Vibrational spectra, hydrogen bonding interactions and chemical reactivity analysis of nicotinamide-citric acid cocrystal by an experimental and theoretical approach

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Electronic Supplementary Information

Part 1. FIGURES

PXRD and DSC pattern of nicotinamide-citric acid (NIC-CA) cocrystal are shown in Fig. S1 and S2, respectively. Optimized structure of NIC and CA are shown in Fig. S3, S4, respectively. Crystallographic structure of NIC and NIC-CA cocrystal is given in Fig. S5 and S6, respectively. Experimental and calculated IR and Raman spectra of NIC and CA are shown in Fig. S7, S8 and S9, S10, respectively. The molecular graph of monomer using AIM2000 program is given in Fig. S11. HOMO and LUMO plot of NIC, CA and NIC-CA (monomer) model with its energy gap is shown in Fig. S12-S14. The molecular electrostatic potential (MESP) surface of NIC, CA and NIC-CA (monomer) model are given in Fig. S15-S17, respectively.

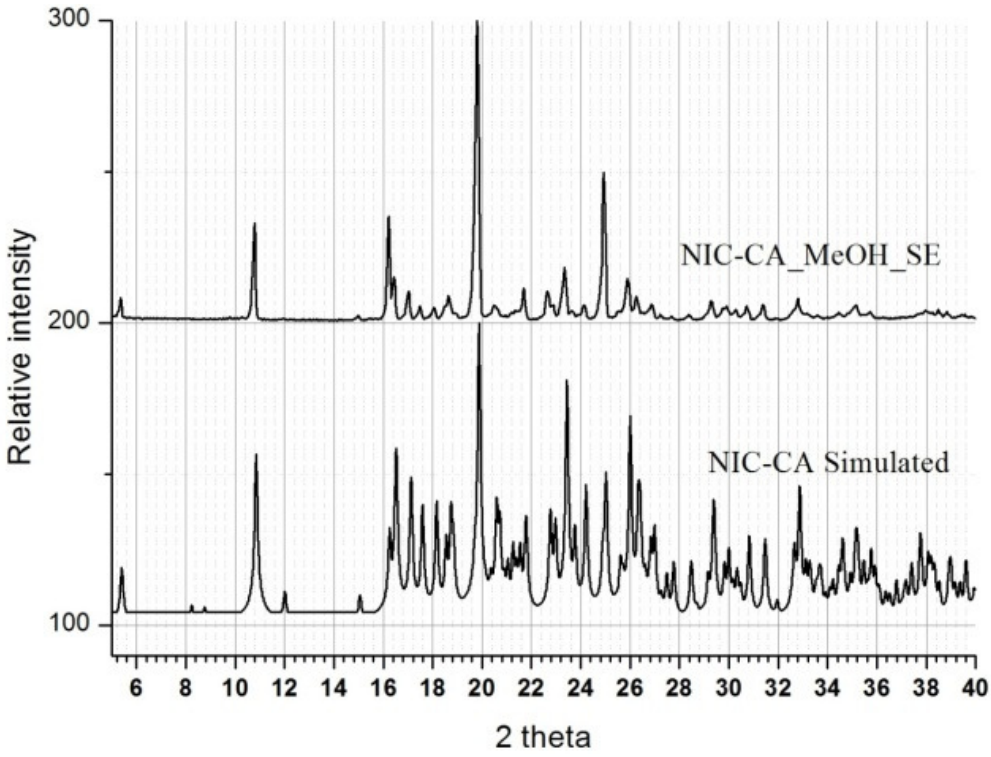

Fig. S1 Powder X-Ray Diffraction (PXRD) pattern of NIC-CA cocrystal.

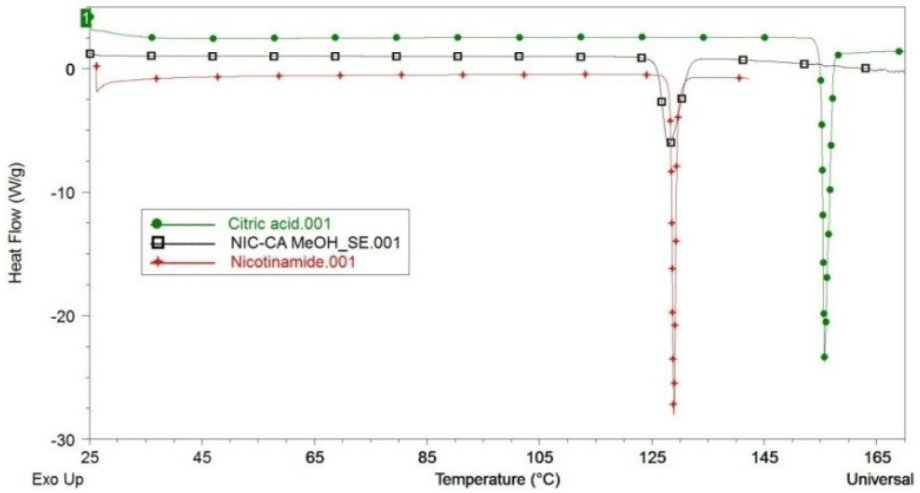

Fig. S2 Differential scanning calorimetry (DSC) of NIC-CA cocrystal.

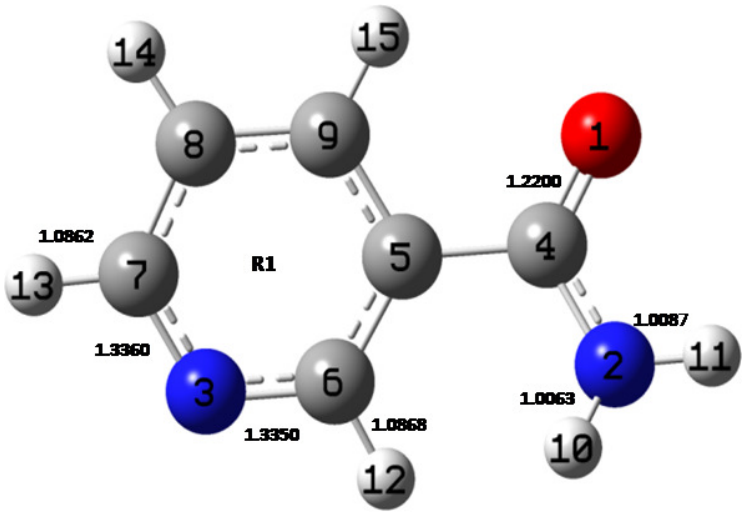

Fig. S3 Optimized structure for NIC and the atom numbering scheme adopted in this study.

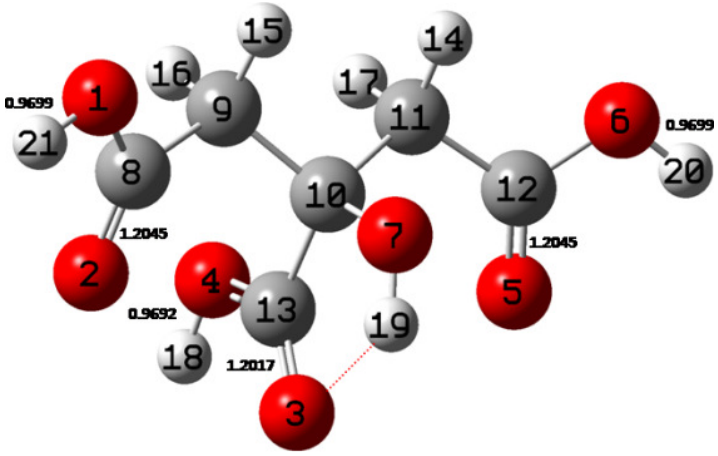

Fig. S4 Optimized structure for CA and the atom numbering scheme adopted in this study.

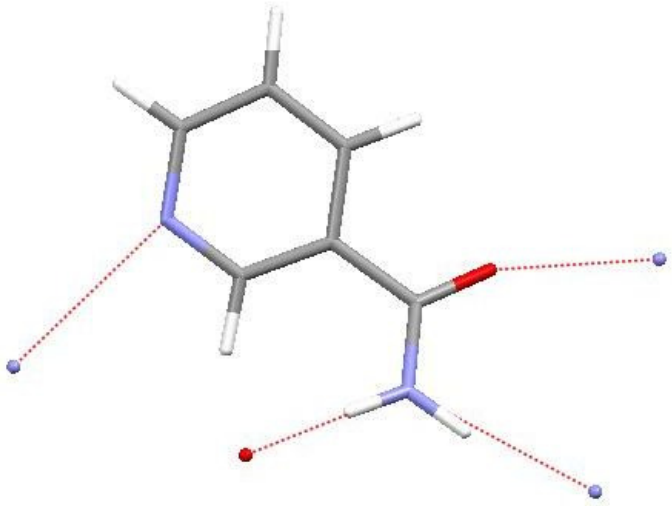

Fig. S5 Crystallographic structure of NIC showing all the interactions.

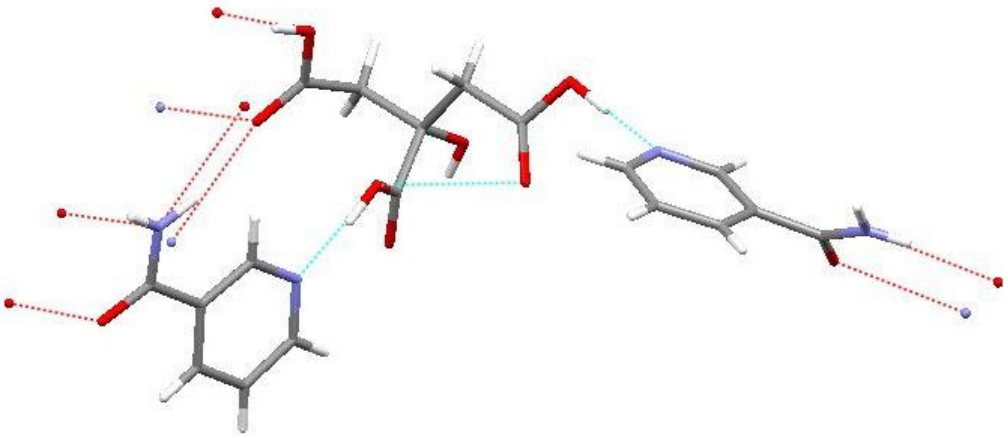

Fig. S6 Crystallographic structure of NIC-CA cocrystal showing all the interactions.

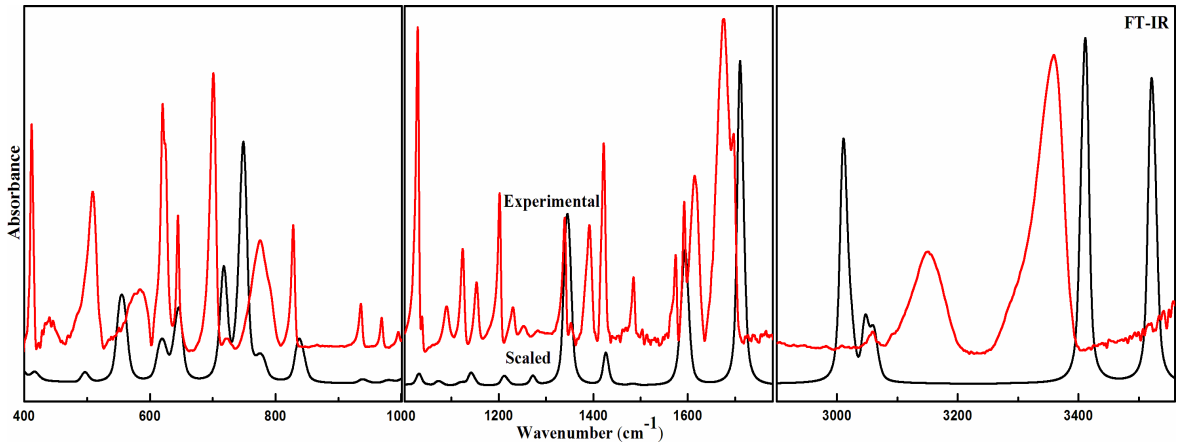

Fig. S7 Experimental and calculated (scaled) IR absorbance spectra of NIC in the region 400-1001 cm^{-1}, 1001-1780 cm^{-1} and 2900-3560 cm^{-1}.

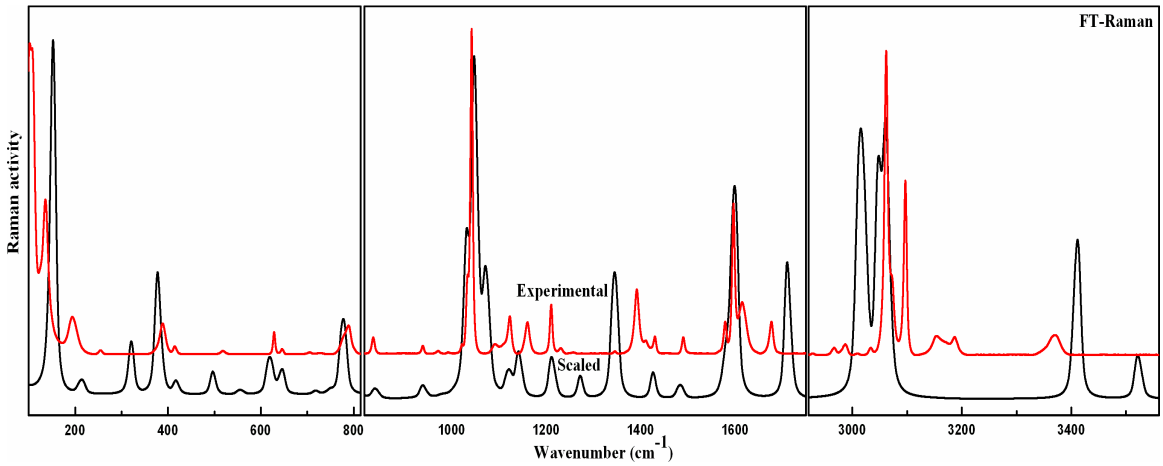

Fig. S8 Experimental and calculated (scaled) Raman scattering spectra of NIC in the region 100-815 cm^{-1}, 815-1750 cm^{-1} and 2920-3560 cm^{-1}.

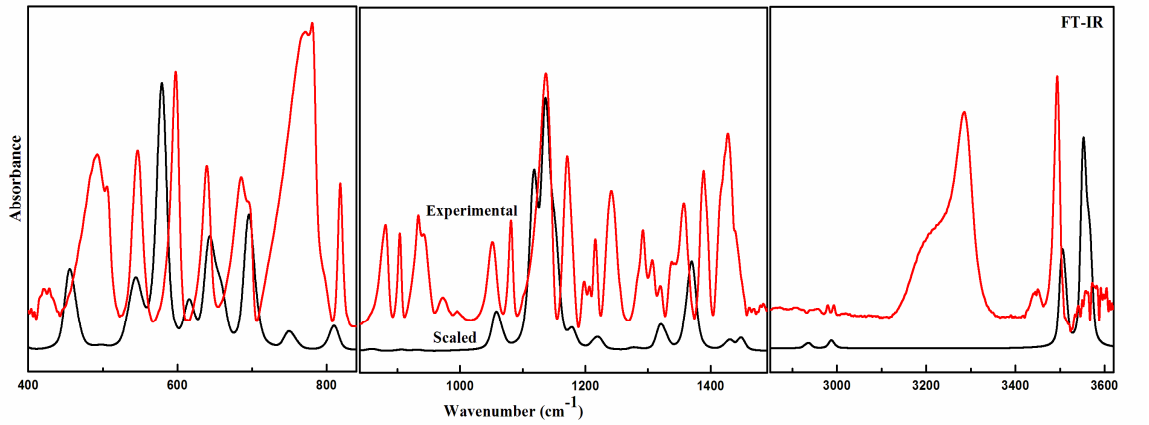

Fig. S9 Experimental and calculated (scaled) IR absorbance spectra of CA in the region 400-840 cm^{-1}, 840-1490 cm^{-1} and 2850-3620 cm^{-1}.

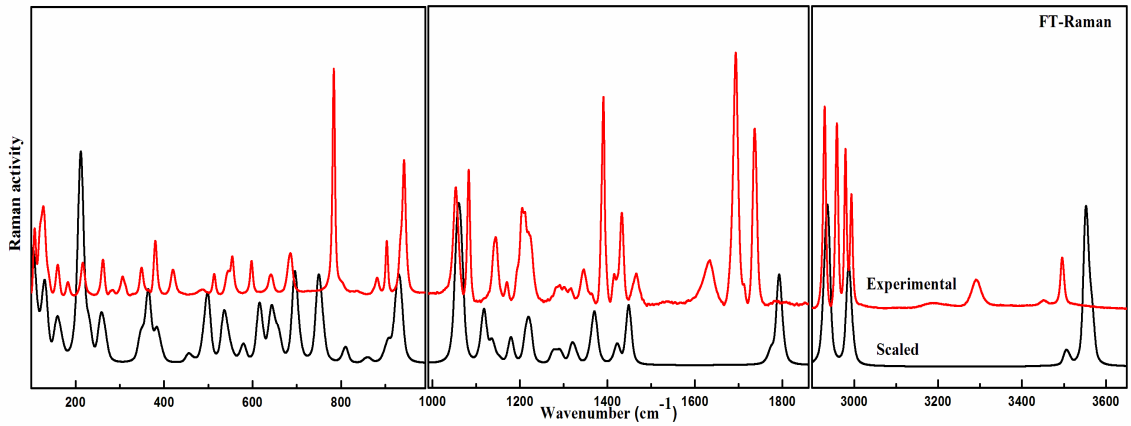

Fig. S10 Experimental and calculated (scaled) Raman scattering spectra of CA in the region 100-990 cm^{-1}, 990-1860 cm^{-1} and 2900-3650 cm^{-1}.

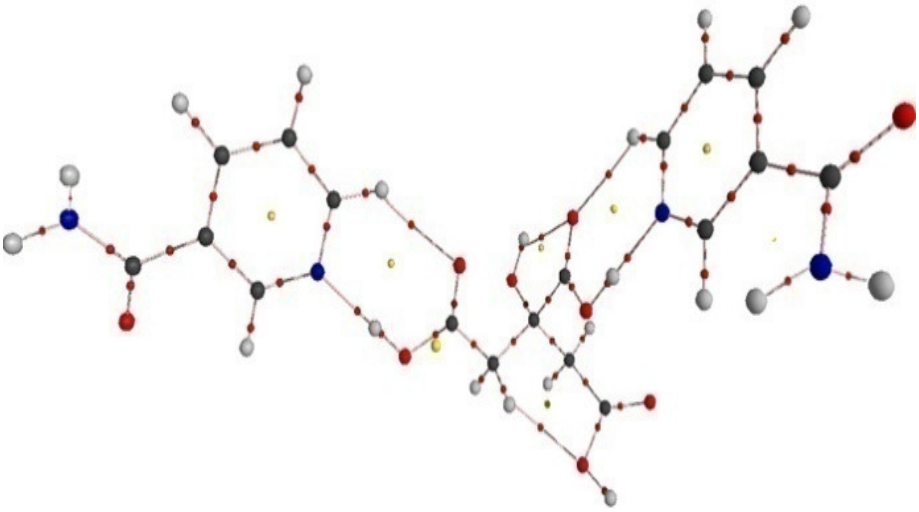

Fig. S11 Molecular graph of NIC-CA (monomer): bond critical points (small red spheres), ring critical points (small yellow sphere), bond paths (pink lines).

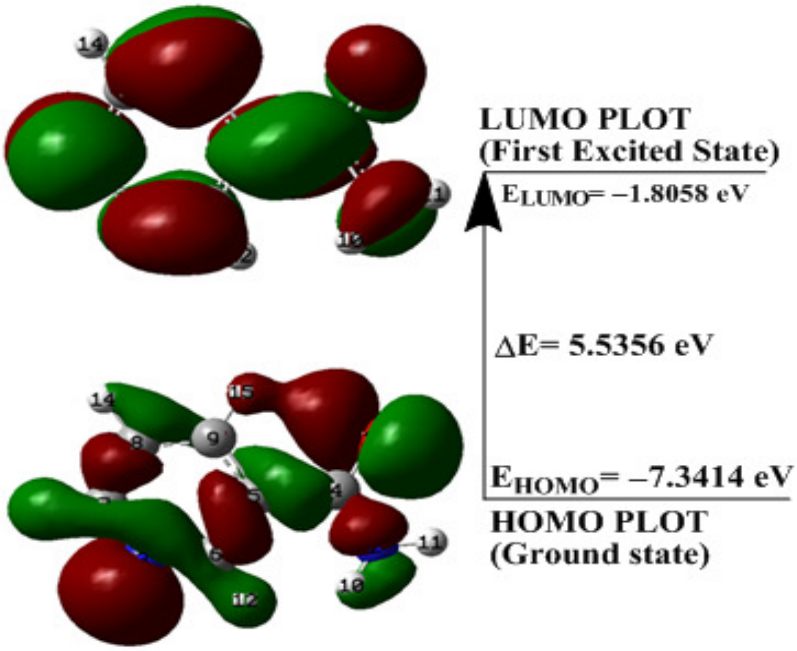

Fig. S12 HOMO-LUMO plot of NIC with orbital involved in electronic transitions.

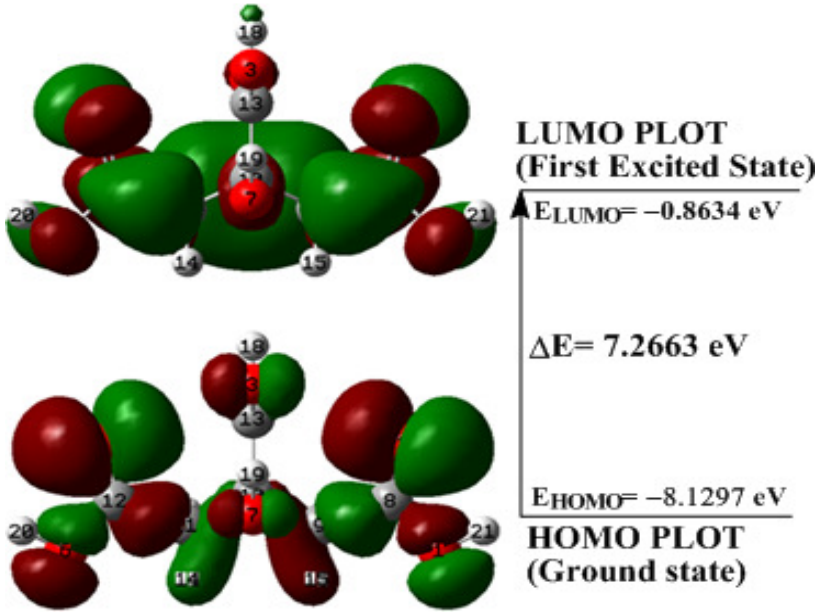

Fig. S13 HOMO-LUMO plot of CA with orbital involved in electronic transitions.

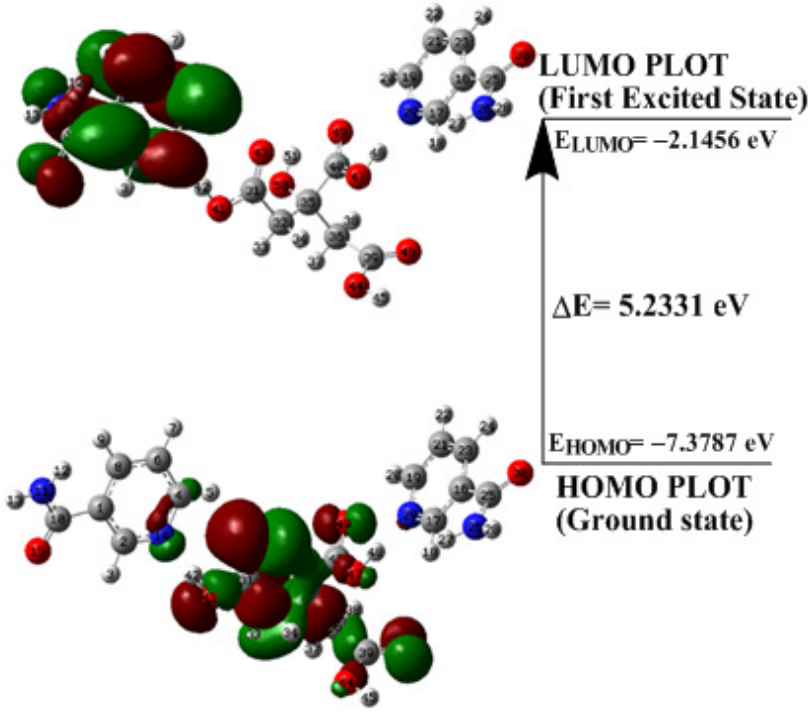

Fig. S14 HOMO-LUMO plot of NIC-CA (monomer) with orbital involved in electronic transitions.

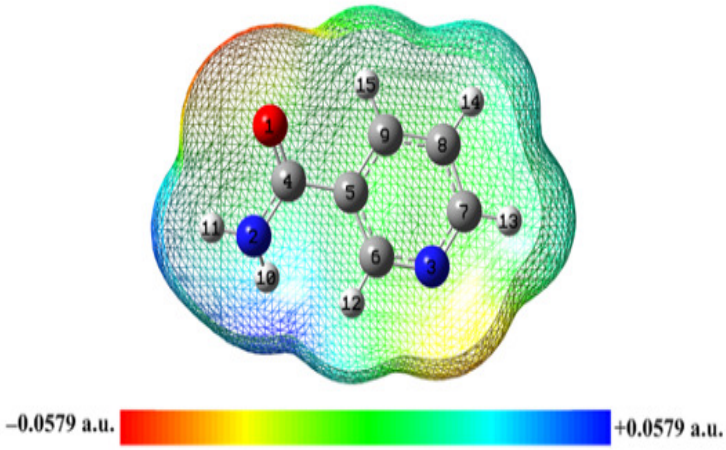

Fig. S15 Molecular electrostatic potential (MESP) formed by mapping of total density over electrostatic potential in gas phase for NIC.

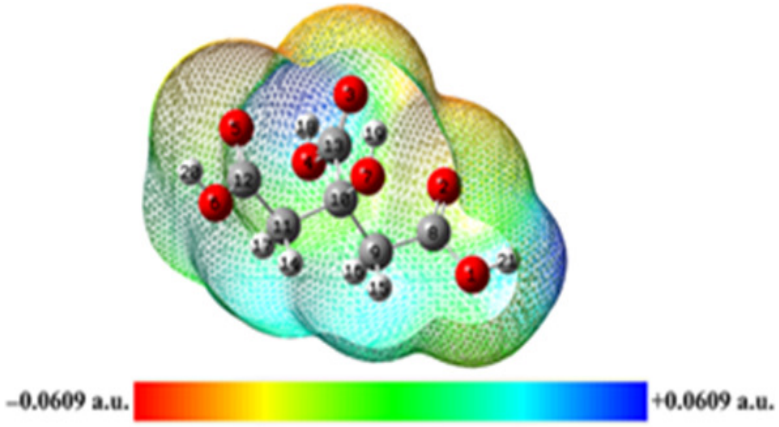

Fig. S16 Molecular electrostatic potential (MESP) formed by mapping of total density over electrostatic potential in gas phase for CA.

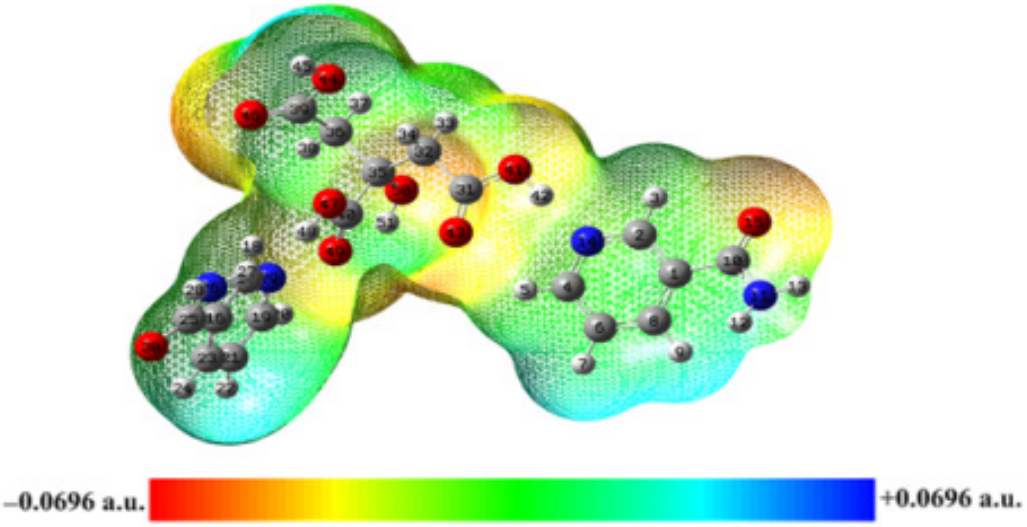

Fig. S17 Molecular electrostatic potential (MESP) formed by mapping of total density over electrostatic potential in gas phase for NIC-CA (monomer).

Part 2. TABLES

The experimental and calculated geometric parameters of NIC, NIC-CA (monomer) and NIC-CA (cluster) model are given in Table S1. Theoretical and experimental vibrational wavenumber along with potential energy distribution (PED) of NIC, CA, NIC-CA (monomer) and NIC-CA (cluster) model are listed in Table S2-S5, respectively. Topological parameters for intra- and inter- molecular interactions in NIC-CA (monomer) are given in Table S6. Geometrical parameters for intra- and inter-molecular hydrogen bonds of NIC-CA (cluster) model are given in Table S7. Second-order perturbation theory analyses of the Fock Matrix, in the NBO basis for intra- molecular interactions in NIC-CA (cluster) model and intra- with inter- molecular interactions in NIC-CA (monomer) is given in Table S8 and S9, respectively. Reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softnesses (s_K^+, s_K^-), local electrophilicity indices (ω_k^+, ω_k^-) for NIC-CA (monomer) and NIC-CA (cluster) model using Hirshfeld atomic charges are given in Table S10 and S11, respectively.

Table S1 The experimental and calculated geometric parameters of NIC-CA cocrystal and calculated geometric parameters of NIC and NIC-CA (cluster) model using DFT/6-311++G(d,p), bond-lengths in angstroms (Å) and bond-angles in degrees (°).

Geometrical parameters	**Experimental**	**Computational optimized parameter**	**Experimental**	**Computational optimized parameter**	
	NIC	**NIC (monomer)**	**NIC-CA cocrystal**	**NIC-CA (monomer)**	**NIC-CA (cluster) model**
			Bond-length (Å)		
R(C1-C2)	1.396	1.399	1.385	1.398	1.398
R(C1-C8)	1.391	1.397	1.388	1.397	1.397
R(C1-C10)	1.498	1.503	1.496	1.503	1.503
R(C2-H3)	1.083	1.087	0.930	1.084	1.084
R(C2-N14)	1.341	1.335	1.329	1.335	1.335
R(C4-H5)	1.083	1.086	0.931	1.085	1.086
R(C4-C6)	1.391	1.395	1.369	1.391	1.392
R(C4-N14)	1.341	1.336	1.339	1.341	1.341
R(C6-H7)	1.083	1.083	0.930	1.083	1.083
R(C6-C8)	1.389	1.388	1.386	1.391	1.391
R(C8-H9)	1.083	1.083	0.930	1.085	1.085
R(C10-N11)	1.340	1.369	1.324	1.371	1.349
R(C10=O15)	1.237	1.220	1.227	1.219	1.234
R(N11-H12)	1.010	1.006	0.922	1.007	1.006
R(N11-H13)	1.011	1.009	0.858	1.009	1.027
R(N14-H42)	-	-	1.632	1.761	1.764
R(C16-C17)	1.396	1.399	1.387	1.395	1.396
R(C16-C23)	1.391	1.397	1.381	1.398	1.398
R(C16-C25)	1.498	1.503	1.490	1.505	1.504
R(C17-H18)	1.083	1.087	0.930	1.086	1.086
R(C17-N29)	1.341	1.335	1.330	1.337	1.337
R(C19-H20)	1.083	1.086	0.930	1.085	1.085
R(C19-C21)	1.391	1.395	1.378	1.393	1.393
R(C19-N29)	1.341	1.336	1.322	1.339	1.339
R(C21-H22)	1.083	1.084	0.930	1.083	1.083
R(C21-C23)	1.389	1.388	1.376	1.388	1.388
R(C23-H24)	1.083	1.083	0.930	1.083	1.083
R(C25-N26)	1.340	1.369	1.323	1.368	1.368
R(C25=O30)	1.237	1.220	1.237	1.219	1.219
R(N26-H27)	1.010	1.006	0.907	1.006	1.007
R(N26-H28)	1.011	1.009	0.893	1.009	1.009
R(N29-H48)	-	-	1.646	1.699	1.705
R(C31-C32)	-	-	1.505	1.515	1.514
R(C31-O41)	-	-	1.329	1.332	1.332
R(C31=O43)	-	-	1.204	1.215	1.216
R(C32-H33)	-	-	0.970	1.092	1.092
R(C32-H34)	-	-	0.970	1.092	1.092
R(C32-C35)	-	-	1.516	1.533	1.533
R(C35-C36)	-	-	1.555	1.565	1.564
R(C35-C40)	-	-	1.533	1.540	1.539
R(C35-O50)	-	-	1.416	1.416	1.418
R(C36-H37)	-	-	0.971	1.093	1.093
R(C36-H38)	-	-	0.970	1.089	1.089

R(C36-C39)	-	-	1.500	1.512	1.514
R(C39-O44)	-	-	1.307	1.359	1.327
R(C39=O46)	-	-	1.223	1.205	1.221
R(C40-O47)	-	-	1.308	1.319	1.319
R(C40=O49)	-	-	1.211	1.216	1.217
R(O41-H42)	-	-	1.015	1.003	1.003
R(O44-H45)	-	-	0.928	0.969	1.000
R(O47-H48)	-	-	0.934	1.013	1.011
R(O50-H51)	-	-	0.827	0.971	0.971
Bond-angle (˚)					
A(C2-C1-C8)	118.13	117.74	117.72	117.78	117.72
A(C2-C1-C10)	124.08	123.94	119.47	117.80	118.08
A(C8-C1-C10)	117.77	118.30	122.75	124.40	124.18
A(C1-C2-H3)	121.36	120.84	118.23	119.47	119.47
A(C1-C2-N14)	123.02	123.89	123.62	123.11	123.16
A(H3-C2-N14)	115.56	115.25	118.15	117.42	117.37
A(H5-C4-C6)	120.36	120.51	118.50	122.32	122.33
A(H5-C4-N14)	116.22	116.05	118.56	115.31	115.31
A(C6-C4-N14)	123.41	123.45	122.94	122.37	122.35
A(C4-C6-H7)	120.28	120.28	120.54	120.07	120.08
A(C4-C6-C8)	118.03	118.56	118.99	118.81	118.81
A(H7-C6-C8)	121.67	121.16	120.48	121.12	121.10
A(C1-C8-C6)	119.51	118.92	118.90	119.20	119.24
A(C1-C8-H9)	118.70	119.00	120.54	120.91	120.95
A(C6-C8-H9)	121.79	122.07	120.56	119.86	119.78
A(C1-C10-N11)	117.58	116.49	116.65	116.22	117.37
A(C1-C10=O15)	119.27	121.46	120.24	121.54	119.88
A(N11-C10=O15)	123.15	122.04	123.11	122.23	122.74
A(C10-N11-H12)	120.44	121.91	120.84	121.54	121.25
A(C10-N11-H13)	117.84	116.70	118.45	116.35	118.95
A(H12-N11-H13)	120.38	117.79	119.90	117.34	118.85
A(C2-N14-C4)	117.86	117.43	117.78	118.72	118.70
A(C2-N14-H42)	-	-	134.20	126.24	126.49
A(C4-N14-H42)	-	-	107.90	115.00	114.79
A(C17-C16-C23)	118.13	117.74	117.55	117.77	117.77
A(C17-C16-C25)	124.08	123.94	122.76	123.91	123.82
A(C23-C16-C25)	117.77	118.30	119.69	118.30	118.38
A(C16-C17-H18)	121.36	120.84	118.48	121.41	121.42
A(C16-C17-N29)	123.02	123.89	122.96	123.08	123.07
A(H18-C17-N29)	115.56	115.25	118.56	115.48	115.48
A(H20-C19-C21)	120.36	120.51	118.73	122.35	122.37
A(H20-C19-N29)	116.22	116.05	118.76	115.35	115.35
A(C21-C19-N29)	123.41	123.45	122.51	122.30	122.28
A(C19-C21-H22)	120.28	120.28	120.67	119.99	120.00
A(C19-C21-C23)	118.03	118.56	118.73	118.83	118.83
A(H22-C21-C23)	121.67	121.16	120.60	121.18	121.17
A(C16-C23-C21)	119.51	118.92	119.55	119.25	119.25
A(C16-C23-H24)	118.70	119.00	120.21	118.79	118.82
A(C21-C23-H24)	121.79	122.07	120.24	121.97	121.93
A(C16-C25-N26)	117.58	116.49	118.51	116.54	116.49
A(C16-C25=O30)	119.27	121.46	119.64	121.19	121.21
A(N26-C25=O30)	123.15	122.04	121.86	122.26	122.30
A(C25-N26-H27)	120.44	121.91	123.77	122.06	121.99
A(C25-N26-H28)	117.84	116.70	119.28	116.68	116.67
A(H27-N26-H28)	120.38	117.79	116.30	117.66	117.62
A(C17-N29-C19)	117.86	117.43	118.70	118.75	118.78
A(C17-N29-H48)	-	-	117.62	125.02	124.74
A(C19-N29-H48)	-	-	123.42	116.22	116.46
A(C32-C31-O41)	-	-	112.68	111.97	112.03
A(C32-C31=O43)	-	-	124.12	124.10	124.15
A(O41-C31=O43)	-	-	123.20	123.91	123.79
A(C31-C32-H33)	-	-	109.15	108.89	108.92
A(C31-C32-H34)	-	-	109.12	107.78	107.90

A(C31-C32-C35)	-	-	112.38	113.43	113.49
A(H33-C32-H34)	-	-	107.82	106.93	106.89
A(H33-C32-C35)	-	-	109.13	108.79	108.73
A(H34-C32-C35)	-	-	109.13	110.81	110.70
A(C32-C35-C36)	-	-	112.27	111.82	111.70
A(C32-C35-C40)	-	-	113.46	113.38	113.30
A(C32-C35-O50)	-	-	105.98	108.33	108.35
A(C36-C35-C40)	-	-	106.80	108.39	108.50
A(C36-C35-O50)	-	-	107.85	106.20	106.38
A(C40-C35-O50)	-	-	110.37	108.41	108.33
A(C35-C36-H37)	-	-	108.59	106.50	106.44
A(C35-C36-H38)	-	-	108.57	107.37	107.38
A(C35-C36-C39)	-	-	114.71	118.34	118.11
A(H37-C36-H38)	-	-	107.56	108.32	108.38
A(H37-C36-C39)	-	-	108.57	108.91	108.72
A(H38-C36-C39)	-	-	108.62	107.06	107.49
A(C36-C39-O44)	-	-	113.85	112.68	113.80
A(C36-C39=O46)	-	-	122.93	125.23	122.43
A(O44-C39=O46)	-	-	123.22	122.05	123.74
A(C35-C40-O47)	-	-	114.21	113.51	113.48
A(C35-C40=O49)	-	-	120.95	120.88	121.03
A(O47-C40=O49)	-	-	124.52	125.47	125.35
A(C31-O41-H42)	-	-	108.44	110.04	110.03
A(C39-O44-H45)	-	-	113.65	106.86	111.13
A(C40-O47-H48)	-	-	110.28	110.53	110.48
A(C35-O50-H51)	-	-	112.51	106.19	106.17
L(14,42,41,16,-1)	-	-	-	-	-
L(29,48,47,7,-1)	-	-	-	-	-
L(14,42,41,16,-2)	-	-	-	-	-
L(29,48,47,7,-2)	-	-	-	-	-
Dihedral-angle (˚)					
D(C8-C1-C2-H3)	176.18	177.01	179.53	-178.68	-178.75
D(C8-C1-C2-N14)	-0.77	-1.20	-0.51	1.20	1.22
D(C10-C1-C2-H3)	-2.20	-1.42	-3.40	-0.17	-0.18
D(C10-C1-C2-N14)	-179.14	-179.62	176.55	179.70	179.79
D(C2-C1-C8-C6)	2.21	1.33	2.41	-0.68	-0.63
D(C2-C1-C8-H9)	-176.83	-178.50	-177.64	177.42	177.53
D(C10-C1-C8-C6)	-179.32	179.85	-174.55	-179.08	-179.11
D(C10-C1-C8-H9)	1.65	0.02	5.40	-0.98	-0.94
D(C2-C1-C10-N11)	-22.76	-19.64	136.73	159.49	157.80
D(C2-C1-C10=O15)	157.65	159.48	-44.48	-21.68	-22.46
D(C8-C1-C10-N11)	158.86	161.94	-46.36	-22.11	-23.73
D(C8-C1-C10=O15)	-20.73	-18.93	132.43	156.72	156.00
D(C1-C2-N14-C4)	-1.05	0.13	-1.62	-0.82	-0.91
D(C1-C2-N14-H42)	-	-	-176.93	-178.35	-179.13
D(H3-C2-N14-C4)	-178.16	-178.16	178.33	179.06	179.07
D(H3-C2-N14-H42)	-	-	3.03	1.53	0.84
D(H5-C4-C6-H7)	-1.27	-0.36	-0.01	0.84	0.73
D(H5-C4-C6-C8)	-179.61	179.72	-179.99	-179.78	-179.86
D(N14-C4-C6-H7)	178.30	179.30	180.00	-178.83	-178.88
D(N14-C4-C6-C8)	-0.03	-0.62	0.01	0.54	0.53
D(H5-C4-N14-C2)	-178.94	-179.53	-178.11	-179.78	-179.63
D(H5-C4-N14-H42)	-	-	-1.65	-1.98	-1.20
D(C6-C4-N14-C2)	1.46	0.81	1.88	-0.08	0.00
D(C6-C4-N14-H42)	-	-	178.35	177.72	178.43
D(C4-C6-C8-C1)	-1.83	-0.50	-2.19	-0.13	-0.19
D(C4-C6-C8-H9)	177.18	179.33	177.86	-178.26	-178.38
D(H7-C6-C8-C1)	179.86	179.59	177.82	179.24	179.22
D(H7-C6-C8-H9)	-1.13	-0.59	-2.13	1.11	1.03
D(C1-C10-N11-H12)	-10.99	-17.01	-7.01	-19.69	-9.82
D(C1-C10-N11-H13)	-177.84	-175.15	-176.66	-174.56	-178.53
D(O15=C10-N11-H12)	168.59	163.87	174.25	161.48	170.46

D(O15=C10-N11-H13)	1.74	5.74	4.59	6.61	1.74
D(C2-N14-O41-C31)	-	-	108.93	-178.21	-179.11
D(C4-N14-O41-C31)	-	-	-68.69	4.93	3.17
D(C23-C16-C17-H18)	176.18	177.01	-179.97	176.90	177.04
D(C23-C16-C17-N29)	-0.77	-1.20	0.09	-1.32	-1.23
D(C25-C16-C17-H18)	-2.20	-1.42	0.23	-1.28	-1.02
D(C25-C16-C17-N29)	-179.14	-179.62	-179.71	-179.49	179.29
D(C17-C16-C23-C21)	2.21	1.33	0.39	1.44	1.48
D(C17-C16-C23-H24)	-176.83	-178.50	-179.59	-178.33	-178.34
D(C25-C16-C23-C21)	-179.32	179.85	-179.81	179.73	179.65
D(C25-C16-C23-H24)	1.65	0.02	0.21	-0.05	-0.17
D(C17-C16-C25-N26)	-22.76	-19.64	-7.34	-19.88	-20.72
D(C17-C16-C25=O30)	157.65	159.48	172.20	159.20	158.26
D(C23-C16-C25-N26)	158.86	161.94	172.86	161.95	161.22
D(C23-C16-C25=O30)	-20.73	-18.93	-7.60	-18.97	-19.79
D(C16-C17-N29-C19)	-1.05	0.13	-0.54	0.22	0.05
D(C16-C17-N29-H48)	-	-	173.81	-179.50	-178.26
D(H18-C17-N29-C19)	-178.16	-178.16	179.52	-178.10	-178.32
D(H18-C17-N29-H48)	-	-	-6.13	2.19	3.37
D(H20-C19-C21-H22)	-1.27	-0.36	0.01	-0.35	-0.43
D(H20-C19-C21-C23)	-179.61	179.72	179.99	179.82	179.69
D(N29-C19-C21-H22)	178.30	179.30	179.96	179.24	179.28
D(N29-C19-C21-C23)	-0.03	-0.62	-0.05	-0.58	-0.60
D(H20-C19-N29-C17)	-178.94	-179.53	-179.52	-179.62	-179.38
D(H20-C19-N29-H48)	-	-	6.47	0.12	-0.93
D(C21-C19-N29-C17)	1.46	0.81	0.52	0.76	0.90
D(C21-C19-N29-H48)	-	-	-173.48	-179.50	179.34
D(C19-C21-C23-C16)	-1.83	-0.50	-0.41	-0.56	-0.62
D(C19-C21-C23-H24)	177.18	179.33	179.57	179.21	179.19
D(H22-C21-C23-C16)	179.86	179.59	179.58	179.62	179.50
D(H22-C21-C23-H24)	-1.13	-0.59	-0.44	-0.62	-0.69
D(C16-C25-N26-H27)	-10.99	-17.01	-2.26	-17.41	-17.79
D(C16-C25-N26-H28)	-177.84	-175.15	-172.65	-175.52	-175.50
D(O30=C25-N26-H27)	168.59	5.74	178.22	163.52	163.24
D(O30=C25-N26-H28)	1.74	5.74	7.83	5.41	5.53
D(C17-N29-O47-C40)	-	-	-149.44	-179.93	177.49
D(C19-N29-O47-C40)	-	-	23.67	0.42	-0.34
D(O41-C31-C32-H33)	-	-	35.76	34.24	33.19
D(O41-C31-C32-H34)	-	-	-81.84	-81.42	-82.49
D(O41-C31-C32-C35)	-	-	156.97	155.52	154.46
D(O43=C31-C32-H33)	-	-	-144.32	-147.51	-148.60
D(O43=C31-C32-H34)	-	-	98.08	96.83	95.71
D(O43=C31-C32-C35)	-	-	-23.11	-26.23	-27.34
D(C32-C31-O41-H42)	-	-	173.79	178.72	178.34
D(O43-O31-O41-H42)	-	-	-6.13	0.48	0.13
D(C31-C32-C35-C36)	-	-	178.81	179.55	179.45
D(C31-C32-C35-C40)	-	-	57.59	56.64	56.54
D(C31-C32-C35-O50)	-	-	-63.68	-63.75	-63.70
D(H33-C32-C35-C36)	-	-	-59.96	-59.12	-59.18
D(H33-C32-C35-C40)	-	-	178.82	177.97	177.91
D(H33-C32-C35-O50)	-	-	57.54	57.58	57.67
D(H34-C32-C35-C36)	-	-	57.63	58.17	57.94
D(H34-C32-C35-C40)	-	-	-63.59	-64.74	-64.96
D(H34-C32-C35-O50)	-	-	175.14	174.87	174.80
D(C32-C35-C36-H37)	-	-	45.02	55.56	54.98
D(C32-C35-C36-H38)	-	-	161.69	171.42	170.88
D(C32-C35-C36-C39)	-	-	-76.63	-67.39	-67.51
D(C40-C35-C36-H37)	-	-	169.99	-178.74	-179.43
D(C40-C35-C36-H38)	-	-	-73.35	-62.88	-63.53
D(C40-C35-C36-C39)	-	-	48.34	58.31	58.08

D(O50-C35-C36-H37)	-	-	-71.37	-62.43	-63.07
D(O50-C35-C36-H38)	-	-	45.29	53.43	52.83
D(O50-C35-C36-C39)	-	-	166.98	174.62	174.45
D(C32-C35-C40-O47)	-	-	39.10	49.60	49.83
D(C32-C35-C40=O49)	-	-	-147.17	-134.53	-134.13
D(C36-C35-C40-O47)	-	-	-85.14	-75.19	-74.82
D(C36-C35-C40=O49)	-	-	88.60	100.69	101.21
D(O50-C35-C40-O47)	-	-	157.88	169.94	170.08
D(O50-C35-C40=O49)	-	-	-28.39	-14.19	-13.89
D(C32-C35-O50-H51)	-	-	166.11	131.25	130.86
D(C36-C35-O50-H51)	-	-	-73.46	-108.49	-108.91
D(C40-C35-O50-H51)	-	-	42.87	7.81	7.57
D(C35-C36-C39-O44)	-	-	84.02	71.91	70.37
D(C35-C36-C39=O46)	-	-	-95.42	-110.29	-111.69
D(H37-C36-C39-O44)	-	-	-37.64	-49.82	-50.95
D(H37-C36-C39=O46)	-	-	142.92	127.98	126.99
D(H38-C36-C39-O44)	-	-	-154.32	-166.74	-168.07
D(H38-C36-C39=O46)	-	-	26.24	11.06	9.87
D(C36-C39-O44-H45)	-	-	-177.82	179.94	-179.26
D(O46=C39-O44-H45)	-	-	1.61	2.05	2.83
D(C35-C40-O47-H48)	-	-	162.07	176.36	177.98
D(O49=C40-O47-H48)	-	-	-11.41	0.71	2.15

Table S2 Theoretical and experimental vibrational wavenumbers (cm^{-1}) of NIC and their assignments using B3LYP/6-311++G(d,p).

Unscaled	Scaled	IR	Raman	Potential Energy Distribution (≥ 5%)
3715	3523	3359	3370	$[\nu_a(N2H_2)](99)$
3589	3410	3150	3149	$[\nu_s(N2H_2)](99)$
3202	3063	3058	3061	R1[ν(CH)](99)
3186	3049		3034	R1[ν(CH)](99)
3155	3020			R1[ν(CH)](97)
3144	3010			R1[ν(C6H12)](97)
1746	1712	1676	1678	[ν(C4=O1)](71)+[ν(C4N2)](8)+[ρ(C4N2)](6)+[δ_{sci}(C4N2)](3)
1629	1600	1614	1615	R1[ν(CC)](45)+R1[δ_{in}(CH)](17)+R1[ν(C6N3)](15)+R1[δ'_a](8)
1621	1592	1592	1596	[δ_{sci}(C4N2)](85)+[ν(C4=O1)](5)+[ν(C4N2)](5)
1606	1578	1573	1579	R1[ν(CC)](51)+R1[ν(C7N3)](15) R1[δ_{in}(C7H13)](12)+R1[δ_a](7)
1508	1484	1485	1490	R1[δ_{in}(CH)](54)+R1[ν(C7N3)](10)+R1[ν(CC)](17)
1448	1427	1421	1431	R1[δ_{in}(C7H13)](46)+R1[ν(C6N3)(14)+R1[ν(CC)](26)
1364	1346	1352	1346	[ν(C4N2)](31)+R1[ν(C4C5)](21)+[δ_{sym}(C4N2)](12)+[ρ(C4N2)](7)+R1[δ_{in}(CH)](11)
1360	1341	1339		R1[δ_{in}(CH)](78)
1288	1272	1253	1256	R1[ν(C6N3)](24)+R1[ν(C7N3)](19)+R1[ν(CC)(48)
1227	1213	1200	1210	R1[δ_{in}(CH)](49)+R1[ν(C7N3)](20)+R1[ν(C7C8)](11)+R1[ν(C6N3)](8)
1155	1143	1153	1160	R1[δ_{in}(C8H14)](22)+R1[ν(CC)](36)+R1[δ_{tri}](14)+[ν(C4N2)](9)+[ρ(C4N2)](9)
1132	1121	1123	1124	R1[δ_{in}(CH)](45)+R1[ν(C6N3)](14)+R1[ν(CC)](22)
1083	1074	1089	1090	[ρ(C4N2)](56)+[ν(C4N2)](24)+[ν(C4=O1)](8)
1058	1049	1037	1042	R1[ν(CC)](55)+R1[ν(C7N3)](17)+R1[δ_{in}(C8H14)](7)+R1[ν(C6N3)](6)
1039	1031	1028	1033	R1[δ_{tri}](70)+R1[ν(CC)](17)
1014	1006	995	994	R1[oop(CH)](86)+R1[puck](8)
988	980	968	969	R1[oop(CH)](90)
947	940	935	939	R1[oop(CH)](82)+R1[puck](12)
843	839	828	834	R1[oop(CH)](51)+R1[puck](20)+[ω(C4N2)](12)+R1[oop(C4C5)](12)
780	777	774	789	R1[δ'_a](34)+R1[ν(CC)](30)+R1[δ_{tri}](7)+[ρ(C4N2)](5)+[ν(C4N2)](5)
750	748	721	754	[ω(C4N2)](51)+R1[oop(CH)](38)
719	717	700	705	R1[puck](79)+R1[oop(C8H14)](13)+R1[oop(C4C5)](5)
646	644	644	646	R1[δ'_a](32)+R1[δ_a](27)+[δ_{sym}(C4N2)](18)+[ρ(C4N2)](12)
620	619	620	628	R1[δ_a](48)+[ρ(C4N2)](23)+[δ_{sym}(C4N2)](12)
556	556	579		[τ(C4N2)](71)+R1[oop(C4C5)](8)+R1[τ'_a](5)
497	497	508	519	[ρ(C4N2)](29)+[δ_{sym}(C4N2)](17)+R1[δ_{in}(C4C5)](12)+R1[oop(C4C5)](8)+R1[τ_a](7)
417	418	414	413	R1[τ_a](71)+R1[oop(C4C5)](7)
385	386	-		R1[τ'_a](63)+R1[oop(C4C5)](17)
377	378	-	386	R1[ν(C4C5)](27)+[ρ(C4N2)](24)+R1[δ'_a](17)+R1[δ_a](7)

319	321	-		[ω(C4N2)](69)+[τ(C4N2)](17)+[ν(C4N2)](6)
213	214	-	252	R1[δ_{in}(C4C5)](58)+[δ_{sym}(C4N2)](13)+[ω(C4N2)](11)+[ρ(C4N2)](5)+[τ(C4N2)](5)
151	152	-	192	R1[oop(C4C5)](42)+R1[τ'_a](26)+[ω(C4N2)](9)+R1[oop(C9H15)](7)+R1[τ_a](5)
55	55	-	-	[τ(C4C5)](77)+R1[δ_{in}(C4C5)](6)+[ρ(C4N2)](5)

Table S3 Theoretical and experimental vibrational wavenumbers (cm^{-1}) of CA and their assignments using B3LYP/6-311++G(d,p).

Unscaled	Scaled	IR	Raman	Potential Energy Distribution (≥ 5%)
3763	3565	3493	3496	[ν(O4H18)](100)
3750	3553	3286	3291	[ν(O6H20)](61)+[ν(O1H21)](39)
3750	3553			[ν(O1H21)](61)+[ν(O6H20)](39)
3698	3507	3224		[ν(O7H19)](100)
3120	2989	2992	2993	[ν_a(C9H_2)] (50)+[ν_a(C11H_2)](49)
3114	2983	2979	2979	[ν_a(C11H_2)](51)+[ν_a(C9H_2)](49)
3061	2935		2930	[ν_s(C11H_2)](50)+[ν_s(C9H_2)](50)
3054	2929			[ν_s(C9H_2)](50)+[ν_s(C11H_2)](50)
1833	1794	1744	1737	[ν(C13=O3)](45)+[ν(C12=O5)](18)+[ν(C8=O2)](17)
1813	1776			[ν(C8=O2)](40)+[ν(C12=O5)](40)
1810	1772			[ν(C13=O3)](36)+[ν(C8=O2)](22)+[ν(C12=O5)](22)
1472	1449	1439	1433	[δ_{sci}(C9H_2)](41)+[δ_{sci}(C11H_2)](41)
1453	1431			[δ_{sci}(C11H_2)](45)+[δ_{sci}(C9H_2)](44)
1442	1421	1427	1416	[δ(C10H19O7)](20)+[ω(C11H_2)](12)+[ω(C9H_2)](12)+[ν(C10C13)(10)+[γ(C9H_2)](5)+[γ(C11H_2)](5)+[ν(C13O4)](5)
1392	1373	1388	1389	[δ(C10H19O7)](21)+[ω(C11H_2)](11)+[ω(C9H_2)](11)+[ν(CC)](10)+[δ_{sci}(C11H_2)](5)
1386	1367	1357	1365	[ω(C9H_2)](18)+[ω(C11H_2)](17)+[ν(CC)](16)+[ν(CO)](12)+[δ(C8H21O1)](5)+[δ(C12H20O6)](5)
1340	1322	1320	1316	[δ(C13H18O4)](30)+[δ(C10H19O7)](26)+[ν(C13O4)](16)+[δ_{sym}(O4C13)](10)
1311	1294	1292	1292	[ω(C9H_2)](19)+[ω(C11H_2)](19)+[δ(C8H21O1)](13)+[δ(C12H20O6)](13)+[γ(C9H_2)](6)+ [γ(C11H_2)](6)
1307	1290		1282	[ω(C11H_2)](20)+[ω(C9H_2)](19)+[δ(C12H20O6)](16)+[δ(C8H21O1)](16)+[ν(CC)](10)
1295	1278	1241		[γ(C11H_2)](21)+[γ(C9H_2)](21)+[ν(C10O7)](12)+[δ(C8H21O1)](7)+[δ(C12H20O6)](7)+ [δ(C13H18O4)](6)+[δ(C10H19O7)](6)
1233	1219	1216	1219	[γ(C9H_2)](35)+[γ(C11H_2)](35)+[δ(C8H21O1)](7)+[δ(C12H20O6)](7)
1192	1179	1169	1170	[ν(CO)](35)+[δ(C13H18O4)](20)+[δ(C8H21O1)](6)+[δ(C12H20O6)](6) +[δ_{sym}(C13O4)](5)
1161	1149			[ν(CO)](43)+[δ(C12H20O6)](7)+[δ(C8H21O1)](7)+[δ(C13H18O4)](7)
1148	1137	1136	1145	[ν(CO)](44)+[δ(C12H20O6)](11)+[δ(C8H21O1)](11)+[γ(C9H_2)](7)+[γ(C11H_2)](7)
1127	1116			[ν(CO)](43)+[δ(C13H18O4)](8)+[ν(CC)](16)+[δ(C10H19O7)](8)
1075	1066	1080	1082	[ω(C10C13O7)](27)+[ν(CC)](48)+[ω(C9H_2)](5)+[ω(C11H_2)](5)+[ω(C13O4)](5)
1065	1056	1051	1052	[ν(CC)](29)+[ρ(C10C13O7)]+10)+[ρ(C9H_2)](8)+[ρ(C11H_2)](8)+[ν(CO)](10)+[δ(C10H19O7)](5)
942	936	942	942	[ρ(C11H_2)](32)+[ρ(C9H_2)](32)+[γ(C10C13O7)](7)+[ω(CO)](12)
936	929	932	933	[ν(C11C12)](50)+[δ_{sci}(C10C9C11)](9)+[ν(CO)](14)
910	904	904	904	[ν(C10O7)](40)+[ρ(C11H_2)](13)+[ρ(C9H_2)](13)+[ω(CO)](12)+[ν(C10C13)](5)
864	859	880	881	[ν(CC)](48)+[δ_{sci}(CCC)](12)+[ν(CO)](10)
812	809	818	803	[ω(CO)](39)+[ω(C10C13O7)](11)+[ν(C9C10)](7)+[ν(C10C11)](7)+δ_{sci}(CCC)](12)
754	752	781	783	[ν(C10C13)](34)+[ρ(C13O4)](17)+[ν(C13O4)](9)+[δ(C13H18O4)](7)
699	698		686	[τ(CO)](40)+[ω(CO)](31)
697	695			[ω(CO)](39)+[τ(CO)](31)+[ρ(C11H_2)](5)+[ρ(C9H_2)](5)
658	656		661	[τ(CO)](61)+[ω(C13O4)](8)+δ_{sym}(CO)](10)
645	644	639	639	[ρ(CO)](30)+[τ(CO)](24)+[δ_{sym}(CO)](20)
618	617	614	615	[δ_{sym}(C13O4)](22)+[δ_{sci}(C10C13O7)](14)+[ρ(CO)](28)+[ν(C13O4)](5)
578	578	598	597	[τ(C13O4)](42)+[ρ(CO)](32)
547	547	547	548	[ω(CO)](28)+[τ(CO)](26)+[ρ(C13O4)](12)+[ρ(C10C13O7)](8)
536	536			[τ(CO)](33)+[ω(CO)](24)+[ρ(C11H_2)](5)+[ρ(C9H_2)](5)
497	497	505	513	[τ(C13O4)](19)+[ω(C13O4)](14)+[ρ(CO)](16)+[ω(C10C13O7)](8)+[ω(CO)](13)+[γ(C10C13O7)](6)
495	495	493	487	[ρ(C13O4)](27)+[ρ(C10C13O7)](11)+[δ_{sci}(C10C13O7)](10)+[ρ(C9H_2)](7)+[ρ(C11H_2)](7)+[δ_{sym}(C13O4)](7)
457	458	428	420	[τ(C10O7)](78)
385	386	-	381	[ρ(C10C13O7)](19)+[δ_{sci}(C10C13O7)](11)+[δ_{sym}(CO)](18)

				[ρ(CO)](16)+[ρ(C9H$_2$)](5)+[ρ(C11H$_2$)](5)+[δ_{sci}(C10C9C11)](5)
363	364	-	365	[δ_{sym}(CO)](39)+[δ_{sci}(C10C13O7)](15)+[ρ(C10C13O7)](13)+[ν(C10C13)](12)+ [ρ(C8O1)](6)+[ρ(C12O6)](6)
348	349	-	349	[γ(C10C13O7)](19)+[ω(C10C13O7)](16)+[τ(C10O7)](15)+[δ_{sym}(CO)](18)+ [ρ(CO)](12)
260	261	-	262	[δ_{sci}(C10C9C11)](18)+[δ_{sym}(C13O4)](15)+[ρ(C10C13O7)](14)+[ρ(C13O4)](12)+ [ν(CC)](12)
227	228	-	242	[δ_{sci}(C10C13O7)](23)+[δ_{sci}(C10C9C11)](21)+[ρ(C10C13O7)](11)+[ρ(C13O4)](8)+ [δ_{sym}(C13O4)](6)
210	211	-	217	[γ(C10C13O7)](42)+[ω(C13O4)](11)+[δ_{sci}(CCC)](18)+[τ(C10O7)](6)+[δ_{sym}(CO)] (10)
160	161	-	161	[ω(C10C13O7)](22)+[δ_{sci}(CCC)](44)+[γ(C10C13O7)](12)+[ω(C13O4)](5)
128	129	-	127	[τ(C10C13)](73)+[τ(C10O7)](11)+[δ_{sci}(CCC)](10)
105	106	-	108	[δ_{sci}(C10C9C11)](84)
75	75	-	-	[τ(CC)](78)+[τ(C10O7)](5)
58	58	-	-	[τ(CC)](79)
36	36	-	-	[τ(C8C9)](73)+[δ_{sci}(CCC)](12)
21	22	-	-	[τ(C11C12)](82)

Table S4 Theoretical and experimental vibrational wavenumbers (cm^{-1}) of NIC-CA (monomer) and their assignments using B3LYP/6-311++G(d,p).

Unscaled	Scaled	IR	Raman	Potential Energy Distribution (≥ 5%)
3758	3561			[ν(O44H45)](100)
3713	3521	3491	3494	[ν_a(N26H$_2$)](100)
3709	3517			[ν_a(N11H$_2$)](100)
3700	3509			[ν(O50H51)](100)
3588	3409	3413	3418	[ν_s(N26H$_2$)](100)
3585	3406			[ν_s(N11H$_2$)](100)
3205	3066	3066	3066	R2[ν(CH)](96)
3199	3060			R1[ν(CH)](91)
3193	3055	3048	3048	R2[ν(CH)](100)
3189	3051			R1[ν(C2H3)](97)
3178	3041			R2[ν(CH)](97)
3178	3041			R1[ν(CH)](97)
3172	3036	3034	3033	R1[ν(C8H9)](99)
3161	3026	3027	3030	R2[ν(C17H18)](99)
3131	2999	2986	2984	[ν_a(C36H$_2$)](99)
3117	2985			[ν_a(C32H$_2$)](99)
3077	2949	2944	2947	[ν(O41H42)](41)+[ν_s(C32H$_2$)](55)
3071	2944			[ν(O41H42)](62)+[ν_s(C32H$_2$)](32)
3064	2938	2860	2858	[ν_s(C36H$_2$)](97)
2896	2784	2813		[ν(O47H48)](93)+[ν(N29H48)](7)
1810	1773	1721	1729	[ν(C39=O46)](79)+[ρ(C39O44)](6)+[ν(C36C39)](5)
1770	1734			[ν(C31 =O43)](55)+[ν(C40=O49)](14)+[δ(C31H42O41)](6)+[ρ(C31O41)](5)
1757	1722			[ν(C40=O49)](51)+[ν(C31=O43)](13)+[δ(C40H48O47)](6)+[ν(C40O47)](6)
1752	1717	1685	1680	[ν(C10=O15)](70)+[ν(C10N11)](8)+[ρ(C10N11)](5)
1751	1716			[ν(C25=O30)](67)+[ν(C25N26)](8)+[ρ(C25N26)](5)
1638	1608	1610	1614	R2[ν(CC)](46)+R2[ν(C17N29)](16)+R2[δ_{in}(CH)](16)+R2[δ_a](9)
1635	1606			R1[ν(CC)](44)+R1[ν(C2N14)](18)+R1[(δ_{in}(CH)](20)+R1[δ_a](9)
1624	1595	1605	1605	[δ_{sci}(C25N26)](67)+[δ_{sci}(C10N11)](17)
1623	1595			[δ_{sci}(C10N11)](62)+[δ_{sci}(C25N26)](18)
1614	1586	1581	1571	R1[ν(CC)](40)+R1[ν(C4N14)](15)+R1[δ_{in}(CH)](18)+R1[δ'_a](7)+[δ_{sci}(C10N11)](6)
1614	1586			R2[ν(CC)](45)+R2[ν(C19N29)](18)+R2[δ_{in}(CH)](18)+R2[δ'_a](7)
1525	1500	1503	1522	[δ(C40H48O47)](52)+[ν(C40O47)](7)+R2[δ_{in}(C17H18)](6)+[ν(C40=O49)](5)
1506	1482	1488	1489	R2[δ_{in}(C21H22)](29)+R1[δ_{in}(CH)](14)+R2[ν(C21C23)](6) +[δ(C40H48O47)](6)+ R2[ν(C19N29)](5)
1506	1482			R1[δ_{in}(CH)](25)+R2[δ_{in}(CH)](15)+R1[ν(C4N14)](7)+R1[ν(C6C8)](5)+ [δ(C31H42O41)](5)
1488	1465	1470	1476	[δ(C31H42O41)](45)+R1[δ_{in}(CH)](14)+ν(C31O41)](6))+R1[ν(C6C8)](5)
1474	1451	1462	1460	[δ_{sci}(C36H$_2$)](91)
1456	1434	1440	1440	[δ_{sci}(C32H$_2$)](25)+R2[δ_{in}(C19H20)](18)+R2[ν(C16C17)](7)+R1[δ_{in}(C4H5)](6)+

				R2[ν(C17N29)](6)
1455	1433			R1[δ_{in}(C4H5)](17)+R2[δ_{in}(C19H20)](11)+R1[ν(C1C2)](10)+R1[ν(C2N14)](7)+ [δ(C31H42O41)](7)
1447	1426	1426	1418	[δ_{sci}($C32H_2$)](64)+[δ(C40H48O47)](6)+R2[δ_{in}(C19H20)](5)
1420	1400	1407	1408	[δ(C35H51O50)](42)+[δ(C40H48O47)](10)+[ν(C35C40)](9)+[γ($C36H_2$)](6)+ [δ_{sci}($C32H_2$)](6)
1386	1367	1360	1359	[ω($C32H_2$)](46)+[ν(CC)](22)+[δ(C31H42O41)](11)+[ν(C31O41)](7)
1366	1348			[ν(C25N26)](33)+R2[ν(C16C25)](24)+[δ_{sym}(C25N26)](11)+R2[ρ(CN)](13)
1363	1344	1344	1347	R1[(δ_{in}(CH)](49)+[ν(C10N11)](15)+R1[ν(C1C10)](11)+[δ_{sym}(C10N11)](6)
1361	1343			R2[δ_{in}(CH)](85)
1355	1337	1335	1338	[ω($C36H_2$)](21)+[δ(C39H45O44)](19)+[ν(C36C39)](16)+[ν(C39O44)](12)+ [δ_{sym}(C39O44)](6)
1353	1335			R1[δ_{in}(CH)](34)+[ν(C10N11)](18)+R1[ν(C1C10)](13)+[ρ(C10N11)](5)
1339	1322	1303	1307	[ω($C36H_2$)](34)+[ν(C40O47)](10)+[γ($C36H_2$)](10)+[ν(C39O44)](7)+ [δ(C39H45O44)](7)
1295	1279	1260	1270	R2[ν(CN)](41)+R2[ν(CC)](44)
1290	1274			R1[ν(CC)](45)+R1[ν(CN)](43)
1288	1273	1243	1243	[ν(C40O47)](30)+[ω($C36H_2$)](14)+[δ(C35H51O50)](11)+[δ_{sym}(C40O47)](6)+ [ν(C35C40)](5)+[δ(C40H48O47)](5)
1270	1254			[γ($C32H_2$)](39)+[ν(C31O41)](20)+[ω($C32H_2$)](12)
1247	1232	1232	1236	[γ($C36H_2$)](39)+[δ(C39H45O44)](23)+[δ(C35H51O50)](6)+[ω($C36H_2$)](6)+ [ν(C31O41)](6)
1233	1219	1221	1228	[ν(C31O41)](22)+[γ($C32H_2$)](20)+[ω($C32H_2$)](5)
1227	1214	1213	1203	R2[δ_{in}(CH)](28)+R2[ν(C19N29)](12)+R2[ν(C17N29)](5)+R2[ν(C19C21)](8)
1225	1211			R1[δ_{in}(CH)](31)+R1[ν(C4N14)](11)+R1[ν(C4C6)](9)+[ν(C31O41)](6)
1182	1170	1186	1189	[ν(C39O44)](18)+[δ(C39H45O44)](15)+[ν(C32C35)](13)+[δ(C35H51O50)](9)+ [ρ($C36H_2$)](8)+[δ_{sym}(C39O44)](5)+[ω(C35O50C40)](5)
1157	1145	1163	1158	R2[δ_{in}(C21H22)](18)+R2[δ_{tri}](16)+R2[ν(CC)](36)+[ν(C25N26)](10)+ R2[ρ(C25N26)](9)
1156	1144			R1[δ_{in}(CH)](25)+R1[ν(CC)](34)+R1[δ_{tri}](16) +[ν(C10N11)](10)+[ρ(C10N11)](5)
1148	1136	1136	1131	R1[δ_{in}(CH)](34)+R1[ν(C2N14)](14)+R1[ν(CC)](19)+[ρ(C10N11)](8)
1136	1125	1123	1120	R2[δ_{in}(CH)](40)+R2[ν(C17N29)](14)+R2[ν(CC)](17)
1125	1114	1109	1104	[ν(C35O50)](34)+[ρ(C35O50C40)](8)+[ρ($C32H_2$)](7)+[γ($C32H_2$)](6)+ [γ($C36H_2$)](6)+[ν(C32C35)](5)+[ν(C39O44)](5)
1085	1075	1070	1074	[ρ(C10N11)](54)+[ν(C10N11)](27)+[ν(C10=O15)](7)
1084	1075			[ρ(C25N26)](56)+[ν(C25N26)](25)+[ν(C25=O30)](8)
1068	1059	1054	1052	[ν(C35C36)](15)+[ν(C32C35)](10)+[ω(C35O50C40)](10)+[γ($C36H_2$)](9)+ [ν(C39O44)](7)+[ν(C35O50)](7)+[ρ($C32H_2$)](6)+[ν(C36C39)](5)+ [ρ(C35O50C40)](5)
1064	1055			R2[ν(CC)](37)+R2[ν(C19N29)](20)+R2[δ_{tri}](9)+R2[δ_{in}(C21H22)](8)+ R2[ν(C17N29)](5)
1063	1053			R1[ν(CC)](35)+R1[ν(C19N29)](25)+R1[δ_{in}(C6H7)](9)
1056	1047			[ν(C35C36)](23)+[τ(C40O47)](9)+[ν(C35C40)](8)+[δ_{sci}(C35C32C36)](6)+ [δ_{sci}(C32C31C35)](5)+[ρ($C36H_2$)](5)
1046	1037	1039	1033	R2[δ_{tri}](63)+R2[ν(CC)](28)
1045	1036			R1[δ_{tri}](66)+R1[ν(CC)](23)
1041	1032	1025	1024	[τ(C40O47)](70)+R2[oop(C19H20)](7)+[ν(C35C36)](5)
1028	1020	1017	1011	R1[oop(CH)](74)+[τ(H5C4N14O41)](7)
1027	1019			R1[oop(CH)](38)+R2[oop(C19H20)](29)+R2[puck](6)
1021	1012	1007	999	[τ(C31O41)](86)+R1[oop(C2H3)](7)
1007	999			R2[oop(C23H24)](48)+R1[oop(C19H20)](31)+[τ(H20C19N29O47)](6)
987	979	971	970	R1[oop(CH)](83)+R1[puck](5)
967	960			R1[oop(CH)](75)+R1[puck](11)
949	943	946	946	[ρ($C36H_2$)](24)+[ρ($C32H_2$)](15)+[ν(C32C32)](9)+[ω(C31O41)](7)+[ν(C35O50)] (5)
944	938	930	931	R2[oop(CH)](79)+R2[puck](11)
927	921	918	916	[ν(C32C32)](23)+[ρ($C32H_2$)](22)+[ν(C35O50)](10)+[ω(C31O41)](7)+ [ν(C31O41)](6)
907	901			[ν(CC)](28)+[ν(C35O50)](10)+[ω(C39O44)](9)+ν(C39O44)](9)+ [δ_{sci}(C36C35C39)](7)+[ρ($C36H_2$)](6)+[δ_{sci}(C32C31C35)](5)
883	878	890	893	[ν(C39O44)](22)+[ν(CC)](22)+[ρ($C36H_2$)](16)+[ω(C31O41)](5)+ [δ_{sci}(C32C31C35)](5)
850	845	838	839	R2[oop(CH)](42)+R2[puck](15)+R1[oop(C19H20)](13)+R2[oop(C23C25C16)]

				(10)+[ω(C25N26)](10)
840	836			R1[oop(CH)](56)+R1[puck](16)+[ω(C10N11)](11)+R1[oop(C1C10)](11)
806	802	807	807	[ρ(C40O47)](19)+[ν(C35C40)](17)+[ω(C40O47)](10)+[δ(C40O47N29)](9)+ [ν(C40O47)](8)+[δ_{sym}(C31O41)](5)
802	798			[ω(C40O47)](26)+[ω(C39O44)](15)+[δ_{sci}(C36C35C39)](7)+[ρ($C36H_2$)](5)+ [ω(C35O50C40)](5)
785	782	792	791	R2[δ_a](26)+R2[ν(CC)](22)+R1[δ_a](10)+R1[ν(C1C10)](6)
784	781			R1[δ_a](26)+R1[ν(CC)](20)+R2[δ_a](10)+R2[ν(C16C25)](6)
754	751	765	751	[ω(C25N26)](53)+R2[oop(CH)](22)+R1[oop(C16H25)](6)+ R2[oop(C23C25C16)](6)
753	750	748		[ω(C10N11)](50)+R1[oop(CH)](42)
718	716	716	722	[ω(C39O44)](37)+[τ(C39O44)](10)+R1[puck](10)+[ν(C35C36)](8)+R2[puck](6)
717	715	713	712	R1[puck](75)+R1[oop(C6H7)](11)
716	714			R2[puck](77)+R2[oop(C21H22)](11)
689	687	694	695	[δ_{sym}(C31O41)](21)+[ρ(C31O41)](13)+[ω(C40O47)](11)+[δ_{sci}(C32C31C35)](7)+ [ν(C31O41)](7)+[δ(C31O41N14)](7)+[ω(C31O41)](7)
659	657	655	652	R2[δ'_a](77)+[δ_{sym}(C25N26)](5)
657	656			R1[δ'_a](74)+[ν(N14H42)](5)
639	638	640	638	[ρ(C31O41)](18)+[δ_{sym}(C40O47)](14)+[δ_{sci}(C35O50C40)](11)+[τ(C39O44)](9)+ [ν(C35C40)](7)
631	630	629	629	[δ_{sym}(C25N26)](16)+R2[ρ(C25N26)](21)+R2[δ_a](13)+[ρ(C39O44)](10)+ [τ(C39O44)](7)
629	628			[ρ(C39O44)](15)+[τ(C39O44)](14)+[δ_{sym}(C25N26)](10)+[ρ(C25N26)](9)+R2[δ_a] (9)+[δ_{sym}(C39O44)](6)
626	625	625	625	[δ_{sym}(C10N11)](26)+R1[δ_a](22)+[ρ(C10N11)](31)+R1[δ'_a](5)
595	594	578	587	[ω(C31O41)](41)+[τ(C39O44)](15)+[ρ($C32H_2$)](9)
584	583			[τ(C39O44)](26)+[ω(C31O41)](11)+[ω(C39O44)](8)+[δsym(C39O44)](7)+ [ω(C35O50C40)](7)+[ω(C40O47)](7)+[ρ(C39O44)](7)+[ρ(C31O41)](6)
557	556	560	555	[τ(C10N11)](63)+R1[τ_a](9)+R1[oop(C1C10)](9)+[ω(C10N11)](5)
556	556	548	541	[τ(C25N26)](68)+R2[τ_a](9)+R2[oop(C16C25)](8)
526	526	528	531	[ρ(C40O47)](21)+[ρ($C32H_2$)](13)+[δ_{sym}(C40O47)](10)+[δ_{sci}(C35O50C40)](8)+ [ω(C31O41)](8)+[ρ(C35O50C40)](5)+[ν(C35C40)](5)+[τ(C32C35)](5)
507	507	514	514	[ρ(C10N11)](22)+[δ_{sym}(C10N11)](18)+R1[δ_{in}(C1C10)](12)+R1[τ_a](11)+ R1[oop(C1C10)](8)+[τ(C10N11)](5)
500	500			[ρ(C25N26)](24)+[δ_{sym}(C25N26)](16)+R2[δ_{in}(C16C25)](11)+R2[τ_a](10)+ R2[oop(C16C25)](8)+[ρ(C25N26)](5)
462	462	467	463	[ρ(C39O44)](16)+[δ_{sym}(C39O44)](13)+[τ(C35O50)](12)+[ω(C39O44)](10)+ [ρ($C36H_2$)](5)+[τ(C35C36)](5)
448	449	448	437	[τ(C35O50)](73)
421	422	420	422	R2[τ'_a](54) +R2[τ_a](12)+R2[oop(C16C25)](6)
420	421			R1[τ'_a](62)+R1[τ_a](9)+R1[oop(C1C10)](5)
410	411	413	411	[δ_{sym}(C39O46)](23)+[δ_{sym}(C31O41)](9)+[ν(C35C36)](7)+[ρ(C31O41)](13)+ [δ_{sym}(C39O44)](6)+[ν(C32C35)](5)
393	394	-	391	R2[τ_a](33)+R2[τ'_a](20) +R2[oop(C16C25)](13)+R1[τ_a](9)
393	394	-		R1[τ_a](35)+R1[oop(C1C10)](13)+R1[τ'_a](13)+R2[τ_a](9)+R2[τ'_a](5)
378	379	-	375	[ρ(C25N26)](17)+R2[δ_a](17)++R2[ν(C16C25)](17)+[ρ(C35O50C40)](7)+ [δ_{sci}(C35O50C40)](5)
376	377	-		[ρ(C10N11)](22)+R1[ν(C1C10)](15)+R1[δ_a](14)+R1[τ_a](9)+R1[ω(C10N11)](6)
375	376	-	370	[ρ(C35O50C40)](20)+[δ_{sci}(C35O50C40)](10)+[ρ($C32H_2$)](7)+[τ(C32C35)](7)+ [δ_{sym}(C31O41)](5)+[ω(C35O50C40)](5)
358	359	-	364	[ω(C10N11)](51)+[τ(C10N11)](14)+[ν(C10N11)](5)
356	357	-		[ω(C10N11)](23)+[ω(C35O50C40)](11)+[δ_{sym}(C31O41)](10)+[τ(C10N11)](6)+ [δ_{sci}(C35O50C40)](5)+[δ_{sym}(C40O47)](5)
326	327	-	329	[ω(C25N26)](67)+[τ(C25N26)](18)+[ν(C25N26)](5)
318	319	-	314	[δ_{sym}(C40O47)](13)+[ν(N29H48)](9)+[ρ(C39O44)](8)+[ρ(C35O50C40)](7)+ [γ(C35O50C40)](6)+[δ_{sci}(CCC)](12)
268	269	-	-	[γ(C35O50C40)](15)+[δ_{sci}(C35O50C40)](12)+[δ_{sci}(CCC)](17)+[ν(N29H48)](7)+ [δ_{sym}(C31O41)](5)+[ρ(C35O50C40)](5)
229	230	-	-	[δ_{sci}(C35C32C36)](19)+[γ(C35O50C40)](19)+[ν(N14H42)](9)+[ω(C40O47)](7)+ [ω(C35O50C40)](7)+[τ(C40O47)](6)
221	222	-	-	R1[δ_{in}(C1C10)](29)+R2[δ_{in}(C16C25)](13)+[δ(C2N14O41)](9)+[δ_{sym}(C10N11)] (7)
219	221	-		R2[δ_{in}(C16C25)](31)+R1[δ_{in}(C1C10)](14)+[δ_{sym}(C25N26)](8)

180	181	-	-	[δ_{sci}(CCC)](42)+[δ(C31O41N14)](14)+[δ(C31H42O41)](5)+[ν(N29H48)](5)
163	164	-	-	R2[oop(C16C25)](10)+[ν(N14H42)](10)+[τ(C40O47)](8) [τ(C35C40O47N29)](7)+R2[τ_a](7)+R1[oop(C1C10)](7)+[τ(C32C35)](6)+ [δ_{sci}(C36C35C39)](5)
159	160	-		R1[oop(C1C10)](24)+R1[τ_a](15)+R2[oop(C16C25)](14)+R2[τ_a](9)+ R1[ω(C10N11)](5)
153	154	-	-	[ν(N14H42)](16)+R2[oop(C16C25)](10)+[δ_{sci}(C36C35C39)](7) [τ(C35C40O47N29)](7)+[τ(C40O47)](6)+[γ(C35O50C40)](5)+R2[τ_a](5)+ [δ(C31H42O41)](5)
136	137	-	-	[τ(CC)](25)+[τ(C35C40O47N29)](7)+[τ(C40O47)](6)+[ν(N29H48)](6)+ [τ(C35O50)](5)+[δ_{sci}(C35C32C36)](5)+[δ(C19N29O47)](5)
122	123	-	-	[τ(C32C31O41N14)](22)+[τ(C31O41)](17)+[τ(C32C35)](15)+[ν(N29H48)](7)
105	106	-	-	[τ(C32C31O41N14)](15)+[τ(C31O41)](14)+[τ(CC)](17)+[δ(C40H48O47)](7)+ [δ(C19N29O47)](7)+[δ(C40O47N29)](5)
101	102	-	-	[ν(N14H42)](19)+[τ(C35C40)](15)+[τ(C32C31O41N14)](7)+[δ_{sci}(C36C35C39)] (6)+[τ(CO)](12)+[τ(C35C40O47N29)](5)+[δ_{sci}(C35C32C36)](5)
90	91	-	-	[δ(C40O47N29)](29)+[ν(N29H48)](13)+[τ(C31O41)](11)+[τ(H5C4N14O41)](9) +[τ(C32C31O41N14)](7)+[δ(C40H48O47)](5)+[τ(C31C32)](5)
80	80	-	-	[δ(C40O47N29)](13)+[τ(C40O47)](11)+[τ(H20C19N29O47)](10)+ [δ(C31O41N14)](9)+[τ(C16C25)](8)+[ν(N29H48)](6)+[τ(C35C40O47N29)](5)+ [ν(N14H42)](5)
76	76	-	-	[δ(C40O47N29)](11)+[τ(C40O47)](10)+[τ(CC)](30)+[τ(C35C40O47N29)](8)+ [τ(H5C4N14O41)](8)+[τ(H20C19N29O47)](8)+[ν(N29H48)](5)
66	66	-	-	[τ(CC)](32)+[δ(C31O41N14)](15)+[ν(N14H42)](10)+[δ(C2N14O41)](6)
59	60	-	-	[δ(C2N14O41)](20)+[τ(CC)](26)+[δ(C31O41N14)](10)+[ν(N14H42)](8)+ [τ(C2N14O41C31)](6)
56	56	-	-	[τ(CC)](42)+[τ(C32C31O41N14)](13)+[δ(C2N14O41)](10)+[τ(C31O41)](10)
50	51	-	-	[τ(CC)](52)+[δ(C19N29O47)](19)
47	47	-	-	[τ(CC)](34)+[τ(C35C40O47N29)](16)+[τ(C40O47)](15)
38	38	-	-	[τ(CC)](68)+[τ(C2N14O41C31)](10)+[τ(H20C19N29O47)](6)+[τ(H5C4N14O41)] (6)
34	34	-	-	[τ(C2N14O41C31)](14)+[δ(C19N29O47)](12)+[δ(C2N14O41)](10)+ [ν(N29H48)](9)+[δ_{sci}(C32C31C35)](5)
28	28	-	-	[τ(C35C40O47N29)](15)+[δ(C2N14O41)](14)+[τ(CC)](18)+[δ(C31O41N14)](8) +[τ(H20C19N29O47)](7)
20	20	-	-	[τ(C32C31O41N14)](47)+[τ(H5C4N14O41)](15)+[τ(C31O41)](14)+ [τ(C35C40O47N29)](8)
16	16	-	-	[τ(C19N29O47C40)](54)+[τ(C35C40O47N29)](11)+[τ(C35C40)](9)+ [τ(H20C19N29O47)](7)
12	12	-	-	[τ(C35C40O47N29)](29)+[τ(C2N14O41C31)](18)+[τ(C40O47)](17)+ [τ(C31C32)](15)
6	6	-	-	[τ(C35C40O47N29)](37)+[τ(C40O47)](18)+[τ(CC)](19)+[τ(C32C31O41N14)](6) +[τ(C2N14O41C31)](5)

Table S5 Theoretical and experimental vibrational wavenumbers (cm^{-1}) of NIC-CA (cluster) model and their assignments using B3LYP/6-311++G(d,p).

Unscaled	Scaled	IR	Raman	Potential Energy Distribution (≥ 5%)
3713	3521			[$\nu_a(N26H_2)$](100)
3701	3510			[ν(O50H51)](100)
3684	3495	3491	3494	[$\nu_a(N55H_2)$](66)+[δ(H79N55O46)](29)
3680	3491			[$\nu_a(N53H_2)$](63)+[δ(H66N53O15)](27)
3680	3491			[$\nu_a(N11H_2)$](62)+[δ(C2N14O41)](33)
3588	3409	3413	3418	[$\nu_s(N26H_2)$](100)
3341	3188	3185	3110	[$\nu_s(N55H_2)$](61)+[ν(O46H80)](28)
3339	3186			[$\nu_s(N53H_2)$](48)+[ν(O15H67)](20)+[$\nu_s(N11H_2)$](14)
3288	3140			[$\nu_s(N11H_2)$](53)+[ν(O52H13)](14)+[δ(C56C65H13)](12)+[$\nu_s(N53H_2)$](12)+[ν(O15H67)](5)
3205	3065	3066	3066	R2[ν(CH)](97)
3204	3065			R3[ν(CH)](99)
3199	3060			R1[ν(CH)](96)
3193	3055			R4[ν(CH)](94)
3193	3055			R2[ν(CH)](99)
3192	3054			R1[ν(C2H3)](96)

3188	3050			R3[ν(CH)](99)
3183	3046	3048	3048	R4[ν(C57H58)](97)
3177	3040			R2[ν(CH)](97)
3175	3038			R1[ν(CH)](99)
3170	3034	3034	3033	R1[ν(CH)](99)
3170	3034		3032	R4[ν(CH)](96)
3162	3027	3027	3030	R2[ν(C17H18)](98)
3159	3024	3018	3018	[ν(O44H45)](70)+[ν(O54H45)](22)
3156	3021			R3[ν(C72H73)](94)
3154	3019	3014	3014	R4[ν(C59H60)](98)
3142	3008	3007	3010	R3[ν(C70H71)](97)
3130	2998	2986	2984	[ν_a(C36H_2)](97)
3115	2984			[ν_a(C32H_2)](99)
3083	2955	2944	2947	[ν(O41H42)](84)+[ν(N14H42)](6)+[ν_s(C32H_2)](5)
3073	2946	2860	2858	[ν_s(C32H_2)](85)+[ν(O41H42)](12)
3062	2936			[ν_s(C36H_2)](97)
2930	2816	2813		[ν(O47H48)](91)+[ν(N29H48)](8)
1769	1733	1721	1729	[ν(C31=O43)](52)+[ν(C40=O49)](12)+[δ(C31H42O41)](6)
1755	1720			[ν(C40=O49)](50)+[ν(C31=O43)](13)+[δ(C40H48O47)](6)+[ν(C40O47)](6)+ [ν(C25=O30)](5)
1750	1715	1685	1680	[ν(C25=O30)](64)+[ν(C25N26)](8)+[ν(C40=O49)](5)+[ρ(C25N26)](5)
1749	1714			[δ(C39O44O54)](33)+[ν(C39=O46)](23)+[ν(C78=O54)](11)+[ν(C39O44)](9)+ [δ(C78O54O44)](7)+[ρ(C39O44)](6)
1729	1695			[δ(H65N53O15)](25)+[ν(C65N53)](16)+[δ_{sci}(C10N11)](9)+[ν(C10=O15)](9)+ [ρ(C65N53)](8)+[ρ(C10N11)](7)+[ν(C10N11)](5)+[ν(C65=O52)](5)
1718	1685	1650	1648	[δ(H65N53O15)](26)+[ν(C65N53)](15)+[δ(C56C65H13)](14)+[δ_{sci}(C65N53)](11)+ [δ_{sci}(C10N11)](9)+[ρ(C65N53)](6)+[δ(C2N14O41)](5)
1707	1674			[ν(C78=O54)](27)+[δ_{sci}(C78N55)](21)+[δ(C78O54O44)](20)+[δ(H79N55O46)](10)+ [ρ(C78N55)](7)
1650	1620			[δ_{sci}(C10N11)](28)+[δ(C2N14O41)](21)+[δ_{sci}(C65N53)](20)+[δ(H66N53O15)](12)+ [δ(C56C65H13)](8)
1637	1608	1610	1614	R1[ν(CC)](24)+[δ_{sci}(C65N53)](14)+[δ(H66N53O15)](8)+[ρ(C65N53)](7)+[δ_{sci}(C10N11)](7)
1637	1608			R2[ν(CC)](35)+R2[ν(C17N29)](12)+R2[δ_{in}(C17H18)](8)+R2[δ_a](7)
1630	1601	1605	1605	[δ_{sci}(C10N11)](16)+[δ_{sci}(C65N53)](14)+[δ(C2N14O41)](11)+[ρ(C65N53)](9)+ [δ(H66N53O15)](7)+[ν(C10=O15)](5)+[δ(H65N53O15)](5)
1630	1601			R3[ν(CC)](43)+ R3[δ_{in}(C76H77)](16)+R3[ν(C70N81)](15)+R3[δ_a](10)
1629	1600			R4[ν(CC)](39)+R4[ν(C57N68)](15)+R4[δ_a](10)+R4[δ_{in}(C63H64)](9)+R4[δ_{in}(C57H58)](7)
1622	1593			[δ_{sci}(C25N26)](49)+[δ_{sci}(C78N55)](14)+[δ(H79N55O46)](10)+[ν(C78=O54)](7)
1622	1593			[δ_{sci}(C78N55)](32)+[δ(H79N55O46)](23)+[ν(C78=O54)](16)+[δ(C78O54O44)](8)+ [ρ(C78N55)](7)
1614	1586	1581	1571	R2[ν(CC)](46)+R2[ν(C19N29)](18)+R2[δ_{in}(CH)](18)+R2[δ'_a](8)
1611	1583			R1[ν(C1C8)](23)+[δ_{sci}(C10N11)](10)+R1[ν(C4N14)](10)+[ν(C10=O15)](8)+ R1[δ_{in}(CH)](13)+[δ(C2N14O41)](8)+R1[δ'_a](5)
1603	1575			[δ(H65N53O15)](12)+R4[ν(CC)](24)+R4[ν(C65=O52)](7)+R4[ν(C59N68)](7)+ R4[δ_{in}(C59H60)](6)+[δ_{sci}(C65N53)](5)+[ρ(C65N53)](5)
1600	1572			[ν(C78=O54)](30)+[δ(C78O54O44)](13)+[δ_{sci}(C78N55)](12)+[δ(H79N55O46)](10)+ R3[ν(C72C74)](6)+[ρ(C78N55)](5)
1522	1497	1503	1522	[δ(C40H48O47)](47)+R2[δ_{in}(CH)](12)+[ν(C40O47)](7)
1512	1488	1488	1489	R3[δ_{in}(CH)](34)+[δ(C78O54O44)](8)+R3[ν(C72N81)](8)+R3[ν(CC)](18)+[δ_{sym}(C78N55)](5)+ R3[oop(C72H73)](5)
1507	1483			R1[δ_{in}(CH)](41)+R1[ν(C4N14)](11)+R1[ν(CC)](12)+ [δ(C31H42O41)](7)
1505	1481			R2[δ_{in}(CH)](42)+[δ(C40H48O47)](13)+R2[ν(CC)](16)+ R2[ν(C19N29)](6)
1505	1481			R4[δ_{in}(CH)](41)+ R4[ν(CC)](17)+[ν(C65N53)](10)+R4[ν(C59N68)](10)
1487	1464	1470	1476	[δ(C31H42O41)](41)+R1[δ_{in}(CH)](14)+[ν(C31O41)](6)
1477	1454	1462	1460	[δ_{sci}(C36H_2)](73)+[ν(C39O44)](7)
1462	1440			[ν(C39O44)](18)+[δ(C39H45O44)](17)+[δ_{sci}(C32H_2)](10)
1459	1437	1440	1441	[ν(C65N53)](14)+[ρ(C10N11)](8)+[δ_{sym}(C65N53)](6)+[ν(C39O44)](6)+ [δ(C39H45O44)](5)+R1[δ_{in}(C4H5)](5)+[ν(C10N11)](5)
1456	1434			[δ(C56C65H13)](33)+[ν(C65N53)](18)+[δ_{sym}(C65N53)](11)+R4[δ_{in}(C59H60)](6)
1455	1433			R2[δ_{in}(C19H20)](23)+R2[ν(C16C17)](9)+[δ_{sci}(C32H_2)](7)+R2[ν(C17N29)](7)+ [δ(C39H45O44)](6)+[ν(C39O44)](5)
1449	1427	1427	1418	[δ_{sci}(C32H_2)](25)+R3[oop(C72H73)](19)+R3[ν(C70N81)](7)+R3[ν(C69C70)](6)
1448	1426			[δ_{sci}(C32H_2)](32)+R3[oop(C72H73)](13)+R3[ν(C70N81)](5)+[δ(C39H45O44)](5)

1422	1401	1407	1408	[δ(C78O54O44)](30)+[ρ(C78N55)](16)+[ρ(C78N55)](15)+[δ_{sym}(C78N55)](10)+ [ν(C78N55)](9)
1417	1397			[δ(C35H51O50)](24)+[δ(C78O54O44)](14)+[ρ(C78N55)](7)+[ρ(C78N55)](7)+ [δ(C40H48O47)](6)+[ν(C35C40)](5)
1410	1390			[ν(C65N53)](33)+[ρ(C10N11)](15)+[δ(H65N53O15)](10)+[ν(C10N11)](10)+ [ρ(C65N53)](7)
1401	1381			[ν(C65N53)](37)+[δ(C56C65H13)](19)+[ρ(C65N53)](10)+[δ(H65N53O15)](7)+ [ρ(C10N11)](6)+[δ_{sym}(C65N53)](5)
1385	1366	1360	1359	[ω(C32H_2)](44)+[ν(C31C32)](12)+[δ(C31H42O41)](11)+[ν(C32C35)](9)+ [ν(C31O41)](6)
1367	1348			[ν(C25N26)](33)+R2[ν(C16C25)](25)+[δ_{sym}(C25N26)](11)+[ρ(C25N26)](8)+[ρ(C25N26)](5)
1362	1344	1344	1347	R2[δ_{in}(CH)](82)
1362	1344			R3[δ_{in}(C70H71)](69)+R3[oop(C72H73)](9)
1356	1338			R1[δ_{in}(CH)](66)
1356	1338			R4[δ_{in}(C57H58)](28)+[ν(C65N53)](6)+[ρ(C65N53)](6)
1343	1325	1337	1338	[ω(C36H_2)](53)+[ν(C40O47)](7)
1320	1303	1303	1307	[ν(C39O44)](48)+[δ(C39O44O54)](27)+[δ(C39H45O44)](6)
1295	1279			R2[ν(CC)](44)+R2[ν(CN)](42)
1290	1274			R1[ν(CC)](45)+R1[ν(CN)](41)
1289	1273			R3[ν(CC)](43)+R3[ν(CN)](40)
1287	1271			[ν(C40O47)](29)+[ω(C36H_2)](12)+[δ(C35H51O50)](10)+[δ_{sym}(C40O47)](6)+ [δ(C40H48O47)](6)+[ν(C35C40)](5)+[ν(C39O44)](5)
1286	1270	1260	1270	R4[ν(CN)](33)+[δ(C56C65H13)](14)+R4[ν(CC)](37)+[δ_{sym}(C65N53)](5)
1269	1254	1243	1243	[γ(C32H_2)](37)+[ν(C31O41)](20)+[ω(C32H_2)](12)
1233	1219			[ν(C31O41)](24)+[γ(C32H_2)](18)+[ν(C40O47)](6)+[ω(C32H_2)] (6)
1230	1216	1221	1228	R3[ν(CN)](21)+[R3[oop(C72H73)](18)+R3[δ_{in}(CH)](18)+ρ(C78N55)](11)+ R3[ν(C72C74)](8)+[δ(H79N55O46)](7)
1227	1213	1213	1203	R2[δ_{in}(CH)](34)+R2[ν(CN)](17)+R2[ν(C19C21)](8)
1225	1211			R4[δ_{in}(CH)](45)+R4[ν(C59N68)](14)+R4[ν(C59C61)](9)+R4[ν(C56C63)](5)
1224	1210			R1[δ_{in}(CH)](29)+R1[ν(C4N14)](10)+R1[ν(C4C6)](8)+ [ν(C31O41)](6)
1217	1203			[ν(C39O44)](28)+[γ(C36H_2)](23)+[δ(C39O44O54)](17)+[δ(C35H51O50)](6)+ [ν(C32C35)](5)+[ω(C36H_2)](5)
1172	1160	1163	1158	[ρ(C78N55)](35)+[δ(H79N55O46)](24)+R3[δ_{in}(C74H75)](8)+R3[ν(C69C78)](6)+ R3[δ_{tri}](5)+R3[ν(C74C76)](5)
1171	1159			[ρ(C10N11)](38)+[δ(C2N14O41)](15)+[δ(C56C65H13)](14)
1167	1155			[ν(C65N53)](20)+[ρ(C65N53)](16)+[δ(H66N53O15)](12)+[ρ(C10N11)](8)+ [δ(H65N53O15)](7)+R4[ν(C56C65)](7)
1157	1145			R2[ν(CC)](36)+R2[δ_{in}(C21H22)](18)+R2[δ_{tri}](16)+[ν(C25N26)](10)+ρ(C25N26)](9)
1152	1140			[ρ(C10N11)](37)+[δ(C2N14O41)](20)+R1[δ_{in}(CH)](11)+R1[ν(C6C8)](7)+ [δ(C56C65H13)](6)
1150	1138	1136	1131	R2[ν(CC)](36)+[ρ(C65N53)](21)+[δ(H66N53O15)](19)+[δ(H65N53O15)](11)+ R4[ν(C61C63)](8)+[ν(C65N53)](5)
1137	1126	1123	1120	R2[δ_{in}(CH)](44)+R2[ν(CC)](17)+R2[ν(C17N29)](14)
1134	1123			[ρ(C78N55)](23)+[δ(H79N55O46)](20)+R3[δ_{in}(C76H77)](13)+[ν(C78=O54)](10)+ [δ(C78O54O44)](7)+R3[ν(C70N81)](5)
1131	1120			[ν(C35O50)](27)+[ν(C32C35)](11)+[ν(C39O44)](9)+[γ(C36H_2)](7)+[ρ(C35O50C40)](5)+ [δ(C39O44O54)](5)
1118	1107	1109	1104	[ρ(C78N55)](45)+[δ(H79N55O46)](37)+[ν(C78=O54)](5)
1118	1107			[ρ(C10N11)](35)+[δ(C2N14O41)](21)+[ν(C65N53)](9)+[δ(H65N53O15)](9)+ [δ(H66N53O15)](8)+[ρ(C65N53)](6)
1114	1103			[δ(H65N53O15)](23)+[ρ(C10N11)](23)+[ν(C65N53)](15)+[ρ(C65N53)](13)+ [δ(H66N53O15)](10)+[δ(C2N14O41)](9)
1084	1074	1070	1074	[ρ(C25N26)](56)+[ν(C25N26)](25)+[ν(C25=O30)](8)
1079	1069			[ν(C39O44)](14)+[ν(C32C35)](9)+[ν(C35O50)](8)+[ρ(C32H_2)](7)+[ρ(C35O50C40)](7)+ [δ(C39O44O54)](7)+[γ(C36H_2)](7)+[ω(C35O50C40)](6)+[ρ(C36H_2)](6)+[ν(C35C36)](5)
1064	1055	1054	1052	R2[ν(CC)](37)+R2[ν(CN)](24)+R2[δ_{tri}](9)+R2[δ_{in}(C21H22)](8)
1063	1054			R1[ν(CC)](32)+R1[ν(CN)](26)+R1[δ_{in}(C6H7)](9)
1061	1052			R4[ν(CC)](42)+R4[ν(CN)](22)+R4[δ_{in}(C61H62)](8)+[δ(H65N53O15)](8)+ [ν(C65N53)](7)
1060	1051			R3[ν(CC)](53)+R3[ν(CN)](23)+R3[δ_{in}(C74H75)](8)
1058	1049			[ν(C35C36)](31)+[ω(C35O50C40)](7)+[ν(C35C40)](6) [δ_{sci}(C35C32C36)](6)+ [δ_{sci}(C32C31C35)](5)
1045	1036	1039	1033	R2[δ_{tri}](62)+R2[ν(CC)](28)
1045	1036			R1[δ_{tri}](64)+R1[ν(CC)](23)

1039	1030			R3[δ_{tri}](68)+R3[ν(CC)](17)
1039	1030			R4[δ_{tri}](60)+R4[ν(CC)](15)+[ν(C65N53)](6)+[δ(H65N53O15)](6)
1032	1024			[τ(C40O47)](39)+R2[oop(C19H20)](29)+[τ(C19N29)](11)+R2[oop(C21H22)](9)+ R2[puck](5)
1028	1020	1017	1011	R1[oop(C4H5)](85)
1026	1018			R2[oop(CH)](67)+[τ(C40O47)](18)
1015	1007	1007	999	[τ(C31O41)](88)+R1[oop(C2H3)](6)
1013	1005			R3[oop(CH)](85)+R3[puck](8)
1006	998			R2[oop(CH)](79)
1005	997			R4[oop(CH)](90)
988	981			R3[oop(CH)](87)+R3[τ_a](6)
986	979			R1[oop(CH)](81)+R1[puck](6)
979	972			[τ(C39O44)](88)
979	972	971	970	R4[oop(CH)](75)+R4[puck](10)
966	959			R1[oop(CH)](75)+R1[puck](11)
958	951			R4[oop(CH)](84)+R4[puck](8)
953	946	946	946	[ρ(C36H_2)](22)+[ρ(C32H_2)]13)+[ρ(C39O44)](7)+[ν(C31C32)](7)+[ω(C31O41)](6)
946	940	930	931	R2[oop(C17H18)](52)+R3[oop(C70H71)](20)+R2[puck](8)
946	940			R3[oop(CH)](52)+R2[oop(CH](28)+R3[puck](9)
931	925			[δ(C39O44O54)](52)+[ν(C39O44)](18)+[ν(C36C39)])(7)
926	920	918	916	[δ(C39O44O54)](47)+[ν(C39O44)](17)+[ν(C31C32)](7)+[ν(C36C39)](6)
895	890	890	893	[δ(C39O44O54)](24)+[ρ(C36H_2)](12)+[ν(C39O44)](11)+[ν(C32C35)](6)+ [ν(C31C32)](6)+[ω(C31O41)](6)+[δ_{sci}(C32C31C35)](6)+[ν(C35O50)](5)
855	851			[ω(C10N11)](21)+[τ(C10N11)](20)+[τ(C65N53)](11)+[ω(C65N53)](10)+ [δ(C56C65H13)](8)+[ω(C10N11)](8)+[δ(C2N14O41)](7)+[ω(C65N53)](6)
850	846	838	839	R2[oop(CH)](56)+R2[puck](16)+R2[oop(C16C25)](10)+[ω(C25N26)](10)
843	839			R3[oop(CH)](48)+R3[puck](18)+[ω(C78N55)](14)+ R3[oop(C69C78)](11)
840	836			R1[oop(CH)](54)+R1[puck](17)+R1[oop(C1C10)](11)+ [ω(C10N11)](9)
834	830			R4[oop(CH)](39)+R4[puck](17)+[ω(C65N53)](12)+R4[oop(C56C65)](10)+ [δ(H65N53O15)](6)+[δ_{sym}(C65N53)](5)
821	817			[τ(C78N55)](30)+[ω(C78N55)](27)+[δ(H79N55O46)](7)+[δ(C78O54O44)](7)
808	804	807	807	[ω(C40O47)](21)+[δ(C39O44O54)](13)+[ρ(C39O44)](10)+[ω(C39O44)](7)+ [ω(C35O50C40)](5)
806	802			[δ(C56C65H13)](17)+[τ(C65N53)](17)+[ω(C65N53)](14)+[ω(C10N11)](10)+ [τ(C10N11)](10)+[δ(H65N53O15)](8)+[ρ(C65N53)](5)
804	800			[ρ(C40O47)](18)+[ν(C35C40)]17)+[δ(C40O47N29)](9)+[ν(C40O47)](9)+[ω(C39O44)](8) +[ν(C32C35)](6)
799	796			[δ(H65N53O15)](22)+[δ(C2N14O41)](19)+[ρ(C10N11)](10)+[δ(C56C65H13)](8)+ [ρ(C10N11)](7)+R1[δ_a](5)+[ρ(C65N53)](5)
795	792			[δ(C78O54O44)](40)+[ρ(C78N55)](17)+[δ(H79N55O46)](16)+[ρ(C78N55)](6)+R3[δ_a](5)
792	789			[δ(H65N53O15)](38)+[ρ(C65N53)](14)+[δ(C56C65H13)](10)+[ν(C65N53)](8)+ [δ(H66N53O15)](7)
785	782	792	791	R2[δ_a](36)+R2[ν(CC)](30)+ρ(C25N26)](5)+R2[δ_{tri}](5)
754	751	765	751	[ω(C25N26)](53)+R2[oop(CH)](33)+R2[oop(C16C25)](6)
747	744			[ω(C10N11)](39)+R1[oop(CH)](25)+[ω(C65N53)](7)+ R1[oop(C1C10)](6)
741	738			[ω(C78N55)](35)+R3[oop(CH)](27)+[δ(C78O54O44)](6)+ R3[oop(C69C78)](6)
740	738			[ω(C65N53)](34)+R4[oop(CH)](26)+[ω(C10N11)](5)
722	720	716	722	[δ(C39O44O54)](53)+[ρ(C39O44)](13)+[δ(C78O54O44)](8)+[ω(C39O44)](5)+ [ω(C40O47)](5)
717	715	713	712	R4[puck](69)+R4[oop(C61H62)](10)+R1[puck](6)
716	714			R2[puck](61)+R3[puck](19)+R2[oop(C21H22)](9)
716	714			R3[puck](55)+R2[puck](19)+R3[oop(C74H75)](7)
715	713			R1[puck](73)+R1[oop(C6H7)](8)+R4[puck](5)
692	690	694	695	[δ(C39O44O54)](18)+[δ_{sym}(C31O41)](12)+[ω(C40O47)](10)+[ρ(C31O41)](10) + [δ(C78O54O44)](6)+[ν(C31O41)](5)+[δ_{sci}(C32C31C35)](5)+[ω(C31O41)](5)+ [δ(C31O41N14)](5)+[ρ(C39O44)](5)
664	663			[δ(H65N53O15)](38)+[ρ(C65N53)](19)+[δ(C2N14O41)](10)+ρ(C10N11)](7)+ [δ(H66N53O15)](5)
663	662			[δ(C78O54O44)](49)+[ρ(C78N55)](17)+[δ(H79N55O46)](11)+[δ_{sym}(C78N55)](9)+ [δ(C39O44O54)](7)
658	657	655	652	R2[δ'_a](36)+[δ(C78O54O44)](17)+[ρ(C78N55)](9)+[δ(H79N55O46)](6)+[δ_{sym}(C78N55)](5)
657	656			[ρ(C65N53)](34)+[δ(H65N53O15)](34)+[δ(H66N53O15)](8)+[δ_{sym}(C65N53)](7)
651	650			[δ(C39O44O54)](27)+[ρ(C39O44)](15)+[ρ(C78N55)](5)

645	644	640	638	[δ(C2N14O41)](24)+[ρ(C10N11)](14)+[δ(C56C65H13)](14)+[ρ(C10N11)](10)+ [δ_{sym}(C10N11)](8)+[ρ(C65N53)](6)+R1[δ'_a](5)
630	629	629	629	[δ_{sym}(C65N53)](20)+[δ(H65N53O15)](19)+[δ(C56C65H13)](18)+[ρ(C65N53)](15) +R4[δ'_a](11)+[δ(H66N53O15)](6)
630	629			[δ_{sym}(C25N26)](23)+[ρ(C25N26)](20)+R2[δ_a](19)+[ρ(C25N26)] (10)
628	627	625	625	[δ(C78O54O44)](32)+[ρ(C78N55)](28)+R3[δ'_a](15)+ [δ(H79N55O46)](11)
624	623			[δ(C39O44O54)](19)+[ρ(C31O41)](13)+[ω(C39O44)](8)+[ρ(C39O44)](7)
594	593	578	587	[ω(C31O41)](38)+[δ(C39O44O54)](11)+[ρ(C39O44)](6)+[ρ($C32H_2$)](6)
560	560	560	555	[τ(C25N26)](68)+R2[τ_a](8)+R2[oop(C16C25)](8)
534	534			[ρ(C65N53)](19)+[δ(C56C65H13)](18)+[δ(C2N14O41)](13)+[δ_{sym}(C65N53)](11)+ [δ(H66N53O15)](8)+[ν(O15H67)](7)+[ρ(C10N11)](6)+[ν(O52H13)](5)
529	529	528	531	[ρ(C40O47)](15)+[ρ(C32H2)](9)+[δ_{sym}(C40O47)](7)+[ω(C31O41)](6)+[δ_{sci}(C35O50C40)](6) +[ν(O46H80)](5)
523	523	514	514	[ρ(C78N55)](39)+[δ(H79N55O46)](20)+[δ_{sym}(C78N55)](15)+[ν(O46H80)](10)
521	521			[ρ(C65N53)](29)+[δ(C56C65H13)](20)+[δsym(C65N53)](15)+[δ(H65N53O15)](7)+ [ρ(C10N11)](6)
501	501			[ρ(C25N26)](23)+[δ_{sym}(C25N26)](15)+R2[τ_a](11)+R2[δ_{in}(C16C25)](11)+ R2[oop(C16C25)](8)+[ρ(C25N26)](5)
485	485	467	463	[ρ(C39O44)](21)+[δ_{sym}(C39O44)](19)+[δ(C39O44O54)](15)+[ν(O54H45)](6)
454	455			[ω(C65N53)](17)+[δ(H65N53O15)](16)+[ω(C10N11)] 10)+[δ(H66N53O15)](9)+ [δ(C2N14O41)](6)+[τ(C65N53)](5)+[ν(O15H67)](5)
454	455			[ω(C78N55)](42)+[δ(H79N55O46)](12)+[τ(C78N55)](10)+[δ(C39O44O54)](5)
450	451	448	437	[τ(C35O50)](51)+[ω(C78N55)](9)
448	449			[ω(C10N11)](30)+[ω(C65N53)](17)+[τ(C10N11)](8)+ [τ(C65N53)](5)+R1[τ_a](5)
427	428			[ν(O46H80)](39)+[δ(H79N55O46)](12)+[δ_{sym}(C39O44)](10)+ [δ(C39O44O54)](9)
420	421	420	422	R2[τ'_a](50)+R2[τ_a](11)+R2[oop(C16C25)](5)
418	419			[δ(C2N14O41)](21)+R1[τ'_a](16)+R3[τ'_a](8)+[ω(C10N11)](8)+[ν(O52H13)](7)
418	419			R3[τ'_a](15)+[δ(C2N14O41)](14)+R1[τ'_a](10)+[δ(H79N55O46)](7)+[ω(C78N55)](6)+ [δ(C39O44O54)](6)+[ω(C10N11)](5)
416	417	413	411	δ(H66N53O15)](21)+R4[τ'_a](21)+[ρ(C65N53)](15)+[ν(O15H67)](12)+ [δ(C56C65H13)](6)+[ω(C65N53)](6)
399	400			[ρ(C78N55)](27)+[ν(O46H80)](19)+[δ(H79N55O46)](10)+[δ(C39O44O54)](10)+ [ν(O54H45)](6)
399	400			[ν(O52H13)](15)+[δ(C56C65H13)](13)+[ρ(C65N53)](12)+[ν(O15H67)](11)+ [δ(C2N14O41)](9)+[ρ(C78N55)](6)+[ρ(C10N11)](5)
393	394	-	391	[ν(O15H67)](19)+[δ(C2N14O41)](14)+[ω(C10N11)](13)+R1[τ_a](11)+ [δ(H65N53O15)](7)+[ρ(C65N53)](6)+[δ(C56C65H13)](5)
393	394	-		R2[τ_a](42)+R2[τ'_a](22)+R2[oop(C16C25)](16)
385	386	-		[δ(H66N53O15)](19)+R4[τ_a](17)+[δ_{sym}(C65N53)](11)+R4[τ'_a](9)+[ω(C65N53)](8)+ R4[oop(C56C65)](7)+[ρ(C65N53)](5)
385	386	-		[δ(H79N55O46)](16)+R3[τ'_a](13)+[δ(C78O54O44)](13)+[ω(C78N55)](12)+R3[τ_a](12)+ [δ(C39O44O54)](9)+[ν(O54H45)](6)+R3[oop(C69C78)](5)
379	380	-	370	[ρ(C35O50C40)](10)+[δ(C78O54O44)](10)+[δ(C39O44O54)](7)+[ρ(C65N53)](7)+ [δ_{sci}(C35O50C40)](5)+[δ(H65N53O15)](5)
377	378	-		[ρ(C65N53)](31)+[δ(H65N53O15)](25)+[δ(C56C65H13)](6)+[ρ(C10N11)](6)
376	377	-		[ρ(C65N53)](19)+[δ(H65N53O15)](16)+R2[ν(C16C25)](5)+[ρ(C25N26)](5)
360	361	-	364	[ν(O46H80)](16)+[δ_{sym}(C31O41)](11)+[ω(C35O50C40)](9)+[δ_{sym}(C40O47)](8)+ [δ_{sci}(C35O50C40)](8)+[δ(C78O54O44)](5)
338	339	-	329	[ω(C25N26)](67)+[τ(C25N26)](17)+[ν(C25N26)](5)
328	329	-		[δ(C78O54O44)](36)+[ν(O54H45)](14)+[ρ(C39O44)](6)+[δ_{sym}(C40O47)](5)+ [δ(C39O44O54)](5)
276	277	-	-	[ν(O46H80)](18)+[ν(O54H45)](17)+[δsci(C35O50C40)](9)+[δ_{sci}(C35C32C36)](7)+ [ν(N29H48)](6)+[δ(H79N55O46)](5)
255	256	-	-	[ν(O15H67)](28)+[ν(O52H13)](23)+[δ(C2N14O41)](16)+[δ(C56C65H13)](12)+ [δ(H66N53O15)](6)
254	255	-	-	[δ(C78O54O44)](55)+[ν(O46H80)](18)+[δ(C39O44O54)](10)+[δ(H79N55O46)](9)
237	238	-	-	[δ(C39O44O54)](31)+[δ(H65N53O15)](22)+[δ(C78O54O44)](21)
236	237	-		[δ(H65N53O15)](74)+[δ(C56C65H13)](10)
219	220	-	-	R2[δ_{in}(C16C25)](42)+[δ_{sym}(C25N26)](11)+[δ(C17N29O47)](11)+[ω(C25N26)](6)+ [τ(C25N26)](5)+[ω(C25N26)](5)+[ρ(C25N26)](4)
197	198	-		[δ(C78O54O44)](62)+[δ(C39O44O54)](16)+[ν(O54H45)](7)
178	179	-	-	[δ(H65N53O15)](48)+[δ(C2N14O41)](26)+[δ(C56C65H13)](5)+[δ(H66N53O15)](5)
171	172	-	-	[δ(H79N55O46)](32)+[δ(C78O54O44)](30)+[ν(O46H80)](11)+[ω(C78N55)](5)

171	172	-	-	[δ(H66N53O15)](22)+[δ(C56C65H13)](16)+[δ(C78O54O44)](10)+[ν(O15H67)](9)+ [δ(H65N53O15)](7)+[ν(O52H13)](7)+[δ(C39O44O54)](7)
168	169	-	-	[δ(C78O54O44)](27)+[δ(C39O44O54)](20)+[δ(H65N53O15)](19)+[δ(C56C65H13)](6) +[δ(H66N53O15)](5)
158	159	-	-	[δ(C39O44O54)](47)+[δ(C78O54O44)](28)+[ν(O46H80)](5)
152	153	-		[δ(C39O44O54)](59)+[δ(C78O54O44)](15)+[ν(O46H80)](13)
127	128	-	-	[δ(C78O54O44)](38)+[δ(C39O44O54)](32)+[τ(C31O41)](5)
122	123	-	-	[δ(C39O44O54)](57)+[ν(O46H80)](27)
119	120	-		[δ(C78O54O44)](58)+[ν(O46H80)](13)+[ν(O54H45)](5)+[ν(O52H13)](5)+ [δ(H79N55O46)](5)
109	110	-	-	[δ(C78O54O44)](35)+[ν(O46H80)](15)+[δ(H65N53O15)](15)+[δ(C2N14O41)](7)+ [ν(O54H45)](6)
106	107	-	-	[δ(H65N53O15)](40)+[ν(O15H67)](19)+[δ(C56C65H13)](16)+[ν(O52H13)](9)+ [δ(C39O44O54)](6)
96	97	-	-	[δ(H65N53O15)](58)+[δ(C56C65H13)](24)+[δ(C39O44O54)](5)
94	95	-	-	[δ(H65N53O15)](27)+[δ(C78O54O44)](15)+[δ(C56C65H13)] (15)+[δ(C39O44O54)](13) +[δ(C2N14O41)](6)+[δ(H66N53O15)](6)
91	92	-	-	[δ(H65N53O15)](44)+[δ(C56C65H13)](28)+[δ(C2N14O41)](8)+ [δ(H66N53O15)](5)
84	85	-	-	[δ(C78O54O44)](23)+[δ(H65N53O15)](17)+[δ(C56C65H13)](7)+[δ(C39O44O54)](7)+ [ν(O54H45)](5)+[ν(O46H80)](5)
81	82	-	-	[δ(C78O54O44)](34)+[δ(H65N53O15)](16)+[δ(C56C65H13)](13)+[δ(H66N53O15)](6)+ [δ(C39O44O54)](5)
77	78	-	-	[δ(H65N53O15)](27)+[δ(C56C65H13)](14)+[δ(C78O54O44)](11)+[δ(C39O44O54)](9)+ [δ(H79N55O46)](7)
76	77	-	-	[δ(C78O54O44)](39)+[δ(C39O44O54)](26)+[ν(O54H45)](6)+[δ(H79N55O46)](5)
69	70	-	-	[δ(C78O54O44)](38)+[δ(C56C65H13)](16)+[ν(O46H80)](13)+[δ(H79N55O46)](10)+ [δ(H65N53O15)](6)
61	61	-	-	[δ(C56C65H13)](39)+[δ(H65N53O15)](14)+[ν(O52H13)](9)+[δ(H66N53O15)](6)+ [ν(O46H80)](6)
58	58	-	-	[δ(C78O54O44)](15)+[ν(O15H67)](12)+[δ(C56C65H13)](11)+[δ(C2N14O41)](8) + [ω(C10N11)](5)+[τ(N14O41)](5)+[ω(C65N53)](5)
57	57	-	-	[δ(C56C65H13)](42)+[δ(H65N53O15)](18)+[δ(C78O54O44)](10)+[ν(O52H13)](9)
54	54		-	[δ(C56C65H13)](48)+[δ(C2N14O41)](13)+[ρ(C65N53)](8)+[ν(O15H67)](6)
52	52	-	-	[ν(O15H67)](20)+[δ(C56C65H13)](17)+[δ(H79N55O46)](10)+[τ(C16C25)](8)+ [δ(C2N14O41)](6)
46	46	-	-	[δ(H65N53O15)](38)+[δ(C56C65H13)](15)+[τ(C31C32)](6)+[ω(C65N53)](5)
41	41	-	-	[δ(H79N55O46)](20)+[ω(C78N55)](8)+[δ(C39O44O54)](7)+[δ(C17N29O47)](6)+ [τ(C16C25)](6)+[τ(C39O44)](6)+[τ(C39O44)](5)+[δ(H65N53O15)](5)
36	36	-	-	[δ(H65N53O15)](41)+[ν(O15H67)](15)+[δ(C17N29O47)](5)+[δ(H66N53O15)](5)
34	34	-	-	[δ(C56C65H13)](17)+[τ(C31O41)](8)+[δ(H65N53O15)](7)+[ν(O15H67)](7)+ [τ(N14O41)](7)+[ν(O54H45)](5)
26	26	-	-	[δ(C56C65H13)](29)+[δ(H65N53O15)](12)+[δ(C2N14O41)](10)
23	23	-	-	[δ(H65N53O15)](26)+[δ(H79N55O46)](13)+[δ(C2N14O41)](10)+[ν(O15H67)](8)+ [ω(C78N55)](7)
18	18	-	-	[ω(C78N55)](11)+[ρ(C78N55)](8)+[δ(H66N53O15)](8)+[τ(C69C78)](8)+[τ(C36C39)](8) +[δ(C2N14O41)](8)+ [ω(C10N11)](6)+[τ(C39O44)](5)+[δ(C78O54O44)](5)
16	16	-	-	[δ(H65N53O15)](10)+[τ(C31O41)](10)+[ω(C10N11)](10)+[δ(C2N14O41)](9)+ [δ(H66N53O15)](8)+[τ(C1C10)](7)
14	14	-	-	[δ(H65N53O15)](38)+[τ(C40O47)](10)+[ν(O15H67)](7)+[δ(C2N14O41)](5)
12	12	-	-	[τ(CN29O47)](29)+[τ(C35C40)](13)+[δ(H65N53O15)](10)+[τ(C19N29)](7)
10	10	-	-	[δ(C39O44O54)](17)+[τ(C31O41)](10)+[ν(O46H80)](9)+[δ(C2N14O41)](9)+ [δ(H65N53O15)](7)+[τ(N14O41)](7)+ [δ(C78O54O44)](6)
7	7	-	-	[τ(C40O47)](16)+[δ(C39O44O54)](14)+[τ(C39O44)](9)+[τ(C40O47)](8)+ [δ(H65N53O15)](8)+[ν(O46H80)](6)+[δ(C78O54O44)](6)
5	5	-	-	[τ(C40O47)](25)+[τ(C39O44)](20)+[τ(C40O47)](13)+[δ(H79N55O46)](9)+ [τ(C39O44)](9)+[τ(CN29O47)](9)
4	4	-	-	[τ(N14O41)](16)+[τ(C31C32)](13)+[δ(C39O44O54)](13)+[τ(C31O41)](13)+[τ(C31O41)](7) +[τ(N14O41)](6)+[δ(C78O54O44)](6)+[τ(C32C35)](6)+[ν(O46H80)](5)

Table S6 Topological parameters for bonds of interacting atoms of inter- and intra- molecular hydrogen bonding of NIC-CA (monomer): bond length (Å), electron density (ρ_{BCP}), Laplacian of electron density ($\nabla^2\rho_{BCP}$), electron kinetic energy density (G_{BCP}), electron potential energy density (V_{BCP}), total electron energy density (H_{BCP}) at bond critical point (BCP) and estimated interaction energy (E_{int}).

Interactions	Bond length (Å)	ρ_{BCP} (a.u.)	$\nabla^2\rho_{BCP}$ (a.u.)	G_{BCP} (a.u.)	V_{BCP} (a.u.)	H_{BCP} (a.u.)	E_{int} (kcal mol^{-1})
O47-H48···N29	1.6988	0.0542	0.0998	0.0121	-0.0491	-0.037	-15.4054
O41-H42···N14	1.7607	0.0466	0.0995	0.0074	-0.0398	-0.0324	-12.4874
O50-H51···O49	2.0264	0.0254	0.1045	-0.0026	-0.0210	-0.0236	-6.5889
C4-H5···O43	2.3782	0.0117	0.0378	-0.0013	-0.0069	-0.0082	-2.1649
C32-H34···O44	2.4577	0.0107	0.0371	-0.0013	-0.0067	-0.0080	-2.1022
C19-H20···O49	2.4210	0.0107	0.0345	-0.0012	-0.0063	-0.0075	-1.9767

Table S7 Geometrical parameters for intra- and inter- molecular hydrogen bonds in NIC-CA (cluster) model: bond-length (Å), bond-angle (°) and the sum of van der Waal radii of interacting atoms ($r_H + r_A$) in Å.

Interactions (D-H···A)	$d_{D\text{-}H}$ (Å)	$d_{H\cdots A}$ (Å)	$d_{D\cdots A}$ (Å)	D-H···A (°)	(r_H+ r_A) (Å)
C19-H20···O49	1.08535	2.44671	3.27909	132.49943	2.72
C32-H34···O44	1.09219	2.44266	3.10431	117.66392	2.72
C4-H5···O43	1.08547	2.37232	3.22551	134.31284	2.72
O50-H51···O49	0.97063	2.02627	2.64560	119.73979	2.72
O41-H42···N14	1.00282	1.76425	2.76690	178.68099	2.75
O47-H48···N29	1.01063	1.70488	2.71535	178.72785	2.75
O44-H45···O54	0.99950	1.68330	2.68111	175.80132	2.72
O52-H13···N11	1.85274	1.02717	2.87646	174.13852	2.75
O15-H67···N53	1.87814	1.02541	2.89921	173.44336	2.75
O46-H80···N55	1.86180	1.02513	2.86994	167.00076	2.75

Table S8 Second-order perturbation theory analyses of the Fock Matrix, in the NBO basis for intra- molecular interactions in NIC-CA (cluster) model.

Donor NBO(i)	ED(i)/e	Acceptor NBO(j)	ED(j)/e	$E^{(2)a}$(kcal mol^{-1})	E(j) -E(i)^b (a.u.)	F(i,j)^c(a.u.)
Nicotinamide (within unit 1)						
πC1-C8	1.63741	π*C2-N14	0.36216	29.38	0.27	0.079
πC1-C8	1.63741	π*C4-C6	0.27687	15.75	0.29	0.062
πC1-C8	1.63741	π*C10=O15	0.32843	17.31	0.30	0.065
σC2-H3	1.97939	σ*C4-N14	0.01765	5.10	1.05	0.065
πC2-N14	1.73027	π*C1-C8	0.34334	11.62	0.33	0.057
πC2-N14	1.73027	π*C4-C6	0.27687	26.22	0.33	0.084
σC4-H5	1.98003	σ*C2-N14	0.01572	5.18	1.06	0.066
πC4-C6	1.60671	π*C1-C8	0.34334	24.43	0.28	0.075
πC4-C6	1.60671	π*C2-N14	0.36216	15.88	0.26	0.058
n(1)N11	1.76421	π*C10=O15	0.32843	59.52	0.29	0.118
n(1)N14	1.87543	σ*C1-C2	0.02808	8.24	0.91	0.079
n(1)N14	1.87543	σ*C4-C6	0.02314	7.86	0.92	0.078
n(2)O15	1.86606	σ*C1-C10	0.06568	18.72	0.68	0.103
n(2)O15	1.86606	σ*C10-N11	0.05518	18.73	0.74	0.107
π*C1-C8	0.34432	π*C10=O15	0.32843	151.75	0.01	0.069
π*C2-N14	0.35970	π*C1-C8	0.34334	139.80	0.02	0.086
π*C2-N14	0.35970	π*C4-C6	0.27687	101.80	0.02	0.077
π*C10=O15	0.27126	σ*C10=O15	0.02877	5.84	0.52	0.116
Nicotinamide (within unit 2)						
πC16-C17	1.63269	π*C19-N29	0.38003	15.75	0.27	0.058
πC16-C17	1.63260	π*C21-C23	0.26785	21.58	0.29	0.073
πC16-C17	1.63260	π*C25=O30	0.27574	16.44	0.31	0.065
σC17-H18	1.97989	σ*C19-N29	0.01729	5.00	1.06	0.065
σC19-H20	1.98007	σ*C17-N29	0.01769	5.38	1.05	0.067
πC19-N29	1.72475	π*C16-C17	0.32187	26.54	0.33	0.084
πC19-N29	1.72475	π*C21-C23	0.26785	11.12	0.34	0.055
πC21-C23	1.62770	π*C16-C17	0.32187	17.41	0.28	0.063
πC21-C23	1.62770	π*C19-N 29	0.38003	31.90	0.26	0.081
n(1)N26	1.75805	π*C25=O30	0.27574	46.06	0.32	0.109

n(1)N29	1.86412	σ*C19-C21	0.02283	7.64	0.92	0.077
n(2)O30	1.86628	σ*C16-C25	0.07124	19.02	0.66	0.102
n(2)O30	1.86628	σ*C25-N26	0.06681	24.80	0.70	0.119
π*C16-C17	0.32187	π*C25=O30	0.27574	71.08	0.02	0.068
π*C19-N29	0.38003	π*C16-C17	0.32187	123.98	0.02	0.077
π*C19-N29	0.38003	π*C21-C23	0.26785	104.35	0.03	0.086
Citric acid (within unit 3)						
σC32-H34	1.95636	π*C31=O43	0.23490	5.90	0.52	0.052
n(1)O41	1.97031	σ*C31=O43	0.02689	8.85	1.17	0.091
n(2)O41	1.78914	π*C31=O43	0.23490	52.40	0.33	0.119
n(2)O43	1.85493	σ*C31-C32	0.06074	17.85	0.65	0.098
n(2)O43	1.85493	σ*C31-O41	0.08324	28.85	0.66	0.091
n(1)O44	1.96840	σ*C39=O46	0.02708	8.94	1.17	0.081
n(2)O44	1.77993	π*C39=O46	0.24758	55.37	0.33	0.121
n(2)O46	1.86323	σ*C36-C39	0.05555	17.44	0.68	0.118
n(2)O46	1.86323	σ*C39-O44	0.08095	24.94	0.60	0.130
n(1)O47	1.96467	σ*C40=O49	0.02680	10.03	1.18	0.097
n(2)O47	1.78049	π*C40=O49	0.24364	55.95	0.33	0.122
n(2)O49	1.85143	σ*C35-C40	0.08768	18.12	0.62	0.096
n(2)O49	1.85143	σ*C40-O47	0.07848	27.43	0.68	0.124
n(2)O50	1.94778	σ*C35-C36	0.03761	7.14	0.63	0.060
Nicotinamide (within unit 4)						
πC56-C63	1.64328	π*O52=C65	0.32542	17.39	0.30	0.065
πC56-C63	1.64328	π*C57-N68	0.33612	26.63	0.28	0.077
πC56-C63	1.64328	π*C59-C61	0.29627	16.46	0.29	0.063
πC57-N68	1.70382	π*C56-C63	0.34770	13.23	0.32	0.059
πC57-N68	1.70382	π*C59-C61	0.29627	27.45	0.32	0.084
πC59-C61	1.62355	π*C56-C63	0.34770	23.98	0.28	0.074
πC59-C61	1.62355	π*C57-N68	0.33612	15.84	0.27	0.059
n(2)O52	1.86983	σ*N53-C65	0.05567	18.51	0.75	0.107
n(2)O52	1.86983	σ*C56-C65	0.06455	18.64	0.69	0.103
n(1)N53	1.70150	π*O52=C65	0.32542	56.93	0.30	0.117
n(1)N68	1.91839	σ*C56-C57	0.03114	9.23	0.89	0.082
n(1)N68	1.91839	σ*C59-C61	0.02596	8.99	0.91	0.082
π*O52=C65	0.32542	σ*O52=C65	0.32542	6.98	0.51	0.126
π*C56-C63	0.34770	π*O52=C65	0.32542	110.38	0.02	0.070
π*C57-N68	0.33612	π* C59-C61	0.29627	203.43	0.01	0.079
Nicotinamide (within unit 5)						
πC69-C70	1.62911	π*O54=C78	0.34015	19.14	0.30	0.068
πC69-C70	1.62911	π*C74-C76	0.27820	22.43	0.30	0.076
σC72-N81	1.98652	π*C72-N81	0.36678	5.85	3.90	0.149
πC72-N81	1.70308	π*C69-C70	0.33576	27.47	0.32	0.084
πC72-N81	1.70308	π*C74-C76	0.27820	12.31	0.34	0.058
πC74-C76	1.63417	π*C69-C70	0.33576	17.68	0.28	0.063
n(2)O54	1.86149	σ*N55-C78	0.05193	15.27	0.78	0.100
n(2)O54	1.86149	σ*C69-C78	0.06255	18.07	0.72	0.104
n(1)N55	1.68991	π*O54=C78	0.34015	61.12	0.29	0.120
n(1)N81	1.91712	σ*C69-C70	0.03254	9.30	0.90	0.083
n(1)N81	1.91712	σ*C72-C74	0.02606	8.72	0.90	0.080
π*C69-C70	0.33576	π*O54=C78	0.34015	201.21	0.01	0.070
π*C69-C70	0.33576	π*C74-C76	0.27820	116.88	0.02	0.077
π*C74 -C76	0.27820	π*C72-N81	0.36678	11.59	3.04	0.295

Table S9 Second-order perturbation theory analysis of the Fock matrix, in the NBO basis for intra- and inter- molecular interactions in NIC-CA (monomer).

Donor NBO(i)	ED(i)/e	Acceptor NBO(j)	ED(j)/e	$E^{(2)a}$ (kcal mol^{-1})	E(j) -E(i)[b] (a.u.)	F(i,j)[c](a.u.)
Within unit 1 (NIC)						
πC1-C8	1.63741	π*C2-N14	0.35970	29.31	0.27	0.079
πC1-C8	1.63741	π*C4-C6	0.27571	15.65	0.29	0.062
πC1-C8	1.63741	π*C10=O15	0.27126	16.01	0.31	0.064
σC2-H3	1.97939	σ*C4-N14	0.01767	5.11	1.05	0.065
πC2-N14	1.73027	π*C1-C8	0.34432	11.74	0.33	0.056

πC2-N14	1.73027	π*C4-C6	0.27571	26.24	0.33	0.084
σC4-H5	1.98003	σ*C2-N14	0.01563	5.17	1.06	0.066
πC4-C6	1.60671	π*C1-C8	0.34432	24.86	0.28	0.075
πC4-C6	1.60671	π*C2-N14	0.35970	15.82	0.26	0.058
n(1)N11	1.76421	π*C10=O15	0.27126	43.99	0.32	0.107
n (1)N14	1.87543	σ*C1-C2	0.02802	8.27	0.91	0.079
n(1)N14	1.87543	σ*C4-C6	0.02308	7.86	0.92	0.078
n (2)O15	1.86606	σ*C1-C10	0.07061	19.01	0.66	0.102
n(2)O15	1.86606	σ*C10-N11	0.06812	25.01	0.69	0.119
π*C1-C8	0.34432	π*C10=O15	0.27126	71.40	0.03	0.069
π*C2-N14	0.35970	π*C1-C8	0.34432	179.77	0.02	0.087
π*C2-N14	0.35970	π*C4-C6	0.34432	101.20	0.02	0.077
From unit 1 (NIC) to unit 3 (CA)						
σC1-C2	1.97703	σ*O41-H42	0.07297	0.20	1.13	0.014
σC2-N14	1.73027	σ*O41-H42	0.07297	0.31	1.26	0.018
σC4-C6	1.98420	σ*O41-H42	0.07297	0.17	1.14	0.013
σC4-N14	1.98699	σ*O41-H42	0.07297	0.29	1.25	0.017
n(1)N14	1.87543	σ*O41-H42	0.07297	27.06	0.78	0.131
Within unit 2 (NIC)						
πC16-C17	1.63269	π*C19-N29	0.38090	15.72	0.26	0.058
πC16-C17	1.63269	π*C21-C23	0.26719	21.55	0.29	0.073
πC16-C17	1.63269	π*C25=O30	0.27608	16.52	0.31	0.065
σC17-H18	1.97991	σ*C19-N29	0.01732	5.00	1.06	0.065
σC19-H20	1.98003	σ*C17-N29	0.01772	5.38	1.05	0.067
πC19-N29	1.72538	π*C16-C17	0.32169	26.54	0.33	0.084
πC19-N29	1.72538	π*C21-C23	0.26719	11.07	0.34	0.055
πC21-C23	1.62684	π*C16-C17	0.32169	17.41	0.28	0.063
πC21-C23	1.62684	π*C19-N29	0.38090	32.09	0.26	0.081
n(1)N26	1.75837	π*C25=O30	0.27608	46.49	0.32	0.109
n(1)N29	1.86238	σ*C16-C17	0.02938	8.18	0.92	0.080
n(1) N29	1.86238	σ*C19-C21	0.02279	7.60	0.92	0.077
n(2)O30	1.86609	σ*C16-C25	0.07130	19.02	0.66	0.102
n(2)O30	1.86609	σ*C25-N26	0.06683	24.80	0.70	0.119
π*C16-C17	0.32169	π*C25=O30	0.27608	73.95	0.02	0.068
π*C19-N29	0.38090	π*C16-C17	0.32169	121.27	0.02	0.077
π*C19-N29	0.38090	π*C21-C23	0.26719	101.53	0.03	0.086
From unit 2 (NIC) to unit 3 (CA)						
σC16-C17	1.97948	σ*O47-H48	0.08864	0.22	1.12	0.014
σC17-N29	1.98697	σ*O47-H48	0.08864	0.46	1.24	0.022
σC19-C21	1.98439	σ*O47-H48	0.08864	0.21	1.11	0.014
σC19-N29	1.98699	σ*O47-H48	0.08864	0.47	1.23	0.022
n(1)N29	1.86238	σ*O47-H48	0.08864	34.12	0.76	0.146
From unit 3 (CA) to unit 1 (NIC)						
σO41-H42	1.98435	σ*C2-N14	0.01563	0.15	1.26	0.012
σO41-H42	1.98435	σ*C4-N14	0.01767	0.08	1.24	0.009
n(1)O41	1.97012	σ*C2-N14	0.01563	0.05	1.09	0.007
n(2)O41	1.78848	π*C2-N14	0.35970	0.09	0.29	0.005
n(1)O43	1.97491	σ*C4-H5	0.02272	0.66	1.12	0.024
n(2)O43	1.85457	σ*C4-H5	0.02272	0.85	0.69	0.022
n(2)O43	1.85457	σ*C4-C6	0.02308	0.13	0.80	0.010
From unit 3 (CA) to unit 2 (NIC)						
σO47-H48	1.98373	σ*C17-N29	0.01772	0.19	1.25	0.014
σO47-H48	1.98373	σ*C19-N29	0.01732	0.12	1.25	0.011
n(2)O47	1.77990	π*C19-N29	0.38090	0.09	0.29	0.005
n(1)O49	1.97552	σ*C19-H20	0.02191	0.53	1.13	0.022
n(2)O49	1.85089	σ*C19-H20	0.02191	0.75	0.70	0.021
n(2)O49	1.85089	σ*C19-C21	0.02279	0.11	0.82	0.009
Within unit 3 (CA)						
σC32-H34	1.95712	π*C31=O43	0.23516	5.90	0.52	0.052
σC36-H38	1.97452	σ*C39-O44	0.10417	4.57	0.84	0.056
n(1)O41	1.97012	σ*C31=O43	0.02665	8.85	1.17	0.091
n(2)O41	1.78848	π*C31=O43	0.23516	52.40	0.33	0.119

n(2)O43	1.85457	σ*C31-C32	0.06130	17.85	0.65	0.098
n(2) O43	1.85457	σ*C31-O41	0.08305	28.85	0.66	0.125
n(1)O44	1.97715	σ*C39=O46	0.02191	6.51	1.25	0.081
n(2)O44	1.82844	π*C39=O46	0.20139	42.74	0.35	0.111
n(2)O46	1.85035	σ*C36-C39	0.05887	17.44	0.65	0.097
n(2)O46	1.85035	σ*C39-O44	0.10417	34.18	0.60	0.130
n(1)O47	1.96470	σ*C40=O49	0.02683	10.03	1.18	0.097
n(2)O47	1.77990	π*C40=O49	0.24385	55.95	0.33	0.122
n(2)O49	1.85089	σ*C35-C40	0.08805	18.12	0.62	0.096
n(2)O49	1.85089	σ*C40-O47	0.07851	27.43	0.68	0.124
n(2)O50	1.94695	σ*C35-C36	0.03834	7.14	0.63	0.060

[a] $E^{(2)}$ means energy of hyper conjugative interaction (stabilization energy).
[b] Energy difference between donor (i) and acceptor NBO orbital.
[c] F(i,j) is the Fock matrix element between i and j NBO orbitals.

Table S10 Reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softness (s_k^+, s_k^-), local electrophilicity indices (ω_k^+, ω_k^-) for NIC-CA (monomer) using Hirshfeld atomic charges.

Atom no.	f_k^+	s_k^+	ω_k^+	Atom no.	f_k^-	s_k^-	ω_k^-
10 C	0.02543	0.004763	0.051832	1 C	0.040118	0.007514	0.081769
11 N	0.027428	0.005137	0.055904	4 C	0.05776	0.010819	0.117728
15 O	0.08926	0.016719	0.181931	8 C	0.05652	0.010587	0.1152
25 C	0.024219	0.004536	0.049364	10 C	0.036356	0.00681	0.074101
26 N	0.022942	0.004297	0.046761	15 O	0.053192	0.009963	0.108417
30 O	0.089715	0.016804	0.182859	16 C	0.039769	0.007449	0.081058
41 O	0.029222	0.005473	0.059561	19 C	0.061469	0.011514	0.125287
43 O	0.056179	0.010523	0.114505	23 C	0.050743	0.009505	0.103425
46 O	0.058987	0.011049	0.120228	25 C	0.037348	0.006996	0.076123
50 O	0.06338	0.011873	0.129197	30 O	0.050905	0.009535	0.103756

f_k^+, f_k^- (in e); s_k^+, s_k^- in eV^{-1} and ω_k^+, ω_k^- in (eV)

Table S11 Reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softness (s_k^+, s_k^-), local electrophilicity indices (ω_k^+, ω_k^-) for NIC-CA (cluster) model using Hirshfeld atomic charges.

Atom no.	f_k^+	s_k^+	ω_k^+	Atom no.	f_k^-	s_k^-	ω_k^-
O 15	0.03402	0.006372	0.06934	C 10	0.494745	0.092669	1.008399
O 30	0.05349	0.010019	0.109024	C 25	0.491229	0.092011	1.001232
O 43	0.06633	0.012424	0.135195	C 31	0.606942	0.113684	1.237081
O 46	0.052	0.00974	0.105987	C 39	0.606769	0.113652	1.236728
O 50	0.06657	0.012469	0.135684	C 40	0.598509	0.112105	1.219892
O 52	0.05977	0.011195	0.121824	H 48	0.378621	0.070918	0.771713
O 54	0.02985	0.005591	0.060841	H 51	0.349716	0.065504	0.712798
H 60	0.02132	0.003993	0.043455	C 65	0.498732	0.093416	1.016525
N 68	0.09248	0.017322	0.188494	H 67	0.339488	0.063588	0.691951
N 81	0.06849	0.012829	0.139598	C 78	0.499827	0.093621	1.018757

f_k^+, f_k^- (in e); s_k^+, s_k^- in eV^{-1} and ω_k^+, ω_k^- in (eV)