Table S3 - Calculated [scaled, DFT(B3LYP)/6-311++G(d,p)] wavenumbers, IR intensities and Potential Energy Distributions (PED) for conformer **I** of MCPIC.[a]

Approximate description	Wavenumber	Intensity	PED[b]
ν(C-H1)	3159	1.7	$S_{37}(95)$
ν(C-H5)	3146	3.0	$S_{41}(86)$
ν(C-H2)	3132	16.9	$S_{38}(84)$
ν(C-H3)	3121	9.9	$S_{39}(93)$
ν(C-H4)	3111	0.1	S_{40} (94)
νCH_3 as´	3107	11.0	$S_8(97)$
νCH_3 as´´	3070	16.3	$S_9(100)$
νCH_3 s	2998	34.3	$S_7(97)$
ν(C=O)	1753	237.5	$S_2(87)$
νPh3	1614	1.0	$S_{33}(63)$, $S_{44}(10)$
νPh4	1591	4.8	$S_{34}(55)$, $S_{22}(11)$
νIsox3	1570	13.1	$S_{24}(44)$, $S_6(13)$, $S_{34}(12)$
δ(C-H4)	1499	1.8	$S_{35}(26)$, $S_{49}(14)$, $S_{24}(12)$, $S_{52}(16)$, $S_{50}(11)$
δCH_3 as´	1469	5.2	$S_{11}(73)$, $S_{10}(13)$
δ(C-H1), νIsox1	1459	83.7	$S_{10}(12)$, $S_{49}(11)$, $S_{22}(11)$, $S_{11}(11)$, $S_1(10)$
δCH_3 as´´	1457	11.6	$S_{12}(90)$
δCH_3 s	1448	29.7	$S_{10}(35)$, $S_{36}(14)$, $S_{49}(12)$, $S_{51}(12)$
νIsox2	1446	53.1	$S_{23}24)$, $S_{10}(14)$, $S_{22}(12)$
νIsox4	1416	25.5	$S_{25}(29)$, $S_{10}(24)$, $S_1(15)$
δ(C-H2)	1339	5.6	$S_{50}(31)$, $S_{52}(28)$, $S_{49}(16)$
νPh2	1312	12.1	$S_{32}(51)$, $S_{36}(16)$
νIsox2,ν(C-C_{IR})	1258	94.7	$S_{23}(16)$, $S_6(13)$, $S_{28}(10)$, $S_{32}(10)$
ν(C-O)	1215	465.5	$S_3(38)$, $S_{13}(11)$
δ(C-H3)	1190	5.8	$S_{33}(24)$, $S_{50}(19)$, $S_{52}(18)$, $S_{49}(15)$, $S_{51}(12)$, $S_{53}(12)$
γCH_3´	1182	34.2	$S_{13}(65)$
δ(C-H5)	1165	0.5	$S_{53}(48)$, $S_{51}(24)$
γCH_3´´	1149	0.9	$S_{14}(92)$
νIsox1	1121	19.6	$S_{26}(22)$, $S_{22}(17)$
νPh6	1084	14.7	$S_{36}(29)$, $S_{32}(13)$, $S_{49}(12)$, $S_{52}(10)$
δIsox2	1060	111.5	$S_{28}(25)$, $S_4(15)$, $S_5(12)$
νPh5	1031	0.5	$S_{35}(45)$, $S_{31}(20)$
δPh1, νPh1	997	0.6	$S_{42}(61)$, $S_{31}(38)$
γ(C-H2)	989	0.1	$S_{45}(26)$, $S_{56}(23)$, $S_{57}(21)$, $S_{55}(16)$
νIsox5	978	53.5	$S_{26}(32)$, $S_{25}(17)$, $S_4(14)$
γ(C-H4)	973	1.0	$S_{47}(26)$, $S_{53}(21)$, $S_{58}(17)$, $S_{57}(17)$, $S_{54}(16)$
ν(O-CH_3)	953	5.5	$S_4(48)$, $S_{26}(18)$
δIsox1	932	8.1	$S_{27}(44)$, $S_{23}(12)$
γ(C-H5)	924	2.6	$S_{56}(28)$, $S_{54}(28)$, $S_{58}(26)$, $S_{46}(12)$
γ(C-H1)	840	0.4	$S_{54}(28)$; $S_{58}(26)$, $S_{57}(24)$, $S_{55}(22)$
δ(OCO)	809	31.9	$S_{19}(36)$, $S_3(17)$, $S_{63}(14)$
γ(C=O)	791	9.5	$S_{21}(62)$, $S_{60}(22)$
γ(C-H3)	769	23.2	$S_{56}(29)$, $S_{62}(24.1)$
δPh3	696	6.1	$S_{44}(46)$, $S_6(11)$, $S_{27}(10)$
τPh1	691	44.0	$S_{45}(41)$, $S_{57}(23)$, $S_{55}(23)$
τIsox1	680	23.4	$S_{29}(35)$, $S_{61}(25)$
τIsox2	632	4.3	$S_{30}(72)$, $S_{21}(10)$
δPh2	621	0.1	$S_{43}(86)$
w(Isox-E),w(Isox-Ph),w(C-Cl)	573	1.1	$S_{66}(16)$, $S_{65}(16)$, $S_{64}(16)$, $S_{20}(11)$
ν(C-Cl)	540	2.7	$S_5(39)$, $S_{20}(10)$, $S_{22}(12)$
γ(Ph-Isox)	485	2.7	$S_{62}(34)$, $S_{46}(19)$, $S_{29}(11)$
ν(C-C_α)	447	0.02	$S_1(22)$, $S_{44}(16)$, $S_{19}(10)$
τPh3	401	0.05	$S_{47}(72)$
δ(CC=O)	362	10.3	$S_{20}(22)$, $S_{63}(18)$, $S_5(13)$, $S_{48}(11)$
γ(Isox-E)	326	4.2	$S_{46}(19)$, $S_{61}(16)$, $S_{60}(13)$
δ(C-O-CH_3)	302	13.7	$S_{63}(38)$, $S_{60}(10)$, $S_{19}(10)$
γ(C-Cl)	278	3.0	$S_{59}(51)$, $S_{60}(10)$
ν(C-Cα),ν(C-C_{IR})	250	0.4	$S_6(19)$, $S_1(14)$, $S_{44}(12)$, $S_{28}(12)$
w(C-Cl)	215	1.1	$S_{64}(47)$, $S_{20}(15)$, $S_{48}(11)$
τIsox1, γ(C-Cl)	178	0.8	$S_{17}(26)$, $S_{29}(16)$, $S_{59}(15)$, $S_{46}(13)$
w(C-Cl),w(Ph-Isox)	150	1.1	$S_{64}(18)$, $S_{65}(17)$, $S_{66}(15)$, $S_{48}(12)$, $S_{20}(10)$
τCH_3	135	0.1	$S_{15}(75)$
τ(C-O)	116	1.1	$S_{17}(42)$, $S_{15}(16)$
w(Isox-Ph)	85	1.8	$S_{66}(29)$, $S_{65}(28)$, $S_{48}(13$, $S_{20}(10)$
γ(Isox-E), γ(Isox-Ph)	45	0.5	$S_{60}(28)$, $S_{61}(27)$, $S_{29}(20)$
τ(C-C_{IR})	29	0.1	$S_{18}(95)$
τ(C-C_α)	20	2.6	$S_{16}(100)$

[a] Wavenumbers (cm^{-1}, scaled by 0.9817), ν, bond stretching, δ, bending, γ, rocking, w, wagging, τ, torsion, s, symmetric, as, anti-symmetric, IR, inter–ring; Isox, isoxazole ring; Ph, phenyl ring; E, ester. See Table S2 for definition of internal coordinates. [b] Only PED values greater than 10% are given.