Supplementary Information for the article entitled

The solid state of anti-inflammatory morniflumate diniflumate: a cocrystalline salt

by

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Tables

Table S1a. Fractional coordinates and isotropic temperature factors of the hydrogen atoms absent in the CSD CIF NIFLUM10 of the niflumic acid crystal structure after the original article by Krishna Murthy and Vijayan [1]

atom[a,b]	x	y	z	B
H(3)	0.332(24)	0.407(9)	0.739(8)	5(3)
H(4)	0.397(24)	0.401(9)	0.894(9)	6(3)
H(5)	0.734(24)	0.482(9)	0.962(9)	6(3)
H(2)	0.343(30)	0.457(10)	0.523(11)	8(5)
H(1)[c]	0.092(32)	0.608(12)	0.676(12)	8(5)
H(9)	0.186(22)	0.653(7)	0.888(7)	4(3)
H(11)	0.729(22)	0.815(8)	0.812(8)	5(3)
H(12)	0.589(23)	0.782(8)	0.664(8)	5(3)
H(13)	0.280(19)	0.680(7)	0.662(7)	3(2)

[a] The hydrogen atoms have the same numbers as those of the carbon atoms to which they are attached in NIFLUM10.

[b] H(1) and H(2) are attached to N(1) and O(2), respectively, in NIFLUM10.

[c] atom H(1) is more realistically located with coordinates x = 0.28, y = 0.68, and z = 0.622.

Table S1b. Temperatures and heats of fusion of morniflumate and niflumic acid determined in this work[a] and found in the literature

Morniflumate (M = 395.380 g·mol^{-1})		
T_{fus} /K	$\Delta_{fus}H$ /J·g^{-1}; kJ·mol^{-1}	Reference
348.10	89.40; 35.34	[2]
347.91	87.77; 34.70	this work
348.03	88.73; 35.08	this work
347.82	88.20; 34.87	this work
347.93	91.58; 36.21	this work
347.92	90.20; 35.66	this work
348.06	91.50; 36.18	this work
348.55	91.50; 36.18	this work
348.63	90.50; 35.78	this work
348.52	90.55; 35.80	this work
348.1(3)	90.0(1.4); 35.6(6)	mean, this work

Niflumic acid (M = 282.218 g·mol^{-1})		
T_{fus} /K	$\Delta_{fus}H$ /J·g^{-1}; kJ·mol^{-1}	Reference
476.00	134.65; 38.00	[3]
476.40	126.50; 35.70	[4]
478.00	129.33; 36.50	[5]
475.15	129.50; 36.55 131.22; 37.03	[6]
475.42 475.52	133.65; 37.72 133.35; 37.63	[7]
476.85	131.18; 37.02	this work
476.18	132.11; 37.28	this work
476.20	130.18; 36.74	this work
476.22	132.20; 37.31	this work
476.28	130.50; 36.83	this work
476.24	133.30; 37.62	this work
476.2(7)	131(2); 37.1(6)	mean, this work

[a] morniflumate heating rates from 0.5 to 10 K min^{-1} and niflumic acid heating rate of 10 K min^{-1}

Table S2a. Atom coordinates and isotropic displacement parameters of morniflumate diniflumate at 297 K[a]

Atom label[b]	$x(\sigma)$	$y(\sigma)$	$z(\sigma)$	$U_{eq}(\sigma)$ /Å^2
F1A	0.4434(10)	0.8317(5)	0.7103(6)	0.183(4)
F2A	0.2491(5)	0.8618(3)	0.7161(3)	0.1306(17)
F3A	0.3821(6)	0.9542(3)	0.6239(3)	0.127(2)
F1AA	0.3624(10)	0.8177(5)	0.7368(3)	0.137(4)
F2AA	0.3328(11)	0.9426(5)	0.6375(7)	0.189(5)
F3AA	0.5168(4)	0.8852(4)	0.6413(4)	0.1154(17)
F1B	0.5564(12)	0.0668(5)	0.6966(3)	0.137(4)
F2B	0.4014(11)	0.0061(11)	0.7964(6)	0.198(5)
F3B	0.5920(19)	-0.0428(7)	0.7938(9)	0.215(6)
F1BB	0.6083(7)	0.0420(6)	0.7076(5)	0.151(3)
F2BB	0.4077(7)	0.0657(5)	0.7440(6)	0.138(3)
F3BB	0.4957(8)	-0.0501(3)	0.8195(3)	0.122(2)
F1C	0.8021(11)	0.0273(9)	0.8686(8)	0.164(3)
F2C	0.8695(12)	-0.0400(5)	0.9753(4)	0.148(2)
F3C	0.9985(5)	0.0272(4)	0.8618(5)	0.1329(19)
F1CC	1.0033(12)	0.0209(16)	0.887(2)	0.210(10)
F3CC	0.813(3)	-0.0267(17)	0.9741(14)	0.206(9)
F2CC	0.839(3)	0.041(2)	0.8450(13)	0.174(8)
O2B	0.67005(11)	0.49342(8)	0.61329(6)	0.0584(3)
O1B	0.70558(11)	0.66173(8)	0.58746(7)	0.0582(3)
O1C	0.95564(11)	0.48197(8)	0.65241(7)	0.0606(3)
O2A	0.11702(12)	0.24231(8)	0.66561(7)	0.0643(3)
O2C	1.02664(11)	0.64250(8)	0.59542(7)	0.0600(3)
O1A	0.23437(11)	0.36387(9)	0.56616(6)	0.0641(3)
O3C	0.91174(19)	1.01711(9)	0.42091(12)	0.0998(5)
N3C	1.00999(12)	0.80263(9)	0.42769(8)	0.0553(3)
N1B	0.57159(14)	0.48906(10)	0.87999(8)	0.0619(3)
N1A	0.29517(13)	0.48294(11)	0.76241(9)	0.0628(3)
N2B	0.60533(12)	0.39111(9)	0.77570(8)	0.0523(3)
N2A	0.31146(13)	0.51178(10)	0.61766(8)	0.0571(3)
N2C	0.89576(14)	0.41906(14)	0.82447(9)	0.0710(4)
N1C	0.92751(18)	0.53499(19)	0.89850(10)	0.0970(6)
C11A	0.19783(14)	0.28905(13)	0.79198(10)	0.0563(3)
C8B	0.60403(12)	0.48521(10)	0.79737(8)	0.0458(3)
C12B	0.64051(12)	0.57481(10)	0.73127(8)	0.0444(3)
C13A	0.19074(13)	0.31661(10)	0.64226(9)	0.0485(3)
C12A	0.22388(12)	0.35186(11)	0.71078(8)	0.0476(3)
C13B	0.67225(12)	0.57159(10)	0.63967(8)	0.0457(3)
C3B	0.4707(2)	0.09816(13)	0.91305(11)	0.0723(5)
C4B	0.55875(15)	0.21919(11)	0.78132(10)	0.0555(3)
C2B	0.51414(17)	0.12222(11)	0.82483(10)	0.0617(4)
C11B	0.64504(15)	0.66733(11)	0.75535(9)	0.0554(3)
C13C	0.98294(13)	0.56348(12)	0.66212(9)	0.0534(3)
C16C	0.92650(17)	0.84252(12)	0.50550(11)	0.0623(4)
C12C	0.97384(15)	0.58803(14)	0.74496(10)	0.0629(4)
C5B	0.4778(2)	0.17190(13)	0.95669(11)	0.0757(5)
C6B	0.52418(18)	0.26891(12)	0.91462(10)	0.0636(4)
C8A	0.27711(13)	0.44935(11)	0.69812(9)	0.0501(3)
C10B	0.6149(2)	0.67056(13)	0.84053(11)	0.0722(5)
C6A	0.41401(15)	0.64264(13)	0.50034(11)	0.0594(3)
C10A	0.21893(17)	0.32306(15)	0.85772(11)	0.0675(4)

C4A	0.34806(16)	0.68239(12)	0.64067(11)	0.0601(4)
C7B	0.56215(13)	0.29473(10)	0.82567(9)	0.0493(3)
C14C	1.04709(16)	0.62121(12)	0.51148(10)	0.0555(3)
C1B	0.5110(2)	0.04273(14)	0.77565(13)	0.0851(6)
C8C	0.93159(15)	0.51399(17)	0.82343(10)	0.0707(5)
C9B	0.5776(2)	0.58054(13)	0.89947(10)	0.0759(5)
C5A	0.45806(18)	0.74134(14)	0.46458(12)	0.0689(4)
C7A	0.35779(13)	0.61184(11)	0.58877(9)	0.0523(3)
C7C	0.85996(16)	0.33313(19)	0.89303(10)	0.0754(5)
C3A	0.4461(2)	0.81247(14)	0.51542(13)	0.0741(5)
C9A	0.26526(18)	0.41994(15)	0.83959(11)	0.0694(4)
C15C	1.10587(16)	0.71366(13)	0.44525(12)	0.0622(4)
C17C	1.0806(2)	0.89045(15)	0.36244(15)	0.0787(5)
C4C	0.88165(17)	0.23552(19)	0.87284(12)	0.0784(5)
C11C	1.0085(2)	0.68387(19)	0.74784(15)	0.0822(5)
C2C	0.84891(19)	0.1460(2)	0.93650(13)	0.0924(7)
C2A	0.39186(18)	0.78145(12)	0.60295(12)	0.0662(4)
C6C	0.8012(2)	0.3413(3)	0.97862(13)	0.0959(7)
C5C	0.7686(3)	0.2515(3)	1.04087(14)	0.1128(10)
C3C	0.7938(2)	0.1542(3)	1.02098(16)	0.1119(10)
C18C	0.9850(3)	0.98128(15)	0.34496(17)	0.0949(7)
C9C	0.9634(3)	0.6273(3)	0.89764(18)	0.1159(10)
C10C	1.0034(3)	0.7039(3)	0.82624(19)	0.1079(8)
C19C	0.8385(2)	0.93539(15)	0.48001(17)	0.0853(6)
C1A	0.3827(3)	0.85644(15)	0.65900(16)	0.0906(6)
C1C	0.8774(3)	0.0422(3)	0.91097(19)	0.1119(8)
H4B	0.5868(16)	0.2362(13)	0.7177(12)	0.064(5)
H3B	0.5300(19)	0.3203(16)	0.9443(13)	0.080(6)
H5B	0.6713(15)	0.7281(13)	0.7117(10)	0.054(4)
H2B	0.453(2)	0.1557(18)	1.0160(16)	0.100(7)
H1B	0.4379(19)	0.0320(16)	0.9432(13)	0.084(6)
H15C	0.8794(16)	0.7837(13)	0.5440(11)	0.059(4)
H5A	0.284(2)	0.4495(17)	0.8808(15)	0.093(6)
H9C	0.9634(16)	0.6087(12)	0.5065(10)	0.056(4)
H18C	0.776(2)	0.9122(16)	0.4536(14)	0.085(6)
H2A	0.4984(17)	0.7646(14)	0.4042(13)	0.066(5)
H14C	0.9871(18)	0.8624(15)	0.5310(12)	0.074(5)
H13C	1.126(2)	0.8639(17)	0.3139(15)	0.087(7)
H1C	0.773(3)	0.087(2)	1.0645(19)	0.120(9)
H7C	1.043(2)	0.7331(19)	0.6965(17)	0.100(8)
H7A	0.1632(17)	0.2197(14)	0.8015(11)	0.065(5)
H17C	0.927(2)	0.9596(17)	0.3181(14)	0.090(6)
H2NC	0.9559(19)	0.7811(15)	0.4015(13)	0.078(5)
H8C	1.1059(16)	0.5611(13)	0.5067(10)	0.059(4)
H11C	1.1700(18)	0.7419(14)	0.4620(12)	0.070(5)
H2C	0.9221(19)	0.2255(16)	0.8158(14)	0.082(6)
H6A	0.2015(19)	0.2808(16)	0.9134(14)	0.086(6)
H4C	0.784(2)	0.4052(19)	0.9917(16)	0.096(8)
H12C	1.142(2)	0.9092(16)	0.3844(14)	0.089(6)
H19C	0.786(2)	0.9652(18)	0.5326(16)	0.099(7)
H3A	0.4220(17)	0.5948(14)	0.4654(12)	0.065(5)
H6B	0.556(2)	0.5785(16)	0.9602(15)	0.093(6)
H4A	0.3145(18)	0.6628(15)	0.7007(14)	0.075(5)
H7B	0.620(2)	0.7315(17)	0.8564(14)	0.085(6)

H1NA	0.3086(17)	0.4773(15)	0.5775(13)	0.072(5)
H10C	1.1513(19)	0.6908(16)	0.3916(14)	0.079(6)
H1NB	0.6243(17)	0.3985(13)	0.7203(12)	0.064(5)
H1A	0.482(2)	0.8813(17)	0.4889(13)	0.085(6)
H5C	0.965(3)	0.639(2)	0.953(2)	0.132(9)
H16C	1.034(2)	1.0386(19)	0.3071(16)	0.105(7)
H6C	1.030(3)	0.773(2)	0.8296(18)	0.120(8)
H1NC	0.911(2)	0.4041(16)	0.7767(14)	0.080(6)
H3C	0.730(3)	0.263(2)	1.0977(19)	0.114(8)
H1OB	0.725(2)	0.6540(16)	0.5315(15)	0.089(6)

[a] esd in parentheses

[b] A, B, and C refer to niflumic acid A and B, and morniflumate (C), respectively (see **Figure S1** below)

Table S2b. Atom coordinates and isotropic displacement parameters of morniflumate diniflumate at 100 K[a]

Atom label[b]	$x(\sigma)$	$y(\sigma)$	$z(\sigma)$	Ueq(σ) /Å^2
F1A	0.45169(18)	0.83400(10)	0.71222(11)	0.0558(5)
F2A	0.24797(12)	0.85972(9)	0.72087(7)	0.0407(4)
F3A	0.38379(13)	0.95903(9)	0.61730(9)	0.0341(3)
F1AA	0.5106(7)	0.8778(7)	0.6487(6)	0.0659(19)
F2AA	0.3356(11)	0.9515(7)	0.6318(7)	0.0659(19)
F3AA	0.3389(9)	0.8239(6)	0.7406(4)	0.0659(19)
F1B	0.5847(7)	0.0608(5)	0.6921(5)	0.0252(16)
F2B	0.3766(13)	0.0409(11)	0.7732(8)	0.0400(16)
F3B	0.5347(15)	-0.0543(7)	0.8148(6)	0.0507(19)
F1BB	0.5864(10)	0.0567(7)	0.6997(8)	0.057(3)
F2BB	0.3856(14)	0.0591(15)	0.7533(15)	0.050(2)
F3BB	0.5110(15)	-0.0530(7)	0.8163(4)	0.0457(18)
F1C	0.79358(10)	0.01534(8)	0.87589(7)	0.0466(2)
F2C	0.86332(10)	-0.05143(8)	0.98905(6)	0.0453(2)
F3C	0.99875(9)	0.01911(7)	0.86717(6)	0.0392(2)
O2B	0.67068(8)	0.49876(6)	0.60901(5)	0.01895(17)
O1B	0.71150(9)	0.66847(7)	0.58149(5)	0.01977(17)
O1C	0.95909(8)	0.47833(7)	0.65070(5)	0.01925(17)
O2A	0.11439(9)	0.23589(7)	0.67617(5)	0.02025(17)
O2C	1.03372(8)	0.64067(6)	0.59294(5)	0.01882(17)
O1A	0.23632(9)	0.35825(7)	0.57309(5)	0.02150(18)
O3C	0.91892(13)	1.02166(7)	0.41094(7)	0.0366(3)
N3C	1.01703(10)	0.80520(7)	0.42012(6)	0.01803(19)
N1B	0.58115(10)	0.48759(8)	0.88150(6)	0.01904(19)
N1A	0.29727(10)	0.47998(8)	0.77215(7)	0.01918(19)
N2B	0.61035(10)	0.39230(7)	0.77452(6)	0.01657(18)
N2A	0.31460(10)	0.50757(8)	0.62354(6)	0.01812(19)
N2C	0.89812(10)	0.41084(9)	0.82656(6)	0.0203(2)
N1C	0.93422(11)	0.52439(9)	0.90325(7)	0.0248(2)
C11A	0.19767(11)	0.28327(9)	0.80548(7)	0.0170(2)
C8B	0.61187(10)	0.48565(8)	0.79686(7)	0.0149(2)
C12B	0.64885(10)	0.57747(8)	0.72889(7)	0.0148(2)
C13A	0.19020(11)	0.31093(9)	0.65176(7)	0.0155(2)
C12A	0.22457(10)	0.34666(9)	0.72129(7)	0.0152(2)
C13B	0.67710(10)	0.57652(9)	0.63540(7)	0.0153(2)
C3B	0.46562(12)	0.09684(9)	0.91551(8)	0.0199(2)
C4B	0.55752(11)	0.22095(9)	0.77980(7)	0.0172(2)
C2B	0.50923(11)	0.12313(9)	0.82467(7)	0.0181(2)

C11B	0.65800(11)	0.66963(9)	0.75295(7)	0.0176(2)
C13C	0.98837(11)	0.55985(9)	0.66093(7)	0.0166(2)
C16C	0.93714(13)	0.84455(9)	0.49947(8)	0.0210(2)
C12C	0.97946(11)	0.58224(9)	0.74588(7)	0.0183(2)
C5B	0.47719(12)	0.16904(9)	0.96079(7)	0.0202(2)
C6B	0.52757(11)	0.26678(9)	0.91744(7)	0.0176(2)
C8A	0.27910(10)	0.44529(9)	0.70696(7)	0.0159(2)
C10B	0.62990(13)	0.67086(9)	0.84046(8)	0.0215(2)
C6A	0.41863(11)	0.64012(9)	0.50227(8)	0.0190(2)
C10A	0.21862(12)	0.31809(10)	0.87272(8)	0.0199(2)
C4A	0.34674(12)	0.68134(9)	0.64477(8)	0.0196(2)
C7B	0.56461(10)	0.29504(8)	0.82587(7)	0.0154(2)
C14C	1.05354(12)	0.62026(9)	0.50733(7)	0.0180(2)
C1B	0.49991(13)	0.04506(10)	0.77510(8)	0.0227(2)
C8C	0.93647(11)	0.50601(10)	0.82623(7)	0.0195(2)
C9B	0.59122(13)	0.57834(10)	0.90137(8)	0.0220(2)
C5A	0.46141(12)	0.74096(10)	0.46423(8)	0.0221(2)
C7A	0.36006(11)	0.60910(9)	0.59280(7)	0.0170(2)
C7C	0.85929(11)	0.32415(10)	0.89725(8)	0.0218(2)
C3A	0.44540(13)	0.81428(10)	0.51486(8)	0.0242(2)
C9A	0.26629(12)	0.41726(10)	0.85235(8)	0.0208(2)
C15C	1.11423(12)	0.71453(10)	0.43897(8)	0.0202(2)
C17C	1.08832(14)	0.89426(10)	0.35241(9)	0.0274(3)
C4C	0.88234(12)	0.22480(11)	0.87780(8)	0.0226(2)
C11C	1.01527(12)	0.67847(10)	0.74994(8)	0.0226(2)
C2C	0.84618(12)	0.13503(11)	0.94402(8)	0.0261(3)
C2A	0.38818(13)	0.78288(9)	0.60453(8)	0.0225(2)
C6C	0.79597(13)	0.33250(12)	0.98378(8)	0.0267(3)
C5C	0.76010(13)	0.24190(13)	1.04855(8)	0.0312(3)
C3C	0.78543(13)	0.14256(13)	1.02998(9)	0.0310(3)
C18C	0.98956(18)	0.98635(10)	0.33354(10)	0.0334(3)
C9C	0.97117(13)	0.61713(12)	0.90362(9)	0.0281(3)
C10C	1.01049(14)	0.69731(12)	0.82999(9)	0.0280(3)
C19C	0.84578(15)	0.93843(10)	0.47317(10)	0.0300(3)
C1A	0.37369(16)	0.85888(10)	0.66124(9)	0.0305(3)
C1C	0.87514(14)	0.03027(12)	0.91991(9)	0.0310(3)
H4B	0.5837(15)	0.2402(12)	0.7167(11)	0.022(4)
H3B	0.5375(15)	0.3142(12)	0.9493(10)	0.019(4)
H5B	0.6806(16)	0.7313(13)	0.7092(11)	0.025(4)
H2B	0.4515(16)	0.1509(13)	1.0248(11)	0.028(4)
H1B	0.4323(16)	0.0292(13)	0.9455(11)	0.026(4)
H15C	0.8868(15)	0.7888(12)	0.5395(10)	0.020(4)
H5A	0.2791(16)	0.4465(13)	0.8969(11)	0.027(4)
H9C	0.9704(15)	0.6082(12)	0.5001(10)	0.019(4)
H18C	0.7834(17)	0.9166(14)	0.4477(11)	0.030(4)
H2A	0.5019(15)	0.7630(12)	0.4018(10)	0.019(4)
H14C	1.0008(16)	0.8640(13)	0.5241(10)	0.024(4)
H13C	1.1343(17)	0.8668(13)	0.2999(12)	0.029(4)
H1C	0.7623(18)	0.0784(15)	1.0758(13)	0.038(5)
H7C	1.0439(16)	0.7294(13)	0.6983(11)	0.025(4)
H7A	0.1628(15)	0.2158(12)	0.8168(10)	0.021(4)
H17C	0.9285(17)	0.9663(13)	0.3084(11)	0.027(4)
H2NC	0.9590(19)	0.7829(15)	0.3920(13)	0.040(5)
H8C	1.1159(15)	0.5594(12)	0.5018(10)	0.020(4)

H11C	1.1818(15)	0.7392(12)	0.4560(10)	0.019(3)
H2C	0.9263(16)	0.2192(13)	0.8194(11)	0.026(4)
H6A	0.2037(16)	0.2744(13)	0.9313(11)	0.025(4)
H4C	0.7768(18)	0.3992(15)	0.9972(12)	0.034(4)
H12C	1.1522(17)	0.9143(14)	0.3758(12)	0.032(4)
H19C	0.7949(18)	0.9657(14)	0.5256(12)	0.036(5)
H3A	0.4285(16)	0.5902(13)	0.4668(11)	0.025(4)
H6B	0.5688(17)	0.5747(13)	0.9637(11)	0.029(4)
H4A	0.3095(16)	0.6612(13)	0.7079(11)	0.024(4)
H7B	0.6374(17)	0.7331(14)	0.8579(12)	0.031(4)
H1NA	0.3098(16)	0.4746(13)	0.5839(11)	0.026(4)
H10C	1.1554(16)	0.6930(13)	0.3846(11)	0.025(4)
H1NB	0.6260(16)	0.4029(13)	0.7178(12)	0.027(4)
H1A	0.4755(18)	0.8841(15)	0.4900(12)	0.034(4)
H5C	0.9701(18)	0.6253(14)	0.9601(12)	0.035(5)
H16C	1.038(2)	1.0445(16)	0.2918(13)	0.044(5)
H6C	1.0329(18)	0.7640(14)	0.8355(12)	0.034(4)
H1NC	0.9118(17)	0.3989(14)	0.7747(12)	0.031(4)
H3C	0.7166(19)	0.2488(15)	1.1067(13)	0.039(5)
H1OB	0.729(2)	0.6623(16)	0.5270(14)	0.046(5)

[a] esd in parentheses

[b] A, B, and C refer to niflumic acid A and B, and morniflumate (C), respectively (see **Figure S1** below)

Table S3. Hydrogen bonding in morniflumate diniflumate at 297 K and at 100K

A···H-D T/K	*d*(H···A) /Å	*d*(H-D) /Å	*d*(A···D) /Å	Angle (A ··· H-D) /°	Symmetry code A	Symmetry code D
O1A···H1NA-N2A						
297	1.869	0.911	2.644	141.49	x,y,z	x,y,z
100	1.881	0.890	2.637	141.72		
O1A···H10B-O1B						
297	1.627	0.926	2.552	176.98	x,y,z	1-x,1-y,1-z
100	1.665	0.885	2.548	176.04		
O2A···H2NC-N3C						
297	1.677	0.945	2.606	166.89	x,y,z	1-x,1-y,1-z
100	1.634	0.988	2.604	165.86		
O1A···H2NC-N3C						
297	2.841	0.945	3.628	141.50	x,y,z	1-x,1-y,1-z
100	2.804	0.988	3.627	141.22		
O2B···H1NB-N2B						
297	1.896	0.873	2.662	145.46	x,y,z	x,y,z
100	1.878	0.877	2.657	147.06		
O1C···H1NC-N2C						
297	2.036	0.834	2.706	136.92	x,y,z	x,y,z
100	1.990	0.875	2.708	138.52		

[a] For atom labels, see **Figure S1**.

Table S4. Fractional site occupancies for the F-atoms in the structure of morniflumate diniflumate at 297 K and 100 K

Atom label[b]	297 K	100 K
F1A	0.554(6)	0.837(3)
F2A	0.554(6)	0.837(3)
F3A	0.554(6)	0.837(3)
F1AA	0.446(6)	0.163(3)
F2AA	0.446(6)	0.163(3)
F3AA	0.446(6)	0.163(3)
F1B	0.443(10)	0.49(4)
F2B	0.443(10)	0.49(4)
F3B	0.443(10)	0.49(4)
F1BB	0.557(10)	0.51(4)
F2BB	0.557(10)	0.51(4)
F3BB	0.557(10)	0.51(4)
F1C	0.70(3)	1
F2C	0.70(3)	1
F3C	0.70(3)	1
F1CC	0.30(3)	0
F2CC	0.30(3)	0
F3CC	0.30(3)	0

[a] esd in parentheses

[b] A, B, and C refer to niflumic acids A and B, and morniflumate (C), respectively (see **Figure S1**).

Table S5a. Calorimetric data for the cocrystal diniflumate morniflumate at various heating rates[a]

Sample mass /mg	T_1 /K	Area peak A[a,b] / J·g^{-1}	T_2 /K	Complete area[a,c] /J·g^{-1}
Heating rate 0.5 K·min^{-1}				
3.052	381.61	-	432.67	-
3.022	381.76	-	434.40	-
3.000	381.78	-	434.80	-
Heating rate 1.25 K·min^{-1}				
3.17	381.82		-	-
4.71	380.88		433.5	87.65
Heating rate 2 K·min^{-1}				
3.025	382.04	-	436.79	-
3.071	381.87	-	436.64	-
7.690	381.71	-	437.36	79.33
Heating rate 5 K·min^{-1}				
4.59	382.02	77.45	434.81	90.72
4.28	381.55	76.71	436.92	90.32
Heating rate 10 K·min^{-1}				
2.88	381.90	77.00	437.18	80.20
3.27	381.94	76.60	438.02	80.90
7.38	381.79	78.55	-	82.54
2.80	382.52	78.38	-	85.12
3.074	382.69	78.34	438.91	89.25
3.078	382.96	78.58	438.88	91.39
3.028	383.22	78.11	439.03	87.60
3.89	383.64	77.20	-	88.59
3.96	382.54	77.16	438.20	87.86
2.77	382.64	77.06	437.33	84.54
Heating rate 20 K·min^{-1}				
4.34	383.07	77.96	436.91	85.31
4.50	384.26	77.80	436.80	86.20
Mean(esd)	382.3(8)	77.6(7)	436.6(1.9)	86.1(3.8)

[a] Refer to scheme S1 below this table for the definition of the quantities in the table.

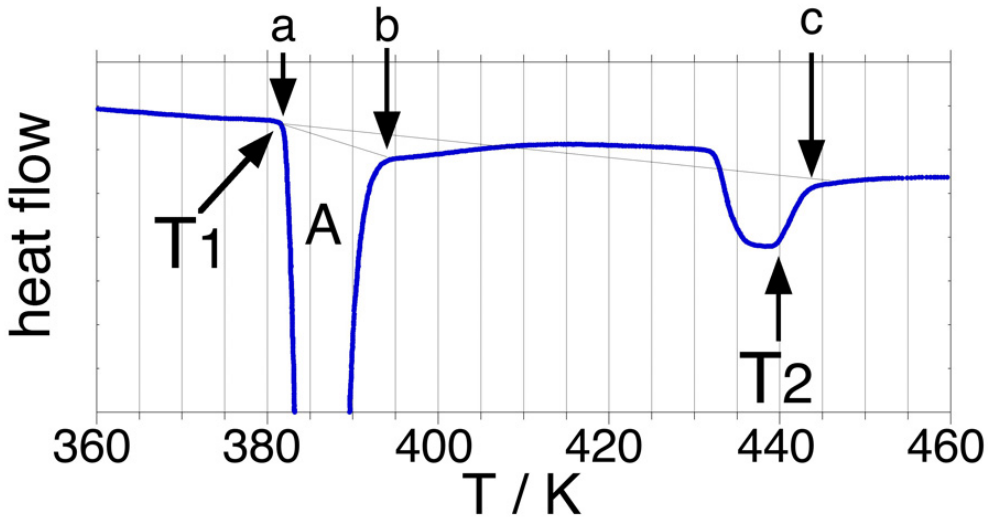
[b] The area of endothermic peak A (see figure below) recorded at rates ≥ 5 K·min^{-1} is obtained by integration between the limits 'a' and 'b'.

[c] The enthalpy of the complete thermal transition sequence from the solid cocrystal to the homogeneous molten state is obtained by integration between the limits 'a' and 'c'.

Table S5b. Calorimetric data for the cocrystal diniflumate morniflumate at 50 K·min^{-1} [d]

Heating rate 50 K·min^{-1}		
Sample mass /mg	**T_{fus} /K**	**$\Delta_{fus}H$ /J·g^{-1}**
3.045	386.81	77.77
3.076	387.94	81.22
3.047	388.61	81.03
Mean(esd)	387.8(9)	80.0(2.0)

[d] A single endothermic peak is recorded, which indicates that the melting transition has become congruent.



Scheme S1. illustrating the peaks and integration limits mentioned in **Table S5**.

Table S6. Lattice parameters and unit-cell volume of monoclinic niflumic acid as a function of the temperature[a]

T /K	a /Å	b /Å	c /Å	β /°	V_{cell} /Å^3
100	5.0789(6)	14.9969(14)	15.4029(14)	96.65(1)	1165.3(2)
200	5.0959(5)	15.1708(15)	15.4587(12)	96.20(1)	1188.1(2)
350	5.1217(4)	15.5302(9)	15.5306(8)	95.07(1)	1230.5(2)
400	5.1295(5)	15.6547(17)	15.5554(16)	94.78(1)	1244.7(2)
425	5.1319(6)	15.7128(18)	15.5653(15)	94.69(2)	1250.9(2)
450	5.1350(7)	15.7715(19)	15.5764(17)	94.59(2)	1257.4(3)

[a] esd in parentheses

Table S7. Temperatures and mole fractions (*x*) for the construction of the niflumic acid – morniflumate T-x diagram (see main text Figure 7)

x **(niflumic acid)**	**Peritexy onset** ***T*** **/K**	**Liquidus maximum** ***T*** **/K**	**Fusion onset components** T_{fus} **/K**	**Eutexy onset** ***T*****/K**
1.0000			476.33	
0.8233	382.85	464.45		
0.6666	382.3	436.60	387.80[a]	
0.9046	382.85	471.85		
0.6887	382.85	447.15		
0.7022	382.85	450.15		
0.2100		373.85		347.85
0.3920		380.65		345.85
0.4650	380.15	385.15		346.15
0.5680		418.15		345.85
0.6030	381.85	433.15		345.85
0.6000	382.85	433.15		346.65
0.6110	382.85	433.15		345.85
0.6340	382.85	436.15		345.85
0.0360		350.65		345.35
0.0000			348.16	

[a] metastable congruent fusion (see **Table S5b**)

Table S8. Weak N···H-C interactions in morniflumate diniflumate at 297 K and comparison with similar compounds from the literature

N(π)···H-C(φ)	d(H···N) /Å	d(H-C) /Å	d(N···C) /Å	Angle (N ··· H-C) /°	CF_3 / COO Orientation[a]	reference[b]
Morniflumate diniflumate at 297 K						
Morniflumate ion	2.387	0.901	2.892	115.64	cis	This work
Acid A ionized	2.363	0.942	2.927	118.07	trans	This work
Acid B neutral	2.271	0.953	2.909	123.62	cis	This work
Data from the literature for niflumic acid-based cocrystals						
Niflumic acid	2.405	0.902	2.886	112.58	trans	NIFLUM10[1]
	2.303	0.950	2.903	120.50		NIFLUM11[8]
Morniflumate	2.398	0.973	2.910	113.02	cis	GAKWIY[9]
Niflumic acid (ionized)-ethanolamine	2.408	1.001	2.950	113.25	trans	CAGXEN[10]
Niflumic acid-sulfamethazine	2.309	0.931	2.886	119.69	trans	DARGEL[11]
	2.305	0.930	2.885	119.98		DARGEL01[12]
Niflumic acid-nicotinamide	2.239	0.929	2.881	125.57	cis	EXAQEA[13]
Niflumic acid-L-proline	2.303	0.950	2.882	118.68	trans	LIRSEN[14]
Niflumic acid-caprolactam	2.346	0.929	2.940	121.39	cis	RIQXAT[15]
Niflumic acid-pyridinone	2.372	0.929	2.958	120.90	cis	RIQXEX[15]
Talniflumate	2.308	0.930	2.893	120.46	trans	PABBUR[16]

[a] Cis / trans indicate that the CF_3 and COO groups point in the same direction or in the opposite direction, respectively.

[b] The uppercase letters are the ref-codes of the structures in the CCDC (Cambridge Crystallographic Data Centre)

Figures

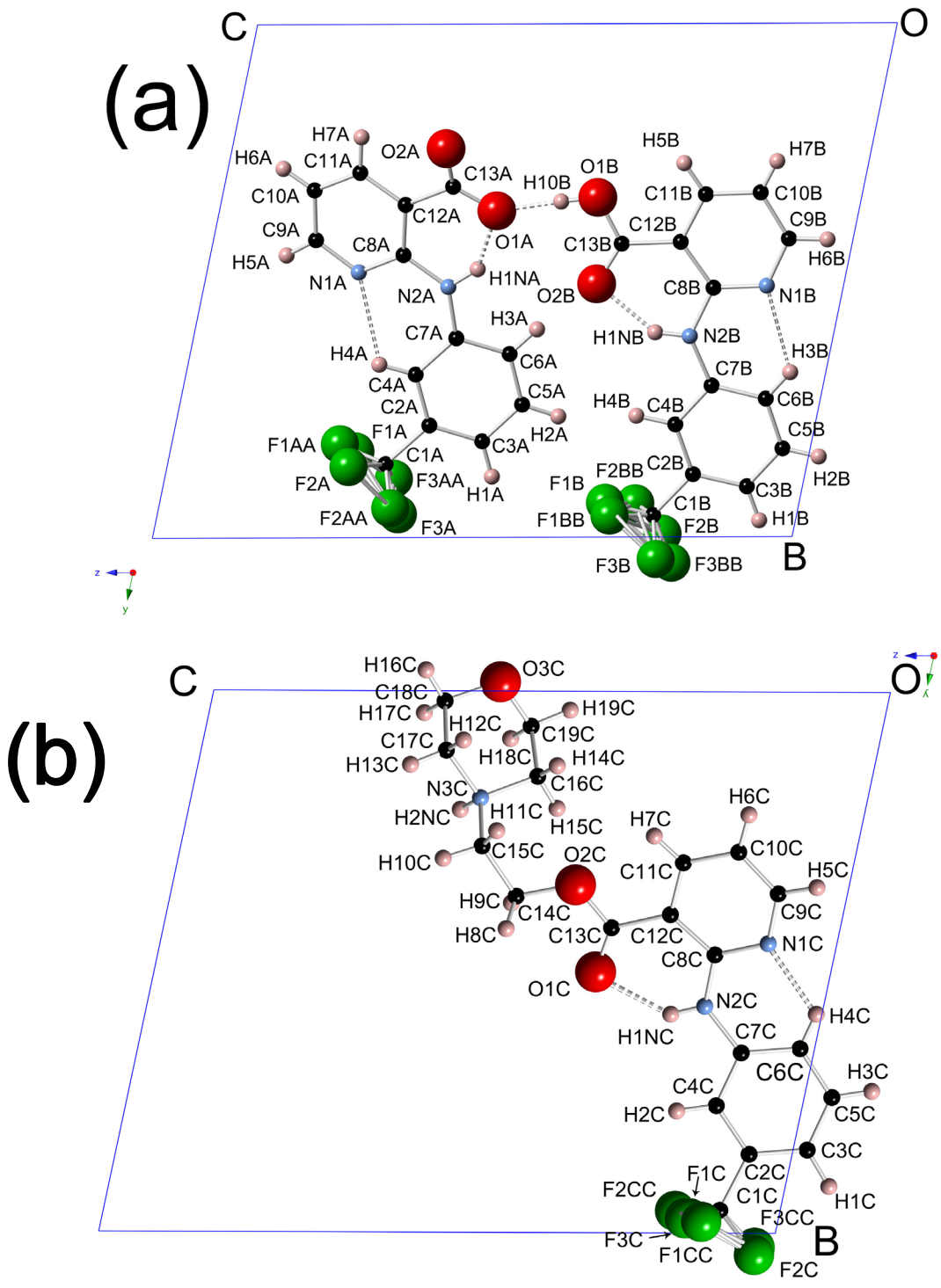


Figure S1. Atom labels in the unit-cell of morniflumate diniflumate: **(a)** niflumic acid A (left-hand side) and B (right-hand side) and **(b)** morniflumate. The molecules are projected on the *bc* plane. Intra- and intermolecular hydrogen bonds are indicated with dashed lines.

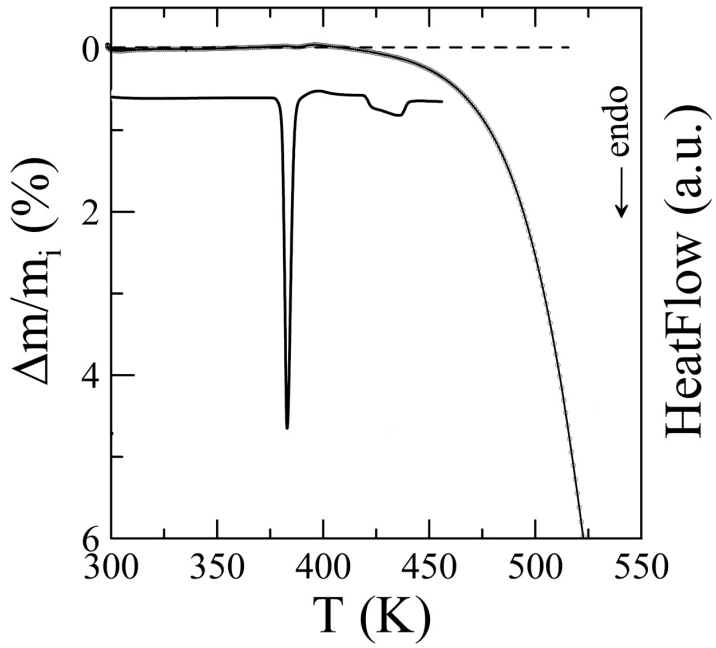


Figure S2. Differential scanning calorimetry and Thermogravimetric analysis curves of morniflumate diniflumate showing that, at 450 K, at the end of the DSC curve with the compound in the molten state, the weight loss is at most 0.5%. Heating rate: 10 K min^{-1}, sample masses: TG = 7.35 mg, DSC = 4.14 mg.

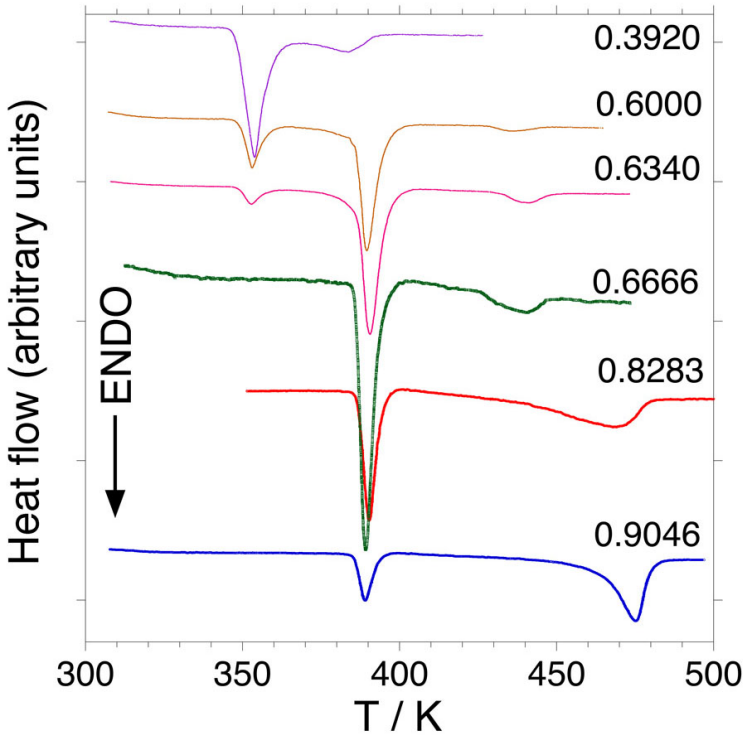


Figure S3. Typical DSC curves recorded on heating with mixtures of niflumic acid and morniflumate in various ratios at a rate of 10 K·min^{-1}. Mole fractions of niflumic acid are indicated on the right-hand side of the figure.

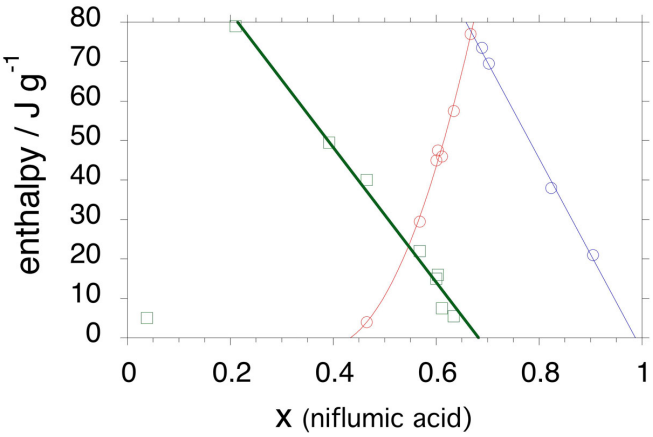


Figure S4. Tammann plots of the invariant lines of the niflumic acid – morniflumate phase diagram. Open circles = peritectic equilibrium whose left-hand side ends at about x = 0.40, the mol fraction of the peritectic liquid. Open squares = eutectic equilibrium whose right-hand side ends at about x = 0.66, the mol fraction of morniflumate diniflumate.

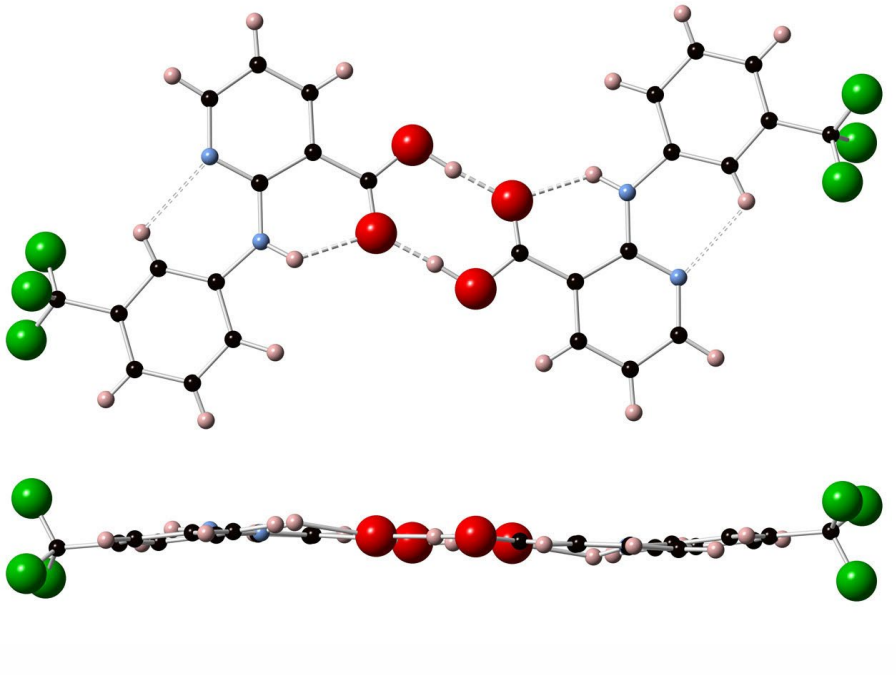


Figure S5. The niflumic acid hydrogen-bonded dimer viewed from the top (top) and from the side (bottom).[1] The C=O group is the acceptor of a bifurcated hydrogen bond. The dimer is almost planar due to the N-H···O bonds and C-H···N interactions that result in pseudo-cycles that are coplanar with the phenyl and pyridyl cycles (hydrogen bonds and weak interactions drawn as dashed lines).

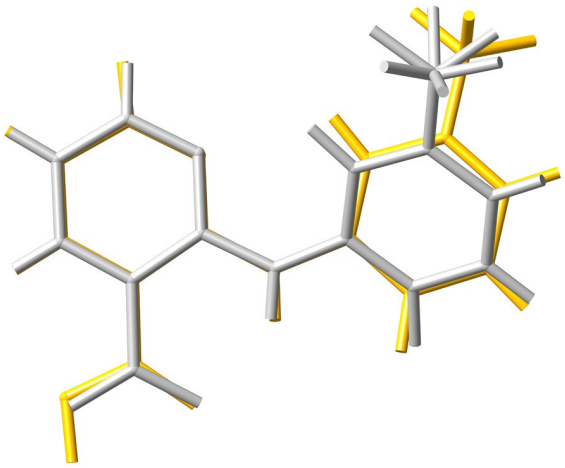


Figure S6. Niflumic acid molecule in its original crystal structure (yellow)[1] in comparison with the deprotonated ion in the niflumic acid-ethanolamine complex (grey)[10]. In both cases, the –COO and $-CF_3$ groups are oriented in opposite directions ('trans conformation').

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