

## عنوان مقاله:

Structure and Geometry of Isomers of Nano N<sub>20</sub> Clusters

## محل انتشار:

دومین همایش ملی نانو مواد و نانو تکنولوژی (سال: 1389)

تعداد صفحات اصل مقاله: 4

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## خلاصه مقاله:

Among the high-energy density materials (HEDMs), nitrogen clusters as the good synthetic targets have been the subject of intense interest in the past 20 years. In these investigations, the studies of stability and bonding have received great attentions. In the present study, we report new quantum chemical calculations for nano nitrogen clusters of N<sub>20</sub> by the density functional theory (DFT) with B3LYP method and aug-ccpVDZ basis set. Since the decomposition mechanism is closely depends on the bonding pattern, therefore this concept was searched via (modern quantum theory of atoms in molecules (QTAIM

## کلمات کلیدی:

Nitrogen Clusters, QTAIM, Structure, Bond

## لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/84427>

