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UCRL-ID- 115050

A Database of Selected Transport Coefficients for Combustion Studies

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August 1993

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A DATABASE OF SELECTED TRANSPORT COEFFICIENTS FOR COMBUSTION STUDIES

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ABSTRACT

COYOTE and similar combustion programs based on the multicomponent Navier-Stokes equations require the mixture viscosity, thermal conductivity, and species transport coefficients as input. This report documents a significant improvement to the calculation of these molecular transport coefficients in COYOTE and provides a self-contained and easy-to-use source of such data in a format suitable for use by such programs. We present the data for various species in two forms. The first is a simple functional fit to the transport coefficients. The second is the use of tabulated Lennard-Jones parameters in simple theoretical expressions for the gas-phase transport coefficients. Tables are given for a number of chemical species.

I. Introduction

Viscosity, thermal conductivity, and species transport coefficients are an important part of any effort to make realistic numerical simulations of reactive flows, especially in the laminar regime. Unfortunately, the available data are scattered widely throughout the literature of chemistry, physics, and engineering in a wide variety of formats. This information must be collected into one place, assessed for accuracy, and put into the appropriate format before it can be used in any particular computational fluid dynamics (CFD) program. Due to the large number of species of potential interest in combustion studies (potentially a thousand or more for a single problem), creating and maintaining such a database can become a major task. The program system CHEMKIN [1-4] is an excellent example of a computerized database designed to address this need. It is difficult to overstate the importance of such a program system to users who are willing to live with the constraints and limitations inherent in using software developed by someone else. The obvious advantages are avoidance of the effort required to independently collect the data in a usable form and the ability to use the same gas physics as a wide community of researchers. However, there are also disadvantages. First, there is the effort of obtaining and porting the programs to the user's system and learning to use them. Second, there is the need to validate, maintain, and update the programs. This can be a major task, especially if local modifications have been made to the program system. Third, an interface with the user's hydrodynamics program must be created and maintained. Fourth, users are constrained by the physics and output formats provided unless they make local modifications.

This report presents a simpler solution to the problem of supplying transport coefficients to the COYOTE reactive-flow CFD program [5]. The first step is to select a representation of the transport coefficients for use in the CFD program. Two of the many possible choices are described in the following sections. These two choices are a simple parametric fitting function (a slightly generalized Sutherland equation) and the use of the Lennard-Jones parameters in simple analytical expressions for the transport coefficients. Sample data for both approaches are given in the tables in this report. A text editor may be used to put these parameter values into the COYOTE input file.

In both cases, simple mixture rules are used to get viscosity and conductivity for a mixture with an arbitrary composition. These formulas are described in detail in the following sections. This is similar to the approach used in COYOTE with respect to the caloric equation of state. The JANAF tables [6-8] provide a homogeneous set of thermochemical data for a large collection of materials. The enthalpy tables and heats of formation for all species of interest are stored in a simple database program, GASMAK, which is run at the start of each problem to generate an input file containing the data on each species included in that problem. COYOTE then uses interpolation in the enthalpy table.

In Section II, we present the data for the coefficient of viscosity. Section III presents the thermal conductivities. Species diffusion coefficients are given in Section IV. Section V describes the input variables used by COYOTE's implementation of the transport coefficient data described in the previous sections. Section VI contains some concluding comments.

II. The Coefficient of Viscosity

Let $\mathcal{T}$ be the viscous stress tensor for a Newtonian fluid,

$$\begin{aligned}\mathcal{T} &= -\mu[\nabla\vec{u} + (\nabla\vec{u})^T] - \mu_1(\nabla \cdot \vec{u})\mathcal{U} \\ &= -\mu[\nabla\vec{u} + (\nabla\vec{u})^T] + \left(\frac{2\mu}{3} - \mu_b\right)(\nabla \cdot \vec{u})\mathcal{U}.\end{aligned}\tag{1}$$

Here $\vec{u}$ is the velocity of the fluid mixture, $\mathcal{U}$ is the unit tensor, μ is the coefficient of viscosity, μ_1 is the second coefficient of viscosity, and μ_b is the bulk viscosity. In almost all studies, the bulk viscosity is set to zero, which is correct, strictly speaking, only for perfect monatomic gases. What we require is a procedure for specifying the coefficient of viscosity for the mixture of species composing the fluid.

The first step in calculating the mixture viscosity is to evaluate the viscosity for each species. At the pressures and temperatures found in typical combustion systems, the species coefficients of viscosity are almost independent of density, so we assume they are functions only of temperature.

Table 1.
Coefficient of Viscosity

Species	n_α	A_α	B_α	C_α	T Range	Ref.
Air	1.5	1.457×10^{-5}	110.	0.0	Unknown	-
Air	1.51	1.387×10^{-5}	105.1	0.0	79-1407	12
He	1.695	3.614×10^{-6}	-9.549	0.0	81-1090	12
N ₂	1.52	1.186×10^{-5}	86.54	0.0	251-1098	12
O ₂	1.46	2.294×10^{-5}	164.4	0.0	273-1102	12
O ₂	1.5	1.16×10^{-5}	0.0	0.0	-	13
C ₃ H ₈	1.72	1.802×10^{-6}	101.0	0.0	290-472	12
SF ₆	1.7	3.526×10^{-6}	73.1	0.0	223-573	17
H ₂	1.67	1.963×10^{-6}	2.187	0.0	89-1098	12
H	1.5	3.95×10^{-6}	0.0	0.0	-	13
O	1.5	1.15×10^{-5}	0.0	0.0	-	13
OH	1.5	1.10×10^{-5}	0.0	0.0	-	13
H ₂ O	1.5	1.60×10^{-5}	0.0	0.0	-	13
HO ₂	1.5	1.16×10^{-5}	0.0	0.0	-	13
H ₂ O ₂	1.5	1.16×10^{-5}	0.0	0.0	-	13

We allow two ways of specifying the coefficient of viscosity. The first is a simple three-parameter analytic function that is suitable for fitting tabulated viscosity data. The second form is based on the Lennard-Jones parameters for each gas species.

The first approach is based on a fitting function that takes advantage of the fact that simple kinetic theory predicts that the viscosity of a gas is proportional to $T^{1/2}$, where T is the absolute temperature. We adopt a slightly more complex parameterization, a generalized Sutherland formula as our fitting function:

$$\mu_\alpha = \frac{A_\alpha T^{n_\alpha}}{B_\alpha + T} + C_\alpha, \quad (2)$$

where α denotes the particular species, and A_α , B_α , C_α , and n_α are constants. Values of the constants are given in Table 1 for a selection of species. The units are all cgs, that is poise (g/cm-s) for the viscosity and kelvins for T . To convert to SI units, multiply the cgs viscosity by 0.1. The

constants in Table 1 were evaluated by setting $C_\alpha = 0.0$ and fitting the viscosity data in the references at three temperatures (usually at the extremes and middle of the temperature range provided). The constant C_α is provided mostly as a convenience in setting the viscosity to a constant value in the CFD code for certain numerical experiments, although it could also have been used to fit a fourth data point. A least squares fit also could have been used.

The accuracy of the fits varies somewhat. Most of the fits in Table 1 have errors of at most a few percent in the temperature range given in the table, and they are often better than one percent over wide temperature ranges. Extrapolation beyond the given temperature range is always risky, although much less so on the high temperature end. Strong non-ideal gas effects can occur at low temperature that are not accounted for in the fits. For example, the He fit is approximately a factor of two in error around 20 K, and it gets worse rapidly as the singularity at 9.549 K is approached.

The second approach uses the Lennard-Jones parameters to estimate the viscosity (in cgs units),

$$\mu_\alpha = \frac{5}{16} \left(\frac{m_H k_B}{\pi} \right)^{1/2} \frac{(M_\alpha T)^{1/2}}{\sigma_\alpha^2 \Omega_\nu} = 2.6693 \times 10^{-5} \frac{(M_\alpha T)^{1/2}}{\sigma_\alpha^2 \Omega_\nu}, \quad (3)$$

where M_α is the molecular weight, m_H is the mass of one atomic mass unit in grams, k_B is the Boltzmann constant, σ_α is the collision diameter in Å, and Ω_ν is the collision integral approximated by

$$\Omega_\nu = 1.147 (T/T_{e\alpha})^{-0.145} + (T/T_{e\alpha} + 0.5)^{-2}, \quad (4)$$

where $T/T_{e\alpha} = T k_B / \epsilon_\alpha$ is the reduced temperature and ϵ_α is the Lennard-Jones potential well depth [9, 10]. Kee, *et al.* [2] recommend interpolation in Table V of Monchick and Mason [11], which includes dependence of the collision integral on the reduced dipole moment of the molecule, δ , as well as dependence on $T_{e\alpha}$. Equation (4) is accurate to a few percent for Monchick and Mason's $\delta < 0.5$ at low temperatures, and it becomes valid for larger values of δ at higher temperatures.

Once the species viscosities have been calculated, they must be combined to provide the viscosity of the fluid mixture. We adopt Wilke' law [12] as modified by Bird *et al.* [13]. For N species,

$$\mu = \sum_{\alpha=1}^N \frac{X_\alpha \mu_\alpha}{\sum_{\beta=1}^N X_\beta \Phi_{\alpha\beta}}, \quad (5)$$

where X_α is the mole fraction of species α and where

$$\Phi_{\alpha\beta} = 8^{-1/2} \left(1 + \frac{M_\alpha}{M_\beta}\right)^{-1/2} \left[1 + \left(\frac{\mu_\alpha}{\mu_\beta}\right)^{1/2} \left(\frac{M_\beta}{M_\alpha}\right)^{1/4}\right]^2. \quad (6)$$

III. Thermal Conductivities

The heat flux is a complicated function, and COYOTE uses

$$\vec{q} = -K\nabla T + \sum_{\alpha} h_{\alpha}(T)\vec{J}_{\alpha} - \sum_{\alpha} \frac{RT}{M_{\alpha}X_{\alpha}} D_{\alpha}^T \left[\nabla X_{\alpha} + (X_{\alpha} - Y_{\alpha}) \frac{\nabla P}{P} \right], \quad (7)$$

where K is the mixture thermal conductivity, h_{α} is the specific enthalpy of species α , $\vec{J}_{\alpha}$ is the species mass flux, and D_{α}^T is the thermal diffusion coefficient [2]. Calculation of the species mass fluxes and thermal diffusion coefficients will be considered in the next section.

In the original COYOTE program, K was calculated from the mixture viscosity μ and a constant mixture Prandtl number. This capability has been expanded to allow calculation of the conductivity based on the local composition and temperature, just as was done for the viscosity. One option is to fit species conductivity data using the same functional form as for the viscosity (that is, Eq. (2)). Results of a few fits are given in Table 2.

The second option is based on the Lennard-Jones parameters. Following the procedure of Hayashi and Hishida [9], we calculate the conductivity from the viscosity using the Eucken correction, which is discussed also by Ferziger and Kaper [14]:

$$K_{\alpha} = 0.25(9\gamma_{\alpha} - 5)\mu_{\alpha} C_{v\alpha}, \quad (8)$$

where $C_{v\alpha}$ is the specific heat at constant volume and γ_i is the ratio of specific heats. Kee, *et al.* [2] describe a more complex approximation that we have not implemented. Their model accounts more accurately for the internal quantum states of the molecules.

There are two possible mixture rules for the conductivity. The first is to use Eq. (5) with μ_{α} replaced by K_{α} , but with the same values of $\Phi_{\alpha\beta}$ as used for the mixture viscosity [13]. The second

Table 2.
Species Thermal Conductivities

Species	n_α	A_α	B_α	C_α	T Range	Ref.
Air	1.5	2.255×10^2	150.0	0.0	233-322	16
He	1.63	4.167×10^2	2.635	0.0	33-322	16
N ₂	1.51	1.935×10^2	110.4	0.0	88-322	16
O ₂	1.86	2.126×10^1	22.26	0.0	88-366	16
C ₃ H ₈	2.69	1.167×10^{-1}	2.409	0.0	233-366	16
SF ₆	1.8	2.296×10^1	140.5	0.0	300-4000	17
H ₂	1.5	1.522×10^3	124.4	0.0	88-322	16
H	1.5	1.173×10^3	0.0	0.0	-	18
O	1.5	2.134×10^2	0.0	0.0	-	18
OH	1.5	2.69×10^2	0.0	0.0	-	18
H ₂ O	1.5	4.596×10^2	1036.2	0.0	255-367	16

rule is due to Mathur *et al.* [15] and is recommended by Kee, *et al.* [2]:

$$K = \frac{1}{2} \left[\sum_{\alpha=1}^N X_\alpha K_\alpha + \left(\sum_{\alpha=1}^N X_\alpha / K_\alpha \right)^{-1} \right]. \quad (9)$$

We presently use the latter rule in COYOTE.

IV. Species Diffusion Coefficients

Calculation of the exact diffusional mass fluxes is an extremely complicated task (for example, [13], [19], and [20]). Many combustion studies simply use Fick's law,

$$\tilde{J}_\alpha = -\rho D_\alpha \nabla(\rho_\alpha/\rho), \quad (10)$$

where ρ is the total density, and D_α is the species diffusivity. The original version of COYOTE used this approximation with the same value of D_α for all species, and this value was given as the kinematic viscosity of the mixture divided by a constant mixture Schmidt number. This simple model has the advantages that it is easy to program, computationally inexpensive, and the species mass

fluxes properly add up to zero when summed over species. Experience suggests that it is adequate for turbulent flows (where molecular transport is overwhelmed by the turbulent eddy diffusion) and in some laminar cases using global chemical kinetics (where the detailed chemical composition is not being modeled all that accurately in any case). In cases where the flow is laminar or nearly so and a detailed chemical reaction network is included, a more accurate model is required.

Ramshaw [21] has developed an effective binary diffusion approximation that we have adopted. He begins with the assumption that multicomponent diffusion in gases is governed by the Stefan-Maxwell equations

$$\sum_{\beta} (X_{\alpha} X_{\beta} / D_{\alpha\beta}) (\vec{u}_{\beta} - \vec{u}_{\alpha}) = \vec{G}_{\alpha} \quad (\alpha = 1, \dots, N), \quad (11)$$

where N is the number of species in the mixture, $\vec{u}_{\alpha}$ is the velocity of species α , X_{α} is the mole fraction of species α , $D_{\alpha\beta}$ is the binary diffusivity for the pair of species (α, β) , and the driving forces $\vec{G}_{\alpha}$ are given by

$$\vec{G}_{\alpha} = \nabla X_{\alpha} + (X_{\alpha} - Y_{\alpha}) \nabla \ln P + \chi_{\alpha} \nabla \ln T - \frac{1}{P} \left[\rho_{\alpha} \vec{F}_{\alpha} - Y_{\alpha} \sum_{\beta} \rho_{\beta} \vec{F}_{\beta} \right]. \quad (12)$$

Here ρ_{α} is the mass density of species α , ρ is the total density of the mixture, Y_{α} is the mass fraction of species α , and $\vec{F}_{\alpha}$ is the body force per unit mass acting on species α . The χ_{α} are related to the species thermal diffusion coefficients. The diffusive mass fluxes are given by

$$\vec{J}_{\alpha} = \rho_{\alpha} (\vec{u}_{\alpha} - \vec{u}), \quad (13)$$

where $\vec{u}$ is the mass-weighted mixture velocity calculated by COYOTE,

$$\rho \vec{u} = \sum_{\alpha} \rho_{\alpha} \vec{u}_{\alpha}. \quad (14)$$

The diffusional fluxes could be found by solving the coupled system (11) through (13) for each cell on each time step, a complex and expensive process when more than two species are present. Another approach is to decouple the fluxes from one another with what is called the “effective binary diffusion approximation,” which exists in a variety of forms. In the absence of thermal, forced, and

pressure diffusion, Eq. (10) is a commonly used approximation. However, this approximation has the serious disadvantage that the fluxes do not sum to zero unless all values of D_α are the same.

Ramshaw's contribution is the development of an effective binary diffusion approximation that simultaneously accounts for all four types of diffusion, and for which the fluxes correctly sum to zero. The resulting model is

$$\vec{J}_\alpha = -cM_\alpha D_\alpha \vec{G}_\alpha + Y_\alpha c \sum_\beta M_\beta D_\beta \vec{G}_\beta, \quad (15)$$

where M_α is the molecular weight of species α ,

$$c = \sum_\alpha \rho_\alpha / M_\alpha \quad (16)$$

is the total molar concentration of the mixture, and

$$D_\alpha = (1 - X_\alpha) \left(\sum_{\beta \neq \alpha} X_\beta / D_{\alpha\beta} \right)^{-1}. \quad (17)$$

The interested reader is referred to Ramshaw [21] for details.

We follow Hayashi and Hishida [9] in evaluation of the binary diffusion coefficients:

$$D_{\alpha\beta} = 1.8829 \times 10^3 \frac{\left[T^3 \left(\frac{M_\alpha + M_\beta}{M_\alpha M_\beta} \right) \right]^{1/2}}{P \sigma_{\alpha\beta}^2 \Omega_D}, \quad (18)$$

where P is the total pressure of the mixture. We also use

$$\sigma_{\alpha\beta} = 0.5(\sigma_\alpha + \sigma_\beta), \quad (19)$$

$$\Omega_D = (T/T_{e\alpha\beta})^{-0.145} + (T/T_{e\alpha\beta} + 0.5)^{-2}, \quad (20)$$

and

$$T_{e\alpha\beta} = (T_{e\alpha} T_{e\beta})^{1/2}. \quad (21)$$

COYOTE presently uses $\chi_\alpha = D_\alpha^T = 0$. Not only are thermal diffusion effects small, there are practical difficulties associated with obtaining the required values of χ_α . There is a shortage of experimental data, and the traditional theory is so complex as to hinder its application by the

nonspecialist. However, Ramshaw has developed an approximate simplified theory [22] that will be incorporated into COYOTE. The first step is to estimate the collision cross section between molecules of types α and β as

$$\sigma^{\alpha\beta} = 0.25\pi(\sigma_\alpha + \sigma_\beta)^2. \quad (22)$$

We define

$$\gamma_{\alpha\beta} = \frac{m_H}{2k_B T} \frac{M_\alpha M_\beta}{M_\alpha + M_\beta}. \quad (23)$$

With these two parameters we calculate the collision time

$$\tau_\alpha = \frac{1}{2} \left[\sum_{\beta=1}^N \frac{n_\beta \sigma^{\alpha\beta}}{(\pi \gamma_{\alpha\beta})^{1/2}} \right]^{-1}, \quad (24)$$

where n_β is the number density of species β . We can now calculate the conventional multicomponent thermal diffusion coefficients

$$D_\alpha^T = k_B T \left(n_\alpha \tau_\alpha - Y_\alpha \sum_{\beta=1}^N n_\beta \tau_\beta \right), \quad (25)$$

which are in turn used to calculate

$$\chi_\alpha = \sum_{\beta=1}^N \frac{X_\alpha X_\beta}{D_{\alpha\beta}} \left(\frac{D_\alpha^T}{\rho_\alpha} - \frac{D_\beta^T}{\rho_\beta} \right) \quad (26)$$

for use in the Stefan-Maxwell equations (12), which in turn are used with Eq. (15) to calculate the diffusion fluxes.

V. COYOTE Input for Transport Coefficients

The transport coefficient data is input into COYOTE as part of the NAMELIST input deck for each problem. The data are found in Tables 1, 2, and 3. Table 3 contains the Lennard-Jones parameters for the set of species used in Glarborg's skeletal mechanism for methane combustion and NO_x chemistry [23], which provides a selection of some of the most important species in combustion. Also included are several species that have been encountered on occasion, including the use of the data of Bzowski, *et al.* [24] to test the models proposed in this report. The format of the table

follows the practice of CHEMKIN [2]. The Index variable is 0, 1, or 2 if the molecules are a single atom, a linear molecule, or a nonlinear molecule. Parameters for additional species may be found in CHEMKIN and scattered throughout the literature. For example, Bird, Stewart, and Lightfoot [13] and Dean, Bozzelli, and Ritter [25] provide short lists of parameters. The latter paper also presents a theoretical model that estimates Lennard-Jones parameter values for other species.

The viscosity parameters are read into COYOTE in the NAMELIST blocks *coydat* and *tranco*. The following variables are set in *coydat*.

airmu = 0., no Sutherland equation for air; = 1., use the Sutherland equation for

air ($A_\alpha = 1.457 \times 10^{-5}$, $B_\alpha = 110$, $n_\alpha = 1.5$, and $C_\alpha = 0.0$) for the

mixture viscosity.

xnumol = constant molecular mixture kinematic viscosity.

jdrflg = 0, use simple Fick's law with species diffusivities given by the mixture

viscosity divided by the mixture Schmidt number *scmol*; = 1, use the detailed binary

diffusion coefficients and Ramshaw's algorithm for computing the species fluxes

without thermal diffusion; = 2, include thermal diffusion.

prmol = constant molecular Prandtl number, used only with *xnumol* and the *airmu*=1.0

viscosity formula.

scmol = constant molecular Schmidt number used when *jdrflg* = 0.

The following variables are set in NAMELIST block *tranco*.

mizvis = 0, use original transport coefficients (that is, use the parameters *airmu* and

xnumol set in *coydat*); = 1, use the species Sutherland formula fits for all species;

= 2, use the Lennard-Jones model for all species.

visfa, *visfb*, *visfc*, *visfn* = arrays containing the parameters A_α , B_α , C_α , and n_α for

mizvis = 1; *visfa* and *visfb* contain the Lennard-Jones parameters σ_α (in Å) and

$T_{\epsilon\alpha} = \epsilon_\alpha / k_B$ if *mizvis* = 2.

confa, *confb*, *confc*, *confn* = arrays containing the parameters analogous to *visfa*,
visfb, *visfc*, *visfn* for the species conductivities. Used only for *mirvis* = 1.
jtdiff = 0, no radiative transfer; = 1, include gray 1T radiation diffusion; = 2, include
gray 2T diffusion; = 3, include emission model radiative heat losses.
jtco, *jtco2*, *jth2o* = species numbers for CO, CO₂, and H₂O for use when *jtdiff* = 3.

VI. Concluding Comments

This simplified, self-contained, and homogeneous data base has proved to be useful in combustion studies. The improved accuracy of the transport coefficients in COYOTE allows more detailed simulations of a wide variety of flows, especially in the laminar regime. For truly large numbers of species, a more automated program system such as CHEMKIN might be preferable, but for a typical COYOTE run with less than about 30 species, the present data base is much simpler to use. The option of direct usage of the Lennard-Jones parameters in COYOTE is preferred over the CHEMKIN approach of using the same theoretical expressions to calculate transport coefficients that are subsequently fit with polynomials, thereby introducing unnecessary truncation errors.

Acknowledgements

I thank J. D. Ramshaw for many useful discussions on various aspects of including molecular transport effects into computational fluid dynamics programs. I also thank Bob Kee, Lila Chase, and Bill Pitz for their help with CHEMKIN. This work was supported by the California Institute for Energy Efficiency and Southern California Gas Company. It was performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

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Table 3.
Selected Lennard-Jones Parameters

Species	Index	ϵ/k_B (K)	σ (Å)	μ (Debye)	α (Å ³)
Ar	0	136.500	3.330	0.000	0.000
C	0	71.400	3.298	0.000	0.000
CH	1	80.000	2.750	0.000	0.000
CH ₂	1	144.000	3.800	0.000	0.000
CH ₃	1	144.000	3.800	0.000	0.000
CH ₄	2	141.400	3.746	0.000	2.600
C ₂ H ₂	1	209.000	4.100	0.000	0.000
CH ₂ O	2	498.000	3.590	0.000	0.000
CH ₂ OH	2	417.000	3.690	1.700	0.000
CN	1	75.000	3.856	0.000	0.000
CO	1	98.100	3.650	0.000	1.950
CO ₂	1	244.000	3.763	0.000	2.650
H	0	145.000	2.050	0.000	0.000
H ₂	1	38.000	2.920	0.000	0.790
HCN	1	569.000	3.630	0.000	0.000
HCO	2	498.000	3.590	0.000	0.000
H ₂ O	2	809.100	2.641	1.850	0.000
H ₂ O ₂	2	107.400	3.458	0.000	0.000
HO ₂	2	107.400	3.458	0.000	0.000
N	0	71.400	3.298	0.000	0.000
N ₂	1	97.530	3.621	0.000	1.760
NCO	1	232.400	3.828	0.000	0.000
NH	1	80.000	2.650	0.000	0.000
N ₂ O	1	232.400	3.828	0.000	0.000
NO	1	97.530	3.621	0.000	1.760
NO ₂	2	200.000	3.500	0.000	0.000
O	0	80.000	2.750	0.000	0.000
O ₂	1	107.400	3.458	0.000	1.600
OH	1	80.000	2.750	0.000	0.000
C ₂ H ₄	2	280.800	3.971	0.000	0.000
C ₂ H ₆	2	252.300	4.302	0.000	0.000
C ₃ H ₈	2	266.800	4.982	0.000	0.000
CF ₄	2	156.500	4.579	-	-
SF ₆	2	207.700	5.252	-	-
He	0	10.200	2.576	0.000	0.000
Kr	0	176.0	3.679		
Ne	0	35.60	2.749		
Xe	0	229.8	3.937		

END

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