SIMULATION OF ^{13}C-^{13}C J-COUPLING TENSORS IN DIAMOND CLUSTERS HOSTING THE NV COLOR CENTER

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In the past decade there was rapid progress in development of quantum magnetic sensing technologies based on nitrogen-vacancy (NV) color centers in diamond (see, e.g. [1,2] for recent reviews). Magnetometer based on single NV center can have nanometer-scale spatial resolution and exceptional sensitivity allowing to detect target single ^{13}C nuclear spins or coupled ^{13}C-^{13}C pairs located within the diamond which can be used as long-lived quantum memory [3]. In these respects, predicting of high-resolution NMR characteristics for studied spin systems is essential. Among them, those of indirect nuclear spin–spin coupling (the *J*-coupling), that arise due to second-order hyperfine interactions with the ^{13}C-^{13}C bond electrons, are important. Here we are presenting our recent results (see also [4]) of simulation of ***full tensors*** $\boldsymbol{J_{KL}}$ ($K,L=X,Y,Z$) describing the *J*-couplings of nucler spins ^{13}C in H-terminated NV-hosting diamond clusters.

We have optimized the cluster geometry using the ORCA 5.0.1 software package with the B3LYP/def2/J/RIJCOSX level of theory and then simulated the n-bond *J*-coupling ***tensors*** $\boldsymbol{^nJ_{KL}}$ for all possible ^{13}C-^{13}C pairs in the clusters using B3LYP/TZVPP/AUTOAUX/decontract level of theory. We found that, in addition to usually considered isotropic Fermi-contact contribution to $\boldsymbol{J_{KL}}$, the anisotropic contributions resulted from dia- and paramagnetic, spin-dipolar and spin-dipolar/Fermi-contact cross terms are essential and can manifest in NMR spectra of ^{13}C dimers recorded using the NV centers.

The calculated values of scalar *J*-constants ^nJ=Sp($\boldsymbol{^nJ_{KL}}$)/3 for different $^{13}C_i$-$^{13}C_j$ pairs in the examplary $C_{33}[NV]^-H_{36}$ cluster are shown in the Fig. 1. The highest ones are those for neighboring ^{13}C: one-bond constant ^1J were 30-37 Hz depending on the position of the ^{13}C dimer in the cluster with respect to the NV center.

Using the same theory level we also simulated full tensors $\boldsymbol{^nJ_{KL}}$ for the adamantane and found that for this molecule the calculated value ^1J = Sp($\boldsymbol{^1J_{KL}}$)/3=29.9 Hz correlates well with the isotropic constant ^1J=31.4 Hz obtained experimentally in [5].

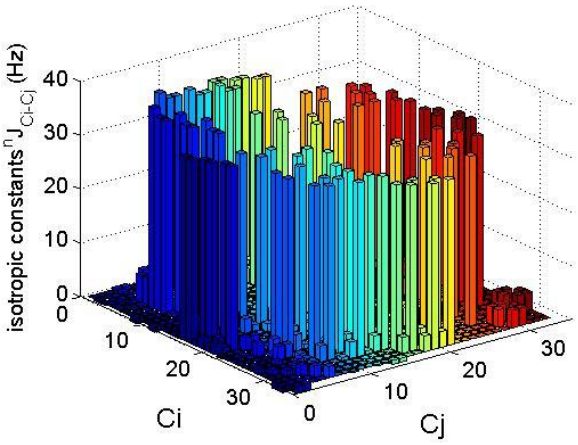

Figure1. Simulated isotropic ^nJ constants for all possible ^{13}C dimers in the $C_{33}[NV]^-H_{36}$ cluster.

References

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