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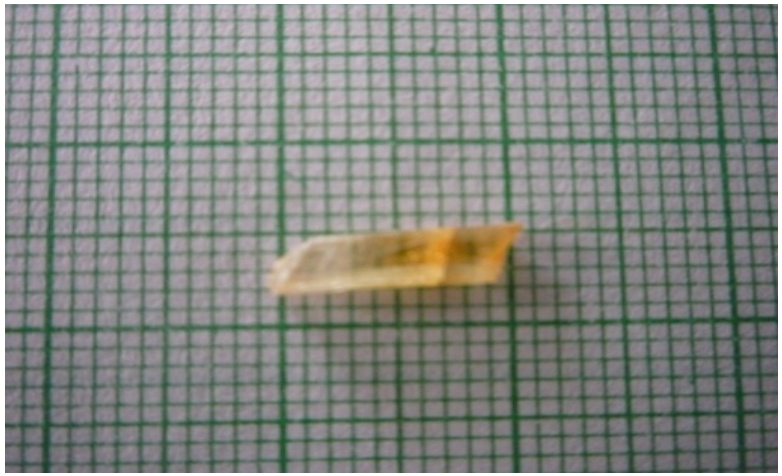

Fig. S1 The grown crystal of 3NCA

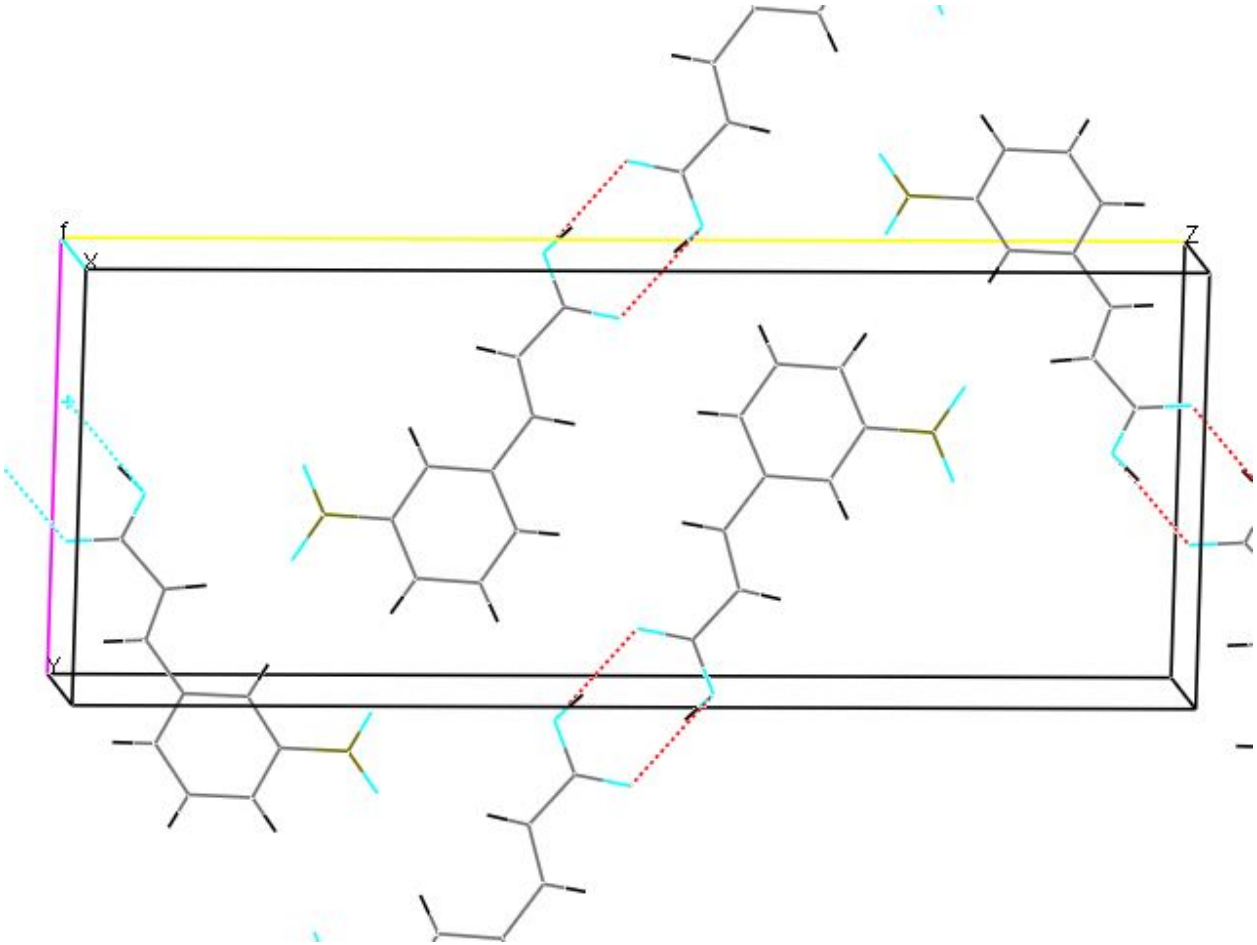

Fig. S2 Crystal packing when viewed along the a-axis

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Crystal packing in 3nitrocinnamic acid

In the crystal, the independent 3nitrocinnamic acid molecules are linked by complimentary intermolecular O-H···O hydrogen bonds. Atom O_{20} acts as a hydrogen bond donor to carbonyl atom O_{19} of another 3nitrocinnamic acidmolecule (–x+1, –y–1, –z). The D···A distance being 2.636(3) Å and the D-H···A angle of 169^{o}. This hydrogen bonding interaction leads to the formation of centrosymmetric dimers with a graph set notation of $R_2^2(8)$. The packing diagram exhibits stacking of such dimers along the crystallographic a axis.

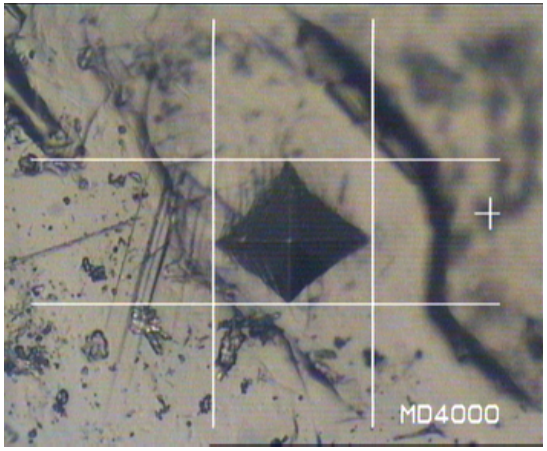

Fig.S3 Indentation mark for 10gm

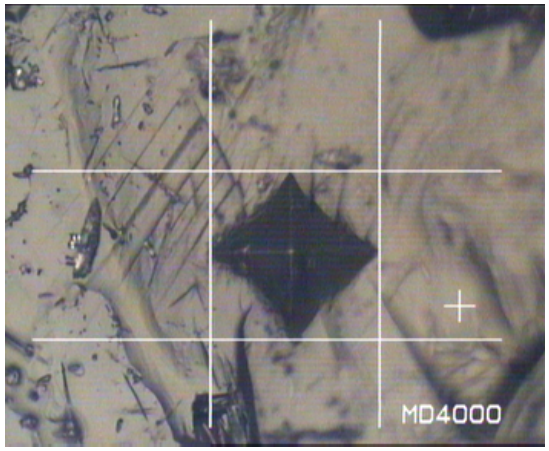

Fig.S4 Indentation mark for 30 gm

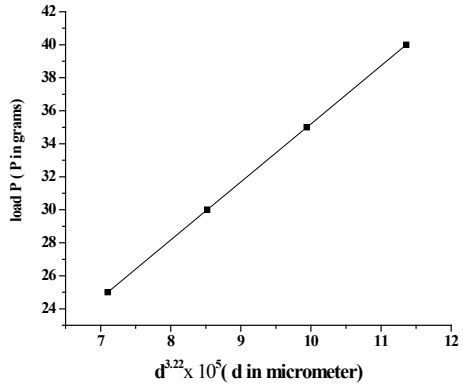

Fig. S5 load P Vs d^n

Table S1. Optimized geometrical parameters of 3NCA

Bond Length (Å)				Bond Angle(^{0})				Dihedral Angle(^{0})			
Parameter	Monomer	Dimer	Exp.	Parameter	Monomer	Dimer	Exp.	Parameter	Monomer	Dimer	Exp.
C_1-C_2	1.407	1.407	1.389	C_1-C_2-H_3	122.10	122.13	120.52	C_9-C_1-C_2-C_4	0.003	-0.004	0.98
C_2-H_3	1.088	1.088	0.930	C_1-C_2-C_4	119.36	119.35	118.80	C_1-C_2-C_4-C_5	-0.002	0.001	-0.86
C_2-C_4	1.389	1.388	1.368	C_2-C_4-C_5	122.65	122.65	123.26	C_2-C_4-C_5-H_6	179.99	179.99	179.97
C_4-C_5	1.397	1.397	1.381	C_4-C_5-H_6	119.46	119.46	121.20	C_2-C_4-C_5-C_7	0.00	0.002	-0.06
C_5-H_6	1.088	1.088	0.930	C_4-C_5-C_7	118.08	118.09	117.70	C_4-C_5-C_7-H_8	-179.99	179.99	179.22
C_5-C_7	1.394	1.394	1.378	C_5-C_7-H_8	119.79	119.78	119.83	C_4-C_5-C_7-C_9	0.001	-0.001	0.83
C_7-H_8	1.091	1.091	0.929	C_5-C_7-C_9	120.23	120.22	120.37	C_5-C_7-C_9-H_{10}	179.99	179.99	179.30
C_7-C_9	1.396	1.396	1.366	C_7-C_9-H_{10}	119.65	119.65	119.18	H_3-C_2-C_4-N_{11}	-0.003	0.003	0.09
C_9-H_{10}	1.092	1.092	0.929	C_2-C_4-N_{11}	118.58	118.57	118.87	C_4-C_2-C_1-C_{12}	-179.99	179.99	-179.56
C_4-N_{11}	1.483	1.483	1.471	C_2-C_1-C_{12}	122.75	122.73	122.06	C_2-C_1-C_{12}-H_{13}	-179.98	179.92	179.40
C_1-C_{12}	1.465	1.465	1.463	C_1-C_{12}-H_{13}	116.18	116.16	115.92	C_2-C_1-C_{12}-C_{14}	0.01	-0.09	-0.60
C_{12}-H_{13}	1.095	1.095	0.929	C_1-C_{12}-C_{14}	127.5	127.36	128.09	H_{13}-C_{12}-C_{14}-H_{15}	179.99	179.99	179.55
C_{12}-C_{14}	1.345	1.346	1.322	C_{12}-C_{14}-H_{15}	123.41	123.41	118.96	H_{13}-C_{12}-C_{14}-C_{16}	-0.00	-0.01	-0.45
C_{14}-H_{15}	1.091	1.091	0.980	C_{12}-C_{14}-C_{16}	119.68	120.53	122.17	C_2-C_4-N_{11}-O_{17}	-179.98	179.99	171.97
C_{14}-C_{16}	1.480	1.478	1.459	C_4-N_{11}-O_{17}	117.43	117.33	118.30	C_2-C_4-N_{11}-O_{18}	0.02	0.002	8.57
N_{11}-O_{17}	1.224	1.224	1.218	C_4-N_{11}-O_{18}	117.53	117.51	118.43	H_{15}-C_{14}-C_{16}-	-179.99	-179.99	177.44

								O_{19}			
N_{11}-O_{18}	1.225	1.225	1.212	C_{14}-C_{16}-O_{19}	126.03	122.75	120.68	H_{15}-C_{14}-C_{16}-O_{20}	0.006	-0.001	-2.01
C_{16}-O_{19}	1.214	1.237	1.244	C_{14}-C_{16}-O_{20}	111.20	112.93	115.69	O_{19}-C_{16}-O_{20}-H_{21}	-0.001	-0.059	-2.90
C_{16}-O_{20}	1.355	1.319	1.278	C_{16}-O_{20}-H_{21}	105.91	110.03	109.49				
O_{20}-H_{21}	0.974	1.012	0.820								

Table S2. Experimental and calculated absorption wavelengths, energies and oscillator strengths of 3NCA using the TD-DFT method at the B3LYP/cc-pvdz and BHHLYP/cc-pvdz level

Excitation	CI expansion coefficient	Wavelen-gth (nm) Calc. gas phase	Oscillator strength (*f*)	Excitation	CI expansion coefficient	Wavelen-gth (nm) Calc. ethanol B3LYP/cc-pvdz	Oscillator strength (*f*)	Excitation	CI expansion coefficient	Wavelength (nm) Calc. ethanol BHandHLYP	Oscillator strength (*f*)	Expt. (nm)
Excited state1	Singlet A			Excited state1	Singlet A			Excited state1	Singlet A			
47 → 51	0.65951			48 → 52	-0.11850			45 -> 51	-0.64248		0.0000	
47 → 52	-0.21927	324.50	0.0000	50 → 51	0.67757	335.44	0.0170	45 -> 52	-0.17808	287.36		
47 → 53	0.10476			50 → 52	0.12637			45 -> 53	-0.17649			
								45 -> 54	-0.13867			

Excited state2 48 → 51 48 → 52 50 → 51 50 → 52	Singlet A 0.11714 0.13375 0.63601 -0.24472	320.04	0.0129	Excited state2 47 → 51 47 → 52	Singlet A 0.68872 0.11237	315.46	0.0000	Excited state2 49 -> 51 49 -> 52 50 -> 51 50 -> 52	Singlet A -0.14866 0.17241 -0.63071 -0.16601	278.59	0.0212	261
Excited state3 49 → 51 49 → 52 49 → 54	Singlet A 0.32658 0.61076 0.10018	296.28	0.0000	Excited state3 49 → 51 49 → 52 49 → 54	Singlet A -0.21175 0.65877 -0.10441	284.03	0.0000	Excited state3 43 -> 51 43 -> 52 43 -> 53 43 -> 54	Singlet A 0.63899 0.17611 0.16492 0.12962	259.39	0.0000	

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Table S3: Definition of internal co-ordinates of 3NCA

No.	Symbol	Type	Definition
Stretching			
1-8	Ri	C-H (ring)	C_2-H_3,C_5-H_6,C_7-H_8,C_9-H_{10},C_{20}-H_{21},C_{23}-H_{24}, C_{25}-H_{26}, C_{27}-H_{28}.
9-12	Ri	C-H (SUB)	C_{12}-H_{13}, C_{14}-H_{15}, C_{30}-H_{31}, C_{32}-H_{33}.
13-24	r_i	C-C (ring)	C_1-C_2,C_2-C_4,C_4-C_5,C_5-C_7,C_7-C_9,C_9-C_1,C_{19}-C_{20}, C_{20}-C_{22}, C_{22}-C_{23}, C_{23}-C_{25}, C_{25}-C_{27}, C_{27}-C_{19}.
25-30	ri	C-C (SUB)	C_1-C_{12}, C_{12}-C_{14}, C_{14}-C_{16}, C_{19}-C_{30}, C_{30}-C_{32}, C_{32}-C_{34}.
31-34	qi	N-O	N_{11}-O_{17}, N_{11}-O_{18}, N_{29}-O_{35}, N_{29}-O_{36}
35-38	Qi	C-O	C_{16}-O_{40}, C_{16}-O_{41}, C_{34}-O_{37}, C_{34}-O_{38}
39-40	Ri	C-N	C_4-N_{11},C_{22}-N_{29}
41-44	qi	O-H	O_{41}-H_{42},O_{38}-H_{39},O_{40}-H_{39},O_{37}-H_{42}
Bending			
45-56	βi	C-C-H (Ring1)	C_1-C_2-H_3,C_4-C_2-H_3,C_4-C_5-H_6,C_7-C_5-H_6, C_5-C_7-H_8,C_9-C_7-H_8,C_7-C_9-H_{10},C_1-C_9-H_{10}, C_1-C_{12}-H_{13}, C_{14}-C_{12}-H_{13}, C_{12}-C_{14}-H_{15}, C_{16}-C_{14}-H_{15}.
57-68	βi	C-C-H (Ring2)	C_{19}-C_{20}-H_{21}, C_{22}-C_{20}-H_{21}, C_{22}-C_{23}-H_{24}, C_{25}-C_{23}-H_{24}, C_{23}-C_{25}-H_{26}, C_{27}-C_{25}-H_{26}, C_{25}-C_{27}-H_{28}, C_{19}-C_{27}-H_{28}, C_{19}-C_{30}-H_{31}, C_{32}-C_{30}-H_{31}, C_{30}-C_{32}-H_{33}, C_{34}-C_{32}-H_{33}.
69-70	βi	C-O-H	C_{16}-O_{41}-H_{42}, C_{34}-O_{38}-H_{39}
71-72	θi	O-H-O	O_{38}-H_{39}-O_{40}, O_{41}-H_{42}-O_{37}
73-76	αi	C-C-C (SUB)	C_9-C_1-C_{12}, C_2-C_1-C_{12}, C_{27}-C_{19}-C_{30}, C_{20}-C_{19}-C_{30}.
77-81	αi	b(C-C-C)	C_2-C_1-C_{12},C_1-C_{12}-C_{14},C_{12}-C_{14}-C_{16},C_{19}-C_{30}-C_{32}, C_{30}-C_{32}-C_{34},

82-85	θi	C-N-O	C_4-N_{11}-O_{17}, C_4-N_{11}-O_{18}, C_{22}-N_{29}-O_{35} ,C_{22}-N_{29}-O_{36}
86-89	αi	C-C-O	C_{14}-C_{16}-O_{40}, C_{14}-C_{16}-O_{41} ,C_{32}-C_{34}-O_{37}, C_{32}-C_{34}-O_{38}
90-95	δi	C-C-C (Ring1)	C_1-C_2-C_4, C_2-C_4-C_5, C_4-C_5-C_7, C_5-C_7-C_9, C_7-C_9-C_1, C_9-C_1-C_2.
96-101	δi	C-C-C (Ring2)	C_{19}-C_{20}-C_{22}, C_{20}-C_{22}-C_{23}, C_{22}-C_{23}-C_{25}, C_{23}-C_{25}-C_{27}, C_{25}-C_{27}-C_{19}, C_{27}-C_{19}-C_{20}.
102-105	βi	C-C-N	C_2-C_4-N_{11}, C_5-C_4-N_{11}, C_{20}-C_{22}-N_{29} , C_{23}-C_{22}-N_{29}.
Out of plane bending			
106-111	ω_i	C-H (Ring1)	H_3-C_2-C_4-C_1, H_6-C_5-C_7-C_4, H_8-C_7-C_9-C_5, H_{10}-C_9-C_1-C_7, H_{13}-C_{12}-C_{14}-C_1, H_{15}-C_{14}-C_{12}-C_{16}.
112-117	ω_i	C-H (Ring 2)	H_{21}-C_{20}-C_{22}-C_{19}, H_{24}-C_{23}-C_{25}-C_{22}, H_{26}-C_{25}-C_{27}-C_{23}, H_{28}-C_{27}-C_{19}-C_{25}, H_{31}-C_{30}-C_{32}-C_{19}, H_{33}-C_{32}-C_{30}-C_{34}.
118-119	ω_i	C-N	N_{11}-C_4-C_2-C_5, N_{29}-C_{22}-C_{23}-C_{20}.
120-121	ω_i	N-O	C_4-N_{11}-O_{17}-O_{18},C_{22}-N_{29}-O_{35}-O_{36}
122-123	ω_i	C-O	C_{14}-C_{16}-O_{40}-O_{41},C_{32}-C_{34}-O_{37}-O_{38}
124-125	ω_i	C-C (SUB)	C_{12}-C_1-C_2-C_9, C_{30}-C_{19}-C_{20}-C_{27}
Torsion			
126-131	τ_i	t(C-C) Ring1	C_1-C_2-C_4-C_5, C_2-C_4-C_5-C_7, C_4-C_5-C_7-C_9, C_5-C_7-C_9-C_1, C_7-C_9-C_1-C_2, C_9-C_1-C_2-C_4.
132-137	τ_i	t(C-C) Ring2	C_{19}-C_{20}-C_{22}-C_{23}, C_{20}-C_{22}-C_{23}-C_{25}, C_{22}-C_{23}-C_{25}-C_{27}, C_{23}-C_{25}-C_{27}-C_{19}, C_{25}-C_{27}-C_{19}-C_{20}, C_{27}-C_{19}-C_{20}-C_{22}.
138-141	τ_i	t(C-O)	C_{12}-C_{14}-C_{16}-O_{40}, H_{15}-C_{14}-C_{16}-O_{41}, C_{30}-C_{32}-C_{34}-O_{37}, H_{33}-C_{32}-C_{34}-O_{38}
142-145	τ_i	t(N-O)	C_5-C_4-N_{11}-O_{18}, C_2-C_4-N_{11}-O_{18}, C_{20}-C_{22}-N_{29}-O_{36}, C_{20}-C_{22}-N_{29}-O_{36}.
146-147	τ_i	t(CCOH)	C_{14}-C_{16}-O_{41}-H_{42},C_{32}-C_{34}-O_{38}-H_{39}
148-153	τ_i	t(CCCC)	C_9-C_1-C_{12}-C_{14}, C_2-C_1-C_{12}-C_{14}, C_{27}-C_{19}-C_{30}-C_{32},

			C_{20}-C_{19}-C_{30}-C_{32}, C_1-C_{12}-C_{14}-C_{16}, C_{19}-C_{30}-C_{32}-C_{34}.
153-156	τ_i	t(OHO)	C_{16}-O_{41}-H_{42}-O_{37}, C_{34}-O_{37}-H_{42}-O_{41}, C_{16}-O_{40}-H_{39}-O_{38}, C_{34}-O_{38}-H_{39}-O_{40}.

Table S4: Definition of local symmetry coordinates (much like the natural internal coordinates) and the corresponding force constant (mdyne/A°) with scale factors used

No.	Symbol	Definition	Scale factors	Force constant
		Stretching		
1-8	νC-H	R_1, R_2,R_3,R_4,R_5,R_6,R_7,R_8	0.9220	5.17
9-12	νC-H(SUB)	R_9, R_{10}, R_{11}, R_{12}.	0.9220	5.17
13-24	νC-C	r_{13},r_{14},r_{15},r_{16},r_{17},r_{18},r_{19},r_{20},r_{21},r_{22}, r_{23}, r_{24}.	0.9110	6.29
25-30	νC-C(SUB)	r_{25}, r_{26}, r_{27}, r_{28}, r_{29}, r_{30}.	0.9202	5.73
31-32	ν NO2ss	$(q_{31}+q_{32})/\sqrt{2}$, $(q_{33}+q_{34})/\sqrt{2}$	0.9532	11.42
33-34	ν NO2as	$(q_{31}-q_{32})/\sqrt{2}$, $(q_{33}-q_{34})/\sqrt{2}$	0.9532	8.79
35-36	ν CO2ss	$(Q_{35}+Q_{36})/\sqrt{2}$, $(Q_{37}+Q_{38})/\sqrt{2}$	0.9532	10.84
37-38	ν CO2as	$(Q_{35}-Q_{36})/\sqrt{2}$, $(Q_{37}-Q_{38})/\sqrt{2}$	0.9212	7.91
39-40	νCN	R_{39}, R_{40}	0.9460	3.81
41-44	νOH	q_{41},q_{42},q_{43},q_{44}	0.9220	6.02
		Bending		
45-50	bCH (Ring1)	$(\beta_{45}-\beta_{46})/\sqrt{2}$, $(\beta_{47}-\beta_{48})/\sqrt{2}$, $(\beta_{49}-\beta_{50})/\sqrt{2}$, $(\beta_{51}-\beta_{52})/\sqrt{2}$, $(\beta_{53}-\beta_{54})/\sqrt{2}$,$(\beta_{55}-\beta_{56})/\sqrt{2}$.	0.9245	0.47
51-56	bCH (Ring2)	$(\beta_{57}-\beta_{58})/\sqrt{2}$, $(\beta_{59}-\beta_{60})/\sqrt{2}$, $(\beta_{61}-\beta_{62})/\sqrt{2}$, $(\beta_{63}-\beta_{64})/\sqrt{2}$, $(\beta_{65}-\beta_{66})/\sqrt{2}$,$(\beta_{67}-\beta_{68})/\sqrt{2}$.	0.9245	0.47
57-58	bCOH	β_{69}, β_{70}	0.9561	4.84
59-60	bOHO	θ_{71}, θ_{72}	0.9561	1.67
61-62	bCC SUB	$(\alpha_{73}-\alpha_{74})/\sqrt{2}$, $(\alpha_{75}-\alpha_{76})/\sqrt{2}$.	0.9562	0.85
63-67	bCCC	α_{77}, α_{78}, α_{79}, α_{80}, α_{81}.	0.9562	1.08
68-69	bNO2ro	$(\theta_{82}-\theta_{83})/\sqrt{2}$, $(\theta_{84}-\theta_{85})/\sqrt{2}$	0.9561	1.32
70-71	bNO2tw	$(\theta_{82}+\theta_{83})/\sqrt{2}$, $(\theta_{84}+\theta_{85})/\sqrt{2}$	0.9561	4.62
72-73	bCO2ro	$(\alpha_{86}-\alpha_{87})/\sqrt{2}$, $(\alpha_{88}-\alpha_{89})/\sqrt{2}$	0.9561	1.00
74-75	bCO2tw	$(\alpha_{86}+\alpha_{87})/\sqrt{2}$, $(\alpha_{88}+\alpha_{89})/\sqrt{2}$	0.9561	7.73
76	bRtri(Ring1)	$(\delta_{90}-\delta_{91}+\delta_{92}-\delta_{93}+\delta_{94}-\delta_{95})/\sqrt{6}$	0.9630	1.21
77	bRtri(Ring2)	$(\delta_{96}-\delta_{97}+\delta_{98}-\delta_{99}+\delta_{100}-\delta_{101})/\sqrt{6}$	0.9630	1.21

78-79	bRsym	$(-\delta_{90}-\delta_{91}+2\delta_{92}-\delta_{93}-\delta_{94}+2\delta_{95})/\sqrt{6}$, $(-\delta_{96}-\delta_{97}+2\delta_{98}-\delta_{99}+\delta_{100}+2\delta_{101})/\sqrt{6}$	0.9630	1.24
80	bRasy(Ring1)	$(\delta_{90}-\delta_{91}+\delta_{93}-\delta_{94})/2$	0.9630	1.22
81	bRasy(Ring2)	$(\delta_{96}-\delta_{97}+\delta_{99}-\delta_{100})/2$	0.9630	1.22
82-83	bCN	$(\beta_{102}-\beta_{103})/\sqrt{2}$, $(\beta_{104}-\beta_{105})/\sqrt{2}$	0.9561	1.19
		Out-of-Plane bending (wagging)		
84-89	gCH(Ring 1)	$\omega_{106}, \omega_{107}, \omega_{108}, \omega_{109}, \omega_{110}, \omega_{111}.$	0.9532	0.46
90-95	gCH(Ring 2)	$\omega_{112}, \omega_{113}, \omega_{114}, \omega_{115}, \omega_{116}, \omega_{117}.$	0.9532	0.46
96-97	gCN	$\omega_{118}, \omega_{119}.$	0.9715	0.55
98-99	gNO2	$\omega_{120}, \omega_{121}.$	0.9715	0.52
100-101	gCO2	$\omega_{122}, \omega_{123}.$	0.9715	0.76
102-103	gccsub	$\omega_{124}, \omega_{125}.$	0.9715	0.54
Torsion				
104	tRtri(Ring1)	$(\tau_{126}-\tau_{127}+\tau_{128}-\tau_{129}+\tau_{130}-\tau_{131})/\sqrt{6}$	0.9707	3.66
105	tRtri(Ring2)	$(\tau_{132}-\tau_{133}+\tau_{134}-\tau_{135}+\tau_{136}-\tau_{137})/\sqrt{6}$	0.9707	3.66
106	tRsym(Ring1)	$(\tau_{126}-\tau_{128}+\tau_{129}-\tau_{131})/2$	0.9707	5.71
107	tRsym(Ring2)	$(\tau_{132}-\tau_{134}+\tau_{135}-\tau_{137})/2$	0.9707	5.71
108-109	tRasy	$(-\tau_{132}+2\tau_{133}-\tau_{134}-\tau_{135}+2\tau_{136}-\tau_{137})/\sqrt{6}$, $(-\tau_{132}+2\tau_{133}-\tau_{134}-\tau_{135}+2\tau_{136}-\tau_{137})/\sqrt{6}$	0.9707	12.90
110-111	tCO2	$(\tau_{138}+\tau_{139})/2$, $(\tau_{140}+\tau_{141})/2$	1.000	0.11
112-113	tNO2	$(\tau_{142}+\tau_{143})/2$, $(\tau_{144}+\tau_{145})/2$	1.000	0.07
114-115	tCCOH	$\tau_{146}, \tau_{147}.$	1.000	0.335
116-119	tCCCC	$(\tau_{148}+\tau_{149})/2$, $(\tau_{150}+\tau_{151})/2$, τ_{152}, τ_{153}	1.000	0.28
120-121	tOHO	$(\tau_{153}+\tau_{154})/2$, $(\tau_{155}+\tau_{156})/2$	1.000	0.85

Table S5: Detailed vibrational assignment of 3NCA dimer by normal mode analysis based on SQM force field calculations

Experimental wavenumbers (cm^{-1})		Scaled wavenumbers (cm^{-1})	[a]IR intensity	[b]Raman intensity	[c]Characterization of normal modes with PED (%)
IR	Raman				
		3103	0.0020	2.42	2 VCH (99)
		3066	0.0032	3.19	13VCH (99)
		3049	0.0025	1.43	VCH (99)
		3049	0.0025	1.43	VCH (99)
		3033	0.0022	0.844	VCH (99)
		1618	0.0689	78.2	vNO2as (59), VCC (14), bNO2ro (10)
		1615	0.0899	100	bCOH (41), VCCSUB (17), bOHO (16), vCO2as (10)
		1611	0.1170	61.2	VCCSUB (58), bCH (12), bCOH (11)
		1454	0.00299	22.3	bCOH (43), bOHO (39), vCO2as (11)
		1440	0.0208	3.72	bCOH (29), bOHO (19), bCH (19), VCC
		1435	0.0142	3.27	bCH (35), VCC (30), bCOH (12), bOHO
1308 s	1305	1313	0.0489	3.14	bCOH (28), bOHO (28), vCO2ss (12)
		1294	0.0182	1.90	14 VCC (58), bCH (10)
		1268	0.00418	0.706	3 bCH (61), VCCSUB (18)
		1226	0.00568	2.07	9b bCH (67)
		1192	0.0255	58.9	bCH (27), VCCSUB (21), vCO2ss (10),
		1154	0.00092	5.46	bCH (66), VCC (14)
		1153	0.00090	5.51	bCH (66), VCC (14)
1109 m	1110	1123	0.00081	0.811	18a bCH (80), VCC (18)

		1123	0.00081	0.811	18a bCH (80), VCC (18)
1076		1055	0.00778	2.53	VCC (41), bCH (36), VCN (13)
		1055	0.00778	2.53	VCC (41), bCH (37), VCN (13)
		1041	0.0107	0.842	bCH (46), VCC (38), VCN (10)
		1041	0.0107	0.842	bCH (46), VCC (38), VCN (10)
		1019	0.0148	0.759	gcH (89)
		1019	0.0148	0.759	gcH (52), tRtri (30), tRasy (13)
		1014	0.0234	0.578	tCCOH (66), bOHO (30)
1001 w	1001 s	1000	0.00328	0.613	gcH (85), tRtri (11)
		1000	0.00328	0.613	tRtri (47), tRsym (30), gcH (22)
973 w		968	0.00091	13.4	bRtri (64), VCC (32)
		968	0.00091	13.4	bRtri (64), VCC (32)
		950	0.00414	5.10	VCCSUB (35), vCO2ss (16), bCCC (15), bOHO (15)
935 m		948	0.00370	5.54	VCCSUB (42), bCCC (17), vCO2ss (13)
		932	0.000729	1.50	tRasy (59), tRtri (23), tRsym (10)
		910	0.00187	2.25	VCC (22), VCN (20), VCCSUB (16),
	909	910	0.00187	2.25	VCC (22), VCN (20), VCCSUB (15),
		891	0.00304	2.55	gcH (83), gCO2 (12)
		816	0.0115	1.02	tRasy (53), tRtri (33), gcH (10)
		812	0.0137	1.03	bNO2tw(55), VCC(10), bRtri(10)
		742	0.00268	0.427	tRtri (31), tRasy (20), gNO2 (18), gCO2 (12)
		714	0.004780	0.289	tRasy (36), tRtri (32), gCO2 (11)
		682	0.000779	1.23	bCO2tw (38), bOHO (12), bRasy (12)
		669	0.00189	0.478	tRtri (54), tRasy (45)
		655	0.00313	1.54	bRasy (42), bCO2tw (19)
596 m		649	0.00149	3.30	bCO2tw (33), bRasy (29), bOHO (11)
		573	0.00226	0.405	bRsym (39), bCO2tw (20), bOHO (16
568 m		572	0.00219	0.428	bRsym (39), bCO2tw (23)
		544	0.00825	0.210	bCO2ro (22), bNO2ro (14), vOH (12), bOHO (12), bCCsub (10)

		522	0.00174	0.633	tRsym (25), tRtri (22), tRasy (17), gccsub
		521	0.00179	0.597	tRsym (34), tRtri (28), tRasy (11), gccsub (11)
		500	0.0108	0.397	bNO2ro (37), bCO2ro (13), vOH (11), bCN (10)
487 m		489	0.00199	1.65	bNO2ro (29), bCO2ro (26), bCCC (17)
425 w	403 vw	428	0.000240	0.180	tRsym (58), gCN (21)
		424	0.000253	0.185	tRasy (53), tRsym (46)
405 w		385	0.00566	0.766	VCN (19), bRasy (19), vOH (16), bOHO (10)
		379	0.00263	1.78	VCN (38), bRasy (27)
		361	0.00521	0.509	vOH (21), bCCsub (17), bOHO (15)
	333 vw	345	0.000570	2.96	vOH (25), bCCsub (15), bCO2ro (14), VCCSUB (12)
		291	0.000154	7.91	vOH 52), bCCC (11)
	288 w	287	0.000191	6.25	tRasy (44), tRsym (40
	275 w	285	0.000204	4.74	tRasy (45), tRsym (43)
		255	0.00126	0.449	VCCSUB (22), bCCC (21), bCN (17), bRsym (13)
		240	0.00424	0.509	vOH (41), bCN (18), bCCC (15), bOHO (12)
	225 w	224	0.000427	1.63	bCOH (34), bOHO (29), bCN (16), bCCC (11)
	187 m	186	0.000101	3.00	tRasy (36), tOHO (14), tCCCC (13), tRsym (10)
		175	0.000229	4.47	tRasy (58), tRsym (21)
		167	0.000121	13.7	tRasy (53), tRsym (23)
		161	0.00011	8.66	tCO2 (28), tOHO (19), tCCCC (12), tRasy (11)
		153	0.00007	11.8	bCOH (37), vOH (35), bOHO (17)
		110	0.000574	3.46	tRasy (25), tOHO (12), tRtri (11), tCCOH (11)

		104	0.00147	2.57	vOH (33), bCCsub (22), bOHO (11)
		93	0.000347	2.83	tCCCC(29), gcH (14), tRasy (13), tOHO (12), gccsub (10)
		74	0.000152	9.83	vOH (59), bOHO (11)
		68	0.000244	10.4	tOHO (89)
		60	0.000101	18.8	tRsym (31), tRasy (25), tNO2 (18)
		49	0.000085	44.4	tRasy (35), tRsym (31), tNO2(13), tOHO (13)
		44	0.000064	10.2	bCCC (38), bCOH (21), bCCsub (14), bOHO (10)
		38	0.000052	25.1	tRasy (27), tCCCC (20), tRsym (19)
		34	0.000052	18.4	tCCCC (49), tRsym (10), tCCOH (10
		18	0.00015	17.5	bCCC (40), vOH (30), bCO2ro (13)
		9	0.00042	8.67	tOHO (57), tCCCC (17)
		8	0.00042	8.11	tOHO (31), tCCOH (26), tCCCC (19)

[a]Calculated IR intensities.

[b]Relative Raman intensities calculated by Eq. (1) and normalized to 100.

[c]Only PED contributions>10% are listed.

Abbreviations: vs – very strong, s – strong, m – medium, w – weak, vw – very weak, br- broad, sh- shoulder, ν – stretching, ss – symmetric stretching, as- asymmetric stretching, R- phenyl ring, b-bending, asy- asymmetric deformation, tri- trigonal deformation, b-inplane bending, t- torsion, g- out of plane bending, W- wagging, bRtri- trigonal ring in-plane bending bRasy- asymmetric ring in-plane bending, bRsy- symmetric ring in-plane bending, tRtri- trigonal ring torsion, tRasy- asymmetric ring torsion, tRsym- symmetric ring torsion.