Communication

Reaction of 4,5-Dichloro-1,2,3-dithiazolium Chloride with 2-(Phenylsulfonyl)acetonitrile

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Abstract: The reaction of 4,5-dichloro-1,2,3-dithiazolium chloride with 2-(phenylsulfonyl)acetonitrile (1 equiv) in the presence of pyridine (2 equiv) gave S-(3-chloro-5-cyanoisothiazol-4-yl)benzene sulfonothioate and (Z)-2-(4-chloro-5H-1,2,3-dithiazol-5-ylidene)-2-(phenylsulfonyl)acetonitrile in 19% and 23% yield, respectively. The compounds were fully characterized and the mechanistic rationale is proposed for the formation of the benzensulfonate.

Keywords: heterocycle; polyfunctionalized; 1,2,3-dithiazole; sulfone; isothiazole

1. Introduction

Monocyclic 1,2,3-dithiazoles are sulfur-rich heterocycles that act as fungicides [1–3], antibacterials [4–6], antivirals [7,8] or anticancer agents [9–11]. Moreover, 1,2,3-dithiazolyls are potential organic magnets and/or conductors [12,13]. The field of monocyclic 1,2,3-dithiazoles took off over 35 years ago with the preparation of 4,5-dichloro-1,2,3-dithiazolium chloride 1 (aka Appel’s salt, Scheme 1) [14], which has been used extensively for the preparation of many neutral 5H-1,2,3-dithiazoles 2 [15]. The chemistry and applications of 1,2,3-dithiazoles have been reviewed [16–19].

![Scheme 1. Structure of Appel’s salt 1 and its neutral 5H-1,2,3-dithiazoles 2.](https://example.com/scheme1.png)

2. Results and Discussion

Recently, we investigated the biological activity of (5H-1,2,3-dithiazol-5-ylidene)-2-acetonitriles and required access to analogues that can be prepared from the condensation of Appel’s salt 1 with active methylenes [14,20,21]. While preparations for ylidene-acetonitriles 3–7 [14,20–23] and their derivatives 8–12 [24] are reported and the compounds are fully characterized, little is known about the only sulfone analogue 13 (Scheme 2). This compound was reported by Rees in 1992, quoting a low yield (exact number not reported) [25], but the reaction conditions or any characterization data of the product were not reported. We therefore repeated this synthesis to obtain and characterize the desired product 13. Interestingly, the carbonyl-containing (5H-1,2,3-dithiazol-5-ylidene)-2-acetonitriles 4–7 were assigned as the Z isomers due to stabilizing “non-bonding” interactions between the carbonyl oxygen and the dithiazole [26].

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The reaction of Appel’s salt 1 with 2-(phenylsulfonyl)acetonitrile (1 equiv) in DCM, for 1 h, followed by the addition of pyridine (2 equiv) and further stirring for 2 h gave two main products, the colorless S-[3-chloro-5-cyanothiazol-4-yl]benzenesulfonothioate (14) in 19% yield and the yellow colored (Z)-2-(4-chloro-5H-1,2,3-dithiazol-5-ylidene)-2-(phenylsulfonyl)acetonitrile (13) in 23% yield (Scheme 3).

Product 14 was isolated as colorless needles, m.p. 146–147 °C (from c-hexane). FTIR spectroscopy showed a cyano ν(C≡N) stretch at 2236 cm⁻¹ along with sulfone ν(S=O) stretches at 1335 and 1148 cm⁻¹, while mass spectrometry revealed a molecular ion [M + Na⁺] peak of m/z 339 (100%) along with a [M + Na⁺ +2] peak at 341 (45%), which supported the presence of a single chlorine. ¹³C NMR spectroscopy showed the presence of three CH resonances and five quaternary carbon resonances (see Supplementary Materials for the complete spectra), while a correct elemental analysis (CHN) was obtained for the molecular formula C₁₀H₅ClN₂O₂S₃. Structural support was also provided by single-crystal X-ray diffraction studies (Figure 1).

Product 13 was isolated as yellow needles, m.p. 181–183 °C (from c-hexane). UV–vis spectroscopy supports an intact dithiazole ring (λmax 433 nm, log ε 4.26). FTIR spectroscopy showed a cyano ν(C≡N) stretch at 2197 cm⁻¹ along with sulfone ν(S=O) stretches at 1315 and 1144 cm⁻¹, while mass spectrometry revealed a molecular ion [M + Na⁺] peak of m/z 339 (100%) along with a [M + Na⁺ +2] peak at 341 (44%) that supported the presence of a single chlorine. ¹³C-NMR spectroscopy showed the presence of three CH resonances and five quaternary carbon resonances (see Supplementary Materials for the complete spectra), while a correct elemental analysis (CHN) was obtained for the molecular formula C₁₀H₅ClN₂O₂S₃. We tentatively assigned the alkene geometry as Z owing to steric and electronic repulsion between the C-4 chloride and the sulfonyl group, while a “non-bonding” interaction between the sulfonyl oxygen and the dithiazole S1 is also possible [26].
The formation of isothiazole 14, which is a structural isomer of ylide 13, is mechanistically interesting. The conversion of (5H-1,2,3-dithiazol-5-ylidene)-2-acetonitriles to isothiazoles occurs in the presence of catalytic chloride [20] or anhydrous HCl or HBr [24], while isothiazoles can also be formed from the reaction of Appel’s salt 1 with enamines [21,27,28]. Tentatively, the reaction herein proceeds via the thiophilic attack of chloride at the S-1 position of dithiazole 13 to form the ring-opened disulfide 15 (Scheme 4). Rotation of the double bond in disulfide 15 enabled by resonance can give the more stable 1,2 alkene 16, which can then add chloride to the nitrile and cyclize onto sulfur to give isothiazole 17 with elimination of ‘SCI’. While isothiazole 17 was not observed, we propose that once formed it rapidly reacted its C-4 position with the electrophilic sulfur of either disulfide 15 or 16 to give intermediate 18. Subsequent attack by chloride on the disulfide group can lead to the stepwise migration of the phenylsulfone unit onto the sulfur via the spirocycle 19 and the formation of isothiazole 14. A few examples of such migrations leading to benzene-sulfonothioates have been reported and include a thermal rearrangement of aziridines [29], a chlorotropic rearrangement [30] and a photochemical reaction of diphenyl sulfone [31].

**3. Materials and Methods**

The reaction mixture was monitored by TLC using commercial glass-backed thin-layer chromatography (TLC) plates (Merck Kieselgel 60 F<sub>254</sub>). The plates were observed under UV light at 254 and 365 nm. The melting point was determined using a PolyTherm-A, Wagner & Munz, Kofler—Hotstage Microscope apparatus (Wagner & Munz, Munich,
The IR spectrum was recorded on a Shimadzu FTIR-NIR Prestige-21 spectrometer (Shimadzu, Kyoto, Japan) with Pike Miracle Ge ATR accessory (Pike Miracle, Madison, WI, USA) and strong, medium and weak peaks are represented by s, m and w, respectively. $^{1}$H and $^{13}$C NMR spectra were recorded on a Bruker Avance 500 machine at 500 and 125 MHz, respectively, (Bruker, Billerica, MA, USA). Deuterated solvents were used for homonuclear lock and the signals are referenced to the deuterated solvent peaks. Attached proton test (APT) NMR studies were used for the assignment of the $^{13}$C peaks as CH$_{3}$, CH$_{2}$, CH and C$_{q}$ (quaternary). The matrix-assisted laser desorption/ionization-time of flight (MALDI-TOF) mass spectrum (+ve mode) was recorded on a Bruker Autoflex III Smartbeam instrument (Bruker). 4,5-Dichloro-1,2,3-dithiazolium chloride (1) was prepared according to the literature procedure [14].

Reaction of Appel’s Salt 1 with 2-(Phenylsulfonyl)acetonitrile.

To a stirred suspension of 4,5-dichloro-1,2,3-dithiazolium chloride (1) (104.3 mg, 0.50 mmol) in DCM (2 mL) was added 2-(phenylsulfonyl)acetonitrile (90.6 mg, 0.50 mmol) and the reaction mixture was stirred at ca. 20 °C for 1 h. Pyridine (81 µL, 1.00 mmol) was then added and the reaction mixture was stirred for another 2 h. The mixture was then adsorbed onto silica and chromatographed (n-hexane/DCM 50:50) to give S-(3-chloro-5-cyanoisothiazol-4-yl)benzenesulfonothioate (14) (30.7 mg, 19%) as colorless needles, m.p. 146–147 °C (from c-hexane); Rf 0.33 (n-hexane/DCM 50:50); (found: C, 38.02; H, 1.70; N, 8.65). C$_{10}$H$_{7}$Cl$_{2}$N$_{2}$O$_{2}$S$_{2}$ requires C, 37.91; H, 1.59; N, 8.84%); $\lambda_{\text{max}}$(DCM)/nm 2236 (C≡N), 1454m, 1447m, 1335s (S=O), 1314w, 1294m, 1148s (S=O), 1076m, 997w, 959w, 827w, 758m, 718s; $\delta_{H}$ (500 MHz; CDCl$_{3}$) 7.76-7.71 (3H, m, Ar CH), 7.58 (2H, dd, J 8.4, 7.5, Ar CH); $\delta_{C}$ (125 MHz; CDCl$_{3}$) 165.1 (Cq), 143.9 (Cq), 142.7 (Cq), 135.2 (CH), 130.0 (CH), 129.0 (Cq), 127.5 (CH), 108.1 (Cq); m/z (MALDI-TOF) 357 (M + K$^{+}$+2, 40%), 355 (M + K$^{+}$, 48), 341 (M + Na$^{+}$+2, 45), 339 (M + Na$^{+}$, 100), 298 (22), 274 (40), 180 (18), 153 (15), 133 (18). Further elution (n-hexane/DCM 25:75) gave (Z)-2-(4-chloro-5H-1,2,3-dithiazol-5-ylidene)-2-(phenylsulfonyl)acetonitrile (13) (36.8 mg, 23%) as yellow needles, mp 181–183 °C (from c-hexane); Rf 0.37 (n-hexane/DCM 25:75); (found: C, 38.09; H, 1.42; N, 8.61). C$_{10}$H$_{7}$Cl$_{2}$N$_{2}$O$_{2}$S$_{2}$ requires C, 37.91; H, 1.59; N, 8.84%); $\lambda_{\text{max}}$(DCM)/nm 2243 (log $\varepsilon$ 4.16), 283 inf (3.78), 433 (4.26); $\nu_{\text{max}}$/cm$^{-1}$ 2197m (C≡N), 1481m, 1470s, 1447m, 1315m (S=O), 1294m, 1190m, 1144s (S=O), 1082m, 1045m, 997w, 916w, 860s, 799w, 760w, 721s; $\delta_{H}$ (500 MHz; CDCl$_{3}$) 8.03 (2H, dd, J 7.8, 1.3, Ar CH), 7.76 (1H, ddd, J 7.6, 6.1, 1.2, Ar CH), 7.63 (2H, dd, J 7.9, 7.9, Ar CH); $\delta_{C}$ (125 MHz; CDCl$_{3}$) 158.7 (Cq), 143.6 (Cq), 138.1 (Cq), 135.2 (CH), 129.7 (CH), 128.0 (Cq), 121.2 (Cq), 103.1 (Cq); m/z (MALDI-TOF) 357 (M + K$^{+}$+2, 9%), 355 (M + K$^{+}$, 22), 341 (M + Na$^{+}$+2, 44), 339 (M + Na$^{+}$, 100), 319 (MH$^{+}$+2, 5), 317 (MH$^{+}$, 17), 133 (35).

X-ray crystallographic studies on S-(3-chloro-5-cyanoisothiazol-4-yl)benzenesulfonothioate (14).

Data were collected on an Oxford-Diffraction Supernova diffractometer, equipped with a CCD area detector utilizing Cu-Kα radiation (λ = 1.5418 Å). A suitable crystal was attached to glass fibers using paratone-N oil and transferred to a goniostat where they were cooled for data collection. Unit cell dimensions were determined and refined by using 2397 (4.159° ≤ θ ≤ 71.800°) reflections. Empirical absorption corrections (multi-scan based on symmetry-related measurements) were applied using CrysAlis RED software [32]. The structures were solved by direct method and refined on F$^{2}$ using full-matrix least squares using SHELXL97 [35]. Software packages used: CrysAlis CCD [32] for data collection, CrysAlis RED [32] for cell refinement and data reduction, WINGX for geometric calculations [34], and DIAMOND [35] for molecular graphics. The non-H atoms were treated anisotropically. The hydrogen atoms were placed in calculated, ideal positions and refined as riding on their respective carbon atoms.
Crystal refinement data for S-(3-chloro-5-cyanoisothiazol-4-yl)benzenesulfonothioate (14): isolated as colorless needles (from DCE/n-pentane vapor diffusion), C_{9}H_{13}ClN_{2}O_{3}S_{2}, M = 316.79, orthorhombic, space group Pna21, a = 14.6164(12) Å, b = 15.4871(8) Å, c = 5.3576(3) Å, a = 90°, β = 90°, γ = 90°, V = 1212.63(14) Å³, Z = 4, T = 100(2) K, ρ_{calc} = 1.735 g cm^{-3}, ϕ_{max} = 71.800°. Refinement of 163 parameters on 1529 independent reflections out of 2397 measured reflections (R_{int} = 0.0358) led to R_{1} = 0.0431 (I > 2σ(I)), wR_{2} = 0.1141 (all data), and S = 1.211 with the largest difference peak and hole of 0.357 and −0.367 e Å^{-3}, respectively. (CCDC: 2132438).

Supplementary Materials: The following are available online: mol file, ¹H and ¹³C NMR spectra.

Author Contributions: A.S.K. and P.A.K. conceived the experiments; A.S.K. designed the experiments; K.P. performed the experiments and collected the data; P.A.K. grew the X-ray crystals; A.K. collected the X-ray crystallography data; A.S.K. wrote the paper; A.S.K. and P.A.K. edited the manuscript. All authors have read and agreed to the published version of the manuscript.

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References
1. Moore, J.E. Certain 4-Halo-5-Aryl-1,2,3-Dithiazole Compounds and Their Preparation. U.S. Patent 4,059,590, 22 November 1977.
2. Appel, R.; Janssen, H.; Haller, I.; Plempel, M. 1,2,3-Dithiazolderivate, Verfahren zu ihrer Herstellung Sowie ihre Verwendung als Arzneimittel. DE Patent 2,848,221, 14 May 1980.
3. Besson, T.; Rees, C.W.; Cottenceau, G.; Pons, A.-M. Antimicrobial evaluation of 3,1-benzoxazin-4-ones, 3,1-benzothiazin-4-ones, 4-alkoxyquinazolin-2-carbonitriles and N-arylimino-1,2,3-dithiazoles. Bioorg. Med. Chem. Lett. 1996, 6, 2343–2348. [CrossRef]
4. Cottenceau, G.; Besson, T.; Gautier, V.; Rees, C.W.; Pons, A.-M. ChemInform Abstract: Antibacterial Evaluation of Novel N-Arylimino-1,2,3-dithiazoles and N-Arylcyanothioformamides. Bioorg. Med. Chem. Lett. 1996, 6, 529–532. [CrossRef]
5. Thiéry, V.; Rees, C.W.; Besson, T.; Cottenceau, G.; Pons, A.-M. Antimicrobial activity of novel N-quinolinyl and N-naphthylimino-1,2,3-dithiazoles. Eur. J. Med. Chem. 1998, 33, 149–153. [CrossRef]
6. Joseph, R.W.; Antes, D.L.; Osei-Gyimah, P. Antimicrobial Compounds with Quick Speed of Kill. U.S. Patent 5,688,744, 3 November 1995.
7. Asquith, C.R.M.; Konstantinova, L.S.; Laitinen, T.; Meli, M.L.; Poso, A.; Rakitin, O.A.; Hofmann-Lehmann, R.; Hilton, S.T. Evaluation of Substituted 1,2,3-Dithiazoles as Inhibitors of the Feline Immunodeficiency Virus (FIV) Nucleocapsid Protein via a Proposed Zinc Ejection Mechanism. ChemMedChem 2016, 11, 2119–2126. [CrossRef]
8. Asquith, C.R.; Meeli, T.; Laitinen, T.; Baranovsky, I.V.; Konstantinova, L.S.; Poso, A.; Rakitin, O.A.; Hofmann-Lehmann, R. Synthesis and comparison of substituted 1,2,3-dithiazole and 1,2,3-thiaseleazene as inhibitors of the feline immunodeficiency virus (FIV) nucleocapsid protein as a model for HIV infection. Bioorg. Med. Chem. Lett. 2019, 29, 1765–1768. [CrossRef]
9. Konstantinova, L.S.; Bol’Shakov, O.I.; Obruchnikova, N.V.; Laborie, H.; Tanga, A.; Sopéna, V.; Lanneluc, I.; Picot, L.; Sablé, S.; Thiéry, V.; et al. One-pot synthesis of 5-phenylimino, 5-thieno or 5-oxo-1,2,3-dithiazoles and evaluation of their antimicrobial and antitumor activity. Bioorg. Med. Chem. Lett. 2009, 19, 136–141. [CrossRef]
10. Oppedisano, F.; Catto, M.; Koutentis, P.A.; Nicolotti, O.; Pochini, L.; Koyioni, M.; Introcaso, A.; Michaelidou, S.S.; Carotti, A.; Indiveri, C. Inactivation of the glutamine/amino acid transporter ASC2 by 1,2,3-dithiazoles: Proteoliposomes as a tool to gain insights in the molecular mechanism of action and of antigenicity. Toxicon. Appl. Pharmacol. 2012, 265, 93–102. [CrossRef]
11. Napoliolato, L.; Scalise, M.; Koyioni, M.; Koutentis, P.; Catto, M.; Eberini, I.; Parravincini, C.; Palazzolo, L.; Pisani, L.; Galluccio, M.; et al. Potent inhibitors of human LAT1 (SLC7A5) transporter based on dithiazole and dithiazine compounds for development of anticancer drugs. Biochem. Pharmacol. 2017, 143, 39–52. [CrossRef]
12. Barclay, T.M.; Cordes, A.W.; Beer, L.; Oakley, R.T.; Preuss, K.E.; Taylor, N.J.; Reed, R.W. Sterically protected 1,2,3-dithiazolyl radicals: Preparation and structural characterization of 4-chloro-5-pentafluorphenyl-1,2,3-dithiazolyl. Chem. Commun. 1999, 531–532. [CrossRef]
13. Beer, L.; Cordes, A.W.; Haddon, R.C.; Itkis, M.E.; Oakley, R.T.; Reed, R.W.; Robertson, C.M. A π-stacked 1,2,3-dithiazolyl radical. Preparation and solid state characterization of (C12C3NS)(C12CNS2). Chem. Commun. 2002, 1872–1873. [CrossRef]
14. Appel, R.; Janssen, H.; Siray, M.; Knoch, F. Synthese und Reaktionen des 4,5-Dichlor-1,2,3-dithiazolium-chlorids. Chem. Ber. 1985, 118, 1632–1643. [CrossRef]
15. Koutentis, P.A. The Preparation and Characterization of 5-Substituted-4-chloro-1,2,3-dithiazolium Salts and their Conversion into 4-Substituted-3-chloro-1,2,5-thiadiazoles. Molecules 2005, 10, 346–359. [CrossRef] [PubMed]
16. Rakitin, O.A. 1,2-Oxa/thia-3-azoles. In Comprehensive Heterocyclic Chemistry III; Katritzky, A.R., Ramsden, C.A., Scriven, E.F.V., Taylor, R.J.K., Zhedankin, V.V., Eds; Elsevier: Oxford, UK, 2008; Volume 6, Chapter 6.01; pp. 1–36.
17. Konstantinova, L.S.; Rakitin, O.A. Synthesis and properties of 1,2,3-dithiazoles. Russ. Chem. Rev. 2008, 77, 521–546. [CrossRef]
18. Kim, K. Recent Advances in 1,2,3-Dithiazole Chemistry. J. Chem. Soc. Perkin Trans. 1 1997, 2505–2510. [CrossRef]
19. Kim, K. Synthesis and Reactions of 1,2,3-Dithiazoles. Sulfur Rep. 1998, 21, 147–207. [CrossRef]
20. Emayan, K.; English, R.F.; Koutentis, P.A.; Rees, C.W. New routes to benzothiophenes, isothiazoles and 1,2,3-dithiazoles. J. Chem. Soc. Perkin Trans. 1 1997, 3345–3350. [CrossRef]
21. Clarke, D.; Emayan, K.; Rees, C.W. New synthesis of isothiazoles from primary enamines. J. Chem. Soc. Perkin Trans. 1 1998, 77–82. [CrossRef]
22. Kalogirou, A.S.; Koutentis, P.A. The reaction of 4,5-dichloro-1,2,3-dithiazolium chloride with dimethylsulfoxonium dicyanomethylene: An improved synthesis of (4-chloro-1,2,3-dithiazolylidene)malononitrile. Tetrahedron 2009, 65, 6850–6854. [CrossRef]
23. Koutentis, P.A.; Rees, C.W. Reactions of tetracyanoethylene oxide with 1,2,3-dithiazoles. J. Chem. Soc. Perkin Trans. 1 1998, 2505–2510. [CrossRef]
24. Kalogirou, A.S.; Christoforou, I.C.; Ioannidou, H.A.; Manos, M.J.; Koutentis, P.A. Ring transformation of (4-chloro-5H-1,2,3-dithiazol-5-ylidene)acetonitriles to 3-haloisothiazole-5-carbonitriles. RSC Adv. 2014, 4, 7735–7748. [CrossRef]
25. Rees, C.W. Polysulfur-nitrogen heterocyclic chemistry. J. Heterocycl. Chem. 1992, 29, 639–651. [CrossRef]
26. Jeon, M.-K.; Kim, K. Synthesis of new 5-alkylidene-4-chloro-5H-1,2,3-dithiazoles and their stereochemistry. Tetrahedron 1999, 55, 9651–9667. [CrossRef]
27. Chang, Y.-G.; Cho, H.S.; Kim, K. Novel Synthesis and Reactions of 5,7-Dialkyl-4,6-dioxo-4,5,6,7-tetrahydro-isothiazolo[3,4-d]pyrimidine-3-carbonitriles and 6-Methyl-4-oxo-4H-1-aza-5-oxa-2-thiaindene-3-carbonitrile. Org. Lett. 2003, 5, 507–510. [CrossRef] [PubMed]
28. Koyioni, M.; Manoli, M.; Manolis, M.J.; Koutentis, P.A. Reinvestigating the Reaction of 1H-Pyrazol-5-amines with 4,5-Dichloro-1,2,3-dithiazolium Chloride: A Route to Pyrazolo[3,4-c]isothiazoles and Pyrazolo[3,4-d]thiazoles. J. Org. Chem. 2014, 79, 4025–4037. [CrossRef] [PubMed]
29. Gaillot, J.-M.; Gelas-Mialhe, Y.; Vessiere, R. Synthèse et réactivité des halogéno-2 sulfonyl-2 aziridines. Can. J. Chem. 1979, 57, 1958–1966. [CrossRef]
30. El-Sayed, I.; Belsky, V.K.; Zavodnik, V.E.; Jørgensen, K.A.; Senning, A. Chlorotropic rearrangements of an α-sulfanyl-α-sulfonylalkanesulfenyl chloride to an α-chloroalkyl disulfide and an S-(α-chloroalkyl) thiosulfonate. J. Chem. Soc. Perkin Trans. 1 1994, 1251–1252. [CrossRef]
31. Bruni, M.C.; Ponterini, G.; Scoponi, M. Photophysics and photochemistry of diphenyl sulfone. 2. Investigation of the S1 decay pathways. J. Phys. Chem. 1989, 93, 678–683. [CrossRef]
32. CrysAlis CCD and CrysAlis RED; version 1.171.32.15; Oxford Diffraction Ltd.: Abingdon, UK, 2008.
33. Sheldrick, G.M. SHELXL-97: A Program for the Refinement of Crystal Structure; University of Göttingen: Göttingen, Germany, 1997.
34. Farrugia, L.J. WinGXsuite for small-molecule single-crystal crystallography. J. Appl. Crystallogr. 1999, 32, 837–838. [CrossRef]
35. Brandenburg, K. Diamond; version 3.1d; Crystal Impact GbR: Bonn, Germany, 2006.