VI I-PROPATH: Ideal Gases and Ideal Gas Mixtures

I-PROPATH is a program package for the properties of ideal gases and ideal gas mixtures based on database by Daubert and Danner[1]. This package provides 11 SUBROUTINE SUBPROGRAMs and 19 FUNCTION SUBPROGRAMs for 54 substances, their mixtures, air as a mixture of ideal gases, and complete combustion-by-air products of $C_XH_YO_Z$. In addition to these SUBPROGRAMs there are 5 single shot programs (ideal gases, air, complete combustion-by-air products, Keenan-Chao-Kaye-style gas tables [2] and JANAF-style tables [3]).

In calculating the properties of air as a mixture of ideal gases and complete combustion-by-air products of $C_XH_YO_Z$, the composition of air is assumed to be that shown in reference [2] (78.03 % nitrogen, 20.99 % oxygen and 0.98 % argon by volume).

1. SUBPROGRAM REFERENCE

1.1 Initialization process

Every I-PROPATH user has to make initialization process by the following procedures.

1.1.1 Reservation of VARIABLEs (required)

A PROGRAM UNIT which is going to CALL the I-PROPATH SUBPROGRAMs should include the following LINEs before the first EXECUTABLE STATEMENT.

```
INTEGER KPA,KMOL,MESS
CHARACTER*25 ANAME
REAL GASCON
COMMON /UNIT/KPA,KMOL,MESS
COMMON /CNST/GASCON
```

`KPA` specifies the units of temperature and pressure and `KMOL` the unit of amount of substance. The system of units which a user can select and the relation between the values of `KPA` and `KMOL` specified by a user and the units are shown in Chapter 3.

`MESS` specifies whether messages to the erroneous SUBPROGRAM REFERENCE are to be printed out to the standard output device or not. I-PROPATH does not return any messages when `MESS`$= 0$, while it does when `MESS`$\neq 0$.

`GASCON` is a reserved NAME as a REAL CONSTANT for the universal gas constant.

`ANAME` is a reserved NAME as a CHARACTER for the name of substance identified by the substance index of an ideal gas.

1.1.2 Initialization of the reserved CONSTANTs (required)

I-PROPATH offers the automatic initialization SUBROUTINE PROGRAM `IPINIT`. A user has to initialize parameters mentioned above by writing

```
CALL IPINIT(KPA,KMOL,MESS,KGAS,GASC)
```

before the first REFERENCE to a I-PROPATH SUBPROGRAM in the MAIN PROGRAM. See section **7.2.9**

1.1.3 Re-initialization (optional)

If a user happens to want to use other settings for parameters `KPA`, `KMOL`, `MESS` and `GASCON` in any places of his or her PROGRAM UNIT, he or she is supposed to write the similar statement as the one described in section **1.1.2** at those places.

1.2 Specification of substance

Each SUBPROGRAMs has an ARGUMENT `ISUB` or an ARRAY `ISUB`(i) named as **substance index(es)** for each ideal gas or ideal gas mixture. Every user has to specify the substance index when he/she wishes to make REFERENCE to the SUBPROGRAMs looking up the following table.

Table VI-1-1 List of substance indexes : ISUB

Chemical Symbol(∗)	Molecular Formula	IUPAC Name of Substance (Synonym)	**ISUB**
Ar	Ar	Argon	23
C	C	Carbon	18
CClF2H	$CHClF_2$	Chlorodifluoromethane (HCFC 22)	24
CClF3	$CClF_3$	Chlorotrifluoromethane (CFC 13)	25
CClH3	CH_3Cl	Methyl Chloride (Chloromethane)	41
CCl2FH	$CHCl_2F$	Dichlorofluoromethane (HCFC 21)	27
CCl2F2	CCl_2F_2	Dichlorodifluoromethane (CFC 12)	28
CCl2H2	CH_2Cl_2	Dichloromethane (Methylene Chloride)	29
CCl3H	$CHCl_3$	Chloroform (Trichloromethane)	26
CF4	CF_4	Carbon Tetrafluoride (Tetrafluoromethane)	30
CH4	CH_4	Methan	10
CH4O	CH_3OH	Methanol	31
CO	CO	Carbon Monoxide	8
CO2	CO_2	Carbon Dioxide	9
C2ClF2H3	CH_3CClF_2	1-Chloro-1,1-Difluoroethane (HCFC 142B)	32
C2ClH5	CH_3CH_2Cl	Ethyl Chloride (Chloroethane)	33
C2Cl2F4	$CClF_2CClF_2$	1,2-Dichlorotetrafluoroethane (CFC 114)	34
C2F2H4	CH_3CHF_2	1,1-Difluoroethane (HFC 152A)	35
C2H2	CHCH	Ethyne (Acetylene)	36
C2H4	CH_2CH_2	Ethylene (Ethene)	12
C2H4O	CH_3CHO	Acetaldehyde	42
C2H4O2	CH_3COOH	Acetic Acid	43
C2H6	CH_3CH_3	Ethane	37
C2H6O	CH_3CH_2OH	Ethanol	44
C3H6	CH_3CHCH_2	Propylene (Propene)	45
C3H6O	CH_3COCH_3	Acetone	46
C3H8	$CH_3CH_2CH_3$	Propane	11
C4H10	$CH_3(CH_2)_2CH_3$	Butane (n-Butane)	38
C4H10	$(CH_3)_3CH$	Isobutane	39
C5H12	$CH_3(CH_2)_3CH_3$	Pentane (n-Pentane)	47
C5H12	$(CH_3)_2CHCH_2CH_3$	Isopentane	40
C6H6	C_6H_6	Benzene	48
C6H14	$CH_3(CH_2)_4CH_3$	Hexane (n-Hexane)	49
C7H8	$(C_6H_5)CH_3$	Toluene (Methylbenzene)	50
C7H16	$CH_3(CH_2)_5CH_3$	Heptane (n-Heptane)	51
C8H18	$CH_3(CH_2)_6CH_3$	Octane (n-Octane)	52
C8H18	$(CH_3)_2CH(CH_2)_4CH_3$	2-Methylheptane (Iso-Octane)	53
C10H8	$(C_6H_4)(C_4H_4)$	Naphthalene	54
ClH	HCl	Hydrogen Chloride	19
Cl2	Cl_2	Chlorine	13
F2	F_2	Fluorine	20
HI	HI	Hydrogen Iodide	21
H2	H_2	Hydrogen	3
H2O	H_2O	Water	2
H3N	NH_3	Ammonia	14
He	He	Helium (Helium-4)	22
NO	NO	Nitric Oxide (Nitrogen Monoxide)	4
NO2	NO_2	Nitrogen Dioxide	5
N2	N_2	Nitrogen	1
N2O	N_2O	Nitrous Oxide (Dinitrogen Monoxide)	6
Ne	Ne	Neon	16
O2	O_2	Oxygen	7
O2S	SO_2	Sulfur Dioxide	15
O3	O_3	Ozone	17

(∗) according to the alphabetical order of elements and increasing order of number of atoms.

2. Operations to Manage Erroneous SUBPROGRAM REFERENCE

A predetermined sequence of operations will occur to process an erroneous SUBPROGRAM REFERNCE when improper SUBPROGRAM REFERENCE has been done. Erroneous SUBPROGRAM REFERENCEs are grouped into 3 levels, with the ascending severity of user's mistake. A user has committed a more serious mistake when level 3 ERROR ocurrs than when a level 2 ERROR does, for example.

2.1 Level 1 ERROR (No error)

When a I-PROPATH SUBROUTINE SUBPROGRAM returns the values of ARGUMENTs correctly to the MAIN PROGRAM, the SUBPROGRAM returns the value 0 of error detection code `IERR`.

2.2 Level 2 ERROR (Invalid ARGUMENT(s))

A level 2 ERROR will occur when the ARGUMENT(s) a user transferred to I-PROPATH SUBPROGRAM from his or her MAIN PROGRAM fail to drop in the proper range.

A level 2 ERROR is processed as below.

value of error detection cord, one of the arguments of SUBROUTINE : `IERR`= -2

value of FUNCTION or values of ARGUMENTs of SUBROUTINE returned to the CALLing program : -1.0E+20

output to the standard output device :

`*** OUT OF RANGE AT` (name of SUBPROGRAM CALLed) `FOR` (name of substance)

2.3 Level 3 ERROR (Substance Unavailable)

A user will encounter a level 3 ERROR when the INTEGER CONSTANT `ISUB` a user specified for the substance index fails to coincide with any of the allowable values.

The level 3 error is processed as shown below.

value of error detection cord, one of the arguments of SUBROUTINE : `IERR`= -3

value of FUNCTION or values of ARGUMENTs of SUBROUTINE returned to the CALLing program : -1.0E+30

output to the standard output device :

`*** SUBSTANCE INDEX * ISUB =` (value of substance index) `* IS NOT INCLUDED IN I-PROPATH ***`

3. System of Units

All REAL quantities are in the fundamental SI or in the coherent derived SI with three exceptions. Temperature can be in the unit of Kelvin [K] or degree Celsius [°C], pressure in the unit of Pascal [Pa] or bar [bar], and the amount of substance in the unit of kilomole [kmol] or kilogram [kg]. These depend on the values of INTEGER CONSTANTs, `KPA` and `KMOL`, which a user assigned to. See 1.1 and 7.2.9.

Table VI-3-1 Units of Pressure and Temperature Specified by `KPA`

`KPA`	unit of pressure	unit of temperature	
0	Pa	K	(default)
1	bar	°C	
2	bar	K	
3	Pa	°C	
others	Pa	K	

Table VI-3-2 Amount of Substance Specified by `KMOL`

`KMOL`	unit of the amount of substance	
0	kmol	(default)
1	kg	
others	kmol	

4. Reference Values of Enthalpy and Entropy

At the reference temperature of 298.15 [K] (25 [°C]), 0 is assigned to enthalpy. At the reference state of 0.1 [MPa] (1 [bar]) and 298.15 [K] (25 [°C]), the absolute entropy cited from reference [1] is assigned to the specific entropy. Thus, the value of enthalpy is relative to the reference temperature while that of entropy is absolute.

5. Reserved NAMEs of COMMON BLOCKs, FUNCTIONs and SUBROUTINEs

I-PROPATH uses a lot of NAMEs, listed below, for its own purpose. These are the NAMEs of SUBPROGRAMs, NAMED COMMON BLOCKs, and ARGUMENTs. A user is supposed to use the NAMEs of SUBPROGRAMs and COMMON BLOCKs only when he/she does so in the original meaning.

Thses are listed below. The letters in the first column are the fist LETTERs in the NAMES listed in the same line.

A	`AKG2KM,AKM2KG, AIRTP`
C	`CHOTBL, COMMON /CNST/`
F	`FUELML`
G	`GASCON`
I	`IDENTI, IDGCMM, IDGFND, IDGT, IDGTBL, IDGTP, IPINIT`
K	`KMOL, KPA`
M	`MIXCMM, MIXTP, MESS`
P	`PTSAIR, PTSIDG, PTVAIR, PTVIDG`
T	`T68,T90, THAIR, THIDG, TPSAIR, TPSIDG, TPVAIR, TPVIDG, TVSAIR, TVSIDG, TUAIR, TUIDG`
U	`COMMON /UNIT/`

6. NAMEs of FUNCTION and SUBROUTINE SUBPROGRAMs

NAMEs of FUNCTIONs and SUBROUTINEs are shown below and the full description of these SUBPROGRAMs is given in chapter 7.

6.1 FUNCTION SUBPROGRAMs

6.1.1 REAL valued FUNCTIONs (conversion of temperature scale and mole-mass conversion)

T68 = conversion from ITS-1990 to ITPS-1968
T90 = conversion from ITPS-1968 to ITS-1990
AKM2KG = conversion from mole to mass
AKG2KM = conversion from mass to mole

6.1.2 REAL valued FUNCTIONs (ideal gas)

PTSIDG = pressure as a function of temperature and entropy
PTVIDG = pressure as a function of temperature and volume
THIDG = temperature as a function of enthalpy
TPSIDG = temperature as a function of pressure and entropy
TPVIDG = temperature as a function of pressure and volume
TVSIDG = temperature as a function of volume and entropy
TUIDG = temperature as a function of internal energy

6.1.3 REAL valued FUNCTIONs (air as a mixture of ideal gases)

PTSAIR = pressure as a function of temperature and entropy
PTVAIR = pressure as a function of temperature and volume
THAIR = temperature as a function of enthalpy
TPSAIR = temperature as a function of pressure and entropy
TPVAIR = temperature as a function of pressure and volume
TVSAIR = temperature as a function of volume and entropy
TUAIR = temperature as a function of internal energy

6.1.4 CHARACTER valued FUNCTION

IDENTI = name of an ideal gas, or version number of PROPATH

6.2 SUBROUTINE SUBPROGRAMs

6.2.1 initialization and conversion

IPINIT = initialization
IDGCMM = conversion from mass to mole, or reverse, for ideal gas.
MIXCMM = conversion from mass fractions to mole fractions, or reverse, for mixture of ideal gases.

6.2.2 ideal gas

IDGFND = critical and fundamental constants
IDGT = properties of ideal gases as a function of temperature at 0.1 MPa (JANAF-style table)
IDGTBL = properties of ideal gases as a function of temperature at 0.1 MPa (Keenan-Chao-Kaye-style gas table)
IDGTP = properties of ideal gases as a function of temperature

6.2.3 mixture of ideal gases

MIXTP = properties of ideal gas mixture as a function of temperature and pressure

6.2.4 air as a mixture of ideal gases

AIRTP = properties of air (78.03 % nitrogen, 20.99 % oxygen and 0.98 % argon by volume) as a function of temperature and pressure

6.2.5 complete combustion-by-air product of $C_XH_YO_Z$

CHOTBL = properties of complete combustion-by-air products of $C_XH_YO_Z$ at 0.1 MPa (Keenan-Chao-Kaye-style gas table) as a function of temperature

FUELML = mole fractions of complete combustion-by-air products of the mixture of $C_XH_YO_Z$ fuels.

7. Descriptions of FUNCTIONs and SUBROUTINEs

Shown in alphabetical order of NAMEs.

7.1 FUNCTIONs

7.1.1 AKM2KG

mole to mass conversion for ideal gas

```
REAL FUNCTION AKM2KG(ISUB,Z)
```

Input
INTEGER `ISUB` : substance index of the gas
REAL `Z` : mole [kmol]

Returned
REAL `AKM2KG` : mass [kg]

7.1.2 AKG2KM

mass to mole conversion for ideal gas

```
REAL FUNCTION AKG2KM(ISUB,Z)
```

Input
INTEGER `ISUB` : substance index of gas
REAL `Z` : mass [kg]

Returned
REAL `AKG2KM` : mole [kmol]

7.1.3 IDENTI

name of an ideal gas, or version number

```
CHARACTER*25 FUNCTION IDENTI(ISUB,A)
```

Input
INTEGER `ISUB` : substance index
CHARACTER*1 `A` : a character to control output

Returned
`IDENTI` : name of substance when `A='S'`, or version number when `A≠'S'`

7.1.4 PTSAIR

pressure of air as a function of temperature and entropy

```
REAL FUNCTION PTSAIR(T,S)
```

Input
REAL `T` : temperature [K],[°C]
REAL `S` : absolute entropy [J/(kmol·K)], [J/(kg·K)]

Returned
REAL `PTSAIR` : pressure [Pa], [bar]

7.1.5 PTSIDG

pressure of ideal gas as a function of temperature and entropy

```
REAL FUNCTION PTSIDG(ISUB,T,S)
```

Input
INTEGER `ISUB` : substance index of the gas
REAL `T` : temperature [K],[°C]
REAL `S` : absolute entropy [J/(kmol·K)], [J/(kg·K)]

Returned
REAL `PTSIDG` : pressure [Pa],[bar]

7.1.6 PTVAIR

pressure of air as a function of temperature and volume

```
REAL FUNCTION PTVAIR(T,V)
```

Input
REAL `T` : temperature [K],[°C]
REAL `V` : volume [m^3/kmol], [m^3/kg]

Returned
REAL `PTVAIR` : pressure [Pa],[bar]

7.1.7 PTVIDG

pressure of ideal gas as a function of temperature and volume

```
REAL FUNCTION PTVIDG(ISUB,T,V)
```

Input
INTEGER `ISUB` : substance index of the gas
REAL `T` : temperature [K],[°C]
REAL `V` : volume [m^3/kmol], [m^3/kg]

Returned
REAL `PTVIDG` : pressure [Pa],[bar]

7.1.8 THAIR

temperature of air as a function of enthalpy

```
REAL FUNCTION THAIR(H)
```

Input
REAL `H` : enthalpy [J/kmol], [J/kg]

Returned
REAL `THAIR` : temperature [K],[°C]

7.1.9 THIDG

temperature of ideal gas as a function of enthalpy

```
REAL FUNCTION THIDG(ISUB,H)
```

Input
INTEGER `ISUB` : substance index of the gas
REAL `H` : enthalpy [J/kmol], [J/kg]

Returned
REAL `THIDG` : temperature [K],[°C]

7.1.10 TPSAIR

temperature of air as a function of pressure and entropy

```
REAL FUNCTION TPSAIR(P,S)
```

Input
REAL `P` : pressure [Pa],[bar]
REAL `S` : absolute entropy [J/(kmol·K)], [J/(kg·K)]

Returned
REAL TPSAIR : temperature [K],[°C]

7.1.11 TPSIDG

temperature of ideal gas as a function of pressure and entropy

```
REAL FUNCTION TPSIDG(ISUB,P,S)
```

Input
INTEGER ISUB : substance index of the gas
REAL P : pressure [Pa],[bar]
REAL S : absolute entropy [J/(kmol·K)], [J/(kg·K)]

Returned
REAL TPSIDG : temperature [K],[°C]

7.1.12 TPVAIR

temperature of air as a function of pressure and volume

```
REAL FUNCTION TPVAIR(P,V)
```

Input
REAL P : pressure [Pa],[bar]
REAL V : volume [m^3/kmol],[m^3/kg]

Returned
REAL TPVAIR : temperature [K],[°C]

7.1.13 TPVIDG

temperature of ideal gas as a function of pressure and volume

```
REAL FUNCTION TPVIDG(ISUB,P,V)
```

Input
INTEGER ISUB : substance index of the gas
REAL P : pressure [Pa],[bar]
REAL V : volume [m^3/kmol],[m^3/kg]

Returned
REAL TPVIDG : temperature [K],[°C]

7.1.14 TVSAIR

temperature of air as a function of volume and entropy

```
REAL FUNCTION TVSAIR(V,S)
```

Input
REAL V : volume [m^3/kmol],[m^3/kg]
REAL S : absolute entropy [J/(kmol·K)], [J/(kg·K)]

Returned
REAL TVSAIR : temperature [K],[°C]

7.1.15 TVSIDG

temperature of ideal gas as a function of volume and entropy

```
REAL FUNCTION TVSIDG(ISUB,V,S)
```

Input
INTEGER ISUB : substance index of the gas
REAL V : volume [m^3/kmol],[m^3/kg]
REAL S : absolute entropy [J/(kmol·K)], [J/(kg·K)]

Returned
REAL `TVSIDG` : temperature [K],[°C]

7.1.16 TUAIR
temperature of air as a function of internal energy

```
REAL FUNCTION TUAIR(U)
```

Input
REAL `U` : internal energy [J/kmol], [J/kg]

Returned
REAL `TUAIR` : temperature [K],[°C]

7.1.17 TUIDG
temperature of ideal gas as a function of internal energy

```
REAL FUNCTION TUIDG(ISUB,U)
```

Input
INTEGER `ISUB` : substance index of the gas
REAL `U` : internal energy [J/kmol], [J/kg]

Returned
REAL `TUIDG` : temperature [K],[°C]

7.2 SUBROUTINEs

7.2.1 AIRTP
properties of air as a function of temperature and pressure

```
SUBROUTINE AIRTP(IERR,AMM,T,P,V,CP,CV,W,U,H,S)
```

Input
REAL `T` : temperature [K],[°C]
REAL `P` : pressure [Pa],[bar]

Output
INTEGER `IERR` : error detection code
0 : no error
-2 : invalid ARGUMENT(s)
REAL `AMM` : molar mass [kg/kmol]
REAL `V` : volume [m^3/kmol], [m^3/kg]
REAL `CP` : isobaric specific heat [J/(kmol·K)], [J/(kg·K)]
REAL `CV` : isochoric specific heat [J/(kmol·K)], [J/(kg·K)]
REAL `W` : speed of sound [m/s]
REAL `U` : internal energy [J/kmol], [J/kg]
REAL `H` : enthalpy [J/kmol], [J/kg]
REAL `S` : absolute entropy [J/(kmol·K)], [J/(kg·K)]

7.2.2 CHOTBL
properties of comlplete combustion-by-air product of $C_XH_YO_Z$ at 0.1MPa, Keenan-Chao-Kaye-style gas table.

```
SUBROUTINE CHOTBL(IERR,X,Y,Z,AF,AMM,T,H,PR,U,VR,SO)
```

Input
REAL `AF` : air factor (≥ 1)
REAL `T` : temperature [K],[°C]
REAL `X` : value of `X`
REAL `Y` : value of `Y`
REAL `Z` : value of `Z`

Output
INTEGER IERR : error detection code
0 : no error
-2 : invalid ARGUMENT(s)
REAL AMM : molar mass [kg/kmol]
REAL H : enthalpy [J/kmol], [J/kg]
REAL PR : relative pressure, $= \exp\left(\frac{1}{R}\int_{T_{ref}}^{T}\frac{c_p}{T}dt\right)$ [-]
REAL U : internal energy [J/kmol], [J/kg]
REAL VR : relative volume, $= \exp\left(-\frac{1}{R}\int_{T_{ref}}^{T}\frac{c_v}{T}dt\right)$ [-]
REAL SO : entropy function, $= \int_{Tref}^{T}\frac{c_p}{T}dT$ [J/(kmol·K)], [J/(kg·K)]
where T_{ref} is the reference temperature 298.15K(25°C).

7.2.3 FUELML

mole fractions of comlplete combustion-by-moist-air products of the mixture of $C_XH_YO_Z$ fuels.

```
SUBROUTINE FUELML(IERR,A,IR,AF,XW,XC,XH,XN,XO)
```

Input
REAL ARRAY A(1:4,1:IR) : parameters for a component fuel of the mixture of $C_XH_YO_Z$ fuels.
REAL ARRAY A(1,I) : mole fraction of the ith component fuel
REAL A(2,I) : value of X of the ith component fuel
REAL A(3,I) : value of Y of the ith component fuel
REAL A(4,I) : value of Z of the ith component fuel
INTEGER IR : number of component fuels of the mixture
REAL AF : air factor (≥ 1)
REAL XW : absolute humidity of the moist air [kg/kg of dry air]

Output
INTEGER IERR : error detection code
0 : no error
-2 : invalid ARGUMENT(s)
REAL XC : mole fraction of CO_2 in the combustion products [-]
REAL XH : mole fraction of H_2O in the combustion products [-]
REAL XN : mole fraction of N_2 in the combustion products [-]
REAL XO : mole fraction of O_2 in the combustion products [-]

7.2.4 IDGCMM

conversion from mole to mass, or reverse, for ideal gas

```
SUBROUTINE IDGCMM(IERR,ITRNS,ISUB,X,Y)
```

Input
INTEGER ITRNS : direction of conversion
$= 0$: conversion from mole to mass
$\neq 0$: conversion from mass to mole
INTEGER ISUB : substance index of the gas
REAL X: mole (for ITRNS $= 0$) or mass (for ITRNS$\neq 0$)

Output
INTEGER IERR : error detection code
0 : no error
-3 : invalid substance index ISUB specified
REAL Y : mass (for ITRNS $= 0$) or mole (for ITRNS $\neq 0$)

7.2.5 IDGFND

critical fundamental constants

```
SUBROUTINE IDGFND(IERR,ISUB,C,ANAME)
```

Input
INTEGER `ISUB` : substance index

Output
INTEGER `IERR` : error detection code
0 : no error
-3 : invalid substance index `ISUB` specified
REAL ARRAY `C(1:10)`
`C(1)` : molar mass [kg/kmol]
`C(2)` : critical temperature [K], [°C]
`C(3)` : critical pressure [Pa], [bar]
`C(4)` : critical volume [m^3/kmol], [m^3/kg]
`C(5)` : ideal gas absolute entropy at reference state of 0.1MPa and 25°C, [J/(kmol· K)], [J/(kg · K)]
`C(6)` : ideal gas enthalpy of formation at reference state of 0.1MPa and 25°C, [[J/kmol], [J/kg]
`C(7)` : ideal gas Gibbs energy of formation at reference state of 0.1MPa and 25°C, [J/(kmol· K)], [J/(kg · K)]
`C(8)` : lower bound of temperature for the ideal gas isobaric specific heat equation [K], [°C]
`C(9)` : upper bound of temperature for the ideal gas isobaric specific heat equation [K], [°C]
`C(10)` : type of state
= 10 : ideal gas and reference state
= 11 : ideal gas
= 19 : ideal gas (not included in JANAF Table [3])
CHARACTER*25 `ANAME` : name of substance

7.2.6 IDGT

properties of ideal gases at 0.1 MPa, JANAF-style table

```
SUBROUTINE IDGT(IERR,ISUB,T,A,ANAME)
```

Input
INTEGER `ISUB` : substance index
REAL `T` : temperature [K],[°C]

Output
INTEGER `IERR` : error detection code
0 : no error
-2 : invalid ARGUMENT(s)
-3 : invalid substance index `ISUB` specified
REAL ARRAY `A(1:4)`
`A(1)` : isobaric specific heat [J/(kmol·K)], [J/(kg·K)]
`A(2)` : absolute entropy [J/(kmol·K)], [J/(kg·K)]
`A(3)` : $-gref^\circ(T) = -\dfrac{g^\circ(T) - h^\circ(T_{ref})}{T}$ [J/(kmol·K)], [J/(kg·K)]
where $g^\circ(T)$ and $h^\circ(T_{ref})$ are the Gibbs free energy at a temperature T and the enthalpy at the reference temperature of 298.15K, respectively.
`A(4)` : enthalpy [J/kmol], [J/kg]
CHARACTER*25 `ANAME` : name of substance

7.2.7 IDGTBL

properties of ideal gases at 0.1MPa, Keenan-Chao-Kaye-style gas table

```
SUBROUTINE IDGTBL(IERR,ISUB,T,H,PR,U,VR,SO)
```

Input
INTEGER `ISUB` : substance index of the gas
REAL `T` : temperature [K],[°C]

Output
INTEGER `IERR` : error detection code
0 : no error
-2 : invalid ARGUMENT(s)

-3 : invalid substance index `ISUB` specified
REAL `AMM` : molar mass [kg/kmol]
REAL `H` : enthalpy [J/kmol], [J/kg]
REAL `PR` : relative pressure $= \exp\left(-\frac{1}{R}\int_{T_{ref}}^{T}\frac{c_p}{T}dt\right)$ [-]
REAL `U` : internal energy [J/kmol], [J/kg]
REAL `VR` : relative volume $= \exp\left(-\frac{1}{R}\int_{T_{ref}}^{T}\frac{c_v}{T}dt\right)$ [-]
REAL `S0` : entropy function, $= \int_{Tref}^{T}\frac{c_p}{T}dT$ [J/(kmol·K)], [J/(kg·K)]
where T_{ref} is the reference temperature 298.15K.

7.2.8 IDGTP

properties of ideal gas as a function of temperature and pressure.

```
SUBROUTINE IDGTP(IERR,ISUB,T,P,V,CP,CV,WS,U,H,S,ANAME)
```

Input
INTEGER `ISUB` : substance index
REAL `T` : temperature [K],[°C]
REAL `P` : pressure [Pa],[bar]

Output
INTEGER `IERR` : error detection code
0 : no error
-2 : invalid ARGUMENT(s)
-3 : invalid substance index `ISUB` specified
REAL `AMM` : molar mass [kg/kmol]
REAL `V` : volume [m^3/kmol], [m^3/kg]
REAL `CP` : isobaric specific heat [J/(kmol·K)], [J/(kg·K)]
REAL `CV` : isochoric specific heat [J/(kmol·K)], [J/(kg·K)]
REAL `W` : speed of sound [m/s]
REAL `U` : internal energy [J/kmol], [J/kg]
REAL `H` : enthalpy [J/kmol], [J/kg]
REAL `S` : absolute entropy [J/(kmol·K)], [J/(kg·K)]
CHARACTER*25 `ANAME` : name of substance

7.2.9 IPINIT

Initialization

```
SUBROUTINE IPINIT(K1,K2,K3,KGAS,GASC)
```

Input
INTEGER `K1` : value of `KPA` for the units of pressure and temperature
INTEGER `K2` : value of `KMOL` for the unit of amount of substance
INTEGER `K3` : value of `MESS` for error message
INTEGER `KGAS` : universal gas constant = 8.31451×10^3 J/(kmol·K) (built-in value) when `KGAS`=0
REAL `GASC` : universal gas constant = `GASC` (user's selection) when `KGAS`$\neq$ 0

Output
The values of `KPA`, `KMOL`, `MESS` and `GASCON` are sent to COMMON BLOCK `UNIT` and `CNST`. See section 1.1 and chapter 3.

7.2.10 MIXCMM

conversion from mass fraction to mole, or reverse, for mixture of ideal gases

```
SUBROUTINE MIXCMM(IERR,ITRNS,ISUBNO,ISUB,X,Y)
```

Input
INTEGER `ITRNS` : direction to conversion
= 0 : mole fraction to mass fraction
≠ 0 : mass fraction to mole fraction
INTEGER `ISUBNO` : number of component gases
INTEGER ARRAY `ISUB(1:ISUBNO)` : substance index of the `ISUBNO` components
REAL ARRAY `X(1:ISUBNO)` : mole fraction (for `ITRNS`=0) or mass fraction (for `ITRNS` ≠ 0) of the ith component

Output
INTEGER `IERR` : error detection code
0 : no error
-3 : invalid substance index, or invalid number of components
REAL ARRAY `Y(1:ISUBNO)` : mass fraction (for `ITRNS`=0) or mole fraction (for `ITRNS` ≠ 0) of the ith component

7.2.11 MIXTP

properties of a mixture of ideal gases as a function of temperature and pressure

```
SUBROUTINE MIXTP(IERR,ISUBNO,ISUB,AM,AMM,TI,PI,V,CP,CV,W,U,H,S)
```

Input
REAL `T` : temperature [K],[°C]
REAL `P` : pressure [Pa],[bar]
INTEGER `ISUBNO` : number of component gases
INTEGER ARRAY `ISUB(1:ISUBNO)` : substance index of the `ISUBNO` components
REAL ARRAY `AM(1:ISUBNO)` : molar fraction of the `ISUBNO` components

Output
INTEGER `IERR` : error detection code
0 : no error
-2 : invalid ARGUMENT(s)
-3 : invalid substance index `ISUB` specified
REAL `AMM` : molar mass [kg/kmol]
REAL `V` : volume [m^3/kmol], [m^3/kg]
REAL `CP` : isobaric specific heat [J/(kmol·K)], [J/(kg·K)]
REAL `CV` : isochoric specific heat [J/(kmol·K)], [J/(kg·K)]
REAL `W` : speed of sound [m/s]
REAL `U` : internal energy [J/kmol], [J/kg]
REAL `H` : enthalpy [J/kmol], [J/kg]
REAL `S` : absolute entropy [J/(kmol·K)], [J/(kg·K)]