Chemical Shift Anisotropy of the Mg on (MgO)₁₈ and Urea/(MgO)₁₈

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The understanding of the catalytic processes of the urea molecule (CH₄N₂O) in magnesium oxides has been of great importance both for the industrial area and for studies of soil fertilization. We use quantum chemistry followed by the Density Functional Theory (DFT) for principal components of the chemical shift tensor (σ) and chemical shift anisotropy analysis applied to the optimized structures of the urea compound at the corner, edge and vacant/surface of (MgO)₁₈, respectively, as in the following figure.

The all calculations being evaluated adopting a 6-31G(d,p) basis set and WP04 functional implemented in the Gaussian 09 code. The tensor σ expresses the fact that the resonance frequency of a nucleus at specific positions of a molecule, agglomerates of atoms or materials depends on the orientation of the molecule relative to the field applied. It is these interactions that determine the position and line widths of the spectrum, containing valuable information about the geometry and motions in the molecules. The table shows the values of σ and $\Delta\sigma$ in parts per million (ppm).

Principal Components of the Chemical Shift Tensor (σ) and Chemical Shift Anisotropy

Mg				
Mg (corner-core)	564.9613	579.1819	587.3912	15.3196
Mg (edge-core)	549.5240	574.1393	586.0962	24.2646
Mg (surface-core)	560.4599	568.0349	568.1100	3.8626
Mg (core/vac)	471.9135	563.9498	709.1838	191.2522
Mg (corner -urea)	540.4981	574.1739	575.2932	17.9572
Mg (edge -urea)	557.8032	573.2104	579.9954	14.4886
Mg (vac/urea)	537.2107	563.5891	654.9529	104.5530

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