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Excitations of the B¹Δ, C¹Π, and D¹∑+ States of N_2O Molecule by Positron Impact

*JLS Lino**

Assessoriae Orientação Estudantil, Núcleode Pesquisas, São José dos Campos, São Paulo, Brazil

Abstract

We report cross-sections for excitations of the B¹Δ, C¹Π, and D¹∑+ states of N_2O molecule by positron impact using the scaling Born positron (SBP) method [J LS Lino, Chin. J. Phys. 54 223(2016)]. The SBP method is applicable only to dipole-allowed excitations and to our knowledge, up to date no experimental data and theoretical results are available for comparison. Similarities and differences with electron-N2O scattering case are discussed. A study to check convergence characteristics using the annihilation parameter Z_{eff} (classical Z) is tested.

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Keywords

Born, Positron, Scaling

Introduction

Fundamental uses of positrons include the formation of neutral antihydrogen atoms, astrophysics process, phenomena including plasmas, molecular clusters and nanoparticles. Many, if not most, of these uses of positrons depend on a quantitative understanding of the basic interactions of positron with molecules [1]. Several processes are of interest and include, for example, electronic excitation, positronium formation, polarization, multichannel effects, and ionization. In our atmosphere, nitrogen oxides are generated as a product of the combustion of fossil fuels and N_2O is known to be generated in selective catalytic reduction reactions and is a known cause of global warning. The N_2O molecule is considered one of the major air pollutants in Earth´s atmosphere [2]. In particularly, N_2O is a linear triatomic molecule with a small permanent dipole and represent a strong challenge for the study of positron as incident particle. From the theoretical point of view, we note that work on positron-N_2O scattering are very scarce when compared with electron scattering case. For example, Arretche, et al. [3] reported elastic cross-sections for positron-N_2O scattering using the Schwinger multichannel method (SMC). Baluja and Jain reported (elastic+inelastic) cross-sections using the parameter-free model potential [4]. On the experimental side relative differential cross-sections for quasielastic including rotational and vibrational excitations positron-N_2O scattering in the 4-100 eV range were measured and reported by Przybyla, et al. [5]. Still on the experimental side, Kwan, et al. [6] reported total cross sections for positron-N_2O scattering in the 1-500 eV incident energy range. Studies on the theoretical side and experimental data including positron-N_2O scattering are widely discussed by Surko, et al. [7].

We recently reported electronic excitation cross sections for positron-CO [8], N_2 [8], NO [8] and C_6H_6 [9] scattering using the called scaled Born positron method [8,9]. The results obtained for these molecules using the SBP method are in excellent agreement when compared with sophisticate methods which suggest that the SBP method can be a reliable tool for the study of positron-molecule scattering. Motivated by these results using the SBP method we will investigated the electronic excitation by positron impact of N_2O molecule considering the B¹Δ, C¹Π, and D¹∑⁺ states. As far as we know, this is the first time that inelastic cross-sections are reports for N_2O molecule using the SBP method and a comparison of our cross-sections with electron-N_2O scattering case are necessary and can provide a interesting insight on differences and similarity of e± - N_2O scattering. In the present study the positronium formation channel is not considered.

In Sec.2 we will identify the SBP method for investigated

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cross sections for the B^{1}Δ, C^{1}Π, and D^1∑$^+$ states of N$_2$O molecule. In Sec.3 computational procedures and results are discussed. Conclusions are presented in Sec.4.

Theory

Recently, Lino proposed [9] the scaled Born positron (SBP) based on the original scaling plane wave Born for electron-molecule collision [10]. The SBP method was found to convert the traditional first Born approximation integral cross sections to reliable cross-sections when compared with sophisticate methods. The traditional first Born approximation (FBA) is used here as the main step, *i.e*, the plane wave is the correct function at infinity. The FBA can be written as

$$\sigma_{Born} = \left[\left(4\pi a_o^2 R\right)\middle/ E\right] f_{FBA} \qquad (1)$$

The SBP method represent a optimization of Eq.(1), *i.e.*, the SBP method replaces the E (energy) that appears in the denominator of Eq.(1) by E + (E$_{exc}$ + E$_{Ps}$). The Eq.(1) can be rewritten as

$$\sigma_{SBP} = \left(f_{accur}/f_{Born}\right).f\left(E\right).\sigma_{Born} \qquad (2)$$

where

$$f\left(E\right) = \left[\left(\frac{E}{E + \left(Eps + Eex\right)}\right)\right] \qquad (3)$$

The Eq. (2) has some important aspects. First, E$_{ps}$ is the positronium energy of the target and is used only when the incident particle is the positron which is not identical to the target electrons. Second, E$_{exc}$ is the excitation energy, f_{accur} is an accurate dipole value from experiments or from accurate wave functions, and f_{Born} is the dipole value from the

traditional FBA and these parameters are free of adjustable. Third, the constant (E$_{Ps}$ + E$_{ex}$) has some consequences practical to the performance of the SBP method [8,9]. For example, the constant is related with energy of the incident positron in the field of the nucleus and the bound electrons of the target. The Eq. (3) also can be seen as the scaling factor to represent the correlation between the positron and electrons of the target. Furthermore, the "scaling factor" here proposed suggests a similarity with polarization effects [9]. The positronium (Ps) energy used in the eq. (3) is written as
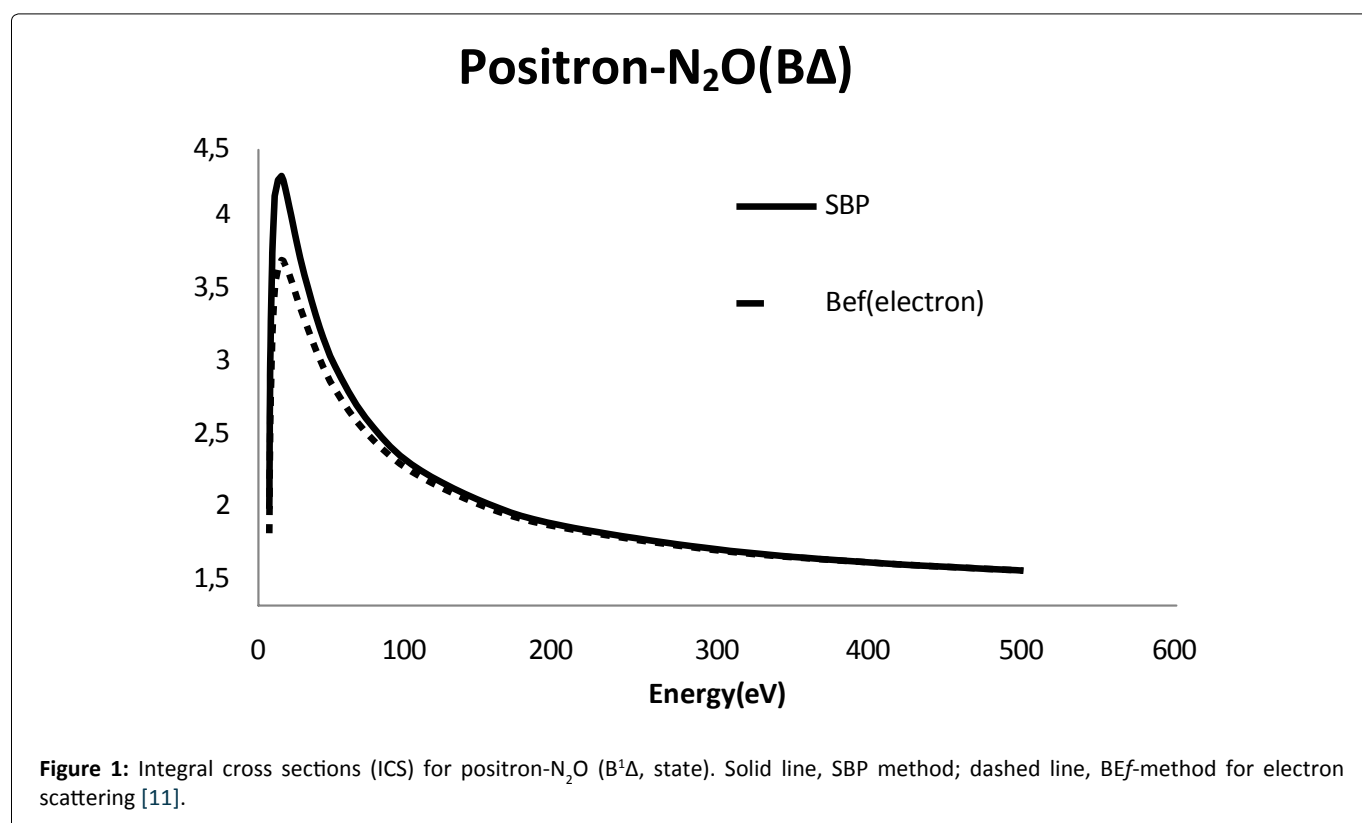
$$E_{ps} = B - 6.8\,eV \qquad (4)$$

where B is the binding energy of the electron of target. Finally, the f (E) factor reduces the FBA at low energies while keeping the validity of the Born approximation at high energies and the SBP method has the effect of correcting the FBA.

Computational Aspects and Results

Following Arretche, et al. [3] the experimental equilibrium geometry of the ground state R$_{(N-N)}$ = 2.127 a$_o$ and R$_{(N-O)}$ = 2.242 a$_o$ is here used. The basis set used (9s5p/4s3p) is the same investigated by Arretche, et al. [3] using the SMC method for elastic positron-N$_2$O scattering [3]. This basis set given a ground state value of -183.727 a.u and a dipole moment of 0.6531D computed using the GAMESS code as in Ref. [3]. Table 1 shows vertical excitation energies compared to experimental data. The appropriated $f_{accur}(f_{Born})$ values to use in the SBP method were deduced from the GOS [10] and the positronium eneqy value is 6.1 eV.

In Figure 1 we report cross sections for the B^{1}Δ state using the SBP method. Also included in Figure 1, for purposes

Positron-N$_2$O(BΔ)

Figure 1: Integral cross sections (ICS) for positron-N$_2$O (B^{1}Δ, state). Solid line, SBP method; dashed line, BEf-method for electron scattering [11].

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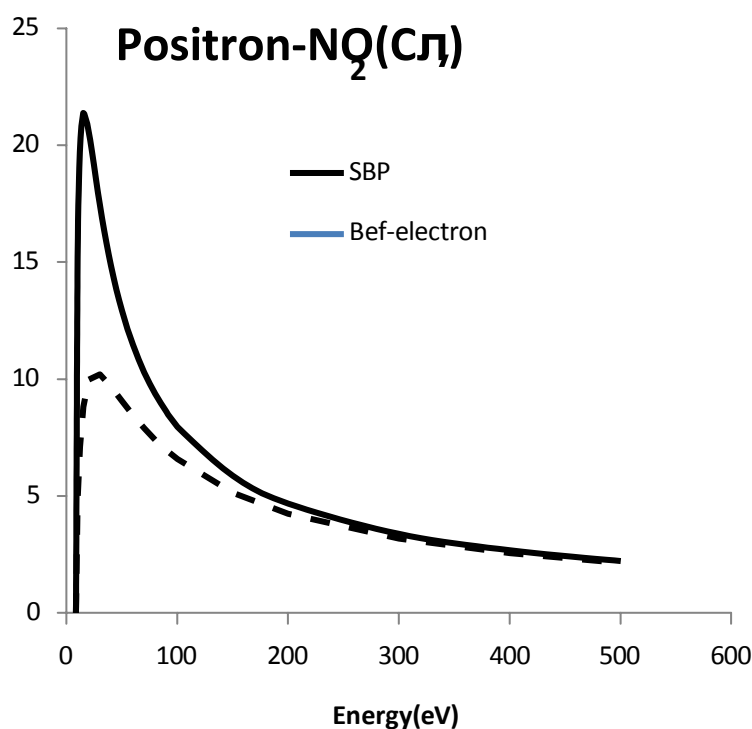
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Figure 2: Integral cross sections (ICS) for positron-N$_2$O (C$^1\Pi$, state). Solid line, SBP method; dashed line, BE*f*-method for electron scattering [11].

Table 1: Vertical excitation energies for N$_2$O molecule in electron volts (eV).

Molecule (state)	E$_{exc}$(eV)	Expt. [10]
N$_2$O (B$^1\Delta$)	6.80	
N$_2$O (C$^1\pi$)	8.50	8.51
N$_2$O (D$^1\sum^+$)	9.50	9.60

Table 2: ICS (10^{-18} cm^2) for the B$^1\Delta$, C$^1\pi$, and D$^1\sum^+$ electronic state using SBP method.

E(eV)	SBP (B$^1\Delta$)	SBP (C$^1\pi$)	SBP (D$^1\sum^+$)
8.5	0.0	0.0	0.0
10	2.98	6.19	7.31
12	3.19	8.90	21.72
15	3.41	10.84	35.22
20	3.27	11.92	47.96
30	2.82	11.75	57.65
40	2.43	10.89	59.41
50	2.13	10.01	58.47
70	1.71	8.52	54.29
100	1.32	6.95	47.73
150	0.96	5.35	39.34
200	0.76	4.37	33.51
300	0.54	3.23	26.00
400	0.42	2.59	21.52
500	0.34	2.16	18.41
600	0.29	1.88	16.16

of comparison only, the called BE*f*-method for electron scattering case. As observed in Figure 1, at low energies the cross-section for positron scattering is larger when compared with electron case using the BE*f*-method. Is interesting to point out that a similar behavior between the cross sections can be observed, *i.e.*, the SBP method not only increase the cross sections magnitude at low energies but also shifts the peak to higher energy. As observed also in Figure 1 at higher energies cross sections for positrons and electrons are very similar. As a first analysis Figure 1 shows a behavior expected.

In Figure 2 we report integral cross-sections for the C$^1\pi$ state using the SBP method. For clarity our results, we choose to compare again the BE*f*-method [11] used for electron- N$_2$O scattering. This scenario is specially important since it can define the quality and validity of the FBA used (BE*f*-method also close for FBA at higher energies) and as observed at low energies the SBP cross sections is larger when compared with electron case. Examination of Figure 1 and Figure 2 indicates that, cross sections for the B$^1\Delta$, and C$^1\Pi$ states are very different in magnitude but with shape similar. As cited in Figure 1 at higher energies cross sections for positrons and electrons are also very similar.

In Figure 3 we report cross sections for the C$^1\pi$ state and in the absence of experimental data the SBP method is compared with experimental data for electron case and again the BE*f*-method [11]. First, at low energies the SBP method shows cross sections with different magnitude when compared with experimental data for electron case. In fact, is seem from this figure that there is a significant difference between the SBP
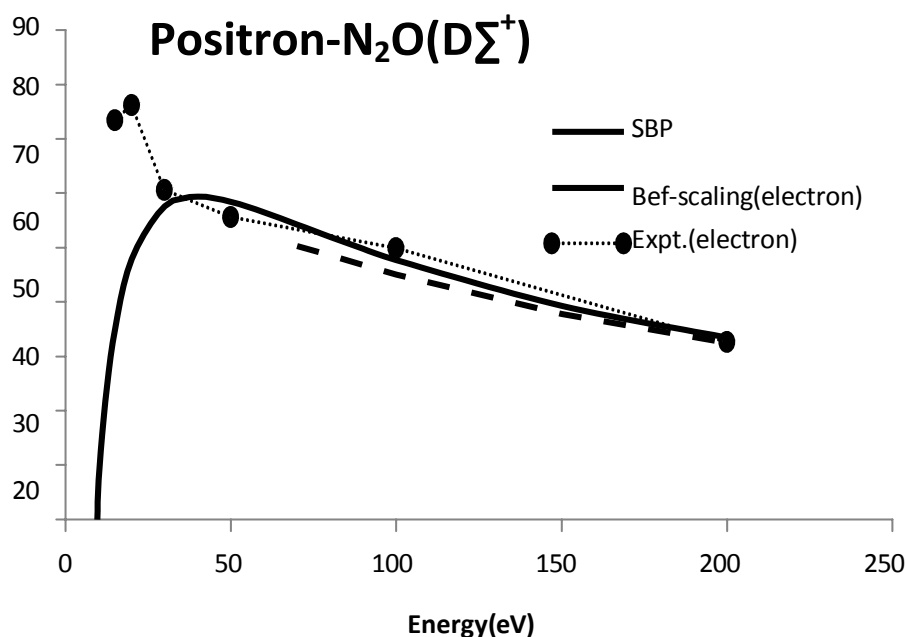
Figure 3: Integral cross-sections (ICS) for positron-N$_2$O (^{1}DΣ^+, state). Solid line, SBP method; dashed line, BEf-method for electron [11]; black circle, experimental data for electron [10].

Figure 4: Integral cross-sections (ICS) for positron-N$_2$O (^{1}DΣ^+,state). Solid line, SBP method; dashed line, BEf-method for electron [11]; black circle, experimental data for electron [10].
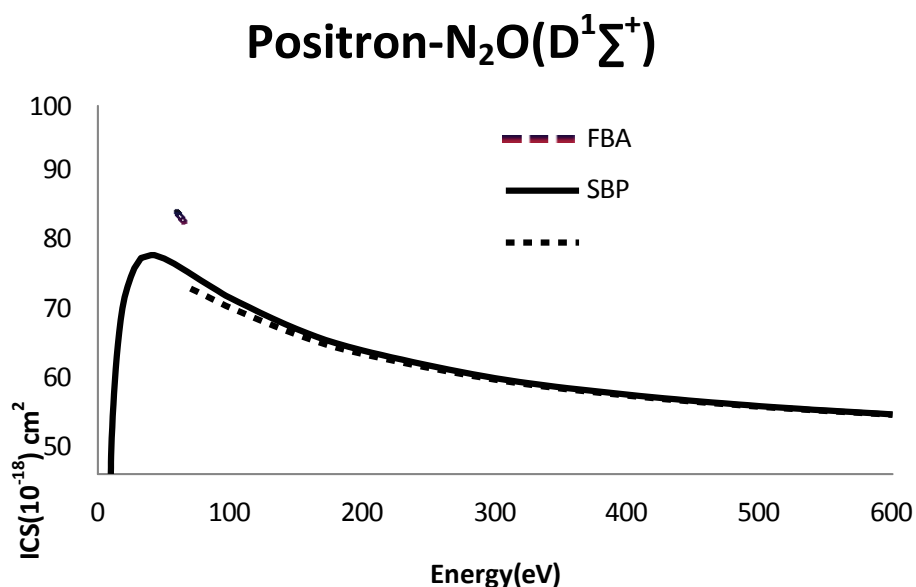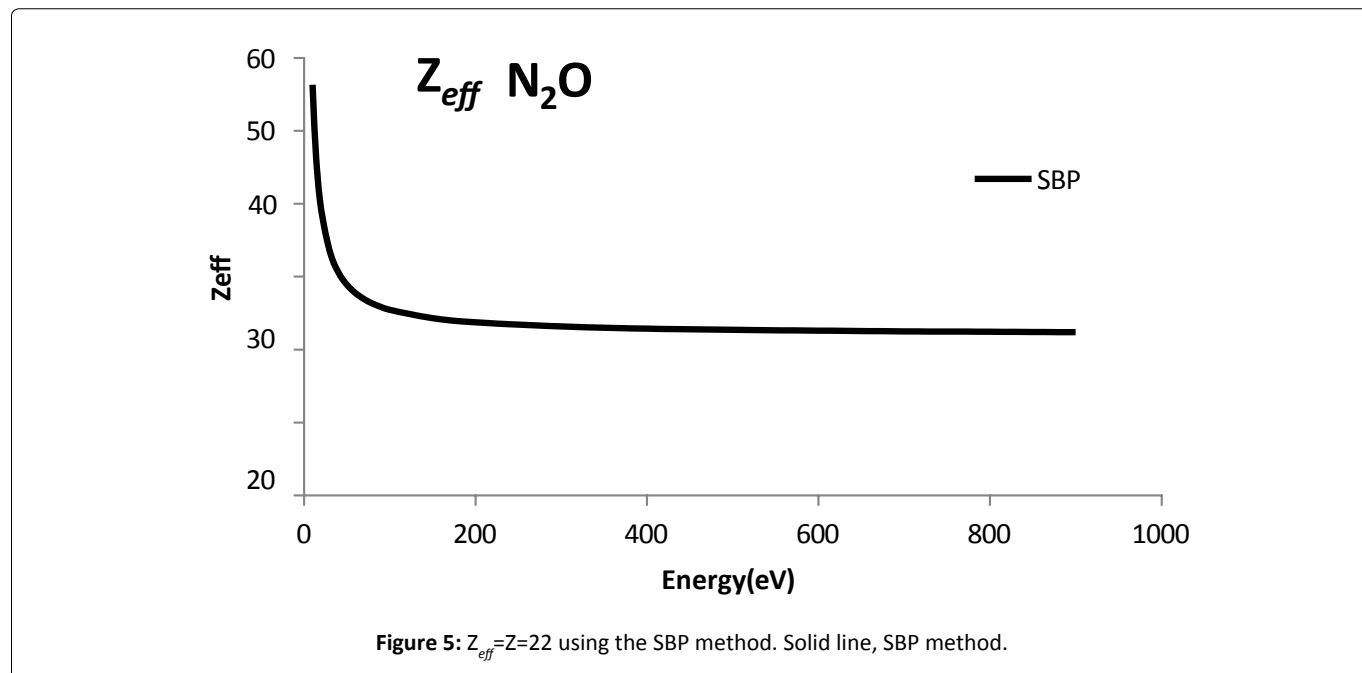
method and experimental data for electron scattering case at low energies (is expect that the positron inelastic cross-section to be larger in magnitude than the corresponding electron inelastic cross-section). It is interesting to point that a similar behavior was observed by Arretche, et al. [3] for the elastic positron-N$_2$O scattering cross-section and reason for this behavior remains as a problem to be better understood. The present study suggests that further development of the current scattering models is needed.

In Figure 4 were port integral cross-sections for the ^{1}DΣ^+

state using the SBP method now in the10-600 eV incident energy range. The results are compared with the BEf-method [11] and the traditional FBA. As observed in Figure 4 the SBP method and BEf method closed with the FBA at higher energies (as expected). The good agreement with the FBA at higher energies is the aspect that basically determines the level of numerical convergence.

In the Table 2 integral crosssections for B$^1\Delta$, C$^1\pi$, and D$^1\Sigma^+$ electronic state using the SBP method are listed for future reference.

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Figure 5: Z_{eff}=Z=22 using the SBP method. Solid line, SBP method.

Finally, a convenient way of dealing also with convergence aspects of SBP method is the analysis of the annihilation Z_{eff} parameter classical, which is traditionally written as

$$Z_{eff} = \int \sum_{i=1}^{z} \delta(r - r_i)\left|\psi(r_1, \ldots, r_z, r)\right|^2 d\,r_1 \ldots dr_z, dr \tag{5}$$

The Eq.(5) represent the effective number of electrons that contribute to the annihilation process, and $\psi(r_1,\ldots,r_z,r)$ is the total wave function of the Z electron and one positron coordinates [7]. If substitutes the asymptotic, plane wave function into equation (5), one obtains Z_{eff} = Z. We have noted that the SBP method can determine the Z_{eff} = Z classical based on the Born approximation, i.e., the $Z_{eff}^{(SBP)}$ represent also a criteria to check the quality of SBP method. The accuracy of the Z_{eff} Born approximation can be given by eq(6) (Figure 5)

$$Z_{eff}^{(SBP)} = \left[\left(\sigma_{Born}/\sigma_{SBP}\right)\right].Z \tag{6}$$

Conclusion

We have discussed a recently developed method for investigate inelastic positron-target scattering. The scaled Born positron (SBP) method improved was tested to electronic excitation of N$_2$O (B$^1\Delta$, C$^1\pi$ and D$^1\Sigma^+$ state) with cross sections substantially, in principle, adequate when compared with electron case (as far as we know, this is the first time that cross-sections are reported using the SBP method). Calculated cross-sections using the SBP method agree well with electron case at higher energies. On the other hand, the not expected behavior between our results and experimental data at small energies when of electron incident still remains as a problem to be better understood (similar effect may be observed also in the elastic case). In order to check the numerical convergence of the SBP method the Z_{eff} classical (Z parameter) was appropriately obtained, giving confidence that the SBP method is significant for positron-N$_2$O scattering.

As observed the literature for inelastic positron-N$_2$O molecule is less clear, and however new results are welcome.

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