Supplementary Material (ESI) for Analyst

Mechanisms Underlying a Non-Covalent Imprinted Polymer System: New Detail from Correlated Theoretical, Spectroscopic and X-ray Crystallographic Studies of Pre-polymerisation Events

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Figure s1. Distance between two naproxen molecules during 10ns simulation of system containing template, functional monomer, crosslinker and solvent, indicating a dimer with a lifetime of 2ns+ is formed.

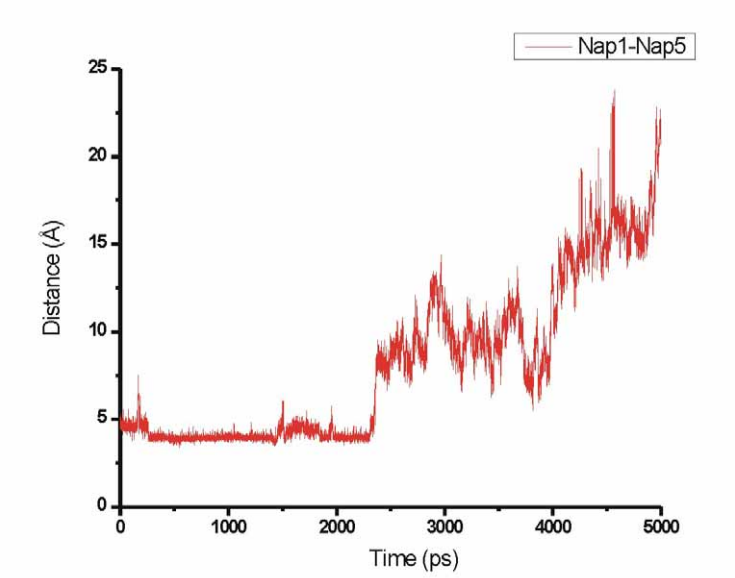

Figure s2. A naproxen unit interacting consecutively with 3 separate functional monomer units during the 10ns simulation including EGDMA.

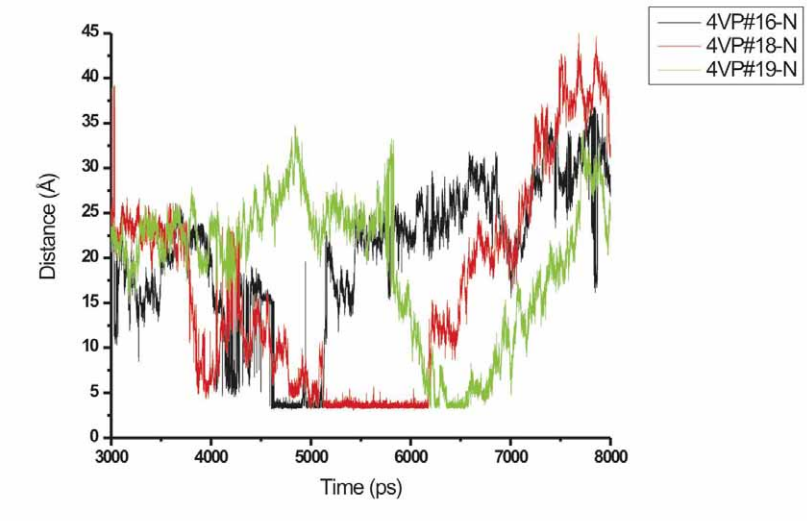

Figure s3. A naproxen unit interacts consecutively with the carbonyl groups of a EGDMA molecule during the 10ns simulation including crosslinker.

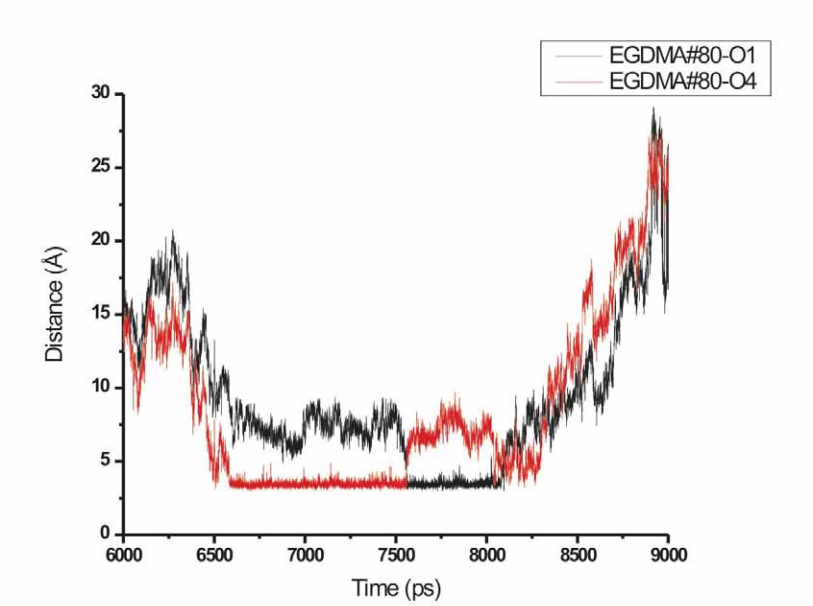

Figure s4. ^{1}H-NMR Titration of ethylene glycol dimethacrylate with 50mM naproxen in $CDCl_3$; protons studied were proton 3 and 2' on naproxen, as indicated in figure 2. The methine (2') proton displays no change, while proton 3 shows some very slight change (KD=0.79±0.2M).

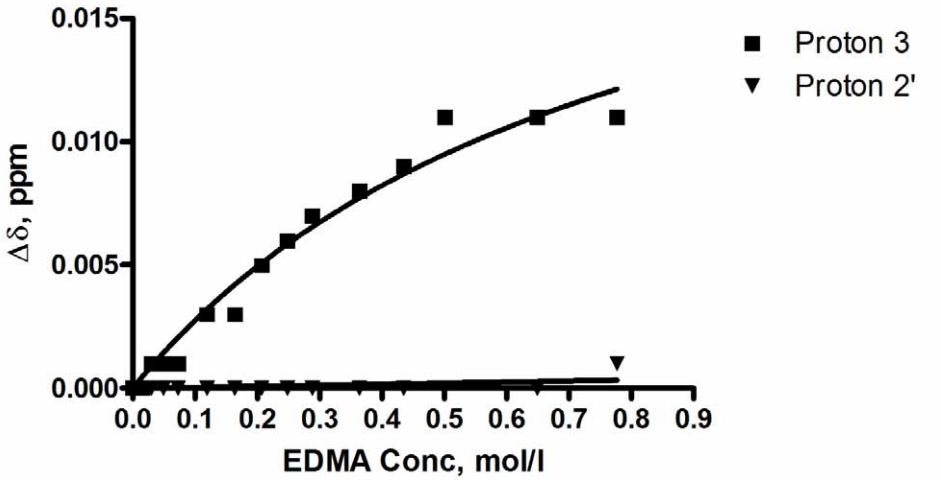

Figure s5. Front (left) and side (right) views of the grid representations of monomer density around a naproxen molecule (red). 4-VP nitrogen density is shown in blue, and EGDMA carbonyl oxygen is shown in green. A contour (i.e. frequency during simulation) level of 4 was chosen to examine the data.

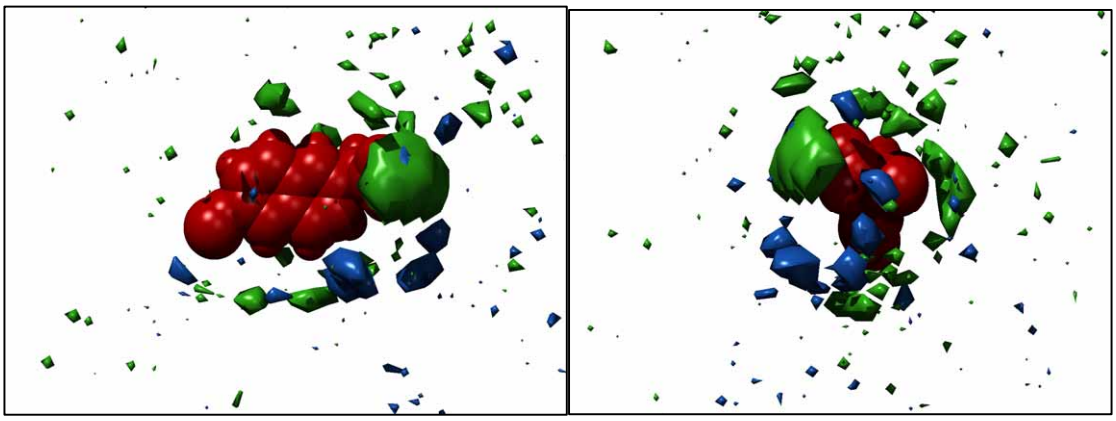

Table s1. Crystal data and structure refinement for naproxen-pyridine co-crystal.

Identification code	jmm01
Empirical formula	$C_{19}\ H_{19}\ N\ O_3$
Molecular formula	$[C_5\ H_6\ N]^+[C_{14}\ H_{13}\ O_3]^-$
Formula weight	309.35
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$ (#4)
Unit cell dimensions	a = 9.5594(12) Å α= 90°.
	b = 5.8786(7) Å β= 96.345(2)°.
	c = 29.704(4) Å γ = 90°.
Volume	1659.0(4) $Å^3$
Z	4
Density (calculated)	1.239 Mg/m^3
Absorption coefficient	0.084 mm^{-1}
F(000)	656
Crystal size	0.50 x 0.30 x 0.20 mm^3
Theta range for data collection	1.38 to 24.00°.
Index ranges	–10<=h<=10, –6<=k<=6, –33<=l<=33
Reflections collected	21891
Independent reflections	2886 [R(int) = 0.0239]
Completeness to theta = 24.00°	99.9 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.9834 and 0.8914
Refinement method	Full–matrix least–squares on F^2
Data / restraints / parameters	2886 / 1 / 419
Goodness–of–fit on F^2	1.067
Final R indices [I>2sigma(I)]	R1 = 0.0532, wR2 = 0.1493
R indices (all data)	R1 = 0.0609, wR2 = 0.1628
Largest diff. peak and hole	0.439 and –0.238 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jmm01. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	6742(4)	453(8)	10055(1)	63(1)
C(2)	6794(4)	1793(9)	10428(1)	66(1)
O(1)	6084(3)	1422(7)	10798(1)	79(1)
C(11)	5169(5)	–480(10)	10782(2)	86(1)
C(3)	7641(5)	3764(9)	10454(2)	80(1)
C(4)	8370(4)	4386(9)	10106(2)	77(1)
C(5)	8298(4)	3084(7)	9710(1)	60(1)
C(6)	8971(4)	3736(8)	9328(1)	66(1)
C(7)	8848(4)	2497(8)	8937(1)	64(1)
C(12)	9511(4)	3229(9)	8518(2)	74(1)
C(13)	11034(5)	3939(17)	8619(2)	126(3)
C(14)	8630(5)	5009(9)	8263(2)	78(1)
O(2)	7356(4)	5235(9)	8281(2)	130(2)
O(3)	9226(4)	6286(10)	8012(2)	147(2)
C(8)	8067(5)	467(8)	8926(2)	74(1)
C(9)	7419(4)	–237(8)	9285(1)	71(1)
C(10)	7494(4)	1066(7)	9685(1)	57(1)
C(15)	3150(4)	9768(8)	4889(1)	61(1)
C(16)	3148(4)	8666(9)	4480(1)	67(1)
O(4)	3838(3)	9338(7)	4129(1)	88(1)
C(25)	4838(5)	11112(11)	4207(2)	91(2)
C(17)	2368(4)	6649(9)	4404(1)	70(1)
C(18)	1649(4)	5741(8)	4729(1)	64(1)
C(19)	1664(3)	6796(7)	5154(1)	54(1)
C(20)	993(4)	5816(7)	5509(1)	60(1)
C(21)	1034(4)	6813(7)	5929(1)	58(1)
C(26)	335(4)	5672(9)	6301(1)	68(1)
C(27)	–669(5)	7227(12)	6521(2)	108(2)
C(28)	1378(4)	4635(8)	6659(1)	67(1)
O(5)	820(3)	3130(8)	6903(1)	101(1)
O(6)	2597(4)	5052(10)	6711(1)	128(2)

C(22)	1761(4)	8892(8)	5995(1)	64(1)
C(23)	2415(4)	9887(7)	5663(1)	63(1)
C(24)	2409(4)	8856(7)	5233(1)	54(1)
N(1)	2627(6)	3855(12)	2549(1)	106(2)
C(29)	2302(6)	5752(14)	2740(2)	100(2)
C(30)	3141(7)	6767(12)	3062(2)	106(2)
C(31)	4358(7)	5832(15)	3205(2)	107(2)
C(32)	4742(7)	3913(16)	3023(2)	114(2)
C(33)	3823(9)	2938(12)	2689(3)	115(2)
N(2)	7472(4)	6360(9)	2433(1)	84(1)
C(34)	6321(5)	7471(10)	2297(2)	85(1)
C(35)	5375(6)	6768(12)	1947(2)	95(2)
C(36)	5653(6)	4815(13)	1733(2)	102(2)
C(37)	6838(6)	3663(12)	1866(2)	110(2)
C(38)	7730(5)	4463(12)	2218(2)	97(2)

Table 3. Bond lengths [Å] and angles [°] for jmm01.

C(1)–C(2)	1.357(6)
C(1)–C(10)	1.424(5)
C(1)–H(1)	0.9300
C(2)–O(1)	1.371(5)
C(2)–C(3)	1.410(7)
O(1)–C(11)	1.417(6)
C(11)–H(11A)	0.9600
C(11)–H(11B)	0.9600
C(11)–H(11C)	0.9600
C(3)–C(4)	1.359(6)
C(3)–H(3)	0.9300
C(4)–C(5)	1.399(6)
C(4)–H(4)	0.9300
C(5)–C(10)	1.411(6)
C(5)–C(6)	1.418(5)
C(6)–C(7)	1.363(6)
C(6)–H(6)	0.9300
C(7)–C(8)	1.406(6)
C(7)–C(12)	1.522(6)
C(12)–C(14)	1.495(7)
C(12)–C(13)	1.513(7)
C(12)–H(12)	0.9800
C(13)–H(13A)	0.9600
C(13)–H(13B)	0.9600
C(13)–H(13C)	0.9600
C(14)–O(2)	1.232(5)
C(14)–O(3)	1.240(6)
C(8)–C(9)	1.356(6)
C(8)–H(8)	0.9300
C(9)–C(10)	1.407(5)
C(9)–H(9)	0.9300
C(15)–C(16)	1.377(6)
C(15)–C(24)	1.411(5)
C(15)–H(15)	0.9300

C(16)–O(4)	1.354(5)
C(16)–C(17)	1.406(7)
O(4)–C(25)	1.416(6)
C(25)–H(25A)	0.9600
C(25)–H(25B)	0.9600
C(25)–H(25C)	0.9600
C(17)–C(18)	1.356(6)
C(17)–H(17)	0.9300
C(18)–C(19)	1.404(5)
C(18)–H(18)	0.9300
C(19)–C(24)	1.411(5)
C(19)–C(20)	1.417(5)
C(20)–C(21)	1.374(5)
C(20)–H(20)	0.9300
C(21)–C(22)	1.409(6)
C(21)–C(26)	1.512(5)
C(26)–C(28)	1.504(6)
C(26)–C(27)	1.524(7)
C(26)–H(26)	0.9800
C(27)–H(27A)	0.9600
C(27)–H(27B)	0.9600
C(27)–H(27C)	0.9600
C(28)–O(6)	1.184(5)
C(28)–O(5)	1.296(5)
C(22)–C(23)	1.359(5)
C(22)–H(22)	0.9300
C(23)–C(24)	1.414(5)
C(23)–H(23)	0.9300
N(1)–C(33)	1.290(8)
N(1)–C(29)	1.304(9)
N(1)–H(1A)	0.8600
C(29)–C(30)	1.322(8)
C(29)–H(29)	0.9300
C(30)–C(31)	1.314(9)
C(30)–H(30)	0.9300
C(31)–C(32)	1.321(11)

C(31)–H(31)	0.9300
C(32)–C(33)	1.375(10)
C(32)–H(32)	0.9300
C(33)–H(33)	0.9300
N(2)–C(34)	1.305(6)
N(2)–C(38)	1.322(7)
N(2)–H(2)	0.8600
C(34)–C(35)	1.364(7)
C(34)–H(34)	0.9300
C(35)–C(36)	1.352(9)
C(35)–H(35)	0.9300
C(36)–C(37)	1.341(8)
C(36)–H(36)	0.9300
C(37)–C(38)	1.359(7)
C(37)–H(37)	0.9300
C(38)–H(38)	0.9300

C(2)–C(1)–C(10)	120.5(4)
C(2)–C(1)–H(1)	119.7
C(10)–C(1)–H(1)	119.7
C(1)–C(2)–O(1)	125.8(4)
C(1)–C(2)–C(3)	119.3(4)
O(1)–C(2)–C(3)	114.8(4)
C(2)–O(1)–C(11)	117.2(4)
O(1)–C(11)–H(11A)	109.5
O(1)–C(11)–H(11B)	109.5
H(11A)–C(11)–H(11B)	109.5
O(1)–C(11)–H(11C)	109.5
H(11A)–C(11)–H(11C)	109.5
H(11B)–C(11)–H(11C)	109.5
C(4)–C(3)–C(2)	121.3(4)
C(4)–C(3)–H(3)	119.3
C(2)–C(3)–H(3)	119.3
C(3)–C(4)–C(5)	120.7(4)
C(3)–C(4)–H(4)	119.6
C(5)–C(4)–H(4)	119.6

C(4)–C(5)–C(10)	118.7(4)
C(4)–C(5)–C(6)	122.7(4)
C(10)–C(5)–C(6)	118.5(4)
C(7)–C(6)–C(5)	122.1(4)
C(7)–C(6)–H(6)	118.9
C(5)–C(6)–H(6)	118.9
C(6)–C(7)–C(8)	118.0(4)
C(6)–C(7)–C(12)	122.7(4)
C(8)–C(7)–C(12)	119.2(4)
C(14)–C(12)–C(13)	112.6(5)
C(14)–C(12)–C(7)	110.5(4)
C(13)–C(12)–C(7)	113.2(4)
C(14)–C(12)–H(12)	106.7
C(13)–C(12)–H(12)	106.7
C(7)–C(12)–H(12)	106.7
C(12)–C(13)–H(13A)	109.5
C(12)–C(13)–H(13B)	109.5
H(13A)–C(13)–H(13B)	109.5
C(12)–C(13)–H(13C)	109.5
H(13A)–C(13)–H(13C)	109.5
H(13B)–C(13)–H(13C)	109.5
O(2)–C(14)–O(3)	118.9(5)
O(2)–C(14)–C(12)	123.9(5)
O(3)–C(14)–C(12)	117.2(4)
C(9)–C(8)–C(7)	121.8(4)
C(9)–C(8)–H(8)	119.1
C(7)–C(8)–H(8)	119.1
C(8)–C(9)–C(10)	120.8(4)
C(8)–C(9)–H(9)	119.6
C(10)–C(9)–H(9)	119.6
C(9)–C(10)–C(5)	118.6(4)
C(9)–C(10)–C(1)	122.0(4)
C(5)–C(10)–C(1)	119.4(4)
C(16)–C(15)–C(24)	120.5(4)
C(16)–C(15)–H(15)	119.8
C(24)–C(15)–H(15)	119.8

O(4)–C(16)–C(15)	126.1(4)
O(4)–C(16)–C(17)	114.6(4)
C(15)–C(16)–C(17)	119.3(4)
C(16)–O(4)–C(25)	117.7(4)
O(4)–C(25)–H(25A)	109.5
O(4)–C(25)–H(25B)	109.5
H(25A)–C(25)–H(25B)	109.5
O(4)–C(25)–H(25C)	109.5
H(25A)–C(25)–H(25C)	109.5
H(25B)–C(25)–H(25C)	109.5
C(18)–C(17)–C(16)	121.2(4)
C(18)–C(17)–H(17)	119.4
C(16)–C(17)–H(17)	119.4
C(17)–C(18)–C(19)	120.7(4)
C(17)–C(18)–H(18)	119.6
C(19)–C(18)–H(18)	119.6
C(18)–C(19)–C(24)	118.9(4)
C(18)–C(19)–C(20)	121.9(4)
C(24)–C(19)–C(20)	119.1(3)
C(21)–C(20)–C(19)	122.2(4)
C(21)–C(20)–H(20)	118.9
C(19)–C(20)–H(20)	118.9
C(20)–C(21)–C(22)	117.5(4)
C(20)–C(21)–C(26)	120.2(4)
C(22)–C(21)–C(26)	122.2(4)
C(28)–C(26)–C(21)	112.7(3)
C(28)–C(26)–C(27)	109.9(4)
C(21)–C(26)–C(27)	113.4(4)
C(28)–C(26)–H(26)	106.8
C(21)–C(26)–H(26)	106.8
C(27)–C(26)–H(26)	106.8
C(26)–C(27)–H(27A)	109.5
C(26)–C(27)–H(27B)	109.5
H(27A)–C(27)–H(27B)	109.5
C(26)–C(27)–H(27C)	109.5
H(27A)–C(27)–H(27C)	109.5

H(27B)–C(27)–H(27C)	109.5
O(6)–C(28)–O(5)	121.9(4)
O(6)–C(28)–C(26)	125.1(4)
O(5)–C(28)–C(26)	113.0(4)
C(23)–C(22)–C(21)	122.0(4)
C(23)–C(22)–H(22)	119.0
C(21)–C(22)–H(22)	119.0
C(22)–C(23)–C(24)	121.1(4)
C(22)–C(23)–H(23)	119.4
C(24)–C(23)–H(23)	119.5
C(15)–C(24)–C(19)	119.4(3)
C(15)–C(24)–C(23)	122.6(4)
C(19)–C(24)–C(23)	118.0(4)
C(33)–N(1)–C(29)	117.5(6)
C(33)–N(1)–H(1A)	121.2
C(29)–N(1)–H(1A)	121.2
N(1)–C(29)–C(30)	123.1(6)
N(1)–C(29)–H(29)	118.5
C(30)–C(29)–H(29)	118.5
C(31)–C(30)–C(29)	119.4(6)
C(31)–C(30)–H(30)	120.3
C(29)–C(30)–H(30)	120.3
C(30)–C(31)–C(32)	120.1(6)
C(30)–C(31)–H(31)	120.0
C(32)–C(31)–H(31)	120.0
C(31)–C(32)–C(33)	117.9(6)
C(31)–C(32)–H(32)	121.1
C(33)–C(32)–H(32)	121.1
N(1)–C(33)–C(32)	122.1(6)
N(1)–C(33)–H(33)	119.0
C(32)–C(33)–H(33)	119.0
C(34)–N(2)–C(38)	117.9(4)
C(34)–N(2)–H(2)	121.0
C(38)–N(2)–H(2)	121.0
N(2)–C(34)–C(35)	123.4(5)
N(2)–C(34)–H(34)	118.3

C(35)–C(34)–H(34)	118.3
C(36)–C(35)–C(34)	117.8(5)
C(36)–C(35)–H(35)	121.1
C(34)–C(35)–H(35)	121.1
C(37)–C(36)–C(35)	119.6(5)
C(37)–C(36)–H(36)	120.2
C(35)–C(36)–H(36)	120.2
C(36)–C(37)–C(38)	119.4(6)
C(36)–C(37)–H(37)	120.3
C(38)–C(37)–H(37)	120.3
N(2)–C(38)–C(37)	121.9(5)
N(2)–C(38)–H(38)	119.0
C(37)–C(38)–H(38)	119.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for jmm01. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	65(2)	52(2)	67(2)	1(2)	–6(2)	–6(2)
C(2)	60(2)	64(3)	71(2)	–4(2)	–8(2)	1(2)
O(1)	79(2)	88(2)	69(2)	–11(2)	8(1)	–12(2)
C(11)	90(3)	82(3)	86(3)	6(3)	14(2)	–8(3)
C(3)	79(3)	73(3)	85(3)	–24(3)	–3(2)	–12(3)
C(4)	72(3)	62(3)	96(3)	–18(3)	3(2)	–17(2)
C(5)	51(2)	49(2)	78(2)	–1(2)	–4(2)	–2(2)
C(6)	53(2)	52(2)	91(3)	2(2)	1(2)	–5(2)
C(7)	57(2)	57(3)	78(3)	5(2)	–2(2)	5(2)
C(12)	74(3)	66(3)	81(3)	8(2)	9(2)	2(2)
C(13)	74(3)	184(8)	120(4)	52(5)	9(3)	–9(4)
C(14)	93(3)	70(3)	72(3)	2(3)	11(2)	2(3)
O(2)	81(2)	108(3)	192(4)	57(3)	–24(2)	–10(2)
O(3)	117(3)	157(5)	178(4)	90(4)	73(3)	43(3)
C(8)	86(3)	61(3)	72(3)	–8(2)	1(2)	–6(2)
C(9)	89(3)	50(2)	73(2)	–7(2)	1(2)	–18(2)
C(10)	58(2)	43(2)	67(2)	–2(2)	–8(2)	3(2)
C(15)	59(2)	51(2)	70(2)	0(2)	–8(2)	–9(2)
C(16)	62(2)	70(3)	67(2)	–3(2)	–4(2)	–7(2)
O(4)	90(2)	104(3)	70(2)	–9(2)	11(2)	–33(2)
C(25)	85(3)	92(4)	96(3)	3(3)	17(3)	–28(3)
C(17)	68(2)	69(3)	71(2)	–15(2)	0(2)	–9(2)
C(18)	56(2)	52(2)	82(3)	–14(2)	–9(2)	–8(2)
C(19)	48(2)	45(2)	64(2)	0(2)	–9(2)	5(2)
C(20)	55(2)	45(2)	78(2)	6(2)	–10(2)	–3(2)
C(21)	54(2)	49(2)	68(2)	9(2)	–7(2)	2(2)
C(26)	59(2)	70(3)	73(2)	9(2)	0(2)	1(2)
C(27)	90(3)	101(5)	140(5)	36(4)	43(3)	29(3)
C(28)	62(2)	65(3)	73(2)	8(2)	3(2)	–5(2)
O(5)	86(2)	115(3)	101(2)	46(2)	7(2)	–17(2)
O(6)	82(2)	160(4)	134(3)	86(3)	–24(2)	–28(3)

C(22)	70(2)	54(2)	63(2)	–1(2)	–6(2)	5(2)
C(23)	73(2)	41(2)	70(2)	1(2)	–8(2)	–6(2)
C(24)	54(2)	45(2)	61(2)	1(2)	–7(2)	3(2)
N(1)	112(4)	133(5)	75(3)	–28(3)	17(3)	–37(4)
C(29)	93(4)	118(5)	88(4)	9(4)	8(3)	21(4)
C(30)	138(5)	77(4)	108(4)	–17(4)	39(4)	3(4)
C(31)	104(4)	133(6)	83(3)	–17(4)	3(3)	–27(5)
C(32)	89(4)	138(7)	118(5)	30(5)	25(4)	33(4)
C(33)	145(6)	71(3)	145(6)	–14(4)	85(5)	–1(4)
N(2)	79(2)	99(3)	73(2)	–29(2)	2(2)	4(2)
C(34)	98(3)	78(3)	83(3)	–15(3)	25(3)	16(3)
C(35)	93(3)	114(5)	79(3)	15(4)	14(3)	35(4)
C(36)	99(4)	126(5)	76(3)	–16(4)	–11(3)	5(4)
C(37)	138(5)	102(5)	86(3)	–40(4)	–6(3)	27(4)
C(38)	92(3)	108(5)	86(3)	–26(4)	–3(3)	26(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for jmm01.

Atom	x	y	z	U(eq)
H(1)	6212	–877	10040	75
H(11A)	4503	–385	10516	129
H(11B)	4677	–490	11046	129
H(11C)	5708	–1854	10772	129
H(3)	7701	4656	10714	96
H(4)	8922	5691	10131	93
H(6)	9513	5053	9344	79
H(12)	9498	1895	8319	89
H(13A)	11422	4238	8341	189
H(13B)	11557	2739	8780	189
H(13C)	11091	5289	8802	189
H(8)	7992	–418	8665	88
H(9)	6920	–1598	9268	85
H(15)	3644	11124	4939	73
H(25A)	4358	12523	4244	136
H(25B)	5376	11228	3954	136
H(25C)	5456	10788	4476	136
H(17)	2344	5924	4124	84
H(18)	1140	4405	4670	77
H(20)	508	4453	5457	72
H(26)	–231	4419	6160	82
H(27A)	–155	8493	6661	162
H(27B)	–1102	6394	6747	162
H(27C)	–1383	7775	6294	162
H(22)	1794	9605	6276	76
H(23)	2875	11269	5719	75
H(1A)	2065	3237	2338	127
H(29)	1438	6423	2645	120
H(30)	2874	8130	3187	127
H(31)	4950	6522	3435	128
H(32)	5606	3242	3117	137

H(33)	4071	1575	2560	138
H(2)	8044	6847	2656	101
H(34)	6136	8812	2445	103
H(35)	4565	7604	1858	114
H(36)	5026	4275	1495	122
H(37)	7047	2331	1719	132
H(38)	8546	3651	2311	116

Table 6. Torsion angles [°] for jmm01.

C(10)–C(1)–C(2)–O(1)	177.8(4)
C(10)–C(1)–C(2)–C(3)	–2.2(6)
C(1)–C(2)–O(1)–C(11)	–2.7(6)
C(3)–C(2)–O(1)–C(11)	177.3(4)
C(1)–C(2)–C(3)–C(4)	2.1(7)
O(1)–C(2)–C(3)–C(4)	–177.9(4)
C(2)–C(3)–C(4)–C(5)	0.2(7)
C(3)–C(4)–C(5)–C(10)	–2.3(6)
C(3)–C(4)–C(5)–C(6)	176.1(4)
C(4)–C(5)–C(6)–C(7)	–177.4(4)
C(10)–C(5)–C(6)–C(7)	0.9(6)
C(5)–C(6)–C(7)–C(8)	–2.4(6)
C(5)–C(6)–C(7)–C(12)	177.3(4)
C(6)–C(7)–C(12)–C(14)	–79.5(5)
C(8)–C(7)–C(12)–C(14)	100.1(5)
C(6)–C(7)–C(12)–C(13)	47.7(7)
C(8)–C(7)–C(12)–C(13)	–132.7(6)
C(13)–C(12)–C(14)–O(2)	–152.9(6)
C(7)–C(12)–C(14)–O(2)	–25.3(7)
C(13)–C(12)–C(14)–O(3)	29.0(7)
C(7)–C(12)–C(14)–O(3)	156.6(5)
C(6)–C(7)–C(8)–C(9)	1.6(6)
C(12)–C(7)–C(8)–C(9)	–178.1(4)
C(7)–C(8)–C(9)–C(10)	0.7(7)
C(8)–C(9)–C(10)–C(5)	–2.2(6)
C(8)–C(9)–C(10)–C(1)	175.4(4)
C(4)–C(5)–C(10)–C(9)	179.8(4)
C(6)–C(5)–C(10)–C(9)	1.4(5)
C(4)–C(5)–C(10)–C(1)	2.1(5)
C(6)–C(5)–C(10)–C(1)	–176.3(3)
C(2)–C(1)–C(10)–C(9)	–177.5(4)
C(2)–C(1)–C(10)–C(5)	0.1(5)
C(24)–C(15)–C(16)–O(4)	–178.5(4)
C(24)–C(15)–C(16)–C(17)	1.7(6)

C(15)–C(16)–O(4)–C(25)	11.1(7)
C(17)–C(16)–O(4)–C(25)	–169.1(4)
O(4)–C(16)–C(17)–C(18)	178.5(4)
C(15)–C(16)–C(17)–C(18)	–1.7(6)
C(16)–C(17)–C(18)–C(19)	0.0(6)
C(17)–C(18)–C(19)–C(24)	1.7(5)
C(17)–C(18)–C(19)–C(20)	–176.1(4)
C(18)–C(19)–C(20)–C(21)	178.3(3)
C(24)–C(19)–C(20)–C(21)	0.5(5)
C(19)–C(20)–C(21)–C(22)	0.8(5)
C(19)–C(20)–C(21)–C(26)	–178.4(3)
C(20)–C(21)–C(26)–C(28)	106.4(4)
C(22)–C(21)–C(26)–C(28)	–72.8(5)
C(20)–C(21)–C(26)–C(27)	–128.0(4)
C(22)–C(21)–C(26)–C(27)	52.9(5)
C(21)–C(26)–C(28)–O(6)	16.1(7)
C(27)–C(26)–C(28)–O(6)	–111.4(6)
C(21)–C(26)–C(28)–O(5)	–161.4(4)
C(27)–C(26)–C(28)–O(5)	71.0(6)
C(20)–C(21)–C(22)–C(23)	–0.7(5)
C(26)–C(21)–C(22)–C(23)	178.5(4)
C(21)–C(22)–C(23)–C(24)	–0.8(6)
C(16)–C(15)–C(24)–C(19)	0.1(5)
C(16)–C(15)–C(24)–C(23)	178.0(4)
C(18)–C(19)–C(24)–C(15)	–1.7(5)
C(20)–C(19)–C(24)–C(15)	176.2(3)
C(18)–C(19)–C(24)–C(23)	–179.8(3)
C(20)–C(19)–C(24)–C(23)	–1.8(5)
C(22)–C(23)–C(24)–C(15)	–175.9(3)
C(22)–C(23)–C(24)–C(19)	2.0(5)
C(33)–N(1)–C(29)–C(30)	0.7(9)
N(1)–C(29)–C(30)–C(31)	–0.8(10)
C(29)–C(30)–C(31)–C(32)	1.0(10)
C(30)–C(31)–C(32)–C(33)	–1.0(10)
C(29)–N(1)–C(33)–C(32)	–0.7(9)
C(31)–C(32)–C(33)–N(1)	0.9(10)

C(38)–N(2)–C(34)–C(35)	0.4(8)
N(2)–C(34)–C(35)–C(36)	0.1(9)
C(34)–C(35)–C(36)–C(37)	–0.7(9)
C(35)–C(36)–C(37)–C(38)	1.0(10)
C(34)–N(2)–C(38)–C(37)	–0.1(8)
C(36)–C(37)–C(38)–N(2)	–0.5(10)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for jmm01 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
N(2)–H(2)...O(5)#1	0.86	1.77	2.631(5)	174.3
N(1)–H(1A)...O(3)#2	0.86	1.91	2.747(6)	165.1

Symmetry transformations used to generate equivalent atoms:

#1 –x+1,y+1/2,–z+1 #2 –x+1,y–1/2,–z+1