

# Precision calculations of atoms with few valence electrons

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## Toy 3-electron atom

Comparison of the 3-e “exact” calculation with the 1-electron calculations in different approximations. Frozen core [ $1s^2$ ] approximation (FC) and effective Hamiltonian calculated with MBPT-II (II), SD, and SD with MBPT-III corrections (SD+III).

$H_{\text{eff}}$	3-e ( $\text{cm}^{-1}$ )	1-e (errors)			
	—	FC	II	SD	SD+III
$2s_{1/2}$	0.0	0.0	0.0	0.0	0.0
$2p_{1/2}$	64870.1	329.9	46.1	16.0	2.2
$2p_{3/2}$	64999.6	328.6	45.2	15.1	1.5
$3s_{1/2}$	302411.3	-256.1	-49.5	-11.1	-1.2
$3p_{1/2}$	319727.1	-189.4	-40.8	-8.1	-1.1
$3p_{3/2}$	319765.1	-189.7	-40.9	-8.4	-1.4
$3d_{3/2}$	324342.0	-284.9	-61.7	-13.9	-2.2
$3d_{5/2}$	324351.2	-284.9	-61.7	-13.8	-2.2
av.err.		-78	-24	-4	-1
max err.		+330	+50	+16	2

## Toy 4-electron atom

Comparison of the 4-e “exact” calculation with the 2-electron calculations in different approximations. Frozen core [ $1s^2$ ] approximation (FC) and effective Hamiltonian calculated with MBPT-II (II), SD, and SD with one-electron MBPT-III corrections (SD+III).

$H_{\text{eff}}$	4-e ( $\text{cm}^{-1}$ )	2-e (errors)			
	—	FC	II	SD	SD+III
$^1S_0(2s^2)$	0.0	0.0	0.0	0.0	0.0
$^3P_0(2s2p)$	52535.9	222.0	31.6	8.3	-3.3
$^3P_1(2s2p)$	52569.7	221.9	31.8	8.5	-3.3
$^3P_2(2s2p)$	52637.5	221.7	31.8	8.8	-3.1
$^1P_1(2s2p)$	104969.2	865.4	80.3	58.8	47.9
$^3P_0(2p^2)$	138303.7	1016.9	111.0	61.2	36.0
$^3P_1(2p^2)$	138337.0	1016.3	110.7	60.8	35.6
$^3P_2(2p^2)$	138402.9	1015.3	110.4	60.6	35.3
$^1D_2(2p^2)$	147954.8	698.6	70.1	26.0	2.3
$^1S_0(2p^2)$	186561.7	845.5	63.7	25.3	4.4
$^3S_1(2s3s)$	239752.9	79.5	11.7	49.9	64.8
$^1S_0(2s3s)$	251971.5	59.8	0.9	35.8	49.6
av. err.	0	569	60	37	24
max err.	0	1017	111	62	65