Structural and Magnetic Properties of Gd$_3$N@C$_{80}$[1] JING LU,
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of Nebraska at Lincoln, Lincoln, Nebraska 68588 — Using relativistic and on-site cor-
relation corrected density functional theory, we have investigated the structural and
magnetic properties of recently synthesized Gd$_3$N@C$_{80}$. The most stable structure
of Gd$_3$N@C$_{80}$ has the three magnetic Gd ions pointing to the centers of hexagons in
C$_{80}$. The magnetic ground state of this structure has the three coplanar spins ($S = 7/2$) offset by 120° angles. At the same time, the state with the highest multiplic-
ity, where all the spins are parallel aligned, is found only about 4.5 meV higher in
energy. Therefore, at room temperature, we expect Gd$_3$N@C$_{80}$ to be paramagnetic
with spin fluctuating between different multiplicities.

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