

Supplementary Information to the paper entitled: “Competition between folded and extended structures of alanylalanine (Ala-Ala) in a molecular beam”

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TABLE TS1. Gibbs free energies for Ala-Ala conformers at different temperatures obtained with G4MP2 single point energy calculations performed for the ω 97X-D/6-311++G(d,p) optimized geometries. The values are presented relative to the C5C7-conformer in cm^{-1} units.

T (K)	15	50	100	150	200	250	300	350	400	450	500	550	600
C5C7-	0	0	0	0	0	0	0	0	0	0	0	0	0
C5C7+	187	185	178	172	166	159	152	145	137	129	122	114	106
C5-trans-	194	180	139	86	28	-34	-100	-168	-239	-312	-386	-461	-538
C5-trans+	446	432	388	335	277	214	148	79	8	-65	-139	-215	-291
C5g(s)-	437	409	343	267	187	104	18	-71	-161	-253	-346	-440	-535
C5g(s)+	644	618	553	478	397	313	226	135	42	-52	-148	-246	-345
C5g(a)-	842	809	733	647	557	462	365	265	164	60	-44	-150	-256
C5g(a)+	983	954	885	807	724	638	549	457	363	267	169	71	-29
C5-trans(a)-	853	817	735	641	542	439	333	223	112	-1	-116	-232	-349
C5-trans(a)+	1079	1043	962	870	772	669	564	455	345	232	118	2	-115
trans-trans	735	717	670	611	543	469	390	308	224	137	49	-41	-131
g-trans-trans+	925	906	858	799	732	659	582	500	417	330	242	153	62
g-trans-trans-	1184	1167	1130	1085	1037	984	928	870	808	745	681	615	548
sc-cis-trans	1066	1052	1009	959	903	843	779	711	640	566	490	413	333
trans-trans(a)-	1496	1459	1370	1265	1150	1028	900	768	633	495	355	214	71

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TABLE TS2. Relative abundances of Ala-Ala conformers at different temperatures obtained from the Boltzmann distribution with the energies presented in Tab. TS1.

T (K)	15	50	100	150	200	250	300	350	400	450	500	550	600
C5C7-	1.00	0.99	0.82	0.57	0.38	0.25	0.18	0.13	0.10	0.08	0.06	0.05	0.04
C5C7+	0.00	0.00	0.06	0.11	0.11	0.10	0.09	0.07	0.06	0.05	0.04	0.04	0.03
C5-trans-	0.00	0.01	0.11	0.25	0.31	0.31	0.29	0.26	0.23	0.21	0.18	0.17	0.15
C5-trans+	0.00	0.00	0.00	0.02	0.05	0.07	0.09	0.09	0.09	0.09	0.09	0.09	0.09
C5g(s)-	0.00	0.00	0.01	0.04	0.10	0.14	0.16	0.17	0.17	0.17	0.16	0.16	0.15
C5g(s)+	0.00	0.00	0.00	0.01	0.02	0.04	0.06	0.07	0.08	0.09	0.09	0.10	0.10
C5g(a)-	0.00	0.00	0.00	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.07	0.08
C5g(a)+	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.02	0.03	0.03	0.04	0.04	0.05
C5-trans(a)-	0.00	0.00	0.00	0.00	0.01	0.02	0.04	0.05	0.06	0.08	0.08	0.09	0.10
C5-trans(a)+	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.02	0.03	0.04	0.04	0.05	0.06
trans-trans	0.00	0.00	0.00	0.00	0.01	0.02	0.03	0.04	0.04	0.05	0.05	0.06	0.06
g-trans-trans+	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.02	0.02	0.03	0.03	0.03	0.04
g-trans-trans-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01
sc-cis-trans	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.02	0.02
trans-trans(a)-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.02	0.02	0.03	0.04