

Molecular structure, spectral analysis and hydrogen bonding analysis of ampicillin trihydrate: A combined DFT and AIM approach

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†Electronic supplementary information

3D MEP of the monomer of AT calculated from optimized structure is shown in Fig. S1. Fig. S2 shows the HOMO and LUMO of monomer and its energy gap. The molecular graph of monomer of AT using AIM program is given in Fig. S3. The experimental and calculated geometric parameters of monomer and dimer of AT is given in Table S1. Selected Lewis orbitals with percentage ED over bonded atoms, hybrid NBOs with s and p character in % for monomer of AT are listed in Table S2. The calculated static dipole moment (μ_0), the mean polarizability ($\langle\alpha_0\rangle$), the anisotropy of the polarizability ($\Delta\alpha$), the mean first order hyperpolarizability (β_0) and their components for monomer and dimer of AT, using B3LYP/6-311++G(d,p) are given in Table S3. The thermodynamic properties at different temperatures for monomer of AT is given in Table S4. Table S5 gives the information about the theoretically calculated total energy (eV), zero-point energy (J/mol), enthalpy (kcal/mol), specific heat ($\text{cal}\cdot\text{mol}^{-1}\text{K}^{-1}$), entropy ($\text{cal}\cdot\text{mol}^{-1}\text{K}^{-1}$) and rotational constants (GHz) at 298.15 K for monomer and dimer of AT. The geometrical parameters for hydrogen bonds in dimer of AT are given in Table S6. Table S7 gives the theoretical and experimental vibrational wavenumbers (cm^{-1}) of AT with potential energy distribution (PED).

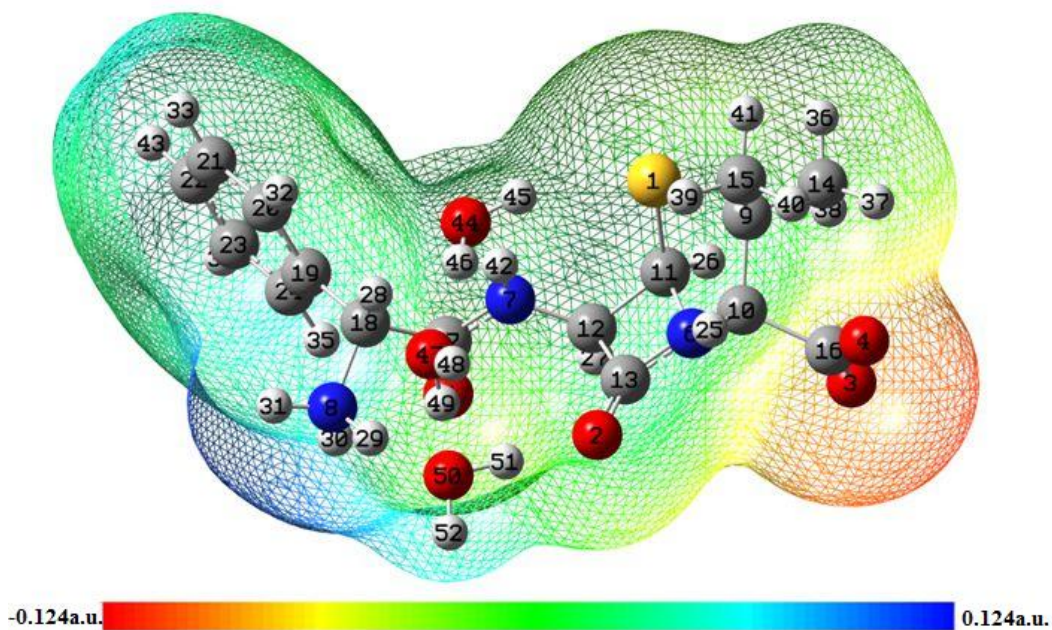


Fig. S1. Molecular electrostatic potential (MEP) formed by mapping of total density over electrostatic potential in gas phase for monomer of AT.

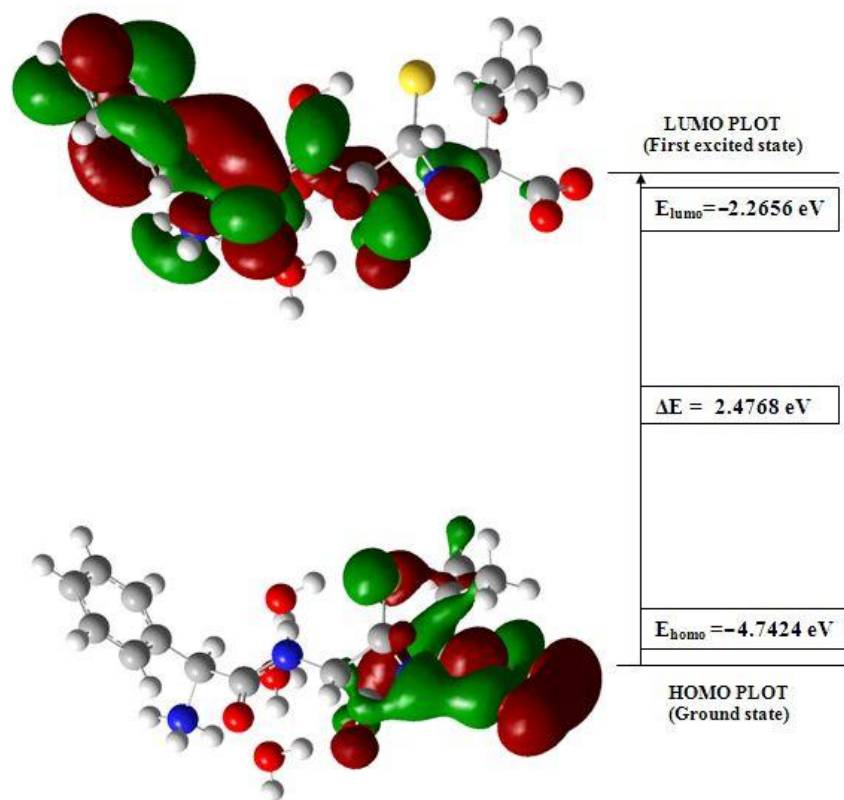


Fig. S2. HOMO-LUMO plot of monomer of AT with orbitals involved in electronic transitions in isolated (gaseous) phase.

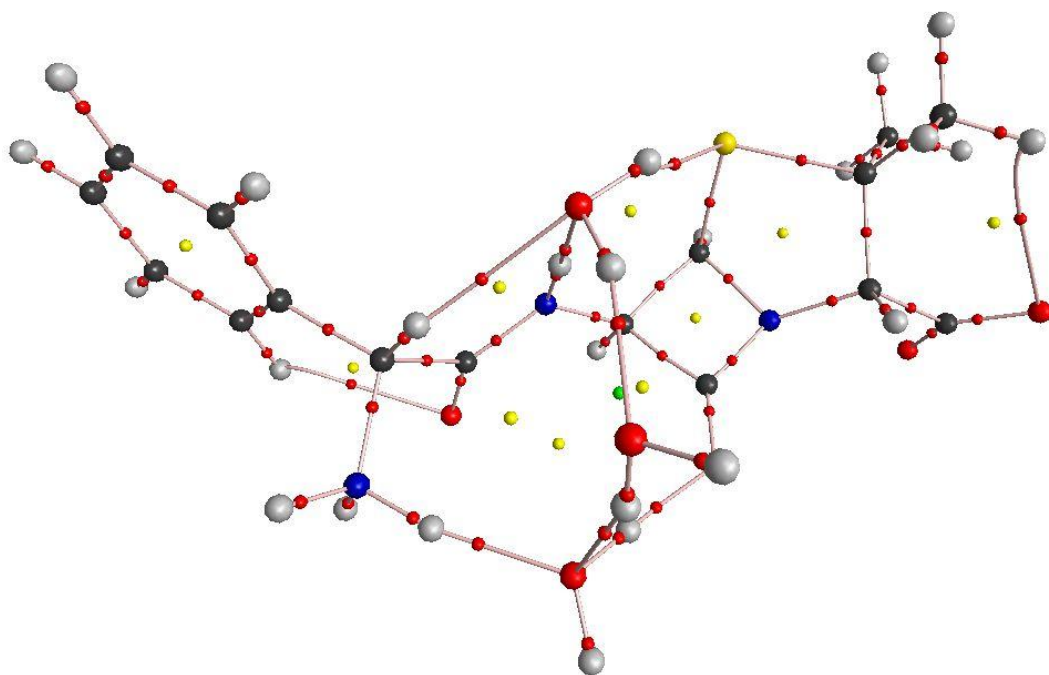


Fig. S3. Molecular graph of monomer of AT: bond critical points (small red spheres), ring critical points (small yellow sphere), bond paths (pink lines).

Table S1 The experimental and calculated geometric parameters of monomer and dimer of AT using DFT/6-311++g(d,p), bond lengths in angstrom (Å) and bond angles and dihedral angles in degrees (°).

Geometrical Parameters	Experimental	Calculated	
		Optimized parameters	
		Monomer	Dimer
Bond lengths(Å)			
S1-C9	1.859	1.926	1.919
S1-C11	1.797	1.837	1.830
O2-C13	1.201	1.229	1.221
O3-C16	1.222	1.239	1.223
O4-C16	1.273	1.245	1.278
O5-C17	1.213	1.229	1.226
N6-C10	1.473	1.459	1.475
N6-C11	1.506	1.467	1.485
N6-C13	1.384	1.339	1.355
N7-C12	1.433	1.445	1.447
N7-C17	1.348	1.341	1.350
N7-H42	1.002	1.026	1.028
N8-C18	1.475	1.525	1.520
N8-H29	1.001	1.056	1.064
N8-H30	1.000	1.027	1.026
N8-H31	1.000	1.020	1.020
C9-C10	1.576	1.570	1.551
C9-C14	1.511	1.535	1.532
C9-C15	1.493	1.527	1.529
C10-C16	1.555	1.597	1.581
C10-H25	1.000	1.092	1.093

C11-C12	1.570	1.560	1.566
C11-H26	1.000	1.089	1.089
C12-C13	1.534	1.554	1.552
C12-H27	1.001	1.088	1.088
C14-H36	1.080	1.092	1.092
C14-H37	1.081	1.092	1.091
C14-H38	1.083	1.091	1.090
C15-H39	1.081	1.093	1.092
C15-H40	1.078	1.093	1.093
C15-H41	1.076	1.093	1.092
C17-C18	1.530	1.544	1.544
C18-C19	1.527	1.512	1.514
C18-H28	1.080	1.089	1.089
C19-C20	1.387	1.399	1.399
C19-C24	1.390	1.401	1.401
C20-C21	1.385	1.393	1.393
C20-H32	1.078	1.085	1.085
C21-C22	1.376	1.393	1.393
C21-H33	1.079	1.084	1.084
C22-C23	1.384	1.395	1.395
C22-H43	1.081	1.084	1.084
C23-C24	1.386	1.392	1.392
C23-H34	1.079	1.084	1.084
C24-H35	1.080	1.084	1.084
O44-H45	0.980	0.969	0.966
O44-H46	0.980	0.977	0.983
O47-H48	0.980	0.962	0.977
O47-H49	0.980	0.970	0.974
O50-H51	0.980	1.012	0.982
O50-H52	0.980	0.964	0.977

Bond angles(°)

C9-S1-C11	90.10	88.75	89.26
C10-N6-C11	117.04	120.03	118.63
C10-N6-C13	128.12	132.81	125.75
C11-N6-C13	93.09	95.33	94.30
C12-N7-C17	123.25	120.25	119.69
C12-N7-H42	118.51	117.56	117.63
C17-N7-H42	118.09	116.35	116.24
C18-N8-H29	109.66	109.71	109.45
C18-N8-H30	109.54	106.77	107.78
C18-N8-H31	109.72	111.56	111.42
H29-N8-H30	109.40	106.88	107.50
H29-N8-H31	108.93	111.27	110.66
H30-N8-H31	109.57	110.42	109.88
S1-C9-C10	104.63	105.65	102.91
S1-C9-C14	109.99	107.26	108.43
S1-C9-C15	107.54	109.11	108.36
C10-C9-C14	111.85	113.13	114.70
C10-C9-C15	112.88	110.91	111.01
C14-C9-C15	109.73	110.51	110.90
N6-C10-C9	105.59	105.72	105.44
N6-C10-C16	112.80	114.64	113.06
N6-C10-H25	103.84	107.15	106.41
C9-C10-C16	114.33	111.64	116.61
C9-C10-H25	112.00	109.74	107.16
C16-C10-H25	107.84	107.79	107.55

S1-C11-N6	103.63	102.96	104.56
S1-C11-C12	119.49	121.84	123.28
S1-C11-H26	108.63	110.87	110.40
N6-C11-C12	87.12	87.61	88.07
N6-C11-H26	116.82	114.85	113.68
C12-C11-H26	118.73	115.58	114.10
N7-C12-C11	116.49	119.71	118.97
N7-C12-C13	115.51	112.87	111.25
N7-C12-H27	112.92	109.76	109.96
C11-C12-C13	85.12	83.64	83.85
C11-C12-H27	108.02	113.95	114.82
C13-C12-H27	115.79	114.88	115.90
O2-C13-N6	130.95	133.19	131.70
O2-C13-C12	135.44	133.74	133.96
N6-C13-C12	93.01	92.57	93.50
C9-C14-H36	109.39	110.24	109.64
C9-C14-H37	109.15	108.81	109.78
C9-C14-H38	109.77	112.27	112.44
H36-C14-H37	109.28	109.19	109.46
H36-C14-H38	109.57	108.96	108.95
H37-C14-H38	109.66	107.27	106.46
C9-C15-H39	109.44	111.73	112.03
C9-C15-H40	109.42	107.49	109.19
C9-C15-H41	109.34	111.50	110.91
H39-C15-H40	109.99	108.23	108.03
H39-C15-H41	109.43	108.92	108.75
H40-C15-H41	109.19	108.83	107.77
O3-C16-O4	126.34	132.86	128.93
O3-C16-C10	117.97	115.33	117.77
O4-C16-C10	115.59	111.77	113.29
O5-C17-N7	124.53	126.78	126.00
O5-C17-C18	122.14	118.13	118.83
N7-C17-C18	113.21	114.96	115.12
N8-C18-C17	109.99	101.81	103.33
N8-C18-C19	112.88	111.08	111.33
N8-C18-H28	107.88	106.85	106.75
C17-C18-C19	110.10	115.45	114.57
C17-C18-H28	109.00	110.94	110.59
C19-C18-H28	106.83	110.10	109.82
C18-C19-C20	119.50	118.69	118.72
C18-C19-C24	120.59	121.74	121.72
C20-C19-C24	119.49	119.56	119.54
C19-C20-C21	119.83	120.23	120.26
C19-C20-H32	119.98	119.78	119.80
C21-C20-H32	119.98	119.96	119.92
C20-C21-C22	120.09	120.01	120.00
C20-C21-H33	119.43	119.74	119.75
C22-C21-H33	119.58	120.23	120.24
C21-C22-C23	119.52	119.96	119.95
C21-C22-H43	120.32	120.03	120.04
C23-C22-H43	119.99	119.99	120.00
C22-C23-C24	119.84	120.27	120.27
C22-C23-H34	120.06	120.08	120.07
C24-C23-H34	120.08	119.63	119.64
C19-C24-C23	119.99	119.94	119.94
C19-C24-H35	119.90	120.11	120.16

C23-C24-H35	119.87	119.92	119.87
C18-H28-H44	143.37	144.63	143.74
H45-O44-H46	112.78	107.06	106.12
H48-O47-H49	128.40	106.39	104.80
H51-O50-H52	102.90	105.43	103.53
Dihedral angles(°)			
C11-S1-C9-C10	-39.79	-34.62	-40.89
C11-S1-C9-C14	80.48	86.33	81.00
C11-S1-C9-C15	-160.05	-153.93	-158.53
C9-S1-C11-N6	37.10	36.16	31.65
C9-S1-C11-C12	131.56	131.49	129.07
C9-S1-C11-H26	-87.76	-87.15	-90.98
C11-N6-C10-C9	-2.60	6.40	-15.80
C11-N6-C10-C16	-128.13	-117.00	-144.32
C11-N6-C10-H25	115.38	123.42	97.81
C13-N6-C10-C9	-121.11	-126.61	-135.70
C13-N6-C10-C16	113.35	109.97	95.77
C13-N6-C10-H25	-3.12	-9.59	-22.08
C10-N6-C11-S1	-26.46	-32.48	-15.17
C10-N6-C11-C12	-146.13	-154.65	-139.13
C10-N6-C11-H26	92.94	88.15	105.30
C13-N6-C11-S1	109.72	114.91	119.95
C13-N6-C11-C12	-9.94	-7.24	-4.00
C13-N6-C11-H26	-130.86	-124.44	-119.56
C10-N6-C13-O2	-33.49	-24.75	-36.16
C10-N6-C13-C12	138.56	147.80	134.31
C11-N6-C13-O2	-161.88	-165.28	-166.43
C11-N6-C13-C12	-161.88	7.27	4.04
C17-N7-C12-C11	136.04	168.59	173.39
C17-N7-C12-C13	-126.32	-95.52	-91.78
C17-N7-C12-H27	10.17	34.02	38.01
H42-N7-C12-C11	-48.45	-39.26	-35.76
H42-N7-C12-C13	49.16	56.60	59.05
H42-N7-C12-H27	-174.33	-173.83	-171.14
C12-N7-C17-O5	0.30	-15.83	-15.36
C12-N7-C17-C18	-175.90	160.06	162.48
H42-N7-C17-O5	-175.20	-168.29	-166.59
H42-N7-C17-C18	8.58	7.60	11.25
H29-N8-C18-C17	59.61	64.28	66.79
H29-N8-C18-C19	-176.97	-172.25	-169.74
H29-N8-C18-H28	-59.16	-52.13	-49.88
H30-N8-C18-C17	-60.45	-51.19	-49.84
H30-N8-C18-C19	62.95	72.25	73.62
H30-N8-C18-H28	-179.24	-167.62	-166.51
H31-N8-C18-C17	179.22	-171.92	-170.48
H31-N8-C18-C19	-57.37	-48.47	-47.01
H31-N8-C18-H28	60.43	71.64	72.84
S1-C9-C10-N6	29.56	21.82	37.32
S1-C9-C10-C16	154.15	147.11	163.70
S1-C9-C10-H25	-82.80	-93.42	-75.76
C14-C9-C10-N6	-89.47	-95.22	-80.23
C14-C9-C10-C16	35.11	30.06	46.14
C14-C9-C10-H25	158.15	149.52	166.67
C15-C9-C10-N6	146.19	139.94	153.07
C15-C9-C10-C16	-89.21	-94.76	-80.54
C15-C9-C10-H25	33.82	24.69	39.97

S1-C9-C14-H36	22.37	59.20	59.50
S1-C9-C14-H37	141.89	178.92	179.79
S1-C9-C14-H38	-97.88	-62.48	-61.87
C10-C9-C14-H36	138.18	175.30	173.87
C10-C9-C14-H37	-102.28	-64.97	-65.82
C10-C9-C14-H38	17.93	53.62	52.50
C15-C9-C14-H36	-95.73	-59.64	-59.36
C15-C9-C14-H37	23.79	60.07	60.92
C15-C9-C14-H38	144.00	178.67	179.25
S1-C9-C15-H39	61.93	57.14	57.81
S1-C9-C15-H40	-177.47	175.75	177.46
S1-C9-C15-H41	-57.91	-65.02	-63.90
C10-C9-C15-H39	-52.96	-58.85	-54.50
C10-C9-C15-H40	67.63	59.75	65.136
C10-C9-C15-H41	-172.81	178.97	-176.23
C14-C9-C15-H39	-178.45	174.84	176.73
C14-C9-C15-H40	-57.85	-66.53	-63.62
C14-C9-C15-H41	61.69	52.67	55.00
N6-C10-C16-O3	-3.58	14.12	60.31
N6-C10-C16-O4	179.68	-167.41	-119.67
C9-C10-C16-O3	-124.24	-106.06	-62.17
C9-C10-C16-O4	59.02	72.39	117.84
H25-C10-C16-O3	110.48	133.33	177.50
H25-C10-C16-O4	-66.24	-48.20	-2.47
S1-C11-C12-N7	21.08	15.20	8.24
S1-C11-C12-C13	-95.05	-97.54	-102.68
S1-C11-C12-H27	149.38	148.01	141.57
N6-C11-C12-N7	125.12	119.00	114.43
N6-C11-C12-C13	8.98	6.25	3.50
N6-C11-C12-H27	-106.57	-108.18	-112.23
H26-C11-C12-N7	-115.68	-124.48	-130.40
H26-C11-C12-C13	128.17	122.76	118.67
H26-C11-C12-H27	12.61	8.32	2.93
N7-C12-C13-O2	44.58	46.02	47.53
N7-C12-C13-N6	-126.87	-126.47	-122.58
C11-C12-C13-O2	161.66	165.64	166.27
C11-C12-C13-N6	-9.78	-6.85	-3.84
H27-C12-C13-O2	-90.65	-80.86	-79.07
H27-C12-C13-N6	97.88	106.64	110.80
O5-C17-C18-N8	37.84	43.83	41.55
O5-C17-C18-C19	-87.16	-76.59	-79.74
O5-C17-C18-H28	155.94	157.24	155.47
N7-C17-C18-N8	-145.83	-132.43	-136.46
N7-C17-C18-C19	89.14	107.12	102.23
N7-C17-C18-H28	-27.74	-19.02	-22.53
N8-C18-C19-C20	132.83	111.18	109.11
N8-C18-C19-C24	-54.61	-68.72	-70.20
C17-C18-C19-C20	-103.81	-133.56	-134.08
C17-C18-C19-C24	68.73	46.52	46.59
H28-C18-C19-C20	14.41	-6.98	-8.91
H28-C18-C19-C24	-173.03	173.09	171.77
N8-C18-H28-O44	139.12	131.12	135.00
C17-C18-H28-O44	19.70	20.93	23.25
C19-C18-H28-O44	-99.24	-108.13	-104.17
C18-C19-C20-C21	172.01	-179.43	-178.88
C18-C19-C20-H32	-13.05	1.73	1.88

C24-C19-C20-C21	-0.61	0.47	0.44
C24-C19-C20-H32	174.31	-178.34	-178.78
C18-C19-C24-C23	-174.77	179.21	178.72
C18-C19-C24-H35	-0.25	-2.50	-2.53
C20-C19-C24-C23	-2.22	-0.70	-0.58
C20-C19-C24-H35	172.29	177.57	178.15
C19-C20-C21-C22	8.53	0.07	-0.00
C19-C20-C21-H33	177.71	-179.53	-179.85
H32-C20-C21-C22	-166.39	178.89	179.23
H32-C20-C21-H33	2.78	-0.71	-0.62
C20-C21-C22-C23	-13.52	-0.40	-0.30
C20-C21-C22-H43	171.01	-179.85	-179.97
H33-C21-C22-C23	177.30	179.20	179.54
H33-C21-C22-H43	1.84	-0.24	-0.12
C21-C22-C23-C24	10.61	0.18	0.16
C21-C22-C23-H34	-168.85	-179.08	-179.38
H43-C22-C23-C24	-173.91	179.63	179.83
H43-C22-C23-H34	6.61	0.36	0.28
C22-C23-C24-C19	-2.75	0.37	0.28
C22-C23-C24-H35	-177.27	-177.90	-178.46
H34-C23-C24-C19	176.71	179.64	179.83
H34-C23-C24-H35	2.19	1.36	1.09

Table S2 Selected Lewis orbitals (occupied bond orbital) with percentage ED over bonded atoms (ED_X , ED_Y in %), hybrid NBOs with s and p character in % for monomer of AT.

Bond (X-Y) (ED_{X-Y})	ED_X (%) ED_Y (%)	Hybrid NBOs	s (%)	p (%)
σ (S1-C9) (1.95607)	51.19 48.81	$0.7154(sp^{5.86})_S +$ $0.6987(sp^{5.70})_C$	14.51 14.90	85.09 84.97
σ (S1-C11) (1.97627)	45.65 54.35	$0.6757(sp^{6.30})_S +$ $0.7372(sp^{3.20})_C$	13.62 23.77	85.84 76.11
σ (O2-C13) (1.99479)	65.53 34.47	$0.8095(sp^{1.55})_{O+}$ $0.5871(sp^{2.08})_C$	39.25 32.46	60.65 67.38
σ (O3-C16) (1.99393)	64.91 35.09	$0.8057(sp^{1.58})_{O+}$ $0.5924(sp^{1.85})_C$	38.68 35.07	61.19 64.77
σ (O4-C16) (1.99246)	65.05 34.95	$0.8065(sp^{1.65})_{O+}$ $0.5912(sp^{1.84})_C$	37.65 35.20	62.23 64.61
σ (O5-C17) (1.99250)	64.49 35.51	$0.8031(sp^{1.49})_{O+}$ $0.5959(sp^{2.07})_C$	40.17 32.51	59.71 67.33
σ (N6-C10) (1.98365)	65.59 34.41	$0.8099(sp^{1.61})_{N+}$ $0.5866(sp^{3.85})_C$	38.32 20.57	61.65 79.11
σ (N6-C11) (1.97338)	62.13 37.87	$0.7882(sp^{2.72})_{N+}$ $0.6154(sp^{3.76})_C$	26.85 20.99	73.09 78.84
σ (N6-C13) (1.98493)	63.02 36.98	$0.7939(sp^{1.98})_{N+}$ $0.6081(sp^{2.01})_C$	33.49 33.17	66.44 66.73
σ (N7-C12) (1.98136)	62.05 37.95	$0.7877(sp^{2.06})_{N+}$ $0.6160(sp^{3.12})_C$	32.70 24.25	67.27 75.63
σ (N7-C17) (1.98817)	61.68 38.32	$0.7854(sp^{1.81})_{N+}$ $0.6190(sp^{1.88})_C$	35.56 34.67	64.38 65.24
σ (N7-H42) (1.97566)	74.07 25.93	$0.8607(sp^{2.54})_{N+}$ $0.5092(sp^{0.00})_H$	28.23 99.91	71.72 0.09
σ (N8-C18) (1.98527)	65.10 34.90	$0.8068(sp^{2.47})_{N+}$ $0.5908(sp^{4.56})_C$	28.85 17.96	71.13 81.90
σ (N8-H29) (1.99103)	75.79 24.21	$0.8706(sp^{2.89})_{N+}$ $0.4920(sp^{0.00})_H$	25.68 99.90	74.27 0.10

$\sigma(\text{N8-H30})$	72.65	$0.8523(\text{sp}^{3.46})_{\text{N}+}$	22.41	77.53
(1.99157)	27.35	$0.5230(\text{sp}^{0.00})_{\text{H}}$	99.92	0.08
$\sigma(\text{N8-H31})$	71.21	$0.8439(\text{sp}^{3.34})_{\text{N}+}$	23.02	76.93
(1.99250)	28.79	$0.5365(\text{sp}^{0.00})_{\text{H}}$	99.94	0.06
$\sigma(\text{O44-H45})$	75.01	$0.8661(\text{sp}^{3.00})_{\text{O}+}$	24.99	74.92
(1.99673)	24.99	$0.4999(\text{sp}^{0.00})_{\text{H}}$	99.89	0.11
$\sigma(\text{O44-H46})$	76.19	$0.8728(\text{sp}^{2.71})_{\text{O}+}$	26.93	72.99
(1.99830)	23.81	$0.4880(\text{sp}^{0.00})_{\text{H}}$	99.85	0.15
$\sigma(\text{O47-H48})$	74.00	$0.8602(\text{sp}^{3.22})_{\text{O}+}$	23.70	76.21
(1.99846)	26.00	$0.5099(\text{sp}^{0.00})_{\text{H}}$	99.90	0.10
$\sigma(\text{O47-H49})$	75.67	$0.8699(\text{sp}^{2.77})_{\text{O}+}$	26.53	73.38
(1.99843)	24.33	$0.4933(\text{sp}^{0.00})_{\text{H}}$	99.85	0.15
$\sigma(\text{O50-H51})$	79.20	$0.8900(\text{sp}^{2.40})_{\text{O}+}$	29.40	70.52
(1.99659)	20.80	$0.4560(\text{sp}^{0.00})_{\text{H}}$	99.81	0.19
$\sigma(\text{O50-H52})$	74.58	$0.8636(\text{sp}^{3.36})_{\text{O}+}$	22.91	77.00
(1.99789)	25.42	$0.5042(\text{sp}^{0.00})_{\text{H}}$	99.92	0.08

Table S3 Calculated static dipole moment (μ_0), the mean polarizability ($\langle\alpha_0\rangle$), the anisotropy of the polarizability ($\Delta\alpha$), the mean first order hyperpolarizability (β_0) and their components for monomer and dimer of AT, using B3LYP/6–311++G(d,p).

Property	Monomer	Dimer	Property	Monomer	Dimer
μ_x	23.5241 Debye	13.6220 Debye	β_{xxx}	817.8269 a.u.	421.0636 a.u.
μ_y	2.8235 Debye	4.2407 Debye	β_{xyy}	71.7618 a.u.	423.8009 a.u.
μ_z	5.4360 Debye	0.6309 Debye	β_{xzz}	28.8111 a.u.	-2.2618 a.u.
μ_0	24.3085 Debye	14.2807 Debye	β_{yyy}	165.0919 a.u.	209.9770 a.u.
α_{xx}	-222.2791 a.u.	-379.2294 a.u.	β_{xxy}	-101.8628 a.u.	-192.1753 a.u.
α_{yy}	-147.4717 a.u.	-386.3897 a.u.	β_{yzz}	11.8080 a.u.	5.9548 a.u.
α_{zz}	-172.4446 a.u.	-313.8598 a.u.	β_{zzz}	59.2442 a.u.	119.5703 a.u.
α_{xy}	27.4927 a.u.	117.6228 a.u.	β_{xxz}	95.8612 a.u.	-0.7569 a.u.
α_{xz}	-19.4991 a.u.	0.5393 a.u.	β_{yyz}	32.1325 a.u.	-84.0154 a.u.
α_{yz}	10.1137 a.u.	-8.5047 a.u.	β_{xyz}	-21.4163 a.u.	-10.3840 a.u.
$ \alpha_0 $	-26.7844*10⁻²⁴ esu	-53.3262*10⁻²⁴ esu	β_0	8.12345*10⁻³⁰ esu	7.28859*10⁻³⁰ esu
$\Delta\alpha$	9.77629*10⁻²⁴ esu	10.2596*10⁻²⁴ esu			

Table S4 Theoretically calculated thermodynamic properties at different temperatures using 6-311++G(d,p) basis set for monomer of AT.

Temperature (K)	Enthalpy (kcal/mol)	Specific Heat (cal/mol K)	Entropy (cal/mol K)
100	265.501	49.191	113.875
125	266.844	58.139	126.267
150	141.535	43.703	118.812
175	142.687	48.537	126.217
200	272.137	82.610	159.924
300	281.935	113.031	200.040
400	294.649	140.615	236.999
500	309.911	163.847	271.401

Table S5 Theoretically calculated total energy (eV), zero-point energy (J/mol), enthalpy (kcal/mol), specific heat (cal/mol K), entropy (cal/mol K) and rotational constants (GHz) at 298.15 K at the B3LYP/6–311++G(d,p) level for monomer and dimer of AT.

Parameters	Monomer	Dimer
Total energy	-46645.79	-93293.60
Zero point energy	1098890.2	2201135.6
Enthalpy	281.726	564.986

Specific heat	112.487	228.767
Entropy	199.336	353.758
Rotational constants	0.31995	0.04870
	0.08833	0.03280
	0.08430	0.02326

Table S6 Geometrical parameters for intra and inter molecular hydrogen bonds in dimer of AT: bond length (Å), bond angle ($^{\circ}$) and sum of van der Waal radii of interacting atoms ($r_H + r_A$) in Å.

D-H...A	D-H (Å)	H...A (Å)	D-H...A ($^{\circ}$)	($r_H + r_A$) (Å)
N7-H42...O44	1.0281	1.8707	167.26	2.72
N8-H29...O50	1.0644	1.6493	164.16	2.72
C24-H35...O5	1.0841	2.5531	117.77	2.72
O44-H45...S1	0.9659	2.7588	130.37	3.00
C14-H37...O3	1.0908	2.4918	104.02	2.72
N53-H84...O4	1.1192	1.4558	170.15	2.72
N53-H83...O2	1.0268	2.1177	142.67	2.72
O50-H51...O2	0.9817	1.7948	164.10	2.72
C18-H28...O44	1.0887	2.3330	143.75	2.72
N53-H82...O47	1.0292	2.1158	157.88	2.72
O44-H46...O47	0.9835	1.7874	168.19	2.72
O47-H48...O54	0.9774	1.8896	166.97	2.72
O47-H49...O50	0.9740	2.0631	153.87	2.72
O50-H52...O59	0.9773	1.8935	143.11	2.72
N61-H95...O97	1.0290	1.8539	169.63	2.72
C71-H81...O97	1.0896	2.4895	141.98	2.72
O97-H99...O100	0.9792	1.8083	173.48	2.72
O100-H102...O54	0.9768	1.8447	167.33	2.72
O54-H103...O56	0.9886	1.7134	156.13	2.72
C77-H88...O59	1.0840	2.6590	112.71	2.72
O97-H98...S55	0.9687	2.5735	140.43	3.00

Table S7 Theoretical and experimental vibrational wavenumbers (cm^{-1}) of AT with potential energy distribution (PED).

Frequency monomer (cm^{-1})				Potential Energy Distribution ($\geq 5\%$)	Calc. Scaled	Simplified description of modes of dimer
Calculated	Experimental				Freq. (cm^{-1})	
Unscaled	Scaled	Raman	FT-IR	Dimer		
3878	3666	-	-	$\nu_a(\text{O47H}_2)(100)$	3675, 3492	OH ₂ asym stretch
3849	3641	-	-	$\nu_a(\text{O50H}_2)(99)$	3656, 3334	OH ₂ asym stretch
3757	3560	-	3506	$\nu_a(\text{O44H}_2)(100)$	3549, 3286	OH ₂ asym stretch
3645	3460	-	3442	$\nu_s(\text{O47H}_2)(91)+\nu_s(\text{O44H}_2)(6)$	3431, 3403	OH ₂ sym stretch
3573	3396	-	-	$\nu_s(\text{O44H}_2)(90)+\nu_s(\text{O47H}_2)(7)$	3427, 3361	OH ₂ sym stretch
3516	3345	-	3367	$\nu_a(\text{NH}_3)(99)$	3340, 3247	NH ₃ asym stretch
3391	3233	-	3207	$\nu_s(\text{NH}_3)(99)$	3250, 3186	NH ₃ sym stretch
3323	3172	-	3207	$\nu(\text{NH}_4)(95)$	3139, 3129	NH stretch
3198	3059	3089	3039	R3[$\nu(\text{CH})$](96)	3060, 3056	Ring 3 CH stretch
3190	3052	3045	3039	R3[$\nu(\text{CH})$](98)	3052, 3049	Ring 3 CH stretch
3182	3045	3045	3039	R3[$\nu(\text{CH})$](99)	3044, 3042	Ring 3 CH stretch
3174	3038	3045	3039	R3[$\nu(\text{CH})$](99)	3038, 3036	Ring 3 CH stretch
3168	3032	3024	3039	R3[$\nu(\text{CH})$](97)	3033, 3030	Ring 3 CH stretch
3129	2997	2996	2991	R2[$\nu(\text{CH}_2)$](97)	2997, 2985	Ring 3 CH stretch
3125	2993	2996	2991	$\nu(\text{CH}_2)(94)$	2993, 2981	Ring 3 CH stretch
3118	2987	2985	2991	$\nu_a(\text{C14H}_3)(98)$	2993, 2983	CH ₃ asymstr

3111	2981	2958	2991	$\nu_a(\text{C14H}_3)(95)$	2989, 2980	$\text{CH}_3\text{asymstr}$
3104	2974	2976	-	$\text{R1}[\nu(\text{CH26})](95)$	2970, 2954	CH stretch
3099	2970	2971	2970	$\nu_a(\text{C15H}_3)(95)$	2976, 2973	$\text{CH}_3\text{asymstr}$
3091	2963	2971		$\nu_a(\text{C15H}_3)(96)$	2970, 2966	$\text{CH}_3\text{asymstr}$
3071	2944	2939	2929	$\text{R1}[\nu(\text{CH25})](98)$	2921, 2921	CH stretch
3040	2916	2935	2929	$\nu_s(\text{C14H}_3)(98)$	2924, 2909	CH_3symstr
3022	2900	2907	-	$\nu_s(\text{C15H}_3)(98)$	2915, 2902	CH_3symstr
2992	2872	2866	2866	$\nu(\text{OH51})(60)+\nu(\text{NH}_3)(37)$	2707	OH stretch
2861	2753	2754	2742	$\nu(\text{NH}_3)(60)+\nu(\text{OH51})(38)$	2666	NH_3str
1764	1729	1777	1768	$\text{R2}[\nu(\text{C=O})(53)+\nu(\text{CN})(17)+\nu(\text{CC13})(4)]+\nu(\text{C=O5})(7)$	1745, 1737	In plane C=O str
1737	1703	1691	1685	$\nu_a(\text{C16O}_2)(91)+\text{R1}[\rho(\text{CC16})](5)$	1712, 1699	$\text{CO}_2\text{ symmetric str}$
1735	1701	1691	1685	$\nu(\text{C=O5})(36)+\rho(\text{C=O5})(11)+\nu(\text{C17N})(8)+\text{R2}[\nu(\text{C=O})](5)+\delta(\text{N7H42O44})(5)$	1705, 1686	$\text{C=O str} + \text{C=O rock}$
1699	1667	1691	1685	$\delta_a(\text{NH}_3)(27)+\tau(\text{O2H51})(23)+\text{R2}[\delta(\text{C13O2H51})](17)+\delta(\text{O50H49})(15)+\tau(\text{H29O50})(8)+\delta(\text{N8H29O50})(5)$	1668, 1638	$\text{NH}_3\text{ scissoring}$
1679	1648	-	-	$\delta_a(\text{NH}_3)(24)+\tau(\text{O2H51})(18)+\delta(\text{N8H29O50})(15)+\text{R2}[\delta(\text{C13O2H51})](13)+\delta(\text{O50H49})(12)+\tau(\text{H29O50})(7)$	1648, 1624	$\text{NH}_3\text{asym deformation}$
1658	1628	-	1624	$\delta(\text{O44H42})(33)+\delta(\text{O44H46O47})(28)+\delta(\text{O47H46})(17)+\tau(\text{H46O47})(8)+\delta(\text{O47H49O50})(6)$	1625, 1619	OH deformation
1644	1614	1607	1606	$\delta(\text{N8H29O50})(33)+\rho(\text{NH}_3)(13)+\delta'_a(\text{NH}_3)(12)+\delta_s(\text{NH}_3)(5)+\text{R3}[\nu(\text{C20C21})(5)+\nu(\text{C23C24})(5)]$	1607, 1595	NHO deformation
1639	1609	1607	1606	$\delta(\text{N8H29O50})(33)+\rho(\text{NH}_3)(12)+\delta'_a(\text{NH}_3)(12)+\text{R3}[\nu(\text{C23C24})(5)+\nu(\text{C20C21})(5)]+\delta_s(\text{NH}_3)(5)$	1619, 1579	NHO deformation
1629	1600	1607	1606	$\delta(\text{O47H46})(30)+\delta(\text{O47H49O50})(17)+\delta(\text{N8H29O50})(11)+\delta(\text{O44H42})(9)+\delta(\text{O44H46O47})(7)+\rho(\text{NH}_3)(6)+\delta'_a(\text{NH}_3)(5)$	1607, 1596	OH deformation
1624	1595	1594	1606	$\text{R3}[\nu(\text{CC})(61)+\delta_{\text{in}}(\text{C22H})(9)+\delta'_a(8)]+\rho'(\text{C18H})(5)$	1598, 1595	Ring 3 CC stretch
1607	1579	1594	1572	$\rho(\text{N7H})(42)+\delta(\text{N7H42O44})(31)+\tau(\text{H42O44})(12)+\nu(\text{C17N})(5)$	1579, 1571	NH rock
1526	1502	-	-	$\text{R3}[\delta_{\text{in}}(\text{CH})(62)+\nu(\text{CC})(32)]$	1503, 1501	In plane ring def
1519	1495	-	1493	$\delta_s(\text{NH}_3)(59)+\delta(\text{N8H29O50})(28)+\delta'_a(\text{NH}_3)(6)$	1538, 1511	NH_3symdef
1511	1487	-	1493	$\delta_a(\text{C14H}_3)(31)+\delta_a(\text{C15H}_3)(31)+\delta'_a(\text{C14H}_3)(23)+\rho(\text{C14H}_3)(5)$	1486, 1477	$\text{CH}_3\text{asymdef}$
1496	1473	-	1458	$\delta'_a(\text{C15H}_3)(28)+\delta_a(\text{C14H}_3)(27)+\delta_a(\text{C15H}_3)(24)+\delta'_a(\text{C14H}_3)(8)+\rho'(\text{C15H}_3)(5)$	1476, 1476	$\text{CH}_3\text{asymdef}$
1492	1468	1466	1458	$\delta'_a(\text{C15H}_3)(30)+\delta_a(\text{C15H}_3)(29)+\delta'_a(\text{C14H}_3)(21)+\delta_a(\text{C14H}_3)(11)$	1467, 1455	$\text{CH}_3\text{asymdef}$
1490	1467	1466	1458	$\rho'(\text{C18H})(23)+\text{R3}[\delta_{\text{in}}(\text{CH})(33)+\nu(\text{CC})(23)]+\rho(\text{C18H})(5)$	1467, 1466	CH rocking
1474	1452	1438	1458	$\delta'_a(\text{C14H}_3)(37)+\delta'_a(\text{C15H}_3)(27)+\delta_a(\text{C14H}_3)(19)+\delta_a(\text{C15H}_3)(8)$	1454, 1453	$\text{CH}_3\text{asymdef}$
1424	1403	1405	1402	$\delta_s(\text{C14H}_3)(33)+\text{R2}[\nu(\text{CN})(15)+\delta_{\text{in}}(\text{C=O})(11)]+\text{R1}[\nu(\text{C10N})](6)+\delta_s(\text{C15H}_3)(6)$	1410, 1403	CH_3symdef
1420	1400	1405	1402	$\delta_s(\text{C14H}_3)(27)+\text{R2}[\nu(\text{CN})(17)+\delta_{\text{in}}(\text{C=O})(14)+\delta(\text{C13O2H51})(5)]+\text{R1}[\nu(\text{C10N})](7)+\delta_s(\text{C15H}_3)(6)$	1400, 1390	CH_3symdef
1405	1385	1387	1385	$\rho(\text{C18H})(44)+\delta(\text{C18H28O44})(38)$	1393, 1392	CH rocking
1398	1379	1379	1373	$\rho'(\text{C18H})(51)+\delta(\text{C18H28O44})(13)+\rho(\text{C18H})(5)$	1376, 1371	CH rocking
1396	1376	1379	1361	$\delta_s(\text{C15H}_3)(73)+\delta_s(\text{C14H}_3)(16)+\text{R1}[\nu(\text{CC15})](6)$	1380, 1390	CH_3symdef
1366	1348	-	1361	$\text{R1}[\omega(\text{C10CH})(32)+\gamma(\text{C10CH})(22)+\delta(\text{C16CH})(5)]+\text{R2}[\delta(\text{N7C12H})](7)+\nu(\text{C11N})(5)$	1365, 1345	CCH wagging
1357	1339	1337	1334	$\text{R3}[\delta_{\text{in}}(\text{CH})(37)+\nu(\text{CC})(27)]+\rho'(\text{C18H})(8)+\rho(\text{C18H})(7)$	1338, 1338	In plane ring def
1347	1330	1337	1334	$\text{R2}[\delta(\text{N7C12H})(31)+\rho(\text{CNH})(12)]+\delta(\text{C18H28O44})(9)+\delta(\text{N7H42O44})(7)+\rho'(\text{C18H})(5)$	1329, 1326	NCH deformation
1320	1304	1312	1306	$\rho(\text{NH}_3)(13)+\text{R3}[\nu(\text{CC})](30)+\delta(\text{N7H42O44})(7)$	1301, 1275	$\text{NH}_3\text{ rocking}$
1312	1295	1298	1306	$\nu(\text{C=O4})(39)+\nu(\text{C=O3})(30)+\text{R1}[\delta(\text{CC16})](11)$	1296, 1269	C=O stretching
1282	1266	1266	1263	$\delta(\text{C11H})(32)+\text{R2}[\omega(\text{CNH})(14)+\gamma(\text{CNH})(9)]+\rho(\text{C11H})(10)+\delta(\text{C18H28O44})(8)$	1275, 1266	CH deformation
1273	1258	1252	1263	$\delta(\text{C18H28O44})(21)+\delta(\text{N7H42O44})(13)+\rho'(\text{C18H})(10)+\nu(\text{C17N})(8)+\rho(\text{N7H})(7)+\rho(\text{C18H})(5)+\tau(\text{H42O44})(5)+\rho(\text{NH}_3)(5)$	1252, 1245	CHO deformation
1258	1243	1252	1263	$\text{R1}[\delta(\text{C16CH})(24)+\rho(\text{C10CH})(22)+\nu(\text{CC15})(9)+\nu(\text{CC14})(9)+\rho(\text{C9C})(8)+\omega(\text{C10CH})(5)]$	1246, 1231	$\text{Ring 1 CCH deformation} + \text{CCH rocking}$

1234	1220	1221	1219	$\rho(\text{C11H})(48)+\delta(\text{C11H})(14)+\text{R1}[\nu(\text{C10N})](5)$	1224, 1217	CH rocking
1222	1208	1221	1219	$\rho(\text{C15H}_3)(14)+\text{R1}[\nu(\text{C9C10})(13)+\delta(\text{C14CC15})(10)+\nu(\text{CC14})(6)+\nu(\text{CC15})(6)]+\rho(\text{C14H}_3)(12)+\rho'(\text{C14H}_3)(6)+\rho'(\text{C15H}_3)(5)$	1214, 1196	CH ₃ rocking
1215	1201	1221	1219	$\rho'(\text{C18H})(32)+\delta(\text{C18H28O44})(22)+\text{R3}[\nu(\text{C18C19})](8)+\rho(\text{NH}_3)(6)$	1200, 1189	CHrocking
1209	1196	1198	1194	$\text{R3}[\delta_{\text{in}}(\text{C20H})(47)+\nu(\text{C19C20})(7)+\nu(\text{C18C19})(5)]+\rho'(\text{C18H})(14)+\delta(\text{C18H28O44})(9)$	1199, 1193	Ring 3 in plane deformation
1196	1183	1198	1194	$\text{R2}[\omega(\text{CNH})(55)+\gamma(\text{CNH})(23)+\nu(\text{C11C})(5)]+\delta(\text{C11H})(4)$	1184, 1182	Ring 2 CNH wagging
1189	1176	1177	1169	$\text{R3}[\text{i}_{\text{in}}(\text{CH})(71)+\nu(\text{C21C22})(15)+\nu(\text{C22C23})(7)]$	1176, 1173	Ring 3 in plane deformation
1170	1158	1165	1155	$\text{R2}[\omega(\text{CNH})(18)+\gamma(\text{CNH})(13)]+\text{R1}[\delta(\text{C16CH})(15)+\delta'_{\text{ring}}(6)]+\nu(\text{C11N})(9)$	1160, 1157	Ring 2 CNH wagging
1162	1150	1165	1155	$\rho(\text{NH}_3)(53)+\delta(\text{N8H29O50})(19)$	1149, 1140	NH ₃ rocking
1154	1143	1165	1155	$\rho(\text{NH}_3)(22)+\text{R2}[\nu(\text{C12N})(13)+\omega(\text{CNH})(10)+\gamma(\text{CNH})(6)+\nu(\text{CC13})(5)]+\delta(\text{N8H29O50})(13)$	1140, 1124	NH ₃ rocking
1134	1123	1122	1118	$\rho'(\text{C15H}_3)(18)+\rho'(\text{C14H}_3)(16)+\rho(\text{C15H}_3)(11)+\text{R1}[\omega(\text{C9CC})](10)+\rho(\text{C14H}_3)(9)$	1124, 1114	CH ₃ rocking
1123	1113	1113	1118	$\delta(\text{C18H28O44})(35)+\rho'(\text{NH}_3)(10)+\rho(\text{C18H})(10)+\rho'(\text{C18H})(6)+\delta(\text{N8C18C17})(6)$	1101, 1099	CHO deformation
1110	1100	1100	1118	$\nu(\text{C11N})(21)+\text{R1}[\omega(\text{C10CH})(10)+\nu(\text{C10N})(8)+\nu(\text{CC14})(5)+\nu(\text{CC15})(5)]+\text{R2}[\nu(\text{C12N})](6)+\delta(\text{C18H28O44})(5)$	1099, 1088	CN stretch
1094	1084	1078	1080	$\delta(\text{C18H28O44})(23)+\rho'(\text{NH}_3)(15)+\rho(\text{C18H})(14)+\rho(\text{NH}_3)(7)+\delta(\text{N8C18C17})(6)+\tau(\text{H29O50})(5)+\text{R3}[\nu(\text{C20C21})](5)$	1081, 1065	CHO deformation
1051	1042	1038	1053	$\text{R3}[\nu(\text{CC})(54)+\delta_{\text{trig}}(13)+\delta_{\text{in}}(\text{CH})(20)]$	1042, 1041	Ring3 CC stretch
1031	1023	1024	1020	$\rho(\text{C14H}_3)(28)+\rho'(\text{C15H}_3)(20)+\text{R2}[\delta_{\text{in}}(\text{C=O})(9)+\nu(\text{CC13})(6)]$	1027, 1024	CH ₃ rocking
1022	1014	1024	1020	$\text{R2}[\delta_{\text{in}}(\text{C=O})(19)+\nu(\text{CC13})(10)+\delta(\text{C13O2H51})(7)+\rho(\text{CNH})(5)]+\rho'(\text{C15H}_3)(5)+\omega(\text{N7H})(5)$	1024, 1018	C=O in plane bend
1022	1014	1024	1020	$\text{R3}[\text{oop}(\text{CH})(68)+\text{puck}(13)+\delta_{\text{trig}}(6)]$	1013, 1010	Ring3 CH out of plane bend
1017	1009	1007	1009	$\text{R3}(\delta_{\text{trig}})(21)+\delta(\text{N7H42O44})(9)+\delta(\text{C12NC})(6)+\text{R2}[\gamma(\text{CNH})](5)+\omega(\text{N7H})(5)$	1011, 1002	Ring 3 deformation
1014	1006	1007	1001	$\delta(\text{N7H42O44})(13)+\delta(\text{C12NC})(9)+\omega(\text{N7H})(8)+\text{R3}(\delta_{\text{trig}})(7)+\text{R2}[\gamma(\text{CNH})(7)+\rho(\text{CNH})(5)+\nu(\text{C11C})(5)]$	1002, 998	NHO deformation
1002	994	993	989	$\text{R3}[\text{oop}(\text{CH})(90)+\tau'_a(8)]$	993, 981	Ring3 CH out of plane bend
982	975	965	972	$\delta(\text{O50H51O2})(41)+\text{R2}[\delta(\text{C13O2H51})](22)+\rho(\text{O50H49})(6)+\delta(\text{O50H49})(6)+\omega(\text{O50H49})(6)$	967, 949	OHO deformation
967	960	965	972	$\text{R3}[\text{oop}(\text{CH})](25)+\nu(\text{CN8})(9)+\rho(\text{NH}_3)(6)+\omega(\text{C=O5})(6)+\delta(\text{N8H29O50})(6)+\delta(\text{C18H28O44})(5)+\delta(\text{O50H51O2})(5)+\nu(\text{C17C18})(5)$	905, 924	Ring3 CH out of plane bend
958	951	955	951	$\text{R1}[\nu(\text{C9C10})(14)+\nu(\text{CC14})(12)+\nu(\text{CC15})(7)]+\rho(\text{C15H}_3)(12)+\text{R2}[\nu(\text{CC13})(9)+\gamma(\text{CNH})(7)+\nu(\text{C11C})(5)]$	863, 879	Ring 1 CC stretch
955	948	955	951	$\rho'(\text{C14H}_3)(34)+\text{R1}[\nu(\text{CC15})(26)+\nu(\text{CC14})(5)]+\rho(\text{C15H}_3)(19)+\rho(\text{C14H}_3)(5)$	874, 887	CH ₃ rocking
941	935	955	929	$\text{R3}[\text{oop}(\text{CH})](20)+\nu(\text{C17C18})(8)+\omega(\text{N7H})(7)+\nu(\text{CN8})(6)$	849, 861	Ring3 CH out of plane bend
912	906	880	875	$\delta(\text{N7H42O44})(21)+\nu(\text{CN8})(13)+\omega(\text{N7H})(10)+\omega(\text{O44H42})(7)+\delta(\text{N8C18C17})(7)$	858, 850	NHO deformation
882	877	880	875	$\delta(\text{N7H42O44})(33)+\omega(\text{N7H})(17)+\omega(\text{O44H42})(13)+\tau(\text{C17N})(7)+\tau(\text{H42O44})(6)+\rho(\text{O44H42})(5)$	838, 843	NHO scissoring + NH wagging
874	869	880	875	$\nu(\text{C11N})(13)+\text{R2}[\nu(\text{CC13})(12)+\text{oop}(\text{C=O})(9)]+\text{R1}[\nu(\text{C10N})](8)+\tau(\text{C17N})(5)$	834, 839	CN stretch
867	863	850	875	$\text{R3}[\text{oop}(\text{CH})](96)$	774, 789	Ring3 CH out of plane bend
860	855	850	847	$\delta(\text{N7H42O44})(17)+\omega(\text{N7H})(11)+\text{R1}[\nu(\text{CC16})(9)+\nu(\text{C9C10})(6)]+\text{R2}[\text{oop}(\text{C=O})](5)$	790, 828	NHO deformation + NH wagging
848	843	841	847	$\text{R1}[\nu(\text{CC16})(17)+\nu(\text{CC14})(12)+\omega(\text{CC16})(10)+\delta(\text{CC16})(8)+\rho(\text{C10CH})(7)]+\text{R2}(\delta_{\text{ring}})(5)+\delta(\text{N8H29O50})(5)$	808, 811	Ring 1 CC stretch

837	833	841	847	$\omega(\text{C}=\text{O}5)(23)+\delta(\text{C}17\text{C}18\text{C}19)(11)+\delta(\text{N}8\text{H}29\text{O}50)(9)+\delta(\text{N}8\text{C}18\text{C}19)(8)+\rho(\text{C}=\text{O}5)(7)+\nu(\text{CN}8)(5)+\rho(\text{NH}_3)(5)$	771, 773	C=O wagging
814	810	811	806	$\text{R}2[\delta_{\text{in}}(\text{C}=\text{O})(13)+\delta_{\text{ring}}(10)+\nu(\text{CC}13)(7)+\text{oop}(\text{C}=\text{O})(5)]+\text{R}1[\omega(\text{CC}16)(7)+\nu(\text{CC}14)(5)]$	675, 770	Ring 2 C=O in plane bend
789	786	783	791	$\tau(\text{H}46\text{O}47)(13)+\omega(\text{O}44\text{H}42)(11)+\delta(\text{O}44\text{H}46\text{O}47)(8)+\rho(\text{O}47\text{H}46)(8)+\text{R}3(\text{puck})(6)+\omega(\text{C}=\text{O}5)(5)$	706, 713	OH torsion
774	771	783	791	$\tau(\text{H}46\text{O}47)(18)+\rho(\text{O}47\text{H}46)(11)+\delta(\text{N}7\text{H}42\text{O}44)(10)+\delta(\text{O}44\text{H}46\text{O}47)(9)+\omega(\text{O}44\text{H}42)(7)$	755, 757	OH torsion
769	766	783	766	$\delta(\text{N}7\text{H}42\text{O}44)(17)+\tau(\text{H}46\text{O}47)(17)+\rho(\text{O}47\text{H}46)(10)+\omega(\text{N}7\text{H})(9)+\delta(\text{O}44\text{H}46\text{O}47)(8)+\omega(\text{O}44\text{H}42)(7)+\text{R}1[\delta(\text{CC}16)](6)$	729, 742	NHO deformation
759	757	744	737	$\omega(\text{N}7\text{H})(24)+\delta(\text{N}7\text{H}42\text{O}44)(23)+\tau(\text{H}46\text{O}47)(9)+\rho(\text{O}47\text{H}46)(6)$	684, 724	NH wagging
727	725	725	721	$\delta(\text{N}7\text{H}42\text{O}44)(14)+\omega(\text{N}7\text{H})(10)+\rho(\text{C}=\text{O}5)(6)+\omega(\text{C}=\text{O}5)(6)+\text{R}2(\delta_{\text{ring}})(6)+\delta(\text{C}17\text{C}18\text{C}19)(5)+\delta(\text{NC}17\text{C})(5)$	715, 719	NHO scissoring
718	716	725	721	$\delta(\text{N}8\text{C}18\text{C}17)(22)+\omega(\text{C}=\text{O}5)(21)+\rho(\text{C}=\text{O}5)(5)$	636, 661	NCC deformation
715	713	725	721	$\text{R}3[\text{puck}(58)+\text{oop}(\text{C}21\text{H})(12)+\text{oop}(\text{C}23\text{H})(12)+\text{oop}(\text{C}19\text{C}18)(6)]$	630, 631	Ring 3 puckering
689	688	691	696	$\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)(12)+\delta_{\text{in}}(\text{C}=\text{O})(8)+\omega(\text{CNH})(7)]+\delta(\text{N}7\text{H}42\text{O}44)(10)+\text{R}1[\nu(\text{SC}11)(7)+\tau'(5)]+\tau(\text{C}17\text{N})(5)$	657, 668	Ring 2 COH deformation
665	664	-	-	$\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)(15)+\text{oop}(\text{C}=\text{O})(14)+\omega(\text{CNH})(7)]+\text{R}1[\nu(\text{SC}11)(6)+\omega(\text{CC}16)(6)+\tau(\text{C}11\text{N})(5)]+\delta(\text{N}7\text{H}42\text{O}44)(6)$	607, 610	Ring 2 COH deformation
648	647	650	644	$\tau(\text{O}2\text{H}51)(21)+\delta(\text{O}44\text{H}46\text{O}47)(15)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](13)+\omega(\text{O}44\text{H}42)(13)+\tau(\text{H}46\text{O}47)(12)+\rho(\text{O}44\text{H}42)(6)+\tau(\text{H}49\text{O}50)(6)$	573, 599	OH torsion
631	630	621	619	$\text{R}3(\delta'a)(78)$	514, 517	Ring 3 deformation
606	606	621	619	$\delta(\text{N}7\text{H}42\text{O}44)(12)+\text{R}2[\delta_{\text{in}}(\text{C}=\text{O})(9)+\text{oop}(\text{C}=\text{O})(8)]+\text{R}3(\delta_a)(9)+\delta(\text{N}8\text{C}18\text{C}19)(8)+\delta(\text{N}8\text{H}29\text{O}50)(6)+\delta(\text{NC}17\text{C})(5)$	567, 594	NHO deformation
592	591	593	-	$\text{R}2[\text{oop}(\text{C}=\text{O})(19)+\delta_{\text{in}}(\text{C}=\text{O})(8)]+\delta(\text{N}8\text{C}18\text{C}19)(6)+\text{R}3(\delta_a)(5)+\tau(\text{H}49\text{O}50)(5)$	539, 552	Ring 2 C=O out of plane bend
572	572	576	-	$\tau(\text{O}2\text{H}51)(21)+\tau(\text{H}49\text{O}50)(17)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](14)+\delta(\text{O}44\text{H}46\text{O}47)(13)+\omega(\text{O}50\text{H}49)(6)$	526, 550	OH torsion
548	548	576	-	$\tau(\text{H}46\text{O}47)(35)+\omega(\text{O}44\text{H}42)(17)+\delta(\text{O}44\text{H}46\text{O}47)(11)+\delta(\text{O}44\text{H}42)(7)+\text{R}1[\nu(\text{SC}9)](5)$	511, 525	OH torsion
536	536	523	-	$\tau(\text{H}46\text{O}47)(42)+\delta(\text{O}44\text{H}46\text{O}47)(15)+\omega(\text{O}44\text{H}42)(14)+\delta(\text{O}44\text{H}42)(7)+\rho(\text{O}47\text{H}46)(5)$	486, 519	OH torsion
521	521	523	-	$\text{R}3[\tau_a(21)+\text{oop}(\text{C}19\text{C}18)(13)+\text{puck}(5)]+\omega(\text{N}7\text{H})(9)+\omega(\text{C}=\text{O}5)(7)$	411, 415	Ring 3 torsion
512	512	515	-	$\text{R}2[\delta_{\text{in}}(\text{C}=\text{O})(19)+\text{puck}(9)+\text{oop}(\text{C}=\text{O})(8)]+\text{R}1[\delta_{\text{ring}}(15)+\tau(\text{C}11\text{N})(7)]$	462, 464	Ring 2 C=O in plane bend
509	509	501	-	$\delta(\text{N}7\text{H}42\text{O}44)(12)+\text{R}1[\nu(\text{SC}11)(6)+\delta'_{\text{ring}}(5)]+\delta(\text{NC}17\text{C})(6)+\text{R}3(\tau_a)(6)$	430, 484	NHO deformation
485	485	476	-	$\rho(\text{O}44\text{H}42)(30)+\tau(\text{H}46\text{O}47)(14)+\delta(\text{O}44\text{H}46\text{O}47)(9)+\omega(\text{O}44\text{H}42)(9)+\delta(\text{O}47\text{H}49\text{O}50)(7)+\rho(\text{O}47\text{H}46)(7)+\delta(\text{O}44\text{H}42)(6)$	424, 446	OH rocking
457	458	476	-	$\text{R}2[\text{oop}(\text{C}=\text{O})(11)+\delta_{\text{in}}(\text{C}=\text{O})(9)]+\delta(\text{N}7\text{H}42\text{O}44)(6)+\text{R}1[\nu(\text{SC}11)(5)+\delta(\text{C}14\text{CC}15)(5)]+\rho(\text{O}44\text{H}42)(5)$	396, 414	Ring 2 C=O out of plane bend
445	446	444	-	$\omega(\text{O}50\text{H}49)(18)+\delta(\text{O}47\text{H}49\text{O}50)(17)+\delta(\text{O}44\text{H}46\text{O}47)(15)+\tau(\text{H}49\text{O}50)(13)+\delta(\text{O}50\text{H}49)(9)+\rho(\text{O}50\text{H}49)(6)$	407, 411	OH wagging
414	415	-	-	$\text{R}3[\tau'_a(72)+\text{oop}(\text{CH})(14)]+\tau(\text{CN}8)(6)$	368, 381	Ring 3 torsion
411	412	405	-	$\delta(\text{N}8\text{H}29\text{O}50)(31)+\tau(\text{CN}8)(27)+\tau(\text{H}29\text{O}50)(11)+\delta(\text{N}8\text{C}18\text{C}17)(5)$	377, 386	NHO deformation
397	398	405	-	$\tau(\text{CN}8)(40)+\delta(\text{N}8\text{H}29\text{O}50)(16)+\tau(\text{H}29\text{O}50)(13)+\rho(\text{C}=\text{O}5)(7)$	349, 364	CN torsion
378	379	387	-	$\text{R}1[\rho(\text{C}9\text{CC})(30)+\omega(\text{C}9\text{CC})(9)+\rho(\text{CC}16)(8)]+\delta(\text{N}8\text{H}29\text{O}50)(8)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)(7)+\delta_{\text{in}}(\text{C}=\text{O})(5)]$	342, 346	Ring 1 CC rocking
373	374	387	-	$\delta(\text{O}47\text{H}49\text{O}50)(28)+\rho(\text{O}47\text{H}46)(22)+\delta(\text{O}44\text{H}46\text{O}47)(14)+\omega(\text{O}44\text{H}42)(5)$	331, 336	OHO deformation
361	362	363	-	$\delta(\text{O}47\text{H}49\text{O}50)(19)+\delta(\text{N}8\text{H}29\text{O}50)(18)+\rho(\text{O}47\text{H}46)(15)+\delta(\text{O}44\text{H}46\text{O}47)(9)$	309, 327	OHO deformation
343	344	337	-	$\text{R}1[\delta(\text{C}14\text{CC}15)(20)+\nu(\text{SC}9)(18)+\omega(\text{C}9\text{CC})(5)]+\tau(\text{CN}8)(10)$	288, 293	Ring 1 CCC deformation
330	331	337	-	$\tau(\text{CN}8)(23)+\delta(\text{N}8\text{C}18\text{C}17)(16)+\omega(\text{N}7\text{H})(14)+\tau(\text{H}29\text{O}50)(8)+\tau(\text{C}17\text{C}18)(6)$	302, 305	CN torsion

329	330	337	-	$\rho(\text{C}=\text{O}5)(13)+\tau(\text{CN}8)(12)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](11)+\delta(\text{N}8\text{H}29\text{O}50)(8)+\omega(\text{N}7\text{H})(6)+\tau(\text{H}29\text{O}50)(6)+\delta(\text{N}7\text{H}42\text{O}44)(5)+\text{R}3[\delta_{\text{in}}(\text{C}19\text{C}18)](5)$	273, 262	C=O5 rocking
308	309	337	-	$\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](30)+\delta(\text{C}18\text{H}28\text{O}44)(11)+\rho(\text{C}=\text{O}5)(10)$	265, 269	Ring 2 COH deformation
300	302	293	-	$\tau(\text{CC}14)(44)+\tau(\text{CC}15)(10)+\text{R}1[\delta'_{\text{ring}}(7)+\nu(\text{CC}16)(6)+\delta(\text{C}14\text{CC}15)(6)]$	253, 278	CC torsion
299	301	293	-	$\tau(\text{CC}15)(14)+\text{R}1[\delta(\text{C}14\text{CC}15)(12)+\delta'_{\text{ring}}(10)+\rho(\text{C}9\text{CC})(10)+\gamma(\text{C}9\text{CC})(6)+\nu(\text{CC}16)(5)+\nu(\text{SC}9)(5)]+\tau(\text{CC}14)(8)$	237, 252	CC torsion
271	273	260	-	$\omega(\text{N}7\text{H})(15)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)(10)+\text{oop}(\text{C}=\text{O})(7)]+\tau(\text{C}17\text{C}18)(6)+\delta(\text{O}47\text{H}49\text{O}50)(5)+\omega(\text{O}47\text{H}46)(5)+\tau(\text{C}17\text{N})(5)+\tau(\text{H}42\text{O}44)(5)$	248, 243	NH wagging
261	262	260	-	$\omega(\text{O}47\text{H}46)(24)+\delta(\text{O}47\text{H}49\text{O}50)(20)+\rho(\text{O}47\text{H}46)(16)+\tau(\text{H}46\text{O}47)(14)+\delta(\text{O}47\text{H}46)(10)+\delta(\text{O}44\text{H}46\text{O}47)(5)$	228, 231	OH wagging
259	260	260	-	$\omega(\text{O}47\text{H}46)(19)+\rho(\text{O}47\text{H}46)(15)+\delta(\text{O}47\text{H}49\text{O}50)(14)+\tau(\text{H}46\text{O}47)(11)+\delta(\text{O}47\text{H}46)(8)+\tau(\text{CC}15)(7)$	221, 223	OH wagging + OH rocking
246	248	260	-	$\tau(\text{CN}8)(18)+\delta(\text{N}7\text{H}42\text{O}44)(15)+\delta(\text{N}8\text{C}18\text{C}17)(10)+\tau(\text{C}17\text{C}18)(8)+\delta(\text{N}8\text{H}29\text{O}50)(7)+\delta(\text{C}12\text{NC})(6)+\delta(\text{C}18\text{H}28\text{O}44)(5)$	198, 217	CN torsion
238	239	226	-	$\text{R}1[\gamma(\text{C}9\text{CC})](35)+\delta(\text{N}8\text{H}29\text{O}50)(7)+\delta(\text{N}7\text{H}42\text{O}44)(6)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](6)$	206, 208	Ring 1 CC twisting
222	223	226	-	$\delta(\text{C}18\text{H}28\text{O}44)(18)+\tau(\text{CN}8)(13)+\tau(\text{H}46\text{O}47)(13)+\omega(\text{O}47\text{H}46)(9)+\delta(\text{N}8\text{C}18\text{C}17)(7)+\delta(\text{O}47\text{H}49\text{O}50)(6)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](5)+\delta(\text{N}8\text{H}29\text{O}50)(5)+\tau(\text{C}17\text{C}18)(5)$	170, 193	CHO deformation
215	217	226	-	$\text{R}2[\delta_{\text{in}}(\text{C}=\text{O})(13)+\delta(\text{C}13\text{O}2\text{H}51)(12)]+\text{R}1[\omega(\text{C}9\text{CC})(6)+\gamma(\text{C}9\text{CC})(5)]+\tau(\text{CC}15)(5)$	181, 186	Ring 2 C=O in plane bend
206	207	207	-	$\delta(\text{N}7\text{H}42\text{O}44)(13)+\omega(\text{O}44\text{H}42)(13)+\omega(\text{N}7\text{H})(9)+\tau(\text{C}17\text{C}18)(8)+\delta(\text{C}18\text{H}28\text{O}44)(7)$	156, 165	NHO deformation
185	186	207	-	$\delta(\text{C}18\text{H}28\text{O}44)(26)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](10)+\delta(\text{N}8\text{H}29\text{O}50)(7)+\tau(\text{CN}8)(6)+\tau(\text{H}42\text{O}44)(5)$	145, 154	CHO deformation
172	174	207	-	$\tau(\text{CN}8)(26)+\delta(\text{N}8\text{H}29\text{O}50)(15)+\delta(\text{C}18\text{H}28\text{O}44)(12)+\tau(\text{C}17\text{C}18)(9)+\delta(\text{O}47\text{H}49\text{O}50)(7)+\delta(\text{N}8\text{C}18\text{C}17)(6)+\delta(\text{N}7\text{H}42\text{O}44)(5)$	139, 146	CN torsion
172	173	169	-	$\omega(\text{O}44\text{H}42)(15)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](12)+\delta(\text{N}8\text{H}29\text{O}50)(10)+\delta(\text{C}18\text{H}28\text{O}44)(7)+\delta(\text{C}17\text{C}18\text{C}19)(6)+\omega(\text{N}7\text{H})(5)+\tau(\text{H}42\text{O}44)(5)$	131, 135	OH wagging
149	150	159	-	$\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](21)+\text{R}1[\tau(\text{C}11\text{N})](14)+\omega(\text{O}44\text{H}42)(7)$	116, 122	Ring 2 COH deformation
134	135	144	-	$\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](27)+\tau(\text{C}17\text{C}18)(12)+\tau(\text{CN}8)(11)+\delta(\text{C}18\text{H}28\text{O}44)(7)$	101, 113	Ring 2 COH deformation
133	134	127	-	$\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](45)+\delta(\text{N}8\text{H}29\text{O}50)(17)+\tau(\text{C}17\text{C}18)(7)$	77, 80	Ring 2 COH deformation
112	113	108	-	$\tau(\text{C}17\text{C}18)(22)+\delta(\text{N}7\text{H}42\text{O}44)(15)+\delta(\text{C}18\text{H}28\text{O}44)(11)+\omega(\text{N}7\text{H})(11)+\tau(\text{C}12\text{N})(7)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](5)+\rho(\text{O}44\text{H}42)(5)$	94, 100	CC torsion
107	108	108	-	$\tau(\text{C}17\text{C}18)(24)+\text{R}2[\text{puck}(16)+\delta(\text{C}13\text{O}2\text{H}51)(7)]+\text{R}1[\tau(\text{C}11\text{N})](16)+\omega(\text{N}7\text{H})(6)+\delta(\text{C}18\text{H}28\text{O}44)(5)$	70.4, 90	CC torsion
97	97	108	-	$\delta(\text{N}7\text{H}42\text{O}44)(49)+\delta(\text{C}18\text{H}28\text{O}44)(22)+\tau(\text{H}42\text{O}44)(8)$	63, 68	NHO deformation
78	78	70	-	$\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](26)+\omega(\text{N}7\text{H})(20)+\tau(\text{C}17\text{C}18)(14)+\tau(\text{H}42\text{O}44)(8)+\omega(\text{O}44\text{H}42)(8)+\tau(\text{H}46\text{O}47)(5)+\delta(\text{C}18\text{H}28\text{O}44)(5)$	56, 66	Ring 2 COH deformation
68	68	70	-	$\omega(\text{O}44\text{H}42)(35)+\tau(\text{CN}8)(13)+\rho(\text{O}47\text{H}46)(11)+\rho(\text{O}44\text{H}42)(8)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](8)+\omega(\text{N}7\text{H})(5)$	50, 53	OH wagging
64	64	70	-	$\tau(\text{CC}16)(28)+\delta(\text{C}18\text{H}28\text{O}44)(11)+\omega(\text{O}44\text{H}42)(9)+\tau(\text{C}17\text{C}18)(8)+\omega(\text{N}7\text{H})(7)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](6)+\tau(\text{CN}8)(5)$	32, 45	CC torsion
54	54	57	-	$\tau(\text{C}17\text{C}18)(33)+\tau(\text{C}12\text{N})(18)+\tau(\text{C}17\text{N})(7)+\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](7)+\delta(\text{N}8\text{H}29\text{O}50)(6)$	38, 47	CC torsion
52	52	57	-	$\delta(\text{N}7\text{H}42\text{O}44)(24)+\delta(\text{C}18\text{H}28\text{O}44)(23)+\tau(\text{CN}8)(9)+\tau(\text{C}17\text{C}18)(9)+\delta(\text{N}8\text{H}29\text{O}50)(6)+\omega(\text{O}44\text{H}42)(5)$	30, 35	NHO deformation
39	39	57	-	$\tau(\text{C}17\text{C}18)(30)+\tau(\text{CN}8)(18)+\delta(\text{N}8\text{H}29\text{O}50)(10)+\delta(\text{C}18\text{H}28\text{O}44)(6)+\omega(\text{O}44\text{H}42)(5)$	18, 28	CC torsion
36	36	57	-	$\text{R}2[\delta(\text{C}13\text{O}2\text{H}51)](35)+\tau(\text{C}12\text{N})(18)+\omega(\text{O}44\text{H}42)(7)+\text{R}1[\tau(\text{C}18\text{C}19)](5)+\tau(\text{CN}8)(5)+\delta(\text{N}7\text{H}42\text{O}44)(5)$	19, 22	Ring 2 COH deformation

28	28	-	-	$R2[\delta(C13O2H51)](14)+\tau(H46O47)(8)+\delta(C18H28O44)(8)+R1[\tau(7)+\tau(C18C19)(5)]+\delta(N7H42O44)(6)+\tau(C17N)(5)$	27,	Ring 2 COH deformation + OH torsion
25	26	-	-	$\tau(C17C18)(36)+\tau(H46O47)(14)+\delta(O44H46O47)(12)+\delta(N8H29O50)(9)$	8, 13	CC torsion
17	17	-	-	$\tau(H46O47)(49)+\delta(O44H46O47)(20)+\delta(O47H49O50)(7)+\omega(O50H49)(6)$	14	OH torsion
