Macromolecules

Macromolecules, 1996, 29(6), 1904-1909, DOI:10.1021/ma951275f

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4-1909-1

Table I. Fractional atomic cordinates and equivalent isotropic temperature factors for non-hydrogen atoms in methyl crotonate 6mer-**A**

atom	x	y	z	B_{eq}
O(1)	0.4138(8)	0.0070(6)	0.207(2)	5.8(4)
O(2)	0.4162(8)	0.1225(6)	0.336(1)	4.9(4)
O(3)	0.2395(9)	0.2855(7)	-0.009(2)	7.7(4)
O(4)	0.3777(8)	0.2979(6)	0.195(1)	5.4(4)
O(5)	0.5892(9)	0.2638(7)	-0.308(2)	6.6(4)
O(6)	0.5318(9)	0.3810(7)	-0.235(2)	6.2(4)
O(7)	0.5873(9)	0.4043(7)	0.232(2)	6.3(4)
O(8)	0.6977(8)	0.4368(6)	0.096(1)	5.1(4)
O(9)	0.981(1)	0.2221(8)	0.376(2)	13.3(7)
O(10)	1.0014(9)	0.3399(8)	0.492(2)	8.5(5)
O(11)	0.948(1)	0.4861(8)	0.175(2)	10.4(6)
O(12)	1.1067(10)	0.4469(8)	0.272(2)	10.5(6)
C(1)	0.137(1)	0.0644(9)	0.321(2)	4.3(5)
C(2)	0.118(1)	0.042(1)	0.457(2)	6.0(6)
C(3)	0.138(2)	-0.030(1)	0.507(3)	8.2(8)
C(4)	0.183(2)	-0.077(1)	0.400(4)	8.8(9)
C(5)	0.203(2)	-0.053(1)	0.261(3)	7.7(8)
C(6)	0.182(1)	0.021(1)	0.211(2)	4.2(5)
C(7)	0.202(1)	0.0429(9)	0.057(2)	4.1(5)
C(8)	0.288(1)	0.1030(8)	0.098(2)	3.5(5)
C(9)	0.312(1)	0.1319(8)	-0.063(2)	2.7(4)
C(10)	0.379(1)	0.2000(8)	-0.011(2)	3.0(4)
C(11)	0.427(1)	0.2230(9)	-0.148(2)	4.1(5)
C(12)	0.5067(9)	0.2817(9)	-0.083(2)	3.9(5)
C(13)	0.592(1)	0.2524(8)	0.065(2)	3.9(5)
C(14)	0.680(1)	0.3062(9)	0.102(2)	3.9(5)
C(15)	0.776(1)	0.2815(9)	0.244(3)	5.3(6)
C(16)	0.871(1)	0.3230(9)	0.250(2)	4.1(5)
C(17)	0.898(1)	0.326(1)	0.081(3)	6.2(6)
C(18)	1.000(1)	0.360(1)	0.097(3)	9.0(8)
C(19)	0.109(1)	0.072(1)	-0.065(2)	8.5(8)
C(20)	0.377(1)	0.0691(9)	0.210(2)	2.9(4)
C(21)	0.508(1)	0.104(1)	0.447(2)	7.8(7)
C(22)	0.354(1)	0.0657(9)	-0.158(2)	5.4(6)
C(23)	0.324(1)	0.2637(8)	0.059(2)	3.0(5)
C(24)	0.336(1)	0.359(1)	0.273(2)	7.6(7)
C(25)	0.350(1)	0.252(1)	-0.299(2)	6.4(6)
C(26)	0.547(1)	0.307(1)	-0.224(2)	3.7(5)
C(27)	0.574(1)	0.411(1)	-0.355(3)	9.3(8)
C(28)	0.6316(10)	0.1713(9)	0.033(2)	4.7(5)
C(29)	0.647(1)	0.387(1)	0.155(2)	4.7(6)
C(30)	0.674(1)	0.514(1)	0.134(3)	8.1(7)
C(31)	0.753(1)	0.287(1)	0.416(2)	6.3(6)
C(32)	0.958(2)	0.287(1)	0.378(3)	7.7(7)
C(33)	1.087(1)	0.313(1)	0.616(3)	14.0(9)
C(34)	0.896(1)	0.250(1)	-0.019(3)	10.4(8)
C(35)	1.014(2)	0.437(1)	0.182(3)	7.4(8)
C(36)	1.130(2)	0.519(1)	0.346(4)	13(1)

4-1909-2

Table II. Fractional atomic cordinates and equivalent isotropic temperature factors for non-hydrogen atoms in methyl crotonate 7mer-**A**

atom	x	y	z	B_{eq}
O(1)	0.1125(3)	0.3940(2)	0.5717(5)	5.4(1)
O(2)	0.2158(3)	0.3338(2)	0.4533(4)	4.5(1)
O(3)	0.4726(3)	0.3433(2)	0.8436(5)	6.0(1)
O(4)	0.3894(2)	0.2454(2)	0.6582(4)	4.6(1)
O(5)	0.3917(3)	0.1458(2)	1.1778(4)	5.6(1)
O(6)	0.2364(2)	0.1590(2)	1.1608(4)	4.5(1)
O(7)	0.3637(3)	0.0735(2)	0.6384(5)	6.5(1)
O(8)	0.3877(3)	0.0036(2)	0.8223(5)	5.5(1)
O(9)	0.0042(3)	-0.1400(2)	0.6158(5)	5.2(1)
O(10)	0.1215(3)	-0.1887(2)	0.5131(4)	4.8(1)
O(11)	0.3663(4)	-0.1505(3)	0.9169(7)	9.4(2)
O(12)	0.2682(4)	-0.2490(3)	0.7461(6)	8.8(2)
O(13)	0.0309(3)	-0.3024(2)	0.9857(5)	6.3(1)
O(14)	0.1243(3)	-0.3858(2)	0.9265(5)	6.4(1)
C(1)	0.2074(5)	0.5485(3)	0.4887(8)	5.7(2)
C(2)	0.2065(5)	0.5712(4)	0.3432(9)	6.9(2)
C(3)	0.2869(7)	0.5735(4)	0.2796(8)	7.6(3)
C(4)	0.3681(6)	0.5520(4)	0.3563(9)	7.7(3)
C(5)	0.3686(5)	0.5287(3)	0.5018(8)	6.0(2)
C(6)	0.2888(4)	0.5272(3)	0.5701(6)	3.8(1)
C(7)	0.2900(4)	0.5030(3)	0.7301(6)	3.8(1)
C(8)	0.2835(3)	0.4181(2)	0.7028(6)	3.2(1)
C(9)	0.2854(4)	0.3875(3)	0.8596(6)	3.5(1)
C(10)	0.3020(3)	0.3070(2)	0.8327(5)	2.9(1)
C(11)	0.3001(3)	0.2726(3)	0.9852(6)	3.2(1)
C(12)	0.3098(3)	0.1898(3)	0.9511(6)	3.0(1)
C(13)	0.2285(3)	0.1376(2)	0.8115(6)	3.1(1)
C(14)	0.2459(3)	0.0562(2)	0.8021(5)	3.2(1)
C(15)	0.1600(3)	-0.0046(2)	0.6964(6)	3.2(1)
C(16)	0.1733(3)	-0.0824(2)	0.7249(6)	3.0(1)
C(17)	0.1841(3)	-0.0914(3)	0.9041(6)	3.4(1)
C(18)	0.1940(4)	-0.1719(3)	0.9150(6)	3.9(1)
C(19)	0.2013(4)	-0.1874(3)	1.0879(7)	4.5(2)
C(20)	0.2047(4)	-0.2694(3)	1.0843(7)	5.1(2)
C(21)	0.3787(5)	0.5445(3)	0.8619(6)	6.1(2)
C(22)	0.1932(4)	0.3817(3)	0.5720(6)	3.5(1)
C(23)	0.1357(4)	0.3009(3)	0.3158(7)	6.0(2)
C(24)	0.1966(4)	0.3989(3)	0.9333(6)	5.0(2)
C(25)	0.3979(4)	0.3018(3)	0.7822(6)	3.5(1)
C(26)	0.4781(4)	0.2343(3)	0.6068(8)	7.1(2)
C(27)	0.3760(4)	0.3167(3)	1.1355(6)	4.6(2)
C(28)	0.3195(4)	0.1623(3)	1.1081(6)	3.6(1)
C(29)	0.2360(5)	0.1306(3)	1.3052(7)	6.7(2)
C(30)	0.1238(4)	0.1461(3)	0.8248(6)	4.1(1)
C(31)	0.3396(4)	0.0472(3)	0.7435(7)	3.9(2)
C(32)	0.4748(4)	-0.0125(3)	0.7722(9)	8.0(2)
C(33)	0.1433(4)	-0.0034(3)	0.5158(6)	4.7(2)
C(34)	0.0886(4)	-0.1386(3)	0.6141(6)	3.7(1)
C(35)	0.0508(5)	-0.2504(3)	0.4136(7)	6.5(2)
C(36)	0.1016(4)	-0.0665(3)	0.9796(6)	4.7(2)
C(37)	0.2867(5)	-0.1900(4)	0.8514(10)	6.2(2)
C(38)	0.3589(5)	-0.2582(4)	0.6830(10)	10.9(3)
C(39)	0.2857(5)	-0.1387(3)	1.2194(7)	7.1(2)
C(40)	0.1094(5)	-0.3187(3)	0.9936(7)	4.7(2)
C(41)	0.0383(5)	-0.4373(3)	0.8388(9)	7.9(2)

4-1909-3

Table III. Fractional atomic cordinates and equivalent isotropic temperature factors for non-hydrogen atoms in methyl crotonate 7mer-**B**

atom	x	y	z	Beq
O(1)	-0.3783(9)	0.0826(7)	0.277(1)	7.8(4)
O(2)	-0.2351(9)	0.0674(6)	0.191(1)	7.3(4)
O(3)	-0.3017(8)	0.3682(6)	0.493(1)	7.3(4)
O(4)	-0.2581(7)	0.2812(5)	0.676(1)	5.5(3)
O(5)	-0.1065(8)	0.0891(6)	0.540(1)	6.3(4)
O(6)	-0.0592(7)	0.1595(6)	0.744(1)	6.5(4)
O(7)	0.1904(7)	0.2574(6)	0.417(1)	6.8(4)
O(8)	0.2644(7)	0.1784(5)	0.606(1)	4.8(3)
O(9)	0.1361(8)	0.1785(6)	0.942(1)	6.2(4)
O(10)	0.2747(8)	0.2176(5)	0.985(1)	5.8(3)
O(11)	0.1116(8)	0.4984(6)	1.171(1)	6.9(4)
O(12)	0.2380(7)	0.4176(5)	1.297(1)	5.2(3)
O(13)	0.4013(8)	0.5564(6)	0.916(1)	7.0(4)
O(14)	0.4130(7)	0.4478(6)	0.776(1)	5.8(3)
C(1)	-0.344(1)	0.1268(9)	-0.199(2)	5.2(5)
C(2)	-0.328(1)	0.072(1)	-0.319(2)	6.8(6)
C(3)	-0.379(1)	0.0179(10)	-0.341(2)	6.7(6)
C(4)	-0.447(1)	0.0188(8)	-0.248(2)	4.7(5)
C(5)	-0.466(1)	0.0734(9)	-0.128(2)	5.2(5)
C(6)	-0.4141(9)	0.1295(8)	-0.106(2)	3.9(4)
C(7)	-0.4318(9)	0.1917(8)	0.020(2)	4.2(4)
C(8)	-0.3430(9)	0.1844(8)	0.152(2)	3.8(4)
C(9)	-0.359(1)	0.2477(7)	0.285(2)	4.2(4)
C(10)	-0.2689(10)	0.2355(6)	0.412(1)	3.4(4)
C(11)	-0.1680(9)	0.2230(7)	0.354(1)	3.4(4)
C(12)	-0.083(1)	0.2128(7)	0.494(1)	3.6(4)
C(13)	0.0196(9)	0.2048(7)	0.449(1)	3.5(4)
C(14)	0.096(1)	0.2154(7)	0.589(1)	3.2(4)
C(15)	0.0633(8)	0.2861(7)	0.695(1)	2.8(3)
C(16)	0.1455(9)	0.2972(7)	0.829(1)	3.9(4)
C(17)	0.1144(9)	0.3617(7)	0.951(1)	3.1(4)
C(18)	0.2007(9)	0.3937(7)	1.029(2)	3.2(4)
C(19)	0.243(1)	0.4364(7)	0.915(2)	3.7(4)
C(20)	0.3357(9)	0.4581(8)	1.000(2)	4.5(4)
C(21)	-0.462(1)	0.2695(9)	-0.050(2)	9.1(6)
C(22)	-0.321(1)	0.105(1)	0.215(2)	4.6(5)
C(23)	-0.213(1)	-0.0087(10)	0.254(2)	12.5(8)
C(24)	-0.451(1)	0.2545(9)	0.361(2)	7.6(6)
C(25)	-0.279(1)	0.3034(9)	0.526(2)	4.2(5)
C(26)	-0.250(1)	0.3406(9)	0.794(2)	7.5(6)
C(27)	-0.1633(10)	0.2865(8)	0.248(2)	5.7(5)
C(28)	-0.085(1)	0.1452(10)	0.593(2)	5.0(5)
C(29)	-0.056(1)	0.100(1)	0.846(2)	11.0(8)
C(30)	0.0522(10)	0.1298(8)	0.359(2)	5.5(5)
C(31)	0.1867(10)	0.2206(8)	0.521(2)	3.1(4)
C(32)	0.3550(9)	0.1878(9)	0.569(2)	6.9(5)
C(33)	0.0307(10)	0.3586(7)	0.603(2)	5.0(4)
C(34)	0.185(1)	0.222(1)	0.920(2)	4.9(5)
C(35)	0.303(1)	0.1508(10)	1.094(2)	9.5(6)
C(36)	0.0583(10)	0.3385(8)	1.070(1)	4.8(4)
C(37)	0.175(1)	0.4426(8)	1.171(2)	4.2(5)
C(38)	0.220(1)	0.4601(10)	1.441(2)	8.7(6)
C(39)	0.174(1)	0.5074(7)	0.847(2)	5.4(5)
C(40)	0.387(1)	0.4934(9)	0.896(2)	4.8(5)
C(41)	0.464(1)	0.4763(10)	0.674(2)	7.8(6)

Table III. (contd.)

4-1909-4

Table IV. Fractional atomic cordinates and equivalent isotropic temperature factors for non-hydrogen atoms in methyl crotonate 8mer-A

atom	x	y	z	Beq
O(1)	1.4511(2)	1.0478(5)	0.1409(2)	8.3(2)
O(2)	1.4537(2)	0.8488(5)	0.1884(1)	6.1(1)
O(3)	1.5236(2)	0.4963(5)	0.1520(1)	6.1(1)
O(4)	1.4184(2)	0.4999(4)	0.1811(1)	4.8(1)
O(5)	1.2864(2)	0.3681(5)	0.0193(1)	7.0(1)
O(6)	1.2941(2)	0.1924(5)	0.0748(1)	5.1(1)
O(7)	1.2615(2)	0.4055(5)	0.2041(1)	6.4(1)
O(8)	1.2043(2)	0.2233(5)	0.1665(1)	5.1(1)
O(9)	1.0018(2)	0.6428(5)	0.1196(2)	6.6(1)
O(10)	1.0022(2)	0.5617(5)	0.1936(1)	6.9(1)
O(11)	1.0339(2)	0.1539(5)	0.1908(1)	6.3(1)
O(12)	0.9290(2)	0.2534(5)	0.1818(1)	6.2(1)
O(13)	0.9108(2)	-0.0904(5)	0.0212(1)	7.6(1)
O(14)	0.8673(2)	-0.1764(4)	0.0874(1)	4.9(1)
O(15)	0.6840(3)	0.2347(7)	0.0440(2)	11.0(2)
O(16)	0.7388(3)	0.3733(7)	0.0969(2)	9.5(2)
C(1)	1.6148(3)	1.1520(10)	0.1563(3)	6.8(2)
C(2)	1.6566(5)	1.210(1)	0.1912(3)	10.9(4)
C(3)	1.7054(8)	1.113(2)	0.2117(5)	15.0(6)
C(4)	1.7107(8)	0.973(2)	0.1973(5)	13.8(5)
C(5)	1.6694(4)	0.9140(9)	0.1638(3)	8.4(3)
C(6)	1.6221(3)	1.0024(9)	0.1422(2)	5.3(2)
C(7)	1.5775(3)	0.9392(7)	0.1026(2)	5.0(2)
C(8)	1.5222(2)	0.8314(6)	0.1229(2)	3.8(1)
C(9)	1.4825(3)	0.7339(6)	0.0865(2)	4.3(2)
C(10)	1.4320(2)	0.6249(6)	0.1099(2)	3.5(1)
C(11)	1.3984(3)	0.5111(6)	0.0753(2)	4.1(2)
C(12)	1.3333(2)	0.4336(6)	0.0949(2)	3.4(1)
C(13)	1.2779(2)	0.5450(6)	0.1119(2)	3.6(1)
C(14)	1.2137(2)	0.4558(6)	0.1280(2)	3.1(1)
C(15)	1.1504(2)	0.5562(6)	0.1363(2)	3.5(1)
C(16)	1.0859(2)	0.4594(6)	0.1454(2)	3.3(1)
C(17)	1.0691(2)	0.3389(6)	0.1081(2)	3.3(1)
C(18)	0.9996(2)	0.2630(6)	0.1164(2)	3.2(1)
C(19)	0.9853(2)	0.1216(6)	0.0852(2)	3.7(1)
C(20)	0.9104(3)	0.0689(6)	0.0888(2)	3.7(1)
C(21)	0.8580(3)	0.1931(6)	0.0743(2)	4.2(2)
C(22)	0.7839(3)	0.1344(7)	0.0791(2)	5.6(2)
C(23)	1.6196(3)	0.8639(8)	0.0655(2)	8.9(2)
C(24)	1.4725(3)	0.9272(8)	0.1505(2)	4.8(2)
C(25)	1.4002(3)	0.9184(9)	0.2141(2)	10.2(3)
C(26)	1.4469(3)	0.8314(7)	0.0499(2)	7.4(2)
C(27)	1.4649(3)	0.5358(7)	0.1493(2)	4.4(2)
C(28)	1.4399(3)	0.3996(7)	0.2174(2)	7.0(2)
C(29)	1.4479(3)	0.3893(7)	0.0583(2)	6.3(2)
C(30)	1.3028(3)	0.3304(7)	0.0578(2)	4.3(2)
C(31)	1.2588(3)	0.0885(7)	0.0443(2)	8.0(2)
C(32)	1.2599(2)	0.6658(6)	0.0763(2)	5.5(2)

Table IV. (contd.)

atom	x	y	z	Beq
C(33)	1.2307(3)	0.3613(7)	0.1709(2)	3.8(2)
C(34)	1.2142(3)	0.1229(7)	0.2050(2)	7.4(2)
C(35)	1.1620(2)	0.6711(6)	0.1753(2)	5.5(2)
C(36)	1.0256(3)	0.5668(7)	0.1503(2)	4.5(2)
C(37)	0.9435(3)	0.6532(9)	0.2013(2)	11.6(3)
C(38)	1.0708(2)	0.4005(6)	0.0579(2)	4.7(2)
C(39)	0.9919(3)	0.2174(7)	0.1675(2)	4.2(2)
C(40)	0.9160(3)	0.2151(9)	0.2294(2)	10.6(3)
C(41)	1.0347(3)	-0.0086(6)	0.0952(2)	6.0(2)
C(42)	0.8979(3)	-0.0726(7)	0.0613(2)	4.7(2)
C(43)	0.8526(3)	-0.3172(7)	0.0655(2)	6.9(2)
C(44)	0.8678(3)	0.2573(7)	0.0254(2)	6.5(2)
C(45)	0.7316(4)	0.255(1)	0.0720(4)	8.9(4)
C(46)	0.6681(6)	0.451(1)	0.0773(4)	29.2(6)