The paper reports attempts to calculate cross-sections for various collisional processes in atoms and molecules using bound-state and continuum orbitals generated by two methods: from standard pseudopotentials and from Hartree-Fock wave-functions by the depurated inversion approach developed previously by the authors. Considerably better results are obtained with the one-electron effective potentials generated by the authors' method.

The manuscript is fairly clear but has quite a few misprints and moderate problems that need to be addressed.

I am not an expert on collision theory, but surely there exist other published calculations of proton-impact cross-sections for H, Li, C, N, Ne, Ar, and small molecules. If so, they should be reviewed in the introduction.

If not, that fact should be stated clearly. The paper should not give the impression that these are the first ever ab initio calculations of proton-impact cross-sections.

On page 10, the authors state "Many ab initio and semi-empirical theoretical approximations have been developed to this end over the last century".

This statement should be supported with a few citations.

It should be explained why the T-matrix of Eq. (12) involves orbitals rather than N-electron wave-functions. Is this an approximation? If so, what is its justification?

Which Ar pseudopotential is shown in Fig. 1? A label is missing.

Axis labels in similar figures are not very consistent.

Why does Fig. 6 show differential cross-sections whereas Fig. 8-9 show simply cross-sections?

Why is the horizontal axis in Figs. 5 and 7 labeled "Proton Velocity" whereas in Figs. 6 (for another proton collision) it says "Energy"?

Shouldn't the horizontal axis labels in Figs. 8, 9, 13 say "Photon Energy" rather than simply "Energy"?

On page 11, the authors state "we considered the methane molecule, which has a suitable spherical geometry". It is a bad choice of words to call the geometry of CH4 "spherical".

Did the basis set used for molecular calculations in Sec. 4.2 (UGBS) include polarization functions? The UGBS as originally defined has no polarizationfunctions and hence is unsuitable for calculations on molecules.

The analytic form of the second term of Eq. (31) should be justified.

Problems with Figs. 1-3 and 5-8: the line samples in the legends are too short to distinguish between solid and dashed lines. The samples should be at least 2.5 times longer. Also, instead of two dashed curves in the plots, one curve should be dashed and the other dot-and-dash to make it possible to distinguish the curves when printed on a b/w printer.

Misprints that I noticed:

Missing minus sign in front of the first term of Eq. (27)

The last sum in Eq. (27) should have "i<j", not "i=1".

one clever idea emerge (p. 2)

pesudopotentials (p. 2)

infomation (p. 2)

Schrodinger (p. 4)

th spherical (p. 4)

The spatial and momentum representation (p. 4), should be "representations"

closer inspection... show (p. 4)

orbitals produces (p. 5)

significative advantage -> significant advantage (p. 5)

momentum -> momenta (plural), above Eq. (12)

Please proofread the MS carefully.

On page 5 it should say "C. Froese Fischer" (last name = "Froese Fischer"), not "C. F. Fischer"

On page 10, the wording "do to their generally multicentered and highly non-central nature" is awkward. Suggest "due to their nonspherical symmetry and multicenter character".

Do not capitalize "depurated inversion method" when it is not abbreviated.

The references should be formatted in the ACS style, as per AQC instructions.