LIST OF PUBLICATIONS

(i) Publications:

(a) Contributions in books as follows:


2. Polynuclear Aromatic Compounds
   Chapter 17, p. 287-307, jointly with W. C. Herndon.

3. Recent advances of Chemistry and Molecular Biology in Cancer Research
   Q. Dai, M.A. Armour and Q. Zheng (Eds) Springer Verlag,
   Preface and 2 Articles pp. 77, 219.

4. The chemistry sections of the new Grade 9 High School Integrated Science Textbook "Exploring our World: Book 3"
   Ministry of Education Youth and Culture, Kingston, Jamaica, 1998,
   jointly with R. Ghosh.

5. The Chapter "Polycyclic Aromatic Hydrocarbon Carcinogenicity; Experimental Facts and Theoretical Modeling"
   in "Theoretical and Computational Chemistry" Vol. 5,
   jointly with R. Ghosh.

(b) Monographs:


Articles published in refereed journals:


11. Potential Curves for the Alkali Dimers and their Cations:
a New Spectroscopic Rule and its Predictions
L.v. Szentpaly

12. A Proper Account of Core-Polarization with Pseudopotentials:
Single Valence-Electron Alkali Compounds
P. Fuentealba, H. Preuss, H. Stoll and L.v. Szentpaly

13. Pseudopotential Calculations on Rb, Cs, RbH, CsH
and the Mixed Alkali Dimer Ions
L.v. Szentpaly, P. Fuentealba, H. Preuss and H. Stoll

14. Pseudopotential Calculations Including Core-Valence
Correlation: Alkali Compounds
P. Fuentealba, L.v. Szentpaly, H. Stoll, F.-X. Fraschio
and H. Preuss.
J. Mol. Struct. 93 (1983) 213

15. On the Reliability of Semiempirical Pseudopotentials:
Simulation of Hartree-Fock and Dirac-Fock Results
P. Fuentealba, H. Stoll, L.v. Szentpaly, P. Schwerdtfeger
and H. Preuss

16. Cu and Ag as One-Valence-Electron Atoms:
Pseudopotential Results for Cu, Ag, CuH, Ag
H. Stoll, P. Fuentealba, M. Dolg, J. Flad, L.v. Szentpaly

17. Cu and Ag as One-Valence-Electron Atoms: CI Results and
Quadrupole Corrections for Cu, Ag, CuH, AgH
H. Stoll, P. Fuentealba, P. Schwerdtfeger, J. Flad,

18. Pseudopotential Calculations Including Core-Valence
Correlation: Alkali and Noble-Metal Compounds
H. Stoll, L.v. Szentpaly, P. Fuentealba, J. Flad,
M. Dolg, F.-X. Fraschio, P. Schwerdtfeger, G. Igel and
H. Preuss.

19. Carcinogenesis by Polycyclic Aromatic Hydrocarbons:
a Multilinear Regression on New Type PMO Indices.
L.v. Szentpaly

20. A comparison of Pencil and Paper Procedures:
PMO, Free-Electron PMO, and Structure-Resonance Theory
Calculations for Proton Affinities
L.v. Szentpaly and W.C. Herndon
in "Conceptual Quantum Chemistry"
21. Pseudopotential Calculations for Alkaline Earth Atoms
   P. Fuentealba, L.v. Szentpaly, H. Preuss and H. Stoll

22. Correlation and Relativistic Effects in Pseudopotential
    Calculations for Br, I, HBr, HI, Br and I.
    P. Schwerdtfeger, L.v. Szentpaly, Kh. Vogel, H. Silberbach,

23. Quantitative Differences in Biotransformation Between the
    Two Chloroform Analogs Chlorodifluoromethane and
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    H. Peter, J.G. Filser and L.v. Szentpaly,
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25. The MCS-model of Chemical Initiation of Cancer:
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26. Dipole Moments of Indoles in their Ground and Lowest
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    C. Parkanyi, S.R. Oruganti, A.O. Abdelhamid, L.v. Szentpaly,

27. Theoretical Model of Activation of Carcinogenic Polycyclic Aromatic
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30. Relativistic Pseudopotential Calculations for HBr, HBr, HI, HI and HI.
    F. Schwerdtfeger, L.v. Szentpaly, H. Stoll and H. Preuss,

31. Implicationes de la Conjugacion sigma

32. The MCS Model of Chemical Initiation of Cancer:
    PPP Calculations on Heteroaromatic Molecules.
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33. Pseudopotential and MCS-X Calculations of Nuclear Quadrupole Coupling Constants and Other Properties of Diatomic Halogen Molecules and their Monoanions and Monoocations.
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51. Valence States in Molecules.3. Transferable Vibrational Force Constants
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52. Electrophilicity Index.