

Use of Advanced Mass Spectrometry Techniques to Help in the Chemical Storage of Solar Energy

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Storing solar energy represents a major challenge in modern science. Chemical storage with **MO**lecular **SOL**ar **THER**mal systems (**MOST**) appears promising though challenging. The working principle of those systems is based on iterative closed cycles of photoisomerization and back-isomerization between a parent compound and its metastable isomer. Energy is stored within the metastable isomer which possesses a certain half-life time and thermal energy is released during the thermal back-isomerization process. Among the MOST systems, azobenzene with its E→Z photoisomerization has been studied but characteristics such as storage enthalpy and half-life time must be improved. To do so, anchoring chromophores on a macromolecular backbone appears to be an elegant strategy since cooperative effects between chromophores may help enhancing these properties [1]. Our work consists of producing new MOST systems based on a peptoid-type backbone supporting azobenzene chromophores at key positions. This backbone could allow cooperative effects since peptoids belong to foldamers family and can thus adopt specific secondary structures in solution. We synthesized different peptoids containing azobenzene(s) at key positions with solid support protocol. Primary structures of the molecules were confirmed with MS and MS/MS analyses based on B/Y and A/Y fragmentation patterns. With UV irradiation, different isomers are produced and their relative proportions against irradiation time are monitored using LC-MS analyses. LC-MS also allows the determination of the crucial photoisomers half-live times ($t_{1/2}$) by performing continuous analyses while the solutions are kept in the dark at controlled temperatures. Determination of $t_{1/2}$ showed that azobenzene behaves differently depending on its position on the backbone, showing interesting influence from our peptoid support. We will show that repeating $t_{1/2}$ measurement at different temperatures allows to have insights on the activation barrier in solution, which is another crucial MOST parameter. Finally, thermal back-isomerization behaviour of each photoisomer will be further discussed since LC-MS allows their separation and independent analyses.

References

1. Zhang, B.; Feng, Y.; Feng, W. Springer Nature Singapore, **14**, 2022.