A combinatorial method for generating periodic 4-connected frameworks is described. The computer algorithm requires, as input, the number of unique tetrahedral atoms and the crystallographic space group type. The algorithm then searches systematically over all possible combinations of connected crystallographic sites that are consistent with 4-connected nets. The resulting graphs are then relaxed by simulated annealing to identify the regular tetrahedral zeolite topologies.

Results are presented for one unique tetrahedral atom in each of the 230 crystallographic space group types. 5,043 unique 3-dimensional 4-connected unimodal graphs are found. About 5% of these graphs refine to reasonable tetrahedral topologies. All the known unimodal zeolites, and dense silicon dioxide phases are small numbers of unique atoms.

explosion of graphs as of the omeric pairs of space group types.

The mean free channel diameters measure about in the framework is large, because its building unit, zeolite topologies planes. In contrast to space group type. The framework density is when dehydrated, and is stable up to 623 and two other recently found microporous frameworks (1) M. Schindler, W. H. Baer, Inst. für Kristallographie, Goethe-Universität, Senckenberganlage 30, 60604 Main am Germany.

The title compound (short: FVP-1) is one of a new class of frameworks that are more open than all aluminosilicates and Al- or Ga-phosphates known so far. These frameworks exchange ions and their H2O can be reversibly removed. FVP-1 was grown hydrothermally in the Na4[(V11O23)6(V(O,OH))12]4P04[(P04)3(O,H)]1.2-3.4 . ZnH2O (WITHE x=1.5-2.0, y=0-0.17, z=3-4). M. Schindler, W. H. Baer, Inst. für Kristallographie, Goethe-Universität, Senckenberganlage 30, 60604 Main am Germany.

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There is a limited number of five molecules M known so far which direct the sodalite structure via molecular recognition in hydrothermal and H2O-free syntheses conditions. The cubic host structure of the SiO2-SOD-phases, which are well characterized by X-ray and neutron diffraction data, show unlike all the other clathrasil-types no 5-membered but instead 4- and 6-membered rings on the microporous tetrahedral framework structure. We have chosen this group of model clathrasils in order to focus our attention to the crystallography of the organic molecules M of low symmetry which, trapped in the 4668-SOD-cages and isolated by the 3D-periodic SiO2-matrix, cause a typical pattern of multi-stage phase transitions into the host structure as shown by DSC-microrcalorimetry and synchrotron powder diffraction data. We report here on the experimental results of three spectroscopic methods IR-spectroscopy, quasi-elastic neutron scattering and MAS-NMRspectroscopy of the nuclei 1H, 13C, 29Si which reveal the guest/guest- and as well the guest/host-interactions through different time windows of frequencies 1012 to 1015 cps, 108 to 1012 cps and 1012 to 1016 cps, respectively. Starting from the frozen in disorder statistics at 10K up to the critical temperatures of about 800K, where thermal decomposition and/or oxidation of the guest molecules occurs, structural phase transitions at temperatures Tm and as well glass points Tg demonstrate critical characters in the van der Waals guest/host-interactions of molecular recognition.