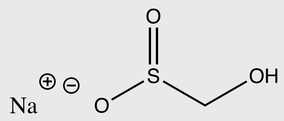
Cyclic Sulfones by Double Conjugate Addition of Rongalite

Melina Goga, Hao Zong, Jazmin Prana, Rudolph Michel, Antonia Muro, and Dr. Magnus Bebbington*
Department of Chemistry and Biochemistry, Montclair State University

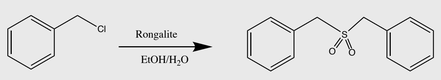
Rongalite Introduction

- Reduced form of SO_2
- Used as bleaching agent
- Very cheap, bulk chemical
- Has low odor
- Environmentally friendly
- Has potential as a sulfur nucleophile

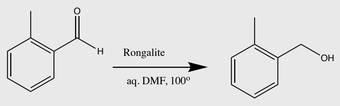


Organic Transformations Mediated by Rongalite

Alkylation of Rongalite

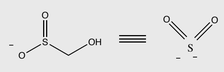


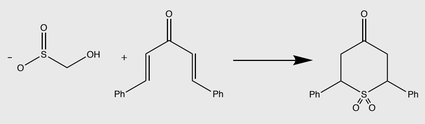
Rongalite serving as a Reducing Agent



Hypothesis

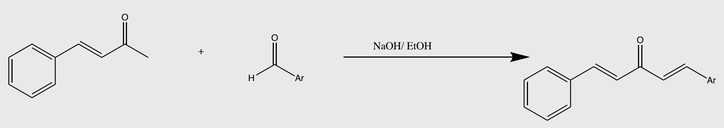
- Rongalite can undergo double conjugate addition in reaction with dienones in order to give cyclic sulfones.



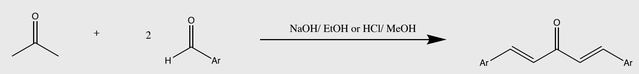


Substrate Synthesis

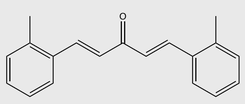
Unsymmetrical



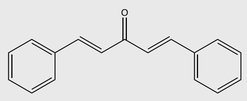
Symmetrical



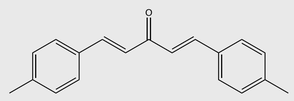
Substrates Synthesized



Yield: 67%

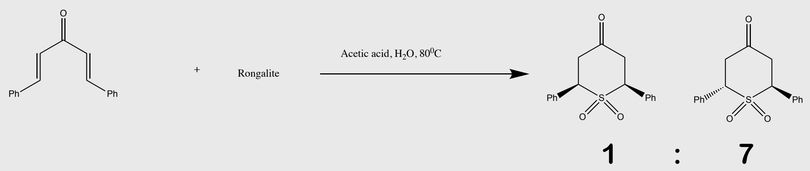


Yield: 77%



Yield: 45%

Results and Optimization - Dibenzalacetone



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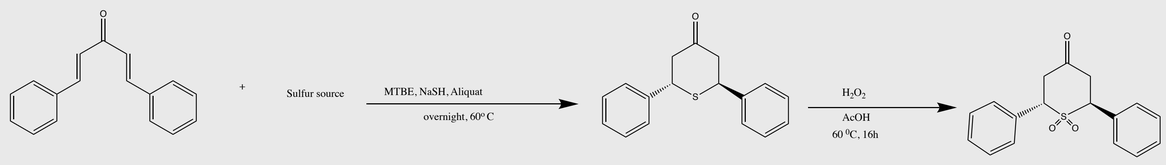
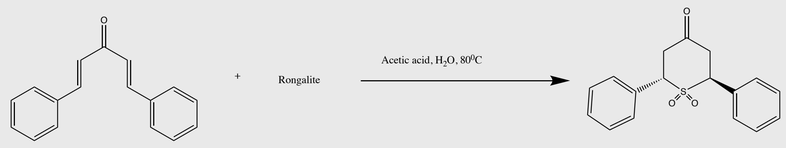
Time	Conditions	Equivalents of Rongalite	% Yield
Overnight	acetic acid	1.5	81
3 hr	acetic acid	1.5	75
18 hr	DMSO	1.5	28
18 hr	DMSO, K_2CO_3	1.5	9
1 hr	DMSO, acetic acid	1.5	28
2 hr	EtOH	1.5	23
Overnight	acetic acid	1.1	64
3 hr	EtOAc, TBAB	1.5	8
3 hr	EtOH, acetic acid	1.5	42

Proof of Structure- Major Diastereomer

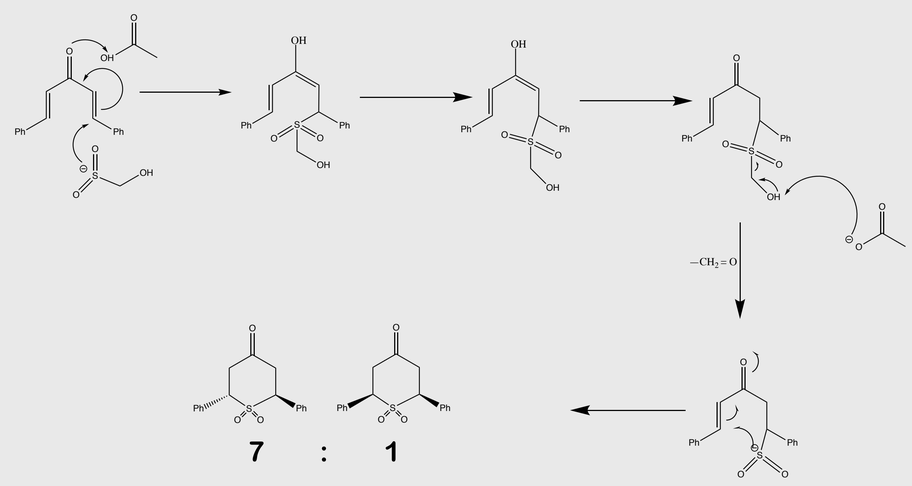


- The oxidation of sulfide was performed and it produced the trans sulfone. The spectroscopic data matched those in literature.

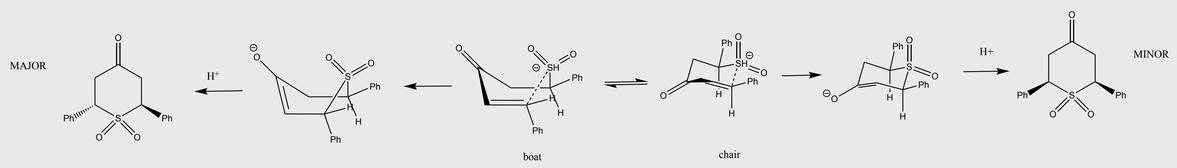


Reference
Gendron, T., Kessedjian, H., Davioud-Charvet, E., & Lanfranchi, D. A. (2015). Diastereoselective Synthesis of 2,6-Diaryltetrahydrothiopyran-4-ones by Phase-Transfer Catalysis. *European Journal of Organic Chemistry*, *2015*(8), 1790–1796.

Proposed Mechanism of Conjugate Addition



Rationalization of Stereochemistry



- For the sulfur heterocycle, boat conformer thought to be preferred
- Feature specific to sulfur: long C-S bond length

Conclusion

Rongalite has the potential to act as a double nucleophile for sulfone synthesis.

Acknowledgments and References

Kotha, S., & Khedkar, P. (2011). Rongalite: A useful green reagent in organic synthesis. *Chemical Reviews*, *112*(3), 1650–1680.