Relativistic Fock Space Coupled Cluster beyond CCSD: Theory and Implementation

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Current problems of the FS-RCC theory

Relativistic Fock space coupled cluster method (FS-RCC)
seems to be one of the most perspective tools for high-precision electronic structure modelling of heavy atoms and molecules

+/− solved problems:

- transition properties (e.g. intensities) → finite-field technique*
- intruder states problem → IH / denominator shifts & extrapolations**

open problems:

- only the FS-CCSD approximation is available now (e.g. DIRAC, TRAFS-3C)
- narrow scope of applicability: max 2 open shells

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How to extend the scope of applicability and increase accuracy of FS-RCC?

*A. Zaitsevskii et al. Opt. Spectrosc., 124, 451 (2018)

**A. Zaitsevskii et al. PRA, 96, 022516 (2017); A. Zaitsevskii, E. Eliav. IJQC, 118, e25772 (2018)

FS-RCC Ansatz and working equations

- Wave operator:

$$\Omega = \{\exp(T)\}_N$$

$$\begin{aligned} \text{CCSD:} \quad & T = T_1 + T_2 \\ \text{CCSDT:} \quad & T = T_1 + T_2 + T_3 \end{aligned}$$

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- Amplitude equations:

$$[T^{(h,p)}, H_0] = (V\Omega - \Omega(V\Omega)_{cl})^{(h,p)}_{conn}$$

complex combination of integrals and amplitudes

- Effective Hamiltonian:

M^{h+p} x M^{h+p} matrix, M – active space dim

$$H^{(h,p)}_{eff} = P^{(h,p)} H\{e^T\} P^{(h,p)}$$

projection onto model space

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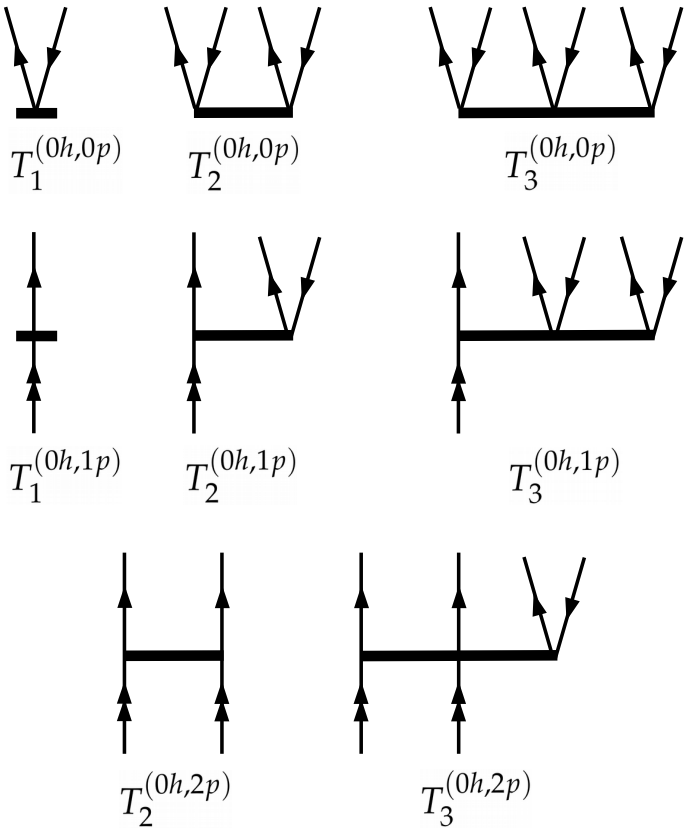
we will work with Brandow diagrams

I. Lindgren. IJQC 14, 33 (1978); U. Kaldor, Theor. Chim. Acta 80, 427 (1991); L. Visscher et al, JCP 115, 9720 (2001)

FS-RCC cluster operator: CCSDT approximation

example: the (0h,2p) sector



- CCSD: no spectator triples = no differential correlation
- model space extension actually does not recover all triples contributions

  Example: Pb atom EEs, IH-FS-CCSD gives errors of order 200 – 600 cm^{-1}*

* A. Landau, E. Eliav, Y. Ishikawa, U. Kaldor, JCP 114, 2977 (2001)

Full CCSDT: the achievable ideal?

Connected $T_3^{(h,p)}$ amplitudes can be defined for all FS sectors up to $h + p = 3$

- similar to the FS-CCSD model:
  $h + p \leq 3 \rightarrow$ iterative solution
  $h + p < 3 \rightarrow$ non-iterative construction of H_{eff}
- *very* high accuracy
  $\rightarrow$ remember about incomplete basis, QED, Breit, ...
- strongly required for high-precision calculations in the (0h,3p) sector

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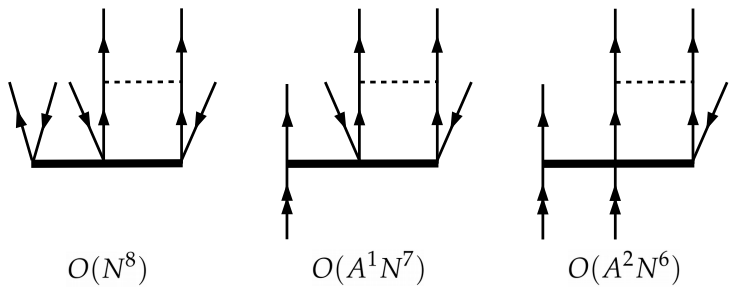
Main problem:

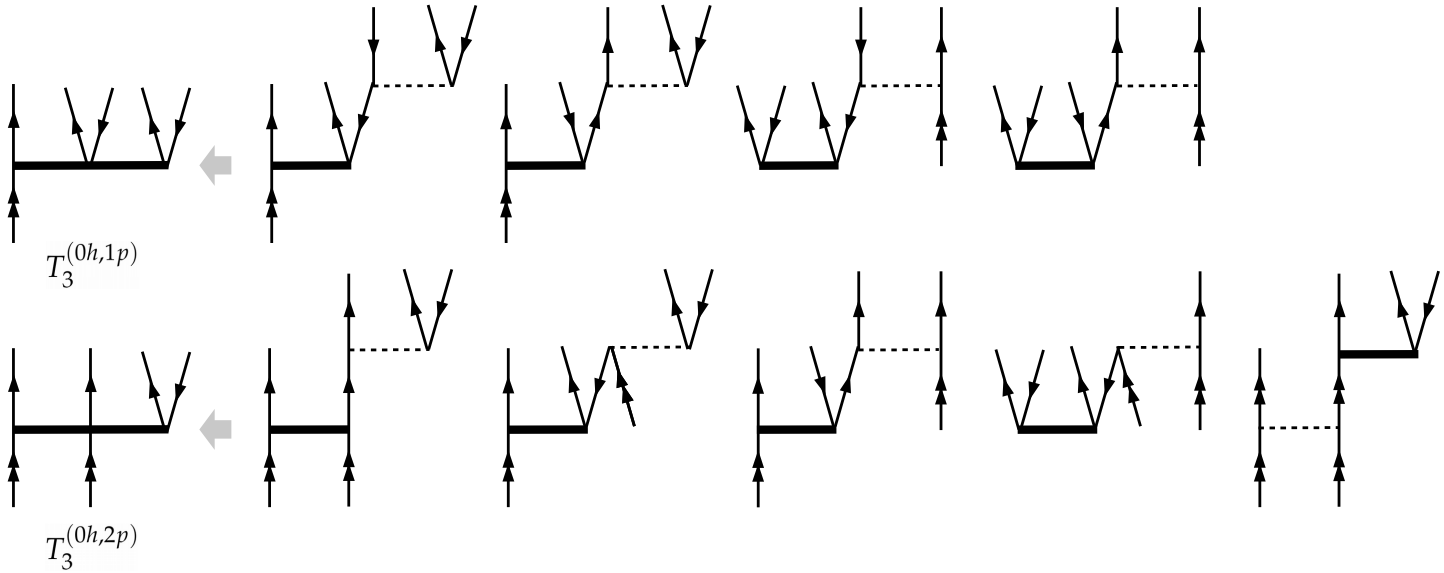


S.R. Hughes, U. Kaldor, CPL 204, 339 (1993)
A. Oleynichenko, A. Zaitsevskii, L. V. Skripnikov, E. Eliav, 2020 *submitted to Symmetry*

The CCSD+T(3) model

Let us try to estimate $T_3^{(h,p)}$ amplitudes using MBPT arguments

T_3 amplitudes are estimated only once, converged T_1 and T_2 amplitudes are used



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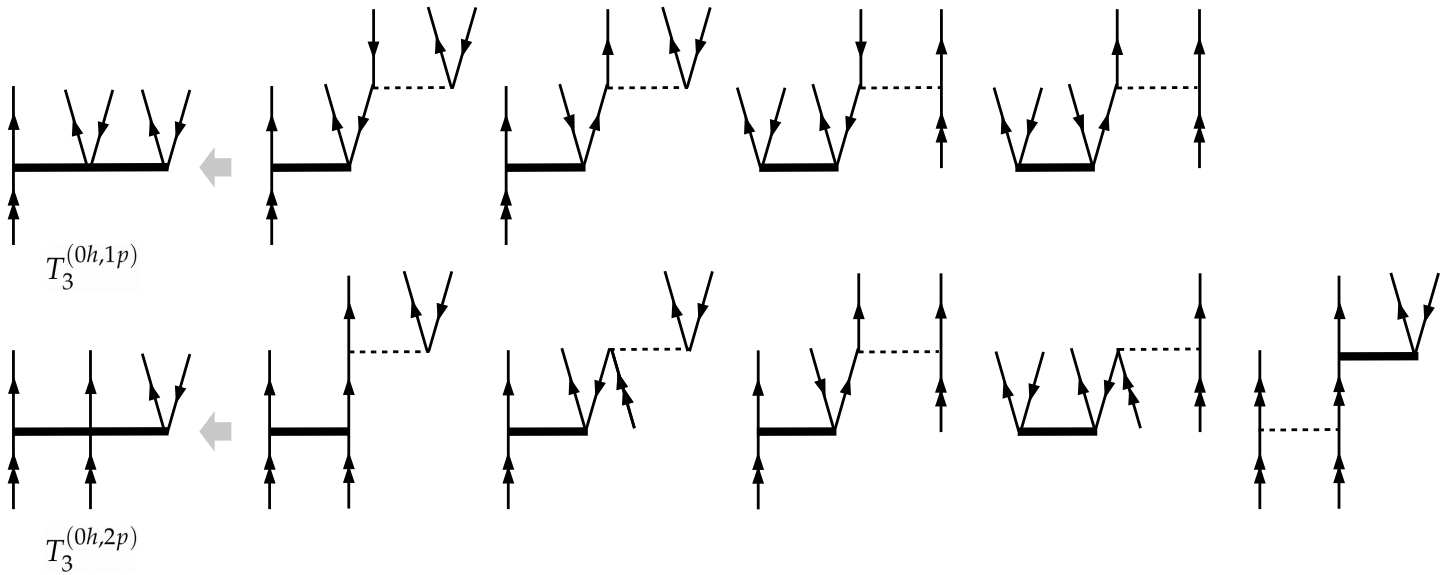

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Main drawback: works *very poorly* except (0h,0p) [Bernholdt, Bartlett, 1999]

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CCSDT-n models

Within the CCSDT-n framework $T_3^{(h,p)}$ amplitudes contribute to T_1 and T_2 equations

CCSDT-1:

$$\left.\begin{aligned} [T_3, H_0] &\approx VT_2 \\ T_1, T_2 &\leftarrow f(V, T_1, T_2, T_3) \end{aligned}\right\} \text{repeat until convergence}$$

- iterative solution only in low FS sectors ($h + p \leq 2$)
- computational complexity is lower than for full CCSDT
- $T_3^{(h,p)}$ are to be recalculated at each iteration

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CCSDT-2, CCSDT-3:

- additional terms including T_1 and T_2 contribute to $T_3^{(h,p)}$
- $O(N^8)$-terms are again avoided

SR-CCSDT-n: J. Noga, R. Bartlett, M. Urban. CPL, 134. 126 (1987)
FS-CCSDT-1: S. R. Hughes, U. Kaldor. CPL, 194, 99 (1992)

modern implementation is required

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the EXP-T program system

The EXP-T program system: efficient and flexible implementation of FS-RCC models

CC models:

- ✔ **CCSD**
- ✔ **CCSD+T(3)**
- ✔ **CCSDT-1,2,3**
- ✔ **CCSDT**

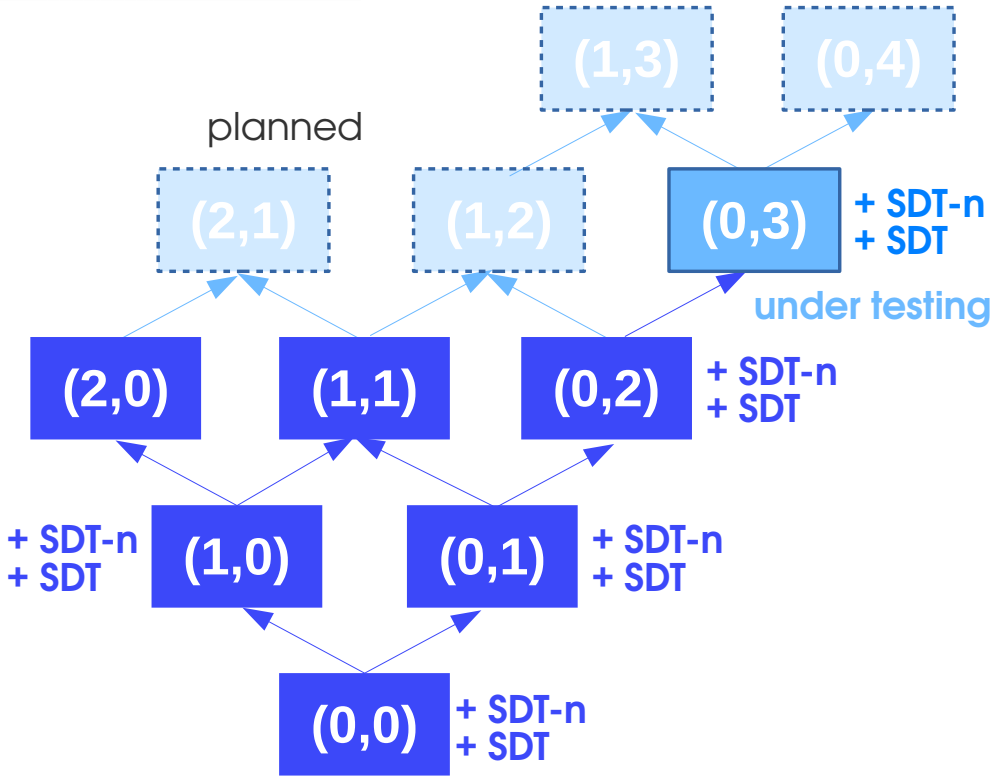
Transformed integrals:

- ✔ **DIRAC**
- ✔ **any abelian groups**
- ✔ **4cDC, X2Cmmf, 2cECP**
- ✔ **Gaunt, properties**
  (D. Maison, L. Skripnikov, PNPI)

Parallelization:

- ✔ **OpenMP**
- ✔ **CUDA**

$$\Omega = \{\exp(\mathbf{T})\}$$



(h,p) – Fock Space sectors

Coming soon:

http://qchem.pnpi.spb.ru/ru/Oleynichenko

The EXP-T program system: technical details

A. Oleynichenko, A. Zaitsevskii, E. Eliav, *Towards High Performance Relativistic Electronic Structure Modelling: The EXP-T Program Package*
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- storage of symmetry and/or formal blocks of tensors: RAM, disk, disk+LZ4

Pilot applications: EEs and IPs of Tl and Pb

Additive scheme:

$$E_{CCSDT} = E_{CCSD,LB} + (E_{CCSDT,SB} - E_{CCSD,SB})$$

Triples contributions are evaluated using smaller basis set

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Tl: $6s7p5d5f4g3h2i$, Pb: $6s6p5d5f4g3h2i$

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Active space: $6p$-spinors only

Pilot applications: EEs and IPs of Tl and Pb

A. Oleynichenko, A. Zaitsevskii, L. V. Skripnikov, E. Eliav

Relativistic Fock-Space Coupled Cluster Method for Many-Electron Systems: Non-Perturbative Account for Connected Triple Excitations

2020, *submitted to Symmetry*

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Table 1. Deviations of the calculated ionization potentials (IP) and excitation energies (EE) of neutral thallium and lead and lead cation (cm^{-1}) from the experimental values. FS-RCCSD/LB+T/SB stands for the combined scheme (8).

	State		Exptl [80]	IH-FS-RCCSD[47]	FS-RCCSD/LB	FS-RCCSD/LB + T/SB SDT-1	SDT-1′	SDT-2	SDT-3	SDT
					Tl, ground state $6s^2 6p\ {}^2P_{1/2}$					
IP			49266		-56	-38	-38	-204	-151	-32
EE	$6s^2 6p$	$^2P_{3/2}$	7793		-112	23	23	1	9	-31
					Pb^+, ground state $6s^2 6p\ {}^2P_{1/2}$					
IP			121245	-168	-143	-28	-28	-190	-158	-59
EE	$6s^2 6p$	$^2P_{3/2}$	14081	-196	-136	25	25	12	14	-42
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IP			59819	-543	364	-44	-285	-347	-336	7
EE	$6s^2 6p^2$	$^3P_1$	7819	-288	-302	76	5	-4	-3	-28
		$^3P_2$	10650	-343	-235	130	129	97	102	13
		$^1D_2$	21458	-605	-394	215	203	158	167	5
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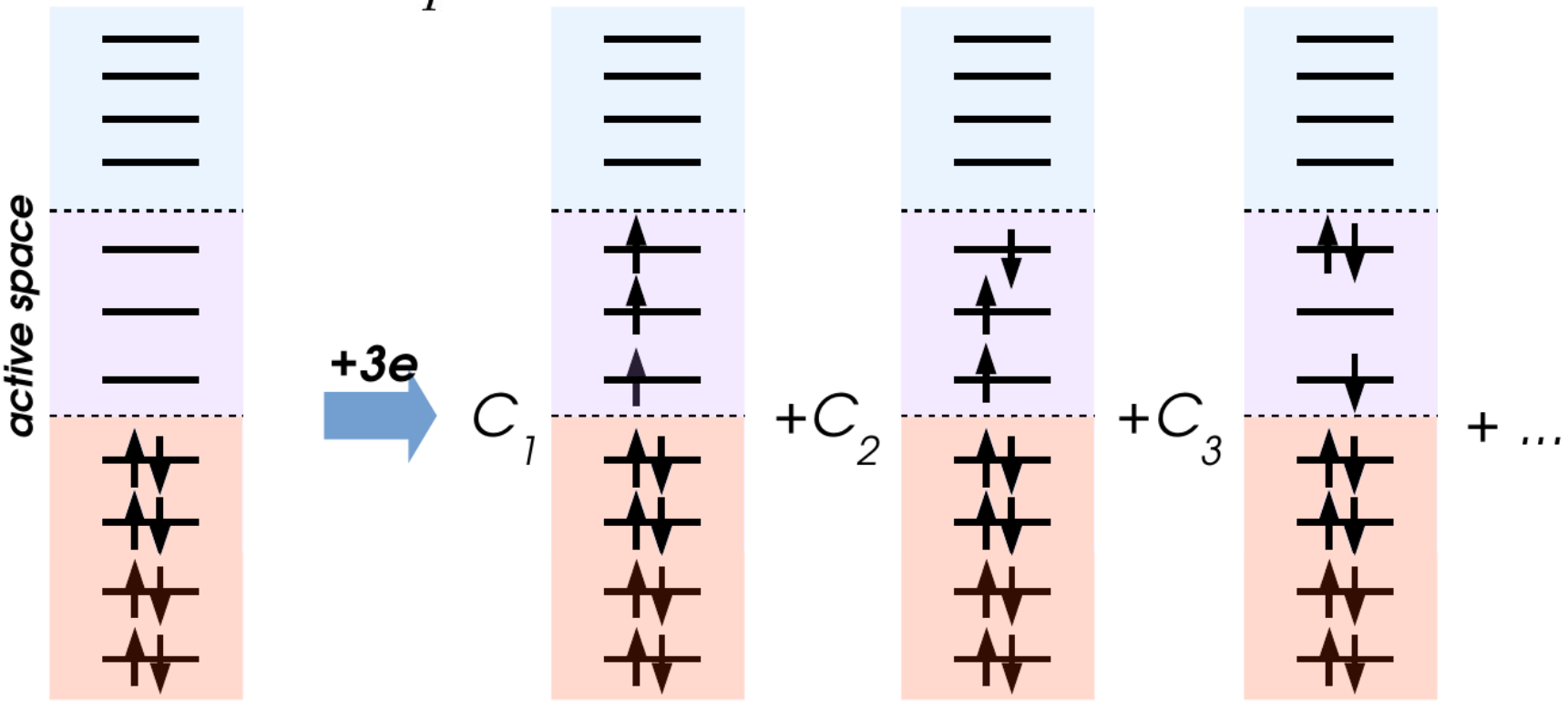
the most accurate *ab initio* results for heavy non-alkali atoms

the (0h,3p) Fock space sector

The (0h,3p) FS sector: three particles over vacuum

$$|\psi_x\rangle = \{e^T\} \sum_I C_I |\Phi_I\rangle$$

"High sectors" of the Fock space



Sector (0,3)
h = 0 p = 3

✔ electonic states of systems with three unpaired electrons

+ Basic theory (Kaldor et al, 1985 - 1993)

- No working code !

- No experience !

The (0h,3p) FS sector: motivation

Protactinium: atomic energy levels

reference state: $Pa^{3+}([Rn]7s^2)$

	Configuration	Term	J	Level(cm^{-1})
0h3p	$5f^2(^3H)6d7s^2$	^4K	11/2	0.000
			13/2	3711.625
			15/2	7512.695
			17/2	11198.270
0h3p	$5f^2(^3H)6d7s^2$	^4I	9/2	825.415
			11/2	4121.450
			13/2	7383.295
			15/2	10049.875
0h3p	$5f^26d7s^2$	$a\ ^4G$	5/2	1618.325
			7/2	4713.870
			9/2	7330.815
0h3p	$5f(^2F)6d^2(^3F)7s^2$	$^4H^\circ$	7/2	1978.220
			9/2	5335.730
			11/2	8419.075
			13/2	11498.725
0h3p	$5f(^2F)6d^2(^3F)7s^2$	$^4I^\circ$	9/2	2659.405

- electronic states can be described only in the (0h,3p) sector
- EOM-CC cannot deal with such electronic states *at all*
- other examples: LiSr dimer, Np, Pu compounds, superactinides atoms

https://physics.nist.gov/PhysRefData/Handbook

The (0h,3p) FS sector: first tests

Almost all electronic states of the **nitrogen atom** can be represented as three particles over the N^{3+} $(1s^2 2s^2)$ vacuum

All electrons were correlated, cc-pVTZ basis set
FSCC: $N^{3+} \rightarrow N^{2+}$ (0h,1p) $\rightarrow N^{+}$ (0h,2p) $\rightarrow N^{0}$ (0h,3p)
Active space: $2p$

Ground state: $^4S^o$ $(2s^2 2p^3)$

			(deviations from FCI, cm^{-1})		
		FCI, cm^{-1}	TEA-EOM-CCSD*	FS-CCSD	FS-CCSDT
$^2D^o$	$2s^2 2p^3$	20275	-1175	-846	-76
$^2P^o$	$2s^2 2p^3$	30038	-6738	-1134	+452

* M. Musial et al, J. Chem. Phys. 137, 174102 (2012)

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All electrons were correlated, cc-pVTZ basis set
FSCC: $N^{3+} \rightarrow N^{2+}$ (0h,1p) $\rightarrow N^{+}$ (0h,2p) $\rightarrow N^{0}$ (0h,3p)
Active space: $2p$

Ground state: $^4S^o$ $(2s^2 2p^3)$

			(deviations from FCI, cm^{-1})		
		FCI, cm^{-1}	TEA-EOM-CCSD*	FS-CCSD	FS-CCSDT
$^2D^o$	$2s^2 2p^3$	20275	-1175	-846	-76
$^2P^o$	$2s^2 2p^3$	30038	-6738	-1134	+452

* M. Musial et al, J. Chem. Phys. 137, 174102 (2012)

to be tested and understood

Ongoing projects

- molecular applications
- high sectors
- MPI parallelization
- triples for properties (with L. V. Skripnikov)
- first public release of EXP-T

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