Table S2 – Definition of internal coordinates used in the normal coordinate analysis of MCPIC.

Nº	Definition [a]	Approximate description
S_1	$\nu(C_3–C_6)$	$\nu(C–C_\alpha)$
S_2	$\nu(C_6=O_7)$	$\nu(C=O)$
S_3	$\nu(C_6–O_8)$	$\nu(C–O)$
S_4	$\nu(O_8–C_9)$	$\nu(O–CH_3)$
S_5	$\nu(C_2–Cl_{13})$	$\nu(C–Cl)$
S_6	$\nu(C_1–C_{14})$	$\nu(C–C_{IR})$
S_7	$\nu(C_9–H_{12})+\nu(C_9–H_{10})+\nu(C_9–H_{11})$	νCH_3 s
S_8	$2\nu(C_9–H_{12})–\nu(C_9–H_{10})–\nu(C_9–H_{11})$	νCH_3 as´
S_9	$\nu(C_9–H_{10})–\nu(C_9–H_{11})$	νCH_3 as´´
S_{10}	$\delta(H_{10}–C_9–H_{11})+\delta(H_{12}–C_9–H_{10})+\delta(H_{12}–C_9–H_{11})–\delta(H_{12}–C_9–O_8)–\delta(H_{10}–C_9–O_8)–\delta(H_{11}–C_9–O_8)$	δCH_3 s
S_{11}	$2\delta(H_{10}–C_9–H_{11})–\delta(H_{12}–C_9–H_{10})–\delta(H_{12}–C_9–H_{11})$	δCH_3 as´
S_{12}	$\delta(H_{12}–C_9–H_{10})–\delta(H_{12}–C_9–H_{11})$	δCH_3 as´´
S_{13}	$2\delta(H_{12}–C_9–O_8)–\delta(H_{10}–C_9–O_8)–\delta(H_{11}–C_9–O_8)$	γCH_3´
S_{14}	$\delta(H_{10}–C_9–O_8)–\delta(H_{11}–C_9–O_8)$	γCH_3´´
S_{15}	$\tau(H_{12}–C_9–O_8–C_6)+\tau(H_{10}–C_9–O_8–C_6)+\tau(H_{11}–C_9–O_8–C_6)$	τCH_3
S_{16}	$\tau(N_4=C_3–C_6=O_7)+\tau(C_2–C_3–C_6=O_7)+\tau(N_4=C_3–C_6–O_8)+\tau(C_2–C_3–C_6–O_8)$	$\tau(C–C_\alpha)$
S_{17}	$\tau(O_7=C_6–O_8–C_9)+\tau(C_3–C_6–O_8–C_9)$	$\tau(C–O)$
S_{18}	$\tau(C_2=C_1–C_{14}–C_{19})+\tau(O_5–C_1–C_{14}–C_{19})+\tau(C_2=C_1–C_{14}–C_{15})+\tau(O_5–C_1–C_{14}–C_{15})$	$\tau(C–C_{IR})$
S_{19}	$2\delta(O_8–C_6=O_7)–\delta(O_8–C_6–C_3)–\delta(O_7=C_6–C_3)$	δ(OCO)
S_{20}	$\delta(O_8–C_6–C_3)–\delta(O_7=C_6–C_3)$	δ(CC=O)
S_{21}	$\gamma(O_7=O_8–O_6–C_3)$	γ(C=O)
S_{22}	$\nu(C_1=C_2)+\nu(C_2–C_3)+\nu(C_3=N_4)+\nu(N_4–O_5)+\nu(O_5–C_1)$	νIsox1
S_{23}	$3\nu(C_1=C_2)+3\nu(C_3=N_4)–2\nu(C_2–C_3)–2\nu(N_4–O_5)–2\nu(O_5–C_1)$	νIsox2
S_{24}	$\nu(C_1=C_2)–\nu(C_3=N_4)$	νIsox3
S_{25}	$2\nu(C_2–C_3)–\nu(N_4–O_5)–\nu(O_5–C_1)$	νIsox4
S_{26}	$\nu(N_4–O_5)–\nu(O_5–C_1)$	νIsox5
S_{27}	$\delta(N_4–O_5–C_1)–0.809\delta(C_3=N_4–O_5)–0.809\delta(O_5–C_1=C_2)+0.309\delta(C_2–C_3=N_4)+0.309\delta(C_1=C_2–C_3)$	δIsox1
S_{28}	$–1.118\delta(C_3=N_4–O_5)+1.118\delta(O_5–C_1=C_2)+1.809\delta(C_2–C_3=N_4)–1.809\delta(C_1=C_2–C_3)$	δIsox2
S_{29}	$\tau(C_3–C_2=C_1–O_5)–0.809\tau(N_4=C_3–C_2=C_1)–0.809\tau(C_2=C_1–O_5–N_4)+0.309\tau(O_5–N_4=C_3–C_2)+$ $+0.309\tau(C_1–O_5–N_4=C_3)$	τIsox1
S_{30}	$1.118\tau(C_2=C_1–O_5–N_4)–1.118\tau(N_4=C_3–C_2=C_1)–1.809\tau(C_1–O_5–N_4=C_3)+1.809\tau(O_5–N_4=C_3–C_2)$	τIsox2
S_{31}	$\nu(C_{14}–C_{15})+\nu(C_{15}–C_{16})+\nu(C_{16}–C_{17})+\nu(C_{17}–C_{18})+\nu(C_{18}–C_{19})+\nu(C_{19}–C_{14})$	νPh1
S_{32}	$\nu(C_{14}–C_{15})+\nu(C_{16}–C_{17})–\nu(C_{17}–C_{18})–\nu(C_{19}–C_{14})$	νPh2
S_{33}	$–\nu(C_{14}–C_{15})+2\nu(C_{15}–C_{16})–\nu(C_{16}–C_{17})–\nu(C_{17}–C_{18})+2\nu(C_{18}–C_{19})–\nu(C_{19}–C_{14})$	νPh3
S_{34}	$\nu(C_{14}–C_{15})–\nu(C_{16}–C_{17})+\nu(C_{17}–C_{18})–\nu(C_{19}–C_{14})$	νPh4
S_{35}	$\nu(C_{14}–C_{15})–\nu(C_{16}–C_{17})–\nu(C_{17}–C_{18})+\nu(C_{19}–C_{14})$	νPh5
S_{36}	$\nu(C_{15}–C_{16})–\nu(C_{18}–C_{19})$	νPh6
S_{37}	$\nu(C_{15}–H_{20})$	ν(C–H1)
S_{38}	$\nu(C_{16}–H_{21})+\nu(C_{17}–H_{22})+\nu(C_{18}–H_{23})$	ν(C–H2)
S_{39}	$\nu(C_{16}–H_{21})–\nu(C_{18}–H_{23})$	ν(C–H3)
S_{40}	$2\nu(C_{17}–H_{22})–\nu(C_{16}–H_{21})–\nu(C_{18}–H_{23})$	ν(C–H4)
S_{41}	$\nu(C_{19}–H_{24})$	ν(C–H5)
S_{42}	$\delta(C_{15}–C_{14}–C_{19})–\delta(C_{14}–C_{19}–C_{18})+\delta(C_{19}–C_{18}–C_{18})–\delta(C_{18}–C_{17}–C_{16})+\delta(C_{17}–C_{16}–C_{15})–\delta(C_{16}–C_{15}–C_{14})$	δPh1
S_{43}	$\delta(C_{15}–C_{14}–C_{19})–\delta(C_{19}–C_{18}–C_{18})+\delta(C_{17}–C_{16}–C_{15})–\delta(C_{16}–C_{15}–C_{14})$	δPh2
S_{44}	$2\delta(C_{15}–C_{14}–C_{19})–\delta(C_{14}–C_{19}–C_{18})–\delta(C_{19}–C_{18}–C_{18})+2\delta(C_{18}–C_{17}–C_{16})–\delta(C_{17}–C_{16}–C_{15})–\delta(C_{16}–C_{15}–C_{14})$	δPh3
S_{45}	$\tau(C_{15}–C_{14}–C_{19}–C_{18})+\tau(C_{15}–C_{14}–C_{19}–H_{24})+\tau(C_1–C_{14}–C_{19}–C_{18})+\tau(C_1–C_{14}–C_{19}–H_{24})–$ $–\tau(C_{14}–C_{19}–C_{18}–C_{17})–\tau(C_{14}–C_{19}–C_{18}–H_{23})–\tau(H_{24}–C_{19}–C_{18}–C_{17})–\tau(H_{24}–C_{19}–C_{18}–H_{23})+$ $+\tau(C_{19}–C_{18}–C_{17}–C_{16})+\tau(C_{19}–C_{18}–C_{17}–H_{22})+\tau(H_{23}–C_{18}–C_{17}–C_{16})+\tau(H_{23}–C_{18}–C_{17}–H_{22})–$ $–\tau(C_{18}–C_{17}–C_{16}–C_{15})–\tau(C_{18}–C_{17}–C_{16}–H_{21})–\tau(H_{22}–C_{17}–C_{16}–C_{15})–\tau(H_{22}–C_{17}–C_{16}–H_{21})+$ $+\tau(C_{17}–C_{16}–C_{15}–C_{14})+\tau(C_{17}–C_{16}–C_{15}–H_{20})+\tau(H_{21}–C_{16}–C_{15}–C_{14})+\tau(H_{21}–C_{16}–C_{15}–H_{20})–$ $–\tau(C_{16}–C_{15}–C_{14}–C_{19})–\tau(C_{16}–C_{15}–C_{14}–C_1)–\tau(H_{20}–C_{15}–C_{14}–C_{19})–\tau(H_{20}–C_{15}–C_{14}–C_1)$	τPh1
S_{46}	$\tau(C_{15}–C_{14}–C_{19}–C_{18})+\tau(C_{15}–C_{14}–C_{19}–H_{24})+\tau(C_1–C_{14}–C_{19}–C_{18})+\tau(C_1–C_{14}–C_{19}–H_{24})–$ $–\tau(C_{19}–C_{18}–C_{17}–C_{16})–\tau(C_{19}–C_{18}–C_{17}–H_{22})–\tau(H_{23}–C_{18}–C_{17}–C_{16})–\tau(H_{23}–C_{18}–C_{17}–H_{22})+$ $+\tau(C_{18}–C_{17}–C_{16}–C_{15})+\tau(C_{18}–C_{17}–C_{16}–H_{21})+\tau(H_{22}–C_{17}–C_{16}–C_{15})+\tau(H_{22}–C_{17}–C_{16}–H_{21})–$ $–\tau(C_{16}–C_{15}–C_{14}–C_{19})–\tau(C_{16}–C_{15}–C_{14}–C_1)–\tau(H_{20}–C_{15}–C_{14}–C_{19})–\tau(H_{20}–C_{15}–C_{14}–C_1)$	τPh2
S_{47}	$–\tau(C_{15}–C_{14}–C_{19}–C_{18})–\tau(C_{15}–C_{14}–C_{19}–H_{24})–\tau(C_1–C_{14}–C_{19}–C_{18})–\tau(C_1–C_{14}–C_{19}–H_{24})+$ $+2\tau(C_{14}–C_{19}–C_{18}–C_{17})+2\tau(C_{14}–C_{19}–C_{18}–H_{23})+2\tau(H_{24}–C_{19}–C_{18}–C_{17})+2\tau(H_{24}–C_{19}–C_{18}–H_{23})+$ $–\tau(C_{19}–C_{18}–C_{17}–C_{16})–\tau(C_{19}–C_{18}–C_{17}–H_{22})–\tau(H_{23}–C_{18}–C_{17}–C_{16})–\tau(H_{23}–C_{18}–C_{17}–H_{22})–$	τPh3

	$-\tau(C_{18}–C_{17}–C_{16}–C_{15})-\tau(C_{18}–C_{17}–C_{16}–H_{21})-\tau(H_{22}–C_{17}–C_{16}–C_{15})-\tau(H_{22}–C_{17}–C_{16}–H_{21})+$ $+2\tau(C_{17}–C_{16}–C_{15}–C_{14})+2\tau(C_{17}–C_{16}–C_{15}–H_{20})+2\tau(H_{21}–C_{16}–C_{15}–C_{14})+2\tau(H_{21}–C_{16}–C_{15}–H_{20})–$ $-\tau(C_{16}–C_{15}–C_{14}–C_{19})-\tau(C_{16}–C_{15}–C_{14}–C_1)-\tau(H_{20}–C_{15}–C_{14}–C_{19})-\tau(H_{20}–C_{15}–C_{14}–C_1)$	
S_{48}	$\delta(C_{15}–C_{14}–C_1)–\delta(C_{19}–C_{14}–C_1)$	w(Ph–Isox)
S_{49}	$\delta(H_{20}–C_{15}–C_{14})–\delta(H_{20}–C_{15}–C_{16})+\delta(H_{21}–C_{16}–C_{15})–\delta(H_{21}–C_{16}–C_{17})+\delta(H_{22}–C_{17}–C_{16})—\delta(H_{22}–C_{17}–C_{18})+$ $+\delta(H_{23}–C_{18}–C_{17})–\delta(H_{23}–C_{18}–C_{19})+\delta(H_{24}–C_{19}–C_{14})–\delta(H_{24}–C_{19}–C_{18})$	δ(C–H1)
S_{50}	$\delta(H_{20}–C_{15}–C_{14})–\delta(H_{20}–C_{15}–C_{16})+\delta(H_{21}–C_{16}–C_{15})–\delta(H_{21}–C_{16}–C_{17})$ $+\delta(H_{23}–C_{18}–C_{17})–\delta(H_{23}–C_{18}–C_{19})+\delta(H_{24}–C_{19}–C_{14})–\delta(H_{24}–C_{19}–C_{18})$	δ(C–H2)
S_{51}	$\delta(H_{20}–C_{15}–C_{14})–\delta(H_{20}–C_{15}–C_{16})–2\delta(H_{22}–C_{17}–C_{16})+2\delta(H_{22}–C_{17}–C_{18})+\delta(H_{24}–C_{19}–C_{14})–\delta(H_{24}–C_{19}–C_{18})$	δ(C–H3)
S_{52}	$\delta(H_{20}–C_{15}–C_{14})–\delta(H_{20}–C_{15}–C_{16})-\delta(H_{21}–C_{16}–C_{15})+\delta(H_{21}–C_{16}–C_{17})+$ $+\delta(H_{23}–C_{18}–C_{17})–\delta(H_{23}–C_{18}–C_{19})–\delta(H_{24}–C_{19}–C_{14})+\delta(H_{24}–C_{19}–C_{18})$	δ(C–H4)
S_{53}	$2\delta(H_{20}–C_{15}–C_{14})–2\delta(H_{20}–C_{15}–C_{16})–3\delta(H_{21}–C_{16}–C_{15})+3\delta(H_{21}–C_{16}–C_{17})+2\delta(H_{22}–C_{17}–C_{16})–$ $–2\delta(H_{22}–C_{17}–C_{18})–3\delta(H_{23}–C_{18}–C_{17})+3\delta(H_{23}–C_{18}–C_{19})+2\delta(H_{24}–C_{19}–C_{14})–2\delta(H_{24}–C_{19}–C_{18})$	δ(C–H5)
S_{54}	$\gamma(H_{20}–C_{14}–C_{15}–C_{16})+\gamma(H_{21}–C_{15}–C_{16}–C_{17})+\gamma(H_{22}–C_{16}–C_{17}–C_{18})+\gamma(H_{23}–C_{17}–C_{18}–C_{19})+$ $+\gamma(H_{24}–C_{18}–C_{19}–C_{14})$ γ(C–H1)	
S_{55}	$\gamma(H_{20}–C_{14}–C_{15}–C_{16})+\gamma(H_{21}–C_{15}–C_{16}–C_{17})–\gamma(H_{23}–C_{17}–C_{18}–C_{19})–\gamma(H_{24}–C_{18}–C_{19}–C_{14})$	γ(C–H2)
S_{56}	$\gamma(H_{20}–C_{14}–C_{15}–C_{16})–2\gamma(H_{22}–C_{16}–C_{17}–C_{18})+\gamma(H_{24}–C_{18}–C_{19}–C_{14})$	γ(C–H3)
S_{57}	$\gamma(H_{20}–C_{14}–C_{15}–C_{16})–\gamma(H_{21}–C_{15}–C_{16}–C_{17})+\gamma(H_{23}–C_{17}–C_{18}–C_{19})–\gamma(H_{24}–C_{18}–C_{19}–C_{14})$	γ(C–H4)
S_{58}	$2\gamma(H_{20}–C_{14}–C_{15}–C_{16})–3\gamma(H_{21}–C_{15}–C_{16}–C_{17})+2\gamma(H_{22}–C_{16}–C_{17}–C_{18})–3\gamma(H_{23}–C_{17}–C_{18}–C_{19})+$ $+2\gamma(H_{24}–C_{18}–C_{19}–C_{14})$	γ(C–H5)
S_{59}	$\gamma(Cl_{13}–C_1=C_2–C_3)$	γ(C–Cl)
S_{60}	$\gamma(C_6–C_2–C_3=N_4)$	γ(Isox–E)
S_{61}	$\gamma(C_{14}–C_2=C_1–O_5)$	γ(Isox–Ph)
S_{62}	$\gamma(C_1–C_{15}–C_{14}–C_{19})$	γ(Ph–Isox)
S_{63}	$\delta(C_6–O_8–C_9)$	$\delta(C–O–CH_3)$
S_{64}	$\delta(Cl_{13}–C_2–C_3)–\delta(Cl_{13}–C_2=C_1)$	w(C–Cl)
S_{65}	$\delta(C_2–C_3–C_6)–\delta(N_4=C_3–C_6)$	w(Isox–E)
S_{66}	$\delta(C_2=C_1–C_{14})–\delta(O_5–C_1–C_{14})$	w(Isox–Ph)

[a] Normalization factors not shown. ν, bond stretching, δ, bending, γ, rocking, w, wagging, τ, torsion, IR, inter–ring; Isox, isoxazole ring; Ph, phenyl ring; E, ester. See Figure 1 for atom numbering. The molecule belongs to the C_1 symmetry point group (all coordinates belong to the A symmetry species).