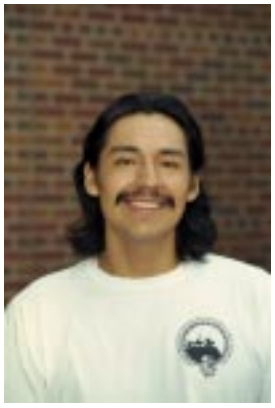
Materials Research Science and Engineering Center
(MRSEC)
Summer 2000 Team



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Different Length Pillars on Host-Guest Interaction

The scope of our work is to investigate the effect of different length of pillars on host-guest interaction. Our host molecules will be guanidinium complexes of disulfostilbene and related compounds with more carbon-carbon double bonds between para-sulfonated phenyl rings. The geometry optimization of these compounds using CACHE revealed S-S distance of 12.347 A, 13.936 A and 16.512 A respectively for disulfostibene, disulfo derivative of trans,trans-diphynylbutadiene (Two C-C double bond) and disulfo derivative with three C-C double bond.

The disulfostilbene and related compounds will be prepared by methods found in the literature as in the attachment. The disulfo-derivatives will be reacted with guanidinium tetra-fluoroborate to obtain their corresponding guanidinium disulfo-complexes. The saturated solution of these complexes in methanol will be carefully added to different host solutions to grow the host-guest crystals. We will use mono- and di-substituted benzene as guest molecules.

We have already prepared the crystals of guanidinium complexes of disulfostilbene with 1,4-divinylbenzene, p-xylene , 3,4-dimethylanisole and 3,5-dimethylanisole as guest. We will determine the crystal structure of these inclusion compounds by single-crystal x-ray crystallography.