Table S2: Definition of internal valence coordinates of LHTFB.

No	Symbol	Type	Definition
		Stretching	
1	R_i	C-C (ring)	C_3-C_2.
2-4	R_i	C-C	C_3-C_4, C_4-C_7, C_7-C_8.
5-6	r_i	C-H (ring)	C_1-H_{19}, C_2-H_{18}.
7-9	r_i	C-H	C_7-H_{21}, C_4-H_5,C_4-H_6.
10-13	Q_i	C-N (ring)	N_{10}=C_1, N_9=C_1, N_{10}-C_3, N_9-C_2.
14	Q_i	C-N	C_7-N_{11}.
15-16	Γ_i	C-O	C_8-O_{13}, C_8-O_{12} .
17	f_i	B-F	F_{25}-B_{26}.
18-20	f_i	B-F	B_{26}-F_{22}, B_{26}-F_{23}, B_{26}-F_{24}.
21	Ω_i	O-H (carboxyl)	O_{12}-H_{15}.
22-23	H_i	F-H(inter bond)	F_{25}-H_{16}, F_{22}-H_{17}.
24-25	λ_i	N-H(ring)	N_9-H_{20}, N_{10}-H_{16}.
26-27	λ_i	N-H	N_{11}-H_{14}, N_{11}-H_{17}.
		Bending	
28	α_i	C-C-C (ring)	C_2-C_3-C_4.
29-30	α_i	C-C-C	C_7-C_4-C_3, C_8-C_7-C_4.
31	β_i	H-C-H	H_6-C_4-H_5.
32-35	β_i	H-C-C	H_6-C_4-C_3, H_6-C_4-C_7, H_5-C_4-C_3, H_5-C_4-C_7.
36-38	β_i	C-C-H	C_8-C_7-H_{21}, C_4-C_7-H_{21}, C_3-C_2-H_{18}.
39-42	γ_i	N-C-H	N_{10}-C_1-H_{19},N_9-C_1-H_{19}, N_9-C_2-H_{18}, N_{11}-C_7-H_{21}.
43-45	δ_i	C-C-N	C_8-C_7-N_{11}, C_4-C_7-N_{11}, C_2-C_3-N_{10}.
46-47	δ_i	N-C-C (ring)	N_{10}-C_3-C_4, N_9-C_2-C_3.
48-49	δ_i	C-N-C (ring)	C_3-N_{10}-C_1, C_1-N_9-C_2.
50	δ_i	N-C-N (ring)	N_{10}-C_1-N_9.
51	μ_i	H-N-H	H_{17}-N_{11}-H_{14}.
52-53	γ_i	C-N-H	C_7-N_{11}-H_{17}, C_7-N_{11}-H_{14}.
54-57	γ_i	C-N-H (ring)	C_1-N_9-H_{20}, C_2-N_9-H_{20}, C_3-$_{10}$-H_{16}, C_1-N_{10}-H_{16}.
58	Ψ_i	C-O-H (carboxyl)	C_8-O_{12}-H_{15}.
59	χ_i	O-C-O (carboxyl)	O_{12} -C_8-O_{13}.
60-61	χ_i	C-C-O (carboxyl)	C_7-C_8-O_{13}, C_7-C_8-O_{12}.
62-67	ϵ_i	F-B-F	F_{23}-B_{26}-F_{24}, F_{22}-B_{26}-F_{23}, F_{22}-B_{26}-F_{24}, F_{25}-B_{26}-F_{22}, F_{25}-B_{26}-F_{24}, F_{25}-B_{26}-F_{23}.
68-69	Σ_i	HFB	H_{16}-F_{25}-B_{26}, H_{17}-F_{22}-B_{26}.
70-71	Π_i	NHF	N_{10}-H_{16}-F_{25}, N_{11}-H_{17}-F_{22}.
		Out-of-Plane bending (wagging)	
72	ω_i	H-C-N-N (ring)	H_{19}-C_1-N_{10}-N_9.
73	ω_i	H-C-N-C (ring)	H_{18}-C_2-N_9-C_3.
74-75	ω_i	H-N-C-C (ring)	H_{20}-N_9-C_1-C_2, H_{16}-N_{10}-C_3-C_1.
76	ω_i	C-C-C-N (ring)	C_4-C_3-C_2-N_{10}.
77	ω_i	C-N-H-H	C_7-N_{11}-H_{14}-H_{17}.
78	ω_i	C-C-O-O (carboxyl)	C_7-C_8-O_{12}-O_{13}.
		Torsion	
79-81	τ_i	tC-N-C-N (Ring puck)	C_3-N_{10}-C_1-N_9, N_{10}-C_1-N_9-C_2, N_9-C_2-C_3-N_{10}.
82-83	τ_i	tC-C-N-C (Ring puck)	C_2-C_3-N_{10}-C_1, C_1-N_9-C_2-C_3.
84-85	τ_i	tC-C-C-O	C_4-C_7-C_8-O_{12}, C_4-C_7-C_8-O_{13}.
86-87	τ_i	tN-C-C-O	N_{11}-C_7-C_8-O_{12}, N_{11}-C_7-C_8-O_{13}.
88-90	τ_i	tH-C-C-O	H_{21}-C_7-C_8-O_{12}, H_{21}-C_7-C_8-O_{13}, C_7-C_8-O_{12}-H_{15}.

91-95	τ_i	tC-C-C-H	C_2-C_3-C_4-H_5, C_2-C_3-C_4-H_6, C_3-C_4-C_7-H_{21}, H_5-C_4-C_7-C_8, H_6-C_4-C_7-C_8.
96-97	τ_i	tC-C-C-C	C_2-C_3-C_4-C_7, C_3-C_4-C_7-C_8.
98-101	τ_i	tN-C-C-H	N_{10}-C_3-C_4-H_5, N_{10}-C_3-C_4-H_6, H_5-C_4-C_7-N_{11}, H_6-C_4-C_7-N_{11}.
102-103	τ_i	tN-C-C-C	N_{10}-C_3-C_4-C_7, C_3-C_4-C_7-N_{11}.
104-105	τ_i	tH-C-C-H	H_5-C_4-C_7-H_{21}, H_6-C_4-C_7-H_{21}.
106-109	τ_i	tC-C-N-H	C_4-C_7-N_{11}-H_{14}, C_4-C_7-N_{11}-H_{17}, C_8-C_7-N_{11}-H_{17}, C_8-C_7-N_{11}-H_{14}.
110-111	τ_i	tH-C-N-H	H_{21}-C_7-N_{11}-H_{14}, H_{21}-C_7-N_{11}-H_{17}.
112-114	τ_i	tH-F-B-F	H_{16}-F_{25}-B_{26}-F_{22}, H_{16}-F_{25}-B_{26}-F_{23}, H_{16}-F_{25}-B_{26}-F_{24}.
115	τ_i	tO-C-O-H	O_{13}-C_8-O_{12}-H_{15}.
116-117	τ_i	tF-H-N-C	F_{25}-H_{16}-N_{10}-C_3, F_{25}-H_{16}-N_{10}-C_1.
118-119	τ_i	tC-N-F-B	C_3-N_{10}-F_{25}-B_{26}, C_1-N_{10}-F_{25}-B_{26}.
120-121	τ_i	tN-H-F-B	N_{10}-H_{16}-F_{25}-B_{26}, N_{11}-H_{17}-F_{22}-B_{26}.