Double resonance structures for NMR and EPR measurements

Abstract
NMR spectroscopy is one of the most important methods to elucidate the structure and dynamics of molecules. The sensitivity of the spectrometer is a limiting factor. The present invention increases the signal sensitivity and spectral resolution. The new double resonance structure is suited for a combined NMR/EPR spectrometer for the investigation of liquid samples applying dynamic nuclear polarization (DNP) and/or electron nuclear double resonance (ENDOR) techniques.

Invention
The new double-resonant structure consists of a strip resonator which generates high-frequency fields for NMR transitions and a microwave resonator for EPR transitions. Part of the strip resonator acts as a flat mirror and reflects irradiating microwaves quasi-optical. The open double-resonant structure offers enough space for measurements of samples with a volume up to 200 nl. The volume is about 10 times larger compared to known helix resonators.

Moreover the flat mirror acts as a sample plate, which can be used as a heat sink due to its good thermal conductivity. This allows investigations of liquid samples with a much larger volume. The arrangement includes a spherical mirror. Through the iris of the mirror microwaves can be fed into the microwave resonator. Simulations show that the new double-resonant structure generates an increased magnetic high-frequency signal. Additionally, a strong and very homogeneous magnetic microwave field within the sample is created. Therefore, the spectrometer provides a high signal sensitivity and high spectral resolution.

In an alternate setup the high-frequency resonator formed from a number of parallel arranged electrically conductive strips. Compared to the use of the single strip resonator the conversion factor is further increased. This provides a higher magnetic field strength and an increased NMR-measuring sensitivity is achieved.

Project Status
A prototype of the invention has been designed and tested.

Customer Benefits
- Approx. 10-fold larger sample volume (200 nl) compared to known helix resonators
- Avoidance of overheating of the samples
- Increased signal sensitivity and spectral resolution for DNP and ENDOR.
- Faster measurements
- Easy to implement

Publications
- Prandolini et al., JACS 2009

Patents
- DE 10 2008 017 135
- DE 10 2009 048 636
- US 8,570,033
- US 8,823,373
- JP 5 399 551
- EP 2 269 045, validated in: DE, GB, FR, CH, SE, NL
- EP 2 414 820, validated in: DE, GB, FR, CH, SE, NL

The technologies can be licensed or assigned. Moreover, collaborations regarding further development are welcome.

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