Table S3: Definition of local symmetry coordinates and the corresponding force constants (mdyne/Å) with scale factors used.

No: of coordinates	Symbol	Definition	Scale factors	Force constants (mdyne/Å)
		Stretching		
1	Imz[νCC]	R_1	0.90	5.15
2-4	νCC	R_2, R_3, R_4	0.90	3.71
5-7	Imz[νCH]	r_5, r_6, r_7	0.90	4.77
8	νCH_{ss}	$(r_8+ r_9) /\sqrt{2}$	0.90	5.30
9	νCH_{as}	$(r_8- r_9) /\sqrt{2}$	0.90	4.94
10-11	Imz[νC=N]	Q_{10}, Q_{11}	0.90	5.28
12-13	Imz[νCN]	Q_{12}, Q_{13}	0.90	5.04
14	νCN	Q_{14}	0.90	5.09
15	νCO_{ss}	$(\Gamma_{15}+ \Gamma_{16}) /\sqrt{2}$	0.94	12.92
16	νCO_{as}	$(\Gamma_{15}- \Gamma_{16}) /\sqrt{2}$	0.94	10.07
17	νBF	f_{17}	0.90	3.47
18	νBF_{ss}	$(f_{18}+ f_{19}+ f_{20}) /\sqrt{3}$	0.90	6.02
19	νBF_{ip}	$(f_{18}- f_{19}- f_{20}) /\sqrt{3}$	0.90	4.37
20	νBF_{op}	$(f_{19}- f_{20}) /\sqrt{2}$	0.90	3.24
21	νOH	Ω_{21}	0.90	1.45
22-23	νFH	H_{22}, H_{23}	0.96	0.24
24-25	Imz[νNH]	λ_{24}, λ_{25}	0.96	5.88
26	νNH_{ss}	$(\lambda_{26}+\lambda_{27}) /\sqrt{2}$	0.96	6.95
27	νNH_{as}	$(\lambda_{26}-\lambda_{27}) /\sqrt{2}$	0.94	5.67
		Bending		
28	Imz[δCC]	$(\alpha_{28}+\delta_{46})/\sqrt{2}$	0.94	0.84
29	δCH_{sci}	$(2\beta_{31}+\alpha_{29})/\sqrt{3}$	0.98	0.93
30	δCXY_{sci}	$(\beta_{31}+2\alpha_{29})/\sqrt{3}$	0.98	1.43
31	δCH_{roc}	$(\beta_{32}+\beta_{33}-\beta_{34}-\beta_{35})/\sqrt{4}$	0.98	1.34
32	δCH_{wag}	$(\beta_{32}-\beta_{33}+\beta_{34}-\beta_{35})/\sqrt{4}$	0.98	1.19
33	δCH_{twi}	$(\beta_{35}-\beta_{32}-\beta_{33}-\beta_{34})/\sqrt{4}$	0.98	2.25
34-35	Imz[δCH]	$(\gamma_{39}+ \gamma_{40}) /\sqrt{2}$, $(\gamma_{41}+ \beta_{38}) /\sqrt{2}$	0.98	0.47
36	δCH_{sy}	$(2\beta_{36}-\beta_{37}-\beta_{38}) /\sqrt{6}$	0.98	1.84
37	δCH_{asy}	$(\beta_{36}-\beta_{37}) /\sqrt{2}$	0.98	0.99
38	δCCN_{xcyd}	$(4\alpha_{30}+\delta_{41}+\delta_{42})/ \sqrt{18}$	0.98	1.91
39	δCCN_{xczd}	$(\alpha_{30}+4\delta_{43}+\delta_{44})/ \sqrt{18}$	0.98	12.85
40	δCCN_{yczd}	$(\alpha_{30}+\delta_{43}+4\delta_{44})/ \sqrt{18}$	0.95	1.06
41	δNH_{sci}	$(2\mu_{51}- \gamma_{52}- \gamma_{53}) /\sqrt{6}$	0.95	0.69
42	δNH_{roc}	$(\gamma_{52}- \gamma_{53}) /\sqrt{2}$	0.95	0.64
43-44	Imz[δCN]	$(\gamma_{54}- \gamma_{55}) /\sqrt{2}$, $(\gamma_{56}- \gamma_{57}) /\sqrt{2}$	1.00	0.59
45	δCOH	Ψ_{58}	0.99	11.84
46	δCO_{syd}	$(2X_{59}- X_{60}-X_{61}) /\sqrt{6}$	0.95	4.92
47	δCO_{roc}	$(X_{60}-X_{61}) /\sqrt{2}$	0.95	12.57
48	δFBF_{syd}	$(\epsilon_{62}+ \epsilon_{63}+ \epsilon_{64} -\epsilon_{65}-\epsilon_{66}-\epsilon_{67}) /\sqrt{6}$	0.94	1.25

49	δFBF_{asyd}	$(2\epsilon_{62}-\epsilon_{63}-\epsilon_{64})/\sqrt{6}$	0.94	0.94
50	δFBF_{asydo}	$(\epsilon_{63}-\epsilon_{64})/\sqrt{2}$	0.94	0.97
51	δFBF_{rock}	$(2\epsilon_{65}-\epsilon_{66}-\epsilon_{67})/\sqrt{6}$	0.94	0.91
52	δFBF_{roco}	$(\epsilon_{66}-\epsilon_{67})/\sqrt{2}$	0.94	1.10
53	$Imz[\delta CN_{syd}]$	$(\delta_{48}+\cos 144^0(\delta_{50}+\delta_{45})$ $+\cos 72^0(\delta_{49}+\delta_{47}))$	1.00	0.59
54	$Imz[\delta CN_{sydo}]$	$(\cos 144^0-\cos 72^0)(\delta_{50}+\delta_{45})$ $+(1-\cos 144^0)(\delta_{49}+\delta_{47})$	1.00	0.73
55-56	δHFB	Σ_{68}, Σ_{69}	0.99	0.72
57-58	δNHF	Π_{70}, Π_{71}	0.99	0.56
		Out-of-Plane bending (wagging)		
59-60	Imz[gCH]	ω_{72}, ω_{73}	1.00	0.08
61-62	Imz[gCN]	ω_{74}, ω_{75}	1.00	0.05
63	Imz[gCC]	ω_{76}	1.00	0.19
64	NH_{wag}	ω_{77}	0.95	0.05
65	CO_{wag}	ω_{78}	0.98	0.52
		Torsion		
66	Imz[τCN]	$(\cos 72^0(\tau_{79}-\tau_{82})+$ $\cos 144^0(\tau_{80}-\tau_{81})+\tau_{83})$	1.00	0.28
67	$Imz[\tau_oCN]$	$(\cos 144^0-\cos 72^0)(\tau_{81}-\tau_{80})+$ $(1-\cos 144^0)(\tau_{82}-\tau_{79})$	1.00	0.39
68	τ_{C7C8}	$(\tau_{84}+\tau_{85}+\tau_{86}+\tau_{87}+$ $\tau_{88}+\tau_{89})/\sqrt{6}$	0.98	0.05
69	τ_{ImzE}	$(\tau_{91}+\tau_{92}+\tau_{96}+\tau_{98}+$ $\tau_{89}+\tau_{102})/\sqrt{6}$	0.98	0.04
70	τ_{C4C7}	$(\tau_{97}+\tau_{103}+\tau_{93}+\tau_{94}+\tau_{100}+$ $\tau_{104}+\tau_{95}+\tau_{101}+\tau_{105})/\sqrt{9}$	0.98	0.02
71	τ_{NF}	$(\tau_{118}+\tau_{119})/\sqrt{2}$	0.98	0.05
72	τ_{NH2}	$(\tau_{106}+\tau_{108}+\tau_{109}+\tau_{110}+$ $\tau_{110}+\tau_{111})/\sqrt{6}$	0.98	0.09
73	τ_{BF4}	$(\tau_{112}+\tau_{113}+\tau_{114})/\sqrt{3}$	0.98	0.13
74	τ_{COOH}	$(\tau_{90}+\tau_{115})/\sqrt{2}$	0.98	1.59
75	$\tau_{FHinter}$	$(\tau_{116}+\tau_{117})/\sqrt{2}$	0.98	0.24
76-77	τ_{CNFB}	τ_{118}, τ_{119}	0.98	0.18
78-79	τ_{NHFB}	τ_{120}, τ_{121}	0.98	0.31