One-pot nitrodebromination and methyl bi-functionalization of 5-bromo 6-methylpyrimidines: a unique simultaneous transformation

Mahsa Mousavi1 · Majid M. Heravi2 · Javad Tajabadi1

Received: 18 May 2020 / Accepted: 22 June 2020 / Published online: 24 July 2020
© Springer-Verlag GmbH Austria, part of Springer Nature 2020

Abstract
A unique one-pot, simultaneous nitrodebromination and methyl bromonitration occurred upon treatment of 5-bromo-2,4-di-tert-amino-6-methylpyrimidine derivatives with a cold mixture of concentrated H2SO4–HNO3 in moderate yields. It is actually a facile and rapid transformation that has been reported neither on pyrimidines nor simultaneously on other organic compounds.

Graphic abstract

Keywords Gem-bromonitromethyl pyrimidine · Bromonitration · Nitrodebromination · Additive free · Catalyst free

Introduction

Organic compounds containing nitro and/or halogen functionalities are considerably important intermediates in organic and total syntheses of natural products [1–3]. Besides their structure-induced properties that have given them a broad range of biological and industrial applications, they can undergo further valuable transformations and; thus, are considered as potential precursors in multistep synthesis [4–6].

In contrast to the frequently reported aromatic C–H nitration, investigation of aliphatic C–H nitration has largely been overlooked, as the latter may require rather challenging and perplexed operation. In this regard, reports on α-nitration of heterocycles mainly involve the use of alkynitrites at − (30–78) °C in the presence of strong bases, such as LDA [7, 8] or KNH2 [9], AgNO3 under oxidative conditions [10], and use of concentrated neat nitric acid [11], or in
combination with a proper anhydride [12]. Moreover, literature survey on α-halogenation reaction revealed that, heterobenzyl halides can generally be obtained from free radical halogenation reaction using N-halosuccinimides [13–15], via a multistep synthetic procedure using SOCl2/PBr3 [16–18], or other systems, such as TBHP/CuX [19] and n-Bu4NI/DCE [20].

Accordingly, while nitrodehalogenation reaction has been observed for a number of reactive arylhalides and pyrazoles in the presence of a proper catalyst [21–25] or an HNO3-containing acid mixture [26, 27], literature survey disclosed that synthesis of gem-halonitro compounds only proceeds through sequential processes involving halogenation of the related nitro-containing intermediates [28–31] or oximes [29, 32, 33].

In continuation of our previous study on hydrodehalogenation of 5-halopyrimidines [34], as well as nitration [35], and bromination [36] of aromatic compounds, herein, we wish to report our interesting and unique finding on a one-pot, nitrodebromination, and α-bromonitration of 2,4-di-tert-amino-5-bromo-6-methylpyrimidine derivatives.

**Results and discussion**

In our previous study on 5-halopyrimidines, we found that under metal/catalyst-free conditions, halogen atom could easily be displaced with S/N nucleophiles through SNAr mechanism [37–41], as well as with radicals [42], or even with electrophilic hydrogen (H+) through electrophilic aromatic substitution mechanism (EAS) [34], to give the ipso-substituted product. This interesting achievement leading to the formation of hydrodehalogenated product, prompted us to examine the possible substitution of halogen with other electrophilic species. To the purpose, a series of 2,4-di-tert-amino-5-bromo-6-methylpyrimidine derivatives 1a–1i were synthesized according to the previously published work (Scheme 1) [42]. Initially, 5-bromo-2,4-dimorpholino-6-methylpyrimidine 1f, as the model derivative, was treated with a mixture of concentrated sulfuric and fuming nitric acids at 0 °C. Interestingly, the elemental and spectral analysis revealed that instead of ipso-product, the product contains two nitro groups and the bromine atom still present in, as the mass spectrum showed a molecular ion peak at m/z = 432. 1H NMR spectrum of this compound exhibited a singlet signal at 7.66 ppm for −CH group; 13C NMR spectrum showed two signals at 78.01 ppm and 120.22 ppm attributed to −C(NO2)(Br) and aromatic C–NO2 groups respectively. Considering of elemental and spectral analysis, the following structure is given to 2f as illustrated in Scheme 1.

Worthy to mention that the formation of other possible isomer, the corresponding 5-bromo-6-dinitromethylpyrimidine 2f’, was ruled out by comparison of calculated 13C NMR values for 2f and 2f’ with the corresponding experimental data, as depicted in Fig. 1 [42–44].

As shown in Fig. 1, a comparison of Gibbs energy difference between 2 and 2f’, indicates that the former is 15.12 kJ mol−1 more stable thermodynamically. Moreover, although the largest difference between unscaled calculated and experimental chemical shifts of structure 2f is only 6.0 ppm for C-6 atom of pyrimidine ring, the calculated chemical shift of carbon atom attached to the two nitro groups in 2f’ deviates 31.6 ppm from the experimental value. It should be noted that there is a well-known heavy-atom effect which is reported without relativistic and spin–orbit coupling corrections. Due to this effect, the results for computed chemical shifts of carbon atoms attached to the halogens, other atoms of the third row or greater, will always be obtained downfield [45]. Accordingly, the de-shielded computed chemical shift value for brominated carbon atom in 2f (12.0 ppm) is normal, while for C-5 of pyrimidine ring attached to Br atom in 2f’, is abnormally 10.2 ppm smaller than the experimental one, despite being de-shielded by the heavy atom. These results clearly rule out the likely formation of 2f’ and cross-validate the results of experimental data for the formation of 2f.

To establish the generality of this strategy for bi-functionalization of methyl group at position 6 of pyrimidine, a wide range of 2- and 4-substituted pyrimidines 1a–1i were successfully examined to afford 2a–2i in satisfactory yields (Scheme 1).

| Entry | Yields % |
|-------|---------|
| 1a–1i | 51      |
| 1b–1i | 58      |
| 1c–1i | 63      |
| 1d–1i | 57      |
| 1e–1i | 62      |
| 1f–1i | 56      |
| 1g–1i | 59      |
| 1h–1i | 55      |

To establish the generality of this strategy for bi-functionalization of methyl group at position 6 of pyrimidine, a wide range of 2- and 4-substituted pyrimidines 1a–1i were successfully examined to afford 2a–2i in satisfactory yields (Scheme 1).

Based on the obtained results, a reasonable mechanism for the observed simultaneous nitrodebrination–bromonitration of 6-methylpyrimidine derivatives is proposed as illustrated in Scheme 2. Accordingly, the reactive electrophile NO2+ is generated upon treatment of concentrated sulfuric...
One-pot nitrodebromination and methyl bi-functionalization of 5-bromo 6-methylpyrimidines:…

acid with fuming nitric acid at 0 °C. The reaction begins by an initial attack of the known electron-rich C-5 atom of pyrimidine to reactive NO$_2^+$ to generate ipso-intermediate A and its mesomeric contributor B. The latter loses a hydrogen atom in the presence of HSO$_4^-$ to create enamine C bearing an exo-methylene group. Subsequent attack of the activated

Fig. 1 Optimized geometries, Gibbs energies, and unscaled GIAO $^{13}$C chemical shift values, in ppm, for compound 2f and its possible isomer 2f' at mPW1PW91/6-31G(d)//mPW1PW91/6-31G(d) level of theory. The experimental chemical shift values are presented in the parentheses

Scheme 2

$\text{H}_2\text{SO}_4 + \text{HNO}_3 \overset{\text{H}_2\text{O}^+\text{NO}_2^- + \text{HSO}_4^-}{\longrightarrow} \overset{\text{H}_2\text{O} + \text{HSO}_4^- + \text{NO}_2^+}{\longrightarrow}$

\[
\begin{align*}
\text{NR}_2\text{N} & \quad \text{NR}_2\text{N} \\
\text{Br} & \quad \text{Br} \\
\text{R}'_2\text{N} & \quad \text{R}'_2\text{N} \\
\text{Me} & \quad \text{Me} \\
\text{NO}_2^+ & \quad \text{NO}_2^+ \\
\text{A} & \quad \text{B} \\
\end{align*}
\]

\[
\begin{align*}
\text{NR}_2\text{N} & \quad \text{NR}_2\text{N} \\
\text{NO}_2 & \quad \text{NO}_2 \\
\text{Me} & \quad \text{Me} \\
\text{Br} & \quad \text{Br} \\
\text{R}'_2\text{N} & \quad \text{R}'_2\text{N} \\
\text{Br} & \quad \text{Br} \\
\text{N}^+ & \quad \text{N}^+ \\
\text{R} & \quad \text{R} \\
\text{C} & \quad \text{D} \\
\end{align*}
\]

\[
\begin{align*}
\text{NR}_2\text{N} & \quad \text{NR}_2\text{N} \\
\text{NO}_2 & \quad \text{NO}_2 \\
\text{Me} & \quad \text{Me} \\
\text{Br} & \quad \text{Br} \\
\text{R}'_2\text{N} & \quad \text{R}'_2\text{N} \\
\text{Br} & \quad \text{Br} \\
\text{N}^+ & \quad \text{N}^+ \\
\text{R} & \quad \text{R} \\
\text{C} & \quad \text{D} \\
\end{align*}
\]
methylene group to nitronium ion, leads to the formation of intermediate D. Further deprotonation of intermediate D followed by a Br [1, 3]-shift [46], affords the gem-bromonitrated product 2.

As could be expected from our previous findings, it seems that 5-halopyrimidines can still undergo EAS reaction at C-5 to afford the ipso-substituted product. In the case of 5-bromo-6-methylpyrimidines, the reaction proceeds further, giving rise to the methyl bi-functionalized product.

It is worthy to note that the formation of the stabilized enamine seems crucial to the formation of products, as the reaction yields were poor with 2,4-dimethylamino and 2,4-diethoxy derivatives. This observation obviously confirms the acidity of methyl group hydrogens in position 6 of certain pyrimidine derivatives.

**Conclusion**

A series of novel gem-bromonitromethyl pyrimidines were synthesized from their corresponding 5-bromo-6-methylpyrimidine derivatives through a unique one-pot, nitrodebronymination and bromonitration reaction in satisfactory yields. The reaction was simply performed in a cold mixture of H2SO4 (conc) − HNO3 (fum) in the absence of any catalyst or other reagents and additives. Short reaction time, easy work-up procedure, and readily availability of reagents were other merits of this approach. To the best of our knowledge, this is the first report of nitrodebronymination and α-methyl bi-functionalization reactions in pyrimidines, as well as first example of one-pot simultaneous nitrodebronymination of a sp3 carbon in an organic compound. In addition, since a stereogenic center is created during the reaction, this protocol can be developed for enantioselective synthesis of pyrimidines with various biological activities in optically pure form which is useful in drug discovery. More studies are underway to expand the scope of this reaction to other reactive electrophilic species or substrates as well as developing a protocol for the synthesis of optically active pyrimidines.

**Experimental**

Melting points were measured by an Electrothermal type 9200 melting point apparatus. The 1H NMR (300 MHz) and 13C NMR (75 MHz) spectra were obtained on a Bruker Advance DRX-300 Fourier transform spectrometer at 25 °C. An Avatar 370 FT-IR Thermo Nicolet spectrometer was employed to record the IR spectra and a Varian Mat CH-7 instrument for scanning mass spectra at 70 eV. Micro analytical data were obtained on a Thermo Finnigan Flash EA 1112 microanalyzer.

**General procedure for the preparation of compounds 1a–1i [42]**

To a solution of 241 mg of commercially available 5-bromo-2,4-dichloro-6-methylpyrimidine (1 mmol) in acetonitrile, secondary amine (4 mmol) was added at room temperature and refluxed for 3 h. After removal of solvent in vacuo, the residue was washed with water, and recrystallized from ethanol to give the desired products.

**General procedure for the preparation of compounds 2a–2i**

To a 1:1 stirring mixture of concentrated H2SO4 (2.2 cm3) and fuming HNO3 (2.2 cm3) at 0 °C in a beaker was added portion-wise pyrimidine derivatives 1a–1i (1 mmol). The mixture was allowed to stir for 30 min. After the completion of reaction monitored by TLC (using n-hexane and ethyl acetate as eluent), the reaction mixture was added dropwise to 180 g crushed ice with vigorous stirring. The yellow precipitate was filtered-off, washed with water, and dried in vacuo to give the desired product. Column chromatography was used where further purification was needed.

4-[5-Bromo-4-methyl-6-(pyrrolidin-1-yl)pyrimidin-2-yl]-morpholine (1a, C13H19BrN4O) White powder; yield: 0.26 g (82%); m.p.: 88–91 °C; 1H NMR (300 MHz, CDCl3): δ = 3.80–3.70 (12H, m, CH2O, CH2N), 2.42 (3H, s, Me), 1.93–1.89 (4H, m, CH2) ppm; 13C NMR (75 MHz, CDCl3): δ = 165.3 (Ar), 159.0 (Ar), 158.9 (Ar), 91.3 (CBr), 66.9, 50.0, 44.4, 25.9, 25.7 ppm; FT-IR (KBr): v = 2932 (s), 2863 (m), 1541 (s) cm−1; MS: m/z = 326 (M+).

5-Bromo-4-methyl-6-(piperidin-1-yl)-2-(pyrrolidin-1-yl)-pyrimidine (1c, C14H21BrN4) Viscous oil; yield: 0.27 g (85%); 1H NMR (300 MHz, CDCl3): δ = 3.56–3.52 (4H, m, CH2N), 3.46–3.42 (4H, m, CH2N), 2.46 (3H, s, Me), 1.98–1.94 (4H, m, CH2), 1.69–1.67 (6H, m, CH2) ppm; 13C NMR (75 MHz, CDCl3): δ = 165.9 (Ar), 164.1 (Ar), 158.1 (Ar), 95.5 (CBr), 49.7 (CH2N), 46.6 (CH2N), 25.7, 25.69, 25.61, 24.7 ppm; FT-IR (KBr): v = 2932 (s), 2855 (m), 1589 (s), 1565 (s) cm−1; MS: m/z = 326 (M+).
4-[5-Bromo-6-methyl-2-](pyrrolidin-1-yl)pyrimidin-4-ylmorpohline (1i, C_{13}H_{19}BrN_{6}O_{4}) Yellow powder; yield: 0.21 g (51%); m.p.: 148–151 °C; 1H NMR (300 MHz, CDCl3): δ = 7.72 (1H, s, CH), 3.82–3.73 (8H, m, CH2 O, CH2 N), 3.54–3.51 (4H, m, CH2 N-piperidin), 3.69 (t, 4H, CH2 O), 3.44 (t, 4H, CH2 N), 1.61–1.50 (6H, m, CH2 C), 1.35 (13H, m, CH2 C), 1.01 (d, 6H, Me, CHMe), 30.9 (CH2 C), 47.9 (CH2 N), 45.9 (CH2 N), 25.6 (CH2 C), 21.6 (Me), 21.5 (Me) ppm; FT-IR (KBr): υ = 2986 (w), 2861 (m), 1576 (s) cm⁻¹; MS: m/z = 430 (M⁺).

4-[Bromo(nitromethyl)-2,6-bis(4-methylpiperidin-1-yl)pyrimidin-1-yl]-5-nitropyrimidine (2e, C_{17}H_{25}BrN_{6}O_{4}) Yellow powder; yield: 0.26 g (62%); m.p.: 59–62 °C; 1H NMR (300 MHz, CDCl3): δ = 7.66 (1H, s, CH), 3.84–3.66 (8H, m, CH2 O, CH2 N), 3.50–3.41 (4H, m, CH2 N), 1.61–1.50 (6H, m, CH2 C) ppm; 13C NMR (75 MHz, CDCl3): δ = 157.9 (Ar), 157.6 (Ar), 157.4 (Ar), 120.2 (CNO2), 78.01 (CBrNO2), 66.6 (CH2 O), 66.2 (CH2 C), 47.7 (CH2 N), 44.5 (CH2 N), 33.8 (CH2 C), 33.6 (CH2 C), 31.0 (CHMe), 30.7 (CHMe), 21.6 (Me), 21.5 (Me) ppm; FT-IR (KBr): υ = 2953 (w) 2925 (m), 1563 (s) cm⁻¹; MS: m/z = 456 (M⁺).

4-[Bromo(nitromethyl)-5-nitropyrimidin-2,4-diyl]morpohline (2f, C_{14}H_{13}BrN_{6}O_{5}) Yellow powder; yield: 0.24 g (56%); m.p.: 112–115 °C; 1H NMR (300 MHz, CDCl3): δ = 7.61 (1H, s, CH), 3.67–3.46 (m, 4H, m, CH2 N), 1.70–1.50 (12H, m) ppm; 13C NMR (75 MHz, CDCl3): δ = 157.9 (Ar), 157.5 (Ar), 157.3 (Ar), 119.3 (CNO2), 78.6 (CBrNO2), 48.7, 45.4, 45.3, 25.5, 24.4, 24.1 ppm; FT-IR (KBr): υ = 2942 (s), 2861 (m), 1567 (s) cm⁻¹; MS: m/z = 417 (M⁺).

4-[Bromo(nitromethyl)-5-nitro-2,6-di(piperidin-1-yl)pyrimidine (2b, C_{13}H_{13}BrN_{6}O_{4}) Yellow powder; yield: 0.24 g (58%); m.p.: 89–92 °C; 1H NMR (300 MHz, CDCl3): δ = 7.72 (1H, s, CH), 3.77–3.74 (4H, m, CH2 N), 3.46–3.43 (4H, m, CH2 C), 1.70–1.50 (12H, m) ppm; 13C NMR (75 MHz, CDCl3): δ = 157.6 (Ar), 156.4 (Ar), 154.6 (Ar), 120.8 (CNO2), 77.8 (CBrNO2), 66.5 (CH2 O), 49.5 (CH2 N), 44.4, 29.7 ppm; FT-IR (KBr): υ = 2986 (s), 2863 (m), 1589 (s), 1565 (s) cm⁻¹; MS: m/z = 417 (M⁺).

4-[Bromo(nitromethyl)-5-nitro-6-piperidin-1-yl)pyrimidine (2c, C_{14}H_{19}BrN_{6}O_{4}) Yellow powder; yield: 0.24 g (57%); m.p.: 145–157 °C; 1H NMR (300 MHz, CDCl3): δ = 7.69 (1H, s, CH), 3.94–3.75 (8H, m, CH2 N), 3.52–3.45 (4H, m, CH2 C), 1.77–1.70 (6H, m, CH2 C) ppm; 13C NMR (75 MHz, CDCl3): δ = 157.7 (Ar), 157.6 (Ar), 157.3 (Ar), 120.1 (CNO2), 78.2 (CBrNO2), 66.6 (CH2 O), 48.7 (CH2 N), 44.4 (CH2 N), 29.7 (CH2 C), 25.5 (CH2 C), 24.0 (CH2 C) ppm; FT-IR (KBr): υ = 3023 (w) 2937 (m), 2855 (m), 1585 (s), 1564 (s), 1336 (m) cm⁻¹; MS: m/z = 430 (M⁺).

4-[Bromo(nitromethyl)-2-[4-methylpiperidin-1-yl]-5-nitropyrimidine (2e, C_{17}H_{25}BrN_{6}O_{4}) Yellow powder; yield: 0.29 g (64%); m.p.: 63–65 °C; 1H NMR (300 MHz, CDCl3): δ = 7.73 (1H, s, CH), 4.77–4.62 (2H, m, CH2 N), 3.94–3.84 (2H, m, CH2 C), 3.04–2.86 (4H, m, CH2 C), 1.78–1.65 (5H, m, CH2 C), 1.31–1.14 (5H, m, CH2 C), 1.01 (d, 6H, Me, J = 6 Hz) ppm; 13C NMR (75 MHz, CDCl3): δ = 157.9 (Ar), 157.5 (Ar), 157.3 (Ar), 119.0 (CNO2), 78.6 (CBrNO2), 48.4 (CH2 N), 48.0 (CH2 N), 44.9 (CH2 N), 44.7 (CH2 N), 33.8 (CH2 C), 33.6 (CH2 C), 31.0 (CHMe), 30.7 (CHMe), 21.6 (Me), 21.5 (Me) ppm; FT-IR (KBr): υ = 2953 (w) 2925 (m), 1563 (s) cm⁻¹; MS: m/z = 456 (M⁺).
4-[6-[Bromo(nitro)methyl]-5-nitro-2-(pyrrolidin-1-yl)pyrindin-4-yl]morpholine (2i, C_{13}H_{17}BrN_{6}O_{5}) Yellow powder; yield: 0.22 g (55%); m.p.: 97–100 °C; 1H NMR (300 MHz, CDCl3): δ = 7.70 (1H, s, CH), 3.80–3.77 (6H, m, CH_{2}O, CH_{2}N), 3.62–3.54 (6H, m, CH_{2}O, CH_{2}N), 2.08–1.98 (4H, m, CH_{2}C) ppm; 13C NMR (75 MHz, CDCl3): δ = 157.5 (Ar), 156.3 (Ar), 155.5 (Ar), 119.7 (CNO2), 78.48 (CBrNO2), 67.30 (CH2O), 66.42 (CH2O), 66.40 (CH2O), 48.0 (CH2N), 47.8 (CH2N), 47.3 (CH_{2}N), 25.3 (CH2C), 25.2 (CH2C) ppm; FT-IR (KBr): ν = 2974 (m), 2870 (m), 1585 (s), 1554 (s), 1524 (s), 1322 (s) cm⁻¹; MS: m/z = 416 (M⁺).

Computational details

The structure of 2f and 2f' were optimized at mPW1PW91/6-31G(d) level of theory in the gas phase and characterized by frequency analysis. The magnetic shielding constants were computed using the gauge including atomic orbitals (GIAO) method [47] at the mPW1PW91/6-31G(d) level of theory in the gas phase. The GIAO 13C chemical shifts were predicted by multi-standard approach (MSTD) [48]. All calculations were carried out with the Gaussian 09 package [49].

Acknowledgements

M. M. acknowledges the Research Council of Ferdowsi University of Mashhad for partial support of this project (333579). M. M. H. is grateful to Alzahra University Research Council as well as appreciates the granted research chair by Iran National Science Foundation (INSF).

References

1. Heravi MM, Zadsirjan V, Malmir M (2018) Molecules 23:943
2. Heravi MM, Zadsirjan V, Hamidi H, Hajiabbas TAP (2017) RSC Adv 7:24470
3. Heravi MM, Lashaki BT, Poorahmad N (2015) Tetrahedron: Asymmetry 26:405
4. Ono N (2001) The nitro group in organic synthesis. Wiley-VCH, New York
5. Soengas RG, Acurcio RC, Silva AM (2014) Eur J Org Chem 2014:6339
6. Hernandes MZ, Cavalcanti SMT, Moreira DRM, de Azevedo J, Filgueira W, Leite ACL (2010) Curr Drug Targets 11:303
7. Sen S, Kamm SR, Potti VR, Murthy YLN, Chaudhary AB (2011) Tetrahedron Lett 52:5585
8. Butler P, Golding BT, Laval G, Loghmani-Khouzani H, Ranjar-Karimi R, Sadeghi MM (2007) Tetrahedron 63:11160
9. Feuer H, Friedman H (1975) J Org Chem 40:187
10. Wu D, Zhang J, Cui J, Zhang W, Liu Y (2014) Chem Commun 50:10857
11. Kurfürst A, Schwarz M (1989) Collect Czech Chem Commun 54:1346
12. Kurfürst A, Racloviá F, Kuthan J (1980) Collect Czech Chem Commun 45:397
13. Stock NS, Bain G, Zunic J, Li Y, Ziff J, Roppe J, Santini A, Darlington J, Prodanovich P, King CD, Baceci C (2011) J Med Chem 54:8013
14. Su N, Bradshaw JS, Zhang XX, Song H, Savage PB, Xue G, Krajkowski KE, Izatt RM (1999) J Org Chem 64:8855
15. Adhikari S, Mandal S, Ghosh A, Das P, Das D (2015) J Org Chem 80:8530
16. Maj AM, Suisse I, Hardouin C, Agbossou-Niedercorn F (2013) Tetrahedron 69:9322
17. Wang L, Hou X, Fu H, Pan X, Xu W, Tang W, Fang H (2015) Bioorg Med Chem 23:4364
18. Shults MD, Imperiali B (2003) J Am Chem Soc 125:14248
19. Bi WZ, Qu C, Chen XL, Wei SK, Qu LB, Liu SY, Sun K, Zhao YF (2018) Tetrahedron 74:1908
20. Xie Y, Li L (2014) Tetrahedron Lett 55:3892
21. Priyadarshini S, Joseph PA, Kantam ML, Sreedhar B (2013) Tetrahedron 69:6409
22. Ravi P, Tewari SP (2013) Catal Commun 42:35
23. Paik SU, Jung MG (2012) Bull Korean Chem Soc 33:689
24. Ravi P, Gure GM, Sikder AK, Tewari SP (2012) Synth Commun 42:3463
25. Wu X, Dube MA, Fry AJ (2006) Tetrahedron Lett 47:7667
26. Chang K, Grimmert MR, Ward DD, Weavers RT (1979) Aust J Chem 32:1727
27. Clewley RG, Fischer A, Henderson GN (1989) Can J Chem 67:1472
28. Reznikov VA, Vishnivetskaya LA, Volodarsky LB (1994) Russ Chem Bull 43:2735
29. Russell G, Dedolph D (1985) J Org Chem 50:2498
30. Feuer H, Vincent EF (1964) J Org Chem 29:939
31. Feuer H, Friedman H (1975) J Org Chem 40:187
32. Terentev AO, Krylov IG, Obigin YN (2006) Synthesis 2006:3819
33. Marchand AP, Arney BE Jr, Dave PR (1988) J Org Chem 53:443
34. Mouavi M, Bakavoli M, Shiri A, Esghii H (2018) ACS Sustainable Chem Eng 6:5852
35. Heravi MM, Benmorad T, Bakhtiari Kh, Bamoharram FF, Oskooie H (2007) J Mol Catal A-Chem 264:318
36. Heravi MM, Abdolhosseini N, Oskooie H (2005) Tetrahedron Lett 46:8959
37. Bakavoli M, Rahimizadeh M, Shiri A, Esghii H, Vaziri-Mehr S, Pordeli P, Nikpour M (2011) Heterocycl Commun 17:49
38. Esghii H, Rahimizadeh M, Saberi S, Abnous K, Bakavoli M (2013) J Chem Res 37:553
39. Bazaar T, Bakavoli M, Rahimizadeh M, Esghii H, Nikpour M (2013) Heterocycl Commun 19:401
40. Ebrahimpour Z, Shiri A, Bakavoli M, Seyed SM, Asghari T, Mague J (2017) J Heterocycl Chem 54:235
41. Igei M, Bakavoli M, Shiri A, Ebrahimpour Z, Azizollahi H, Beyzaei A, Moghadam-Manes M (2016) J Chem Res 40:628
42. Mouavi M, Bakavoli M, Shiri A, Tajabadi J (2018) Chemistry Select 3:5401
43. Tajabadi J, Bakavoli M, Gholizadeh M, Esghii H, Izadyar M (2015) RSC Adv 5:38489
44. Bakavoli M, Esghii H, Shiri A, Afrout H, Tajabadi J (2013) Tetrahedron 69:8470
45. Lodewyk MW, Siebert MR, Tantillo DJ (2012) Chem Rev 112:1839
46. Minkin VI, Mikhailov IE, Dushenko GA, Yudilevich JA, Minyaev RM, Zschunke A, Mögge K (1991) J Phys Org Chem 4:31
47. Ditchfield R (1974) Mol Phys 26:1839
48. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb, MA, Cheeseman JR, Scalmani G, Barone V, Mennucci, B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA, Peralta JE, Ogliaro F, Bearpark M, Moghaddam-Manesh M (1991) J Phys Org Chem 4:31
49. Kucharski RE, Gnanavel G, Porsolt M, Schuurman A, van der Merwe S, Meyer S, van der Helm T, de Jongh KH, van der Vlist MM, Taal TA, van der Velden AE, van der Made AJ, van der Marel PA, van der Marel IA, van der Marel IP, van der Made AL, van der Marel J, van der Made A (2007) J Org Chem 72:8747
50. Sarotti AM, Pellegrinet SCA (2009) J Org Chem 74:7254
51. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb, MA, Cheeseman JR, Scalmani G, Barone V, Mennucci, B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA, Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC,
Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ (2009) Gaussian 09, Revision A.02. Gaussian, Inc, Wallingford, CT

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.