

TABLE IS: Experimental and calculated wavenumbers (cm^{-1}) for 1,6-diaminohexane (C_{2h}), in the low frequency region.

Experimental		^a Calculated (<i>all-trans</i> conformer)				Approximate description
Raman	INS	Raman (^b)	Infrared (^c)	INS	Sym. species	
<i>1,6-diaminohexane</i>						
516				505	Ag	in-plane CCN deformation (LAM 3)
507	506	503 (2)		472	Bu	in-plane CCN deformation (LAM 2)
	477		472 (1)	472	Bu	in-plane CCN deformation (LAM 4)
	383		362 (12)	365	Bg	NH ₂ torsion
394		303 (6)		302	Au	NH ₂ torsion
			302 (106)	302	Ag	in-plane CCN deformation (LAM 1)
286	284	269 (9)		272	Ag	in-plane CCN deformation (LAM 5)
	240	202 (1)		204	Ag	
	205					
	194		174 (0)	174	Au	out-of-plane CCN deformation (TAM)
	177					
	162	141 (0)		141	Bg	out-of-plane CCN deformation (TAM)
149	151	119 (0)		119	Bg	out-of-plane CCN deformation (TAM)
	123		80 (3)	80	Bu	in-plane CCN deformation (LAM 6)
	117		70 (8)	70	Au	out-of-plane CCN deformation (TAM)
	99		50 (1)	50	Au	out-of-plane CCN deformation (TAM)
82	80					
	75					
	59					
	54					
<i>1,6-diaminohexane-N-d₄</i>						
491	487	478 (1)		477	Ag	in-plane CCN deformation (LAM 3)
	467		458 (2)	458	Bu	in-plane CCN deformation (LAM 2)
	368		343 (16)	343	Bu	in-plane CCN deformation (LAM 4)
~300 sh	304	234 (3)		232	Bg	ND ₂ torsion
272	274	261 (8)		261	Ag	in-plane CCN deformation (LAM 1)
	237	193 (1)		193	Ag	in-plane CCN deformation (LAM 5)
			231 (53)	232	Au	ND ₂ torsion
	203					
	194		171 (0)	171	Au	out-of-plane CCN deformation (TAM)
176	179	134 (0)		134	Bg	out-of-plane CCN deformation (TAM)
147	152	116 (0)		116	Bg	out-of-plane CCN deformation (TAM)
132	136					
	128		77 (2)	77	Bu	in-plane CCN deformation (LAM 6)
	115		64 (8)	64	Au	out-of-plane CCN deformation (TAM)
108	104		48 (1)	48	Au	out-of-plane CCN deformation (TAM)
	78					
	63					
	46					

^aB3LYP/6-31G* level of calculation; ^bRaman scattering activities in Å²amu⁻¹; ^cIR intensities in km.mol⁻¹.

TABLE IIS: Experimental and calculated wavenumbers (cm⁻¹) for 1,7-diaminoheptane (C_{2v}), in the low frequency region.

Experimental		^a Calculated (<i>all-trans</i> conformer)				Approximate description
Raman	INS	Raman (^b)	Infrared (^c)	INS	Sym. species	
<i>1,7-diaminoheptane</i>						
525	521	519 (2)	519 (1)	519	A1	in-plane CCN deformation (LAM 3)
	450		450 (3)	449	B2	in-plane CCN deformation (LAM 2)
438	434		428 (5)	428	B2	in-plane CCN deformation (LAM 4)
406		302 (1)	302 (105)	301	B1	NH ₂ torsion
		301 (5)		301	A2	NH ₂ torsion
	320	298 (1)	298 (3)	301	A1	in-plane CCN deformation (LAM 5)
269	256	241 (9)		241	A1	in-plane CCN deformation (LAM 1)
	199	173 (0)	173 (0)	173	A2	out-of-plane CCN deformation (TAM)
	187	163 (2)	163 (2)	163	B1	out-of-plane CCN deformation (TAM)
	178					
170						
	164	162 (3)	162 (3)	163	B2	in-plane CCN deformation (LAM 6)
	152					
148	137	129 (4)	129 (4)	129	B1	out-of-plane CCN deformation (TAM)
93	99	103 (0)	103 (0)	103	A2	out-of-plane CCN deformation (TAM)
82						
	70	73 (0)	73 (0)	73	A2	out-of-plane CCN deformation (TAM)
	119		62 (1)	62	A1	in-plane CCN deformation (LAM 7)
61	64		46 (2)	46	B1	out-of-plane CCN deformation (TAM)
<i>1,7-diaminoheptane-N-d₄</i>						
	503	497 (1)		497	A1	in-plane CCN deformation (LAM 3)
	452		449 (3)	449	B2	in-plane CCN deformation (LAM 2)
415	419		397 (12)	397	B2	in-plane CCN deformation (LAM 4)
306	311		290 (2)	290	A1	in-plane CCN deformation (LAM 5)
284		233 (2)		232	A2	ND ₂ torsion
			233 (50)	232	B1	ND ₂ torsion
255	249	231 (8)		232	A1	in-plane CCN deformation (LAM 1)
	193	169 (0)	169 (0)	168	A2	out-of-plane CCN deformation (TAM)
	183		161 (2)	160	B1	out-of-plane CCN deformation (TAM)
			157 (4)	160	B2	in-plane CCN deformation (LAM 6)
161	161					
146	150		122 (5)	122	B1	out-of-plane CCN deformation (TAM)
	132	101 (0)	101 (0)	101	A2	out-of-plane CCN deformation (TAM)
	116	66 (0)	66 (0)	66	A2	out-of-plane CCN deformation (TAM)
	107		60 (1)	60	A1	in-plane CCN deformation (LAM 7)
	97		45 (2)	45	B1	out-of-plane CCN deformation (TAM)
	63					

^aB3LYP/6-31G* level of calculation; ^bRaman scattering activities in Å.amu⁻¹; ^cIR intensities in km.mol⁻¹.

TABLE IIIS: Experimental and calculated wavenumbers (cm⁻¹) for 1,8-diaminooctane (C_{2h}), in the low frequency region.

Experimental		^a Calculated (<i>all-trans</i> conformer)				Approximate description	
Raman	INS	Raman (^b)	Infrared (^c)	INS	Sym. species		
<i>1,8-diaminooctane</i>							
517	514	514 (3)		514	Ag	in-plane CCN deformation (LAM 3)	
	496		491 (8)	492	Bu	in-plane CCN deformation (LAM 4)	
	407		404 (1)	404	Bu	in-plane CCN deformation (LAM 2)	
397	391	379 (1)		379	Ag	in-plane CCN deformation (LAM 5)	
			315 (106)	315	Au	NH ₂ torsion	
377		314 (6)		315	Bg	NH ₂ torsion	
	269		250 (7)	250	Bu	in-plane CCN deformation (LAM 6)	
236	236	219 (8)		219	Ag	in-plane CCN deformation (LAM 1)	
	207	172 (0)		171	Bg	out-of-plane CCN deformation (TAM)	
	202						
	189		159 (2)	159	Au	out-of-plane CCN deformation (TAM)	
	175	138 (1)		138	Ag	in-plane CCN deformation (LAM 7)	
	163		137 (1)	138	Au	out-of-plane CCN deformation (TAM)	
137	139	113 (0)		113	Bg	out-of-plane CCN deformation (TAM)	
118	122	82 (0)		82	Bg	out-of-plane CCN deformation (TAM)	
	112		58 (1)	58	Bu	in-plane CCN deformation (LAM 8)	
	104		58 (5)	58	Au	out-of-plane CCN deformation (TAM)	
	87		33 (1)	33	Au	out-of-plane CCN deformation (TAM)	
80	79						
63	69						
	52						
33							
<i>1,8-diaminooctane-N-d₄</i>							
500	504	498 (1)		497	Ag	in-plane CCN deformation (LAM 3)	
	487		478 (12)	478	Bu	in-plane CCN deformation (LAM 4)	
	401		389 (3)	389	Bu	in-plane CCN deformation (LAM 2)	
388	381	365 (1)		365	Ag	in-plane CCN deformation (LAM 5)	
	262		242 (8)	241	Bu	in-plane CCN deformation (LAM 6)	
			241 (51)	241	Au	ND ₂ torsion	
273	262	240 (3)		241	Bg	ND ₂ torsion	
229	231	213 (8)		213	Ag	in-plane CCN deformation (LAM 1)	
	204	170 (0)		170	Bg	out-of-plane CCN deformation (TAM)	
	198						
	185		156 (4)	156	Au	out-of-plane CCN deformation (TAM)	
165	167	134 (1)		134	Ag	in-plane CCN deformation (LAM 7)	
	153		135 (1)	134	Au	out-of-plane CCN deformation (TAM)	
148							
135	138	107 (0)		107	Bg	out-of-plane CCN deformation (TAM)	
116	123	80 (0)		80	Bg	out-of-plane CCN deformation (TAM)	
	112		56 (1)	55	Bu	in-plane CCN deformation (LAM 8)	
	102		54 (5)	55	Au	out-of-plane CCN deformation (TAM)	
95							
	89						
	83		32 (1)	32	Au	out-of-plane CCN deformation (TAM)	
79	77						
62	68						
	50						
31							

^aB3LYP/6-31G* level of calculation; ^bRaman scattering activities in Å.amu⁻¹; ^cIR intensities in km.mol⁻¹.

TABLE IVS: Experimental and calculated wavenumbers (cm⁻¹) for 1,9-diaminononane (C_{2v}), in the low frequency region.

Experimental		^a Calculated (<i>all-trans</i> conformer)				Approximate description
Raman	INS	Raman (^b)	Infrared (^c)	INS	Sym. species	
<i>1,9-diaminonane</i>						
504	498	498 (3)		498	A1	in-plane CCN deformation (LAM 3)
495	519		517 (5)	516	B2	in-plane CCN deformation (LAM 4)
450	445	437 (1)	437 (3)	437	A1	in-plane CCN deformation (LAM 5)
		302 (1)	302 (104)	301	B1	NH ₂ torsion
392		301 (5)		301	A2	NH ₂ torsion
379	382	376 (0)	376 (0)	376	B2	in-plane CCN deformation (LAM 2)
	341		323 (6)	323	B2	in-plane CCN deformation (LAM 6)
229	218	199 (8)		199	A1	in-plane CCN deformation (LAM 1)
223	246	211 (1)	211 (2)	211	A1	in-plane CCN deformation (LAM 7)
~203 sh	204	178 (0)	178 (0)	177	B1	out-of-plane CCN deformation (TAM)
	199	170 (0)	170 (0)	170	A2	out-of-plane CCN deformation (TAM)
	182	149 (0)	149 (0)	149	A2	out-of-plane CCN deformation (TAM)
	169		126 (3)	126	B1	out-of-plane CCN deformation (TAM)
	156		112 (2)	112	B2	in-plane CCN deformation (LAM 8)
	148		107 (3)	108	B1	out-of-plane CCN deformation (TAM)
~140	136					
123	124	76 (0)	76 (0)	76	A2	out-of-plane CCN deformation (TAM)
	106	63 (0)	63 (0)	63	A2	out-of-plane CCN deformation (TAM)
95	100	42 (0)	42 (0)	42	A1	in-plane CCN deformation (LAM 9)
	86		33 (1)	33	B1	out-of-plane CCN deformation (TAM)
75	77					
63	65					
56	56					
45						
	27					
<i>1,9-diaminonane-N-d₄</i>						
510	506		501 (12)	500	B2	in-plane CCN deformation (LAM 4)
494	491	490 (1)		491	A1	in-plane CCN deformation (LAM 3)
429	436	418 (1)	418 (2)	418	A1	in-plane CCN deformation (LAM 5)
373	375	369 (0)	369 (0)	369	B2	in-plane CCN deformation (LAM 2)
	325		310 (9)	310	B2	in-plane CCN deformation (LAM 6)
289		233 (0)		233	A2	ND ₂ torsion
			233 (50)	233	B1	ND ₂ torsion
227	213	191 (7)	191 (1)	190	A1	in-plane CCN deformation (LAM 1)
213	235	209 (1)	209 (1)	209	A1	in-plane CCN deformation (LAM 7)
	201		176 (1)	175	B1	out-of-plane CCN deformation (TAM)
~196	196	168 (0)	168 (0)	169	A2	out-of-plane CCN deformation (TAM)
	185					
	176	144 (0)	144 (0)	144	A2	out-of-plane CCN deformation (TAM)
	168		124 (3)	124	B1	out-of-plane CCN deformation (TAM)
	154		109 (2)	109	B2	in-plane CCN deformation (LAM 8)
144	144		102 (4)	102	B1	out-of-plane CCN deformation (TAM)
	135					
120		75 (0)	75 (0)	73	A2	out-of-plane CCN deformation (TAM)
105	104	58 (0)	58 (0)	58	A2	out-of-plane CCN deformation (TAM)
93	99	41 (0)	41 (0)	41	A1	in-plane CCN deformation (LAM 9)
	87		33 (1)	33	B1	out-of-plane CCN deformation (TAM)
75	75					
63	64					
54	55					
43						

^aB3LYP/6-31G* level of calculation; ^bRaman scattering activities in Å.amu⁻¹; ^cIR intensities in km.mol⁻¹.

TABLE VS: Experimental and calculated wavenumbers (cm⁻¹) for 1,10-diaminodecane (C_{2h}), in the low frequency region.

Experimental		^a Calculated (<i>all-trans</i> conformer)				Approximate description
Raman	INS	Raman (^b)	Infrared (^c)	INS	Sym. species	
<i>1,10-diaminodecane</i>						
	527		525 (4)	525	B _u	in-plane CCN deformation (LAM 4)
489	491	489 (0)		489	A _g	in-plane CCN deformation (LAM 5)
476	479	469 (4)		469	A _g	in-plane CCN deformation (LAM 3)
	401		389 (8)	389	B _u	in-plane CCN deformation (LAM 6)
375		301 (6)		301	B _g	NH ₂ torsion
	359		349 (0)	349	B _u	in-plane CCN deformation (LAM 2)
			301 (104)	301	A _u	NH ₂ torsion
297	296	282 (1)		282	A _g	in-plane CCN deformation (LAM 7)
	221		181 (4)	180	B _u	in-plane CCN deformation (LAM 8)
201		185 (8)		180	A _g	in-plane CCN deformation (LAM 1)
	201		179 (0)	180	A _u	out-of-plane CCN deformation (TAM)
		171 (0)		173	B _g	out-of-plane CCN deformation (TAM)
176	180	154 (0)		153	B _g	out-of-plane CCN deformation (TAM)
	170		139 (3)	139	A _u	out-of-plane CCN deformation (TAM)
	157					
	148		110 (2)	109	A _u	out-of-plane CCN deformation (TAM)
132	137	98 (0)		98	A _g	in-plane CCN deformation (LAM 9)
	123	98 (0)		98	B _g	out-of-plane CCN deformation (TAM)
	114	64 (0)		63	B _g	out-of-plane CCN deformation (TAM)
	107		56 (5)	56	A _u	out-of-plane CCN deformation (TAM)
99						
	95		39 (1)	39	B _u	in-plane CCN deformation (LAM 10)
84						
	80		28 (0)	28	A _u	out-of-plane CCN deformation (TAM)
64	64					
51	51					
	44					
32						
<i>1,10-diaminodecane-N-d₄</i>						
	512		511 (8)	511	B _u	in-plane CCN deformation (LAM 4)
487	485	488 (1)		488	A _g	in-plane CCN deformation (LAM 5)
459						
453	456	445 (2)		445	A _g	in-plane CCN deformation (LAM 3)
	392		382 (9)	382	B _u	in-plane CCN deformation (LAM 6)
	345		336 (3)	336	B _u	in-plane CCN deformation (LAM 2)
287	286	274 (1)		274	A _g	in-plane CCN deformation (LAM 7)
269		232 (3)		232	B _g	ND ₂ torsion
			232 (50)	232	A _u	ND ₂ torsion
	203		176 (5)	177	B _u	in-plane CCN deformation (LAM 8)
197						
	198	181 (7)		177	A _g	in-plane CCN deformation (LAM 1)
			178 (0)	177	A _u	out-of-plane CCN deformation (TAM)
		169 (0)		170	B _g	out-of-plane CCN deformation (TAM)
173	177	151 (0)		151	B _g	out-of-plane CCN deformation (TAM)
	164		134 (4)	134	A _u	out-of-plane CCN deformation (TAM)
	152					
	143		108 (2)	108	A _u	out-of-plane CCN deformation (TAM)
132	135	95 (0)		94	A _g	in-plane CCN deformation (LAM 9)
117	120	93 (0)		94	B _g	out-of-plane CCN deformation (TAM)
	113	62 (0)		62	B _g	out-of-plane CCN deformation (TAM)
	107		53 (5)	53	A _u	out-of-plane CCN deformation (TAM)
95						
	90		37 (1)	37	B _u	in-plane CCN deformation (LAM 10)
82						
	76		27 (0)	27	A _u	out-of-plane CCN deformation (TAM)
63						
50	49					
30						

^a B3LYP/6-31G* level of calculation; ^b Raman scattering activities in Å.amu⁻¹; ^c IR intensities in km.mol⁻¹.

Experimental		^a Calculated (<i>all-trans</i> conformer)			Approximate description	
Raman	INS	Raman (^b)	Infrared (^c)	INS	Sym. species	
<i>1,12-diaminodecane</i>						
522	522	523 (1)		523	Ag	in-plane CCN deformation (LAM 5)
	509		510 (0)	510	Bu	in-plane CCN deformation (LAM 4)
	479		474 (7)	474	Bu	in-plane CCN deformation (LAM 6)
433	432	429 (3)		429	Ag	in-plane CCN deformation (LAM 3)
408	407	394 (1)		394	Ag	in-plane CCN deformation (LAM 7)
			315 (106)	314	Au	NH ₂ torsion
373		315 (6)		314	Bg	NH ₂ torsion
	314		310 (2)	314	Bu	in-plane CCN deformation (LAM 2)
			301 (4)	302	Bu	in-plane CCN deformation (LAM 8)
239	237	217 (0)		217	Ag	in-plane CCN deformation (LAM 9)
197	204	173 (0)		172	Bg	out-of-plane CCN deformation (TAM)
	197					
	189		171 (1)	172	Au	out-of-plane CCN deformation (TAM)
175	181	160 (7)		160	Ag	in-plane CCN deformation (LAM 1)
	181		155 (0)	156	Au	out-of-plane CCN deformation (TAM)
		149 (0)		149	Bg	out-of-plane CCN deformation (TAM)
	167		139 (3)	140	Bu	in-plane CCN deformation (LAM 10)
152	153	121 (0)		121	Bg	out-of-plane CCN deformation (TAM)
			116 (3)	117	Au	out-of-plane CCN deformation (TAM)
	138		82 (1)	80	Au	out-of-plane CCN deformation (TAM)
127	132	80 (0)		80	Bg	out-of-plane CCN deformation (TAM)
	118	77 (0)		80	Ag	in-plane CCN deformation (LAM 11)
109		45 (0)		43	Bg	out-of-plane CCN deformation (TAM)
	106		42 (3)	43	Au	out-of-plane CCN deformation (TAM)
89						
	87		34 (0)	35	Bu	in-plane CCN deformation (LAM 12)
	77		18 (0)	18	Au	out-of-plane CCN deformation (TAM)
69	72					
52						
	48					
42						
30						
<i>1,12-diaminodecane-N-d₄</i>						
516	514	513 (0)		513	Ag	in-plane CCN deformation (LAM 5)
	505		506 (1)	506	Bu	in-plane CCN deformation (LAM 4)
	465		457 (13)	457	Bu	in-plane CCN deformation (LAM 6)
427	427	424 (2)		424	Ag	in-plane CCN deformation (LAM 3)
400	399	380 (2)		380	Ag	in-plane CCN deformation (LAM 7)
390						
	311		309 (2)	309	Bu	in-plane CCN deformation (LAM 2)
	300		289 (5)	289	Bu	in-plane CCN deformation (LAM 8)
			241 (55)	241	Au	ND ₂ torsion
275		241 (3)		241	Bg	ND ₂ torsion
231	231	213 (0)		213	Ag	in-plane CCN deformation (LAM 9)
	206					
	202	172 (0)		171	Bg	out-of-plane CCN deformation (TAM)
	196		170 (1)	171	Au	out-of-plane CCN deformation (TAM)
173	177	156 (7)		155	Ag	in-plane CCN deformation (LAM 1)
	181		154 (0)	155	Au	out-of-plane CCN deformation (TAM)
		145 (0)		146	Bg	out-of-plane CCN deformation (TAM)
	161		136 (3)	137	Bu	in-plane CCN deformation (LAM 10)
149	150	120 (0)		119	Bg	out-of-plane CCN deformation (TAM)
	145					
			112 (3)	113	Au	out-of-plane CCN deformation (TAM)
	137		80 (1)	76	Au	out-of-plane CCN deformation (TAM)
131	131	76 (0)		76	Bg	out-of-plane CCN deformation (TAM)
123	119	75 (0)		76	Ag	in-plane CCN deformation (LAM 11)
109		44 (0)		44	Bg	out-of-plane CCN deformation (TAM)
	106		39 (3)	40	Au	out-of-plane CCN deformation (TAM)
89						
	85		33 (0)	34	Bu	in-plane CCN deformation (LAM 12)
			18 (0)	18	Au	out-of-plane CCN deformation (TAM)
68	72					
61						
53	50					
42						
30						

^aB3LYP/6-31G* level of calculation; ^bRaman scattering activities in Å.amu⁻¹; ^cIR intensities in km.mol⁻¹.