6679.013	0.011
6	0	6	5	1	5	7280.228	-0.004
6	1	6	5	1	5	7295.506	0.051
6	0	6	5	0	5	7318.660	-0.003
6	1	6	5	0	5	7333.884	-0.002
7	0	7	6	1	6	8450.718	0.010
7	1	7	6	1	6	8456.507	0.052
7	0	7	6	0	6	8465.941	0.011
7	1	7	6	0	6	8471.655	-0.022
4	3	1	3	2	2	8553.878	0.008
6	2	4	5	2	3	8724.034	0.017
7	1	6	6	2	5	8990.076	0.006
7	2	6	6	2	5	9146.439	0.014
4	4	0	3	3	1	9578.099	-0.002
7	3	5	6	3	4	9597.705	-0.031
8	0	8	7	1	7	9611.657	-0.013
8	0	8	7	0	7	9617.444	0.028
8	1	8	7	0	7	9619.535	0.021
7	2	5	6	2	4	10075.498	-0.053
8	1	7	7	2	6	10267.183	-0.006
8	2	7	7	2	6	10337.607	0.008
9	0	9	8	1	8	10768.752	-0.004
9	1	9	8	1	8	10769.484	-0.018
9	0	9	8	0	8	10770.829	-0.024
9	1	9	8	0	8	10771.591	-0.007
8	3	6	7	3	5	10893.323	0.009
9	1	8	8	2	7	11481.371	-0.004
9	2	8	8	2	7	11511.103	-0.008
9	2	8	8	1	7	11581.477	-0.045

**Table S2.** Measured rotational transitions (in MHz) assigned to conformer  $\alpha$ -G+g/cc/t using CP-FTMW spectroscopy.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$\nu_{\text{obs}}$	$\nu_{\text{obs}} - \nu_{\text{cal}}$
5	2	4	4	2	3	6328.266	0.017
5	3	3	4	3	2	6577.787	0.064
6	0	6	5	1	5	6769.014	0.003
6	1	6	5	1	5	6785.799	0.045
6	0	6	5	0	5	6811.457	0.032
6	1	6	5	0	5	6828.174	0.004
5	2	3	4	2	2	7009.604	-0.008
6	2	5	5	2	4	7497.333	0.051
7	0	7	6	1	6	7848.754	0.003
7	1	7	6	1	6	7855.079	0.028
7	1	7	6	0	6	7871.843	0.048
6	3	4	5	3	3	7874.877	-0.033
6	2	4	5	2	3	8390.817	0.007
7	1	6	6	2	5	8457.100	-0.005
7	2	6	6	2	5	8629.428	0.030
8	0	8	7	1	7	8917.972	0.014
8	1	8	7	1	7	8920.234	-0.016
8	0	8	7	0	7	8924.252	-0.007
8	1	8	7	0	7	8926.555	0.005

7	3	5	6	3	4	9137.467	0.013
7	4	4	6	4	3	9282.154	-0.003
8	1	7	7	2	6	9654.960	0.017
7	2	5	6	2	4	9672.504	-0.051
8	2	7	7	2	6	9732.253	0.002
4	4	1	3	3	0	9786.838	-0.002
4	4	0	3	3	1	9797.798	0.000
9	0	9	8	1	8	9982.884	-0.007
9	1	9	8	1	8	9983.682	-0.021
9	0	9	8	0	8	9985.183	0.001
9	1	9	8	0	8	9985.979	-0.015
8	3	6	7	3	5	10357.322	0.046
8	5	4	7	5	3	10613.756	-0.040
9	1	8	8	2	7	10782.884	0.032
9	2	8	8	2	7	10815.378	-0.007
8	2	6	7	2	5	10834.473	-0.033
10	0	10	9	1	9	11046.177	-0.023
10	1	10	9	1	9	11046.453	-0.030
10	0	10	9	0	9	11047.008	-0.005
10	1	10	9	0	9	11047.265	-0.030
5	4	1	4	3	2	11134.931	-0.006
8	3	5	7	3	4	11249.799	-0.022
9	3	7	8	3	6	11532.592	-0.016

**Table S3.** Measured rotational transitions (in MHz) assigned to conformer  $\alpha$ -Tg+/cc/t using CP-FTMW spectroscopy.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$\nu_{\text{obs}}$	$\nu_{\text{obs}} - \nu_{\text{cal}}$
6	1	6	5	1	5	6822.801	0.023
6	0	6	5	0	5	6869.392	0.024
6	2	5	5	2	4	7467.283	0.005
7	1	7	6	1	6	7905.067	0.023
7	0	7	6	0	6	7927.498	-0.007
6	2	4	5	2	3	8224.086	0.001
7	2	6	6	2	5	8623.150	0.041
8	1	8	7	1	7	8981.471	0.018
8	0	8	7	0	7	8991.615	0.006
7	3	5	6	3	4	9024.174	-0.010
7	2	5	6	2	4	9555.592	0.014
8	2	7	7	2	6	9751.287	-0.005
9	1	9	8	1	8	10054.828	-0.012
9	0	9	8	0	8	10059.2275	-0.011
8	3	6	7	3	5	10265.375	-0.014
9	2	8	8	2	7	10857.373	-0.009
9	1	8	8	1	7	10956.891	-0.011
10	1	10	9	1	9	11126.796	-0.004
10	0	10	9	0	9	11128.595	-0.051
9	3	7	8	3	6	11473.195	-0.007
10	2	9	9	2	8	11947.931	0.016

**Table S4.** Measured rotational transitions (in MHz) assigned to conformer  $\alpha$ -G-g+/cc/t using LA-MB-FTMW spectroscopy.

$J'$	$K'_{-1}$	$K'_{+1}$	$F'$	$J''$	$K''_{-1}$	$K''_{+1}$	$F''$	$\nu_{\text{obs}}$	$\nu_{\text{obs}} - \nu_{\text{cal}}$
4	0	4	3	3	1	3	2	4853.910	0.005
4	0	4	5	3	1	3	4	4853.989	0.003
4	0	4	4	3	1	3	3	4854.143	0.000
4	1	4	4	3	1	3	3	4944.265	0.002
4	1	4	5	3	1	3	4	4944.309	0.004
4	0	4	5	3	0	3	4	5043.431	0.002
4	0	4	3	3	0	3	2	5043.508	0.000
4	1	4	5	3	0	3	4	5133.751	0.003
4	1	4	3	3	0	3	2	5133.881	0.002
4	1	3	4	3	1	2	3	5710.490	0.001
4	1	3	5	3	1	2	4	5710.616	-0.000
4	1	3	3	3	1	2	2	5710.767	-0.002
5	0	5	4	4	1	4	3	6088.312	0.001
5	0	5	6	4	1	4	5	6088.337	0.000
5	0	5	5	4	1	4	4	6088.343	0.001
5	1	5	5	4	1	4	4	6126.717	0.001
5	1	5	4	4	1	4	3	6126.776	-0.000
5	1	5	6	4	1	4	5	6126.787	0.001
5	0	5	5	4	0	4	4	6178.463	0.000
5	0	5	6	4	0	4	5	6178.658	0.002
5	0	5	4	4	0	4	3	6178.680	-0.001
5	1	5	5	4	0	4	4	6216.839	0.002
5	1	5	6	4	0	4	5	6217.106	-0.000
5	1	5	4	4	0	4	3	6217.150	0.003
5	1	4	5	4	1	3	4	6991.716	-0.000
5	1	4	6	4	1	3	5	6991.982	-0.002
5	1	4	4	4	1	3	3	6992.101	0.000
6	1	6	6	5	1	5	5	7295.388	-0.003
6	1	6	5	5	1	5	4	7295.449	-0.006
6	1	6	7	5	1	5	6	7295.458	-0.004
6	0	6	6	5	0	5	5	7318.559	-0.004
6	0	6	7	5	0	5	6	7318.681	-0.002

**Table S5.** Measured rotational transitions (in MHz) assigned to conformer  $\alpha$ -G+g-/cc/t using LA-MB-FTMW spectroscopy.

$J'$	$K'_{-1}$	$K'_{+1}$	$F'$	$J''$	$K''_{-1}$	$K''_{+1}$	$F''$	$\nu_{\text{obs}}$	$\nu_{\text{obs}} - \nu_{\text{cal}}$
4	0	4	3	3	1	3	2	4514.534	0.000
4	0	4	5	3	1	3	4	4514.602	0.001
4	0	4	4	3	1	3	3	4514.659	-0.000
4	1	4	4	3	1	3	3	4614.533	0.001
4	1	4	3	3	1	3	2	4614.562	0.000
4	1	4	5	3	1	3	4	4614.598	0.001
4	0	4	4	3	0	3	3	4724.829	0.000
4	0	4	5	3	0	3	4	4725.048	-0.000
4	1	4	4	3	0	3	3	4824.703	0.002
4	1	4	5	3	0	3	4	4825.046	0.001
4	1	4	3	3	0	3	2	4825.110	0.002
4	1	3	4	3	1	2	3	5474.860	0.000
4	1	3	5	3	1	2	4	5474.983	0.001
4	1	3	3	3	1	2	2	5475.082	0.001
5	0	5	5	4	1	4	4	5665.462	0.003
5	0	5	6	4	1	4	5	5665.482	0.000
5	1	5	5	4	1	4	4	5707.836	0.000
5	1	5	6	4	1	4	5	5707.908	0.002

5	1	5	5	4	0	4	4	5807.708	-0.000
5	1	5	6	4	0	4	5	5807.902	-0.001
5	1	4	5	4	1	3	4	6678.236	-0.001
5	1	4	6	4	1	3	5	6678.441	-0.001
5	1	4	4	4	1	3	3	6678.515	-0.002
6	0	6	6	5	1	5	5	6768.967	-0.003
6	0	6	7	5	1	5	6	6769.015	-0.002
6	0	6	6	5	0	5	5	6811.346	-0.000
6	0	6	5	5	0	5	4	6811.433	-0.002
6	0	6	7	5	0	5	6	6811.442	0.001
6	1	6	6	5	0	5	5	6828.076	-0.000
6	1	6	7	5	0	5	6	6828.188	-0.001

**Table S6.** Measured rotational transitions (in MHz) assigned to conformer  $\alpha$ -*Tg*<sup>+</sup>/*cc*/*t* using LA-MB-FTMW spectroscopy.

$J'$	$K'_{-1}$	$K'_{+1}$	$F'$	$J''$	$K''_{-1}$	$K''_{+1}$	$F''$	$\nu_{\text{obs}}$	$\nu_{\text{obs}} - \nu_{\text{cal}}$
4	0	4	4	3	0	3	3	4761.448	0.002
4	0	4	5	3	0	3	4	4761.766	-0.000
4	0	4	3	3	0	3	2	4761.869	0.001
4	1	3	4	3	1	2	3	5404.677	0.000
4	1	3	5	3	1	2	4	5404.743	0.002
4	1	3	3	3	1	2	2	5404.894	0.001
5	1	5	5	4	1	4	4	5730.265	0.001
5	1	5	6	4	1	4	5	5730.327	-0.001
5	0	5	5	4	0	4	4	5817.484	-0.000
5	0	5	6	4	0	4	5	5817.721	-0.002
5	0	5	4	4	0	4	3	5817.766	0.001
5	0	5	4	4	1	4	3	5643.506	-0.001
5	0	5	6	4	1	4	5	5643.549	0.001
5	0	5	5	4	1	4	4	5643.632	-0.001
5	1	4	5	4	1	3	4	6646.291	-0.002
5	1	4	6	4	1	3	5	6646.492	-0.001
6	1	6	6	5	1	5	5	6822.699	0.001
6	1	6	5	5	1	5	4	6822.765	-0.001