European Journal of Chemistry

View Journal Online
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Crystal structure of 2,4-dinitrophenyl 2,4,6-trimethylbenzenesulfonate

Brock Anton Stenfors and Felix Nyuangem Ngassa *

Department of Chemistry, Grand Valley State University, 1 Campus Drive, Allendale, MI 49401, USA

** Corresponding author at: Department of Chemistry, Grand Valley State University, 1 Campus Drive, Allendale, MI 49401, USA.*
e-mail: ngassaf@gvsu.edu (F.N. Ngassa).

RESEARCH ARTICLE

10.5155/eurjchem.13.2.145-150.2279

Received: 06 April 2022
Received in revised form: 12 April 2022
Accepted: 27 April 2022
Published online: 30 June 2022
Printed: 30 June 2022

KEYWORDS

Crystal
Sulfonate
Sulfonylation
Crystallization
X-ray diffraction
Synthetic methods

ABSTRACT

Arylsulfonates are a useful class of synthetic precursors, affording either their arylamine or arylsulfonamide counterparts upon amination via regioselective C–O/S–O bond cleavage. Herein, the synthesis of 2,4-dinitrophenyl 2,4,6-trimethylbenzenesulfonate is described, utilizing our previously developed synthetic methods, and crystallographic characterization. While the mechanism for nucleophilic substitution at the sulfonyl group remains largely unknown, experimental work within our group and in the literature lend credence to a mechanism analogous to its carbonyl counterpart. Characterization of the molecular structure of the title compound, $C_{15}H_{14}N_2O_7S$, at 173 K, features a sulfonate group with S=O bond lengths of 1.4198(19) and 1.4183(19) Å and a S–O bond length of 1.6387(18) Å. Viewing down the S–O bond reveals *gauche* oriented aromatic rings. Crystal data for $C_{15}H_{14}N_2O_7S$: Monoclinic, space group $P2_1/c$ (no. 14), a = 6.8773(10) Å, b = 8.9070(14) Å, c = 25.557(4) Å, β = 93.0630(18)°, V = 1563.3(4) Å3, Z = 4, T = 173.15 K, μ(MoKα) = 0.251 mm^{-1}, D_{calc} = 1.557 g/cm^3, 12259 reflections measured (3.192° ≤ 2Θ ≤ 50.682°), 2861 unique (R_{int} = 0.0493, R_{sigma} = 0.0419) which were used in all calculations. The final R1 was 0.0457 (I > 2σ(I)) and wR2 was 0.1306 (all data).

Cite this: *Eur. J. Chem.* **2022**, *13(2)*, 145-150 **Journal website**: www.eurjchem.com

1. Introduction

Arylsulfonates are ubiquitous building blocks in synthetic chemistry, utilized as synthetic precursors and protecting groups alike due to the stability of the sulfonate ester leaving group [1,2]. This class of compounds also exhibit medicinal properties [3,4]. While the importance of arylsulfonates is evident, mechanistic details for nucleophilic substitution at the sulfonyl group remain unknown [5-8]. Previous reports suggest a substitution mechanism somewhat analogous to its carbonyl counterpart [9,10]. In our work, our interests are focused on the nucleophilic aromatic substitution (S_NAr) reaction of various arylsulfonate analogs. While the S–O cleavage is responsible for most of the uses currently seen in the literature, a competitive S–O and C–O bond fission of arylsulfonates, in the presence of a nucleophilic amine, lends credence to a facile synthesis of arylamines and arylsulfonamides, two biologically significant classes of compounds [11]. Previously, our group investigated the structure of two unique arylsulfonates [12,13]. A variety of arylsulfonates have been synthesized to gain further insight into the regioselective factors responsible for the S–O/C–O bond cleavage (Scheme 1).

Apart from being useful synthetic precursors, their arylsulfonamide and arylamine counterparts are widely used in medicinal chemistry [14,15]. A regioselective synthesis of these molecules can be carried out via amination of electrophilic arylsulfonate precursors. We aim to investigate the effects of various sulfonate substituents and amines to achieve high regioselectivities for a favorable S–O or C–O bond cleavage. As the title compound is of interest in this ongoing investigation, we report herein the synthesis and crystallographic characterization of this electrophilic arylsulfonate.

2. Experimental

2.1. Instrumentation and materials

Reagents were obtained from commercial sources and used without further purification. Thin-layer chromatography (TLC) was used to track reaction progress and obtain R_f values for the reactions. ^{1}H NMR spectra (400 MHz) were recorded on a JEOL ECZ400 spectrometer using a chloroform-*d* solvent. Chemical shifts are reported in parts per million (ppm, δ) relative to the residual solvent peak, and coupling constants (*J*) are reported in Hertz (Hz). Results were analyzed, and figures were created with the use of MestReNov [16].

2.2. Synthesis

The title compound was prepared via a dropwise addition of 2,4-dinitrophenol (2.02 g, 11.0 mmol) to a stirred mixture of 2,4,6-trimethylsulfonyl chloride (1.00 g, 4.58 mmol) in 10 mL of tetrahydrofuran.

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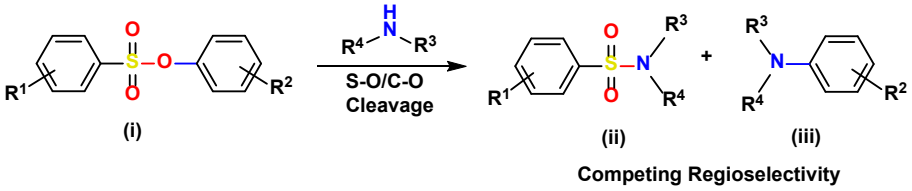
https://dx.doi.org/10.5155/eurjchem.13.2.145-150.2279

Table 1. Crystal data and details of the structure refinement for the title compound.

Parameters	
Empirical formula	$C_{15}H_{14}N_2O_7S$
Formula weight	366.34
Temperature (K)	173.15
Crystal system	Monoclinic
Space group	$P2_1/c$
a, (Å)	6.8773(10)
b, (Å)	8.9070(14)
c, (Å)	25.557(4)
α (°)	90
β (°)	93.0630(18)
γ (°)	90
Volume (Å^3)	1563.3(4)
Z	4
ρ_{calc} (g/cm^3)	1.557
μ (mm^{-1})	0.251
F(000)	760.0
Crystal size (mm^3)	0.216 × 0.138 × 0.117
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection (°)	3.192 to 50.682
Index ranges	$-8 \le h \le 8$, $-10 \le k \le 10$, $-30 \le l \le 30$
Reflections collected	12259
Independent reflections	2861 [R_{int} = 0.0493, R_{sigma} = 0.0419]
Data/restraints/parameters	2861/0/229
Goodness-of-fit on F^2	1.050
Final R indexes [I≥2σ (I)]	R_1 = 0.0457, wR_2 = 0.1146
Final R indexes [all data]	R_1 = 0.0659, wR_2 = 0.1306
Largest diff. peak/hole (e.Å^{-3})	0.34/-0.38



Scheme 1. General reaction for the regioselective S–O/C–O bond cleavage of arylsulfonate (**i**) in the presence of nucleophilic amine to afford the corresponding arylsulfonamide (**ii**) and arylamine (**iii**).

Following another dropwise addition of aqueous potassium carbonate (10 mL, 0.915 M), the mixture was left to stir for 24 h at room temperature. After dilution with 15 mL of dichloromethane, the reaction mixture was washed with water (3×10 mL) and the aqueous layers back extracted with 10 mL of dichloromethane. The organic layers were combined, washed with 10 mL of brine, dried over anhydrous sodium sulfate, and evaporated to yield a crude, yellow residue. Recrystallization in 5 mL of dichloromethane yielded the product as large, pale-yellow crystals.

2,4-Dinitrophenyl 2,4,6-trimethylbenzenesulfonate: Color: Pale-yellow. Yield: 88%. M.p.: 128-132 °C. R_f : 0.86 (CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.75 (d, 1H, *J* = 2.8 Hz, Ar-H), 8.44 (dd, 1H, *J* = 9.0, 2.8 Hz, Ar-H), 7.58 (d, 1H, *J* = 9.0 Hz, Ar-H), 7.03 (2H, s, Ar-H), 2.57 (6H, s, Bn-H), 2.35 (3H, s, Bn-H). ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 146.12, 145.70, 145.16, 142.95, 140.84, 132.39, 129.55, 128.57, 126.21, 121.62, 22.87, 21.34.

2.3. Crystallographic characterization

X-ray diffraction was carried out on a Bruker APEXII CCD diffractometer with Mo *K*α radiation. The software used for data collection is as follows: data collection, APEX2 [17]; cell refinement and data reduction, SAINT [18]; program used to refine the structure, SHELXL [19]; program used to solve the structure, SHELXS [20]; molecular graphics and publication material, OLEX2 [21,22]; program used to generate figures, Mercury [23-27]; absorbance correction, SADABS [28].

3. Results and discussion

3.1. Crystallographic characterization

Crystal data, data collection and structure refinement details are summarized in Table 1. A list of bond distances and angles is given in Table 2. For this structure, hydrogen atoms bonded to carbon atoms were placed in calculated positions and refined as riding: C–H = 0.95–1.00 Å with U_{iso}(H) = 1.2U_{eq}(C) for methine groups and aromatic hydrogen atoms, and U_{iso}(H) = 1.5U_{eq}(C) for methyl groups.

The molecular structure of the title compound is shown in Figure 1. Characterization reveals a monoclinic system ($P2_1/c$ space group). The two aryl rings of the title compound are oriented *gauche* to one another with a C7–S1–O1–C1 torsion angle of 73.8(2) °. The O2=S1=O3 and C7–S1–O1 bond angles of 119.19(12) and 102.13(11)°, respectively, are typical for phenyl arene sulfonates with a *gauche* conformation around the ester S–O bond. Steric hindrance between ortho substituents of the benzene ring results in a 40.8(3)° perturbation of the nitro group relative to the benzene best plane, allowing the shortest contact of 2.760(3) Å between the oxygen atoms of these groups to be close to the sum of the van der Waals radii.

An intermolecular S=O···N interaction between the sulfonyl and nitro groups is responsible for the formation of centro-symmetric dimers, with an O2···N2 distance of 3.077(3) Å. Another centrosymmetric dimer is formed *via* intermolecular π–π stacking interactions between the relatively electron-rich phenyl rings (Figure 2a), with a plane-plane distance of 3.723(3) Å. These dimers are organized into columns, which are then assembled into layers through nonclassical C–H···O interactions between phenyl hydrogen atoms and sulfonyl/nitro group oxygen atoms (Figure 2b; Figure 3). The central sulfur atom, S1, exhibits a slightly distorted tetrahedron geometry, in agreement with the τ_4 descriptor for four-fold coordination [29].

Table 2. Bond lengths and angles for the title compound.

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
S1	O1	1.6387(18)	C2	C3	1.375(4)
S1	O2	1.4198(19)	C3	C4	1.379(4)
S1	O3	1.4183(19)	C4	C5	1.378(4)
S1	C7	1.760(2)	C5	C6	1.383(4)
O1	C1	1.390(3)	C7	C8	1.420(3)
O4	N1	1.226(3)	C7	C12	1.412(4)
O5	N1	1.214(3)	C8	C9	1.383(4)
O6	N2	1.220(3)	C8	C13	1.509(4)
O7	N2	1.225(3)	C9	C10	1.389(4)
N1	C2	1.466(3)	C10	C11	1.378(4)
N2	C4	1.473(3)	C10	C15	1.507(4)
C1	C2	1.395(4)	C11	C12	1.394(4)
C1	C6	1.389(4)	C12	C14	1.515(4)

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
O1	S1	C7	102.13(11)	C3	C4	N2	118.2(2)
O2	S1	O1	107.18(10)	C5	C4	N2	119.2(2)
O2	S1	C7	111.77(12)	C5	C4	C3	122.5(2)
O3	S1	O1	102.30(11)	C4	C5	C6	118.9(2)
O3	S1	O2	119.19(12)	C5	C6	C1	120.0(2)
O3	S1	C7	112.19(12)	C8	C7	S1	117.72(19)
C1	O1	S1	118.56(15)	C12	C7	S1	120.43(19)
O4	N1	C2	117.6(2)	C12	C7	C8	121.8(2)
O5	N1	O4	124.4(2)	C7	C8	C13	124.9(2)
O5	N1	C2	117.9(2)	C9	C8	C7	117.3(2)
O6	N2	O7	124.4(2)	C9	C8	C13	117.9(2)
O6	N2	C4	117.9(2)	C8	C9	C10	122.7(2)
O7	N2	C4	117.7(2)	C9	C10	C15	120.9(2)
O1	C1	C2	121.2(2)	C11	C10	C9	118.3(2)
C6	C1	O1	119.5(2)	C11	C10	C15	120.8(2)
C6	C1	C2	119.3(2)	C10	C11	C12	123.2(2)
C1	C2	N1	121.3(2)	C7	C12	C14	126.2(2)
C3	C2	N1	117.3(2)	C11	C12	C7	116.8(2)
C3	C2	C1	121.3(2)	C11	C12	C14	117.0(2)
C2	C3	C4	117.9(2)				

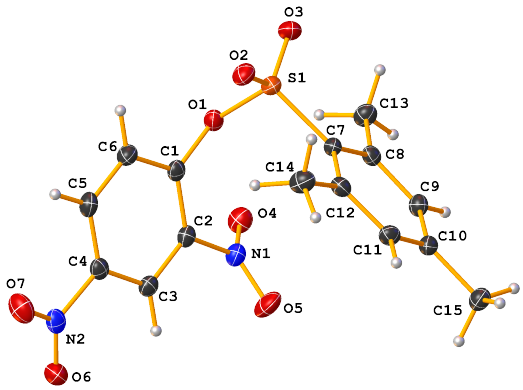


Figure 1. Molecular structure of the title compound.

(**a**) (**b**)

Figure 2. (**a**) Centrosymmetric dimers of the title compound formed via intermolecular π–π stacking interactions (**b**) A depiction of the inter- and intramolecular contacts present in the crystal of the title compound using a capped stick model with standard CPK colors. Contacts are shown in cyan.

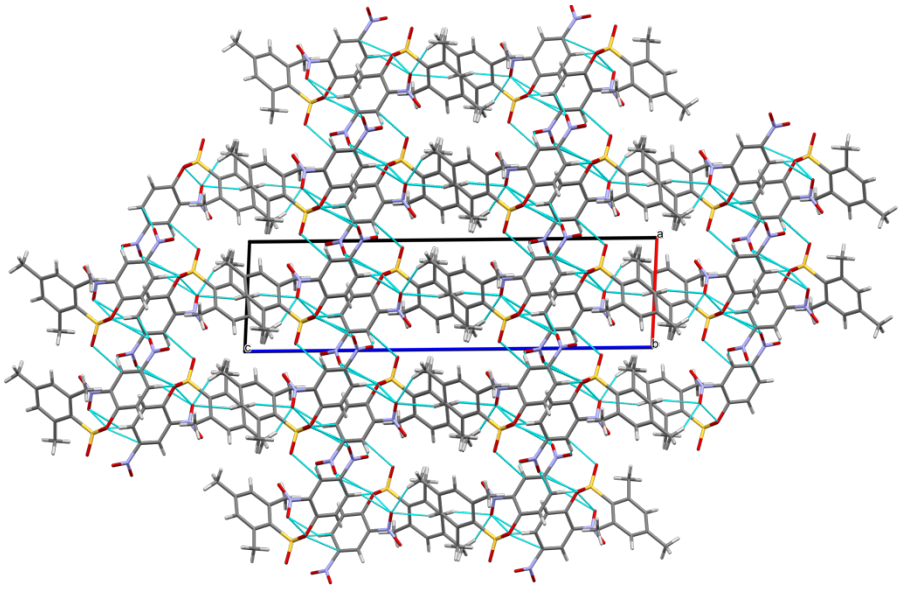
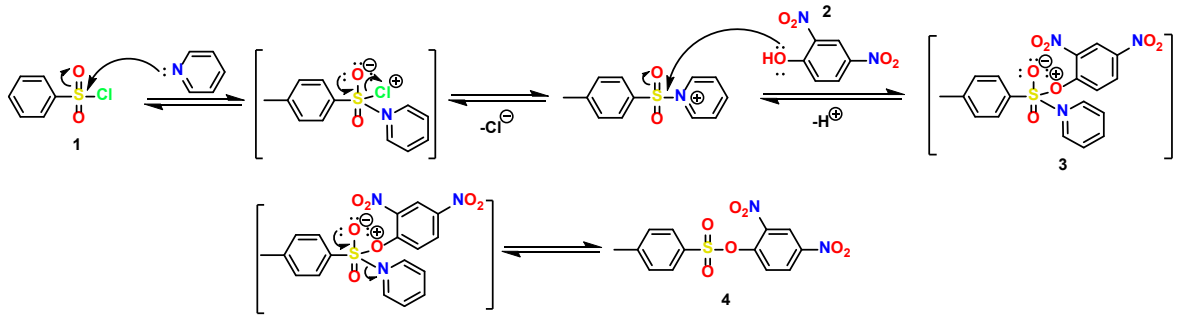
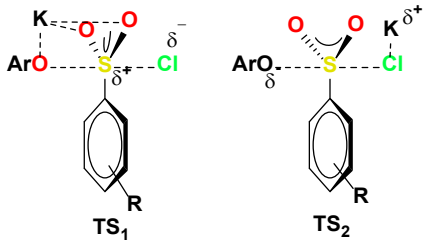


Figure 3. A view down the *b* axis of the crystal packing showing the supramolecular sheets formed *via* non-covalent interactions. Inter- and intramolecular contacts are shown in cyan.



Scheme 2. The previously proposed mechanism for the treatment of *p*-toluenesulfonyl chloride (**1**) with 2,4-dinitrophenol (**2**) in the presence of pyridine and dichloromethane to form, 2,4-dinitrophenylpyridinium *p*-toluenesulfonate (**3**). Shown below, this is the desired rearrangement of compound **3** to give the sulfonate product (**4**).



Scheme 3. Proposed transition states, derived from a previous report by Um *et al.* [31], explaining the role of K^+ in the formation of arylsulfonates.

3.2. Synthetic techniques

The synthetic strategy employed in this work has been previously reported by our group [30]. Initial reaction conditions of dichloromethane in the presence of pyridine resulted in the formation of an undesired pyridinium salt as the only product. Scheme 2 shows the previously proposed mechanism for the formation of this pyridinium salt.

Alternative routes were explored, leading to the development of a semi-miscible biphasic system consisting of 1:1 THF/aqueous K_2CO_3, the same technique employed in this work. These conditions resulted in higher yields, less environmental impact due to the environmentally benign conditions, and shorter reaction times. Outlined in Scheme 3, previous reports suggest a reaction catalyzed by K^+ via increased electrophilicy of the reaction center (**TS$_1$**) or by increased nucleofugality of the leaving group (**TS$_2$**) [31], further supporting the observed increase in yield and decreased reaction time. Additionally, the highly pure sulfonate product can be isolated directly from the reaction mixture. Such conditions have been used to synthesize a variety of arylsulfonates in hopes of studying their regioselective C–O/S–O bond cleavage upon treatment with a nucleophilic amine.

4. Conclusion

In this work, the synthesis and crystallographic characterization of 2,4-dinitrophenyl 2,4,6-trimethylbenzenesulfonate

was discussed. Crystallographic characterization revealed a high correlation of bond angles around the sulfonyl when compared to similar structures exhibiting *gauche* oriented phenyl rings about the S–O bond axis. Two sets of centro-symmetric dimers are formed via intermolecular S=O···N and π–π stacking interactions. Nonclassical C–H···O interactions between phenyl hydrogen atoms further assemble these dimers into layers, affording supramolecular sheets. Apart from characterization, the aforementioned synthetic method offers an efficient and environmentally benign route to arylsulfonate precursors. Subsequent regioselective C–O/S–O bond cleavage upon amination affords either the arylsulfomanide or corres-ponding arylamine, two biologically significant scaffolds. Crystallographic characterization may potentially offer structural insight into such regioselective factors. Various arylsulfonates will be synthesized to further study these factors and the potential for an efficient one-pot synthesis of arylsulfon amides and arylamines from a single synthetic precursor. Furthermore, the results afforded from various reaction conditions will provide insight into the mechanistic details for the nucleophilic substitution of sulfonyls.

Acknowledgements

The authors thank Pfizer Inc. for the donation of a Varian INOVA 400 FT NMR. The CCD-based X-ray diffractometers at Michigan State University were replaced and/or upgraded with departmental funds.

Supporting information

CCDC-2157592 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via https://www.ccdc.cam.ac.uk/structures/, or by e-mailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033.

Disclosure statement

Conflict of interest: The authors declare that they have no conflict of interest.
Ethical approval: All ethical guidelines have been adhered.
Sample availability: Samples of the compounds are available from the author.

CRediT authorship contribution statement

Conceptualization: Brock Anton Stenfors, Felix Nyuangem Ngassa; Methodology: Brock Anton Stenfors, Felix Nyuangem Ngassa; Software: Brock Anton Stenfors, Felix Nyuangem Ngassa; Validation: Brock Anton Stenfors, Felix Nyuangem Ngassa; Formal Analysis: Brock Anton Stenfors, Felix Nyuangem Ngassa; Investigation: Brock Anton Stenfors, Felix Nyuangem Ngassa; Resources: Brock Anton Stenfors, Felix Nyuangem Ngassa; Data Curation: Brock Anton Stenfors, Felix Nyuangem Ngassa; Writing - Original Draft: Brock Anton Stenfors, Felix Nyuangem Ngassa; Writing - Review and Editing: Brock Anton Stenfors, Felix Nyuangem Ngassa; Visualization: Brock Anton Stenfors, Felix Nyuangem Ngassa; Funding acquisition: Felix Nyuangem Ngassa; Supervision: Felix Nyuangem Ngassa; Project Administration: Felix Nyuangem Ngassa.

Funding

Funding for this research was provided by: National Science Foundation, Directorate for Mathematical and Physical Sciences (grant No. MRI CHE-1725699; grant No. MRI CHE-1919817); GVSU Chemistry Department's Weldon Fund.

ORCID and Email

Brock Anton Stenfors
stenforb@mail.gvsu.edu
https://orcid.org/0000-0001-8760-5878
Felix Nyuangem Ngassa
ngassaf@gvsu.edu
https://orcid.org/0000-0001-8246-3639

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