

The Two Missing Conformers of Gas-Phase Alanine: A Jet-Cooled Raman Spectroscopy Study

[Supporting information]

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Table S1. DFT (B3LYP) vibrational analysis of alanine conformers **I-VIIIa**: frequencies (Freq) are in $[\text{cm}^{-1}]$, infrared intensities (Int) are in $[\text{km mol}^{-1}]$.

Ref.[19]. Complete citation for reference **19**.

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Supplementary Material (ESI) for PCCP
This journal is © the Owner Societies 2010**Table S1.** DFT (B3LYP) vibrational analysis of alanine conformers **I-VIIIa**: frequencies (Freq) are in [cm⁻¹], infrared intensities (Int) are in [km mol⁻¹], zero-point energies (ZPE) are in [kcal mol⁻¹].

	I		IIa		IIb		IIIb		IIIa		IVa	
	Freq	Int	Freq	Int	Freq	Int	Freq	Int	Freq	Int	Freq	Int
v₃₃	48	67	62	49	57	26	-	-	33	191	58	52
v₃₂	202	5	231	2	229	1	-	-	223	1	205	3
v₃₁	226	1	246	4	268	2	-	-	234	9	235	3
v₃₀	239	6	272	4	276	4	-	-	259	4	245	8
v₂₉	300	6	334	4	350	7	-	-	287	5	309	2
v₂₈	376	6	388	4	405	2	-	-	369	6	372	6
v₂₇	496	5	529	12	528	12	-	-	529	10	501	5
v₂₆	595	4	632	5	568	11	-	-	595	3	599	5
v₂₅	636	8	742	6	737	9	-	-	611	6	634	6
v₂₄	755	16	798	19	801	20	-	-	773	8	758	14
v₂₃	787	19	840	5	840	2	-	-	777	15	792	14
v₂₂	884	6	864	2	872	3	-	-	859	6	835	8
v₂₁	922	10	937	6	936	5	-	-	917	11	917	11
v₂₀	1018	5	1012	4	1019	2	-	-	1020	4	1031	5
v₁₉	1084	7	1057	6	1074	4	-	-	1044	3	1080	13
v₁₈	1123	3	1127	3	1142	2	-	-	1138	6	1137	2
v₁₇	1165	4	1200	9	1208	8	-	-	1179	6	1170	2
v₁₆	1274	1	1268	4	1233	4	-	-	1267	1	1233	5
v₁₅	1294	8	1332	2	1313	4	-	-	1329	6	1315	4
v₁₄	1354	3	1359	5	1389	5	-	-	1345	1	1352	4
v₁₃	1401	1	1401	4	1404	5	-	-	1401	4	1400	0
v₁₂	1416	4	1411	1	1411	1	-	-	1408	1	1431	4
v₁₁	1495	5	1497	5	1492	4	-	-	1493	6	1494	5
v₁₀	1500	3	1502	4	1501	4	-	-	1499	4	1503	3
v₉	1670	2	1655	4	1657	4	-	-	1664	2	1639	2
v₈	1803	9	1832	10	1829	10	-	-	1800	12	1809	9

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v₇	3036	72	3031	81	3030	79	-	-	3037	66	3028	75
v₆	3052	22	3036	19	3040	15	-	-	3072	30	3040	33
v₅	3104	22	3091	20	3092	23	-	-	3104	16	3096	25
v₄	3124	25	3127	19	3127	21	-	-	3117	28	3103	21
v₃	3492	35	3477	27	3468	26	-	-	3498	35	3500	34
v₂	3564	15	3516	37	3506	30	-	-	3576	14	3584	12
v₁	3731	45	3592	16	3590	18	-	-	3740	32	3736	33
ZPE	68.15		68.55		68.45		-		68.20		68.15	
	IVb		Va		Vb		VI		VII		VIIIa	
	Freq	Int	Freq	Int	Freq	Int	Freq	Int	Freq	Int	Freq	Int
v₃₃	59	9	51	87	43	28	51	87	56	61	57	76
v₃₂	209	2	222	2	213	1	190	5	226	2	209	5
v₃₁	226	2	235	10	250	1	225	1	257	4	242	4
v₃₀	266	2	244	2	275	1	240	5	298	6	245	5
v₂₉	331	7	303	1	322	11	303	6	349	3	314	3
v₂₈	416	3	362	7	406	2	376	10	394	4	375	7
v₂₇	493	4	527	11	495	6	492	4	431	5	499	4
v₂₆	560	9	585	3	553	7	497	15	525	16	504	13
v₂₅	616	4	609	5	610	4	643	5	617	7	643	3
v₂₄	730	21	769	12	734	20	742	5	653	3	744	6
v₂₃	798	20	785	19	795	21	792	15	737	7	795	8
v₂₂	826	4	837	2	851	4	889	3	795	15	834	11
v₂₁	936	7	914	13	936	7	917	10	920	8	914	11
v₂₀	1025	4	1022	4	1023	4	1018	4	993	2	1030	3
v₁₉	1104	5	1075	11	1090	4	1081	4	1055	4	1080	11
v₁₈	1130	2	1096	2	1135	4	1119	6	1142	4	1137	5
v₁₇	1182	2	1184	5	1161	3	1164	5	1181	8	1184	4
v₁₆	1232	5	1244	4	1255	4	1265	6	1243	3	1226	8
v₁₅	1322	2	1342	2	1314	4	1283	2	1318	3	1289	5
v₁₄	1344	6	1345	4	1345	3	1331	3	1323	4	1343	3
v₁₃	1403	2	1402	0	1413	3	1407	3	1376	4	1403	1

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v₁₂	1418	3	1415	6	1421	1	1417	2	1408	0	1418	3
v₁₁	1495	5	1491	5	1491	5	1489	5	1497	5	1495	6
v₁₀	1500	3	1501	3	1498	3	1502	4	1498	4	1499	3
v₉	1635	2	1651	3	1649	3	1672	2	1639	2	1639	2
v₈	1802	11	1812	9	1813	9	1836	11	1830	10	1840	11
v₇	2923	53	3027	70	2914	56	3007	41	3030	72	2976	43
v₆	3042	63	3071	36	3042	62	3037	57	3049	18	3026	71
v₅	3104	23	3095	29	3105	21	3098	16	3101	28	3088	28
v₄	3125	19	3102	15	3128	18	3119	27	3135	20	3104	17
v₃	3512	39	3497	41	3507	45	3490	34	3543	35	3497	34
v₂	3598	13	3578	15	3587	16	3561	14	3649	12	3583	11
v₁	3740	32	3740	32	3741	35	3784	18	3702	18	3786	18
ZPE	68.12		68.12		68.13		68.00		68.02		67.99	

Conformer IIIb geometry has not converged.

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Ref.[19]. Complete citation for reference 19.

[19] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J.E.; Hratchian, H.P.; Cross, J.B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.E.; Yazyev, O.; Austin, A.J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Cliford, J.; Cioslowski, B. B.; Stefanov, G.; Liu, A.; Liashenko, P.; Piskorz, I.; Komaromi, S.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A. Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. (2004) Gaussian 03, Revision C.02, Gaussian, Inc., Wallingford CT.