TABLE S1. DFT(B3LYP)/6-311++G(d,p) and MP2/6-311++G(d,p) optimized structural parameters and experimental geometries for the two conformers of nicotinamide[a]

Parameter	Theoretical				Experimental[b]		Parameter	Theoretical				Experimental[b]	
	E		*Z*					*E*		*Z*			
	DFT	MP2	DFT	MP2	X-ray diffraction	Neutron diffraction		DFT	MP2	DFT	MP2	X-ray diffraction	Neutron diffraction
Bond length / pm							**Bond length / pm**						
N_1-C_2	133.5	134.4	133.3	134.2	133.7	134.1	C_5-C_6	139.5	140.1	139.3	139.9	137.5	138.3
N_1-C_6	133.6	134.4	133.8	134.5	133.2	133.8	C_5-H_9	108.4	108.6	108.3	108.6	93.0	108.2
C_2-C_3	139.9	140.3	140.1	140.3	139.0	138.4	C_6-H_{10}	108.6	108.8	108.6	108.8	100.0	107.7
C_2-H_7	108.7	108.8	108.5	108.7	93.0	107.4	C_{11}-N_{12}	136.9	137.5	137.3	137.8	132.9	133.7
C_3-C_4	139.7	140.0	139.6	140.0	137.9	138.8	C_{11}=O_{15}	122.0	122.2	121.9	122.1	123.4	123.0
C_3-C_{11}	150.3	150.1	150.2	150.0	149.8	149.2	N_{12}-H_{13}	100.6	100.8	100.7	100.9	89.0	100.0
C_4-C_5	138.8	139.4	139.1	139.7	137.6	138.5	N_{12}-H_{14}	100.9	101.1	100.9	101.1	89.0	101.5
C_4-H_8	108.3	108.6	108.5	108.7	102.0	109.2							
Bond angles / °							**Bond angles / °**						
C_2-N_1-C_6	117.4	116.9	117.5	117.0	117.3	118.0	C_4-C_5-H_9	121.2	121.1	121.1	121.1	121.2	121.5
N_1-C_2-C_3	123.9	123.8	123.8	123.8	123.3	123.1	C_6-C_5-H_9	120.3	120.1	120.4	120.1	120.6	120.2
N_1-C_2-H_7	115.2	115.7	117.1	116.8	117.3	115.4	N_1-C_6-C_5	123.4	123.7	123.5	123.7	123.7	123.1
C_3-C_2-H_7	120.8	120.5	119.1	119.4	119.1	121.5	N_1-C_6-H_{10}	116.0	115.9	116.1	115.9	112.3	116.5
C_2-C_3-C_4	117.7	118.4	117.8	118.5	117.7	118.0	C_5-C_6-H_{10}	120.5	120.4	120.4	120.4	123.9	120.4
C_2-C_3-C_{11}	123.9	122.8	118.1	118.4	123.8	124.1	C_3-C_{11}-N_{12}	116.5	115.0	116.1	114.6	117.9	117.8
C_4-C_3-C_{11}	118.3	118.7	124.0	123.1	118.5	117.9	C_3-C_{11}=O_{15}	121.5	121.8	121.9	122.1	119.1	119.7
C_3-C_4-C_5	118.9	118.3	118.9	118.3	119.8	119.5	N_{12}-C_{11}=O_{15}	122.0	123.2	122.1	123.2	123.0	122.5
C_3-C_4-H_8	119.0	119.6	121.0	120.8	117.9	118.5	C_{11}-N_{12}-H_{13}	121.9	118.9	121.2	118.4	120.1	121.3
C_5-C_4-H_8	122.1	122.1	120.1	120.9	122.4	122.0	C_{11}-N_{12}-H_{14}	116.7	115.6	116.2	115.3	122.5	118.5
C_4-C_5-C_6	118.5	118.8	118.5	118.8	118.2	118.3	H_{13}-N_{12}-H_{14}	117.8	116.7	117.3	116.3	-	119.1
Dihedral angles / °							**Dihedral angles / °**						
C_6-N_1-C_2-C_3	-0.1	0.0	-0.8	-0.7	-	0.1	C_4-C_3-C_{11}-N_{12}	-161.9	-151.4	-24.3	-33.3	-	-158.5
C_6-N_1-C_2-H_7	178.2	178.2	179.2	179.2	-	179.0	C_4-C_3-C_{11}=O_{15}	19.0	30.4	154.6	144.8	-	21.0
C_2-N_1-C_6-C_5	-0.8	-1.1	0.1	0.1	-	-1.1	C_3-C_4-C_5-C_6	0.5	-0.1	-0.2	-0.2	-	1.6
C_2-N_1-C_6-H_{10}	179.5	179.6	-179.6	-179.6	-	178.7	C_3-C_4-C_5-H_9	-179.6	-179.7	179.2	179.2	-	-179.5
N_1-C_2-C_3-C_4	1.2	1.1	1.0	0.8	-	0.4	H_8-C_4-C_5-C_6	-179.3	-179.3	-178.3	-178.4	-	-177.0
N_1-C_2-C_3-C_{11}	179.6	-179.9	179.7	-180.0	-	179.0	H_8-C_4-C_5-H_9	0.6	1.0	1.1	0.9	-	2.0
H_7-C_2-C_3-C_4	-177.0	-177.0	-179.0	-179.1	-	-177.5	C_4-C_5-C_6-N_1	0.6	1.2	0.4	0.3	-	-0.2
H_7-C_2-C_3-C_{11}	1.4	2.0	-0.4	0.1	-	1.2	C_4-C_5-C_6-H_{10}	-179.7	-179.5	-179.9	-180.0	-	-180.0
C_2-C_3-C_4-C_5	-1.3	-1.0	-0.5	-0.4	-	-1.7	H_9-C_5-C_6-N_1	-179.3	-179.2	-179.0	-179.0	-	-179.1
C_2-C_3-C_4-H_8	178.5	178.3	177.6	177.9	-	176.9	H_9-C_5-C_6-H_{10}	0.4	0.1	0.7	0.7	-	1.1
C_{11}-C_3-C_4-C_5	-179.8	180.0	-179.71	-179.5	-	179.6	C_3-C_{11}-N_{12}-H_{13}	17.0	24.9	-20.5	-26.4	-	11.3
C_{11}-C_3-C_4-H_8	0.0	-0.7	-1.0	-1.3	-	-1.8	C_3-C_{11}-N_{12}-H_{14}	175.1	171.3	-174.0	-170.8	-	178.6
C_2-C_3-C_{11}-N_{12}	19.7	29.6	157.2	147.6	-	22.9	O_{15}=C_{11}-N_{12}-H_{13}	-163.9	-157.0	160.6	155.6	-	-168.1
C_2-C_3-C_{11}=O_{15}	-159.4	-148.6	-24.0	-34.4	-	-157.7	O_{15}=C_{11}-N_{12}-H_{14}	-5.7	-10.5	7.2	11.2	-	-0.8

[a] See Scheme 1 for atom numbering.
[b] Crystal data [23].

TABLE S2. Definition of internal coordinates used in the normal coordinate analysis of nicotinamide.

	Definition[a]	Approximate description
S_1	$\nu(N_1\text{-}C_2)+\nu(C_4\text{-}C_5)$	ν ring 1
S_2	$\nu(N_1\text{-}C_2)-\nu(C_4\text{-}C_5)$	ν ring 2
S_3	$\nu(C_2\text{-}C_3)+\nu(C_5\text{-}C_6)$	ν ring 3
S_4	$\nu(C_2\text{-}C_3)-\nu(C_5\text{-}C_6)$	ν ring 4
S_5	$\nu(C_3\text{-}C_4)+\nu(C_6\text{-}N_1)$	ν ring 5
S_6	$\nu(C_3\text{-}C_4)-\nu(C_6\text{-}N_1)$	ν ring 6
S_7	$\nu(C_3\text{-}C_{11})$	ν(C-C)
S_8	$\nu(C_2\text{-}H_7)+\nu(C_6\text{-}H_{10})$	ν(C-H)'1
S_9	$\nu(C_2\text{-}H_7)-\nu(C_6\text{-}H_{10})$	ν(C-H)'2
S_{10}	$\nu(C_4\text{-}H_8)+\nu(C_5\text{-}H_9)$	ν(C-H)''1
S_{11}	$\nu(C_4\text{-}H_8)-\nu(C_5\text{-}H_9)$	ν(C-H)''2
S_{12}	$\nu(C_{11}\text{=}O_{15})$	ν(C=O)
S_{13}	$\nu(C_{11}\text{-}N_{12})$	ν(C-N)
S_{14}	$\nu(N_{12}\text{-}H_{13})+\nu(N_{12}\text{-}H_{14})$	$\nu(NH_2)$s
S_{15}	$\nu(N_{12}\text{-}H_{13})-\nu(N_{12}\text{-}H_{14})$	$\nu(NH_2)$as
S_{16}	$\delta(C_2\text{-}N_1\text{-}C_6)-\delta(N_1\text{-}C_6\text{-}C_5)+\delta(C_6\text{-}C_5\text{-}C_4)-\delta(C_5\text{-}C_4\text{-}C_3)+\delta(C_4\text{-}C_3\text{-}C_2)-\delta(C_3\text{-}C_2\text{-}N_1)$	δ ring 1
S_{17}	$\delta(H_7\text{-}C_2\text{-}N_1)-\delta(H_7\text{-}C_2\text{-}C_3)+\delta(H_{10}\text{-}C_6\text{-}C_5)-\delta(H_{10}\text{-}C_6\text{-}N_1)$	δ(C-H)'1
S_{18}	$\delta(H_7\text{-}C_2\text{-}N_1)-\delta(H_7\text{-}C_2\text{-}C_3)-\delta(H_{10}\text{-}C_6\text{-}C_5)+\delta(H_{10}\text{-}C_6\text{-}N_1)$	δ(C-H)'2
S_{19}	$\delta(H_8\text{-}C_4\text{-}C_3)-\delta(H_8\text{-}C_4\text{-}C_5)+\delta(H_9\text{-}C_5\text{-}C_4)-\delta(H_9\text{-}C_5\text{-}C_6)$	δ(C-H)''1
S_{20}	$\delta(H_8\text{-}C_4\text{-}C_3)-\delta(H_8\text{-}C_4\text{-}C_5)-\delta(H_9\text{-}C_5\text{-}C_4)+\delta(H_9\text{-}C_5\text{-}C_6)$	δ(C-H)''2
S_{21}	$\delta(C_{11}\text{-}C_3\text{-}C_2)-\delta(C_{11}\text{-}C_3\text{-}C_4)$	w(C-C)
S_{22}	$2\delta(C_2\text{-}N_1\text{-}C_6)-\delta(N_1\text{-}C_6\text{-}C_5)-\delta(C_6\text{-}C_5\text{-}C_4)+2\delta(C_5\text{-}C_4\text{-}C_3)-\delta(C_4\text{-}C_3\text{-}C_2)-\delta(C_3\text{-}C_2\text{-}N_1)$	δ ring 2
S_{23}	$\delta(N_1\text{-}C_6\text{-}C_5)-\delta(C_6\text{-}C_5\text{-}C_4)+\delta(C_4\text{-}C_3\text{-}C_2)-\delta(C_3\text{-}C_2\text{-}N_1)$	δ ring 3
S_{24}	$\delta(O_{15}\text{=}C_{11}\text{-}N_{12})-\delta(O_{15}\text{=}C_{11}\text{-}C_3)$	δ(C=O)
S_{25}	$2\delta(N_{12}\text{-}C_{11}\text{-}C_3)-\delta(O_{15}\text{=}C_{11}\text{-}N_{12})-\delta(O_{15}\text{=}C_{11}\text{-}C_3)$	δ(C-C-N)
S_{26}	$2\delta(H_{13}\text{-}N_{12}\text{-}H_{14})-\delta(H_{13}\text{-}N_{12}\text{-}C_{11})-\delta(H_{14}\text{-}N_{12}\text{-}C_{11})$	$\delta(NH_2)$
S_{27}	$\delta(H_{13}\text{-}N_{12}\text{-}C_{11})-\delta(H_{14}\text{-}N_{12}\text{-}C_{11})$	$w(NH_2)$
S_{28}	$\tau(N_1\text{-}C_2\text{-}C_3\text{-}C_4)-\tau(C_2\text{-}C_3\text{-}C_4\text{-}C_5)+\tau(C_3\text{-}C_4\text{-}C_5\text{-}C_6)-\tau(C_4\text{-}C_5\text{-}C_6\text{-}N_1)+\tau(C_5\text{-}C_6\text{-}N_1\text{-}C_2)-\tau(C_6\text{-}N_1\text{-}C_2\text{-}C_3)$	τ ring 1
S_{29}	$2\tau(N_1\text{-}C_2\text{-}C_3\text{-}C_4)-\tau(C_2\text{-}C_3\text{-}C_4\text{-}C_5)-\tau(C_3\text{-}C_4\text{-}C_5\text{-}C_6)+2\tau(C_4\text{-}C_5\text{-}C_6\text{-}N_1)-\tau(C_5\text{-}C_6\text{-}N_1\text{-}C_2)-\tau(C_6\text{-}N_1\text{-}C_2\text{-}C_3)$	τ ring 2
S_{30}	$\tau(C_2\text{-}C_3\text{-}C_4\text{-}C_5)-\tau(C_3\text{-}C_4\text{-}C_5\text{-}C_6)+\tau(C_5\text{-}C_6\text{-}N_1\text{-}C_2)-\tau(C_6\text{-}N_1\text{-}C_2\text{-}C_3)$	τ ring 3
S_{31}	$\tau(O_{15}\text{-}C_{11}\text{-}N_{12}\text{-}H_{13})+\tau(O_{15}\text{-}C_{11}\text{-}N_{12}\text{-}H_{14})$	τ(C-N)
S_{32}	$\tau(O_{15}\text{-}C_{11}\text{-}C_3\text{-}C_2)+\tau(O_{15}\text{-}C_{11}\text{-}C_3\text{-}C_4)$	τ(C-C)
S_{33}	$\gamma(C_{11}\text{-}(N_{12}\text{-}H_{14})\text{-}H_{13})$	$\gamma(NH_2)$
S_{34}	$\gamma(H_8\text{-}(C_4\text{-}C_3)\text{-}C_5)+\gamma(H_9\text{-}(C_5\text{-}C_4)\text{-}C_6)$	γ(C-H)'1
S_{35}	$\gamma(H_8\text{-}(C_4\text{-}C_3)\text{-}C_5)-\gamma(H_9\text{-}(C_5\text{-}C_4)\text{-}C_6)$	γ(C-H)'2
S_{36}	$\gamma(H_7\text{-}(C_2\text{-}N_1)\text{-}C_3)+\gamma(H_{10}\text{-}(C_6\text{-}C_5)\text{-}N_1)$	γ(C-H)''1
S_{37}	$\gamma(H_7\text{-}(C_2\text{-}N_1)\text{-}C_3)-\gamma(H_{10}\text{-}(C_6\text{-}C_5)\text{-}N_1)$	γ(C-H)''2
S_{38}	$\gamma(C_{11}\text{-}(C_3\text{-}C_2)\text{-}C_4)$	γ(C-C)
S_{39}	$\gamma(O_{15}\text{=}(C_{11}\text{-}N_{12})\text{-}C_3)$	γ(C=O)

[a] See Scheme 1 for atom numbering.; s, symmetric; as, anti-symmetric. Normalizing factors (N) are not provided; they can be calculated as $N_j = \sqrt{\sum_i {}^{1}\!/_{c_{ji}^2}}$, where j refers to the internal coordinate $S_j = \sum_i c_{ji} s_i$ and s_i are the primitive internal coordinates: ν, bond stretching; δ, bending; γ, rocking; w, wagging; τ, torsion.

TABLE S3. DFT(B3LYP)/6-311++G(d,p) calculated wavenumbers and intensities, and normal coordinate analysis for nicotinamide (conformer *E*)[a]

Approximate Description	Calculated Wavenumber[b]	Intensity	PED[c]
ν(NH_2)as	3568	43	S_{15}(99)
ν(NH_2)s	3446	48	S_{14}(99)
ν(C-H)''1	3074	5	S_{10}(91)
ν(C-H)''2	3059	8	S_{11}(87)
ν(C-H)'1	3029	9	S_8(60)+S_9(33)
ν(C-H)'2	3018	21	S_9(65)+S_8(35)
ν(C=O)	1726	369	S_{12}(77)
ν ring 1	1609	39	S_1(43)+S_5(14)+S_{20}(12)+S_3(10)
δ(NH_2)	1601	142	S_{26}(88)
ν ring 5	1587	6	S_3(35)+S_5(32)+S_{18}(13)
δ(C-H)'2	1490	2	S_{18}(26)+S_{19}(25)+S_6(20)
δ(C-H)'1	1431	29	S_{17}(33)+S_4(19)+S_2(14)
ν(C-N)	1348	216	S_{13}(30)+S_7(18)+S_{24}(14)+S_{19}(13)+S_{27}(10)
δ(C-H)''1	1343	11	S_{17}(46)+S_{19}(24)
ν ring 4	1273	8	S_2(35)+S_6(27)+S_4(24)
ν ring 6	1212	11	S_{18}(31)+S_6(20)+S_{20}(16)
δ(C-H)''2	1141	15	S_{20}(14)+S_{16}(12)+S_1(10)
ν ring 2	1118	4	S_{20}(38)+S_2(24)+S_5(11)
w(NH_2)	1070	6	S_{27}(54)+S_{13}(24)+S_{12}(10)
ν ring 3	1046	1	S_3(23)+S_1(19)+S_4(18)+S_5(12)+S_{19}(10)
δ ring 1	1027	10	S_{16}(68)+S_6(12)
γ(C-H)'2	1002	1	S_{35}(99)+S_{37}(15)
γ(C-H)''2	976	1	S_{37}(66)+S_{34}(19)+S_{35}(11)
γ(C-H)''1	935	1	S_{36}(75)+S_{34}(13)+S_{37}(19)
γ(C-H)'1	833	10	S_{34}(41)+S_{39}(17)+S_{38}(14)+S_{28}(11)
ν(C-C)	771	5	S_{23}(34)+S_7(20)+S_5(12)
γ(C=O)	741	42	S_{39}(49)+S_{34}(21)+S_{31}(13)+S_{36}(10)
τ ring 1	711	17	S_{28}(100)
δ(C=O)	638	14	S_{23}(34)+S_{22}(27)+S_{24}(24)
δ ring 2	613	9	S_{22}(50)+S_{24}(27)
τ(C-N)	549	21	S_{31}(72)
δ(C-C-N)	491	2	S_{25}(41)+S_{21}(14)
τ ring 3	412	1	S_{30}(89)
τ ring 2	380	7	S_{29}(75)+S_{38}(12)
δ ring 3	372	4	S_7(31)+S_{24}(17)+S_{23}(17)+S_{25}(11)
γ(NH_2)	316	176	S_{33}(88)
w(C-C)	210	15	S_{21}(65)+S_{25}(18)
γ(C-C)	149	3	S_{38}(52)+S_{29}(29)
τ(C-C)	54	14	S_{32}(97)

[a] Wavenumbers in cm^{-1}; intensities in km mol^{-1}. ν, bond stretching; δ, bending; γ, rocking; w, wagging; τ, torsion; s, symmetric; as, anti-symmetric. See Table S2 for definition of coordinates. [b] Scaled by 0.960 in the high wavenumbers region and by 0.988 in the low wavenumbers region (below 1800 cm^{-1}). [c] Only PED values greater than 10 % are given.

TABLE S4. DFT(B3LYP)/6-311++G(d,p) calculated wavenumbers and intensities, and normal coordinate analysis for nicotinamide (conformer *Z*)[a]

Approximate Description	Calculated Wavenumbers[b]	Intensity	PED[c]
ν(NH_2)as	3559	38	S_{15}(99)
ν(NH_2)s	3440	44	S_{14}(99)
ν(C-H)''1	3065	11	S_{10}(80)+S_{11}(14)
ν(C-H)'1	3054	2	S_8(53)+S_9(45)
ν(C-H)''2	3044	8	S_{11}(80)+S_{10}(17)
ν(C-H)'2	3028	12	S_9(51)+S_8(41)
ν(C=O)	1730	362	S_{12}(78)
ν ring 1	1608	63	S_1(41)+S_5(15)+S_20(12)
δ(NH_2)	1601	102	S_{26}(87)
ν ring 5	1587	19	S_3(36)+S_5(30)+S_{18}(12)
δ(C-H)''1	1485	4	S_{18}(28)+S_{19}(26)+S_6(20)
ν ring 4	1434	13	S_{17}(23)+S_4(18)+S_2(15)+S_{18}(10)
δ(C-H)'1	1344	99	S_{17}(51)+S_{13}(11)
ν(C-N)	1334	137	S_{19}(26)+S_{13}(20)+S_7(13)
ν ring 6	1270	1	S_2(30)+S_6(29)+S_4(24)
δ(C-H)'2	1210	12	S_{18}(35)+S_6(19)+S_{20}(18)
δ(C-H)''2	1140	6	S_{20}(20)+S_2(12)+S_{16}(12)+S_1(10)
ν ring 2	1126	12	S_{20}(27)+S_2(22)+S_{27}(11)+S_4(10)+S_5(10)
w(NH_2)	1071	10	S_{27}(49)+S_{13}(28)
ν ring 3	1046	1	S_3(25)+S_1(20)+S_5(14)+S_4(13)
δ ring 1	1026	18	S_{16}(66)+S_6(13)
γ(C-H)''2	993	1	S_{37}(67)+S_{35}(43)
γ(C-H)'2	967	1	S_{35}(68)+S_{37}(32)
γ(C-H)''1	947	1	S_{36}(84)+S_{34}(22)
γ(C-H)'1	823	8	S_{34}(42)+S_{39}(19)+S_{38}(13)+S_{28}(11)
ν(C-C)	770	6	S_{23}(33)+S_7(20)+S_5(12)
γ(C=O)	742	46	S_{39}(47)+S_{34}(24)+S_{31}(12)
τ ring 1	710	16	S_{28}(100)
δ(C=O)	635	12	S_{23}(34)+S_{22}(33)+S_{24}(12)
δ ring 2	614	13	S_{22}(44)+S_{24}(38)
τ(C-N)	549	28	S_{31}(66)+S_{33}(12)
δ(C-C-N)	502	1	S_{25}(37)+S_{21}(15)
τ ring 3	411	4	S_{30}(93)
τ ring 2	381	53	S_{29}(44)+S_{33}(23)
δ ring 3	367	61	S_{24}(32)+S_{23}(23)+S_{25}(17)
γ(NH_2)	363	73	S_{33}(43)+S_7(18)
w(C-C)	206	5	S_{21}(66)+S_{25}(17)
γ(C-C)	149	3	S_{38}(52)+S_{29}(25)
τ(C-C)	60	4	S_{32}(97)

[a] Wavenumbers in cm^{-1}; intensities in km mol^{-1}. ν, bond stretching; δ, bending; γ, rocking; w, wagging; τ, torsion; s, symmetric; as, anti-symmetric. See Table S2 for definition of coordinates. [b] Scaled by 0.960 in the high wavenumbers region and by 0.988 in the low wavenumbers region (below 1800 cm^{-1}). [c] Only PED values greater than 10 % are given.

TABLE S5. Definition of symmetry coordinates used in the normal coordinate analysis for *Dimer 1* of nicotinamide.

	Definition[a]	Sym-metry	Approximate description
S_1	$\nu(N_{1A}\text{-}C_{2A})+\nu(N_{1B}\text{-}C_{2B})$	A_g	ν ring 1
S_2	$\nu(N_{1A}\text{-}C_{2A})-\nu(N_{1B}\text{-}C_{2B})$	A_u	ν ring 1
S_3	$\nu(C_{2A}\text{-}C_{3A})+\nu(C_{2B}\text{-}C_{3B})$	A_g	ν ring 2
S_4	$\nu(C_{2A}\text{-}C_{3A})-\nu(C_{2B}\text{-}C_{3B})$	A_u	ν ring 2
S_5	$\nu(C_{3A}\text{-}C_{4A})+\nu(C_{3B}\text{-}C_{4B})$	A_g	ν ring 3
S_6	$\nu(C_{3A}\text{-}C_{4A})-\nu(C_{3B}\text{-}C_{4B})$	A_u	ν ring 3
S_7	$\nu(C_{4A}\text{-}C_{5A})+\nu(C_{4B}\text{-}C_{5B})$	A_g	ν ring 4
S_8	$\nu(C_{4A}\text{-}C_{5A})-\nu(C_{4B}\text{-}C_{5B})$	A_u	ν ring 4
S_9	$\nu(C_{5A}\text{-}C_{6A})+\nu(C_{5B}\text{-}C_{6B})$	A_g	ν ring 5
S_{10}	$\nu(C_{5A}\text{-}C_{6A})-\nu(C_{5B}\text{-}C_{6B})$	A_u	ν ring 5
S_{11}	$\nu(C_{6A}\text{-}N_{1A})+\nu(C_{6A}\text{-}N_{1A})$	A_g	ν ring 6
S_{12}	$\nu(C_{6A}\text{-}N_{1A})-\nu(C_{6A}\text{-}N_{1A})$	A_u	ν ring 6
S_{13}	$\nu(C_{2A}\text{-}H_{7A})+\nu(C_{2B}\text{-}H_{7B})$	A_g	ν(C-H)1
S_{14}	$\nu(C_{2A}\text{-}H_{7A})-\nu(C_{2B}\text{-}H_{7B})$	A_u	ν(C-H)1
S_{15}	$\nu(C_{3A}\text{-}C_{11A})+\nu(C_{3B}\text{-}C_{11B})$	A_g	ν(C-C)
S_{16}	$\nu(C_{3A}\text{-}C_{11A})-\nu(C_{3B}\text{-}C_{11B})$	A_u	ν(C-C)
S_{17}	$\nu(C_{4A}\text{-}H_{8A})+\nu(C_{4B}\text{-}H_{8B})$	A_g	ν(C-H)2
S_{18}	$\nu(C_{4A}\text{-}H_{8A})-\nu(C_{4B}\text{-}H_{8B})$	A_u	ν(C-H)2
S_{19}	$\nu(C_{5A}\text{-}H_{9A})+\nu(C_{5B}\text{-}H_{9B})$	A_g	ν(C-H)3
S_{20}	$\nu(C_{5A}\text{-}H_{9A})-\nu(C_{5B}\text{-}H_{9B})$	A_u	ν(C-H)3
S_{21}	$\nu(C_{6A}\text{-}H_{10A})+\nu(C_{6B}\text{-}H_{10B})$	A_g	ν(C-H)4
S_{22}	$\nu(C_{6A}\text{-}H_{10A})-\nu(C_{6B}\text{-}H_{10B})$	A_u	ν(C-H)4
S_{23}	$\nu(C_{11A}\text{=}O_{15A})+\nu(C_{11B}\text{=}O_{15B})$	A_g	ν(C=O)
S_{24}	$\nu(C_{11A}\text{=}O_{15A})-\nu(C_{11B}\text{=}O_{15B})$	A_u	ν(C=O)
S_{25}	$\nu(C_{11A}\text{-}N_{12A})+\nu(C_{11B}\text{-}N_{12B})$	A_g	ν(C-N)
S_{26}	$\nu(C_{11A}\text{-}N_{12A})-\nu(C_{11B}\text{-}N_{12B})$	A_u	ν(C-N)
S_{27}	$\nu(N_{12A}\text{-}H_{13A})+\nu(N_{12B}\text{-}H_{13B})$	A_g	ν(N-H)1
S_{28}	$\nu(N_{12A}\text{-}H_{13A})-\nu(N_{12B}\text{-}H_{13B})$	A_u	ν(N-H)1
S_{29}	$\nu(N_{12A}\text{-}H_{14A})+\nu(N_{12B}\text{-}H_{14B})$	A_g	ν(N-H)2
S_{30}	$\nu(N_{12A}\text{-}H_{14A})-\nu(N_{12B}\text{-}H_{14B})$	A_u	ν(N-H)2
S_{31}	$\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})-\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})+\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})-\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})+\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})-\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})+\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})-\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})+\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})-\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})+\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})-\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A_g	δ ring 1
S_{32}	$\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})-\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})+\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})-\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})+\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})-\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})-\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})+\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})-\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})+\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})-\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})+\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A_u	δ ring 1
S_{33}	$\delta(H_{7A}\text{-}C_{2A}\text{-}N_{1A})-\delta(H_{7A}\text{-}C_{2A}\text{-}C_{3A})+\delta(H_{7B}\text{-}C_{2B}\text{-}N_{1B})-\delta(H_{7B}\text{-}C_{2B}\text{-}C_{3B})$	A_g	δ(C-H)1
S_{34}	$\delta(H_{7A}\text{-}C_{2A}\text{-}N_{1A})-\delta(H_{7A}\text{-}C_{2A}\text{-}C_{3A})-\delta(H_{7B}\text{-}C_{2B}\text{-}N_{1B})+\delta(H_{7B}\text{-}C_{2B}\text{-}C_{3B})$	A_u	δ(C-H)1
S_{35}	$\delta(H_{8A}\text{-}C_{4A}\text{-}C_{3A})-\delta(H_{8A}\text{-}C_{4A}\text{-}C_{5A})+\delta(H_{8B}\text{-}C_{4B}\text{-}C_{3B})-\delta(H_{8B}\text{-}C_{4B}\text{-}C_{5B})$	A_g	δ(C-H)2
S_{36}	$\delta(H_{8A}\text{-}C_{4A}\text{-}C_{3A})-\delta(H_{8A}\text{-}C_{4A}\text{-}C_{5A})-\delta(H_{8B}\text{-}C_{4B}\text{-}C_{3B})+\delta(H_{8B}\text{-}C_{4B}\text{-}C_{5B})$	A_u	δ(C-H)2
S_{37}	$\delta(H_{9A}\text{-}C_{5A}\text{-}C_{4A})-\delta(H_{9A}\text{-}C_{5A}\text{-}C_{6A})+\delta(H_{9B}\text{-}C_{5B}\text{-}C_{4B})-\delta(H_{9B}\text{-}C_{5B}\text{-}C_{6B})$	A_g	δ(C-H)3
S_{38}	$\delta(H_{9A}\text{-}C_{5A}\text{-}C_{4A})-\delta(H_{9A}\text{-}C_{5A}\text{-}C_{6A})-\delta(H_{9B}\text{-}C_{5B}\text{-}C_{4B})+\delta(H_{9B}\text{-}C_{5B}\text{-}C_{6B})$	A_u	δ(C-H)3
S_{39}	$\delta(H_{10A}\text{-}C_{6A}\text{-}C_{5A})-\delta(H_{10A}\text{-}C_{6A}\text{-}N_{1A})+\delta(H_{10B}\text{-}C_{6B}\text{-}C_{5B})-\delta(H_{10B}\text{-}C_{6B}\text{-}N_{1B})$	A_g	δ(C-H)4
S_{40}	$\delta(H_{10A}\text{-}C_{6A}\text{-}C_{5A})-\delta(H_{10A}\text{-}C_{6A}\text{-}N_{1A})+\delta(H_{10B}\text{-}C_{6B}\text{-}C_{5B})+\delta(H_{10B}\text{-}C_{6B}\text{-}N_{1B})$	A_u	δ(C-H)4
S_{41}	$\delta(C_{11A}\text{-}C_{3A}\text{-}C_{2A})-\delta(C_{11A}\text{-}C_{3A}\text{-}C_{4A})+\delta(C_{11B}\text{-}C_{3B}\text{-}C_{2B})-\delta(C_{11B}\text{-}C_{3B}\text{-}C_{4B})$	A_g	w(C-C)
S_{42}	$\delta(C_{11A}\text{-}C_{3A}\text{-}C_{2A})-\delta(C_{11A}\text{-}C_{3A}\text{-}C_{4A})-\delta(C_{11B}\text{-}C_{3B}\text{-}C_{2B})+\delta(C_{11B}\text{-}C_{3B}\text{-}C_{4B})$	A_u	w(C-C)
S_{43}	$2\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})-\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})-\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})+2\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})-\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})-\delta(C_{3A}\text{-}C_{2A}\text{-}N_{A})+2\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})-\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})-\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})+2\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})-\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})-\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A_g	δ ring 2
S_{44}	$2\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})-\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})-\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})+2\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})-\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})-$	A_u	δ ring 2

	$\delta(C_{3A}\text{-}C_{2A}\text{-}N_A)\text{-}\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})+\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})+\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})\text{-}2\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})+$ $\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})+\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})$		
S_{45}	$\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})\text{-}\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})+\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})\text{-}\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})+\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})\text{-}$ $\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})+\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})\text{-}\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A_g	δ ring 3
S_{46}	$\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})\text{-}\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})+\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})\text{-}\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})\text{-}\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})+$ $\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})\text{-}\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})+\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A_u	δ ring 3
S_{47}	$2\delta(N_{12A}\text{-}C_{11A}\text{-}C_{3A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{3A})+2\delta(N_{12B}\text{-}C_{11B}\text{-}C_{3B})\text{-}$ $\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}C_{3B})$	A_g	δ(C-C-N)
S_{48}	$2\delta(N_{12A}\text{-}C_{11A}\text{-}C_{3A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{3A})\text{-}2\delta(N_{12B}\text{-}C_{11B}\text{-}C_{3B})+$ $\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})+\delta(O_{15B}\text{=}C_{11B}\text{-}C_{3B})$	A_u	δ(C-C-N)
S_{49}	$\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{3A})+\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}C_{3B})$	A_g	δ(C=O)
S_{50}	$\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{3A})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})+\delta(O_{15B}\text{=}C_{11B}\text{-}C_{3B})$	A_u	δ(C=O)
S_{51}	$2\delta(H_{13A}\text{-}N_{12A}\text{-}H_{14A})\text{-}\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})+2\delta(H_{13B}\text{-}N_{12B}\text{-}H_{14B})\text{-}$ $\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})\text{-}\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	A_g	$\delta(NH_2)$
S_{52}	$2\delta(H_{13A}\text{-}N_{12A}\text{-}H_{14A})\text{-}\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})\text{-}2\delta(H_{13B}\text{-}N_{12B}\text{-}H_{14B})+$ $\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})+\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	A_u	$\delta(NH_2)$
S_{53}	$\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})+\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})\text{-}\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	A_g	$w(NH_2)$
S_{54}	$\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})+\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	A_u	$w(NH_2)$
S_{55}	$\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})+\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})\text{-}\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})+$ $\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})+\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})\text{-}\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})+$ $\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})\text{-}\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})+\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})\text{-}\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})$	A_u	τ ring 1
S_{56}	$\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})+\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})\text{-}\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})+$ $\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})\text{-}\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})+\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})\text{-}$ $\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})+\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})\text{-}\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})+\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})$	A_g	τ ring 1
S_{57}	$2\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})\text{-}\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})+2\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{-}$ $\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})+2\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})\text{-}\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})\text{-}$ $\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})+2\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})\text{-}\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})\text{-}\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})$	A_u	τ ring 2
S_{58}	$2\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})\text{-}\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})+2\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{-}$ $\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})\text{-}2\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})+\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})+$ $\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})\text{-}2\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})+\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})+\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})$	A_g	τ ring 2
S_{59}	$\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})\text{-}\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})+\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})+$ $\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})\text{-}\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})+\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})\text{-}\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})$	A_u	τ ring 3
S_{60}	$\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})\text{-}\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})+\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})\text{-}$ $\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})+\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})\text{-}\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})+\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})$	A_g	τ ring 3
S_{61}	$\tau(O_{15A}\text{=}C_{11A}\text{-}N_{12A}\text{-}H_{13A})+\tau(O_{15B}\text{=}C_{11B}\text{-}N_{12B}\text{-}H_{13B})$	A_u	τ(C-N)
S_{62}	$\tau(O_{15A}\text{=}C_{11A}\text{-}N_{12A}\text{-}H_{13A})\text{-}\tau(O_{15B}\text{=}C_{11B}\text{-}N_{12B}\text{-}H_{13B})$	A_g	τ(C-N)
S_{63}	$\tau(O_{15A}\text{=}C_{11A}\text{-}C_{3A}\text{-}C_{2A})+\tau(O_{15B}\text{=}C_{11B}\text{-}C_{3B}\text{-}C_{2B})$	A_u	τ(C-C)1
S_{64}	$\tau(O_{15A}\text{=}C_{11A}\text{-}C_{3A}\text{-}C_{2A})\text{-}\tau(O_{15B}\text{=}C_{11B}\text{-}C_{3B}\text{-}C_{2B})$	A_g	τ(C-C)1
S_{65}	$\tau(C_{11A}\text{-}C_{3A}\text{-}C_{2A}\text{-}N_{1A})+\tau(C_{11B}\text{-}C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A_u	τ(C-C)2
S_{66}	$\tau(C_{11A}\text{-}C_{3A}\text{-}C_{2A}\text{-}N_{1A})\text{-}\tau(C_{11B}\text{-}C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A_g	τ(C-C)2
S_{67}	$\gamma(H_{9A}\text{-}(C_{5A}\text{-}C_{4A})\text{-}C_{6A})+\gamma(H_{9A}\text{-}(C_{5A}\text{-}C_{4A})\text{-}C_{6A})$	A_u	γ(C-H)1
S_{68}	$\gamma(H_{9A}\text{-}(C_{5A}\text{-}C_{4A})\text{-}C_{6A})\text{-}\gamma(H_{9A}\text{-}(C_{5A}\text{-}C_{4A})\text{-}C_{6A})$	A_g	γ(C-H)1
S_{69}	$\gamma(H_{7A}\text{-}(C_{2A}\text{-}N_{1A})\text{-}C_{3A})+\gamma(H_{7B}\text{-}(C_{2B}\text{-}N_{1B})\text{-}C_{3B})$	A_u	γ(C-H)2
S_{70}	$\gamma(H_{7A}\text{-}(C_{2A}\text{-}N_{1A})\text{-}C_{3A})\text{-}\gamma(H_{7B}\text{-}(C_{2B}\text{-}N_{1B})\text{-}C_{3B})$	A_g	γ(C-H)2
S_{71}	$\gamma(H_{10A}\text{-}(C_{6A}\text{-}C_{5A})\text{-}N_{1A})+\gamma(H_{10B}\text{-}(C_{6B}\text{-}C_{5B})\text{-}N_{1B})$	A_u	γ(C-H)3
S_{72}	$\gamma(H_{10A}\text{-}(C_{6A}\text{-}C_{5A})\text{-}N_{1A})\text{-}\gamma(H_{10B}\text{-}(C_{6B}\text{-}C_{5B})\text{-}N_{1B})$	A_g	γ(C-H)3
S_{73}	$\gamma(H_{8A}\text{-}(C_{4A}\text{-}C_{5A})\text{-}C_{6A})+\gamma(H_{8B}\text{-}(C_{4B}\text{-}C_{5B})\text{-}C_{6B})$	A_u	γ(C-H)4
S_{74}	$\gamma(H_{8A}\text{-}(C_{4A}\text{-}C_{5A})\text{-}C_{6A})\text{-}\gamma(H_{8B}\text{-}(C_{4B}\text{-}C_{5B})\text{-}C_{6B})$	A_g	γ(C-H)4
S_{75}	$\gamma(O_{15A}\text{=}(C_{11A}\text{-}N_{12A})\text{-}C_{3A})+\gamma(O_{15B}\text{=}(C_{11B}\text{-}N_{12B})\text{-}C_{3B})$	A_u	γ(C=O)
S_{76}	$\gamma(O_{15A}\text{=}(C_{11A}\text{-}N_{12A})\text{-}C_{3A})\text{-}\gamma(O_{15B}\text{=}(C_{11B}\text{-}N_{12B})\text{-}C_{3B})$	A_g	γ(C=O)
S_{77}	$\gamma(C_{11A}\text{-}(N_{12A}\text{-}H_{14A})\text{-}H_{13A})+\gamma(C_{11B}\text{-}(N_{12B}\text{-}H_{14B})\text{-}H_{13B})$	A_u	$\gamma(NH_2)$
S_{78}	$\gamma(C_{11A}\text{-}(N_{12A}\text{-}H_{14A})\text{-}H_{13A})\text{-}\gamma(C_{11B}\text{-}(N_{12B}\text{-}H_{14B})\text{-}H_{13B})$	A_g	$\gamma(NH_2)$
S_{79}	$\nu(O_{15A}\text{...}H_{14B})+\nu(O_{15B}\text{...}H_{14A})$	A_g	$\nu_{A\text{...}B}$
S_{80}	$\nu(O_{15A}\text{...}H_{14B})\text{-}\nu(O_{15B}\text{...}H_{14A})$	A_u	$\nu_{A\text{...}B}$
S_{81}	$\delta(C_{11A}\text{...}N_{12B}\text{...}C_{11B})\text{-}\delta(C_{11A}\text{…}O_{15B}\text{...}C_{11B})$	A_g	$\delta_{A\text{...}B}$

S_{82}	$\tau(C_{11B}...N_{12A}...C_{11A}...O_{15A})+\tau(C_{11A}...N_{12B}...C_{11B}\ldots O_{15B})$	A_u	$\tau_{A...B}$
S_{83}	$\tau(C_{11B}...N_{12A}...C_{11A}...O_{15A})-\tau(C_{11A}...N_{12B}...C_{11B}\ldots O_{15B})$	A_g	$\tau_{A...B}$
S_{84}	$\gamma(N_{12A}\ldots C_{11A}...C_{11B}...N_{12B})+\gamma(N_{12A}...C_{11A}...C_{11B}...O_{15B})+\gamma(O_{15A}...C_{11A}...C_{11B}...N_{12B})+\gamma(O_{15A}...C_{11A}...C_{11B}...O_{15B})$	A_u	$\gamma_{A...B}$

[a] See Scheme 1 for atom numbering. ν, bond stretching; δ, bending; γ, rocking; w, wagging; τ, torsion. Normalizing factors (N) are not provided; they can be calculated as $N_j = \sqrt{\sum_i {}^{1}/_{c_i^2}}$, where j refer to the vibrational coordinate and c_i are the coefficients associated with each coordinate in which the vibrational coordinate expands.

TABLE S6. DFT(B3LYP)/6-311++G(d,p) calculated wavenumbers and intensities, and normal coordinate analysis for *Dimer 1* of nicotinamide [a]

Approximate Description	Symmetry	Calculated Wavenumber[b]	Intensity	PED[c]
ν(N-H)1	A_u	3535	178	$S_{28}(97)$
ν(N-H)1	A_g	3534	0	$S_{27}(97)$
ν(N-H)2	A_u	3204	2566	$S_{30}(97)$
ν(N-H)2	A_g	3165	0	$S_{29}(99)$
ν(C-H)2	A_g	3075	0	$S_{17}(81)+S_{19}(18)$
ν(C-H)2	A_u	3075	12	$S_{18}(81)+S_{20}(18)$
ν(C-H)3	A_g	3059	0	$S_{19}(75)+S_{17}(19)$
ν(C-H)3	A_u	3059	20	$S_{20}(75)+S_{18}(19)$
ν(C-H)4	A_g	3029	0	$S_{21}(91)$
ν(C-H)4	A_u	3029	21	$S_{22}(91)$
ν(C-H)1	A_u	3017	43	$S_{14}(98)$
ν(C-H)1	A_g	3017	0	$S_{13}(98)$
ν(C=O)	A_u	1707	788	$S_{24}(56)+S_{52}(16)+S_{26}(13)$
$\delta(NH_2)$	A_g	1696	0	$S_{51}(51)+S_{23}(28)$
$\delta(NH_2)$	A_u	1630	135	$S_{52}(77)+S_{24}(17)$
ν(C=O)	A_g	1612	0	$S_{51}(30)+S_{23}(27)+S_5(12)$
δ(C-H)3	A_u	1609	104	$S_8(29)+S_2(15)+S_6(10)+S_{36}(10)$
δ(C-H)3	A_g	1609	0	$S_7(22)+S_1(11)+S_3(11)+S_{33}(10)+S_{51}(10)$
ν ring 3	A_u	1585	18	$S_{10}(21)+S_6(18)+S_{12}(14)+S_4(13)+S_{40}(11)$
ν ring 3	A_g	1582	0	$S_9(18)+S_{23}(18)+S_5(14)+S_{11}(11)+S_3(10)+S_{39}(10)$
δ(C-H)4	A_g	1493	0	$S_{37}(24)+S_{33}(21)+S_{11}(11)+S_7(10)$
δ(C-H)4	A_u	1492	4	$S_{38}(24)+S_{34}(22)+S_{12}(11)$
ν ring 2	A_g	1431	0	$S_{39}(37)+S_1(15)+S_3(13)$
ν ring 2	A_u	1431	69	$S_{40}(39)+S_2(16)+S_4(13)$
ν(C-N)	A_g	1404	0	$S_{25}(43)+S_{15}(15)+S_{53}(14)+S_{49}(11)$
ν(C-N)	A_u	1393	566	$S_{26}(41)+S_{16}(17)+S_{54}(14)+S_{50}(11)$
δ(C-H)1	A_u	1344	5	$S_{34}(44)+S_{36}(25)+S_{38}(10)+S_{40}(10)$
δ(C-H)1	A_g	1344	0	$S_{33}(44)+S_{35}(25)+S_{37}(10)+S_{39}(10)$
ν ring 1	A_g	1273	0	$S_1(30)+S_{11}(19)+S_3(17)+S_5(10)$
ν ring 1	A_u	1273	11	$S_2(30)+S_{12}(18)+S_4(17)+S_6(10)$
ν ring 6	A_g	1215	0	$S_{39}(25)+S_{11}(19)+S_1(10)+S_9(10)+S_{33}(10)$
ν ring 6	A_u	1214	32	$S_{40}(25)+S_{12}(20)+S_2(10)+S_{10}(10)$
ν ring 4	A_g	1157	0	$S_{37}(21)+S_7(14)+S_{15}(14)+S_{53}(13)+S_{31}(12)$
ν ring 4	A_u	1154	12	$S_{38}(21)+S_8(14)+S_{16}(13)+S_{54}(12)+S_{32}(12)$
δ(C-H)2	A_g	1121	0	$S_{35}(31)+S_1(10)+S_7(10)$
δ(C-H)2	A_u	1120	19	$S_{36}(33)+S_2(11)+S_8(10)$
$w(NH_2)$	A_g	1106	0	$S_{53}(43)+S_{25}(16)$
$w(NH_2)$	A_u	1102	8	$S_{54}(50)+S_{26}(16)+S_{24}(11)$
ν ring 5	A_g	1045	0	$S_9(42)+S_{11}(18)+S_7(13)$
ν ring 5	A_u	1047	1	$S_{10}(41)+S_{12}(18)+S_8(14)$
δ ring 1	A_g	1027	0	$S_{31}(68)+S_5(10)+S_3(10)$
δ ring 1	A_u	1026	27	$S_{32}(68)+S_6(10)+S_4(10)$
γ(C-H)1	A_g	1001	0	$S_{68}(46)+S_{74}(32)+S_{72}(17)$
γ(C-H)1	A_u	1001	3	$S_{67}(46)+S_{73}(32)+S_{71}(17)$
γ(C-H)3	A_u	976	2	$S_{71}(59)+S_{73}(29)+S_{69}(14)$
γ(C-H)3	A_g	976	0	$S_{72}(60)+S_{74}(29)+S_{70}(14)$
γ(C-H)2	A_g	934	0	$S_{70}(84)+S_{72}(10)$
γ(C-H)2	A_u	934	2	$S_{69}(84)+S_{71}(10)$
$\gamma(NH_2)$	A_u	843	88	$S_{78}(72)+S_{61}(32)$

γ(C-H)4	A_g	833	0	$S_{68}(35)+S_{56}(23)+S_{76}(17)+S_{74}(14)$
γ(C-H)4	A_u	832	58	$S_{67}(34)+S_{55}(23)+S_{71}(14)+S_{73}(13)$
γ(NH_2)	A_g	796	0	$S_{77}(80)+S_{62}(29)$
ν(C-C)	A_u	786	18	$S_{46}(25)+S_{16}(19)+S_6(12)$
ν(C-C)	A_g	782	0	$S_{45}(28)+S_{15}(20)+S_5(12)$
γ(C=O)	A_g	736	0	$S_{76}(51)+S_{68}(13)+S_{74}(11)$
γ(C=O)	A_u	731	33	$S_{75}(50)+S_{65}(14)+S_{73}(12)$
τ ring 1	A_g	709	0	$S_{56}(84)$
τ ring 1	A_u	708	46	$S_{55}(83)$
δ(C=O)	A_u	658	42	$S_{50}(43)+S_{46}(41)$
δ(C=O)	A_g	649	0	$S_{49}(40)+S_{45}(40)$
δ ring 2	A_u	622	7	$S_{44}(77)$
δ ring 2	A_g	620	0	$S_{43}(71)+S_{49}(11)$
δ(C-C-N)	A_u	521	46	$S_{48}(44)+S_{42}(10)$
δ(C-C-N)	A_g	507	0	$S_{47}(41)+S_{58}(12)+S_{41}(10)$
τ(C-N)	A_g	443	0	$S_{62}(42)+S_{77}(15)+S_{58}(11)$
τ(C-N)	A_u	437	135	$S_{61}(41)+S_{78}(18)+S_{57}(17)+S_{59}(10)$
τ ring 3	A_u	415	73	$S_{59}(68)+S_{61}(17)$
τ ring 3	A_g	412	0	$S_{60}(74)$
δ ring 3	A_g	402	0	$S_{15}(22)+S_{45}(15)+S_{47}(13)+S_{79}(12)$
τ ring 2	A_u	385	18	$S_{57}(50)+S_{16}(12)$
τ ring 2	A_g	374	0	$S_{58}(69)+S_{62}(12)$
δ ring 3	A_u	372	25	$S_{57}(26)+S_{16}(22)+S_{46}(13)+S_{50}(13)+S_{61}(11)$
w(C-C)	A_u	250	92	$S_{42}(58)+S_{80}(25)$
w(C-C)	A_g	234	0	$S_{41}(56)+S_{81}(19)+S_{47}(12)$
τ(C-C)2	A_g	170	0	$S_{66}(65)+S_{83}(16)$
τ(C-C)2	A_u	163	8	$S_{65}(74)$
$\nu_{A...B}$	A_g	98	0	$S_{79}(81)$
$\delta_{A...B}$	A_g	87	0	$S_{81}(68)$
$\gamma_{A...B}$	A_u	79	15	$S_{84}(60)+S_{63}(42)$
τ(C-C)1	A_g	54	0	$S_{64}(59)+S_{83}(31)$
$\nu_{A...B}$	A_u	51	1	$S_{80}(57)+S_{48}(20)+S_{42}(12)$
$\tau_{A...B}$	A_g	48	0	$S_{83}(54)+S_{64}(39)$
τ(C-C)1	A_u	24	2	$S_{63}(59)+S_{84}(37)$
$\tau_{A...B}$'	A_u	14	1	$S_{82}(68)$

[a] Wavenumbers in cm^{-1}; intensities in km mol^{-1}. ν, bond stretching; δ, bending; γ, rocking; w, wagging; τ, torsion. See Table S5 for definition of symmetry coordinates. [b] Scaled by 0.960 in the high wavenumbers region and by 0.988 in the low wavenumbers region (below 1800 cm^{-1}). [c] Only PED values greater than 10 % are given.

TABLE S7. Definition of symmetry coordinates used in the normal coordinate analysis for the *Dimer 2* of nicotinamide.

	Definition[a]	**Sym-metry**	**Approximate description**
S_1	$\nu(N_{1A}\text{-}C_{2A})$	A	ν ring 1_A
S_2	$\nu(C_{4A}\text{-}C_{5A})$	A	ν ring 2_A
S_3	$\nu(C_{2A}\text{-}C_{3A})$	A	ν ring 3_A
S_4	$\nu(C_{5A}\text{-}C_{6A})$	A	ν ring 4_A
S_5	$\nu(C_{3A}\text{-}C_{4A})$	A	ν ring 5_A
S_6	$\nu(C_{6A}\text{-}N_{1A})$	A	ν ring 6_A
S_7	$\nu(C_{3A}\text{-}C_{11A})$	A	$\nu(C\text{-}C)_A$
S_8	$\nu(C_{2A}\text{-}H_{7A})$	A	$\nu(C\text{-}H)1_A$
S_9	$\nu(C_{6A}\text{-}H_{10A})$	A	$\nu(C\text{-}H)2_A$
S_{10}	$\nu(C_{4A}\text{-}H_{8A})$	A	$\nu(C\text{-}H)3_A$
S_{11}	$\nu(C_{5A}\text{-}H_{9A})$	A	$\nu(C\text{-}H)4_A$
S_{12}	$\nu(C_{11A}\text{=}O_{15A})$	A	$\nu(C\text{=}O)_A$
S_{13}	$\nu(C_{11A}\text{-}N_{12A})$	A	$\nu(C\text{-}N)_A$
S_{14}	$\nu(N_{12A}\text{-}H_{13A})$	A	$\nu(N\text{-}H)1_A$
S_{15}	$\nu(N_{12A}\text{-}H_{14A})$	A	$\nu(N\text{-}H)2_A$
S_{16}	$\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})\text{-}\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})\text{+}\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})\text{-}\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})\text{+}\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})\text{-}\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})$	A	δ ring 1_A
S_{17}	$\delta(H_{7A}\text{-}C_{2A}\text{-}N_{1A})\text{-}\delta(H_{7A}\text{-}C_{2A}\text{-}C_{3A})$	A	$\delta(C\text{-}H)1_A$
S_{18}	$\delta(H_{10A}\text{-}C_{6A}\text{-}C_{5A})\text{-}\delta(H_{10A}\text{-}C_{6A}\text{-}N_{1A})$	A	$\delta(C\text{-}H)2_A$
S_{19}	$\delta(H_{8A}\text{-}C_{4A}\text{-}C_{3A})\text{-}\delta(H_{8A}\text{-}C_{4A}\text{-}C_{5A})$	A	$\delta(C\text{-}H)3_A$
S_{20}	$\delta(H_{9A}\text{-}C_{5A}\text{-}C_{4A})\text{-}\delta(H_{9A}\text{-}C_{5A}\text{-}C_{6A})$	A	$\delta(C\text{-}H)4_A$
S_{21}	$\delta(C_{11A}\text{-}C_{3A}\text{-}C_{2A})\text{-}\delta(C_{11A}\text{-}C_{3A}\text{-}C_{4A})$	A	$w(C\text{-}C)_A$
S_{22}	$2\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})\text{-}\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})\text{-}\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})\text{+}2\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})\text{-}\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})\text{-}\delta(C_{3A}\text{-}C_{2A}\text{-}N_A)$	A	δ ring 2_A
S_{23}	$\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})\text{-}\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})\text{+}\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})\text{-}\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})$	A	δ ring 3_A
S_{24}	$2\delta(N_{12A}\text{-}C_{11A}\text{-}C_{3A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{3A})$	A	$\delta(C\text{-}C\text{-}N)_A$
S_{25}	$\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{3A})$	A	$\delta(C\text{=}O)_A$
S_{26}	$2\delta(H_{13A}\text{-}N_{12A}\text{-}H_{14A})\text{-}\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})$	A	$\delta(NH_2)_A$
S_{27}	$\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})$	A	$w(NH_2)_A$
S_{28}	$\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})\text{+}\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})\text{-}\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{+}\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})$	A	τ ring 1_A
S_{29}	$2\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})\text{-}\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})\text{+}2\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{-}\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})$	A	τ ring 2_A
S_{30}	$\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})\text{-}\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})\text{+}\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})$	A	τ ring 3_A
S_{31}	$\tau(O_{15A}\text{=}C_{11A}\text{-}N_{12A}\text{-}H_{13A})\text{+}\tau(O_{15A}\text{=}C_{11A}\text{-}N_{12A}\text{-}H_{14A})$	A	$\tau(C\text{-}N)_A$
S_{32}	$\tau(O_{15A}\text{=}C_{11A}\text{-}C_{3A}\text{-}C_{2A})\text{+}\tau(O_{15A}\text{=}C_{11A}\text{-}C_{3A}\text{-}C_{4A})$	A	$\tau(C\text{-}C)_A$
S_{33}	$\gamma(H_{8A}\text{-}(C_{4A}\text{-}C_{3A})\text{-}C_{5A})$	A	$\gamma(C\text{-}H)1_A$
S_{34}	$\gamma(H_{9A}\text{-}(C_{5A}\text{-}C_{4A})\text{-}C_{6A})$	A	$\gamma(C\text{-}H)2_A$
S_{35}	$\gamma(H_{7A}\text{-}(C_{2A}\text{-}N_{1A})\text{-}C_{3A})$	A	$\gamma(C\text{-}H)3_A$
S_{36}	$\gamma(H_{10A}\text{-}(C_{6A}\text{-}C_{5A})\text{-}N_{1A})$	A	$\gamma(C\text{-}H)4_A$
S_{37}	$\gamma(O_{15A}\text{=}(C_{11A}\text{-}N_{12A})\text{-}C_{3A})$	A	$\gamma(C\text{=}O)_A$
S_{38}	$\gamma(C_{11A}\text{-}(N_{12A}\text{-}H_{14A})\text{-}H_{13A})$	A	$\gamma(NH_2)_A$
S_{39}	$\gamma(C_{11A}\text{-}(C_{3A}\text{-}C_{2A})\text{-}C_{4A})$	A	$\gamma(C\text{-}C)_A$
S_{40}	$\nu(N_{1B}\text{-}C_{2B})$	A	ν ring 1_B
S_{41}	$\nu(C_{4B}\text{-}C_{5B})$	A	ν ring 2_B
S_{42}	$\nu(C_{2B}\text{-}C_{3B})$	A	ν ring 3_B
S_{43}	$\nu(C_{5B}\text{-}C_{6B})$	A	ν ring 4_B
S_{44}	$\nu(C_{3B}\text{-}C_{4B})$	A	ν ring 5_B
S_{45}	$\nu(C_{6B}\text{-}N_{1B})$	A	ν ring 6_B
S_{46}	$\nu(C_{3B}\text{-}C_{11B})$	A	$\nu(C\text{-}C)_B$

S_{47}	$\nu(C_{2B}\text{-}H_{7B})$	A	$\nu(C\text{-}H)1_B$
S_{48}	$\nu(C_{6B}\text{-}H_{10B})$	A	$\nu(C\text{-}H)2_B$
S_{49}	$\nu(C_{4B}\text{-}H_{8B})$	A	$\nu(C\text{-}H)3_B$
S_{50}	$\nu(C_{5B}\text{-}H_{9B})$	A	$\nu(C\text{-}H)4_B$
S_{51}	$\nu(C_{11B}\text{=}O_{15B})$	A	$\nu(C\text{=}O)_B$
S_{52}	$\nu(C_{11B}\text{-}N_{12B})$	A	$\nu(C\text{-}N)_B$
S_{53}	$\nu(N_{12B}\text{-}H_{13B})$	A	$\nu(N\text{-}H)1_B$
S_{54}	$\nu(N_{12B}\text{-}H_{14B})$	A	$\nu(N\text{-}H)2_B$
S_{55}	$\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})\text{-}\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})+\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})\text{-}\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})+\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})\text{-}\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A	δ ring 1_B
S_{56}	$\delta(H_{7B}\text{-}C_{2B}\text{-}N_{1B})\text{-}\delta(H_{7B}\text{-}C_{2B}\text{-}C_{3B})$	A	$\delta(C\text{-}H)1_B$
S_{57}	$\delta(H_{10B}\text{-}C_{6B}\text{-}C_{5B})\text{-}\delta(H_{10B}\text{-}C_{6B}\text{-}N_{1B})$	A	$\delta(C\text{-}H)2_B$
S_{58}	$\delta(H_{8B}\text{-}C_{4B}\text{-}C_{3B})\text{-}\delta(H_{8B}\text{-}C_{4B}\text{-}C_{5B})$	A	$\delta(C\text{-}H)3_B$
S_{59}	$\delta(H_{9B}\text{-}C_{5B}\text{-}C_{4B})\text{-}\delta(H_{9B}\text{-}C_{5B}\text{-}C_{6B})$	A	$\delta(C\text{-}H)4_B$
S_{60}	$\delta(C_{11B}\text{-}C_{3B}\text{-}C_{2B})\text{-}\delta(C_{11B}\text{-}C_{3B}\text{-}C_{4B})$	A	$w(C\text{-}C)_B$
S_{61}	$2\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})\text{-}\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})\text{-}\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})+2\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})\text{-}\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})\text{-}\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A	δ ring 2_B
S_{62}	$\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})\text{-}\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})+\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})\text{-}\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})$	A	δ ring 3_B
S_{63}	$2\delta(N_{12B}\text{-}C_{11B}\text{-}C_{3B})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}C_{3B})$	A	$\delta(C\text{-}C\text{-}N)_B$
S_{64}	$\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}C_{3B})$	A	$\delta(C\text{=}O)_B$
S_{65}	$2\delta(H_{13B}\text{-}N_{12B}\text{-}H_{14B})\text{-}\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})\text{-}\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	A	$\delta(NH_2)_B$
S_{66}	$\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})\text{-}\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	A	$w(NH_2)_B$
S_{67}	$\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})\text{-}\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})+\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})\text{-}\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})+\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})\text{-}\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})$	A	τ ring 1_B
S_{68}	$2\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})\text{-}\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})\text{-}\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})+2\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})\text{-}\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})\text{-}\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})$	A	τ ring 2_B
S_{69}	$\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})\text{-}\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})+\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})\text{-}\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})$	A	τ ring 3_B
S_{70}	$\tau(O_{15B}\text{=}C_{11B}\text{-}N_{12B}\text{-}H_{13B})+\tau(O_{15B}\text{=}C_{11B}\text{-}N_{12B}\text{-}H_{14B})$	A	$\tau(C\text{-}N)_B$
S_{71}	$\tau(O_{15B}\text{=}C_{11B}\text{-}C_{3B}\text{-}C_{2B})+\tau(O_{15B}\text{=}C_{11B}\text{-}C_{3B}\text{-}C_{4B})$	A	$\tau(C\text{-}C)_B$
S_{72}	$\gamma(H_{8B}\text{-}(C_{4B}\text{-}C_{3B})\text{-}C_{5B})$	A	$\gamma(C\text{-}H)1_B$
S_{73}	$\gamma(H_{9B}\text{-}(C_{5B}\text{-}C_{4B})\text{-}C_{6B})$	A	$\gamma(C\text{-}H)2_B$
S_{74}	$\gamma(H_{7B}\text{-}(C_{2B}\text{-}N_{1B})\text{-}C_{3B})$	A	$\gamma(C\text{-}H)3_B$
S_{75}	$\gamma(H_{10B}\text{-}(C_{6B}\text{-}C_{5B})\text{-}N_{1B})$	A	$\gamma(C\text{-}H)4_B$
S_{76}	$\gamma(O_{15B}\text{=}(C_{11B}\text{-}N_{12B})\text{-}C_{3B})$	A	$\gamma(C\text{=}O)_B$
S_{77}	$\gamma(C_{11B}\text{-}(N_{12B}\text{-}H_{14B})\text{-}H_{13B})$	A	$\gamma(NH_2)_B$
S_{78}	$\gamma(C_{11B}\text{-}(C_{3B}\text{-}C_{2B})\text{-}C_{4B})$	A	$\gamma(C\text{-}C)_B$
S_{79}	$\nu(O_{15B}\ldots N_{12A})+\nu(N_{12B}\ldots N_{1A})$	A	$\nu_{A\ldots B}'$
S_{80}	$\nu(O_{15B}\ldots N_{12A})\text{-}\nu(N_{12B}\ldots N_{1A})$	A	$\nu_{A\ldots B}''$
S_{81}	$\delta(N_{12B}\ldots C_{2A}\ldots N_{1A})\text{-}\delta(N_{12B}\ldots C_{6A}\ldots N_{1A})$	A	$\delta_{A\ldots B}$
S_{82}	$\tau(N_{1A}\ldots C_{11B}\ldots N_{12B}\ldots H_{13B})+\tau(N_{12B}\ldots C_{2A}\ldots N_{1A}\ldots C_{6A})$	A	$\tau_{A\ldots B}'$
S_{83}	$\tau(N_{1A}\ldots C_{11B}\ldots N_{12B}\ldots H_{13B})\text{-}\tau(N_{12B}\ldots C_{2A}\ldots N_{1A}\ldots C_{6A})$	A	$\tau_{A\ldots B}''$
S_{84}	$\gamma(C_{11B}\ldots N_{12A}\ldots N_{1A}\ldots C_{6A})+\gamma(C_{11B}\ldots N_{12A}\ldots N_{1A}\ldots C_{2A})+\gamma(H_{13B}\ldots N_{12A}\ldots N_{1A}\ldots C_{6A})+\gamma(H_{13B}\ldots N_{12A}\ldots N_{1A}\ldots C_{2A})$	A	$\gamma_{A\ldots B}$

[a] See Scheme 1 for atom numbering. ν, bond stretching; δ, bending; γ, rocking; w, wagging; τ, torsion. Normalizing factors (N) are not provided; they can be calculated as $N_j = \sqrt{\sum_i {}^{1}\!/_{c_i^2}}$, where j refer to the vibrational coordinate and c_i are the coefficients associated with each coordinate in which the vibrational coordinate expands.

TABLE S8. DFT(B3LYP)/6-311++G(d,p) calculated wavenumbers and intensities, and normal coordinate analysis for *Dimer 2* of nicotinamide [a]

Approximate Description	Symmetry	Calculated Wavenumber[b]	Intensity	PED[c]
ν(N-H)1_B	A	3537	96	S_{53}(94)
ν(N-H)2_A	A	3532	120	S_{15}(78)+S_{14}(22)
ν(N-H)1_A	A	3388	283	S_{14}(78)+S_{15}(22)
ν(N-H)2_B	A	3293	625	S_{54}(94)
ν(C-H)3_B	A	3075	5	S_{49}(78)+S_{50}(21)
ν(C-H)3_A	A	3073	8	S_{10}(66)+S_{11}(31)
ν(C-H)1_A	A	3069	4	S_8(97)
ν(C-H)4_B	A	3059	6	S_{50}(71)+S_{49}(21)
ν(C-H)4_A	A	3059	10	S_{11}(71)+S_{10}(30)
ν(C-H)2_A	A	3032	13	S_9(93)
ν(C-H)2_B	A	3029	10	S_{48}(92)
ν(C-H)1_B	A	3018	21	S_{47}(98)
ν(C=O)$_A$	A	1721	334	S_{12}(78)
ν(C=O)$_B$	A	1697	514	S_{51}(51)+S_{65}(22)+S_{52}(11)
δ(NH_2)$_B$	A	1635	114	S_{65}(71)+S_{51}(23)
δ(NH_2)$_A$	A	1629	105	S_{26}(78)
ν ring 2_A	A	1616	8	S_2(30)+S_1(14)+S_{17}(13)+S_3(13)
ν ring 2_B	A	1609	54	S_{41}(39)+S_{40}(15)+S_{44}(11)+S_{58}(10)
ν ring 5_A	A	1595	18	S_5(37)+S_6(16)+S_4(13)+S_{18}(10)
ν ring 5_B	A	1585	8	S_{43}(21)+S_{42}(14)+S_{44}(17)+S_{45}(14)+S_{57}(10)
δ(C-H)1_A	A	1503	9	S_{17}(39)+S_{20}(34)+S_6(11)
δ(C-H)1_B	A	1491	1	S_{59}(35)+S_{56}(33)+S_{45}(10)
δ(C-H)2_A	A	1434	36	S_{18}(42)+S_1(19)+S_3(11)
δ(C-H)2_B	A	1431	38	S_{57}(39)+S_{40}(19)+S_{42}(13)
ν(C-N)$_B$	A	1377	201	S_{52}(31)+S_{17}(16)+S_{46}(10)
δ(C-H)3_A	A	1364	94	S_{17}(31)+S_{52}(17)+S_{19}(12)
ν(C-N)$_A$	A	1355	130	S_{13}(30)+S_7(16)+S_{25}(13)
δ(C-H)3_B	A	1345	3	S_{56}(44)+S_{58}(25)+S_{57}(10)+S_{59}(10)
ν ring 3_A	A	1277	4	S_1(42)+S_6(18)+S_3(15)
ν ring 3_B	A	1273	6	S_{40}(30)+S_{42}(17)+S_{45}(18)+S_{44}(11)
ν ring 6_A	A	1214	26	S_{18}(52)+S_6(30)
ν ring 6_B	A	1214	5	S_{57}(30)+S_{40}(18)+S_{45}(16)
δ(C-H)4_A	A	1149	2	S_{20}(42)+S_{59}(30)+S_{41}(11)
δ(C-H)4_B	A	1148	20	S_{59}(41)+S_{20}(31)+S_{41}(11)
ν ring 1_B	A	1120	9	S_{58}(55)+S_{40}(12)+S_{41}(12)
ν ring 1_A	A	1117	5	S_{19}(43)+S_1(12)+S_2(11)+S_{20}(10)
w(NH_2)$_B$	A	1092	4	S_{66}(48)+S_{52}(17)+S_{51}(10)
w(NH_2)$_A$	A	1089	6	S_{27}(46)+S_{13}(28)
ν ring 4_A	A	1047	3	S_4(35)+S_6(19)+S_2(10)
ν ring 4_B	A	1047	1	S_{43}(37)+S_{45}(16)+S_{41}(12)
δ ring 1_A	A	1036	8	S_{16}(69)+S_5(10)
δ ring 1_B	A	1027	14	S_{55}(68)+S_{44}(10)
γ(C-H)1_A	A	1002	1	S_{33}(59)+S_{34}(31)+S_{36}(10)
γ(C-H)1_B	A	999	2	S_{73}(48)+S_{72}(42)+S_{75}(10)
γ(C-H)4_A	A	975	4	S_{36}(47)+S_{33}(21)+S_{35}(21)
γ(C-H)4_B	A	974	1	S_{75}(48)+S_{72}(29)+S_{74}(14)
γ(C-H)3_A	A	943	9	S_{35}(73)+S_{36}(19)+S_{34}(13)
γ(C-H)3_B	A	936	1	S_{74}(82)+S_{75}(12)
γ(C-H)2_A	A	833	8	S_{34}(35)+S_{37}(18)+S_{36}(15)+S_{39}(12)+S_{28}(12)

$\gamma(C\text{-}H)2_B$	A	832	12	$S_{73}(34)+S_{76}(17)+S_{75}(14)+S_{78}(14)$
$\nu(C\text{-}C)_B$	A	779	7	$S_{46}(44)+S_{62}(40)$
$\nu(C\text{-}C)_A$	A	776	5	$S_{23}(33)+S_{7}(25)+S_{62}(18)$
$\gamma(C{=}O)_A$	A	754	10	$S_{37}(35)+S_{31}(15)+S_{70}(21)+S_{76}(12)$
$\delta(C{=}O)_B$	A	748	71	$S_{64}(21)+S_{76}(20)+S_{70}(14)+S_{31}(12)$
$\gamma(C{=}O)_B$	A	718	7	$S_{67}(29)+S_{76}(18)+S_{28}(15)+S_{77}(12)$
τ ring 1_A	A	712	41	$S_{28}(70)+S_{67}(26)$
τ ring 1_B	A	700	24	$S_{67}(45)+S_{77}(21)+S_{76}(16)+S_{70}(10)$
δ ring 3_B	A	645	17	$S_{62}(51)+S_{64}(34)$
$\delta(C{=}O)_A$	A	643	13	$S_{23}(34)+S_{22}(23)+S_{25}(20)$
δ ring 2_A	A	621	4	$S_{22}(39)+S_{61}(19)+S_{31}(13)+S_{25}(11)$
δ ring 2_B	A	619	7	$S_{61}(54)+S_{22}(18)+S_{64}(12)$
$\tau(C\text{-}N)_A$	A	615	13	$S_{31}(42)+S_{25}(17)+S_{37}(11)$
$\delta(C\text{-}C\text{-}N)_B$	A	516	9	$S_{63}(61)+S_{78}(11)$
$\delta(C\text{-}C\text{-}N)_A$	A	503	21	$S_{24}(67)+S_{38}(12)$
$\gamma(NH_2)_A$	A	464	179	$S_{38}(84)$
$\gamma(NH_2)_B$	A	433	53	$S_{77}(65)+S_{70}(23)$
τ ring 3_A	A	415	6	$S_{30}(62)+S_{69}(28)$
τ ring 3_B	A	410	25	$S_{69}(57)+S_{30}(20)+S_{77}(15)$
τ ring 2_A	A	394	13	$S_{29}(59)+S_{39}(11)$
$\tau(C\text{-}N)_B$	A	385	10	$S_{52}(50)+S_{29}(18)+S_{46}(10)$
δ ring 3_A	A	375	1	$S_{7}(32)+S_{23}(17)+S_{25}(17)$
τ ring 2_B	A	372	10	$S_{68}(40)+S_{46}(14)+S_{77}(13)$
$w(C\text{-}C)_B$	A	235	26	$S_{60}(76)+S_{83}(17)$
$w(C\text{-}C)_A$	A	220	19	$S_{21}(73)+S_{24}(17)$
$\gamma(C\text{-}C)_B$	A	163	4	$S_{78}(40)+S_{68}(28)+S_{82}(25)$
$\gamma(C\text{-}C)_A$	A	156	2	$S_{39}(60)+S_{29}(30)$
$\nu_{A\ldots B}'$	A	90	2	$S_{79}(63)+S_{32}(21)+S_{82}(13)$
$\tau(C\text{-}C)_A$	A	87	7	$S_{32}(44)+S_{84}(41)+S_{71}(15)$
$\delta_{A\ldots B}$	A	72	1	$S_{81}(81)+S_{84}(19)$
$\tau_{A\ldots B}'$	A	68	1	$S_{82}(62)+S_{71}(21)+S_{32}(17)$
$\tau(C\text{-}C)_B$	A	47	1	$S_{82}(57)+S_{80}(24)+S_{71}(21)$
$\gamma_{A\ldots B}$	A	34	2	$S_{84}(70)+S_{80}(13)+S_{71}(11)$
$\nu_{A\ldots B}''$	A	20	1	$S_{80}(71)+S_{81}(26)$
$\tau_{A\ldots B}''$	A	15	1	$S_{83}(95)$

[a] Wavenumbers in cm^{-1}; intensities in km mol^{-1}. ν, bond stretching; δ, bending; γ, rocking; w, wagging; τ, torsion. See Table S7 for definition of symmetry coordinates. [b] Scaled by 0.960 in the high wavenumbers region and by 0.988 in the low wavenumbers region (below 1800 cm^{-1}). [c] Only PED values greater than 10 % are given.

TABLE S9. Definition of symmetry coordinates used in the normal coordinate analysis for *Dimer 1* of picolinamide.

	Definition[a]	Sym-metry	Approximate description
S_1	$\nu(N_{1A}\text{-}C_{6A})+\nu(N_{1B}\text{-}C_{6B})$	A_g	ν ring 1’
S_2	$\nu(N_{1A}\text{-}C_{6A})-\nu(N_{1B}\text{-}C_{6B})$	B_u	ν ring 1’’
S_3	$\nu(N_{1A}\text{-}C_{2A})+\nu(N_{1B}\text{-}C_{2B})$	A_g	ν ring 2’
S_4	$\nu(N_{1A}\text{-}C_{2A})-\nu(N_{1B}\text{-}C_{2B})$	B_u	ν ring 2’’
S_5	$\nu(C_{2A}\text{-}C_{3A})+\nu(C_{2B}\text{-}C_{3B})$	A_g	ν ring 3’
S_6	$\nu(C_{2A}\text{-}C_{3A})-\nu(C_{2B}\text{-}C_{3B})$	B_u	ν ring 3’’
S_7	$\nu(C_{3A}\text{-}C_{4A})+\nu(C_{3B}\text{-}C_{4B})$	A_g	ν ring 4’
S_8	$\nu(C_{3A}\text{-}C_{4A})-\nu(C_{3B}\text{-}C_{4B})$	B_u	ν ring 4’’
S_9	$\nu(C_{4A}\text{-}C_{5A})+\nu(C_{4B}\text{-}C_{5B})$	A_g	ν ring 5’
S_{10}	$\nu(C_{4A}\text{-}C_{5A})-\nu(C_{4B}\text{-}C_{5B})$	B_u	ν ring 5’’
S_{11}	$\nu(C_{5A}\text{-}C_{6A})+\nu(C_{5B}\text{-}C_{6B})$	A_g	ν ring 6’
S_{12}	$\nu(C_{5A}\text{-}C_{6A})-\nu(C_{5B}\text{-}C_{6B})$	B_u	ν ring 6’’
S_{13}	$\nu(C_{6A}\text{-}H_{10A})+\nu(C_{6B}\text{-}H_{10B})$	A_g	ν(C-H)1’
S_{14}	$\nu(C_{6A}\text{-}H_{10A})-\nu(C_{6B}\text{-}H_{10B})$	B_u	ν(C-H)1’’
S_{15}	$\nu(C_{2A}\text{-}C_{11A})+\nu(C_{2B}\text{-}C_{11B})$	A_g	ν(C-C)’
S_{16}	$\nu(C_{2A}\text{-}C_{11A})-\nu(C_{2B}\text{-}C_{11B})$	B_u	ν(C-C)’’
S_{17}	$\nu(C_{3A}\text{-}H_{7A})+\nu(C_{3B}\text{-}H_{7B})$	A_g	ν(C-H)2’
S_{18}	$\nu(C_{3A}\text{-}H_{7A})-\nu(C_{3B}\text{-}H_{7B})$	B_u	ν(C-H)2’’
S_{19}	$\nu(C_{4A}\text{-}H_{8A})+\nu(C_{4B}\text{-}H_{8B})$	A_g	ν(C-H)3’
S_{20}	$\nu(C_{4A}\text{-}H_{8A})-\nu(C_{4B}\text{-}H_{8B})$	B_u	ν(C-H)3’’
S_{21}	$\nu(C_{5A}\text{-}H_{9A})+\nu(C_{5B}\text{-}H_{9B})$	A_g	ν(C-H)4’
S_{22}	$\nu(C_{5A}\text{-}H_{9A})-\nu(C_{5B}\text{-}H_{9B})$	B_u	ν(C-H)4’’
S_{23}	$\nu(C_{11A}\text{=}O_{15A})+\nu(C_{11B}\text{=}O_{15B})$	A_g	ν(C=O)’
S_{24}	$\nu(C_{11A}\text{=}O_{15A})-\nu(C_{11B}\text{=}O_{15B})$	B_u	ν(C=O)’’
S_{25}	$\nu(C_{11A}\text{-}N_{12A})+\nu(C_{11B}\text{-}N_{12B})$	A_g	ν(C-N)’
S_{26}	$\nu(C_{11A}\text{-}N_{12A})-\nu(C_{11B}\text{-}N_{12B})$	B_u	ν(C-N)’’
S_{27}	$\nu(N_{12}\text{-}H_{13})+\nu(N_{12}\text{-}H_{13})$	A_g	ν(N-H)1’
S_{28}	$\nu(N_{12}\text{-}H_{13})-\nu(N_{12}\text{-}H_{13})$	B_u	ν(N-H)1’’
S_{29}	$\nu(N_{12}\text{-}H_{14})+\nu(N_{12}\text{-}H_{14})$	A_g	ν(N-H)2’
S_{30}	$\nu(N_{12}\text{-}H_{14})-\nu(N_{12}\text{-}H_{14})$	B_u	ν(N-H)2’’
S_{31}	$\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})-\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})+\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})-\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})+\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})-\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})+\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})-\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})+\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})-\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})+\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})-\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})$	A_g	δ ring 1’
S_{32}	$\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})-\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})+\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})-\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})+\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})-\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})-\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})+\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})-\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})+\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})-\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})+\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})$	B_u	δ ring 1’’
S_{33}	$\delta(H_{10A}\text{-}C_{6A}\text{-}C_{5A})-\delta(H_{10A}\text{-}C_{6A}\text{-}N_{1A})+\delta(H_{10B}\text{-}C_{6B}\text{-}C_{5B})-\delta(H_{10B}\text{-}C_{6B}\text{-}N_{1B})$	A_g	δ(C-H)1’
S_{34}	$\delta(H_{10A}\text{-}C_{6A}\text{-}C_{5A})-\delta(H_{10A}\text{-}C_{6A}\text{-}N_{1A})-\delta(H_{10B}\text{-}C_{6B}\text{-}C_{5B})+\delta(H_{10B}\text{-}C_{6B}\text{-}N_{1B})$	B_u	δ(C-H) 1’’
S_{35}	$\delta(H_{7A}\text{-}C_{3A}\text{-}C_{2A})-\delta(H_{7A}\text{-}C_{3A}\text{-}C_{4A})+\delta(H_{7B}\text{-}C_{3B}\text{-}C_{2B})-\delta(H_{7B}\text{-}C_{3B}\text{-}C_{4B})$	A_g	δ(C-H)2’
S_{36}	$\delta(H_{7A}\text{-}C_{3A}\text{-}C_{2A})-\delta(H_{7A}\text{-}C_{3A}\text{-}C_{4A})-\delta(H_{7B}\text{-}C_{3B}\text{-}C_{2B})+\delta(H_{7B}\text{-}C_{3B}\text{-}C_{4B})$	B_u	δ(C-H)2’’
S_{37}	$\delta(H_{8A}\text{-}C_{4A}\text{-}C_{3A})-\delta(H_{8A}\text{-}C_{4A}\text{-}C_{5A})+\delta(H_{8B}\text{-}C_{4B}\text{-}C_{3B})-\delta(H_{8B}\text{-}C_{4B}\text{-}C_{5B})$	A_g	δ(C-H)3’
S_{38}	$\delta(H_{8A}\text{-}C_{4A}\text{-}C_{3A})-\delta(H_{8A}\text{-}C_{4A}\text{-}C_{5A})-\delta(H_{8B}\text{-}C_{4B}\text{-}C_{3B})+\delta(H_{8B}\text{-}C_{4B}\text{-}C_{5B})$	B_u	δ(C-H)3’’
S_{39}	$\delta(H_{9A}\text{-}C_{5A}\text{-}C_{4A})-\delta(H_{9A}\text{-}C_{5A}\text{-}C_{6A})+\delta(H_{9B}\text{-}C_{5B}\text{-}C_{4B})-\delta(H_{9B}\text{-}C_{5B}\text{-}C_{6B})$	A_g	δ(C-H)4’
S_{40}	$\delta(H_{9A}\text{-}C_{5A}\text{-}C_{4A})-\delta(H_{9A}\text{-}C_{5A}\text{-}C_{6A})-\delta(H_{9B}\text{-}C_{5B}\text{-}C_{4B})+\delta(H_{9B}\text{-}C_{5B}\text{-}C_{6B})$	B_u	δ(C-H)4’’
S_{41}	$\delta(C_{11A}\text{-}C_{2A}\text{-}N_{1A})-\delta(C_{11A}\text{-}C_{2A}\text{-}C_{3A})+\delta(C_{11B}\text{-}C_{2B}\text{-}N_{1B})-\delta(C_{11B}\text{-}C_{2B}\text{-}C_{3B})$	A_g	w(C-C)’
S_{42}	$\delta(C_{11A}\text{-}C_{2A}\text{-}N_{1A})-\delta(C_{11A}\text{-}C_{2A}\text{-}C_{3A})-\delta(C_{11B}\text{-}C_{2B}\text{-}N_{1B})+\delta(C_{11B}\text{-}C_{2B}\text{-}C_{3B})$	B_u	w(C-C)’’
S_{43}	$2\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})-\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})-\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})+2\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})-\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})-\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})+2\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})-\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})-\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})+2\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})-\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})-\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})$	A_g	δ ring 2’
S_{44}	$2\delta(N_{1A}\text{-}C_{6A}\text{-}C_{5A})-\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})-\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})+2\delta(C_{4A}\text{-}C_{3A}\text{-}C_{2A})-\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})-$	B_u	δ ring 2’’

	$\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})\text{-}2\delta(N_{1B}\text{-}C_{6B}\text{-}C_{5B})+\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})+\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})\text{-}2\delta(C_{4B}\text{-}C_{3B}\text{-}C_{2B})+\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})+\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})$		
S_{45}	$\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})\text{-}\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})+\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})\text{-}\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})+\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})\text{-}\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})+\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})\text{-}\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})$	A_g	δ ring 3’
S_{46}	$\delta(C_{6A}\text{-}C_{5A}\text{-}C_{4A})\text{-}\delta(C_{5A}\text{-}C_{4A}\text{-}C_{3A})+\delta(C_{3A}\text{-}C_{2A}\text{-}N_{1A})\text{-}\delta(C_{2A}\text{-}N_{1A}\text{-}C_{6A})\text{-}\delta(C_{6B}\text{-}C_{5B}\text{-}C_{4B})+\delta(C_{5B}\text{-}C_{4B}\text{-}C_{3B})\text{-}\delta(C_{3B}\text{-}C_{2B}\text{-}N_{1B})+\delta(C_{2B}\text{-}N_{1B}\text{-}C_{6B})$	B_u	δ ring 3’’
S_{47}	$2\delta(N_{12A}\text{-}C_{11A}\text{-}C_{2A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{2A})+2\delta(N_{12B}\text{-}C_{11B}\text{-}C_{2B})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}C_{2B})$	A_g	δ(C-C-N)’
S_{48}	$2\delta(N_{12A}\text{-}C_{11A}\text{-}C_{2A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{2A})\text{-}2\delta(N_{12B}\text{-}C_{11B}\text{-}C_{2B})+\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})+\delta(O_{15B}\text{=}C_{11B}\text{-}C_{2B})$	B_u	δ(C-C-N)’’
S_{49}	$\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{2A})+\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}C_{2B})$	A_g	δ(C=O)’
S_{50}	$\delta(O_{15A}\text{=}C_{11A}\text{-}N_{12A})\text{-}\delta(O_{15A}\text{=}C_{11A}\text{-}C_{2A})\text{-}\delta(O_{15B}\text{=}C_{11B}\text{-}N_{12B})+\delta(O_{15B}\text{=}C_{11B}\text{-}C_{2B})$	B_u	δ(C=O)’’
S_{51}	$2\delta(H_{13A}\text{-}N_{12A}\text{-}H_{14A})\text{-}\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})+2\delta(H_{13B}\text{-}N_{12B}\text{-}H_{14B})\text{-}\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})\text{-}\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	A_g	δ(NH_2)’
S_{52}	$2\delta(H_{13A}\text{-}N_{12A}\text{-}H_{14A})\text{-}\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})\text{-}2\delta(H_{13B}\text{-}N_{12B}\text{-}H_{14B})+\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})+\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	B_u	δ(NH_2)’’
S_{53}	$\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})+\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})\text{-}\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	A_g	w(NH_2)’
S_{54}	$\delta(H_{13A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{14A}\text{-}N_{12A}\text{-}C_{11A})\text{-}\delta(H_{13B}\text{-}N_{12B}\text{-}C_{11B})+\delta(H_{14B}\text{-}N_{12B}\text{-}C_{11B})$	B_u	w(NH_2)’’
S_{55}	$\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})\text{-}\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})+\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})\text{-}\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})+\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{-}\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})+\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})\text{-}\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})+\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})\text{-}\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})+\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})\text{-}\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})$	A_u	τ ring 1’
S_{56}	$\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})\text{-}\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})+\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})\text{-}\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})+\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{-}\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})+\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})\text{-}\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})+\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})\text{-}\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})+\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})$	B_g	τ ring 1’’
S_{57}	$2\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})\text{-}\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})+2\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})\text{-}\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{-}\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})+2\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})\text{-}\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})\text{-}\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})+2\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})\text{-}\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})\text{-}\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})$	A_u	τ ring 2’
S_{58}	$2\tau(C_{6A}\text{-}N_{1A}\text{-}C_{2A}\text{-}C_{3A})\text{-}\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})+2\tau(C_{3A}\text{-}C_{4A}\text{-}C_{5A}\text{-}C_{6A})\text{-}\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{-}\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}2\tau(C_{6B}\text{-}N_{1B}\text{-}C_{2B}\text{-}C_{3B})+\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})+\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})\text{-}2\tau(C_{3B}\text{-}C_{4B}\text{-}C_{5B}\text{-}C_{6B})+\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})+\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})$	B_g	τ ring 2’’
S_{59}	$\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})+\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{-}\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})+\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})\text{-}\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})+\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})\text{-}\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})$	A_u	τ ring 3’
S_{60}	$\tau(N_{1A}\text{-}C_{2A}\text{-}C_{3A}\text{-}C_{4A})\text{-}\tau(C_{2A}\text{-}C_{3A}\text{-}C_{4A}\text{-}C_{5A})+\tau(C_{4A}\text{-}C_{5A}\text{-}C_{6A}\text{-}N_{1A})\text{-}\tau(C_{5A}\text{-}C_{6A}\text{-}N_{1A}\text{-}C_{2A})\text{-}\tau(N_{1B}\text{-}C_{2B}\text{-}C_{3B}\text{-}C_{4B})+\tau(C_{2B}\text{-}C_{3B}\text{-}C_{4B}\text{-}C_{5B})\text{-}\tau(C_{4B}\text{-}C_{5B}\text{-}C_{6B}\text{-}N_{1B})+\tau(C_{5B}\text{-}C_{6B}\text{-}N_{1B}\text{-}C_{2B})$	B_g	τ ring 3’’
S_{61}	$\tau(O_{15A}\text{=}C_{11A}\text{-}N_{12A}\text{-}H_{13A})+\tau(O_{15B}\text{=}C_{11B}\text{-}N_{12B}\text{-}H_{13B})$	A_u	τ(C-N)’
S_{62}	$\tau(O_{15A}\text{=}C_{11A}\text{-}N_{12A}\text{-}H_{13A})\text{-}\tau(O_{15B}\text{=}C_{11B}\text{-}N_{12B}\text{-}H_{13B})$	B_g	τ(C-N)’’
S_{63}	$\tau(O_{15A}\text{=}C_{11A}\text{-}C_{2A}\text{-}N_{1A})+\tau(O_{15B}\text{=}C_{11B}\text{-}C_{2B}\text{-}N_{1B})$	A_u	τ(C-C)1’
S_{64}	$\tau(O_{15A}\text{=}C_{11A}\text{-}C_{2A}\text{-}N_{1A})\text{-}\tau(O_{15B}\text{=}C_{11B}\text{-}C_{2B}\text{-}N_{1B})$	B_g	τ(C-C)1’’
S_{65}	$\tau(C_{11A}\text{-}C_{2A}\text{-}N_{1A}\text{-}C_{6A})+\tau(C_{11B}\text{-}C_{2B}\text{-}N_{1B}\text{-}C_{6B})$	A_u	τ(C-C)2’
S_{66}	$\tau(C_{11A}\text{-}C_{2A}\text{-}N_{1A}\text{-}C_{6A})\text{-}\tau(C_{11B}\text{-}C_{2B}\text{-}N_{1B}\text{-}C_{6B})$	B_g	τ(C-C)2’’
S_{67}	$\gamma(H_{8A}\text{-}(C_{4A}\text{-}C_{3A})\text{-}C_{5A})+\gamma(H_{8B}\text{-}(C_{4B}\text{-}C_{3B})\text{-}C_{5B})$	A_u	γ(C-H)1’
S_{68}	$\gamma(H_{8A}\text{-}(C_{4A}\text{-}C_{3A})\text{-}C_{5A})\text{-}\gamma(H_{8B}\text{-}(C_{4B}\text{-}C_{3B})\text{-}C_{5B})$	B_g	γ(C-H)1’’
S_{69}	$\gamma(H_{10A}\text{-}(C_{6A}\text{-}N_{1A})\text{-}C_{5A})+\gamma(H_{10B}\text{-}(C_{6B}\text{-}N_{1B})\text{-}C_{5B})$	A_u	γ(C-H)2’
S_{70}	$\gamma(H_{10A}\text{-}(C_{6A}\text{-}N_{1A})\text{-}C_{5A})\text{-}\gamma(H_{10B}\text{-}(C_{6B}\text{-}N_{1B})\text{-}C_{5B})$	B_g	γ(C-H)2’’
S_{71}	$\gamma(H_{9A}\text{-}(C_{5A}\text{-}C_{4A})\text{-}C_{6A})+\gamma(H_{9B}\text{-}(C_{5B}\text{-}C_{4B})\text{-}C_{6B})$	A_u	γ(C-H)3’
S_{72}	$\gamma(H_{9A}\text{-}(C_{5A}\text{-}C_{4A})\text{-}C_{6A})\text{-}\gamma(H_{9B}\text{-}(C_{5B}\text{-}C_{4B})\text{-}C_{6B})$	B_g	γ(C-H)3’’
S_{73}	$\gamma(H_{7A}\text{-}(C_{3A}\text{-}C_{2A})\text{-}C_{4A})+\gamma(H_{7B}\text{-}(C_{3B}\text{-}C_{2B})\text{-}C_{4B})$	A_u	γ(C-H)4’
S_{74}	$\gamma(H_{7A}\text{-}(C_{3A}\text{-}C_{2A})\text{-}C_{4A})\text{-}\gamma(H_{7B}\text{-}(C_{3B}\text{-}C_{2B})\text{-}C_{4B})$	B_g	γ(C-H)4’’
S_{75}	$\gamma(O_{15A}\text{=}(C_{11A}\text{-}N_{12A})\text{-}C_{2A})+\gamma(O_{15B}\text{=}(C_{11B}\text{-}N_{12B})\text{-}C_{2B})$	A_u	γ(C=O)’
S_{76}	$\gamma(O_{15A}\text{=}(C_{11A}\text{-}N_{12A})\text{-}C_{2A})\text{-}\gamma(O_{15B}\text{=}(C_{11B}\text{-}N_{12B})\text{-}C_{2B})$	B_g	γ(C=O)’’
S_{77}	$\gamma(C_{11A}\text{-}(N_{12A}\text{-}H_{14A})\text{-}H_{13A})+\gamma(C_{11B}\text{-}(N_{12B}\text{-}H_{14B})\text{-}H_{13B})$	A_u	γ(NH_2)’
S_{78}	$\gamma(C_{11A}\text{-}(N_{12A}\text{-}H_{14A})\text{-}H_{13A})\text{-}\gamma(C_{11B}\text{-}(N_{12B}\text{-}H_{14B})\text{-}H_{13B})$	B_g	γ(NH_2)’’
S_{79}	$\nu(O_{15A}...H_{14B})+\nu(O_{15B}...H_{14A})$	A_g	$\nu_{A...B}$’
S_{80}	$\nu(O_{15A}...H_{14B})\text{-}\nu(O_{15B}...H_{14A})$	B_u	$\nu_{A...B}$’’
S_{81}	$\delta(C_{11A}...N_{12B}...C_{11B})\text{-}\delta(C_{11A}\ldots O_{15B}...C_{11B})$	A_g	$\delta_{A...B}$

S_{82}	$\tau(C_{11B}...N_{12A}...C_{11A}...O_{15A})+\tau(C_{11A}...N_{12B}...C_{11B}\ldots O_{15B})$	A_u	$\tau_{A...B}$'
S_{83}	$\tau(C_{11B}...N_{12A}...C_{11A}...O_{15A})-\tau(C_{11A}...N_{12B}...C_{11B}\ldots O_{15B})$	B_g	$\tau_{A...B}$''
S_{84}	$\gamma(N_{12A}\ldots C_{11A}...C_{11B}...N_{12B})+\gamma(N_{12A}...C_{11A}...C_{11B}...O_{15B})+\gamma(O_{15A}...C_{11A}...C_{11B}...N_{12B})+\gamma(O_{15A}...C_{11A}...C_{11B}...O_{15B})$	A_u	$\gamma_{A...B}$

[a] See Scheme 1 for atom numbering. ν, bond stretching; δ, bending; γ, rocking; w, wagging; τ, torsion; s, symmetric; as, asymmetric. Normalizing factors (N) are not provided; they can be calculated as $N_j = \sqrt{\sum_i {}^{1}\!/_{c_i^2}}$, where j refer to the vibrational coordinate and c_i are the coefficients associated with each coordinate in which the vibrational coordinate expands.

TABLE S10. DFT(B3LYP)/6-311++G(d,p) calculated wavenumbers and intensities, and normal coordinate analysis for *Dimer 1* of picolinamide[a].

Approximate Description	Symmetry	Calculated Wavenumber[b]	Intensity	PED[c]
ν(N-H)1'	A_g	3492	0	$S_{27}(95)$
ν(N-H)1''	B_u	3491	442	$S_{28}(95)$
ν(N-H)2''	B_u	3224	2265	$S_{30}(96)$
ν(N-H)2'	A_g	3185	0	$S_{29}(97)$
ν(C-H)2'	A_g	3086	0	$S_{17}(95)$
ν(C-H)2''	B_u	3086	5	$S_{18}(95)$
ν(C-H)4'	A_g	3066	0	$S_{21}(76)+S_{19}(18)$
ν(C-H)4''	B_u	3066	33	$S_{22}(76)+S_{20}(18)$
ν(C-H)3'	A_g	3048	0	$S_{19}(77)+S_{21}(17)$
ν(C-H)3''	B_u	3048	17	$S_{20}(77)+S_{22}(17)$
ν(C-H)1'	A_g	3029	0	$S_{13}(92)$
ν(C-H)1''	B_u	3029	35	$S_{14}(92)$
ν(C=O)''	B_u	1719	704	$S_{24}(61)+S_{26}(17)$
ν(C=O)'	A_g	1694	0	$S_{23}(43)+S_{51}(28)+S_{25}(14)$
ν ring 3''	B_u	1609	24	$S_8(20)+S_6(18)+S_{12}(16)+S_2(10)$
ν ring 3'	A_g	1609	0	$S_7(21)+S_5(19)+S_{11}(17)+S_1(10)$
δ(NH_2)''	B_u	1603	213	$S_{52}(80)+S_{24}(11)$
δ(NH_2)'	A_g	1596	0	$S_{51}(33)+S_9(19)$
ν ring 5''	B_u	1591	79	$S_{10}(33)+S_4(15)$
ν ring 5'	A_g	1587	0	$S_{51}(30)+S_{23}(26)+S_9(15)$
ν ring 2'	A_g	1482	0	$S_{33}(30)+S_3(18)+S_{35}(16)+S_{11}(10)$
ν ring 2''	B_u	1482	13	$S_{34}(31)+S_4(19)+S_{36}(16)$
δ(C-H)4'	A_g	1454	0	$S_{39}(28)+S_{37}(13)$
δ(C-H)4''	B_u	1451	21	$S_{40}(30)+S_{38}(17)+S_6(11)$
ν(C-N)'	A_g	1411	0	$S_{25}(33)+S_{53}(14)+S_{37}(12)$
ν(C-N)''	B_u	1398	451	$S_{26}(33)+S_{54}(15)+S_{16}(12)$
δ(C-H) 1''	B_u	1302	8	$S_{34}(41)+S_6(13)+S_{36}(13)+S_4(12)$
δ(C-H)1'	A_g	1302	0	$S_{33}(41)+S_5(13)+S_{35}(13)+S_3(12)$
ν ring 1'	A_g	1283	0	$S_1(41)+S_3(14)+S_{11}(11)$
ν ring 1''	B_u	1282	28	$S_2(40)+S_4(14)+S_{12}(11)$
ν ring 4'	A_g	1177	0	$S_{31}(18)+S_7(17)+S_{15}(15)+S_{53}(14)$
ν ring 4''	B_u	1174	12	$S_{32}(18)+S_8(16)+S_{16}(14)+S_{54}(13)$
δ(C-H)3'	A_g	1156	0	$S_{39}(31)+S_{37}(29)+S_{35}(15)+S_9(13)$
δ(C-H)3''	B_u	1156	2	$S_{40}(31)+S_{38}(29)+S_{36}(16)+S_{10}(12)$
w(NH_2)'	A_g	1123	0	$S_{53}(43)+S_{25}(25)+S_{23}(17)$
w(NH_2)''	B_u	1118	9	$S_{54}(46)+S_{26}(22)+S_{24}(17)$
δ(C-H)2'	A_g	1097	0	$S_{39}(22)+S_{11}(18)+S_{35}(16)+S_7(15)$
δ(C-H)2''	B_u	1096	10	$S_{40}(22)+S_{12}(18)+S_8(15)+S_{36}(15)$
ν ring 6'	A_g	1049	0	$S_9(32)+S_{11}(22)+S_{35}(11)$
ν ring 6''	B_u	1049	17	$S_{10}(33)+S_{12}(22)+S_{36}(12)$
γ(C-H)1'	A_u	1010	1	$S_{67}(60)+S_{73}(24)+S_{71}(17)$
γ(C-H)1''	B_g	1010	0	$S_{68}(60)+S_{74}(24)+S_{72}(17)$
δ ring 1'	A_g	1005	0	$S_{31}(52)+S_3(12)+S_1(10)$
δ ring 1''	B_u	1005	13	$S_{32}(52)+S_4(12)+S_2(10)$
γ(C-H)2'	A_u	975	2	$S_{69}(66)+S_{71}(31)$
γ(C-H)2''	B_g	975	0	$S_{70}(66)+S_{72}(31)$
γ(C-H)4'	A_u	917	4	$S_{73}(38)+S_{69}(27)+S_{67}(18)+S_{71}(16)$
γ(C-H)4''	B_g	917	0	$S_{74}(38)+S_{70}(27)+S_{68}(17)+S_{72}(16)$
γ(NH_2)'	A_u	845	65	$S_{77}(55)+S_{62}(45)$

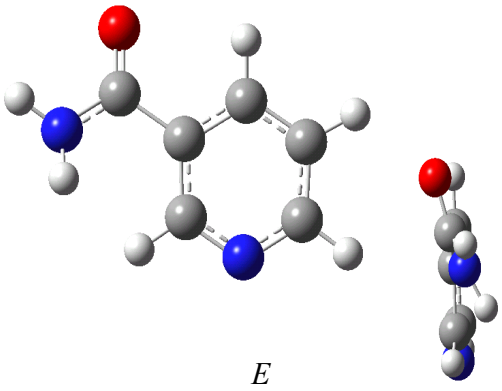
γ(C=O)''	B_g	825	0	$S_{76}(33)+S_{56}(25)+S_{72}(19)$
γ(C=O)'	A_u	824	53	$S_{75}(30)+S_{55}(26)+S_{71}(20)$
γ(NH_2)''	B_g	802	0	$S_{78}(55)+S_{61}(45)$
δ ring 2''	B_u	786	6	$S_{16}(23)+S_{46}(14)+S_{44}(13)+S_6(11)$
δ ring 2'	A_g	781	0	$S_{15}(24)+S_{45}(15)+S_{43}(14)+S_5(12)$
γ(C-H)3''	B_g	754	0	$S_{56}(26)+S_{72}(21)+S_{74}(21)+S_{68}(20)$
γ(C-H)3'	A_u	754	51	$S_{55}(30)+S_{73}(21)+S_{71}(19)+S_{67}(19)$
τ ring 1''	B_g	698	0	$S_{56}(49)+S_{76}(37)$
τ ring 1'	A_u	692	19	$S_{55}(45)+S_{75}(41)$
δ(C=O)''	B_u	653	24	$S_{44}(43)+S_{50}(34)$
δ(C=O)'	A_g	644	0	$S_{43}(54)+S_{49}(25)$
δ ring 3''	B_u	625	33	$S_{46}(52)+S_{44}(26)+S_{50}(13)$
δ ring 3'	A_g	621	0	$S_{45}(53)+S_{49}(24)+S_{43}(13)$
τ(C-N)'	A_u	576	302	$S_{61}(61)+S_{78}(39)$
τ(C-N)''	B_g	573	0	$S_{62}(54)+S_{77}(44)$
δ(C-C-N)''	B_u	517	65	$S_{48}(43)+S_{42}(19)$
δ(C-C-N)'	A_g	499	0	$S_{47}(43)+S_{41}(22)$
τ ring 2''	B_g	445	0	$S_{58}(84)$
τ ring 2'	A_u	442	<0.1	$S_{57}(85)$
τ ring 3'	A_u	411	3	$S_{59}(81)$
τ ring 3''	B_g	410	0	$S_{60}(81)$
ν(C-C)'	A_g	406	0	$S_{15}(27)+S_{45}(17)+S_{47}(14)+S_{79}(13)+S_{49}(11)$
ν(C-C)''	B_u	382	4	$S_{16}(34)+S_{46}(19)+S_{50}(16)+S_{48}(12)$
w(C-C)''	B_u	259	118	$S_{42}(45)+S_{80}(28)$
w(C-C)'	A_g	245	0	$S_{41}(53)+S_{81}(22)+S_{47}(17)$
τ(C-C)2''	B_g	170	0	$S_{66}(61)+S_{83}(18)+S_{60}(13)$
τ(C-C)2'	A_u	162	0.1	$S_{65}(61)+S_{59}(14)$
$\nu_{A...B}$'	A_g	96	0	$S_{79}(86)$
τ(C-C)1'	A_u	92	7	$S_{63}(59)+S_{84}(38)$
$\delta_{A...B}$	A_g	87	0	$S_{81}(78)+S_{41}(10)$
τ(C-C)1''	B_g	79	0	$S_{64}(85)$
$\nu_{A...B}$''	B_u	54	3	$S_{80}(64)+S_{48}(19)+S_{42}(12)$
$\tau_{A...B}$''	B_g	50	0	$S_{83}(82)+S_{66}(11)$
$\gamma_{A...B}$	A_u	35	0.5	$S_{84}(57)+S_{63}(32)$
$\tau_{A...B}$'	A_u	16	3	$S_{82}(87)$

[a] Wavenumbers in cm^{-1}; intensities in km mol^{-1}. ν, bond stretching; δ, bending; γ, rocking; w, wagging; τ, torsion. See Table S9 for definition of symmetry coordinates. [b] Scaled by 0.960 in the high wavenumbers region and by 0.988 in the low wavenumbers region (below 1800 cm^{-1}). [c] Only PED values greater than 10 % are given.

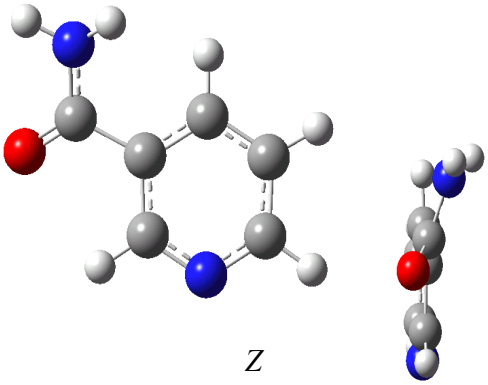
TABLE S11 - Observed wavenumbers for the neat PA solid in the glassy state resulting from fast deposition of the vapor of the compound onto the cryostat's cold substrate at 10 K and in the room temperature (25ºC) crystalline phase (in KBr pellet).[a]

Approximate Description	Symmetry	DIMER 1 (C_{2h})		Glass (film, 10 K)	Crystal (KBr pellet, 25ºC)
		Calculated Wavenumber	Intensity		
ν(N-H)1''	B_u	3491.0	441.5	3448 / 3392	3417 / 3385
ν(N-H)2''	B_u	3223.7	2265.3	3304 / 3256 / 3188	3271 / 3185
ν(C-H)2''	B_u	3086.1	5.0	n.o.	3079
ν(C-H)4''	B_u	3066.0	33.2	3068	3061
ν(C-H)3''	B_u	3048.3	17.2	3013	3042
ν(C-H)1''	B_u	3028.5	34.6		3016
ν(C=O)''	B_u	1718.5	704.4	1686	1662
ν ring 3''	B_u	1608.7	23.5	1591	1587
δ(NH_2)''	B_u	1602.8	212.8	1571	1568
ν ring 5''	B_u	1591.1	79.2	~1583	1603 / ~1583
ν ring 2''	B_u	1481.7	12.5	1471	1468
δ(C-H)4''	B_u	1450.6	21.3	1446	1443
ν(C-N)''	B_u	1397.8	451.4	1397 / 1386	1406 / 1390
δ(C-H) 1''	B_u	1302.1	8.2	1293	1284
ν ring 1''	B_u	1282.2	28.2	1254	1253
ν ring 4''	B_u	1174.2	12.4	1165	1165
δ(C-H)3''	B_u	1156.3	1.9	1147	1143
w(NH_2)''	B_u	1117.8	8.9	1097	1096 / 1084
δ(C-H)2''	B_u	1096.3	10.4	1224	1225
ν ring 6''	B_u	1049.4	16.9	1043	1043
γ(C-H)1'	A_u	1010.4	0.7	n.o.	n.o.
δ ring 1''	B_u	1004.8	13.0	998	996
γ(C-H)2'	A_u	974.8	2.3	974	986
γ(C-H)4'	A_u	917.4	3.5	911	909
γ(NH_2)'	A_u	844.8	64.5	824	826
γ(C=O)'	A_u	823.8	53.3	n.o.	770
δ ring 2''	B_u	786.1	6.0	752	756
γ(C-H)3'	A_u	753.6	50.6	685	694
τ ring 1'	A_u	692.3	19.0	644	649
δ(C=O)''	B_u	652.6	24.3	~779	796
δ ring 3''	B_u	624.8	32.8	615	610
δ(C-C-N)''	B_u	517.0	65.0	512	522
w(C-C)''	B_u	259.3	118.0	~570	630

[a] Wavenumbers in cm^{-1}; intensities in km mol^{-1}. ν, bond stretching; δ, bending; γ, rocking; τ, torsion; w, wagging.



E



Z

Figure S1: Optimized structures of the conformers of nicotinamide. Two perspectives are provided, one with the viewpoint placed above the ring (left) and the other with the viewpoint along the major axis of the molecule.

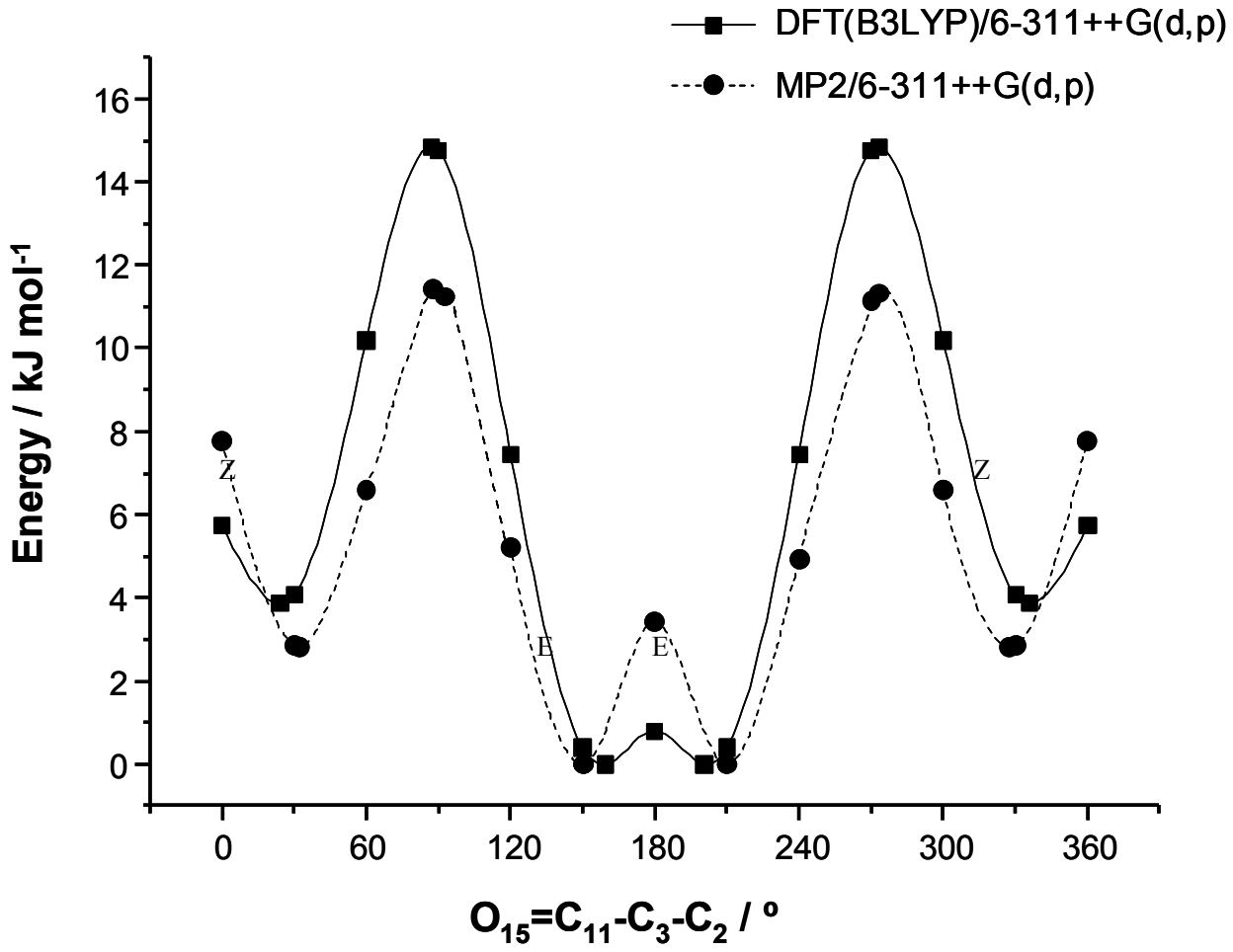


Figure S2: Potential energy profiles calculated at the DFT-B3LYP/6-311++G(d,p) and MP2/6-311++G(d,p) levels for the *E*↔*Z* conformational interconversion in nicotinamide.

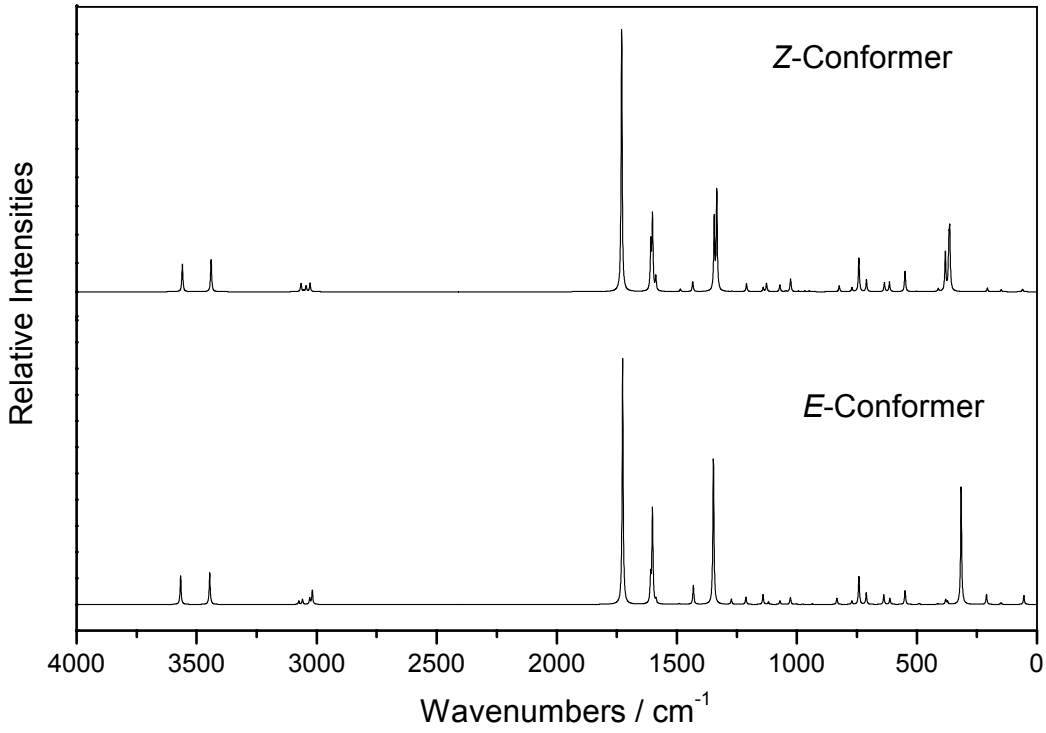


Figure S3: B3LYP/6-311++G(d,p) calculated spectra for the *E* and *Z* conformers of nicotinamide. The spectra were simulated using Lorentzian functions with a halfbandwidth of 5 cm^{-1}, frequencies being scaled by 0.960 in the high frequency range and 0.988 below 1800 cm^{-1}. Ordinate scales in arbitrary units.