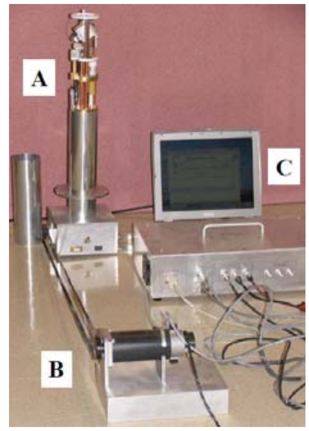
## Best of Both Worlds

*New NMR capability generates structural data, allows in situ control, merits patent*

A new nuclear magnetic resonance capability developed at the Department of Energy's EMSL, called DMAT, holds promise to open new doors in catalysis and biology research. The DMAT, or discrete magic angle turning, apparatus and method was developed by researchers at the Pacific Northwest National Laboratory's Institute for Interfacial Catalysis, EMSL, and PNNL and merited a United States patent.




*The DMAT apparatus consists of three parts: a specialized NMR probe (A), a DC Servo motor (B), and a computer-programmed box that precisely controls the rotation of the motor (C).*

DMAT combines the advantages of two established NMR technologies: magic angle hopping and magic angle turning. MAH and MAT are built from the cornerstone of NMR, magic angle spinning, which produces high-resolution, high-sensitivity isotropic spectra. But traditional MAS at a sample spinning rate of several kHz cannot be adapted for *in situ* investigations that require simultaneous, elevated pressure and flow controls. MAH allows simultaneous control over sample conditions (pressure, flow, and temperature) and generates enhanced structural data, but technical difficulties limit its wide-spread application for *in situ* experiments. MAT overcomes some of the technological challenges of MAH, but cannot be applied to *in situ* investigations that require precise pressure control. DMAT combines the best of both worlds of MAH and MAT and showed great potential in preliminary experiments. For example, DMAT structural data on 1,2,3-trimethoxybenzene were significantly enhanced compared to MAH and similar to that obtained with MAT, and this data quality was coupled with the ability to control sample temperature, pressure, flow conditions, and reactant feed composition *in situ* and simultaneously.

**Scientific Impact:** The simultaneous *in situ* control over sample conditions afforded by DMAT will open new doors for researchers to conduct *in situ* NMR studies of catalytic reactions and biological systems. The invention garnered a U.S. patent, *Discrete Magic Angle Turning System, Apparatus, and Process for in situ Magnetic Resonance Spectroscopy and Imaging*, Patent Number US 7,535,224 B2, and supports EMSL's goals to characterize surfaces and interfaces with unprecedented resolution as well as to predict biological functions from molecular and chemical data.

**Societal Impact:** DMAT will allow researchers to gain new insights into catalytic reactions, which may lead to an improved ability to tailor catalysts for optimal performance for applications such as alternative energy production and environmental remediation. In addition, DMAT can be used to collect novel data for—and, therefore foster a stronger fundamental understanding of—biological systems, such as dense cell systems and cells attached to solid surfaces.

For more information, contact EMSL Communications Manager Mary Ann Showalter (509-371-6017).

**Reference:** Hu JZ, JA Sears, JH Kwak, DW Hoyt, Y Wang, CHF Peden. 2009. "An Isotropic Chemical Shift-Chemical Shift Anisotropic Correlation Experiment using Discrete Magic Angle Turning." *Journal of Magnetic Resonance* 198:105–110.

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