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## Ozonation of Benzotetrazine 1,3-Dioxides. Facile Synthesis of Di(methoxycarbonyl)-1,2,3,4-tetrazine 1,3-Dioxide

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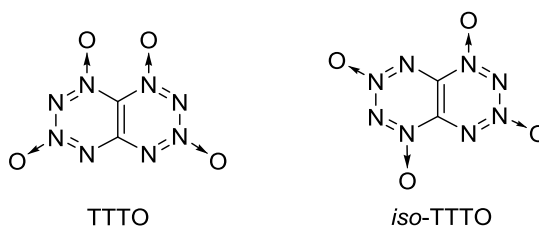
### Abstract

A new method for the synthesis of non-annulated 1,2,3,4-tetrazine-1,3-dioxides, proceeding *via* ozonation of benzotetrazine 1,3-dioxides bearing electron-donating substituents, followed by treatment with MeOH/HCl has been developed. Dimethyl 1,2,3,4-tetrazine-5,6-dicarboxylate 1,3-dioxide (**4**), methyl 5-(1,1-dichloro-2-ethoxy-2-oxoethyl)-1,2,3,4-tetrazine-6-carboxylate 1,3-dioxide (**5**) and methyl 6-formyl-1,2,3,4-tetrazine-5-carboxylate 1,3-dioxide (**6**) were prepared and the structures of tetrazines **4** and **5** were confirmed by X-ray diffraction analysis.

**Keywords:** benzotetrazine 1,3-dioxides, 1,2,3,4-tetrazine 1,3-dioxides, ozonation, ring-opening reaction, X-ray diffraction analysis.

Since reporting the first synthesis of a benzoannulated 1,2,3,4-tetrazine 1,3-dioxide (TDO),<sup>1</sup> our research group has extensively explored the synthesis of these compounds.<sup>2,3</sup> Although benzoannulated TDOs are the most common type, TDOs annulated with furazane,<sup>4</sup> pyridine<sup>5</sup> and triazole<sup>6</sup> rings have been also prepared. Recently, new methods for the synthesis of annulated TDOs have been developed<sup>7,8</sup> and the TDO formation mechanism has been confirmed.<sup>9</sup>

1,2,3,4-Tetrazine 1,3-dioxide derivatives including tetrazino-tetrazine 1,3,6,8-tetraoxide (TTTO) and tetrazino-tetrazine 1,3,5,7-tetraoxide (*iso*-TTTO) are of considerable interest as high energy density materials (HEDM). A number of theoretical studies of these HEDMs have been performed during the last decade.<sup>10</sup>



Non-annulated TDOs are likely to be key sources for the synthesis of TTTO and *iso*-TTTO. Moreover, they are of interest as such for designing new HEDMs.<sup>11</sup> Two representatives of this class of TDOs **2a,b**, have been described and were prepared by the thermolysis of (polyazido)benzotetrazine 1,3-dioxides **1a,b**<sup>12</sup> (Scheme 1).<sup>13</sup> However, this method is rather inconvenient for scale-up and the chemical properties of these compounds have not been studied.

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