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^1^1^3Cd MAS NMR谱表征纳米CdO， CdS在NaY的β笼内 形成的构型

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摘要 通过29^Si,27^Al和^1^1^3CdMASNMR谱，观察到如下结果：(1)在Nayβ笼内形成的CdO和CdS簇，它们的^1^1^3Cd化学位移分别为115.0和100.0这些值接近于体相CdO的化学位移83.5，而远离体相CdS的化学位移583.8，因此它们的构型应归属为体相CdO的立方岩盐构型，而不属于体相CdS的配位数为4的闪锌矿构型。(2)CdO-NaY硫化时，NaY的骨架脱铝原子，脱铝原子使β笼的窗口扩大，这有利于直径大于β笼窗口的硫原子(或H2S)进入β笼对CdO[或Cd(OH)^+]硫化。

关键词 结构表征 纳米相材料 光敏材料 构型 分子筛 簇 硫化镉 笼状结构 氧化镉 核磁共振谱法 镉113核磁共振谱法

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Characterization of configuration of CdO, CdS in Nay β- cage by using ^1^1^3Cd MAS NMR

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Abstract The geometry structure of the guest clusters Cd(OH)^+, CdO and CdS located at βcage of Y zeolite was investigated by ^1^1^3Cd MAS NMR . The results show that there is a chemical shift at 115.0, 114.4 and 100.0 in the 113^Cd MAS NMR spectrum of CdO-NaY, CdS10-NaY and CdS20- NaY(sulphuration time for CdO-NaY is 10 min, 20 min respectively), respectively. These chemical shift values are close to the value of 83.5 which is the resonance signal of cubic halite type of bulk CdO with coordination number of 6, and deviate from the value of 583.8 which is the 113^Cd chemical shift of cubic sphalerite of bulk CdS with coordination number of 4. These results illustrate that the corrdination environment of the Cd^2+ ions located at βcage of Y zeolite is similar to that of bulk CdO with the cubic halite structure. It is also noted that the chemical shift value for CdO-NaY sample decreases with the increase of sulphuration time due to the oxygen atom with larger electronegativity being gradually substituted by sulphur atom. The phenomenon is identical with that substitute of selenium for sulphur of CdS or tellurium for selenium of CdSe. In addition, the 29^Si and 27^Al MAS NMR results show that several aluminum ions were removed from framework of zeolite NaY in the period of preparation of guest cluster with ion exchange and sulfidation treatment bringing about the formation of framework defect position. It is of benefit to sulfur atoms with larger atomic diameter from α cage smoothly into βcage of Y zeolite and sulfate the CdO or Cd(OH)^+ clusters to Cd(O,S) clusters.

Key words STRUCTURE CHARACTERISTICS NANOPHASE MATERIALS PHOTOSENSITIVE MATERIALS CONFIGURATION MOLECULAR SIEVE VARIETY CADMIUM SULFIDE CAGE STRUCTURE CADMIUM OXIDE NMR SPECTROMETRY

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