Thermal Fluctuations and Infrared Spectra of the Formamide–Formamidine Complex

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SUPPORTING INFORMATION

Complete reference records for the citations with more than 10 authors:

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Table 1: Frequencies (in cm^{-1}) and intensities (in $km{\cdot}mol^{-1}$) of the IR vibrational modes calculated at the B3LYP/aug-cc-pVTZ level using harmonic and anharmonic approximation to the electronic potential energy and the band assignments in terms of bond stretching (ν), angle bending (β) and dihedral angle torsions (τ) for the FM and FI monomers and for the FM$\cdots$FI dimer.

Frequency		Intensity	Assignment
Harmonic	Anharmonic		
			FM monomer
3708	3548	39	-96% (ν(NH) $-$ ν(NH))
3577	3430	28	96% (ν(NH) $+$ ν(NH))
3522	3351	8	100% ν(NH)
3042	2866	53	99% ν(CH)
1716	1674	333	60% ν(NC) $-$ 12% ν(NC) $+$ 16% β(HCN)
1623	1578	24	10% ν(NC) $+$ 73% τ(HNCO)
1405	1372	27	-19% ν(NC) $+$ 20% β(HNC) $+$ 41% β(HCN) $+$ 13% β(NCN)
1328	1288	34	-22% ν(NC) $+$ 16% β(HNC) $+$ 18% β(HNC) $-$ 34% β(HCN)
1106	1075	135	37% ν(NC) $+$ 56% β(HNC)
1086	1044	2	18% ν(NC) $+$ 52% β(HNC) $+$ 11% τ(HCNH)
1045	1020	0	79% τ(HCNH)
799	788	53	86% τ(HNCN)
566	514	56	38% β(NCN) $-$ 13% (τ(HNCN) $-$ τ(NCNH)) $+$ 39% (τ(HNCN) $+$ τ(NCNH))
529	462	55	-12% β(HNC) $+$ 39% β(NCN) $-$ 35% (τ(HNCN) $+$ τ(NCNH))
327	168	189	76% (τ(HNCN) $-$ τ(NCNH)) $+$ 18% (τ(HNCN) $+$ τ(NCNH))
			FI monomer
3713	3512	42	98% (ν(NH) $-$ ν(NH))
3575	3401	34	98% (ν(NH) $+$ ν(NH))
2943	2758	92	100% ν(CH)
1786	1752	433	79% ν(OC)
1619	1576	58	90% β(HNH)
1417	1421	6	10% ν(OC) $+$ 84% β(HCO)
1265	1183	112	52% ν(NC) $+$ 25% β(HNC) $-$ 19% β(NCO)
1054	1050	5	-32% ν(NC) $+$ 47% β(HNC)
1043	1020	3	97% β(HNC)
639	555	15	95% (β(HNH) $+$ τ(HNCO))
568	569	11	19% β(HNC) $+$ 73% β(NCO)
246	494	201	-97% (β(HNH) $-$ τ(HNCO))
			FM$\cdots$FI dimer
3595	3385	73	97% ν(NH)
3542	3356	42	98% ν(NH)
3424	3278	5	100% ν(NH)
3211	2983	806	93% ν(NH)
2990	2738	663	90% ν(NH)
2964	2769	236	94% ν(CH)
2861	2665	220	99% ν(CH)
1686	1642	530	40% ν(OC) $+$ 16% β(HNC) $-$ 11% β(HNH)
1660	1604	106	-16% ν(NC) $+$ 12% ν(NC) $+$ 36% β(HNH) $-$ 13%β(CNH)
1607	1562	8	21% ν(OC) $-$ 14% β(HNH) $+$ 56% β(HNH)
1581	1564	2	30% ν(NC) $+$ 33% β(HNH)
1378	1355	42	-16% ν(NC) $-$ 26% β(HNH) $-$ 21% τ(NCOH) $+$ 14% β(NCN)
1375	1373	12	14% ν(OC) $+$ 77% β(HCO)
1324	1300	44	-20% ν(NC) $+$ 49% τ(NCOH) $+$ 10% β(NCN)
1294	1256	85	54% ν(NC) $+$ 28% β(HNC) $-$ 12% β(NCO)
1123	1111	79	-26% ν(NC) $+$ 45% β(HNH) $-$ 11% β(CNH)
1081	1068	1	-12% ν(NC) $-$ 21% ν(NC) $+$ 23% β(CNH)
1069	1050	4	-18% ν(NC) $+$ 33% β(HNC) $+$ 11% β(HNH) $-$ 12% β(CNH)
1023	994	16	-19% β(HNC) $+$ 20% β(HNC) $+$ 41% β(HCN) $-$ 10% τ(CNHN)
1010	997	0	18% β(HNC) $+$ 44% β(HNC) $-$ 18% β(HCN) $+$ 11% τ(CNHN)
872	833	34	49% β(CNH) $-$ 22% τ(CNHN)
781	747	0	28% τ(HNHO) $-$ 26% τ(CONH) $-$ 28% τ(NCNH)
730	736	121	40% β(HNC) $-$ 19% τ(CONH) $-$ 17% τ(NCNH)
625	616	9	64% β(NCO)
572	568	7	60% β(NCN) $+$ 14% β(CNH)
499	499	82	-36% β(CNH) $+$ 46% β(CNH)
354	302	62	-37% τ(HNHO) $+$ 43% τ(CNHN)
216	230	83	-13% ν(OH) $+$ 51% β(HNH) $+$ 24% β(COH)
164	174	2	84% ν(OH)
159	194	3	51% β(HNH) $-$ 24% τ(NCOH)
156	160	1	-16% β(NHO) $+$ 58% β(NCO) $-$ 15% β(CNH)
113	127	84	18% τ(HNHO) $-$ 23% τ(NCNH) $+$ 40% τ(NCNH)
59	98	5	26% β(HNH) $+$ 60% τ(NCOH)