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Study of reagent composition on the reaction between 1,1,2,2-tetrabromethane and imidazole or 1,2,4-triaqzole in a superbasic medium

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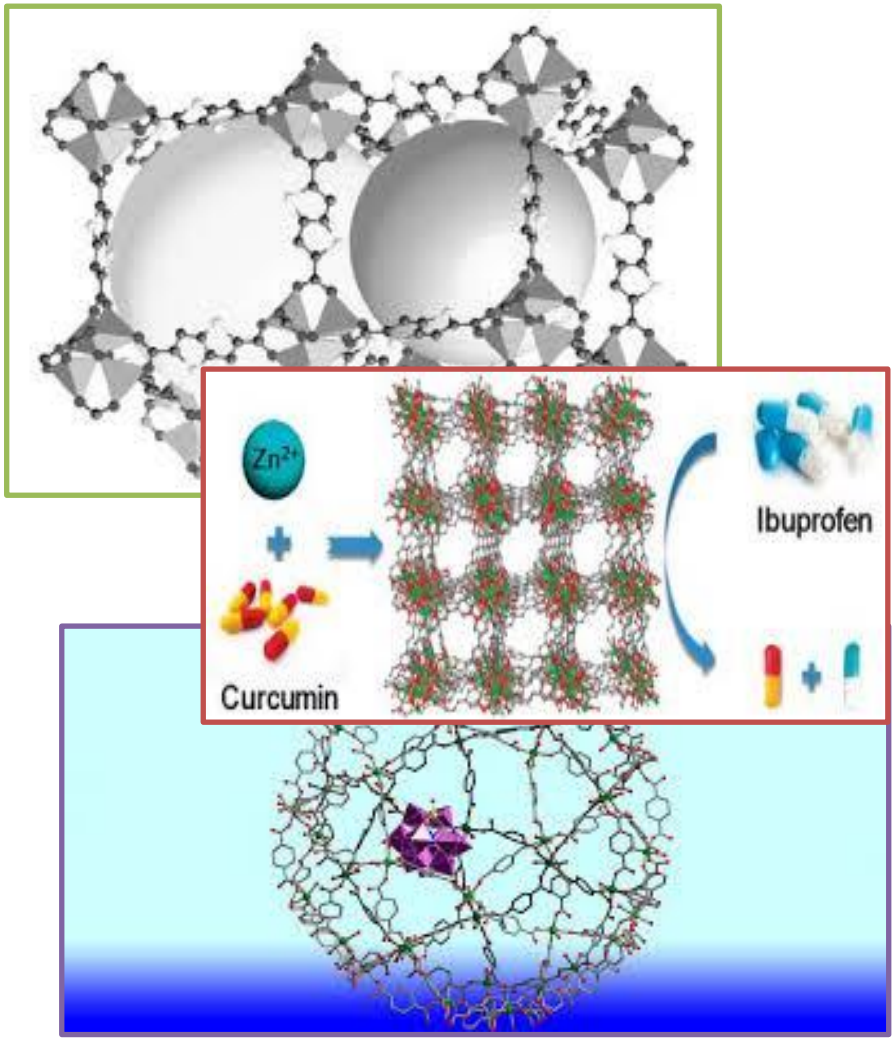
BACKGROUND

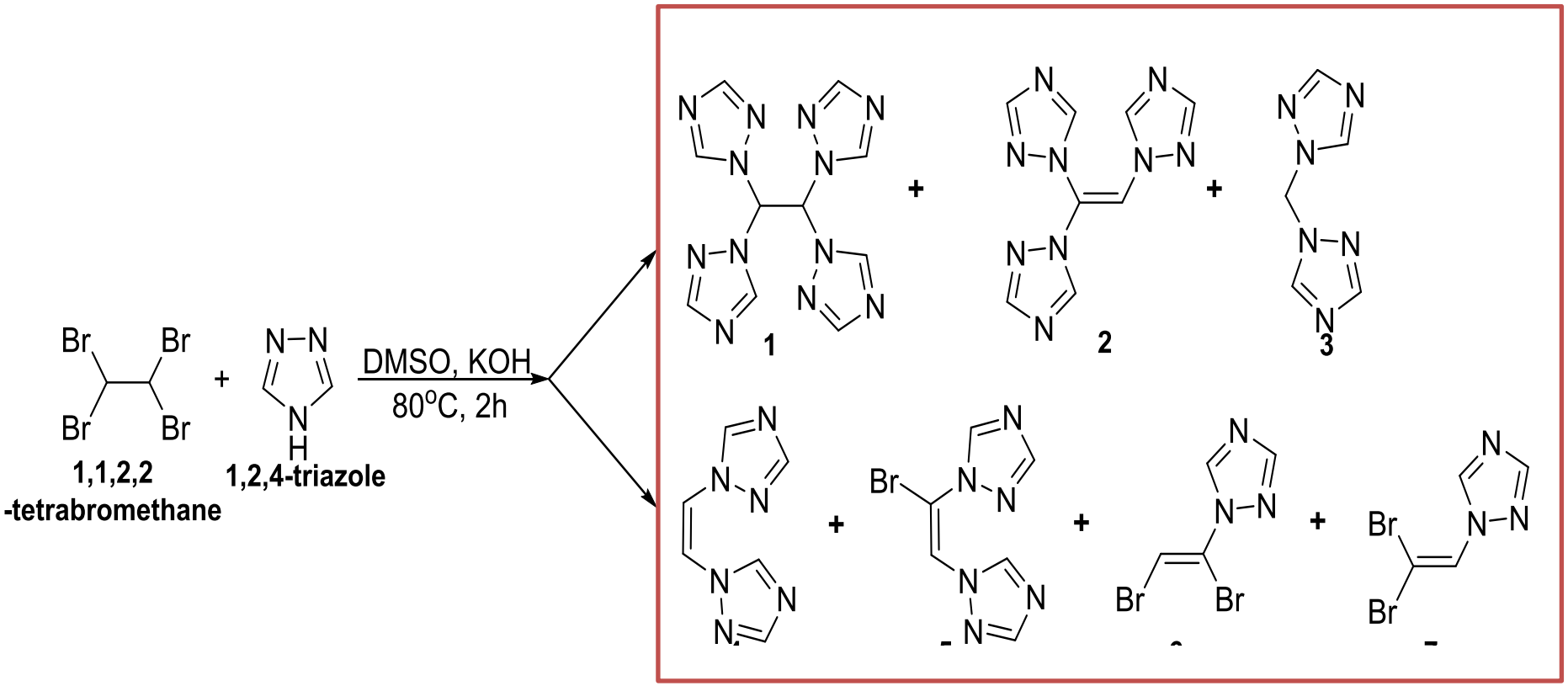
Compounds bearing several heterocyclic moieties can act as multidentate ligands for the construction of metal-organic frameworks (MOFs). Constant design of new MOFs is stimulated by their

- high capacity for gas storage
- photo-physical properties
- sensor capabilities
- excellent catalytic performance

Tetra(pyrazolyl)derivatives were successfully used for preparation of coordination polymers and molecular complexes.

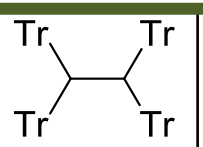
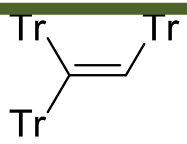
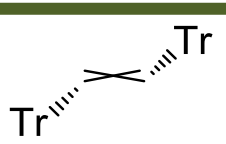
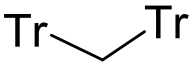
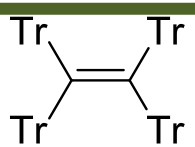


THE SYNTHESIS SCHEME



RESULTS AND DISCUSSION

- The 1,2,4-triazole (TrH) with 1,1,2,2-tetrabromethane (TBE) reaction was carried out using 1:1, 2:1, and 4:1 molar ratios of the reagents
- The resulting mixtures of products were examined by GC/MS

					Tr_2Br_2 (E & Z)	$TrBr_2$ (E or Z)	gem-$TrBr_2$	
1:1	———	9,2%	———	———	30%	56%	———	4,9%
1:2	7%	16%	———	———	19,5%	49%	14,8%	3,7%
1:4	17,6%	33,1%	8,3%	39,5%	———	———	———	———

CONCLUSION

- In all the cases, the reactions yielded complex product mixtures, in which triazolyl- and bromo-substituted ethenes were the dominating components.
- When triazole reacted with TBE in 1:1 ratio, bromoe-thenes containing one or two triazole rings were the major products.
- For 2:1 TrH-TBE reaction, 1,1,2-tris(triazol-1-yl)ethane Tr3 was detected as a second to the dominating product.
- In case of 4:1 TrH-TBE ratio, Tr3 was obtained as a major product, while only little amount of Tr4 was formed and no TrBr2 was detected at all.