Electronic Supplementary Information (ESI) for B814677B

Unusual reactivity of *N*-acyl imides: *N*-aroyl-1,2,4-dithiazolidine-3,5-diones as acyl isocyanate equivalents

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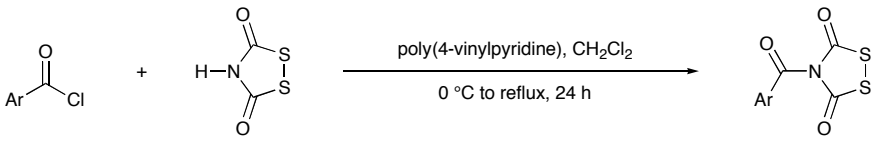
General experimental procedure for the preparation of *N*-aroyl-1,2,4-dithiazolidine-3,5-diones

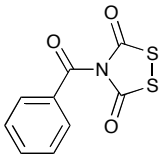


2 **5**

The acid chloride (1.00 mmol) was added dropwise to a stirred solution of 1,2,4-dithiazolidine-3,5-dione (100 mg, 0.74 mmol) in anhydrous dichloromethane (10 cm^3) containing poly(4-vinylpyridine) (116 mg), under a nitrogen atmosphere at 0 °C. The reaction mixture was allowed to warm to room temperature before heating under reflux for 24 h, after which time, the poly(4-vinylpyridine) was filtered off and the solvent was removed *in vacuo*. Recrystallisation by slow diffustion of pentane into a chloroform solution of the resulting residue at room temperature, gave the *N*-aroyl-1,2,4-dithiazolidine-3,5-dione as white needles.

Analytical/spectroscopic data for *N*-aroyl-1,2,4-dithiazolidine-3,5-diones

_N_-Benzoyl-1,2,4-dithiazolidine-3,5-dione 5a



5a

mp 94-96 °C

Found: C, 45.15; H, 1.98; N, 5.91. $C_9H_5NO_3S_2$ requires C, 45.18; H, 2.11; N, 5.85%

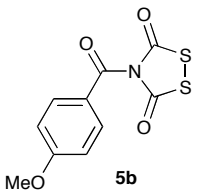
ν_{max}**/cm^{-1}** (KBr disc) 3073-2085 (w), 1763 (m), 1738 (s), 1710 (s), 1698 (s), 1677 (s), 1656 (s), 1259 (s), 1254 (m), 1180 (m), 1165 (m), 775 (m) and 679 (m)

δ_H (300 MHz; $CDCl_3$) 7.58 (2H, *ca* t, *J* = 7.5, phenylC*H*), 7.76 (1H, *ca* t, *J* = 6.0, phenylC*H*) and 7.96 (2H, *ca* d, *J* = 9.0, phenylC*H*)

δ_C (75 MHz; $CDCl_3$) 129.4, 129.5, 132.1 (phenyl*C*H), 136.3 (phenyl *ipso*C), 165.0 (Ph*C*(O)) and 165.2 (*C*(O)N*C*(O))

m/z (EI) 147 (fragmentation to benzoyl isocyanate, 9%), 105 (100), 77 (35) and 64 (10)

_N_-(4-Methoxybenzoyl)-1,2,4-dithiazolidine-3,5-dione 5b



5b

mp 108-109 °C

Found: C, 44.49; H, 2.33; N, 5.30, $C_{10}H_7NO_4S_2$ requires C, 44.60; H, 2.62; N, 5.20%

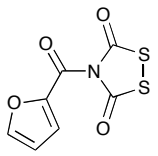
ν_{max}**/cm^{-1}** (Thin film) 2930-2843 (w), 1758 (m), 1735 (m), 1718 (m), 1666 (s), 1596 (s), 1510 (m), 1459 (w), 1425 (w), 1242 (s) and 1167 (s)

δ_H (300 MHz; $CDCl_3$) 3.92 (3H, s, CH_3) and 7.01, 7.90 (2 x 2H, AA'BB', *J* = 6.0, arylC*H*)

δ_C (75 MHz; $CDCl_3$) 55.9 (*C*H_3), 115.0 (aryl*C*H), 121.7 (aryl *ipso**C*-C=O), 133.9 (aryl*C*H), 163.8 (aryl *ipso**C*-O), 165.4 (*C*(O)N*C*(O)) and 166.2 (aryl-*C*(O))

m/z (EI) 177 (fragmentation to 4-methoxybenzoyl isocyanate, 24%), 135 (100), 107 (17), 92 (31), 84 (27), 77 (55), 64 (32), 63 (33), 51 (22), 49 (33) and 44 (18)

***N*-(2-Furoyl)-1,2,4-dithiazolidine-3,5-dione 5c**



5c

mp 115-117 °C

Found: C, 36.59; H, 1.23; N, 6.21%, $C_7H_3NO_4S_2$ requires C, 36.68; H, 1.32; N, 6.11%

ν_{max}**/cm^{-1}** (Thin film) 3144-3098 (w), 1728 (s), 1698 (s), 1656 (s), 1632 (m), 1462 (m), 1397 (w), 1278 (m), 1183 (m) and 995 (w)

δ_H (300 MHz; $CDCl_3$) 6.70 (1H, dd, *J* = 1.6 and 3.8, furoylC*H*), 7.55 (1H, d, *J* = 3.8, furoylC*H*) and 7.76 (1H, m, furoylC*H*)

δ_C (75 MHz; $CDCl_3$) 114.2, 125.1 (furoyl*C*H), 145.2 (furoyl *ipso**C*), 150.2 (furoyl*C*H), 153.3 (furoyl*C*(O)) and 164.9 (*C*(O)N*C*(O))

m/z (EI) 169 ((M-COS)$^+$, 25%), 149 (5), 141 (20), 137 (fragmentation to 2-furoyl isocyanate, 5), 111 (11), 105 (6), 95 (100), 86 (10), 84 (18), 49 (20) and 39 (27)