Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

The effect of N-methylation on the conformational landscape of Alanine: the case of N-Methyl-L-Alanine

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Tables of experimental transition frequencies of all the observed conformer of N-Methyl-L-Alanine.

Table 1. Rotational transitions measured of the conformer Ia of N-MeAla.

J´	*K´-1*	*K´+1*	*J″*	*K″-1*	*K″+1*	*F′*	*F″*	*obs*[a]	*obs - calc*[b]
2	1	2	1	1	1	2	1	7234.576	0.002
2	1	2	1	1	1	3	2	7234.659	0.002
2	0	2	1	0	1	2	1	7616.364	0.010
2	0	2	1	0	1	3	2	7616.546	0.009
3	1	3	2	1	2	3	2	10771.689	0.000
3	1	3	2	1	2	4	3	10771.770	-0.001
3	0	3	2	0	2	3	2	11124.691	0.000
3	0	3	2	0	2	4	3	11124.909	0.000
3	0	3	2	0	2	2	1	11124.938	-0.000
2	2	0	1	1	0	2	1	11861.625	0.002
2	2	0	1	1	0	3	2	11861.891	-0.002
4	1	4	3	1	3	4	3	14242.880	-0.000
4	1	4	3	1	3	3	2	14242.920	-0.003
4	1	4	3	1	3	5	4	14242.956	-0.004
3	2	1	2	1	1	3	2	15731.427	-0.002
3	2	1	2	1	1	4	3	15731.520	0.000
3	2	1	2	1	1	2	1	15731.646	-0.004
5	1	5	4	1	4	4	3	17661.193	0.007
5	1	5	4	1	4	6	5	17661.216	0.007
4	1	3	3	1	2	4	3	16198.804	-0.004
4	1	3	3	1	2	5	4	16198.934	-0.005
4	1	3	3	1	2	3	2	16199.012	0.000
2	2	1	1	1	1	1	0	12242.946	-0.003
2	2	1	1	1	1	3	2	12243.662	0.002
2	2	1	1	1	1	2	1	12244.163	-0.001
4	0	4	3	0	3	4	3	14467.348	-0.006
4	0	4	3	0	3	5	4	14467.526	-0.005
4	0	4	3	0	3	3	2	14467.526	-0.009
3	2	2	2	1	2	2	1	16648.616	0.000
3	2	2	2	1	2	4	3	16648.921	0.006
3	2	2	2	1	2	3	2	16649.454	0.001

[a] Observed.
[b] Observed minus calculated

Table 2. Rotational transitions measured of the conformer IIa of N-MeAla.

J´	*K´-1*	*K´+1*	*J″*	*K″-1*	*K″+1*	*F′*	*F″*	*obs*[a]	*obs - calc*[b]
3	0	3	2	1	2	4	3	10389.240	0.000
3	0	3	2	1	2	2	1	10389.342	0.001
3	0	3	2	1	2	3	2	10389.399	0.001
3	1	3	2	1	2	4	3	10833.941	-0.002
3	1	3	2	1	2	2	1	10834.021	-0.001
3	1	3	2	1	2	3	2	10834.163	-0.000
3	0	3	2	0	2	4	3	11194.338	0.001
3	0	3	2	0	2	2	1	11194.423	0.001
3	0	3	2	0	2	3	2	11194.525	0.001
4	1	3	3	1	2	3	2	16259.157	-0.000
4	1	3	3	1	2	5	4	16259.194	-0.000
4	1	3	3	1	2	4	3	16259.354	0.000
5	0	5	4	1	4	6	5	17691.206	-0.002
5	0	5	4	1	4	4	3	17691.249	-0.002
5	0	5	4	1	4	5	4	17691.293	0.004
5	1	5	4	1	4	6	5	17777.513	0.000
5	1	5	4	1	4	4	3	17777.553	0.000
5	1	5	4	1	4	5	4	17777.608	0.000
4	0	4	3	1	3	5	4	14124.423	0.006
4	0	4	3	1	3	4	3	14124.507	-0.004
4	0	4	3	1	3	3	2	14124.475	-0.006
3	1	3	2	0	2	4	3	11639.040	0.000
3	1	3	2	0	2	2	1	11639.102	-0.000
3	1	3	2	0	2	3	2	11639.288	-0.000

[a] Observed.
[b] Observed minus calculated

Table 3. Rotational transitions measured of the conformer IIc of N-MeAla.

J´	*K´-1*	*K´+1*	*J″*	*K″-1*	*K″+1*	*F′*	*F″*	*obs*[a]	*obs - calc*[b]
2	0	2	1	0	1	1	1	7765.942	0.009
2	0	2	1	0	1	2	1	7765.985	-0.004
2	0	2	1	0	1	3	2	7766.323	0.007
3	0	3	2	0	2	3	2	11258.205	-0.000
3	0	3	2	0	2	4	3	11258.591	-0.001
3	0	3	2	0	2	2	1	11258.738	0.001
3	1	3	2	1	2	2	1	10862.076	-0.005
3	1	3	2	1	2	3	2	10862.188	-0.002
3	1	3	2	1	2	4	3	10862.205	-0.004
3	1	2	2	1	1	3	2	12763.485	-0.002
3	1	2	2	1	1	4	3	12763.500	-0.001
4	1	4	3	1	3	4	3	14327.204	0.002
4	1	4	3	1	3	5	4	14327.294	0.004
4	0	4	3	0	3	4	3	14560.501	-0.001
4	0	4	3	0	3	5	4	14560.790	-0.000
3	2	2	2	2	1	2	1	11938.518	-0.005
3	2	2	2	2	1	4	3	11938.738	-0.001
3	2	2	2	2	1	3	2	11939.137	0.008
1	1	0	0	0	0	2	1	5879.128	0.007
1	1	0	0	0	0	1	1	5879.727	-0.007
2	1	1	1	0	1	3	2	10505.077	-0.000

[a] Observed
[b] Observed minus calculated

Table 4. Rotational transitions measured of the conformer IIIa of N-MeAla.

J´	*K´-1*	*K´+1*	*J″*	*K″-1*	*K″+1*	*F′*	*F″*	*obs*[a]	*obs - calc*[b]
1	1	0	0	0	0	0	1	5433.318	0.003
1	1	0	0	0	0	2	1	5433.925	0.006
1	1	0	0	0	0	1	1	5434.326	0.004
2	1	1	1	0	1	1	0	9983.008	-0.007
2	1	1	1	0	1	3	2	9983.529	0.000
2	1	1	1	0	1	2	2	9983.631	-0.004
2	1	1	1	0	1	2	1	9983.938	0.000
2	2	1	1	1	1	1	0	11751.872	0.000
2	2	1	1	1	1	3	2	11752.206	0.004
2	2	1	1	1	1	2	1	11752.629	0.003
3	2	2	2	1	2	2	1	16301.512	-0.006
3	2	2	2	1	2	4	3	16301.757	0.000
3	2	2	2	1	2	3	2	16302.187	-0.002
3	2	1	2	1	1	2	1	15511.218	0.009
3	2	1	2	1	1	3	2	15511.303	-0.000
2	2	0	1	1	0	3	2	11409.020	-0.006
2	2	0	1	1	0	2	1	11409.042	0.004
2	2	0	1	1	0	2	2	11409.434	-0.006
3	1	2	2	0	2	3	2	14825.175	-0.001
3	1	2	2	0	2	3	3	14824.778	0.006

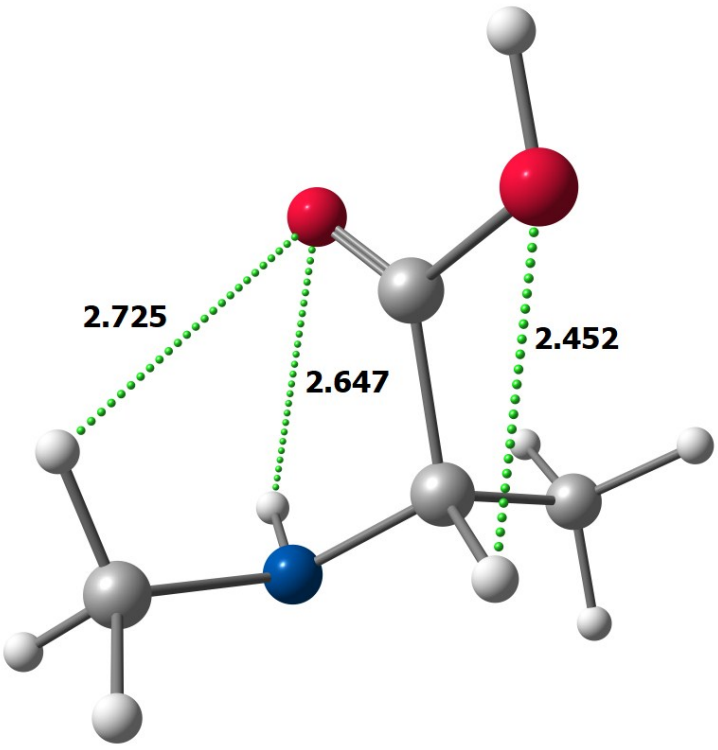
[a] Observed.
[b] Observed minus calculated

Structures of the observed conformers:

Conformer Ia

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.849371	-0.568568	-0.820412
2	8	0	0.838747	-1.024161	1.149512
3	7	0	-1.501888	0.329786	0.167542
4	6	0	-0.171279	0.613067	-0.334295
5	6	0	0.300982	1.981466	0.165455
6	6	0	0.860996	-0.423756	0.097430
7	6	0	-2.054843	-0.922221	-0.348660
8	1	0	-0.209165	0.617164	-1.429124
9	1	0	1.291674	2.222717	-0.229373
10	1	0	-0.412401	2.743986	-0.154040
11	1	0	0.350298	1.982362	1.259376
12	1	0	-1.460298	0.286700	1.182995
13	1	0	-1.438183	-1.806328	-0.127440
14	1	0	-2.166773	-0.836378	-1.433658
15	1	0	-3.047119	-1.077777	0.081002
16	1	0	2.485102	-1.190446	-0.434922

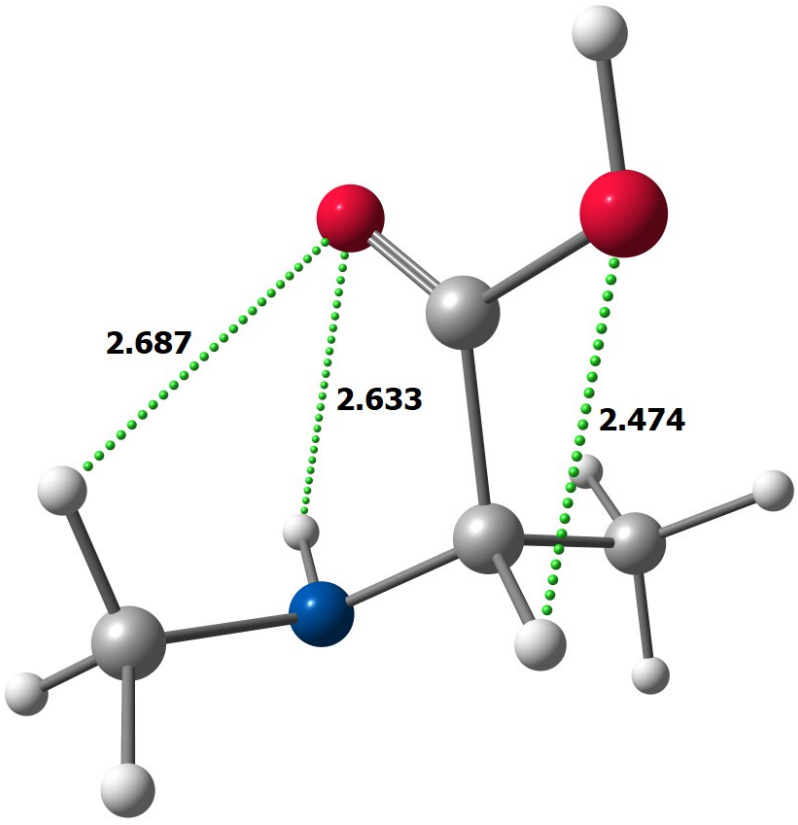


Conformer Ia – quadrupole correction structure

Rotation of N-C-C-OH from -32.6° to -27°

Standard orientation:

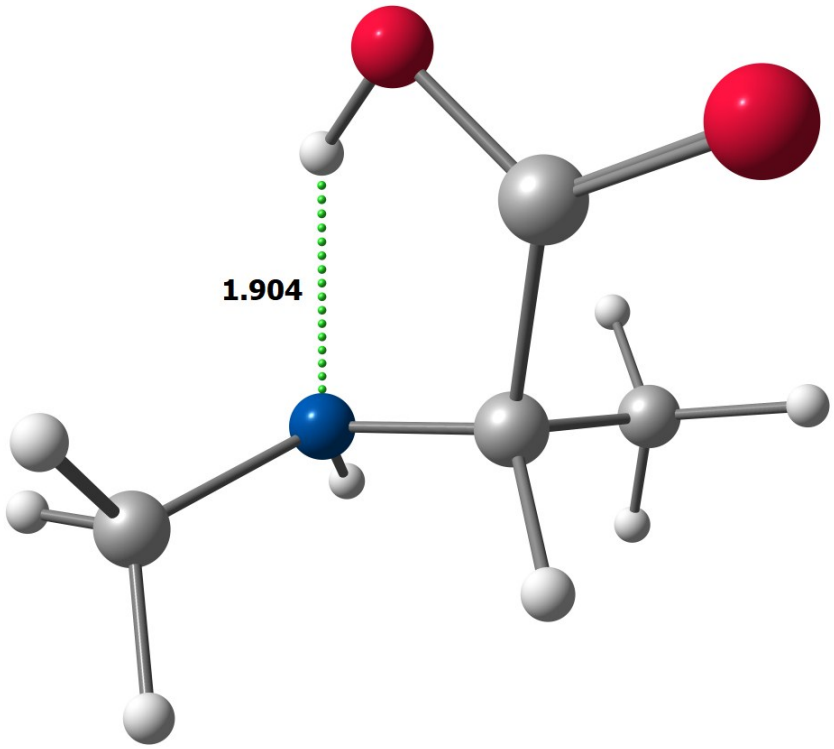
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.774882	-1.145771	1.074815
2	6	0	0.853110	-0.451113	0.085349
3	6	0	-0.159925	0.616790	-0.315986
4	7	0	-1.493907	0.352373	0.185122
5	6	0	0.343842	1.964638	0.210982
6	6	0	-2.092018	-0.856575	-0.381500
7	8	0	1.893356	-0.510687	-0.783834
8	1	0	-0.201022	0.647365	-1.410501
9	1	0	1.337222	2.193765	-0.183494
10	1	0	-0.355954	2.748086	-0.086955
11	1	0	0.397764	1.941156	1.304599
12	1	0	-1.446195	0.262550	1.197120
13	1	0	-1.501265	-1.768420	-0.209781
14	1	0	-2.214518	-0.715705	-1.459626
15	1	0	-3.083772	-1.000664	0.053408
16	1	0	2.509130	-1.165517	-0.421542



Conformer IIa

Standard orientation:

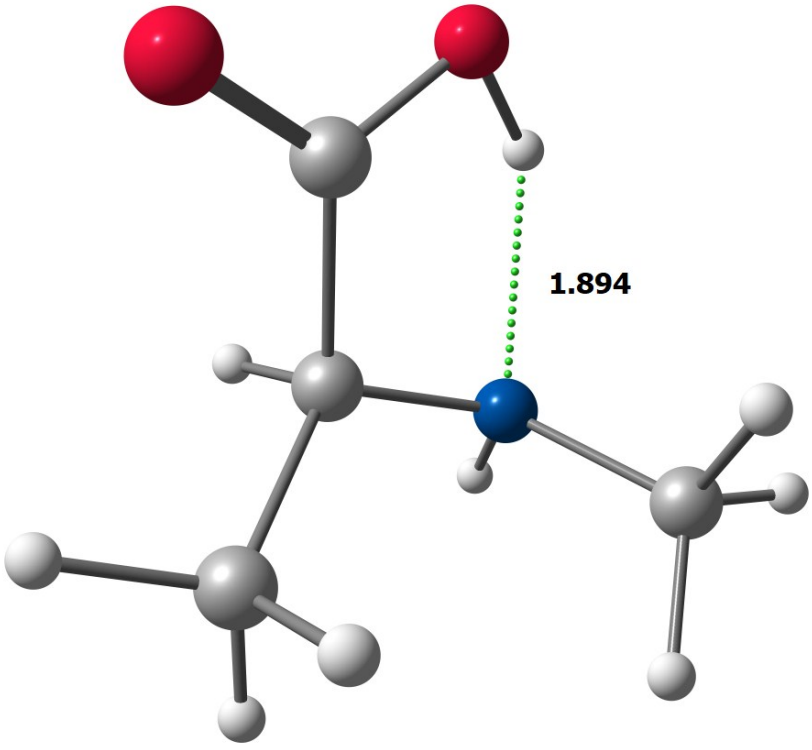
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.777980	-1.206380	1.004992
2	8	0	1.962406	-0.576772	-0.800986
3	7	0	-1.319739	0.191790	0.356800
4	6	0	-0.092282	0.603810	-0.325417
5	6	0	0.412191	1.934475	0.233650
6	6	0	0.989801	-0.460199	-0.093885
7	6	0	-2.148935	-0.710265	-0.451302
8	1	0	-0.229035	0.689671	-1.412629
9	1	0	0.546249	1.864252	1.317657
10	1	0	1.369978	2.192673	-0.223139
11	1	0	-0.304676	2.733148	0.017899
12	1	0	-1.856632	1.011568	0.622946
13	1	0	-3.046223	-0.979409	0.110159
14	1	0	-1.585983	-1.626086	-0.653246
15	1	0	-2.443536	-0.267800	-1.413068
16	1	0	-0.099709	-0.902251	1.325498



Conformer IIc

Standard orientation:

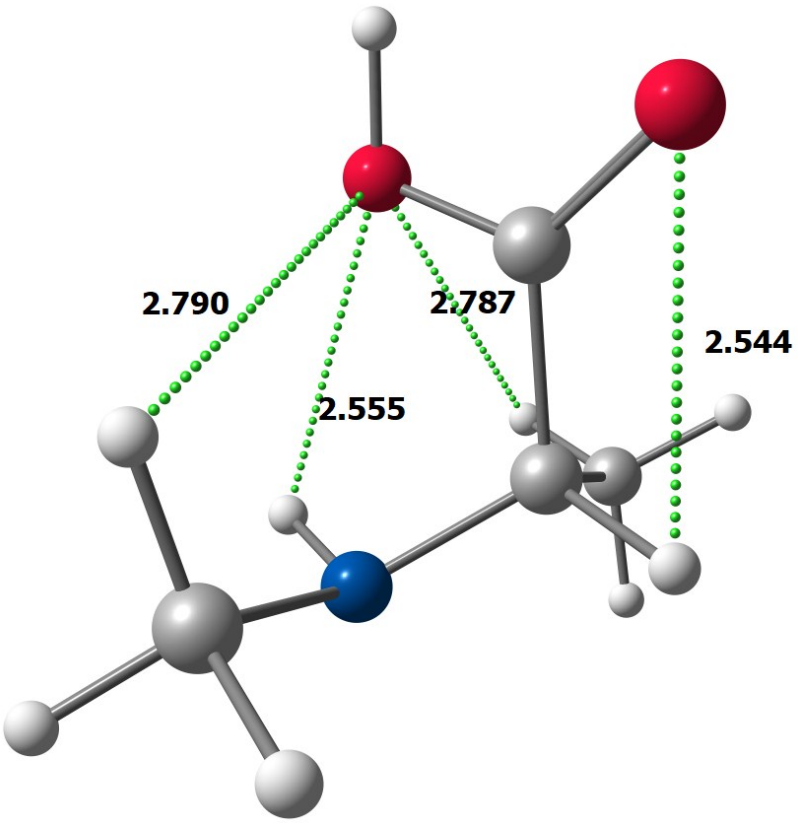
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.115568	-1.536219	0.090553
2	8	0	-2.063019	0.424237	-0.463788
3	7	0	1.216361	-0.503560	0.574872
4	6	0	0.115376	0.471324	0.603976
5	6	0	0.378607	1.832800	-0.034555
6	6	0	-1.135704	-0.194678	0.001516
7	6	0	1.934108	-0.580138	-0.703022
8	1	0	-0.132224	0.619880	1.663521
9	1	0	-0.483165	2.482996	0.126829
10	1	0	1.263456	2.297114	0.411976
11	1	0	0.527867	1.747194	-1.113460
12	1	0	1.867912	-0.309584	1.328220
13	1	0	2.455974	0.346023	-0.972465
14	1	0	1.221409	-0.818548	-1.498460
15	1	0	2.662655	-1.392094	-0.647425
16	1	0	-0.224035	-1.728048	0.455549



Conformer IIIa

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.963567	-0.702117	1.202547
2	8	0	1.694913	-0.835260	-0.931439
3	7	0	-1.466966	0.300375	0.195310
4	6	0	-0.185379	0.630298	-0.406474
5	6	0	0.271017	2.014746	0.056093
6	6	0	0.921254	-0.379497	-0.119139
7	6	0	-1.971682	-1.010139	-0.210697
8	1	0	-0.309530	0.627458	-1.494486
9	1	0	0.402913	2.027073	1.142366
10	1	0	1.220272	2.289294	-0.412884
11	1	0	-0.489990	2.749628	-0.215607
12	1	0	-1.373178	0.331846	1.207072
13	1	0	-1.298299	-1.845881	0.037234
14	1	0	-2.130722	-1.006832	-1.293048
15	1	0	-2.934696	-1.188530	0.273271
16	1	0	1.702898	-1.320119	1.301355



Conformer IIIa – quadrupole correction structure

Rotation of N-C-C-OH from -47.2° to -44.5°

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.923973	-0.768977	1.186292
2	6	0	0.923134	-0.382314	-0.118659
3	6	0	-0.179239	0.635485	-0.395103
4	7	0	-1.465692	0.307288	0.195446
5	6	0	0.286953	2.008892	0.091986
6	6	0	-1.985735	-0.986314	-0.243982
7	8	0	1.729015	-0.790108	-0.925107
8	1	0	-0.297442	0.652354	-1.483655
9	1	0	0.414611	2.001928	1.178948
10	1	0	1.240101	2.283101	-0.369063
11	1	0	-0.467309	2.754297	-0.169565
12	1	0	-1.374352	0.312835	1.207819
13	1	0	-1.321922	-1.835676	-0.017884
14	1	0	-2.145347	-0.953002	-1.325764
15	1	0	-2.950690	-1.166110	0.235619
16	1	0	1.667604	-1.382568	1.280492