Hyperfine characteristics of quantum registers NV-^{13}C in diamond nanocrystals formed by seeding approach from isotopic aza-adamantane and methyl-aza-adamanthane

© *A.P. Nizovtsev* [1,2], *S.Ya. Kilin* [1], *A.L. Pushkarchuk* [3,4], *S.A. Kuten* [4], *A.S. Gusev* [2], *F. Jelezko* [5]

[1] Institute of Physics, National Academy of Sciences of Belarus,
220072 Minsk, Belarus
[2] National Research Nuclear University „MEPhI",
115409 Moscow, Russia
[3] Institute of Physical-Organic Chemistry, National Academy of Sciences of Belarus,
220072 Minsk, Belarus
[4] Institute for Nuclear Problems, Belarusian State University,
220030 Minsk, Belarus
[5] Institute for Quantum Optics, Ulm University,
89069 Ulm, Germany
E-mail: apniz@dragon.bas-net.by, sergei_kilin@yahoo.com, alexp51@bk.ru,
semen_kuten@list.ru, ASGusev@mephi.ru, fedor.jelezko@uni-ulm.de

We predict the characteristics of hyperfine interactions (hfi) for a number of electron-nuclear spin systems NV-^{13}C in diamonds grown by seeding approach from the specific isotopic aza-adamantane or methyl-aza-adamantane molecules differing in ^{13}C position in the precursor as well as in the orientation of the NV center in the post-obtained diamond. For the purpose we have used the spatial and hfi data simulated previously for the cluster $C_{510}[NV]^{-}H_{252}$. The data obtained can be used to identify (and correlate with the precursor used) the specific NV-^{13}C spin system by measuring the hfi-induced splitting in optically detected magnetic resonance spectra being characteristic for the NV-^{13}C system.

Keywords: Nitrogen-vacancy (NV) color center, diamond, ^{13}C nuclear spin, precursor, aza-adamantane, methyl-aza-adamantane, hyperfine interaction, density functional theory.

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