**Numerical Methods for the Evaluation
of the Löwdin α-Function**

Nemanja Sovic and James D. Talman
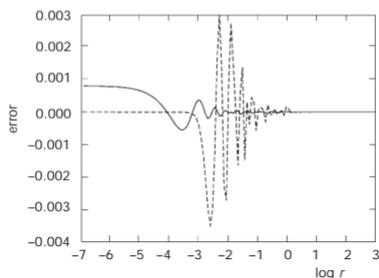
**Electric Properties of
Cyanoborane Isomers**

Miroslav Medveď, Ivan Černušák,
Stanislav Kedžuch and Jozef Noga
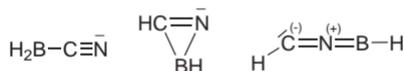
**A Case Study of State-Specific and
State-Averaged Brueckner
Equation-of-Motion Coupled-Cluster
Theory: The Ionic-Covalent Avoided
Crossing in Lithium Fluoride**

Marcel Nooijen and K. R. Shamasundar
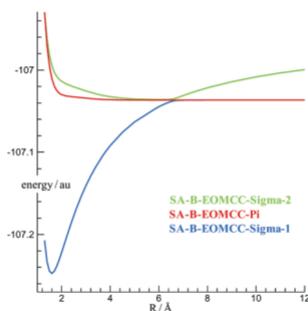
**Time-Independent Coupled-Cluster
Theory of the Polarization Propagator**

Robert Moszynski, Piotr S. Żuchowski and
Bogumil Jeziorski
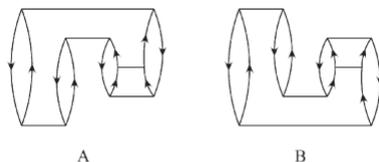
Hydrogen Atom and One-Electron Molecular Systems in a Strong Magnetic Field: Are All of Them Alike
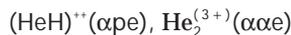
Alexander V. Turbiner, Alexei B. Kaidalov and Juan Carlos López Vieyra

$H_2^{(+)}$(ppe), $H_3^{(2+)}$(pppe)

(HeH)$^{++}$(αpe), $He_2^{(3+)}$(ααe)

***Ab initio* Correlation Effects in Density Functional Theories: An Electron-Distribution-Based Study for Neon**

Karol Jankowski, Ireneusz Grabowski, Krzysztof Nowakowski and Jan Wasilewski
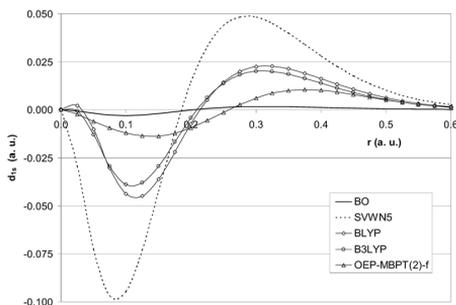
Commutator-Based $(A)[X]_n(SU(2) \times S_n)$ NMR Cluster Systems: Establishment of the Universality of $[\hat{n}](S_n)$ Salients and Constraints on $\hat{\phi}_{\pm 1}^1$(1.1) Polarisations to the $[\hat{1}^n]$ Salient: Permutational Spin Symmetry (PSS) Within NMR Spin Dynamics – an Analytic View

Francis P. Temme

$\lambda_{\pm 1} = \mp J/2 \pm D/2$; whereas $\lambda_{\pm 2} = \pm J/2 \pm D/2$

$\langle\langle F_- \rangle\rangle[t] = (1 - \sin 2\theta) \cos \lambda_{\pm 2} t + (1 + \sin 2\theta) \cos \lambda_{\pm 1} t$

Dipole Oscillator Strength Distributions and Properties for Methanol, Ethanol and Propan-1-ol and Related Dispersion Energies

Ashok Kumar, B. L. Jhanwar and William J. Meath

$$S_k = \int_{E_0}^{\infty} (E/E_H)^k (df/dE)\, dE$$

$$L_k = \int_{E_0}^{\infty} (E/E_H)^k (df/dE) \ln(E/E_H)\, dE$$

$$I_k = E_H \exp(L_k/S_k)$$

**The Spherical Tensor
Gradient Operator**

Ernst Joachim Weniger

$$\mathcal{Y}_l^m(\nabla) = \left[\frac{2l+1}{4\pi}(l+m)!(l-m)!\right]^{1/2}$$

$$\times \sum_{k \geq 0} \frac{\left(-\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)^{m+k}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)^{k}\left(\frac{\partial}{\partial z}\right)^{l-m-2k}}{2^{m+2k}(m+k)!\,k!\,(l-m-2k)!}$$

**Assessment of the Direct Generalized
Bloch Approach B0: Application to
the Li and Be Atoms and the Molecules
LiH, BeH, and the Phenolate Anion**

Holger Meissner

LiH, BeH, PhO⁻

DGB calculation