## **CTR THEORET. CHEM. (KOX) 1976-1979**

## 1. Papers in Refereed Journals

 "Theory and calculation of excited state wave functions and properties", D.R. Beck and C.A. Nicolaides, Int. J. Quantum Chem. Suppl. Y-10, 119 (1976).

2. "Collective excitations in atoms and molecules",C.A. Nicolaides and D.R. Beck,J. Phys. B <u>9</u>, L259 (1976).

3. "Calculation of induced electric and magnetic moments of atoms and molecules", D.R. Beck and C.A. Nicolaides, Chem. Phys. Lett. <u>48</u>, 135 (1977).

4. "Lower bounds to static polarizabilities",D.R. Beck and C.A. Nicolaides,Chem. Phys. Lett. <u>49</u>, 357 (1977).

5. "Comment on mean-square deviation formula for autoionizing states", C.A. Nicolaides,Phys. Rev. A <u>15</u>, 1787 (1977).

6. "Variational method for calculating energies and widths of resonances", C.A. Nicolaides and D.R. Beck,
Phys. Lett. A <u>60</u>, 92 (1977).

7. "High-spin and mixed states in BI and BII",D.R. Beck and C.A. Nicolaides,Phys. Lett. A <u>61</u>, 227 (1977).

 "Continuum and its effect on cascades in beam-foil spectroscopy", C.A. Nicolaides, Phys. Lett. A <u>63</u>, 209 (1977).

Possibility of observing nonexponential decays in autoionizing states", C.A. Nicolaides and D.R. Beck,
Phys. Rev. Lett. <u>38</u>, 683 (1977).

10. "Transfer of oscillator strength in regions of (avoided) crossings - 2-state approximation", C.A. Nicolaides and D.R. Beck,Chem. Phys. Lett. <u>53</u>, 87 (1978).

11. "Transfer of oscillator strength in regions of avoided crossings. Atomic spectra for non-

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12. "Methods for improving spin-densities obtained from unrestricted Hartree-Fock wavefunctions",A.T. Amos, D.R. Beck and I.L. Cooper,Chem. Phys. Lett. <u>56</u>, 95 (1978).

13. "How many bound-states do H<sup>-</sup> and H<sup>2-</sup> have", D.R. Beck and C.A. Nicolaides, Chem. Phys. Lett. <u>59</u>, 525 (1978).

14. "Variational calculation of energies and widths of resonances", C.A. Nicolaides and D.R. Beck, Phys. Lett. A <u>65</u>, 11 (1978).

15. "Transition-probabilities for Vuv resonance lines of Mg-like and Zn-like molybdenum ions",D.R. Beck and C.A. Nicolaides,Phys. Lett. A <u>65</u>, 293 (1978).

16. "Time-dependence, complex scaling, and calculation of resonances in many-electron systems",C.A. Nicolaides and D.R. Beck,

Int. J. Quantum Chem. <u>14</u>, 457 (1978).

17. "Comment on the lifetime of the Li  $1s2p^{2} {}^{2}P$  state: How probable is radiative autoionization?", C.A. Nicolaides and D.R. Beck, Phys. Rev. A <u>17</u>, 2116 (1978).

18. "Theory of atomic structures including electron correlation. 5. Excited-states not lowest of their symmetry and oscillator strengths in neutral and singly ionized atoms - comment", C.A. Nicolaides and D.R. Beck, Phys. Rev. A <u>18</u>, 1307 (1978).

19. "Analysis of maximum entropy principle debate",J.F. Cyranski,Found. Phys. <u>8</u>, 493 (1978).

20. "Quantum measurement as a communication with nature", J.F. Cyranski,Found. Phys. <u>8</u>, 805 (1978).

21. "One-electron binding and Auger energies in atomic and molecular states"

G. Theodorakopoulos, C.A. Nicolaides and D.R. Beck, Int. J. Quantum Chem. Symp. <u>13</u>, 671 (1979).

22. "Configuration interaction methods for improving unrestricted Hartree-Fock spindensities",

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23. "Measurement theory for physics",J.F. Cyranski,Found. Phys. <u>9</u>, 641 (1979).

24. "Measurement, theory, and information",J.F. Cyranski,Inform. and Control <u>41</u>, 275 (1979).

## 2. Book Chapters

1. "Theory of the electronic structure of excited states with numerical applications to atomic states",

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*Excited States in Quantum Chemistry*, C.A. Nicolaides and D.R. Beck, Co-editors, D. Reidel (1978), pp.105-142.

2. "Many body theory of photoabsorption in atoms and molecules",

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3. "Theory of one electron binding energies including correlation, relativistic and radiative effects: application to free atoms and metals",

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4. "Theory of atomic and molecular non-stationary states within the coordinate rotation method",

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