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[e009]

Microwave assisted synthesis of triskelium compounds from 1,3,5-triazines

Julio A. Seijas,,* M. Pilar Vázquez-Tato,* José Crecente-Campo, M. Ara Carballo-Meilán
Departamento de Química Orgánica. Facultad de Ciencias. Universidad de Santiago de Compostela. Aptdo. 27080-Lugo. Spain

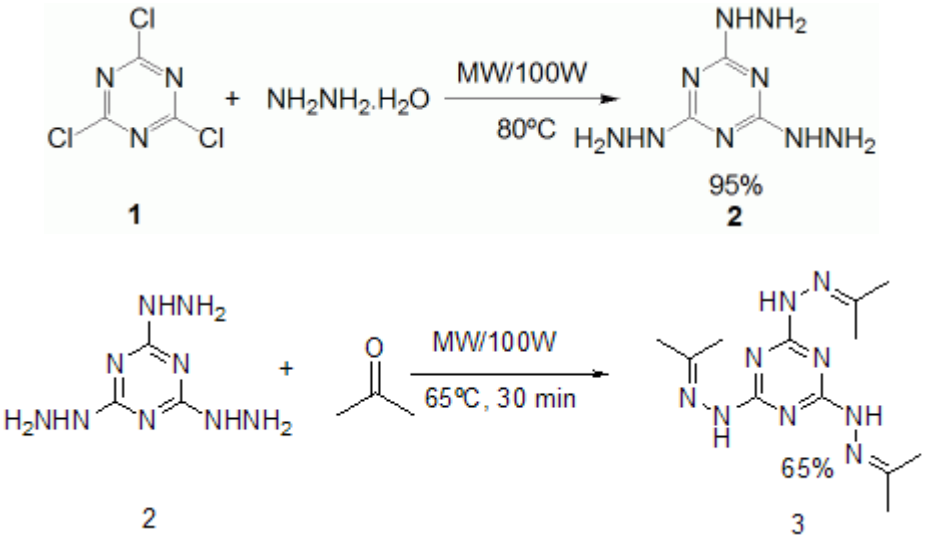
Abstract: *Microwave assisted synthesis of 2,4,6-trishydrazino-1,3,5-triazine from hydrazine and cyanuric chloride is achieved in good yield. Its reaction with acetone and benzaldehyde yields the corresponding trishydrazones in good yields and short reaction times using MAOS.*

s-Triazine chemistry has undergone a revitalization due to the usefulness of melamine derivatives as precursors of a variety of oligomers,[1] polymers,[2] as scavenging resins,[3] components of host–guest,[4] superstructure assemblies,[5] ligand scaffolds for catalysis,[6] in medicinal chemistry,[7] as in encapsulation of anticancer drugs and reduction of its toxicity.[8] 1,3,5-Triazine derivatives have proven their great potential in this rising area of material chemistry, both for their π-interaction abilities,[9] and for their aptitude to be involved in intricate H-bond networks.[10] They can recognize other molecules by the donation and acceptance of hydrogen bonds, metal chelation, and π–π interactions.

The appeal of the s-triazine core is largely due to the ease of sequential substitution of the chloride atoms in cyanuric chloride with amine nucleophiles, to generate a variety of structures. Although for products with C_3 symmetry the substitution of three clorine atoms in cyanuric chloride (**1**) can be achieved in one-pot reaction.

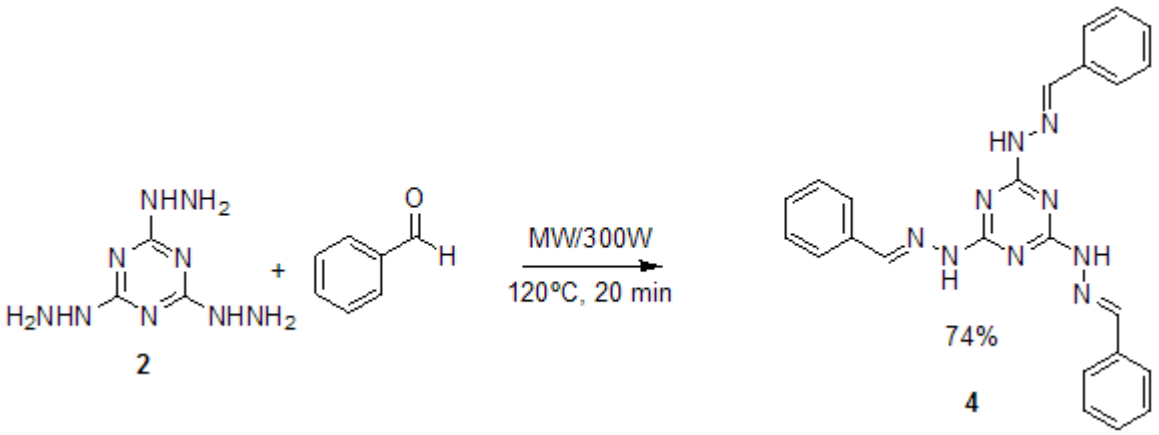
In this communication we report our preliminary results on the application of microwaves to the chemistry of s-triazines.

So, synthesis of 2,4,6-trishydrazino-1,3,5-triazine has been carried out by reacting hydrazine hydrate (80% aqueous solution) with cyanuric chloride under microwave irradiation for 15 minutes. The temperature was maintained at 80ºC irradiating with a power of 100W, with simultaneous cooling, in order to increase the amount of microwaves irradiated. This yielded a 95% yield of hydrazine **2** (scheme1).



Scheme 2

Once checked the utility of microwaves for the preparation of hydrazones of 2,4,6-trihydrazinyl-1,3,5-triazine, hydrazine **2** was irradiated together with benzaldehyde in 1:4 molar ratio for 20 minutes, at 120ºC (irradiation power set at 300W with simultaneous air cooling). this reaction conditions yielded 74% yield of 2,4,6-tris((E/Z)-2-benzylidenehydrazinyl)-1,3,5-triazine.



Scheme 3

Two posible 3D structures for compound 4 were modellized using MOPAC with Hamiltonian PM3. The lowest heat of formation corresponding with a triskelion like form (figure 2).

Hf=229.86487 kcal/mole	Hf=241.56413 kcal/mole

In summary, microwave assisted solvent-free organic synthesis (MASFOS) for triskelium like molecules can be used as a tool to get this compounds with C_3 symmetry.

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A triskelion is a typical celtic symbol. Its stucture consists of three identical curved branches meeting in the center. [triskelia (plural), greek *triskeles*.three-legged].
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