Ring Topology and Strain in pure Silica Zeolites

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Framework stability in zeolites has been the subject of many studies and whether the source of structural instability is or not related with the number of rings and its distribution remains unclear. Only rough estimations of strain associated to 4-, 5- and 6-MR (membered rings) have been given. Also it is argued that 3-MR are utterly unstable although no calculations have been reported.

This study analyses rings in pure silica zeolites and strains associated to rings through the values of OSiO angles. A software code has been updated which calculates: (i) OSiO (and SiOSi) angles against ring size, (ii) strain associated to OSiO angles of each topologically unique Si atom, (iii) individual rings in each structure and ring-strain according to the classical quadratic term in OSiO.

In MEI topology, Si1 is the most strained atom, against the classical explanation that Si4, to which the 3-MR are associated, should be the most unstable. Nevertheless, it is true that amongst the rings, the 3-MR are the most strained. Although 3-MR are formed by Si4 atoms, Si4 atoms are also part of another five rings. The corresponding vertex symbol for Si4 (3 7 5 5 5 5) gives us this information, and our software calculates the strain associated to the six OSiO angles, most of which happen to be very stable. On the other hand, Si1, with vertex symbol (4 7 4 7 4 7) contains six relatively unstable OSiO angles forming part of strained 4-MR and 7-MR, which -overall- make this knot (Si1) more unstable than Si4.

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