

Hans Jørgen Aagaard Jensen

Professor

Department of Physics, Chemistry and Pharmacy
University of Southern Denmark
Campusvej 55
5230 Odense M
Denmark



E-mail : hjj@sdu.dk

Phone : +45 6550 2512

My standard CV : https://minesider.sdu.dk/personal/hjj/hjaa_j_public/docs/HJAAJ-CV-dec2013.pdf

Google scholar profile : <http://scholar.google.com/citations?user=ljHToR8AAAAJ>

Publications

Fuglsbjerg, J. H., Nagy, D., Jensen, H. J. A., & Sauer, S. P. A. (2024). Performance of range-separated long-range SOPPA short-range density functional theory method for vertical excitation energies. *The Journal of Chemical Physics*, *160*(20), Article 204102. <https://doi.org/10.1063/5.0197228>

Teale, A. M., Helgaker, T., Savin, A., Adamo, C., Aradi, B., Arbuznikov, A. V., Ayers, P. W., Baerends, E. J., Barone, V., Calaminici, P., Cancès, E., Carter, E. A., Chattaraj, P. K., Chermette, H., Ciofini, I., Crawford, T. D., De Proft, F., Dobson, J. F., Draxl, C., ... Yang, W. (2022). DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. *Physical Chemistry Chemical Physics*, *24*(47), 28700-28781. <https://doi.org/10.1039/d2cp02827a>

Jørgensen, F. K., Kjellgren, E., Jensen, H. J. A., & Hedegård, E. D. (2022). Multiconfigurational short-range density functional theory for nuclear magnetic resonance shielding constants with gauge-including atomic orbitals. *The Journal of Chemical Physics*, *157*(16), Article 164106. <https://doi.org/10.1063/5.0106422>

Van Den Heuvel, W., Reinholdt, P., Jensen, H. J. A., & Kongsted, J. (2022). Multiconfigurational SCF and short-range DFT combined with polarizable density embedding: Comparison of linear-response and state-specific solvatochromic shifts of acrolein and para-nitrophenolate in water. *Journal of Chemical theory and Computation*, *18*(10), 6231-6239. <https://doi.org/10.1021/acs.jctc.2c00739>

Knecht, S., Repisky, M., Jensen, H. J. A., & Saue, T. (2022). Exact two-component Hamiltonians for relativistic quantum chemistry: Two-electron picture-change corrections made simple. *The Journal of Chemical Physics*, *157*(11), Article 114106. <https://doi.org/10.1063/5.0095112>

Hapka, M., Pernal, K., & Jensen, H. J. A. (2022). An efficient implementation of time-dependent linear-response theory for strongly orthogonal geminal wave function models. *The Journal of Chemical Physics*, *156*(17), Article 174102. <https://doi.org/10.1063/5.0082155>

Pototschnig, J. V., Papadopoulos, A., Lyakh, D. I., Repisky, M., Halbert, L., Severo Pereira Gomes, A., Jensen, H. J. A., & Visscher, L. (2021). Implementation of Relativistic Coupled Cluster Theory for Massively Parallel GPU-Accelerated Computing Architectures. *Journal of Chemical theory and Computation*, *17*(9), 5509-5529. <https://doi.org/10.1021/acs.jctc.1c00260>

Kjellgren, E. R., & Jensen, H. J. A. (2021). Multi-configurational short-range density functional theory can describe spin-spin coupling constants of transition metal complexes. *The Journal of Chemical Physics*, *155*(8), Article 084102. <https://doi.org/10.1063/5.0059128>

Luo, L., Straatsma, T. P., Suarez, L. E. A., Broer, R., Bykov, D., D'Azevedo, E. F., Faraji, S. S., Gottiparthi, K. C., De Graaf, C., Harris, J. A., Havenith, R. W. A., Jensen, H. J. A., Joubert, W., Kathir, R. K., Larkin, J., Li, Y. W., Lyakh, D. I., Messer, O. E. B., Norman, M. R., ... Wibowo, M. (2020). Pre-exascale accelerated application development: The ORNL Summit experience. *IBM Journal of Research and Development*, *64*(3-4), Article 8960361. <https://doi.org/10.1147/JRD.2020.2965881>

Andersen, A. B. A., Pyykkönen, A., Jensen, H. J. A., McKee, V., Vaara, J., & Nielsen, U. G. (2020). Remarkable reversal of ^{13}C -NMR assignment in d^1 , d^2 compared to d^8 , d^9 acetylacetonate complexes: Analysis and explanation based on solid-state MAS NMR and computations. *Physical Chemistry Chemical Physics*, *22*(15), 8048-8059. <https://doi.org/10.1039/d0cp00980f>

Olsen, J. M. H., Reine, S., Vahtras, O., Kjellgren, E., Reinholdt, P., Hjorth Dundas, K. O., Li, X., Cukras, J., Ringholm, M., Hedegård, E. D., Di Remigio, R., List, N. H., Faber, R., Cabral Tenorio, B. N., Bast, R., Pedersen, T. B., Rinkevicius, Z., Sauer, S. P. A., Mikkelsen, K. V., ... Norman, P. (2020). Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. *The Journal of Chemical Physics*, *152*(21), Article 214115. <https://doi.org/10.1063/1.5144298>

Saue, T., Bast, R., Gomes, A. S. P., Jensen, H. J. A., Visscher, L., Aucar, I. A., Di Remigio, R., Dyall, K. G., Eliav, E., Fasshauer, E., Fleig, T., Halbert, L., Hedegård, E. D., Helmich-Paris, B., Iliáš, M., Jacob, C. R., Knecht, S., Laerdahl, J. K., Vidal, M. L., ... van Stralen, J. N. P. (2020). The DIRAC code for relativistic molecular calculations: The Journal of Chemical Physics. *The Journal of Chemical Physics*, *152*(20), Article 152. <https://doi.org/10.1063/5.0004844>

Schnack-Petersen, A. K., Simmermacher, M., Fasshauer, E., Jensen, H. J. A., & Sauer, S. P. A. (2020). The Second-Order-Polarization-Propagator-Approximation (SOPPA) in a four-component spinor basis. *The Journal of Chemical Physics*, *152*(13), Article 134113. <https://doi.org/10.1063/5.0002389>

Pastorczyk, E., Jensen, H. J. A., Kowalski, P. H., & Pernal, K. (2019). Generalized Valence Bond Perfect-Pairing Made Versatile Through Electron-Pairs Embedding. *Journal of Chemical Theory and Computation*, *15*(8), 4430-4439. <https://doi.org/10.1021/acs.jctc.9b00384>

Knecht, S., Jensen, H. J. A., & Saue, T. (2019). Relativistic quantum chemical calculations show that the uranium molecule U_2 has a quadruple bond. *Nature Chemistry*, *11*, 40-44. <https://doi.org/10.1038/s41557-018-0158-9>

Kjellgren, E. R., Hedegård, E. D., & Jensen, H. J. A. (2019). Triplet excitation energies from multiconfigurational short-range density-functional theory response calculations. *The Journal of Chemical Physics*, *151*(12), Article 124113. <https://doi.org/10.1063/1.5119312>

Jensen, H. J. A. (2018). Going from work station computing to exascale computing with the Dirac and Dalton programs. *Journal of the American Chemical Society*, *255*.

Dong, G., Ryde, U., Aa Jensen, H. J., & Hedegård, E. D. (2018). Exploration of H_2 binding to the [NiFe]-hydrogenase active site with multiconfigurational density functional theory. *Physical chemistry chemical physics : PCCP*, *20*(2), 794-801. <https://doi.org/10.1039/c7cp06767d>

Hedegård, E. D., Toulouse, J., & Jensen, H. J. A. (2018). Multiconfigurational short-range density-functional theory for open-shell systems. *The Journal of Chemical Physics*, *148*(21), Article 214103. <https://doi.org/10.1063/1.5013306>

List, N. H., Norman, P., Kongsted, J., & Jensen, H. J. A. (2017). A quantum-mechanical perspective on linear response theory within polarizable embedding. *The Journal of Chemical Physics*, *146*(23), Article 234101. <https://doi.org/10.1063/1.4985565>

Hedegård, E. D., Bast, R., Kongsted, J., Olsen, J. M. H., & Jensen, H. J. A. (2017). Relativistic Polarizable Embedding. *Journal of Chemical Theory and Computation*, *13*(6), 2870-2880. <https://doi.org/10.1021/acs.jctc.7b00162>

Nørby, M. S., Olsen, J. M. H., Kongsted, J., & Jensen, H. J. A. (2016). Multipole moments for embedding potentials: Exploring different atomic allocation algorithms. *Journal of Computational Chemistry*, *37*(20), 1887-1896. <https://doi.org/10.1002/jcc.24403>

Almoukhalalati, A., Knecht, S., Jensen, H. J. A., Dyall, K. G., & Saue, T. (2016). Electron correlation within the relativistic no-pair approximation. *The Journal of Chemical Physics*, *145*(7), 074104-1-074104-15. Article 074104. <https://doi.org/10.1063/1.4959452>

Hubert, M., Jensen, H. J. A., & Hedegård, E. D. (2016). Excitation Spectra of Nucleobases with Multiconfigurational Density Functional Theory. *The Journal of Physical Chemistry Part A*, *120*(1), 36-43. <https://doi.org/10.1021/acs.jpca.5b09662>

Hubert, M., Hedegård, E. D., & Jensen, H. J. A. (2016). Investigation of Multiconfigurational Short-Range Density Functional Theory for Electronic Excitations in Organic Molecules. *Journal of Chemical Theory and Computation*, *12*(5), 2203-2213. <https://doi.org/10.1021/acs.jctc.5b01141>

List, N. H., Jensen, H. J. A., & Kongsted, J. (2016). Local electric fields and molecular properties in heterogeneous environments through polarizable embedding. *Physical Chemistry Chemical Physics*, *18*(15), 10070-10080. <https://doi.org/10.1039/c6cp00669h>

Senjean, B., Knecht, S., Jensen, H. J. A., & Fromager, E. (2015). Linear interpolation method in ensemble Kohn-Sham and range-separated density-functional approximations for excited states. *Physical Review A*, *92*(1), Article 012518. <https://doi.org/10.1103/PhysRevA.92.012518>

Sauer, S. P. A., Pitzner-Frydendahl, H. F., Buse, M., Jensen, H. J. A., & Thiel, W. (2015). Performance of SOPPA-based methods in the calculation of vertical excitation energies and oscillator strengths. *Molecular Physics*, *113*(13-14), 2026-2045. <https://doi.org/10.1080/00268976.2015.1048320>

Denis, M., Norby, M. S., Jensen, H. J. A., Gomes, A. S. P., Nayak, M. K., Knecht, S., & Fleig, T. (2015). Theoretical study on ThF⁺, a prospective system in search of time-reversal violation. *New Journal of Physics*, *17*, Article 043005. <https://doi.org/10.1088/1367-2630/17/4/043005>

Hedegård, E. D., Olsen, J. M. H., Knecht, S., Kongsted, J., & Jensen, H. J. A. (2015). Polarizable embedding with a multiconfiguration short-range density functional theory linear response method. *The Journal of Chemical Physics*, *142*(11), Article 114113. <https://doi.org/10.1063/1.4914922>

List, N. H., Beerepoot, M., Olsen, J. M. H., Gao, B., Ruud, K., Jensen, H. J. A., & Kongsted, J. (2015). Molecular quantum mechanical gradients within the polarizable embedding approach—Application to the internal vibrational Stark shift of acetophenone. *The Journal of Chemical Physics*, *142*(3), Article 034119. <https://doi.org/10.1063/1.4905909>

List, N. H., Kauzcor, J., Saue, T., Jensen, H. J. A., & Norman, P. (2015). Beyond the electric-dipole approximation: A formulation and implementation of molecular response theory for the description of absorption of electromagnetic field radiation. *The Journal of Chemical Physics*, *142*(24), Article 244111. <https://doi.org/10.1063/1.4922697>

Hedegård, E. D., Knecht, S., Kielberg, J. S., Jensen, H. J. A., & Reiher, M. (2015). Density matrix renormalization group with efficient dynamical electron correlation through range separation. *The Journal of Chemical Physics*, *142*(22), 224108. Article 224108. <https://doi.org/10.1063/1.4922295>

Hedegård, E. D., Jensen, H. J. A., & Kongsted, J. (2014). Polarizable Embedding Based on Multiconfigurational Methods: Current Developments and the Road Ahead. *International Journal of Quantum Chemistry*, *114*(17), 1102-1107. <https://doi.org/10.1002/qua.24632>

Aidas, K., Angeli, C., Bak, K. L., Bakken, V., Bast, R., Boman, L., Christiansen, O., Cimraglia, R., Coriani, S., Dahle, P., Dalskov, E. K., Ekström, U., Enevoldsen, T., Eriksen, J. J., Ettenhuber, P., Fernández, B., Ferrighi, L., Fliegl, H., Frediani, L., ... Ågren, H. (2014). The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, *4*(3), 269–284. <https://doi.org/10.1002/wcms.1172>

Fromager, E., Knecht, S., & Jensen, H. J. A. (2013). Multi-configuration time-dependent density-functional theory based on range separation. *The Journal of Chemical Physics*, *138*(8), Article 084101. <https://doi.org/10.1063/1.4792199>

Cornaton, Y., Stoyanova, A., Jensen, H. J. A., & Fromager, E. (2013). Alternative separation of exchange and correlation energies in range-separated density-functional perturbation theory. *Physical Review A*, *88*(2), Article 022516. <https://doi.org/10.1103/PhysRevA.88.022516>

Hedegård, E. D., Jensen, H. J. A., Knecht, S., & Fromager, E. (2013). Assessment of charge-transfer excitations with time-dependent, range-separated density functional theory based on long-range MP2 and multiconfigurational self-consistent field wave functions. *The Journal of Chemical Physics*, *139*(18), Article 184308. <https://doi.org/10.1063/1.4826533>

List, N. H., Jensen, H. J. A., Kongsted, J., & Hedegård, E. D. (2013). A Unified Framework for the Polarizable Embedding and Continuum Methods within Multiconfigurational Self-Consistent-Field Theory. *Advances in Quantum Chemistry*, *66*, 195-238. <https://doi.org/10.1016/B978-0-12-408099-7.00004-0>

Vad, M. S., Pedersen, M. N., Nørager, A., & Jensen, H. J. A. (2013). Correlated four-component EPR g-tensors for doublet molecules. *The Journal of Chemical Physics*, *138*(21), Article 214106. <https://doi.org/10.1063/1.4804352>

Eriksen, J. J., Sauer, S. P. A., Mikkelsen, K. V., Christiansen, O., Jensen, H. J. A., & Kongsted, J. (2013). Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. *Molecular Physics*, *111*(9-11), 1235-1248. <https://doi.org/10.1080/00268976.2013.793841>

Iliáš, M., Jensen, H. J. A., Bast, R., & Saue, T. (2013). Gauge origin independent calculations of molecular magnetisabilities in relativistic four-component theory. *Molecular Physics*, *111*(9-11), 1373-1381. <https://doi.org/10.1080/00268976.2013.798436>

Hedegård, E. D., List, N. H., Jensen, H. J. A., & Kongsted, J. (2013). The Multi-Configuration Self-Consistent Field Method Within a Polarizable Embedded Framework. *The Journal of Chemical Physics*, *139*(4), 044101. Article 044101. <https://doi.org/10.1063/1.4811835>

Sharkas, K., Savin, A., Jensen, H. J. A., & Toulouse, J. (2012). A multiconfigurational hybrid density-functional theory. *The Journal of Chemical Physics*, *137*, 044104. <https://doi.org/10.1063/1.4733672>

List, N. H., Olsen, J. M. H., Jensen, H. J. A., Steindal, A. H., & Kongsted, J. (2012). Molecular-level Insight into the Spectral Tuning Mechanism of the DsRed Chromophore. *The Journal of Physical Chemistry Letters*, *3*, 3513-3521. <https://doi.org/10.1021/jz3014858>

Eriksen, J. J., Sauer, S. P. A., Mikkelsen, K. V., Jensen, H. J. A., & Kongsted, J. (2012). On the importance of excited state dynamic response electron correlation in polarizable embedding methods. *Journal of Computational Chemistry*, *33* (25), 2012-2022. <https://doi.org/10.1002/jcc.23032>. Epub 2012 Jun 8.

Norman, P., & Jensen, H. J. A. (2012). Phosphorescence parameters for platinum (II) organometallic chromophores: A study at the non-collinear four-component Kohn–Sham level of theory. *Chemical Physics Letters*, *531*, 229-235. <https://doi.org/10.1016/j.cplett.2012.02.012>

Bagus, P. S., Ilton, E. S., Martin, R. L., Jensen, H. J. A., & Knecht, S. (2012). Spin–orbit coupling in actinide cations. *Chemical Physics Letters*, *546*, 58-62. <https://doi.org/10.1016/j.cplett.2012.07.035>

Fromager, E., & Jensen, H. J. A. (2011). Analysis of self-consistency effects in range-separated density-functional theory with Møller-Plesset perturbation theory. *The Journal of Chemical Physics*, *135*(034116). <https://doi.org/10.1063/1.3611053>

Knecht, S., Sørensen, L. K., Jensen, H. J. A., Fleig, T., & Marian, C. M. (2010). Accurate calculations of the ground state and low-lying excited states of the (RbBa)⁺ molecular ion: a proposed system for ultracold reactive collisions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, *43*(5), Article 055101. <https://doi.org/10.1088/0953-4075/43/5/055101>

Knecht, S., Jensen, H. J. A., & Fleig, T. (2010). Large-scale parallel configuration interaction. II. Two- and four-component double-group general active space implementation with application to BiH. *The Journal of Chemical Physics*, *132*(014108). <https://doi.org/10.1063/1.3276157>

Fromager, E., Cimiraglia, R., & Jensen, H. J. A. (2010). Merging multireference perturbation and density-functional theories by means of range separation: Potential curves for Be₂, Mg₂, and Ca₂. *Physical Review A*, *81*(024502). <https://doi.org/10.1103/PhysRevA.81.024502>

Ilias, M., Saue, T., Enevoldsen, T., & Jensen, H. J. A. (2009). Gauge origin independent calculations of nuclear magnetic shieldings in relativistic four-component theory. *The Journal of Chemical Physics*, *131*(124119), 1-13. <https://doi.org/10.1063/1.3240198>

Hansen, M. B., Jensen, H. J. A., & Jensen, F. (2009). Modeling Enzymatic Transition States by Force Field Methods. *International Journal of Quantum Chemistry*, *109*, 373-383. <https://doi.org/10.1002/qua.21782>

Fromager, E., Réal, F., Wåhlin, P., Wahlgren, U., & Jensen, H. J. A. (2009). On the universality of the long-/short-range separation in multiconfigurational density-functional theory. II. Investigating f⁰ actinide species. *The Journal of Chemical Physics*, *131*(054107), 1-11. <https://doi.org/10.1063/1.3187032>

Bast, R., Jensen, H. J. A., & Saue, T. (2009). Relativistic Adiabatic Time-Dependent Density Functional Theory Using Hybrid Functionals and Noncollinear Spin Magnetization. *International Journal of Quantum Chemistry*, *109*, 2091-2112. <https://doi.org/10.1002/qua.22065>

Thyssen, J., Fleig, T., & Jensen, H. J. A. (2008). A direct relativistic four-component multiconfiguration self-consistent-field method for molecules. *The Journal of Chemical Physics*, *129*(3), Article 034109. <https://doi.org/10.1063/1.2943670>

Jensen, H. J. A. (2008). Can Electron Propagator Methods Be Used To Improve Polarization Propagator Methods? In T. E. Simos, & G. Maroulis (Eds.), *COMPUTATION IN MODERN SCIENCE AND ENGINEERING: Proceedings of the International Conference on Computational Methods in Science and Engineering (ICCMSE 2007) Corfu, Greece, 25-30 September 2007 Volume 2, Part A* (pp. 191-192). American Institute of Physics.

Knecht, S., Jensen, H. J. A., & Fleig, T. (2008). Large-scale parallel configuration interaction. I. Nonrelativistic and scalar-relativistic general active space implementation with application to (Rb-Ba)⁺. *The Journal of Chemical Physics*, *129*(1), 014108-1-14. <https://doi.org/10.1063/1.2805369>

Fromager, E., & Jensen, H. J. A. (2008). **Self-consistent many-body perturbation theory in range-separated density-functional theory: A one-electron reduced-density-matrix-based formulation.** *Physical Review A. Atomic, Molecular, and Optical Physics*, *78*(2), 022504. <https://doi.org/10.1103/PhysRevA.78.022504>

Fromager, E., Toulouse, J., & Jensen, H. J. A. (2007). On the universality of the long-/short-range separation in multiconfigurational density-functional theory. *The Journal of Chemical Physics*, *126*(7), 074111-074119. <https://doi.org/10.1063/1.2566459>

Hanni, M., Lantto, P., Ilias, M., Jensen, H. J. A., & Vaara, J. (2007). Relativistic effects in the intermolecular interaction-induced nuclear magnetic resonance parameters of xenon dimer. *The Journal of Chemical Physics*, *127*(16), 164313-1-13. <https://doi.org/10.1063/1.2777143>

Rubensson, E. H., & Jensen, H. J. A. (2006). Determination of the Chemical Potential and HOMO/LUMO Orbitals in Density Purification Methods. *Chemical Physics Letters*, *432*(4-6), 591-594. <https://doi.org/10.1016/j.cplett.2006.10.090>

Jensen, H. J. A., Oddershede, J., & Ogilvie, J. F. (2006). Rotational Q Factors Calculated for Diatomic Molecular Cations H₂⁺, HeH⁺ and NeH⁺. *Journal of Physics B: Atomic, Molecular and Optical Physics*, *39*(24), 5215-5223. <https://doi.org/10.1088/0953-4075/39/24/017>

Fleig, T., Jensen, H. J. A., Olsen, J., & Visscher, L. (2006). The Generalized Active Space Concept for the Relativistic Treatment of Electron Correlation. III. Large-scale Configuration Interaction and Multiconfiguration Self-consistent-field Four-component Methods with Application to UO₂. *The Journal of Chemical Physics*, 124(10), 104106-1 - 104106-11. <https://doi.org/10.1063/1.2176609>

Olsen, J., & Jensen, H. J. A. (2005). Preface. In *Advances in Quantum Chemistry 50 Response Theory and Molecular Properties* Academic Press. [https://doi.org/10.1016/S0065-3276\(05\)50017-0](https://doi.org/10.1016/S0065-3276(05)50017-0)

Ogilvie, J. F., Jensen, H. J. A., & Sauer, S. P. A. (2005). Analysis of pure rotational and vibration-rotational spectra of NaCl X¹ Σ^+ and quantum-chemical calculation of related molecular properties. *Journal of the Chinese Chemical Society*, (52), 631-639.

van Stralen, J., Visscher, L., Larsen, C. V., & Jensen, H. J. A. (2005). First-order MP2 molecular properties in a relativistic framework. *Chemical Physics*, (311), 81-95. <https://doi.org/10.1016/j.chemphys.2004.10.018>

Norman, P., Bishop, D. M., Jensen, H. J. A., & Oddershede, J. (2005). Nonlinear response theory with relaxation: The first hyperpolarizability. *The Journal of Chemical Physics*, 123, 194103-194121. <https://doi.org/10.1063/1.2107627>

Sauer, S. P. A., Jensen, H. J. A., & Ogilvie, J. F. (2005). Quantum-chemical Calculations of Radial Functions for Rotational and Vibrational g Factors, Electric Dipolar Moment and Adiabatic Corrections to the Potential Energy for Analysis of Spectra of HeH⁺. *Advances in Quantum Chemistry*, (48), 319-334. [https://doi.org/10.1016/S0065-3276\(05\)48017-X](https://doi.org/10.1016/S0065-3276(05)48017-X)

Jensen, H. J. A., Sabin, J. R., & Brandäs, E. (Eds.) (2005). *Response Theory and Molecular Properties: (A Tribute to Jan Linderberg and Poul Jørgensen)*. Advances in Quantum Chemistry No. 50

Ilias, M., Jensen, H. J. A., Kellö, V., Roos, B. O., & Urban, M. (2005). Theoretical study of PbO and the PbO anion. *Chemical Physics Letters*, (408), 210-215. <https://doi.org/10.1016/j.cplett.2005.04.027>

Henriksson, J., Norman, P., & Jensen, H. J. A. (2005). Two-photon absorption in the relativistic fourcomponent Hartree-Fock approximation. *The Journal of Chemical Physics*, (122), 114106/1-114106/9. <https://doi.org/10.1063/1.1869469>

Norman, P., & Jensen, H. J. A. (2004). Quadratic response functions in the time-dependent four-component Hartree-Fock approximation. *The Journal of Chemical Physics*, 121, 6145-6154. <https://doi.org/10.1063/1.1785774>

Saue, T., & Jensen, H. J. A. (2003). Linear response at the 4-component relativistic level: Application to the frequency-dependent dipole polarizabilities of the coinage metal dimers. *The Journal of Chemical Physics*, 118(2), 522-536. <https://doi.org/10.1063/1.1522407>

Nielsen, S. B., Nielsen, M. B., & Jensen, H. J. A. (2003). The tetrathiafulvalene dication in the gas phase: its formation and stability. *Physical Chemistry Chemical Physics*, 5, 1376-80. <https://doi.org/10.1039/B300537B>

Norman, P., Schimmelpfennig, B., Ruud, K., Jensen, H. J. A., & Ågren, H. (2002). Relativistic effects on linear and nonlinear polarizabilities studied by effective-core potential, Douglas-Kroll, and Dirac-Hartree-Fock response theory. *The Journal of Chemical Physics*, 116(16), 6914-6923. <https://doi.org/10.1063/1.1463437>

Norman, P., Bishop, D. M., Jensen, H. J. A., & Oddershede, J. (2001). Near-resonant absorption in the time-dependent self-consistent field and multiconfigurational self-consistent field approximations. *The Journal of Chemical Physics*, 115 (22), 10323-10334. <https://doi.org/10.1063/1.1415081>

Keszthelyi, T., Grage, M. M. L., Offersgaard, J. F., Wilbrandt, R., Svendsen, C., Mortensen, O. S., Pedersen, J. K., & Jensen, H. J. A. (2000). 2,2'-Bithiophene Radical Cation: An Experimental and Computational Study. *Journal of Physical Chemistry A*, 104, 2808-2823. <https://doi.org/10.1021/jp993913s>

Venkatnathan, A., Mishra, M. K., & Jensen, H. J. A. (2000). An investigation of basis set effects in the characterization of electron: atom scattering resonances using the dilated electron propagator method. *Theoretical Chemistry Accounts*, 104(6), 445-5. <https://doi.org/10.1007/s00214000164>

Carravetta, V., Ågren, H., Vahtras, O., & Jensen, H. J. A. (2000). *Ab initio* calculations of molecular resonant photoemission spectra. *The Journal of Chemical Physics*, 113(18), 7790-98. <https://doi.org/10.1063/1.1316046>

Shigemitsu, Y., Jensen, H. J. A., Koch, H., & Oddershede, J. (2000). Propagator calculations of electronic spectra of photochromic spirooxazines. *Molecular Crystals and Liquid Crystals*, 345, 89-9. <https://doi.org/10.1080/10587250008023900>

Saue, T., & Jensen, H. J. A. (2000). Quaternion symmetry of the Dirac equation. In M. Defranceschi, & C. Le Bris (Eds.), *Mathematical Models and Methods for Ab Initio Quantum Chemistry* (Vol. 3, pp. 227-246). Springer Science+Business Media. https://doi.org/10.1007/978-3-642-57237-1_11

Enevoldsen, T., Visscher, L., Saue, T., Jensen, H. J. A., & Oddershede, J. (2000). Relativistic four-component calculations of indirect nuclear spin-spin couplings in MH_4 ($M=C, Si, Ge, Sn, Pb$) and $Pb(CH_3)_3H$. *The Journal of Chemical Physics*, 112(8), 3493-98. <https://doi.org/10.1063/1.480504>

Visscher, L., Enevoldsen, T., Saue, T., Jensen, H. J. A., & Oddershede, J. (1999). Full four-component relativistic calculations of the NMR shielding and indirect spin-spin coupling tensors in the hydrogen halides. *Journal of Computational Chemistry*, 20, 1262-73. [https://doi.org/10.1016/S0040-4039\(03\)01584-3](https://doi.org/10.1016/S0040-4039(03)01584-3)

Aucar, G. A., Saue, T., Visscher, L., & Jensen, H. J. A. (1999). On the origin and contribution of the diamagnetic term in four-component relativistic calculations of magnetic properties. *The Journal of Chemical Physics*, 110(13), 6208-18. <https://doi.org/10.1063/1.479181>

Saue, T., & Jensen, H. J. A. (1999). Quaternion symmetry in relativistic molecular calculations: The Dirac-Hartree-Fock method. *The Journal of Chemical Physics*, 111, 6211-22. <https://doi.org/10.1063/1.479958>

Ruud, K., Jonsson, D., Norman, P., Ågren, H., Saue, T., Jensen, H. J. A., Dahle, P., & Helgaker, T. (1998). Generalized integral-screening for efficient calculations of nonlinear optical properties of large molecules. *The Journal of Chemical Physics*, 108(19), 7973-7979. <https://doi.org/10.1063/1.476237>

Dalskov, E. K., Jensen, H. J. A., & Oddershede, J. (1997). Does scaling or addition provide the correct frequency dependence of $\beta_{\parallel}(-\omega_{\sigma}; \omega_1, \omega_2)$ at the correlated level? An investigation for six molecules. *Molecular Physics*, 90(1), 3-14.

Kirpekar, S., Jensen, H. J. A., & Oddershede, J. (1997). Spin-orbit corrections to the indirect nuclear spin-spin coupling constants in XH_4 ($X=C, Si, Ge, \text{ and } Sn$). *Theoretical Chemistry Accounts*, 95(1-2), 35-47. <https://doi.org/10.1007/BF02329240>

Ågren, H., Luo, Y., Gelmukhanov, F., & Jensen, H. J. A. (1996). Screening in resonant X-ray emission of molecules. *Journal of Electron Spectroscopy and Related Phenomena*, 82(1-2), 125-134.

Packer, M. J., Dalskov, E. K., Enevoldsen, T., Jensen, H. J. A., & Oddershede, J. (1996). A new implementation of the second-order polarization propagator approximation (SOPPA): The excitation spectra of benzene and naphthalene. *The Journal of Chemical Physics*, 105(14), 5886-5900. <https://doi.org/10.1063/1.472430>

Jensen, H. J. A., Dyal, K. G., Saue, T., & Fægri, K. (1996). Relativistic four-component multiconfigurational self-consistent-field theory for molecules: Formalism. *The Journal of Chemical Physics*, 104(11), 4083-4097. <https://doi.org/10.1063/1.471644>

- Aucar, G. A., Jensen, H. J. A., & Oddershede, J. (1995). Operator representations in Kramers bases. *Chemical Physics Letters*, 232(1-2), 47-53. [https://doi.org/10.1016/0009-2614\(94\)01332-P](https://doi.org/10.1016/0009-2614(94)01332-P)
- Mikkelsen, K. V., Cesar, A., Ågren, H., & Jensen, H. J. A. (1995). Multiconfigurational self-consistent reaction field theory for nonequilibrium solvation. *The Journal of Chemical Physics*, 103(20), 9010-9023. <https://doi.org/10.1063/1.470011>
- Kirpekar, S., Oddershede, J., & Jensen, H. J. A. (1995). Relativistic corrections to molecular dynamic dipole polarizabilities. *The Journal of Chemical Physics*, 103(8), 2983-2990. <https://doi.org/10.1063/1.470486>
- Olsen, J., Minaev, B., Vahtras, O., Ågren, H., Jørgensen, P., Jensen, H. J. A., & Helgaker, T. (1994). The Vegard-Kaplan band and the phosphorescent decay of N₂. *Chemical Physics Letters*, 231(4-6), 387-394. [https://doi.org/10.1016/0009-2614\(94\)01300-4](https://doi.org/10.1016/0009-2614(94)01300-4)
- Kirpekar, S., Jensen, H. J. A., & Oddershede, J. (1994). Correlated calculations of indirect nuclear spin-spin coupling constants for XH₄ (X = Si, Ge, and Sn). *Chemical Physics*, 188(2-3), 171-181. [https://doi.org/10.1016/0301-0104\(94\)00260-6](https://doi.org/10.1016/0301-0104(94)00260-6)
- Ischtwan, J., Schwerdtfeger, P., Peyerimhoff, S. D., Collins, M. A., Helgaker, T., Jørgensen, P., & Jensen, H. J. A. (1994). MCSCF reaction-path energetics and thermal rate-constants for the reaction of ³NH with H₂. *Theoretica Chimica Acta*, 89(2-3), 157-168. <https://doi.org/10.1007/BF01132799>
- Bak, K. L., Jørgensen, P., Helgaker, T., Ruud, K., & Jensen, H. J. A. (1994). Basis set convergence of atomic axial tensors obtained from self-consistent field calculations using London atomic orbitals. *The Journal of Chemical Physics*, 100(9), 6620-6627. <https://doi.org/10.1063/1.467019>
- Vahtras, O., Ågren, H., & Jensen, H. J. AA. (1994). Direct one-index transformations in multiconfiguration response calculations. *Journal of Computational Chemistry*, 15(6), 573-579. <https://doi.org/10.1002/jcc.540150602>
- Hettema, H., Wormer, P. E. S., Jørgensen, P., Jensen, H. J. A., & Helgaker, T. (1994). Frequency-dependent polarizabilities of O₂ and van der Waals coefficients of dimers containing O₂. *The Journal of Chemical Physics*, 100(2), 1297-1302. <https://doi.org/10.1063/1.467256>
- Ruud, K., Helgaker, T., Kobayashi, R., Jørgensen, P., Bak, K. L., & Jensen, H. J. A. (1994). Multiconfigurational self-consistent field calculations of nuclear shieldings using London atomic orbitals. *The Journal of Chemical Physics*, 100(11), 8178-8185. <https://doi.org/10.1063/1.466812>
- Vahtras, O., Ågren, H., Jørgensen, P., Helgaker, T., & Jensen, H. J. A. (1993). The nuclear spin-spin coupling in N₂ and CO. *Chemical Physics Letters*, 209(3), 201-206. [https://doi.org/10.1016/0009-2614\(93\)80093-5](https://doi.org/10.1016/0009-2614(93)80093-5)
- Koch, H., Ågren, H., Jørgensen, P., Helgaker, T., & Jensen, H. J. A. (1993). Large scale random phase calculations for direct self-consistent field wavefunctions. *Chemical Physics*, 172(1), 13-20. [https://doi.org/10.1016/0301-0104\(93\)80102-F](https://doi.org/10.1016/0301-0104(93)80102-F)
- Ågren, H., & Jensen, H. J. A. (1993). Relaxation and correlation contributions to molecular double core ionization energies. *Chemical Physics*, 172(1), 45-57. [https://doi.org/10.1016/0301-0104\(93\)80105-1](https://doi.org/10.1016/0301-0104(93)80105-1)
- Bak, K. L., Jørgensen, P., Helgaker, T., Ruud, K., & Jensen, H. J. A. (1993). Gauge-origin independent multiconfigurational self-consistent-field theory for vibrational circular dichroism. *The Journal of Chemical Physics*, 98(11), 8873-8887. <https://doi.org/10.1063/1.464445>
- Ruud, K., Helgaker, T., Bak, K. L., Jørgensen, P., & Jensen, H. J. A. (1993). Hartree-Fock limit magnetizabilities from London orbitals. *The Journal of Chemical Physics*, 99(5), 3847-3859. <https://doi.org/10.1063/1.466131>

- Ågren, H., Carravetta, V., Jensen, H. J. A., Jørgensen, P., & Olsen, J. (1993). Multiconfiguration linear-response approaches to the calculation of absolute photoionization cross sections: HF, H₂O, and Ne. *Physical Review A*, 47(5), 3810-3823. <https://doi.org/10.1103/PhysRevA.47.3810>
- Jaszuński, M., Jensen, H. J. A., Jørgensen, P., Rizzo, A., Helgaker, T., & Ruud, K. (1992). The magnetic hyperpolarizability anisotropy of the neon atom. *Chemical Physics Letters*, 191(6), 599-602. [https://doi.org/10.1016/0009-2614\(92\)85595-2](https://doi.org/10.1016/0009-2614(92)85595-2)
- Ågren, H., Knuts, S., Mikkelsen, K. V., & Jensen, H. J. A. (1992). Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes. *Chemical Physics*, 159(2), 211-225. [https://doi.org/10.1016/0301-0104\(92\)80071-3](https://doi.org/10.1016/0301-0104(92)80071-3)
- Špirko, V., Jørgensen, P., & Jensen, H. J. A. (1992). Ab initio potential energy function and geometry of the A⁻ state of ammonia. *Journal of Molecular Spectroscopy*, 152(1), 199-204. [https://doi.org/10.1016/0022-2852\(92\)90131-7](https://doi.org/10.1016/0022-2852(92)90131-7)
- Bak, K. L., Jørgensen, P., Jensen, H. J. A., Olsen, J., & Helgaker, T. (1992). First-order nonadiabatic coupling matrix elements from multiconfigurational self-consistent-field response theory. *The Journal of Chemical Physics*, 97(10), 7573-7584. <https://doi.org/10.1063/1.463477>
- Vahtras, O., Ågren, H., Jørgensen, P., Jensen, H. J. A., Padkjær, S. B., & Helgaker, T. (1992). Indirect nuclear spin-spin coupling constants from multiconfiguration linear response theory. *The Journal of Chemical Physics*, 96(8), 6120-6125. <https://doi.org/10.1063/1.462654>
- Stanton, J. F., Gauss, J., Bartlett, R. J., Helgaker, T., Jørgensen, P., Jensen, H. J. A., & Taylor, P. R. (1992). Interconversion of diborane (4) isomers. *The Journal of Chemical Physics*, 97(2), 1211-1216. <https://doi.org/10.1063/1.463247>
- Nordfors, D., Ågren, H., & Jensen, H. J. A. (1992). MCSCF/MCLR Studies of potential energy surfaces, spectra, and properties of the X¹A₁ and a³B₂ states of ozone. *International Journal of Quantum Chemistry*, 44(3), 413. <https://doi.org/10.1002/qua.560440309>
- Vahtras, O., Ågren, H., Jørgensen, P., Jensen, H. J. A., Helgaker, T., & Olsen, J. (1992). Multiconfigurational quadratic response functions for singlet and triplet perturbations: The phosphorescence lifetime of formaldehyde. *The Journal of Chemical Physics*, 97(12), 9178-9187. <https://doi.org/10.1063/1.463344>
- Hettema, H., Jensen, H. J. A., Jørgensen, P., & Olsen, J. (1992). Quadratic response functions for a multiconfigurational self-consistent field wave function. *The Journal of Chemical Physics*, 97(2), 1174-1190. <https://doi.org/10.1063/1.463245>
- Fernandez, B., Jørgensen, P., Byberg, J., Olsen, J., Helgaker, T., & Jensen, H. J. A. (1992). Spin polarization in restricted electronic structure theory: Multiconfiguration self-consistent-field calculations of hyperfine coupling constants. *The Journal of Chemical Physics*, 97(5), 3412-3419. <https://doi.org/10.1063/1.462977>
- Jensen, H. J. A., Jørgensen, P., Hettema, H., & Olsen, J. (1991). The hyperpolarizability dispersion of neon is not anomalous. *Chemical Physics Letters*, 187(4), 387-390. [https://doi.org/10.1016/0009-2614\(91\)80269-4](https://doi.org/10.1016/0009-2614(91)80269-4)
- Sanchez de Merás, A. M., Jensen, H. J. A., Jørgensen, P., & Olsen, J. (1991). Restricted and complete-active-space multiconfiguration linear response calculations of the polarizability of formamide and urea. *Chemical Physics Letters*, 186(4-5), 379-385. [https://doi.org/10.1016/0009-2614\(91\)90195-F](https://doi.org/10.1016/0009-2614(91)90195-F)
- Špirko, V., Daadoch, N. M., Jensen, H. J. A., Jørgensen, P., & Helgaker, T. (1991). An ab initio investigation of the potential energy function and rotation-vibration energies of H₂O·Na⁺. *Chemical Physics Letters*, 185(3-4), 265-269. [https://doi.org/10.1016/S0009-2614\(91\)85058-5](https://doi.org/10.1016/S0009-2614(91)85058-5)

Cesar, A., Ågren, H., Helgaker, T., Jørgensen, P., & Jensen, H. J. A. (1991). Excited state structures and vibronic spectra of H_2CO^+ , HDCO^+ , and D_2CO^+ using molecular gradient and Hessian techniques. *The Journal of Chemical Physics*, *95*(8), 5906-5917. <https://doi.org/10.1063/1.461612>

Nordfors, D., Ågren, H., & Jensen, H. J. A. (1991). MCSCF/MCLR Studies of potential energy surfaces, spectra, and properties of the X^1A_1 and a^3B_2 states of ozone. *International Journal of Quantum Chemistry*, *40*(4), 475-490. <https://doi.org/10.1002/qua.560400404>

Helgaker, T., Uggerud, E., & Jensen, H. J. A. (1990). Integration of the classical equations of motion on ab initio molecular potential energy surfaces using gradients and Hessians: application to translational energy release upon fragmentation. *Chemical Physics Letters*, *173*, 145-150. [https://doi.org/10.1016/0009-2614\(90\)80068-O](https://doi.org/10.1016/0009-2614(90)80068-O)

Špirko, V., Hans, H. J., & Jørgensen, P. (1990). Dipole polarizability surfaces of ammonia. *Chemical Physics*, *144*(3), 343-351. [https://doi.org/10.1016/0301-0104\(90\)80099-J](https://doi.org/10.1016/0301-0104(90)80099-J)

Koch, H., Jensen, H. J. A., Jørgensen, P., Helgaker, T., Scuseria, G. E., & Schaefer, H. F. (1990). Coupled cluster energy derivatives. Analytic Hessian for the closed-shell coupled cluster singles and doubles wave function: Theory and applications. *The Journal of Chemical Physics*, *92*(8), 4924-4940. <https://doi.org/10.1063/1.457710>

Koch, H., Jensen, H. J. A., Jørgensen, P., & Helgaker, T. (1990). Excitation energies from the coupled cluster singles and doubles linear response function (CCSDLR). Applications to Be, CH^+ , CO, and H_2O . *The Journal of Chemical Physics*, *93*(5), 3345-3350. <https://doi.org/10.1063/1.458815>

Carravetta, V., Ågren, H., Jensen, H. J. A., Jørgensen, P., & Olsen, J. (1989). Accurate photodetachment cross sections for Li^- . *Journal of Physics B: Atomic, Molecular and Optical Physics*, *22*(13), 2133-2140. Article 017. <https://doi.org/10.1088/0953-4075/22/13/017>

Jensen, H. J. A., Jørgensen, P., Helgaker, T., & Olsen, J. (1989). Accurate calculations of the dynamic dipole polarizability of N_2 . A multiconfigurational linear response study using restricted active space (RAS) wavefunctions. *Chemical Physics Letters*, *162*(4-5), 355-360. [https://doi.org/10.1016/0009-2614\(89\)87058-7](https://doi.org/10.1016/0009-2614(89)87058-7)

Olsen, J., De Meñas, A. M. S., Jensen, H. J. A., & Jørgensen, P. (1989). Excitation energies, transition moments and dynamic polarizabilities for CH^+ . A comparison of multiconfigurational linear response and full configuration interaction calculations. *Chemical Physics Letters*, *154*(4), 380-386. [https://doi.org/10.1016/0009-2614\(89\)85373-4](https://doi.org/10.1016/0009-2614(89)85373-4)

Ågren, H., Olsen, J., Jensen, H. J. A., & Jørgensen, P. (1989). Accurate static and dynamic polarizabilities of Li^- . *Physical Review A*, *40*(5), 2265-2269. <https://doi.org/10.1103/PhysRevA.40.2265>

Medina-Llanos, C., Ågren, H., Mikkelsen, K. V., & Jensen, H. J. A. (1989). Self-consistent reaction field calculations of photoelectron binding energies for solvated molecules. *The Journal of Chemical Physics*, *90*(11), 6422-6435. <https://doi.org/10.1063/1.456308>

Ågren, H., Medina-Llanos, C., Mikkelsen, K. V., & Jensen, H. J. A. (1988). On the validity of the equivalent core approximation in Born-Haber analyses of liquids and solutions. *Chemical Physics Letters*, *153*(4), 322-327. [https://doi.org/10.1016/0009-2614\(88\)80149-0](https://doi.org/10.1016/0009-2614(88)80149-0)

Jørgensen, P., Jensen, H. J. A., & Helgaker, T. (1988). A gradient extremal walking algorithm. *Theoretica Chimica Acta*, *73*(1), 55-65. <https://doi.org/10.1007/BF00526650>

Mikkelsen, K. V., Ågren, H., Jensen, H. J. A., & Helgaker, T. (1988). A multiconfigurational self-consistent reaction-field method. *The Journal of Chemical Physics*, *89*(5), 3086-3095. <https://doi.org/10.1063/1.454965>

Olsen, J., Roos, B. O., Jørgensen, P., & Jensen, H. J. A. (1988). Determinant based configuration interaction algorithms for complete and restricted configuration interaction spaces. *The Journal of Chemical Physics*, *89*(4), 2185-2192. <https://doi.org/10.1063/1.455063>

Jensen, H. J. A., Jørgensen, P., Ågren, H., & Olsen, J. (1988). Erratum: Second-order Møller-Plesset perturbation theory as a configuration and orbital generator in multiconfiguration self-consistent-field calculations (Journal of Chemical Physics (1988) 88 (3834)). *The Journal of Chemical Physics*, *89*(8). <https://doi.org/10.1063/1.455749>

Jørgensen, P., Jensen, H. J. A., & Olsen, J. (1988). Linear response calculations for large scale multiconfiguration self-consistent field wave functions. *The Journal of Chemical Physics*, *89*(6), 3654-3661. <https://doi.org/10.1063/1.454885>

Olsen, J., Jensen, H. J. A., & Jørgensen, P. (1988). Solution of the large matrix equations which occur in response theory. *Journal of Computational Physics*, *74*(2), 265-282. [https://doi.org/10.1016/0021-9991\(88\)90081-2](https://doi.org/10.1016/0021-9991(88)90081-2)

Ågren, H., & Jensen, H. J. A. (1987). An efficient method for the calculation of generalized overlap amplitudes for core photoelectron shake-up spectra. *Chemical Physics Letters*, *137*(5), 431-436. [https://doi.org/10.1016/0009-2614\(87\)80228-2](https://doi.org/10.1016/0009-2614(87)80228-2)

Jensen, H. J. A., Jørgensen, P., & Ågren, H. (1987). Efficient optimization of large scale MCSCF wave functions with a restricted step algorithm. *The Journal of Chemical Physics*, *87*(1), 451-466. <https://doi.org/10.1063/1.453590>

Jensen, H. J. A., & Ågren, H. (1986). A direct, restricted-step, second-order MC SCF program for large scale ab initio calculations. *Chemical Physics*, *104*(2), 229-250. [https://doi.org/10.1016/0301-0104\(86\)80169-0](https://doi.org/10.1016/0301-0104(86)80169-0)

Flores-Riveros, A., Ågren, H., Brammer, R., & Jensen, H. J. A. (1986). A diabatic model for photoionization. Application to the inner valence x-ray photoelectron spectrum of acetylene. *The Journal of Chemical Physics*, *85*(11), 6270-6275. <https://doi.org/10.1063/1.451456>

Helgaker, T. U., Jensen, H. J. A., & Jørgensen, P. (1986). Analytical calculation of MCSCF dipole-moment derivatives. *The Journal of Chemical Physics*, *84*(11), 6280-6284. <https://doi.org/10.1063/1.450772>

Ågren, H., Flores-Riveros, A., & Jensen, H. J. A. (1986). Evaluation of first- and second-order nonadiabatic coupling elements from large multiconfigurational self-consistent-field wave functions. *Physical Review A*, *34*(6), 4606-4614. <https://doi.org/10.1103/PhysRevA.34.4606>

Helgaker, T. U., Almlöf, J., Jensen, H. J. A., & Jørgensen, P. (1986). Molecular Hessians for large-scale MCSCF wave functions. *The Journal of Chemical Physics*, *84*(11), 6266-6279. <https://doi.org/10.1063/1.450771>

Jensen, H. J. A., Jørgensen, P., & Helgaker, T. (1986). Systematic determination of MCSCF equilibrium and transition structures and reaction paths. *The Journal of Chemical Physics*, *85*(7), 3917-3929. <https://doi.org/10.1063/1.450914>

Ågren, H., Correia, N., Flores-Riveros, A., & Jensen, H. J. AA. (1985). Direct restricted-step MCSCF calculations on the structure and spectrum of cyclobutadiene. *International Journal of Quantum Chemistry*, *28*(19 S), 237-246. <https://doi.org/10.1002/qua.560280823>

Hans, H. J., & Agren, H. (1984). MC SCF optimization using the direct, restricted step, second-order norm-extended optimization method. *Chemical Physics Letters*, *110*(2), 140-144. [https://doi.org/10.1016/0009-2614\(84\)80163-3](https://doi.org/10.1016/0009-2614(84)80163-3)

Davis, C. L., Jensen, H. J. A., & Monkhorst, H. J. (1984). Accurate Hartree-Fock wave functions without exponent optimization. *The Journal of Chemical Physics*, *80*(2), 840-855. <https://doi.org/10.1063/1.446738>

Weiner, B., Jensen, H. J. A., & Öhrn, Y. (1984). Erratum: Polarization propagator calculations with AGP reference state (The Journal of Chemical Physics (1984) 80 (2009)). *The Journal of Chemical Physics*, 81(1). <https://doi.org/10.1063/1.448190>

Jensen, H. J. A., & Jørgensen, P. (1983). A direct approach to second-order MCSCF calculations using a norm extended optimization scheme. *The Journal of Chemical Physics*, 80(3), 1204-1214. <https://doi.org/10.1063/1.446797>

Weiner, B., Jensen, H. J. A., & Öhrn, Y. (1983). Polarization propagator calculations with an AGP reference state. *The Journal of Chemical Physics*, 80(5), 2009-2021. <https://doi.org/10.1063/1.446964>

Hans, H. J., Weiner, B., & Öhrn, Y. (1983). AGP Propagator calculations. *International Journal of Quantum Chemistry*, 23(1), 65-70. <https://doi.org/10.1002/qua.560230107>

Kurtz, H. A., Weiner, B., & Jensen, H. J. A. (1983). The polarization propagator based on an AGP state: Theory and application to the helium atom. *International Journal of Quantum Chemistry*, 24(Suppl. 17), 415-423. <https://doi.org/10.1002/qua.560240846>

Jensen, H. J. A., Weiner, B., Ortiz, J. V., & Öhrn, Y. (1982). A powerful procedure for optimizing AGP states. *International Journal of Quantum Chemistry*, 22(16 S), 615-631. <https://doi.org/10.1002/qua.560220853>