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Recommended Collision Integrals for Transport Property Computations Part 2: Mars and Venus Entries

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A review of the best-available data for calculating a complete set of binary collision integrals for the computation of the mixture transport properties (viscosity, thermal conductivity, ordinary and thermal diffusion) of 17-species weakly ionized CO_2–N_2 mixtures is presented. The fidelity of the data varies considerably, but most of the atom–atom interactions are derived from ab initio methods that are estimated to be accurate to within 5%. The remaining important interactions between neutral species are estimated to be accurate to within about 30% over the temperature range of interest (300–20,000 K) to Mars and Venus reentry plasmas. Collision integrals for important ion–neutral interactions are computed using a modified Tang–Toennies potential and have an estimated accuracy of ±25%, whereas those between trace species are approximated via the polarization (Langevin) potential model. The accuracy and valid temperature range for electron–neutral interactions vary considerably due to scarcity of the required cross section data.

Nomenclature

A^*, B^*, C^* = nondimensional collision integral ratios
C_6 = dispersion coefficient, e^2Å^5
E = interaction energy
e = electron charge, 4.803×10^{-10} esu
T = temperature, K
α = dipole polarizability, Å^3
α_q = quadrupole polarizability, Å^5
α = Buckingham potential parameter
θ = scattering angle, deg
σ = cross section, Å^2
$\Omega^{1,1}$ = diffusion collision integral, Å^2
$\Omega^{2,2}$ = viscosity collision integral, Å^2

Subscripts

elas = elastic
ex = exchange
m = momentum transfer
v = viscosity

I. Introduction

ACCURATE modeling of the transport properties of weakly ionized gases is important in several fields, including the aerothermodynamics of entering spacecraft and the study of laboratory plasmas. To compute the transport properties of a gas mixture, collision data are needed as a function of temperature for all binary interactions that occur in the gas. For weakly ionized CO_2–N_2 mixtures such as would be encountered during entries of Mars or Venus, the gas can be described with 17 chemical species: CO_2, N_2, N_2^+, O_2, CO, CO^+, NO, NO^+, CN, CN^+, C, C^+, N, N^+, O, O^+, and e^-, which leads to a total of 153 possible binary interactions. There are also several additional trace species, including NCO, C_2, and Ar, which are included in some Mars atmosphere kinetic models [1]. However, interactions involving these species will have very little impact on mixture transport properties. Therefore, required collision data for these binary interactions can be taken from the Lennard–Jones potential model without appreciable loss of fidelity.

According to Chapman–Enskog theory [2], the transport properties of a dilute gas mixture can be computed to first-order accuracy with the knowledge of just three binary interaction parameters: the diffusion collision integral $\Omega^{1,1}$, the viscosity collision integral $\Omega^{2,2}$, and the dimensionless collision integral ratio $B^* = (5\Omega^{1,2} - 4\Omega^{1,3})/\Omega^{1,1}$. One additional quantity, $C^* = \Omega^{1,2}/\Omega^{1,1}$, is necessary to evaluate the second term of the expansion as required to compute thermal diffusion coefficients. Higher-order terms of the expansion, which may be required for accurate computations of the electron thermal conductivity and diffusion in a partially ionized gas, introduce additional collision integral ratios. These collision integrals, if required, can be computed by a straightforward extension of the data presented in this article.

Uncertainty in the collision integrals employed has a first-order impact on the uncertainties in the resulting mixture transport properties. In a single species gas, the uncertainties in viscosity and translational thermal conductivity are directly proportional to the uncertainty in $\Omega^{2,2}$, whereas the uncertainties in species diffusion and internal energy thermal conductivity are directly proportional to the uncertainty in $\Omega^{1,1}$. For a gas mixture the relationship between the uncertainty in input collision integrals and mixture transport properties is more complex, and depends on the relative importance of each binary interaction in the gas mixture.

A previous paper [3] reviewed the collision integrals necessary for computing the transport properties of weakly ionized air. No similar comprehensive review for Mars and Venus atmosphere transport property calculations currently exists, although Magin et al. [4] have looked at collision integrals for a weakly ionized pure CO_2 gas mixture. In their work most interactions were modeled using a mix of exponential repulsion (Born–Meyer) potentials for high temperatures and $m, 6$ (generalized Lennard–Jones) potentials at low temperatures. In addition, Riabov [5] has published approximate values for many of the relevant collision integrals in the dissociation regime, based primarily on exponential repulsion potentials obtained from various experimental sources. Finally, the Earth entry review of Park et al. [6] included collision integral data for some carbonaceous ablation product interactions with air species. However, Park's data were primarily based on the Lennard–Jones potential model, which is inappropriate for high temperatures. Also, none of these reviews account for recent high-fidelity computations of key neutral–neutral

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and ion–neutral interactions, as well as collision data for electron–neutral interactions. In addition, none of the previous CO_2 reviews adequately address the accuracy of the collision integrals selected.

The purpose of the current paper is to collect in a single place the best-available published collision integral data, including estimated uncertainties, at temperatures of interest for weakly ionized CO_2–N_2 plasmas (approximately 300–20,000 K). The data presented can be readily fit to an appropriate expression [7,8] for use in existing codes. Data are presented here for ground state species interactions only, which is appropriate for the conditions of interest in most reentry problems. Transport properties for low-lying excited states of carbon atoms have been presented by Biolsi and Biolsi [9], whereas Capitelli et al. have looked at the impact of electronically excited states on the transport properties of local thermodynamic equilibrium hydrogen plasmas [10], oxygen atoms [11], and the interaction between carbon and oxygen atoms [12]. This work could be adapted for other problems of interest if required.

II. Results

A. Neutral–Neutral Interactions

Of the 45 possible interactions between two neutral atomic or molecular species for Mars entries, 15 were reviewed in a previous article on air species [3]; these data are still current and will not be repeated here. Two of the remaining 30 interactions, C–C and C–N, have been recently evaluated via high-fidelity ab initio calculations from quantum mechanical potential energy surfaces that include extensive comparisons to previous theoretical and experimental results [13]. The estimated accuracy of these computations is approximately ±5% over the temperature range 300–20,000 K. However, it should be noted that Stallcop et al. [13] considered only those states of C_2 and CN that dissociate to ground state atoms in their analysis: the transport properties of excited state atoms were not considered. See [9] for a preliminary discussion of the transport properties of excited carbon atoms.

For the CO_2–N interaction, we use the intermolecular potential computed by Amaee and Brown [14], as recommended in the compilation of Murphy [15]. These data were based on median-averaged quantum mechanical ab initio fourth-order Møller–Plesset (MP4) calculations, fit to Buckingham exponential α:6 potentials. Although Amaee and Brown [14] do not give their estimated uncertainty for this interaction, the accuracy of their results can be crudely estimated by comparing their results for the O_2–O interaction to the ab initio computations of Stallcop et al. [16], that have an estimated uncertainty of ±10% [3]. The potentials computed by Amaee and Brown [14] for CO_2–N were extended using scaled Buckingham fits for intermolecular distances smaller than 1.2 Å and larger than 5.2 Å. The O_2–O $\Omega^{1,1}$ collision integrals based on the ab initio potential results were within 10% of the values computed by Stallcop et al. [16], as shown in Fig. 1. However, the Buckingham fit gives values that differ by as much as 15% at higher temperatures, because the Buckingham fit was tailored to match the potential well minimum and is less accurate in the short range repulsive wall region [14]. Given these results, as well as the fact that CO_2–N is a four-atom system, we estimate an accuracy of ±25% for the resulting CO_2–N collision integral.

An intermolecular potential was also calculated in Amaee and Brown [14] for the CO–N interaction based on median-averaged MP4 calculations at interaction angles of 60 and 120 deg. However, analysis of these data indicated that the averaged potential was strongly influenced by a localized resonance at an interaction angle of 60 deg. Therefore, collision integrals for this interaction are computed for this work based on new ab initio potential energy surface calculations using the same methodology employed in [16]. Calculations are performed with MOLPRO using the augmented core Valence Triple Zeta (aug-cc-VTZ) basis [17,18] at the two "magic" interaction angles [16] of 54.74 and 125.3 deg over a range of intermolecular distances between 1.4 and 5.0 Å. The CO bond length is fixed at 1.13085 Å, which is the approximate value of the average bond length in the ground vibrational state. This is computed as $r_e\sqrt{B_e/B_o}$ with molecular constants taken from Huber and Hertzberg [19]. For CO–N, we use the spin-restricted coupled cluster single discharge [RCCSD(T)] method from orbitals determined using the restricted open-shell Hartree–Fock (ROHF) method. Energies for CO–N are computed on the quartet A'' potential energy surface, which is the only surface involving ground state species for this interaction. The approximate one-dimensional potential energy surface was taken as the average of the data at 54.74 and 125.3 deg, and was extended at both long and short range using a scaled Buckingham potential. Transport cross sections and the resulting collision integrals were then computed with the SKATR code [13]. The resulting collision integrals have an estimated accuracy of ±20%, based on prior ab initio computations of the N_2–N and O_2–O interactions [16]. Figure 2 compares the results of the current computations with the collision integrals computed from Amaee and Brown [14], as well as those based on an exponential repulsion potential of Riabov [5]. The current data include the assumed ±20% error bars. As expected the current results are in excellent agreement with the exponential repulsion potentials of Riabov at high temperature, which should be accurate in the limit of large interaction energy. At lower temperatures the agreement is still quite good, with a maximum difference between the two results of 10% at about 4000 K. In contrast, the results of Amaee and Brown [14] differ from the current computations at all temperatures, by as much as a factor of 2 at the higher temperatures. The effects of the overemphasized resonance can be clearly seen in the Amaee and Brown data, resulting in a nonmonotonic decrease of the computed collision integral with temperature.

Where such ab initio calculations are not available, alternate sources are used. For example, Bzowski et al. [20] developed a universal collision integral concept and applied it to binary mixtures of diatomic, polyatomic, and noble gases. The binary interaction constants for each pair were chosen to best match the available experimental and theoretical data for the interaction over a wide temperature range. This method was shown to be in good agreement (within ±15%) with existing pure-species experimental and ab initio data [3,20], although the error should be somewhat larger for interactions between different species due to the somewhat empirical nature of the mixing rules employed. The Bzowski et al. [20]

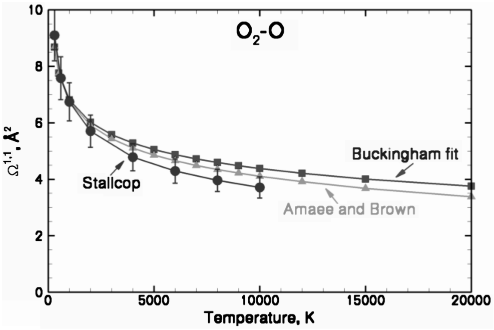

Fig. 1 Comparison of $\Omega^{1,1}$ for O_2–O interactions calculated by various methods.

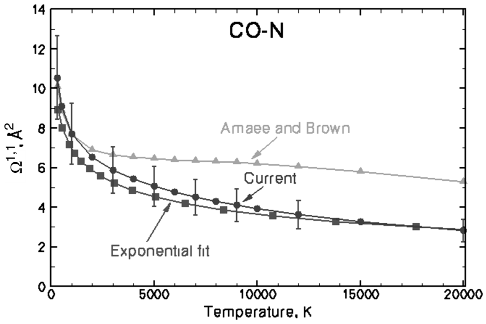

Fig. 2 Comparison of $\Omega^{1,1}$ for CO–N interactions calculated by various methods.

universal collision integrals are used here for the nine binary interactions of CO_2 and CO with each other as well as N_2, O_2, and NO.

For interactions between C and O atoms, we use the tabulations of Capitelli and Ficocelli [12], who computed collision integrals for both ground state and low-lying excited state interactions of these atomic species in the temperature range 2000–20,000 K, based on Morse or exponential repulsion potentials fit to each of the potential energy surfaces. For ground state $C(^3P)$–$O(^3P)$ interactions a total of 18 bound and repulsive states were considered. Interactions involving excited state C or O atoms were not considered in the present paper. The accuracy of the resulting collision integrals is not given in Capitelli and Ficocelli but have an estimated uncertainty of ±25% based on similar analysis of other atom–atom systems as compared to quantum mechanical results. Collision integrals at temperatures below 2000 K were taken from the formula of Bade and Yos [21], discussed in the following paragraph.

For neutral–neutral interactions between dissimilar species for which no high-fidelity data exist, Bade and Yos [21] proposed a simple combining rule, given by

$$\Omega_{A\text{–}B} = \frac{1}{4}\left(\sqrt{\Omega_{A\text{–}A}} + \sqrt{\Omega_{B\text{–}B}}\right)^2 \tag{1}$$

where A and B are generic chemical species (atoms or molecules). Using this expression, the collision integrals of a dissimilar (A–B) interaction are computed from the known values for the two like species (A–A and B–B) interactions. The accuracy of Eq. (1) is best evaluated by direct comparison to available reference ab initio data. Figure 3 shows the error in the $\Omega^{1,1}$ collision integrals computed using Eq. (1) for two atom–atom interactions (C–N and N–O), one atom–molecule interaction (N_2–N), and one molecule–molecule interaction (N_2–H_2). In each case high-fidelity ab initio data are used for the two required same-species interactions [13,16,22,23]. The error in Fig. 3 is defined as the percentage difference between the collision integrals computing using Eq. (1) vs the collision integrals obtained directly from ab initio calculations of the A–B interaction. The maximum error for any of the interactions shown in Fig. 3 is less than 15%. Results for $\Omega^{2,2}$ (not shown) are nearly identical. From the figure we see that Eq. (1), although empirical in nature, is remarkably accurate for a variety of dissimilar interactions. Based on this result, we compute collision integrals for the C–N_2 and low-temperature (below 2000 K) C–O interactions using Eq. (1) and available ab initio data for C–C [13], O–O [22], and N_2–N_2 [16]. The estimated uncertainty in the resulting collision integrals is ±25%.

For the remainder of the neutral–neutral interactions, we rely on the reviews of Riabov [5] and Magin et al. [4] First, Riabov [5] published a review of transport properties for Earth and Mars dissociating gases in which the necessary collision integrals were computed based on Born–Meyer exponential repulsion potentials from experimental sources [24,25] and prior surveys [26,27]. For those interactions for which no experimental data existed, potential parameters were approximated by Riabov using the additive potential method of Amdur et al. [28] Later, Magin et al. [4] revised the data for dissociated CO_2 mixtures based on the data of Leonas [29]. The necessary collision integrals for the 14 remaining neutral–neutral interactions are computed from the exponential repulsion potential parameters of Magin et al. [4] and Riabov [5,26] using the collision integral tables given by Monchick [30]. In all cases the collision integrals computed using the newer Magin et al. data are within 10% of those computed using the data of Riabov. Unfortunately, none of these references provide an estimate of the accuracy of their data. However, most of the interactions were approximated from experimental beam data using additive potentials in a manner analogous to that used by Cubley and Mason [31] for air species. Because the data of [5] for air species interactions correlate well with those of Cubley and Mason, it is reasonable to assume that the resulting accuracy is similar. Based on the comparisons between Cubley and Mason data [31] and ab initio calculations presented in [3], we estimate the accuracy of the collision integrals computed based on data from [4,5] to be ±30%. It should be noted that the exponential repulsion potential is not realistic at low temperatures (below approximately 2000 K), because it neglects long range dispersion forces in the interaction potential. However, all of the interactions that are represented in this work using exponential repulsion data are between species that are only present in significant quantities in the high-temperature region behind the shock layer, and therefore the accuracy of the fit at low temperature is not critical.

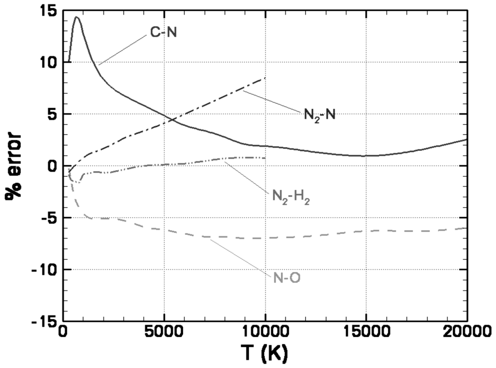

Fig. 3 Comparison of the Bade–Yos mixing rule [21] with the results of ab initio calculations.

Tables 1 and 2 show the recommended values for the collision integrals $\Omega^{1,1}$ and $\Omega^{2,2}$ for all 30 neutral–neutral interactions, as well as an estimate of the accuracy (Acc.) of these data over the temperature range 300–20,000 K. The final column of the tables lists the references (Ref.) used to determine their values. Values are not given for all interactions at all temperatures; this is because for some of the interactions the data were published at discrete temperatures, and the temperatures reported differ between the references. The dimensionless collision integral ratios B^* and C^* are only weak functions of temperature. Therefore, a constant value of $B^* = 1.15$ and $C^* = 0.92$ can be used to represent all neutral–neutral interactions to within 10% accuracy, which is sufficient for reentry aeroheating applications.

B. Ion–Neutral Interactions

A total of 63 possible interactions can occur between an ion and a neutral species. Twenty of these occur between air species and were previously computed in [32]. Fortunately, many of the remaining 43 interactions occur between trace species (including all ion interactions with CO_2 and CN as well as neutral interactions with CO^+ and CN^+), and thus will have minimal impact on computed mixture transport properties. Therefore, collision integrals based on the polarization (Langevin) potential will be sufficient for these interactions [33]. The diffusion collision integral resulting from integration of the polarization potential is a function only of the dipole polarizability of the neutral species and the temperature, and is given by [33]

$$\Omega^{1,1} = 425.4\left(\frac{\alpha}{T}\right)^{\frac{1}{2}} \tag{2}$$

Table 3 lists the value of α for all neutral species in the mixture. The ratio of the viscosity and diffusion collision integrals is assumed to be constant, given by

$$\Omega^{2,2} = 1.1\Omega^{1,1} \tag{3}$$

A constant ratio of 1.1 was used in Eq. (3) rather than the value of 0.87 recommended by Capitelli et al. [33], based on a comparison of the computed collision integral ratio $A^* = \Omega^{2,2}/\Omega^{1,1}$ for several ion–neutral interactions with accurately determined collision integrals for atom–atom and atom–molecule interactions [32], as shown in Fig. 4. Although the results of [32] show that collision integrals computed via this method can be a reasonable approximation (within ±30%) for many interactions, Capitelli [40] has demonstrated that using the polarizability potential can result in a significant overprediction of the collision integrals for some ion–neutral systems, particularly at

Table 1 Diffusion collision integral $\Omega^{1,1}$ (Å^2) as a function of temperature for neutral–neutral, ion–neutral, and electron–neutral interactions

	T, K												Acc.	Ref.
	300	500	600	1000	2000	4000	5000	6000	8000	10,000	15,000	20,000		
CO_2–CO_2	17.35	14.39	13.66	12.12	10.66	9.47	9.13	8.86	8.44	8.12	7.54	7.15	20%	20
CO_2–N_2	14.17	12.36	11.88	10.77	9.52	8.25	7.86	7.54	7.05	6.68	6.04	5.60	20%	20
CO_2–O_2	13.68	11.84	11.36	10.27	9.08	7.97	7.64	7.38	6.98	6.69	6.17	5.82	20%	20
CO_2–CO	14.18	12.36	11.88	10.77	9.52	8.26	7.86	7.54	7.05	6.68	6.04	5.60	20%	20
CO_2–NO	14.03	12.11	11.62	10.49	9.28	8.04	7.67	7.37	6.93	6.61	6.04	5.66	20%	20
CO_2–CN	——	12.41	11.99	10.96	9.59	8.34	7.95	7.65	7.17	6.82	6.19	5.77	30%	5
CO_2–C	——	10.84	10.50	9.52	8.22	7.08	6.72	6.41	6.00	5.67	5.10	4.71	30%	4
CO_2–N	12.00	10.33	——	8.87	7.80	6.89	6.61	6.40	6.05	5.79	5.34	5.02	25%	14
CO_2–O	——	9.15	8.88	8.12	7.11	6.19	5.91	5.68	5.34	5.09	4.62	4.33	30%	4
N_2–CO	14.17	12.36	11.88	10.77	9.52	8.25	7.86	7.54	7.05	6.68	6.04	5.60	20%	20
N_2–CN	——	10.90	10.43	9.29	7.81	6.47	6.07	5.75	5.26	4.90	4.27	3.86	30%	5
N_2–C	12.28	——	10.28	9.22	7.85	6.64	——	5.96	5.47	5.07	——	——	25%	——
O_2–CO	11.60	10.37	10.02	9.15	7.96	6.76	6.40	6.12	5.69	5.36	4.80	4.42	20%	20
O_2–CN	——	9.90	9.56	8.62	7.49	6.44	6.11	5.85	5.45	5.16	4.64	4.29	30%	5
O_2–C	——	8.33	8.01	7.21	6.222	5.26	4.97	4.74	4.40	4.15	3.70	3.40	30%	4
CO–CO	12.12	10.90	10.54	9.63	8.41	7.09	6.67	6.33	5.81	5.42	4.74	4.29	20%	20
CO–NO	11.88	10.60	10.24	9.35	8.12	6.82	6.40	6.12	5.66	5.31	4.71	4.30	20%	20
CO–CN	——	10.07	9.74	8.73	7.55	6.44	6.10	5.83	5.41	5.10	4.56	——	30%	5
CO–C	——	9.01	8.62	7.72	6.57	5.51	5.19	4.94	4.55	4.27	3.77	——	30%	4
CO–N	10.54	9.09	——	7.69	6.53	5.43	5.06	4.76	4.29	3.92	3.26	2.82	20%	——
CO–O	——	7.40	7.11	6.37	5.42	4.55	4.29	4.09	3.77	3.53	3.12	2.85	30%	4
NO–CN	——	10.31	9.91	8.94	7.64	6.47	6.11	5.82	5.39	5.06	4.50	4.12	30%	5
NO–C	——	7.97	7.65	6.86	5.82	4.87	4.58	4.35	4.00	3.74	3.29	3.00	30%	5
CN–CN	——	10.67	10.24	9.19	7.79	6.52	6.13	5.83	5.36	5.01	4.41	4.01	30%	5
CN–C	——	8.25	7.90	7.03	5.91	4.88	4.58	4.34	3.97	3.69	3.21	2.90	30%	5
CN–N	——	8.68	8.30	7.29	6.02	4.87	4.53	4.26	3.85	3.54	3.02	2.68	30%	5
CN–O	——	7.79	7.50	6.69	5.72	4.82	4.55	4.33	4.00	3.75	3.32	3.03	30%	5
C–C	12.34	10.50	9.96	8.66	7.14	5.84	5.43	5.11	4.59	4.17	3.40	2.86	5%	13
C–N	9.17	7.65	7.25	6.43	5.63	4.81	4.54	4.33	3.98	3.69	3.13	2.72	5%	13
C–O	10.35	8.82	——	——	6.49	5.29	——	4.56	4.08	3.70	3.02	2.66	25%	12
C–N^+	29.88	21.86	——	13.82	9.25	6.97	6.50	6.19	5.76	5.47	5.02	——	25%	——
C–O^+	29.77	21.90	——	13.70	8.86	6.45	5.96	5.64	5.20	4.91	4.46	——	25%	——
C–C^+	52.37	46.62	——	40.92	36.78	33.50	32.58	31.86	30.79	29.99	28.63	27.70	30%	42
O_2–C^+	28.30	20.70	——	13.17	9.03	6.96	6.52	6.22	5.80	5.51	5.04	4.73	25%	——
CO–N^+	32.39	23.64	——	14.65	9.46	6.88	6.36	6.00	5.53	5.21	4.70	——	25%	——
CO–O^+	32.38	23.79	——	14.62	9.15	6.42	5.88	5.52	5.03	4.71	4.21	——	25%	——
CO–C^+	31.97	23.48	——	14.82	9.89	7.42	6.91	6.56	6.09	5.76	5.24	——	25%	——
CO–CO^+	40.94	34.48	——	28.47	24.62	22.20	21.61	21.16	20.59	20.23	19.90	——	40%	15
N–C^+	22.94	16.66	——	10..98	8.04	6.54	6.21	5.98	5.65	5.41	5.02	——	25%	——
O–C^+	19.40	13.87	——	9.30	7.03	6.25	5.54	5.34	5.04	4.82	4.46	——	25%	——
CN–CN^+	41.30	34.75	——	28.63	24.71	22.25	21.65	21.20	20.62	20.25	19.92	——	50%	——
e–CO_2	——	——	——	9.61	4.59	2.20	1.83	1.65	1.51	1.48	1.57	1.71	30%	47, 49
e–CO	——	——	——	3.45	4.63	6.30	6.71	6.86	6.68	6.23	5.14	4.39	30%	51, 52
e–CN	——	——	——	3.45	4.63	6.30	6.71	6.86	6.68	6.23	5.14	4.39	50%	——
e–C	——	——	——	——	8.24	6.44	5.63	5.03	4.28	3.87	3.40	——	30%	53

high temperatures. Therefore, we conservatively estimate an average uncertainty of ±40% for collision integrals computed via this method.

Interactions involving C and CO with the atomic ions (C^+, N^+, and O^+) as well as O_2, O, and N with C^+ are computed at a higher fidelity for this work. These interactions are calculated by assuming a modified Tang–Toennies interaction potential [41], in which the long range form is governed by polarization and (to a lesser extent) dispersion forces whereas the short range form is effectively an exponential repulsion. This methodology, discussed in detail in [32], requires knowledge of five constants for each binary interaction: the dipole polarizability and dispersion coefficient (C_6) of the neutral and ion species, and the quadrupole polarizability (α_q) of the neutral. The required constants and their sources are given in Table 3. Collision integrals computed using this methodology were previously found to agree to within 20% with more accurate ab initio data for the N–O^+ and O–N^+ interactions, as well as viscosity collision integral data for the resonant interactions N–N^+ and O–O^+ [32].

Finally, for interactions between an ion and its parent neutral (C–C^+, CO–CO^+, and CN–CN^+), resonant charge transfer can significantly increase the size of the momentum transfer cross section, which directly affects the diffusion collision integral $\Omega^{1,1}$ [42]. Following the work of Murphy [15], we combine the charge-exchange and elastic (polarization) contributions to the diffusion collision integrals for all interactions between and atom or molecule and its ion using the empirical mixing rule

$$\Omega^{1,1} = \sqrt{\left[\Omega_{\mathrm{ex}}^{1,1}\right]^2 + \left[\Omega_{\mathrm{elas}}^{1,1}\right]^2} \tag{4}$$

where $\Omega_{\mathrm{ex}}^{1,1}$ is the collision integral computed by integrating twice the resonant charge-exchange cross section [42] and $\Omega_{\mathrm{elas}}^{1,1}$ is the standard elastic collision integral. As a check on the resulting collision integrals, the value of $\Omega^{1,1}$ should approach the polarization limit at sufficiently low temperature [42].

Charge-exchange cross sections for the C–C^+ interaction are taken from [43]. Resonance charge transfer cross sections for the CO–CO^+ interaction are taken from [15]. Charge-exchange cross sections for CN–CN^+ were not available in the literature. Therefore, diffusion collision integrals for the CN–CN^+ interaction are computed assuming that the charge-exchange portion is identical to that for the CO–CO^+ interaction. Given the relative lack of data we estimate an uncertainty of ±40% for these interactions. The viscosity collision integral ($\Omega^{2,2}$) is unaffected by charge transfer due to symmetry considerations [42], and is computed using Eqs. (2) and

Table 2 Viscosity collision integral $\Omega^{2,2}$ (Å^2) as a function of temperature for neutral–neutral, ion–neutral, and electron–neutral interactions

	T, K												Acc.	Ref.
	300	500	600	1000	2000	4000	5000	6000	8000	10,000	15,000	20,000		
CO_2–CO_2	20.35	16.45	15.50	13.58	11.92	10.69	10.32	10.02	9.57	9.21	8.59	8.15	20%	20
CO_2–N_2	16.24	13.91	13.32	12.03	10.74	9.49	9.08	8.74	8.20	7.79	7.06	6.56	20%	20
CO_2–O_2	15.74	13.35	12.76	11.47	10.23	9.15	8.80	8.53	8.10	7.77	7.19	6.79	20%	20
CO_2–CO	16.24	13.92	13.32	12.03	10.74	9.50	9.08	8.74	8.21	7.79	7.07	6.56	20%	20
CO_2–NO	16.16	13.68	13.05	11.72	10.44	9.30	8.92	8.62	8.14	7.78	7.13	6.68	20%	20
CO_2–CN	——	14.22	13.76	12.64	11.14	9.77	9.33	8.99	8.47	8.07	7.37	6.89	30%	5
CO_2–C	——	12.48	12.08	10.98	9.62	8.36	7.95	7.62	7.15	6.78	6.14	5.71	30%	4
CO_2–N	13.17	11.36	——	9.87	8.81	7.87	7.59	7.35	6.99	6.72	6.22	5.88	25%	14
CO_2–O	——	10.44	10.13	9.29	8.22	7.23	6.92	6.66	6.28	6.01	5.49	5.15	30%	4
N_2–CO	13.67	12.18	11.77	10.81	9.57	8.16	7.70	7.33	6.75	6.31	5.54	5.02	20%	20
N_2–CN	——	12.83	12.30	11.03	9.37	7.86	7.39	7.03	6.47	6.05	5.32	4.84	30%	5
N_2–C	13.58	——	11.36	10.18	8.77	7.46	——	6.78	6.28	5.94	——	——	25%	——
O_2–CO	13.11	11.60	11.19	10.25	9.13	7.93	7.54	7.23	6.73	6.36	5.70	5.25	20%	20
O_2–CN	——	11.42	11.05	10.02	8.78	7.61	7.24	6.95	6.51	6.18	5.59	5.20	30%	5
O_2–C	——	9.62	9.29	8.41	7.31	6.26	5.94	5.69	5.30	5.01	4.50	4.16	30%	4
CO–CO	13.67	12.18	11.77	10.81	9.57	8.16	7.70	7.33	6.75	6.31	5.54	5.01	20%	20
CO–NO	13.43	11.87	11.44	10.48	9.32	8.04	7.61	7.27	6.74	6.33	5.62	5.14	20%	20
CO–CN	——	11.68	11.31	10.20	8.89	7.65	7.27	6.96	6.50	6.15	5.53	——	30%	5
CO–C	——	10.48	10.08	9.07	7.80	6.63	6.26	5.98	5.54	5.21	4.63	——	30%	4
CO–N	11.80	10.24	——	8.85	7.71	6.59	6.24	5.94	5.43	5.02	4.24	3.69	20%	——
CO–O	——	8.61	8.29	7.46	6.42	5.46	5.17	4.93	4.58	4.31	3.84	3.52	30%	4
NO–CN	——	12.00	11.56	10.49	9.05	7.73	7.33	7.01	6.51	6.14	5.50	5.06	30%	5
NO–C	——	9.34	8.98	8.10	6.93	5.86	5.54	5.28	4.88	4.58	4.07	3.72	30%	5
CN–CN	——	12.50	12.02	10.85	9.28	7.85	7.42	7.07	6.54	6.14	5.44	4.98	30%	5
CN–C	——	9.72	9.32	8.36	7.10	5.94	5.59	5.31	4.88	4.56	4.01	3.64	30%	5
CN–N	——	10.33	9.90	8.76	7.32	6.00	5.60	5.29	4.81	4.46	3.84	3.44	30%	5
CN–O	——	9.09	8.76	7.87	6.79	5.78	5.47	5.23	4.85	4.57	4.07	3.74	30%	5
C–C	13.44	11.50	10.93	9.44	7.77	6.31	5.92	5.60	5.11	4.71	3.94	3.38	5%	13
C–N	10.31	8.67	8.33	7.33	6.29	5.33	5.07	4.87	4.53	4.26	3.71	3.27	5%	13
C–O	11.36	9.79	——	——	7.06	5.87	——	5.17	4.69	4.30	3.57	3.18	25%	12
C–N^+	30.52	23.53	——	15.37	10.21	7.70	7.22	6.90	6.46	6.17	5.72	——	25%	——
C–O^+	30.47	23.54	——	15.31	9.86	7.16	6.66	6.33	5.87	5.58	5.13	——	25%	——
C–C^+	30.47	23.59	——	15.60	10.70	8.33	7.87	7.57	7.13	6.84	6.39	——	25%	——
O_2–C^+	29.63	22.64	——	14.68	10.00	7.74	7.30	7.00	6.56	6.27	5.80	5.48	25%	——
CO–N^+	32.65	25.30	——	16.38	10.55	7.69	7.15	6.79	6.29	5.96	5.46	——	25%	——
CO–O^+	32.45	25.23	——	16.37	10.26	7.21	6.64	6.26	5.75	5.42	4.92	——	25%	——
CO–C^+	33.13	25.50	——	16.56	10.98	8.26	7.74	7.39	6.89	6.57	6.05	——	25%	——
CO–CO^+	37.73	29.22	——	20.66	14.61	10.33	9.24	8.44	7.31	6.53	5.34	——	40%	——
N–C^+	24.47	18.36	——	12.11	8.81	7.22	6.89	6.66	6.32	6.06	5.70	——	25%	——
O–C^+	20.85	15.31	——	10.25	7.74	6.49	6.21	6.01	5.70	5.48	5.12	——	25%	——
CN–CN^+	38.21	29.60	——	20.93	14.80	10.46	9.36	8.54	7.40	6.62	5.40	——	40%	——
e–CO_2	——	——	——	6.50	3.10	1.54	1.37	1.32	1.35	1.43	1.62	1.74	30%	47, 49
e–CO	——	——	——	2.94	4.13	6.31	6.81	6.93	6.58	6.01	4.79	4.02	30%	51, 52
e–CN	——	——	——	2.94	4.13	6.31	6.81	6.93	6.58	6.01	4.79	4.02	50%	——
e–C	——	——	——	——	8.86	6.57	5.95	5.56	5.11	4.86	4.30	——	30%	53

Table 3 Dipole polarizabilities, quadrupole polarizabilities, and dispersion coefficients for neutral species and atomic ions

Species	α, Å^3	α_q, Å^5	C_6/e^2, Å^5
CO_2	2.91[b]	——	——
O_2	1.58[a]	3.14[a]	2.56[a]
N_2	1.74[a]	3.60[a]	3.00[a]
CO	1.95[b]	4.86[c]	3.37[c]
CN	2.00[b]	-	
NO	1.70[a]	2.78[a]	2.89[a]
C	1.76[b]	2.35[d]	2.05[e]
N	1.10[a]	1.00[a]	1.14[a]
O	0.80[a]	0.80[a]	0.73[a]
C^+	0.88[f]	——	0.85[a]
N^+	0.56[a]	——	0.37[a]
O^+	0.35[a]	——	0.22[a]

[a] [34]
[b] [35]
[c] [36]
[d] [37]
[e] [38]
[f] [39]

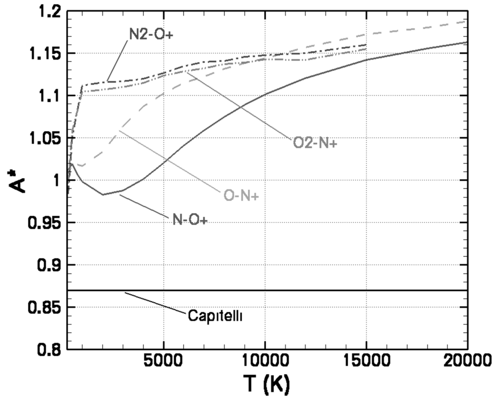

Fig. 4 A^* as a function of temperature computed for several ion–neutral interactions.

(3) for the CO–CO$^+$ and CN–CN$^+$ interactions, and the Tang–Toennies model for the C–C$^+$ interaction.

The ion–neutral diffusion and viscosity collision integrals computed for this work are given in Tables 1 and 2, respectively. Those determined using the polarization potential are not shown in the tables for brevity, but can be readily evaluated using the closed-form expressions given by Eqs. (2) and (3). The required nondimensional collision integral ratios B^* and C^* are assumed to be constant for all ion–neutral interactions and are taken from the collision integral calculations of Levin and Wright [32]:

$$B^* = 1.2; \qquad C^* = 0.85 \tag{5}$$

These values were shown to be accurate to within 10% over the temperature range of interest for multiple ion-neutral interaction pairs [32].

C. Electron–Neutral Interactions

Wright et al. [3] briefly reviewed the procedure for computing the collision integrals for electron–neutral interactions and gave results for those that are important for weakly ionized air. The most accurate method for determining collision integrals for these interactions is by numerical integration of differential elastic cross sections (DCS), if available. These differential cross sections ($d\sigma/d\Omega$) can be numerically integrated over all scattering angles to obtain integral momentum transfer (diffusion) and viscosity cross sections as a function of the interaction energy [2]:

$$\sigma_m(E) = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin\theta(1 - \cos\theta)\,\mathrm{d}\theta \tag{6}$$

$$\sigma_v(E) = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} (\sin^3\theta)\,\mathrm{d}\theta \tag{7}$$

The resulting cross sections can then be integrated again over energy assuming a Boltzmann distribution [22] to obtain the necessary transport collision integrals. In addition to those computed in [3], four additional electron–neutral interactions are required for Mars and Venus applications: e–CO$_2$, e–CO, e–CN, and e–C. The sources used for the necessary cross section data for these interactions and the resulting uncertainty levels in the computed collision integrals are discussed next.

Available cross section data for the e–CO$_2$ interaction were reviewed by Itikawa [44], Trajmar et al. [45], and most recently by Shirai et al. [46]. Unfortunately, considerable discrepancies exist between the available DCS data at low interaction energies, particularly among the theoretical computations. However, the recent experimental measurements of Tanaka et al. [47] and Gibson et al. [48] agree to within 20% over the energy range 1–10 eV. In this work we use the data of Gibson et al. [48], based on the recommendation of Shirai et al. [46]. These DCS have a stated absolute uncertainty of less than 10%; however, the resulting momentum transfer cross sections have an uncertainty of ±25% due to extrapolation of the DCS to scattering angles greater than 130 deg [48]. At energies between 0.5 and 1 eV we use the elastic momentum transfer cross sections based on swarm data presented by Nakamura [49], which are in good agreement (within 10%) with the data of Gibson et al. [48] over the entire energy range from 1 to 10 eV. At still lower energies we rely on Itikawa [44], who recommended the cross section data of Lowke et al. [50]. These data agree with the results of Nakamura [49] to within about 20% over the overlap range 0.5–1 eV, and predict very large cross sections at low (near thermal) energies. This results in large collision integrals at low temperatures. The accuracy of the resulting collision integrals is estimated at ±30%. The momentum transfer collision integrals presented here agree with the results of Murphy [15] and Magin et al. [4] to within 5% below 2000 K because both are based on the Lowke et al. [50] cross section data. At higher temperatures the current results are significantly smaller than those of Murphy [15] and Magin et al. [4] (about 20% at 5000 K, 40% at 10,000 K, and 50% at 15,000 K), due to significant differences between the Lowke et al. [50] and current recommended [46] cross sections in this energy range.

For the e–CO interaction we follow the recommendations of the recent critical reviews of Shirai et al. [46] and Brunger and Buckman [51]. DCS data above 1 eV are taken from Gibson et al. [52]. The estimated uncertainty in the Gibson et al. DCS is less than 15% except at 1 eV and large scattering angles [51]. However, the stated uncertainty in the resulting momentum transfer cross sections is about ±30%, again due to extrapolation of the DCS at high scattering angles [46]. These data are supplemented at lower energies by the integral momentum transfer cross sections from Land [53]. The Land data were based on swarm experiments and agree well (within 15%) with the results of Gibson et al. [52] in the overlap region from 1 to 10 eV, except near the resonance at 1.5 eV. Based on these data, we estimate the uncertainty in the resulting collision integrals at ±30%. The resulting momentum transfer collision integrals agree with the results of Murphy [15] and Magin et al. [4] to within 15%, who each integrated the Land [53] cross section data, over the temperature range 1000–15,000 K.

No experimental or computational data were found in the literature for the e–CN interaction, presumably because of the short lifetime of this radical species. Therefore, we assume that the collision integrals for e–CN are equal to those computed for e–CO. The estimated uncertainty in this assumption is no better than ±50%. However, e–CN interactions will be uncommon for most applications because CN is a trace species, so the high uncertainty is not a major concern.

The only available DCS for the e–C interaction are those computed by Thomas and Nesbet [54] at energies between 0.1 and 7 eV. No uncertainty estimates are given by Thomas and Nesbet, and no experimental data are available to validate the computations. However, we estimate a total uncertainty of ±30% for this interaction based on comparisons of DCS computed by the same authors with experimental data for the e–N and e–O interactions [3]. The resulting collision integrals agree well with those of Magin et al. [4], which is not surprising because both were based on the same cross section data.

Recommended values of $\Omega^{1,1}$ and $\Omega^{2,2}$ for the four required electron–neutral interactions based on the preceding references are given in Tables 1 and 2. In most cases values are not given below 1000 K due to a lack of cross section data at low interaction energies. However, the relative importance of electron–neutral interactions at very low temperatures should be negligible for most applications. The collision integral ratios B^* and C^* derived from these data show more temperature dependence as well as variability between the different electron–neutral interactions than was observed previously for neutral–neutral and ion–neutral interactions. Therefore, B^* and C^* are given for each of the four interactions as a function of temperature in Tables 4 and 5.

Table 4 Collision integral ratio B^* as a function of temperature for electron–neutral interactions

	T, K												Acc.	Ref.
	300	500	600	1000	2000	4000	5000	6000	8000	10,000	15,000	20,000		
e–CO^2	——	——	——	1.41	1.35	1.07	0.92	0.83	0.79	0.77	0.65	0.67	30%	47, 49
e–CO	——	——	——	0.66	0.60	0.91	1.14	1.28	1.41	1.41	1.31	1.24	30%	51, 52
e–CN	——	——	——	0.66	0.60	0.91	1.14	1.28	1.41	1.41	1.31	1.24	50%	——
e–C	——	——	——	——	1.39	1.39	1.30	1.22	1.10	1.05	1.23	——	20%	53

Table 5 Collision integral ratio C^* as a function of temperature for electron–neutral interactions

	T, K												Acc.	Ref.
	300	500	600	1000	2000	4000	5000	6000	8000	10,000	15,000	20,000		
e–CO^2	——	——	——	0.66	0.63	0.69	0.77	0.84	0.95	1.01	1.08	1.12	30%	47, 49
e–CO	——	——	——	1.15	1.15	1.12	1.07	1.01	0.93	0.87	0.82	0.82	30%	51, 52
e–CN	——	——	——	1.15	1.15	1.12	1.07	1.01	0.93	0.87	0.82	0.82	50%	——
e–C	——	——	——	——	0.98	0.81	0.79	0.80	0.83	0.87	0.90	——	20%	53

D. Electron–Electron, Electron–Ion, and Ion–Ion Interactions

Finally, interactions between charged particles must be considered. Once again, the necessary collision integrals for the shielded coulomb potential that governs such interactions have been presented in [3] and will not be repeated here.

III. Conclusions

The data presented in this paper, together with the air data from [3], form a complete set of collision integrals for the computation of the transport properties of 17-species weakly ionized CO_2–N_2 mixtures. Although the fidelity of the data varies, all collision integrals presented herein, with the exception of the electron–neutral interactions, are estimated be accurate to within 30% over the temperature range of interest ($\sim$300–20,000 K). In addition, many of the dominant interactions have been computed via ab initio methods that are estimated be accurate to within 20%.

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