Supporting Information

Geometry Transformation of Ionic Surfactants and Adsorption Behavior on *n*-decane/Water-interface: Calculation by Molecular Dynamics Simulation and DFT Study

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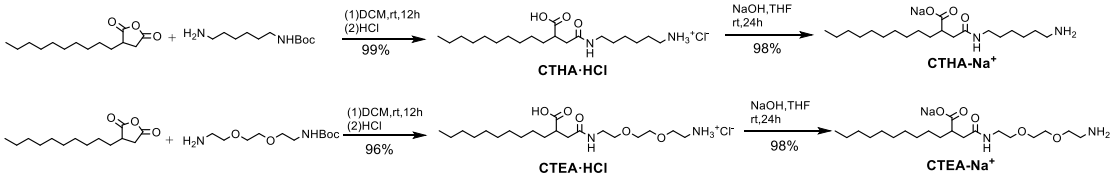
1. Analytical Methods

Nuclear magnetic resonance (NMR) spectra were recorded in D_2O using a NMR spectrometer (an AVANCE III 500; Bruker instrument [Karlsruhe, Baden-Württemberg, Germany]). The chemical shifts are reported as parts per million downfield from tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet.).

2. Synthesis



Synthesis of the CTHA·HCl:

(1) Decylsuccinic anhydride (0.98g, 4.1mmol) and Boc-protected diamine were dissolved in 20 mL of dichloromethane in a 250 mL flask, and the mixture was stirred for 12 h. After the reaction, the product was purified by column chromatography.

(2) Add 6 mol/L HCl 20 mL to the product obtained in the previous step, and stir it at room temperature for 48h, and with the reaction going on, there are flakes formed in the system, and then the system becomes white emulsion. After the reaction is completed, a certain amount of methanol is added to the system to make water and methanol form azeotropes, and the water and methanol was removed under vacuum and the structures of the samples were confirmed using NMR.

Synthesis of the $CTHA^-Na^+$:

(1) **CHTA·HCl** (0.39g, 1mmol) was dissolved in 5mL H_2O, and 80 mg (2mmol) NaOH slowly added. Stirred at room temperature for 24 h. After stopping stirring, remove the solvent and get the product.

Synthesis of the CTEA·HCl:

(1) Decylsuccinic anhydride (0.96g, 4.1mmol) and Boc-protected 1,8-Diamino-3,6-dioxaoctane were dissolved in 20 mL of dichloromethane in a 250 mL flask, and the

mixture was stirred for 12 h. After the reaction, the product was purified by column chromatography.

(2) Add 6 mol/L HCl 20 mL to the product obtained in the previous step, and stir it at room temperature for 48h, and with the reaction going on, there are flakes formed in the system, and then the system becomes white emulsion. After the reaction is completed, the solution was removed under vacuum and the structures of the samples were confirmed using NMR.

Synthesis of the $CTEA^-Na^+$:

(1) **CHTA·HCl** (0.434g, 1mmol) was dissolved in 5mL H_2O, and (80 mg, 2mmol) NaOH slowly added. Stirred at room temperature for 24 h. After stopping stirring, remove the solvent and get the product.

3. Spectra of compounds

The structures of two compounds were characterized as compound **CHTA·HCl** and compound **CETA·HCl** respectively. Compounds **$CTHA^-Na^+$** and **$CTEA^-Na^+$** are derived from compounds **CHTA·HCl** and **CETA·HCl** with a simple acid-base reaction. Therefore, the structures of compounds **$CTHA^-Na^+$** and **$CTEA^-Na^+$** have not been characterized.

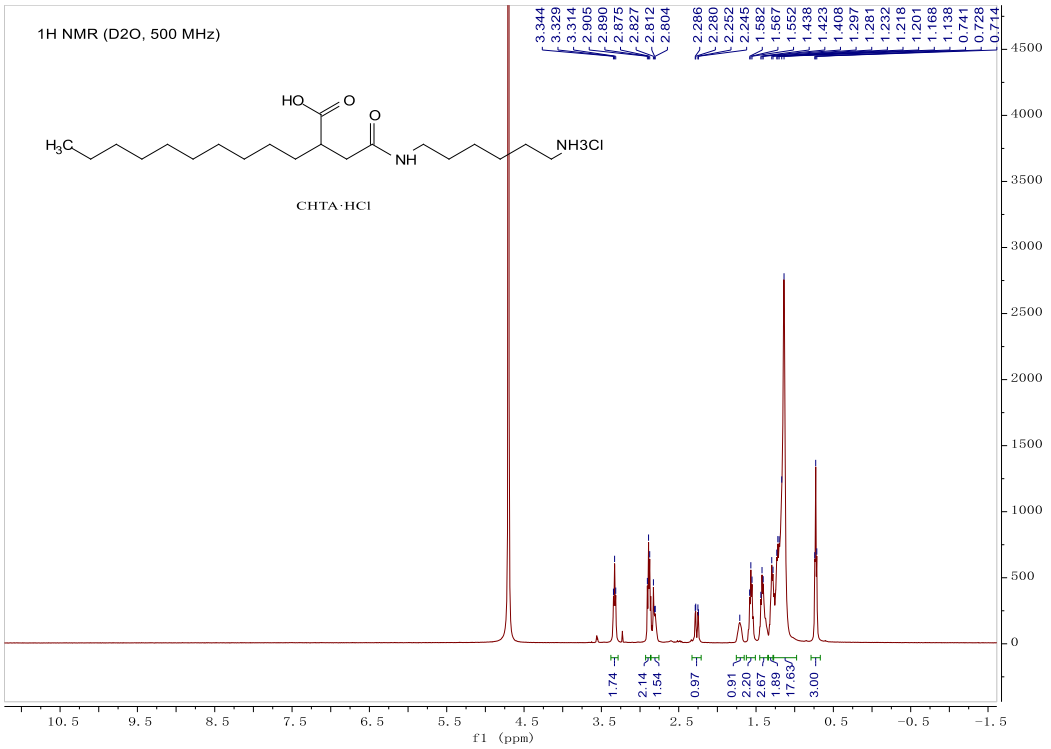


Fig. S1. ^{1}H NMR of compound CTHA·HCl (D_2O)

(**CHTA·HCl**) white solid, (99.7%); R_f = 0.2, DCM : MeOH=5:3; IR (KBr): 3457, 1699, 1466, 3391, 1345, 1609, 1409, 1199 cm^{-1}; ^{1}H NMR (500 MHz, D_2O) δ 3.32 (t, *J* = 7.4 Hz, 2H), 2.89 (t, *J* = 7.5 Hz, 2H), 2.82 (t, *J* = 11.7 Hz, 2H), 2.28-2.24 (m, *J* = 20.5 Hz, 1H), 1.71 (m, 1H), 1.56 (t, *J* = 7.5 Hz, 2H), 1.42 (d, *J* = 8.2 Hz, 3H), 1.29 (d, *J* = 14.8 Hz, 2H), 1.23-1.13 (m, *J* =7 Hz, 18H) 0.73 (t, *J* = 6.6 Hz, 3H).

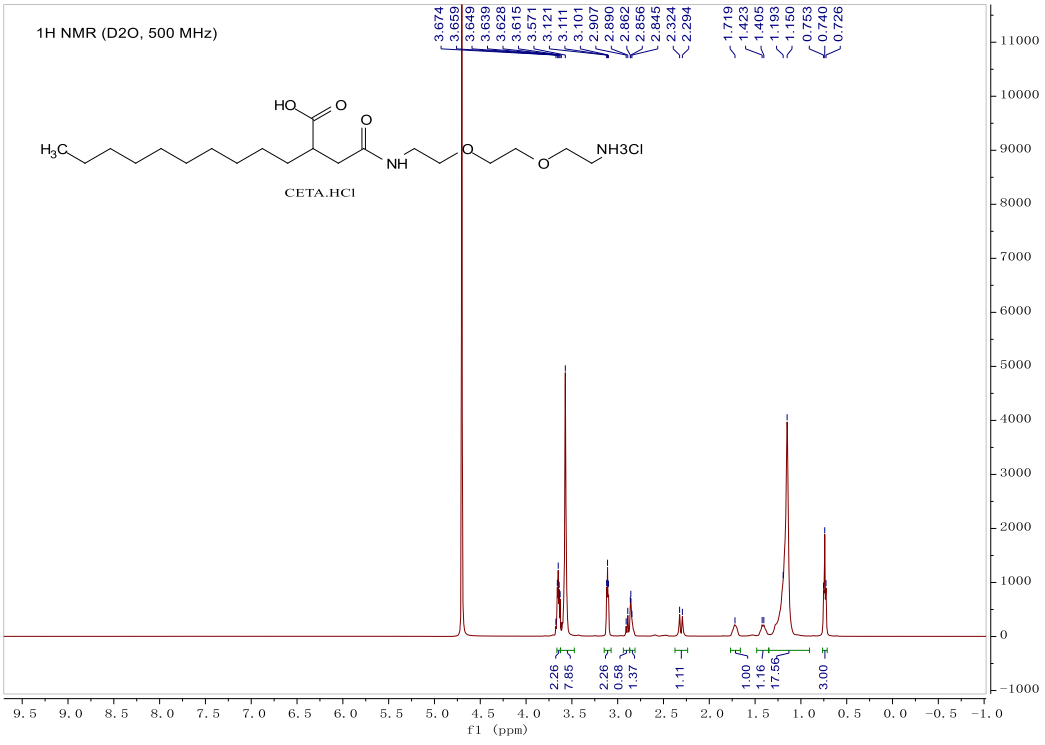


Fig. S2. ^{1}H NMR of compound CTEA·HCl (D_2O)

(**CETA·HCl**) white solid, (96.1%); R_f = 0.2, DCM : MeOH= 5:3; IR (KBr): 3461, 3402, 2929, 2858, 1705, 1609, 1453, 1403, 1336, 1195, 1130, 950 cm^{-1}; ^1H NMR (500 MHz, D_2O) δ 3.64 (dt, *J* = 15.5, 7.5 Hz, 2H), 3.57 (s, 8H), 2.89 (t, *J*=8.5 Hz, 1H), 2.85 (m, *J*=3 Hz, 8.5Hz), 2.32 (d, *J* = 15 Hz, 2H), 1.71 (m, 1H), 1.42(d, *J* = 9 Hz, 1H), 1.193-1.15 (m, *J* = 21.5 Hz, 18H), 0.74 (t, *J* = 13.5 Hz, 3H).

4. System Information

TABLE S1. System Information[a,b]

system	N_{sur}	A_s (nm^2/sur)	γ_{sim} (mN/m)	γ_{cmc} (mN/m)
decane/water	0	-	51.4	51.7[a]
2-1	31	0.81	35.81	34.97[b]
2-2	25	1.00	29.39	28.65[b]
3-1	34	0.73	30.94	30.58[b]
3-2	27	0.92	26.43	25.18[b]

a Experimental γ of decane/water interface.

b Experimental interfacial tensions at the critical micelle concentration provided in the Supporting Information. All literature data and the experimental interfacial tension was measured at 298 K.

5. Equilibrium structures of MD simulation

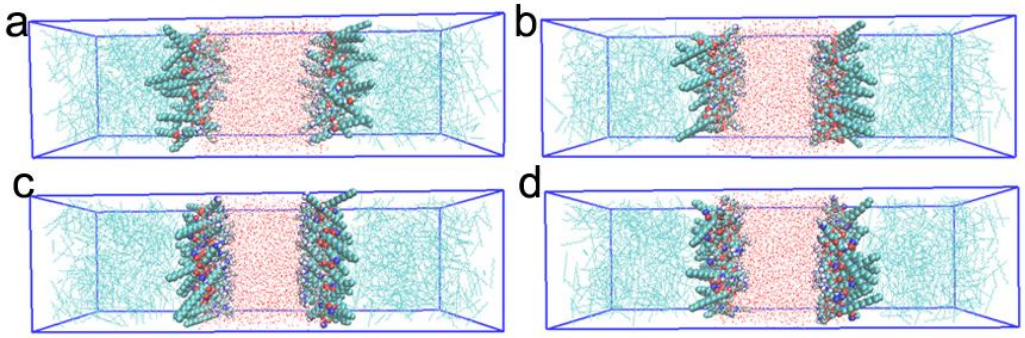


Fig. S3 Equilibrium structures of MD simulation: a) **CTHA·HCl** b) **$CTHA^-Na^+$** c) **CTEA·HCl** d) **$CTEA^-Na^+$.** The initial simulation box for the oil-water-surfactant system measured around 5 × 5 × 17 nm^3. The x and y dimensions (~5 nm) of the systems were kept constant to maintain stable interfaces, leaving the z dimension (~17 nm) adjustable for an appropriate pressure.

6. Equilibrated System: Surfactant Conformation

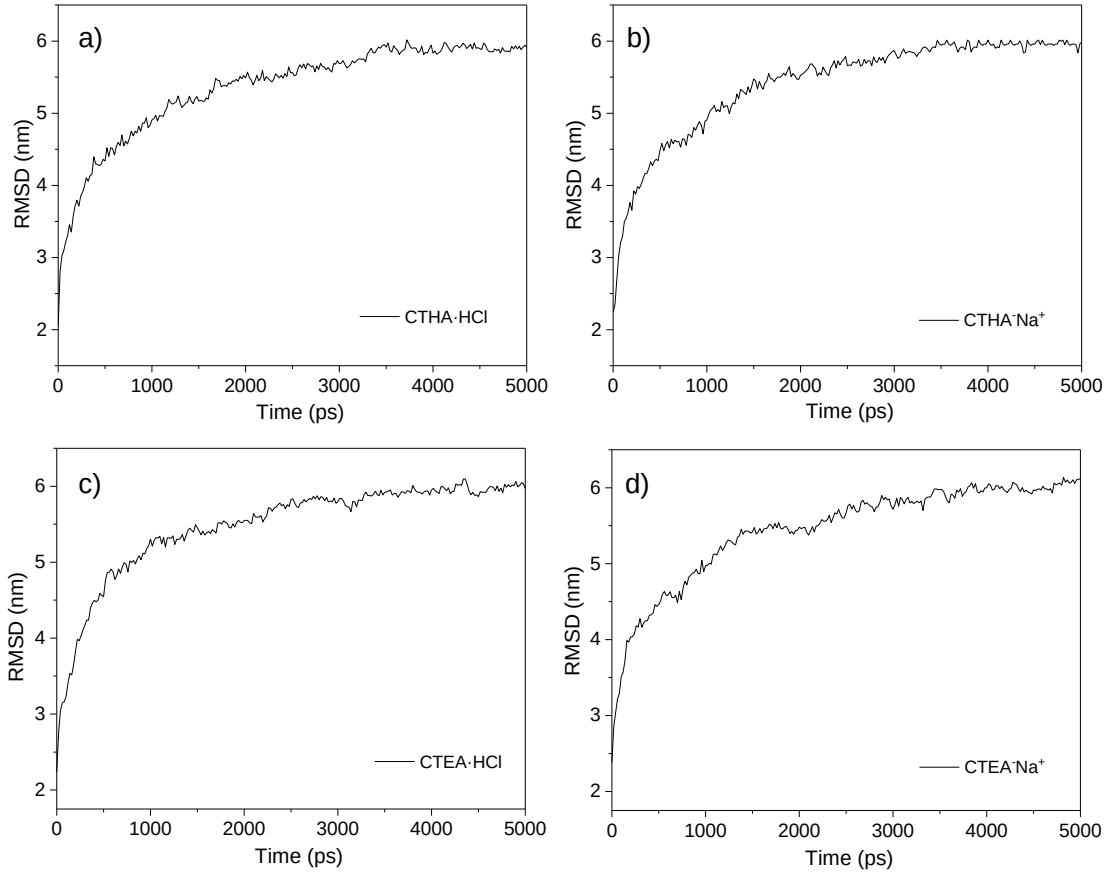


Fig. S4 RMSD of MD simulation: a) **CTHA·HCl** b) **CTHA$^-$Na$^+$** c) **CTEA·HCl** d) **CTEA$^-$Na$^+$**

7. Bonded Forcefield

; Table 2.5.2.1

; GROMOS bond-stretching parameters

;

;

; Bond type code

; Force constant

; Ideal bond length

; Examples of usage in terms of non-bonded atom types

;

;

; ICB(H)[N] CB[N] B0[N]

;

```
#define gb_1              0.1000    1.5700e+07
; H    -    OA           750
;
#define gb_2              0.1000    1.8700e+07
; H    -    N (all) 895
;
#define gb_3              0.1090    1.2300e+07
; HC    -    C           700
;
#define gb_4               0.112    3.7000e+07
; C - O (CO in heme)    2220
;
#define gb_5              0.1230    1.6600e+07
; C    - O              1200
;
#define gb_6              0.1250    1.3400e+07
; C    - OM             1000
;
#define gb_7              0.1320    1.2000e+07
; CR1    -    NR (6-ring)      1000
;
#define gb_8              0.1330    8.8700e+06
; H    -    S            750
;
#define gb_9              0.1330    1.0600e+07
; C    -    NT, NL    900
;
#define gb_10             0.1330    1.1800e+07
; C, CR1    -    N, NR, CR1, C (peptide, 5-ring)            1000
;
```

```
#define gb_11              0.1340    1.0500e+07

; C    -    N, NZ, NE              900

;

#define gb_12              0.1340    1.1700e+07

; C    -    NR (no H) (6-ring)           1000

;

#define gb_13              0.1360    1.0200e+07

; C    -    OA           900

;

#define gb_14              0.1380    1.1000e+07

; C    -    NR (heme)             1000

;

#define gb_15              0.1390    8.6600e+06

; CH2    -    C, CR1 (6-ring)             800

;

#define gb_16              0.1390    1.0800e+07

; C, CR1    -    CH2, C, CR1 (6-ring)             1000

;

#define gb_17              0.1400    8.5400e+06

; C, CR1, CH2    -    NR (6-ring)      800

;

#define gb_18              0.1430    8.1800e+06

; CHn    -    OA       800

;

#define gb_19              0.1430    9.2100e+06

; CHn    -    OM       900

;

#define gb_20              0.1435    6.1000e+06

; CHn    -    OA (sugar)       600

;
```

```
#define gb_21            0.1470    8.7100e+06
; CHn    -    N, NT, NL, NZ, NE          900
;
#define gb_22            0.1480    5.7300e+06
; CHn    -    NR (5-ring)      600
;
#define gb_23            0.1480    7.6400e+06
; CHn    -      NR (6-ring)    800
;
#define gb_24            0.1480    8.6000e+06
; O, OM    -      P          900
;
#define gb_25            0.1500    8.3700e+06
; O    -    S              900
;
#define gb_26            0.1520    5.4300e+06
; CHn    -      CHn (sugar)    600
;
#define gb_27            0.1530    7.1500e+06
; C, CHn    -      C, CHn        800
;
#define gb_28            0.1610    4.8400e+06
; OA    -      P          600
;
#define gb_29            0.1630    4.7200e+06
; OA    -      SI        600
;
#define gb_30            0.1780    2.7200e+06
; FE    -    C (Heme)
;
```

```
#define gb_31           0.1780    5.9400e+06
; CH3    -     S       900
;
#define gb_32           0.1830    5.6200e+06
; CH2    -     S       900
;
#define gb_33           0.1870    3.5900e+06
; CH1    -     SI      600
;
#define gb_34            0.198    0.6400e+06
; NR     -     FE      120
;
#define gb_35            0.200    0.6280e+06
; NR (heme)    -    FE      120
;
#define gb_36           0.2040    5.0300e+06
; S      -     S          1000
;
#define gb_37            0.221    0.5400e+06
; NR     -    FE         126
;
#define gb_38           0.1000    2.3200e+07
; HWat    -     OWat             1110
;
#define gb_39           0.1100    1.2100e+07
; HChl    -     CChl             700
;
#define gb_40           0.1758    8.1200e+06
; CChl    -     CLChl            1200
;
```

```
#define gb_41            0.1530    8.0400e+06
; ODmso    -     SDmso          900
;
#define gb_42         0.193799    4.9500e+06
; SDmso    -     CDmso          890
;
#define gb_43            0.1760    8.1000e+06
; CCl4    -     CLCl4           1200
;
#define gb_44            0.1265    1.3100e+07
; CUrea    -    OUrea           1000
;
#define gb_45             0.135    1.0300e+07
; CUrea    -    NUrea           900
;
#define gb_46         0.163299    8.7100e+06
; HWat    -     HWat            1110
;
#define gb_47         0.233839    2.6800e+06
; HChl    -     CLChl           700
;
#define gb_48         0.290283    2.9800e+06
; CLChl -     CLChl           1200
;
#define gb_49         0.279388    2.3900e+06
; ODmso -     CDmso           890
;
#define gb_50         0.291189    2.1900e+06
; CDmso -     CDmso           890
;
```

#define gb_51 0.2077 3.9700e+06

; HMet - CMet 820

;

#define gb_52 0.287407 3.0400e+06

; CLCl4 - CLCl4 1200

;

;---

; Table 2.5.3.1.

; GROMOS bond-angle bending parameters

;

;

; Bond-angle type code

; Force constant

; Ideal bond angle

; Example of usage in terms of non-bonded atom types

;

;

; ICT(H)[N] CT[N] (T0[N])

;

#define ga_1 90.00 380.00

; NR(heme) - FE - C 90

;

#define ga_2 90.00 420.00

; NR(heme) - FE - NR(heme) 100

;

#define ga_3 96.00 405.00

; H - S - CH2 95

;

#define ga_4 100.00 475.00

; CH2 - S - CH3 110

;

#define ga_5 103.00 420.00

; OA - P - OA 95

;

#define ga_6 104.00 490.00

; CH2 - S - S 110

;

#define ga_7 108.00 465.00

; NR, C, CR1(5-ring) 100

;

#define ga_8 109.50 285.00

; CHn - CHn - CHn, NR(6-ring) (sugar) 60

;

#define ga_9 109.50 320.00

; CHn, OA - CHn - OA, NR(ring) (sugar) 68

;

#define ga_10 109.50 380.00

; H - NL, NT - H, CHn - OA - CHn(sugar) 80

;

#define ga_11 109.50 425.00

; H - NL - C, CHn H - NT - CHn 90

;

#define ga_12 109.50 450.00

; X - OA, SI - X 95

;

#define ga_13 109.50 520.00

; CHn,C - CHn - C, CHn, OA, OM, N, NE 110

;

#define ga_14 109.60 450.00

; OM - P - OA 95

;

#define ga_15 111.00 530.00

; CHn - CHn - C, CHn, OA, NR, NT, NL 110

;

#define ga_16 113.00 545.00

; CHn - CH2 - S 110

;

#define ga_17 115.00 50.00

; NR(heme) - FE - NR 10

;

#define ga_18 115.00 460.00

; H - N - CHn 90

;

#define ga_19 115.00 610.00

; CHn, C - C - OA, N, NT, NL 120

;

#define ga_20 116.00 465.00

; H - NE - CH2 90

;

#define ga_21 116.00 620.00

; CH2 - N - CH1 120

;

#define ga_22 117.00 635.00

; CH3 - N - C, CHn - C - OM 120

;

#define ga_23 120.00 390.00

; H - NT, NZ, NE - C 70

;

#define ga_24 120.00 445.00

; H - NT, NZ - H 80

;

#define ga_25 120.00 505.00

; H - N - CH3, H, HC - 6-ring, H - NT - CHn 90

;

#define ga_26 120.00 530.00

; P, SI - OA - CHn, P 95

;

#define ga_27 120.00 560.00

; N, C, CR1 (6-ring, no H) 100

;

#define ga_28 120.00 670.00

; NZ - C - NZ, NE 120

;

#define ga_29 120.00 780.00

; OM - P - OM 140

;

#define ga_30 121.00 685.00

; O - C - CHn, C CH3 - N - CHn 120

;

#define ga_31 122.00 700.00

; CH1, CH2 - N - C 120

;

#define ga_32 123.00 415.00

; H - N - C 70

;

#define ga_33 124.00 730.00

; O - C - OA, N, NT, NL C - NE - CH2 120

;

#define ga_34 125.00 375.00

; FE - NR - CR1 (5-ring) 60

;

#define ga_35 125.00 750.00

; - 120

;

#define ga_36 126.00 575.00

; H, HC - 5-ring 90

;

#define ga_37 126.00 640.00

; X(noH) - 5-ring 100

;

#define ga_38 126.00 770.00

; OM - C - OM 120

;

#define ga_39 132.00 760.00

; 5, 6 ring connnection 100

;

#define ga_40 155.00 2215.00

; SI - OA - SI 95

;

#define ga_41 180.00 91350.00

; Fe - C - O (heme) 57

;

#define ga_42 109.50 434.00

; HWat - OWat - HWat 92

;

#define ga_43 107.57 484.00

; HChl - CChl - CLChl 105

;

#define ga_44 111.30 632.00

; CLChl - CChl - CLChl 131

;

#define ga_45 97.40 469.00

; CDmso - SDmso - CDmso 110

;

#define ga_46 106.75 503.00

; CDmso - SDmso - ODmso 110

;

#define ga_47 108.53 443.00

; HMet - OMet - CMet 95

;

#define ga_48 109.50 618.00

; CLCl4 - CCl4 - CLCl4 131

;

#define ga_49 107.60 507.00

; FTFE - CTFE - FTFE 100

;

#define ga_50 109.50 448.00

; HTFE - OTFE - CHTFE 85

;

#define ga_51 110.3 524.00

; OTFE - CHTFE - CTFE 97

;

#define ga_52 111.4 532.00

; CHTFE - CTFE - FTFE 95

;

#define ga_53 117.2 636.00

; NUrea - CUrea - NUrea 120

;

#define ga_54 121.4 690.00

; OUrea - CUrea - NUrea 120

```
;
;           Table 2.5.4.1
;           GROMOS improper (harmonic) dihedral angle parameters
;
;
; Improper dihedral-angle type code
; Force constant
; Ideal improper dihedral angle
; Example of usage
;
;
; ICQ(H)[N] CQ[N] (Q0[N])
;
#define gi_1                0.0     167.42309
; planar groups 40
;
#define gi_2          35.26439     334.84617
; tetrahedral centres      80
;
#define gi_3                0.0     669.69235
; heme iron         160
;
#define gi_4              180.0     167.42309
; planar groups 40
;
#define gi_5         -35.26439     334.84617
; tetrahedral centres      80
;
;           Table 2.5.5.1 (Note: changes with respect to the 43A1 table)
;           GROMOS (trigonometric) dihedral torsional angle parameters
```

```
;
;
; Dihedral-angle type code
; Force constant
; Phase shift
; Multiplicity
; Example of usage in terms of non-bonded atom types
;
;
; ICP(H)[N]    CP[N] PD[N] NP[N]
;
#define gd_1        180.000          2.67              1
; CHn-CHn-CHn-OA (sugar)    0.6
;
#define gd_2        180.000          3.41              1
; OA-CHn-OA-CHn,H (beta sugar) 0.8
;
#define gd_3        180.000          4.97              1
; OA-CHn-CHn-OA (sugar)     1.2
;
#define gd_4        180.000          5.86              1
; N-CHn-CHn-OA (lipid) 1.4
;
#define gd_5        180.000          9.35              1
; OA-CHn-CHn-OA (sugar)     2.2
;
#define gd_6        180.000          9.45              1
; OA-CHn-OA-CHn,H (alpha sugar)    2.3
;
#define gd_7          0.000          2.79              1
```

; P-O5*-C5*-C4* (dna) 0.7

;

#define gd_8 0.000 5.35 1

; O5*-C5*-C4*-O4* (dna) 1.3

;

#define gd_9 180.000 1.53 2

; C1-C2-CAB-CBB (heme) 0.4

;

#define gd_10 180.000 5.86 2

; -C-C- 1.4

;

#define gd_11 180.000 7.11 2

; -C-OA,OE- (at ring) 1.7

;

#define gd_12 180.000 16.7 2

; -C-OA,OE- (carboxyl) 4.0

;

#define gd_13 180.000 24.0 2

; CHn-OE-C-CHn (ester lipid) 5.7

;

#define gd_14 180.000 33.5 2

; -C-N,NT,NE,NZ,NR- 8.0

;

#define gd_15 180.000 41.8 2

; -C-CR1- (6-ring) 10.0

;

#define gd_16 0.000 0.0 2

; -CH1(sugar)-NR(base) 0.0

;

#define gd_17 0.000 0.418 2

; O-CH1-CHn-no O 0.1

;

#define gd_18 0.000 2.09 2

; O-CH1-CHn-O 0.5

;

#define gd_19 0.000 3.14 2

; -OA-P- 0.75

;

#define gd_20 0.000 5.09 2

; O-P-O- (dna, lipids) 1.2

;

#define gd_21 0.000 16.7 2

; -S-S-4.0

;

#define gd_22 0.000 1.05 3

; -OA-P- 0.25

;

#define gd_23 0.000 1.26 3

; -CHn-OA(no sugar)- 0.3

;

#define gd_24 0.000 1.30 3

; HTFE-OTFE-CHTFE-CTFE 0.3

;

#define gd_25 0.000 2.53 3

; O5*-C5*-C4*-O4* (dna) 0.6

;

#define gd_26 0.000 2.93 3

; -CH2-S- 0.7

;

#define gd_27 0.000 3.19 3

; O-P-O- (dna, lipids) 0.8

;

#define gd_28 0.000 3.65 3

; OA-CHn-OA-CHn,H (alpha sugar) 0.9

;

#define gd_29 0.000 3.77 3

; -C,CHn,SI- 0.9

;

#define gd_30 0.000 3.90 3

; CHn-CHn-OA-H (sugar) 0.9

;

#define gd_31 0.000 4.18 3

; HC-C-S- 1.0

;

#define gd_32 0.000 4.69 3

; AO-CHn-OA-CHn,H (beta sugar)

;

#define gd_33 0.000 5.44 3

; HC-C-C- 1.3

;

#define gd_34 0.000 5.92 3

; -CHn,SI-CHn- 1.4

;

#define gd_35 0.000 7.69 3

; OA-CHn-CHn-OA (sugar) 1.8

;

#define gd_36 0.000 8.62 3

; N-CHn-CHn-OA (lipid) 2.1

;

#define gd_37 0.000 9.50 3

; OA-CHn-CHn-OA (sugar) 2.3

;

#define gd_38 0.000 0.0 4

; -NR-FE- 0.0

;

#define gd_39 180.000 1.0 6

; -CHn-N,NE- 0.24

;

#define gd_40 0.000 1.0 6

; -CHn-C,NR(ring), CR1-0.24

;

#define gd_41 0.000 3.77 6

; -CHn-NT- 0.9

;

#define gd_42 180.000 3.5 2

; Backbone dihedral angle -N-CA-C-N- 0.84

;

#define gd_43 0.000 2.8 3

; Backbone dihedral angle -C-N-CA-C- 0.67

;

#define gd_44 180.000 0.7 6

; Backbone dihedral angle -C-N-CA-C- 0.17

;

#define gd_45 0.000 0.4 6

; Backbone dihedral angle -N-CA-C-N- 0.096

;

; get the constraint distances for dummy atom constructions

#include "ff_dum.itp"

```
[ constrainttypes ]

; now the constraints for the rigid NH3 groups

 MNH3       C       2      DC_MNC1

 MNH3    CH1       2      DC_MNC2

 MNH3    CH2       2      DC_MNC2

 MNH3 MNH3       2      DC_MNMN

; and the angle-constraints for OH and SH groups in proteins:

   CH2       H       2      DC_CO

   CH1       H       2      DC_CO

      C       H       2      DC_CO

      P       H       2      DC_PO


; bond-, angle- and dihedraltypes for specbonds:

[ bondtypes ]

S          S           2       gb_36

NR         FE          2       gb_34


[ angletypes ]

CH1       CH2       S         2      ga_16

CH2       S         S         2      ga_6

CR1       NR        FE        2    ga_34

NR        FE        NR        2      ga_17


[ dihedraltypes ]

S          S          1      gd_21

NR         FE         1      gd_38

CH2       S          1      gd_26
```

non-bonded forcefield

[atomtypes]

;name	at.num	mass	charge	ptype	c6	c12
O	8	0.000	0.000	A	0.0022619536	1e-06
OM	8	0.000	0.000	A	0.0022619536	7.4149321e-07
OA	8	0.000	0.000	A	0.0022619536	1.505529e-06
OE	8	0.000	0.000	A	0.0022619536	1.21e-06
OW	8	0.000	0.000	A	0.0026173456	2.634129e-06
N	7	0.000	0.000	A	0.0024364096	2.319529e-06
NT	7	0.000	0.000	A	0.0024364096	5.0625e-06
NL	7	0.000	0.000	A	0.0024364096	2.319529e-06
NR	7	0.000	0.000	A	0.0024364096	3.389281e-06
NZ	7	0.000	0.000	A	0.0024364096	2.319529e-06
NE	7	0.000	0.000	A	0.0024364096	2.319529e-06
C	6	0.000	0.000	A	0.0023406244	4.937284e-06
CH0	6	0.000	0.000	A	0.0023970816	0.0002053489
CH1	6	0.000	0.000	A	0.00606841	9.70225e-05
CH2	6	0.000	0.000	A	0.0074684164	3.3965584e-05
CH3	6	0.000	0.000	A	0.0096138025	2.6646244e-05
CH4	6	0.000	0.000	A	0.01317904	3.4363044e-05
CH2r	6	0.000	0.000	A	0.0073342096	2.8058209e-05
CR1	6	0.000	0.000	A	0.0055130625	1.5116544e-05
HC	1	0.000	0.000	A	8.464e-05	1.5129e-08
H	1	0.000	0.000	A	0	0
DUM	0	0.000	0.000	A	0	0
S	16	0.000	0.000	A	0.0099840064	1.3075456e-05
CU1+	29	0.000	0.000	A	0.0004182025	5.1251281e-09
CU2+	29	0.000	0.000	A	0.0004182025	5.1251281e-09
FE	26	0.000	0.000	A	0	0
ZN2+	30	0.000	0.000	A	0.0004182025	9.4400656e-09

MG2+	12	0.000	0.000	A	6.52864e-05	3.4082244e-09
CA2+	20	0.000	0.000	A	0.00100489	4.9801249e-07
P	15	0.000	0.000	A	0.01473796	2.2193521e-05
AR	18	0.000	0.000	A	0.0062647225	9.847044e-06
F	9	0.000	0.000	A	0.0011778624	7.6073284e-07
CL	17	0.000	0.000	A	0.0087647044	1.5295921e-05
BR	35	0.000	0.000	A	0.02765569	6.5480464e-05
CMet	6	0.000	0.000	A	0.0088755241	1.936e-05
OMet	8	0.000	0.000	A	0.0022619536	2.325625e-06
NA+	11	0.000	0.000	A	7.884019264e-05	7.290000e-08
CL-	17	0.000	0.000	A	0.0128097124	6.0466176e-05
CChl	6	0.000	0.000	A	0.0026308693	4.064256e-06
CLChl	17	0.000	0.000	A	0.0083066819	1.3764842e-05
HChl	1	0.000	0.000	A	3.76996e-05	4.2999495e-09
SDmso	16	0.000	0.000	A	0.010561673	2.149806e-05
CDmso	6	0.000	0.000	A	0.0096138025	2.6646244e-05
ODmso	8	0.000	0.000	A	0.0022707131	7.5144626e-07
CCl4	6	0.000	0.000	A	0.0026308693	7.5999462e-06
CLCl4	17	0.000	0.000	A	0.0076040144	1.2767758e-05
FTFE	9	0.000	0.000	A	0.0011778624	1e-06
CTFE	6	0.000	0.000	A	0.0023406244	3.374569e-06
CHTFE	6	0.000	0.000	A	0.0071048041	2.5775929e-05
OTFE	8	0.000	0.000	A	0.0022619536	1.505529e-06
CUrea	6	0.000	0.000	A	0.0048868488	1.3589545e-05
OUrea	8	0.000	0.000	A	0.0023639044	1.5898688e-06
NUrea	7	0.000	0.000	A	0.0033527574	3.9509513e-06
SI	14	0.000	0.000	A	0.01473796	2.2193521e-05
MNH3	0	0.000	0.000	A	0.0	0.0
MW	0	0.000	0.000	D	0.0	0.0
CH3p	6	0.000	0.000	A	0.0096138025	2.6646244e-05

```
      I       0          0.000          0.000        A       0.0455822      0.000148352
  CLOpt       0          0.000          0.000        A      0.00674862      8.24838e-06
      B       0          0.000          0.000        A      0.00234062      4.93728e-06
     SE       0          0.000          0.000        A      0.00998401      1.30755e-05
   HS14       0          0.000          0.000        A               0                0
  CLAro       0          0.000          0.000        A      0.00674862      8.24838e-06
  BROpt       0          0.000          0.000        A       0.0342028      0.000120341
  OEOpt       0          0.000          0.000        A      0.00308914      4.77422e-06
   NOpt       0          0.000          0.000        A      0.00826281        2.916e-05
   CAro       0          0.000          0.000        A      0.00234062      4.45632e-06
   CPos       0          0.000          0.000        A        0.002025            1e-06
   NPri       0          0.000          0.000        A        0.010816          4.9e-05
   NTer       0          0.000          0.000        A      0.00863041        2.025e-05
   OAlc       0          0.000          0.000        A      0.00177494        1.21e-06


[ nonbond_params ]
;      i      j      func  c6     c12
       OM     O      1     2.261954E-03     8.611000E-07
       OA     O      1     2.261954E-03     1.386510E-06
       OA     OM     1     2.261954E-03     2.258907E-06
       OE     O      1     2.261954E-03     1.100000E-06
       OE     OM     1     2.261954E-03     9.472100E-07
       OE     OA     1     2.261954E-03     1.505529E-06
       OW     O      1     2.433170E-03     1.833990E-06
       OW     OM     1     2.433170E-03     2.987943E-06
       OW     OA     1     2.433170E-03     1.991421E-06
       OW     OE     1     2.433170E-03     1.991421E-06
       N      O      1     2.347562e-03     1.943000e-06
       N      OM     1     2.347562E-03     3.577063E-06
       N      OA     1     2.347562E-03     2.384061E-06
```

N	OE	1	2.347562E-03	2.384061E-06
N	OW	1	2.525258E-03	3.153489E-06
NT	O	1	2.347562E-03	2.542500E-06
NT	OM	1	2.347562E-03	4.142250E-06
NT	OA	1	2.347562E-03	2.760750E-06
NT	OE	1	2.347562E-03	2.760750E-06
NT	OW	1	2.525258E-03	3.651750E-06
NT	N	1	2.436410E-03	4.371750E-06
NL	O	1	2.347562E-03	3.466840E-06
NL	OM	1	2.347562E-03	9.412624E-06
NL	OA	1	2.347562E-03	3.764436E-06
NL	OE	1	2.347562E-03	3.764436E-06
NL	OW	1	2.525258E-03	4.979364E-06
NL	N	1	2.436410E-03	2.319529E-06
NL	NT	1	2.436410E-03	6.903000E-06
NR	O	1	2.347562E-03	2.080330E-06
NR	OM	1	2.347562E-03	3.389281E-06
NR	OA	1	2.347562E-03	2.258907E-06
NR	OE	1	2.347562E-03	2.258907E-06
NR	OW	1	2.525258E-03	2.987943E-06
NR	N	1	2.436410E-03	3.577063E-06
NR	NT	1	2.436410E-03	4.142250E-06
NR	NL	1	2.436410E-03	5.648188E-06
NZ	O	1	2.347562E-03	2.427240E-06
NZ	OM	1	2.347562E-03	6.590064E-06
NZ	OA	1	2.347562E-03	2.635596E-06
NZ	OE	1	2.347562E-03	2.635596E-06
NZ	OW	1	2.525258E-03	3.486204E-06
NZ	N	1	2.436410E-03	2.319529E-06
NZ	NT	1	2.436410E-03	4.833000E-06

NZ	NL	1	2.436410E-03	2.319529E-06
NZ	NR	1	2.436410E-03	3.954468E-06
NE	O	1	2.347562E-03	2.241920E-06
NE	OM	1	2.347562E-03	6.086912E-06
NE	OA	1	2.347562E-03	2.434368E-06
NE	OE	1	2.347562E-03	2.434368E-06
NE	OW	1	2.525258E-03	3.220032E-06
NE	N	1	2.436410E-03	2.319529E-06
NE	NT	1	2.436410E-03	4.464000E-06
NE	NL	1	2.436410E-03	2.319529E-06
NE	NR	1	2.436410E-03	3.652544E-06
NE	NZ	1	2.436410E-03	2.319529E-06
C	O	1	2.300953E-03	2.222000E-06
C	OM	1	2.300953E-03	1.913364E-06
C	OA	1	2.300953E-03	2.444200E-06
C	OE	1	2.300953E-03	2.444200E-06
C	OW	1	2.475121E-03	3.606306E-06
C	N	1	2.388037E-03	3.384106E-06
C	NT	1	2.388037E-03	3.384106E-06
C	NL	1	2.388037E-03	3.384106E-06
C	NR	1	2.388037E-03	3.384106E-06
C	NZ	1	2.388037E-03	3.384106E-06
C	NE	1	2.388037E-03	3.384106E-06
CH0	O	1	2.328538E-03	1.433000E-05
CH0	OM	1	2.328538E-03	1.233956E-05
CH0	OA	1	2.328538E-03	1.576300E-05
CH0	OE	1	2.328538E-03	1.576300E-05
CH0	OW	1	2.504794E-03	2.325759E-05
CH0	N	1	2.416666E-03	2.182459E-05
CH0	NT	1	2.416666E-03	2.182459E-05

CH0	NL	1	2.416666E-03	2.182459E-05
CH0	NR	1	2.416666E-03	2.182459E-05
CH0	NZ	1	2.416666E-03	2.182459E-05
CH0	NE	1	2.416666E-03	2.182459E-05
CH0	C	1	2.368685E-03	3.184126E-05
CH1	O	1	3.704924E-03	9.850000E-06
CH1	OM	1	3.704924E-03	8.481835E-06
CH1	OA	1	3.704924E-03	1.083500E-05
CH1	OE	1	3.704924E-03	1.083500E-05
CH1	OW	1	3.985364E-03	1.598655E-05
CH1	N	1	3.845144E-03	1.500155E-05
CH1	NT	1	3.845144E-03	1.500155E-05
CH1	NL	1	3.845144E-03	1.500155E-05
CH1	NR	1	3.845144E-03	1.500155E-05
CH1	NZ	1	3.845144E-03	1.500155E-05
CH1	NE	1	3.845144E-03	1.500155E-05
CH1	C	1	3.768802E-03	2.188670E-05
CH1	CH0	1	3.813984E-03	1.411505E-04
CH2	O	1	4.110135E-03	5.828000E-06
CH2	OM	1	4.110135E-03	5.018491E-06
CH2	OA	1	4.110135E-03	6.410800E-06
CH2	OE	1	4.110135E-03	6.410800E-06
CH2	OW	1	4.421247E-03	9.458844E-06
CH2	N	1	4.265691E-03	8.876044E-06
CH2	NT	1	4.265691E-03	8.876044E-06
CH2	NL	1	4.265691E-03	8.876044E-06
CH2	NR	1	4.265691E-03	8.876044E-06
CH2	NZ	1	4.265691E-03	8.876044E-06
CH2	NE	1	4.265691E-03	8.876044E-06
CH2	C	1	4.181000E-03	1.294982E-05

CH2	CH0	1	4.231123E-03	8.351524E-05
CH2	CH1	1	6.732118E-03	5.740580E-05
CH3	O	1	4.663258E-03	5.162000E-06
CH3	OM	1	4.663258E-03	4.444998E-06
CH3	OA	1	4.663258E-03	5.678200E-06
CH3	OE	1	4.663258E-03	5.678200E-06
CH3	OW	1	5.016238E-03	8.377926E-06
CH3	N	1	4.839748E-03	7.861726E-06
CH3	NT	1	4.839748E-03	7.861726E-06
CH3	NL	1	4.839748E-03	7.861726E-06
CH3	NR	1	4.839748E-03	7.861726E-06
CH3	NZ	1	4.839748E-03	7.861726E-06
CH3	NE	1	4.839748E-03	7.861726E-06
CH3	C	1	4.743659E-03	1.146996E-05
CH3	CH0	1	4.800528E-03	7.397146E-05
CH3	CH1	1	7.638095E-03	5.084570E-05
CH3	CH2	1	8.473481E-03	3.008414E-05
CH4	O	1	5.459888E-03	5.862000E-06
CH4	OM	1	5.459888E-03	5.047768E-06
CH4	OA	1	5.459888E-03	6.448200E-06
CH4	OE	1	5.459888E-03	6.448200E-06
CH4	OW	1	5.873168E-03	9.514026E-06
CH4	N	1	5.666528E-03	8.927826E-06
CH4	NT	1	5.666528E-03	8.927826E-06
CH4	NL	1	5.666528E-03	8.927826E-06
CH4	NR	1	5.666528E-03	8.927826E-06
CH4	NZ	1	5.666528E-03	8.927826E-06
CH4	NE	1	5.666528E-03	8.927826E-06
CH4	C	1	5.554024E-03	1.302536E-05
CH4	CH0	1	5.620608E-03	8.400246E-05

CH4	CH1	1	8.942920E-03	5.774070E-05
CH4	CH2	1	9.921016E-03	3.416374E-05
CH4	CH3	1	1.125614E-02	3.025964E-05
CH2r	O	1	4.073038E-03	5.297000E-06
CH2r	OM	1	4.073038E-03	4.561247E-06
CH2r	OA	1	4.073038E-03	5.826700E-06
CH2r	OE	1	4.073038E-03	5.826700E-06
CH2r	OW	1	4.381342E-03	8.597031E-06
CH2r	N	1	4.227190E-03	8.067331E-06
CH2r	NT	1	4.227190E-03	8.067331E-06
CH2r	NL	1	4.227190E-03	8.067331E-06
CH2r	NR	1	4.227190E-03	8.067331E-06
CH2r	NZ	1	4.227190E-03	8.067331E-06
CH2r	NE	1	4.227190E-03	8.067331E-06
CH2r	C	1	4.143263E-03	1.176993E-05
CH2r	CH0	1	4.192934E-03	7.590601E-05
CH2r	CH1	1	6.671356E-03	5.217545E-05
CH2r	CH2	1	7.401009E-03	3.087092E-05
CH2r	CH3	1	8.397002E-03	2.734311E-05
CH2r	CH4	1	9.831472E-03	3.105101E-05
CR1	O	1	3.531330E-03	3.888000E-06
CR1	OM	1	3.531330E-03	3.347957E-06
CR1	OA	1	3.531330E-03	4.276800E-06
CR1	OE	1	3.531330E-03	4.276800E-06
CR1	OW	1	3.798630E-03	6.310224E-06
CR1	N	1	3.664980E-03	5.921424E-06
CR1	NT	1	3.664980E-03	5.921424E-06
CR1	NL	1	3.664980E-03	5.921424E-06
CR1	NR	1	3.664980E-03	5.921424E-06
CR1	NZ	1	3.664980E-03	5.921424E-06

CR1	NE	1	3.664980E-03	5.921424E-06
CR1	C	1	3.592215E-03	8.639136E-06
CR1	CH0	1	3.635280E-03	5.571504E-05
CR1	CH1	1	5.784075E-03	3.829680E-05
CR1	CH2	1	6.416685E-03	2.265926E-05
CR1	CH3	1	7.280212E-03	2.006986E-05
CR1	CH4	1	8.523900E-03	2.279146E-05
CR1	CH2r	1	6.358770E-03	2.059474E-05
HC	O	1	4.375520E-04	1.230000E-07
HC	OM	1	4.375520E-04	1.059153E-07
HC	OA	1	4.375520E-04	1.353000E-07
HC	OE	1	4.375520E-04	1.353000E-07
HC	OW	1	4.706720E-04	1.996290E-07
HC	N	1	4.541120E-04	1.873290E-07
HC	NT	1	4.541120E-04	1.873290E-07
HC	NL	1	4.541120E-04	1.873290E-07
HC	NR	1	4.541120E-04	1.873290E-07
HC	NZ	1	4.541120E-04	1.873290E-07
HC	NE	1	4.541120E-04	1.873290E-07
HC	C	1	4.450960E-04	2.733060E-07
HC	CH0	1	4.504320E-04	1.762590E-06
HC	CH1	1	7.166800E-04	1.211550E-06
HC	CH2	1	7.950640E-04	7.168440E-07
HC	CH3	1	9.020600E-04	6.349260E-07
HC	CH4	1	1.056160E-03	7.210260E-07
HC	CH2r	1	7.878880E-04	6.515310E-07
HC	CR1	1	6.831000E-04	4.782240E-07
H	O	1	0.000000E+00	0.000000E+00
H	OM	1	0.000000E+00	0.000000E+00
H	OA	1	0.000000E+00	0.000000E+00

H OE 1 0.000000E+00 0.000000E+00

H OW 1 0.000000E+00 0.000000E+00

H N 1 0.000000E+00 0.000000E+00

H NT 1 0.000000E+00 0.000000E+00

H NL 1 0.000000E+00 0.000000E+00

H NR 1 0.000000E+00 0.000000E+00

H NZ 1 0.000000E+00 0.000000E+00

H NE 1 0.000000E+00 0.000000E+00

H C 1 0.000000E+00 0.000000E+00

H CH0 1 0.000000E+00 0.000000E+00

H CH1 1 0.000000E+00 0.000000E+00

H CH2 1 0.000000E+00 0.000000E+00

H CH3 1 0.000000E+00 0.000000E+00

H CH4 1 0.000000E+00 0.000000E+00

H CH2r 1 0.000000E+00 0.000000E+00

H CR1 1 0.000000E+00 0.000000E+00

H HC 1 0.000000E+00 0.000000E+00

DUM O 1 0.000000E+00 0.000000E+00

DUM OM 1 0.000000E+00 0.000000E+00

DUM OA 1 0.000000E+00 0.000000E+00

DUM OE 1 0.000000E+00 0.000000E+00

DUM OW 1 0.000000E+00 0.000000E+00

DUM N 1 0.000000E+00 0.000000E+00

DUM NT 1 0.000000E+00 0.000000E+00

DUM NL 1 0.000000E+00 0.000000E+00

DUM NR 1 0.000000E+00 0.000000E+00

DUM NZ 1 0.000000E+00 0.000000E+00

DUM NE 1 0.000000E+00 0.000000E+00

DUM C 1 0.000000E+00 0.000000E+00

DUM CH0 1 0.000000E+00 0.000000E+00

DUM	CH1	1	0.000000E+00	0.000000E+00
DUM	CH2	1	0.000000E+00	0.000000E+00
DUM	CH3	1	0.000000E+00	0.000000E+00
DUM	CH4	1	0.000000E+00	0.000000E+00
DUM	CH2r	1	0.000000E+00	0.000000E+00
DUM	CR1	1	0.000000E+00	0.000000E+00
DUM	HC	1	0.000000E+00	0.000000E+00
DUM	H	1	0.000000E+00	0.000000E+00
S	O	1	4.752195E-03	3.616000E-06
S	OM	1	4.752195E-03	3.113738E-06
S	OA	1	4.752195E-03	3.977600E-06
S	OE	1	4.752195E-03	3.977600E-06
S	OW	1	5.111907E-03	5.868768E-06
S	N	1	4.932051E-03	5.507168E-06
S	NT	1	4.932051E-03	5.507168E-06
S	NL	1	4.932051E-03	5.507168E-06
S	NR	1	4.932051E-03	5.507168E-06
S	NZ	1	4.932051E-03	5.507168E-06
S	NE	1	4.932051E-03	5.507168E-06
S	C	1	4.834130E-03	8.034752E-06
S	CH0	1	4.892083E-03	5.181728E-05
S	CH1	1	7.783768E-03	3.561760E-05
S	CH2	1	8.635086E-03	2.107405E-05
S	CH3	1	9.797156E-03	1.866579E-05
S	CH4	1	1.147082E-02	2.119699E-05
S	CH2r	1	8.557149E-03	1.915395E-05
S	CR1	1	7.419060E-03	1.405901E-05
S	HC	1	9.192640E-04	4.447680E-07
S	H	1	0.000000E+00	0.000000E+00
S	DUM	1	0.000000E+00	0.000000E+00

CU1+ O	1	9.726020E-04	2.542500E-07
CU1+ OM	1	9.726020E-04	6.903000E-07
CU1+ OA	1	9.726020E-04	2.760750E-07
CU1+ OE	1	9.726020E-04	2.760750E-07
CU1+ OW	1	1.046222E-03	3.651750E-07
CU1+ N	1	1.009412E-03	1.090316E-07
CU1+ NT	1	1.009412E-03	1.090316E-07
CU1+ NL	1	1.009412E-03	1.090316E-07
CU1+ NR	1	1.009412E-03	4.142250E-07
CU1+ NZ	1	1.009412E-03	1.090316E-07
CU1+ NE	1	1.009412E-03	1.090316E-07
CU1+ C	1	9.893710E-04	1.590730E-07
CU1+ CH0	1	1.001232E-03	1.025885E-06
CU1+ CH1	1	1.593055E-03	7.051615E-07
CU1+ CH2	1	1.767289E-03	4.172265E-07
CU1+ CH3	1	2.005122E-03	3.695476E-07
CU1+ CH4	1	2.347660E-03	4.196606E-07
CU1+ CH2r	1	1.751338E-03	3.792122E-07
CU1+ CR1	1	1.518412E-03	2.783419E-07
CU1+ HC	1	1.881400E-04	8.805570E-09
CU1+ H	1	0.000000E+00	0.000000E+00
CU1+ DUM	1	0.000000E+00	0.000000E+00
CU1+ S	1	2.043364E-03	2.588694E-07
CU2+ O	1	9.726020E-04	4.622830E-07
CU2+ OM	1	9.726020E-04	1.255119E-06
CU2+ OA	1	9.726020E-04	5.019657E-07
CU2+ OE	1	9.726020E-04	5.019657E-07
CU2+ OW	1	1.046222E-03	6.639693E-07
CU2+ N	1	1.009412E-03	1.090316E-07
CU2+ NT	1	1.009412E-03	1.090316E-07

CU2+	NL	1	1.009412E-03	1.090316E-07
CU2+	NR	1	1.009412E-03	7.531531E-07
CU2+	NZ	1	1.009412E-03	1.090316E-07
CU2+	NE	1	1.009412E-03	1.090316E-07
CU2+	C	1	9.893710E-04	1.590730E-07
CU2+	CH0	1	1.001232E-03	1.025885E-06
CU2+	CH1	1	1.593055E-03	7.051615E-07
CU2+	CH2	1	1.767289E-03	4.172265E-07
CU2+	CH3	1	2.005122E-03	3.695476E-07
CU2+	CH4	1	2.347660E-03	4.196606E-07
CU2+	CH2r	1	1.751338E-03	3.792122E-07
CU2+	CR1	1	1.518412E-03	2.783419E-07
CU2+	HC	1	1.881400E-04	8.805570E-09
CU2+	H	1	0.000000E+00	0.000000E+00
CU2+	DUM	1	0.000000E+00	0.000000E+00
CU2+	S	1	2.043364E-03	2.588694E-07
CU2+	CU1+	1	4.182025E-04	5.125128E-09
FE	O	1	0.000000E+00	0.000000E+00
FE	OM	1	0.000000E+00	0.000000E+00
FE	OA	1	0.000000E+00	0.000000E+00
FE	OE	1	0.000000E+00	0.000000E+00
FE	OW	1	0.000000E+00	0.000000E+00
FE	N	1	0.000000E+00	0.000000E+00
FE	NT	1	0.000000E+00	0.000000E+00
FE	NL	1	0.000000E+00	0.000000E+00
FE	NR	1	0.000000E+00	0.000000E+00
FE	NZ	1	0.000000E+00	0.000000E+00
FE	NE	1	0.000000E+00	0.000000E+00
FE	C	1	0.000000E+00	0.000000E+00
FE	CH0	1	0.000000E+00	0.000000E+00

FE	CH1	1	0.000000E+00	0.000000E+00
FE	CH2	1	0.000000E+00	0.000000E+00
FE	CH3	1	0.000000E+00	0.000000E+00
FE	CH4	1	0.000000E+00	0.000000E+00
FE	CH2r	1	0.000000E+00	0.000000E+00
FE	CR1	1	0.000000E+00	0.000000E+00
FE	HC	1	0.000000E+00	0.000000E+00
FE	H	1	0.000000E+00	0.000000E+00
FE	DUM	1	0.000000E+00	0.000000E+00
FE	S	1	0.000000E+00	0.000000E+00
FE	CU1+	1	0.000000E+00	0.000000E+00
FE	CU2+	1	0.000000E+00	0.000000E+00
ZN2+	O	1	9.726020E-04	1.097908E-07
ZN2+	OM	1	9.726020E-04	2.980869E-07
ZN2+	OA	1	9.726020E-04	1.192153E-07
ZN2+	OE	1	9.726020E-04	1.192153E-07
ZN2+	OW	1	1.046222E-03	1.576907E-07
ZN2+	N	1	1.009412E-03	1.479747E-07
ZN2+	NT	1	1.009412E-03	1.479747E-07
ZN2+	NL	1	1.009412E-03	1.479747E-07
ZN2+	NR	1	1.009412E-03	1.788716E-07
ZN2+	NZ	1	1.009412E-03	1.479747E-07
ZN2+	NE	1	1.009412E-03	1.479747E-07
ZN2+	C	1	9.893710E-04	2.158895E-07
ZN2+	CH0	1	1.001232E-03	1.392303E-06
ZN2+	CH1	1	1.593055E-03	9.570260E-07
ZN2+	CH2	1	1.767289E-03	5.662485E-07
ZN2+	CH3	1	2.005122E-03	5.015399E-07
ZN2+	CH4	1	2.347660E-03	5.695519E-07
ZN2+	CH2r	1	1.751338E-03	5.146565E-07

ZN2+	CR1	1	1.518412E-03	3.777581E-07
ZN2+	HC	1	1.881400E-04	1.195068E-08
ZN2+	H	1	0.000000E+00	0.000000E+00
ZN2+	DUM	1	0.000000E+00	0.000000E+00
ZN2+	S	1	2.043364E-03	3.513306E-07
ZN2+	CU1+	1	4.182025E-04	6.955684E-09
ZN2+	CU2+	1	4.182025E-04	6.955684E-09
ZN2+	FE	1	0.000000E+00	0.000000E+00
MG2+	O	1	3.842848E-04	6.596940E-08
MG2+	OM	1	3.842848E-04	1.791098E-07
MG2+	OA	1	3.842848E-04	7.163226E-08
MG2+	OE	1	3.842848E-04	7.163226E-08
MG2+	OW	1	4.133728E-04	9.475074E-08
MG2+	N	1	3.988288E-04	8.891274E-08
MG2+	NT	1	3.988288E-04	8.891274E-08
MG2+	NL	1	3.988288E-04	8.891274E-08
MG2+	NR	1	3.988288E-04	1.074776E-07
MG2+	NZ	1	3.988288E-04	8.891274E-08
MG2+	NE	1	3.988288E-04	8.891274E-08
MG2+	C	1	3.909104E-04	1.297204E-07
MG2+	CH0	1	3.955968E-04	8.365854E-07
MG2+	CH1	1	6.294320E-04	5.750430E-07
MG2+	CH2	1	6.982736E-04	3.402386E-07
MG2+	CH3	1	7.922440E-04	3.013576E-07
MG2+	CH4	1	9.275840E-04	3.422236E-07
MG2+	CH2r	1	6.919712E-04	3.092389E-07
MG2+	CR1	1	5.999400E-04	2.269814E-07
MG2+	HC	1	7.433600E-05	7.180740E-09
MG2+	H	1	0.000000E+00	0.000000E+00
MG2+	DUM	1	0.000000E+00	0.000000E+00

MG2+	S	1	8.073536E-04	2.111021E-07
MG2+	CU1+	1	1.652360E-04	4.179424E-09
MG2+	CU2+	1	1.652360E-04	4.179424E-09
MG2+	FE	1	0.000000E+00	0.000000E+00
MG2+	ZN2+	1	1.652360E-04	5.672201E-09
CA2+	O	1	1.507652E-03	7.974410E-07
CA2+	OM	1	1.507652E-03	2.165088E-06
CA2+	OA	1	1.507652E-03	8.658939E-07
CA2+	OE	1	1.507652E-03	8.658939E-07
CA2+	OW	1	1.621772E-03	1.145351E-06
CA2+	N	1	1.564712E-03	1.074781E-06
CA2+	NT	1	1.564712E-03	1.074781E-06
CA2+	NL	1	1.564712E-03	1.074781E-06
CA2+	NR	1	1.564712E-03	1.299194E-06
CA2+	NZ	1	1.564712E-03	1.074781E-06
CA2+	NE	1	1.564712E-03	1.074781E-06
CA2+	C	1	1.533646E-03	1.568065E-06
CA2+	CH0	1	1.552032E-03	1.011268E-05
CA2+	CH1	1	2.469430E-03	6.951145E-06
CA2+	CH2	1	2.739514E-03	4.112820E-06
CA2+	CH3	1	3.108185E-03	3.642823E-06
CA2+	CH4	1	3.639160E-03	4.136813E-06
CA2+	CH2r	1	2.714788E-03	3.738093E-06
CA2+	CR1	1	2.353725E-03	2.743762E-06
CA2+	HC	1	2.916400E-04	8.680110E-08
CA2+	H	1	0.000000E+00	0.000000E+00
CA2+	DUM	1	0.000000E+00	0.000000E+00
CA2+	S	1	3.167464E-03	2.551811E-06
CA2+	CU1+	1	6.482650E-04	5.052106E-08
CA2+	CU2+	1	6.482650E-04	5.052106E-08

CA2+	FE	1	0.000000E+00	0.000000E+00
CA2+	ZN2+	1	6.482650E-04	6.856581E-08
CA2+	MG2+	1	2.561360E-04	4.119877E-08
P	O	1	5.773784E-03	5.323430E-06
P	OM	1	5.773784E-03	1.445335E-05
P	OA	1	5.773784E-03	5.780397E-06
P	OE	1	5.773784E-03	5.780397E-06
P	OW	1	6.210824E-03	7.645953E-06
P	N	1	5.992304E-03	7.174853E-06
P	NT	1	5.992304E-03	7.174853E-06
P	NL	1	5.992304E-03	7.174853E-06
P	NR	1	5.992304E-03	8.672951E-06
P	NZ	1	5.992304E-03	7.174853E-06
P	NE	1	5.992304E-03	7.174853E-06
P	C	1	5.873332E-03	1.046784E-05
P	CH0	1	5.943744E-03	6.750863E-05
P	CH1	1	9.457060E-03	4.640335E-05
P	CH2	1	1.049139E-02	2.745571E-05
P	CH3	1	1.190327E-02	2.431818E-05
P	CH4	1	1.393672E-02	2.761588E-05
P	CH2r	1	1.039670E-02	2.495417E-05
P	CR1	1	9.013950E-03	1.831637E-05
P	HC	1	1.116880E-03	5.794530E-07
P	H	1	0.000000E+00	0.000000E+00
P	DUM	1	0.000000E+00	0.000000E+00
P	S	1	1.213029E-02	1.703498E-05
P	CU1+	1	2.482630E-03	3.372605E-07
P	CU2+	1	2.482630E-03	3.372605E-07
P	FE	1	0.000000E+00	0.000000E+00
P	ZN2+	1	2.482630E-03	4.577208E-07

P	MG2+	1	9.809120E-04	2.750282E-07
P	CA2+	1	3.848380E-03	3.324553E-06
AR	O	1	3.764374E-03	3.138000E-06
AR	OM	1	3.764374E-03	2.702132E-06
AR	OA	1	3.764374E-03	3.451800E-06
AR	OE	1	3.764374E-03	3.451800E-06
AR	OW	1	4.049314E-03	5.092974E-06
AR	N	1	3.906844E-03	4.779174E-06
AR	NT	1	3.906844E-03	4.779174E-06
AR	NL	1	3.906844E-03	4.779174E-06
AR	NR	1	3.906844E-03	4.779174E-06
AR	NZ	1	3.906844E-03	4.779174E-06
AR	NE	1	3.906844E-03	4.779174E-06
AR	C	1	3.829277E-03	6.972636E-06
AR	CH0	1	3.875184E-03	4.496754E-05
AR	CH1	1	6.165785E-03	3.090930E-05
AR	CH2	1	6.840143E-03	1.828826E-05
AR	CH3	1	7.760657E-03	1.619836E-05
AR	CH4	1	9.086420E-03	1.839496E-05
AR	CH2r	1	6.778406E-03	1.662199E-05
AR	CR1	1	5.876887E-03	1.220054E-05
AR	HC	1	7.281800E-04	3.859740E-07
AR	H	1	0.000000E+00	0.000000E+00
AR	DUM	1	0.000000E+00	0.000000E+00
AR	S	1	7.908668E-03	1.134701E-05
AR	CU1+	1	1.618617E-03	2.246494E-07
AR	CU2+	1	1.618617E-03	2.246494E-07
AR	FE	1	0.000000E+00	0.000000E+00
AR	ZN2+	1	1.618617E-03	3.048881E-07
AR	MG2+	1	6.395320E-04	1.831964E-07

AR	CA2+	1	2.509055E-03	2.214487E-06
AR	P	1	9.608810E-03	1.478312E-05
F	O	1	1.632259E-03	8.722000E-07
F	OM	1	1.632259E-03	7.510514E-07
F	OA	1	1.632259E-03	1.505529E-06
F	OE	1	1.632259E-03	9.594200E-07
F	OW	1	1.755811E-03	1.991421E-06
F	N	1	1.694035E-03	2.384061E-06
F	NT	1	1.694035E-03	2.760750E-06
F	NL	1	1.694035E-03	3.764436E-06
F	NR	1	1.694035E-03	2.258907E-06
F	NZ	1	1.694035E-03	2.635596E-06
F	NE	1	1.694035E-03	2.434368E-06
F	C	1	1.660402E-03	1.938028E-06
F	CH0	1	1.680307E-03	1.249863E-05
F	CH1	1	2.673528E-03	8.591170E-06
F	CH2	1	2.965934E-03	5.083182E-06
F	CH3	1	3.365076E-03	4.502296E-06
F	CH4	1	3.939936E-03	5.112836E-06
F	CH2r	1	2.939165E-03	4.620043E-06
F	CR1	1	2.548260E-03	3.391114E-06
F	HC	1	3.157440E-04	1.072806E-07
F	H	1	0.000000E+00	0.000000E+00
F	DUM	1	0.000000E+00	0.000000E+00
F	S	1	3.429254E-03	3.153875E-06
F	CU1+	1	7.018440E-04	2.760750E-07
F	CU2+	1	7.018440E-04	5.019657E-07
F	FE	1	0.000000E+00	0.000000E+00
F	ZN2+	1	7.018440E-04	1.192153E-07
F	MG2+	1	2.773056E-04	7.163226E-08

F	CA2+	1	1.087944E-03	8.658939E-07
F	P	1	4.166448E-03	5.780397E-06
F	AR	1	2.716428E-03	2.736964E-06
CL	O	1	4.452567E-03	3.911000E-06
CL	OM	1	4.452567E-03	3.367762E-06
CL	OA	1	4.452567E-03	4.798797E-06
CL	OE	1	4.452567E-03	4.302100E-06
CL	OW	1	4.789599E-03	6.347553E-06
CL	N	1	4.621083E-03	7.599073E-06
CL	NT	1	4.621083E-03	8.799750E-06
CL	NL	1	4.621083E-03	1.199895E-05
CL	NR	1	4.621083E-03	7.200151E-06
CL	NZ	1	4.621083E-03	8.400828E-06
CL	NE	1	4.621083E-03	7.759424E-06
CL	C	1	4.529336E-03	8.690242E-06
CL	CH0	1	4.583635E-03	5.604463E-05
CL	CH1	1	7.292998E-03	3.852335E-05
CL	CH2	1	8.090640E-03	2.279331E-05
CL	CH3	1	9.179441E-03	2.018858E-05
CL	CH4	1	1.074758E-02	2.292628E-05
CL	CH2r	1	8.017617E-03	2.071657E-05
CL	CR1	1	6.951285E-03	1.520597E-05
CL	HC	1	8.613040E-04	4.810530E-07
CL	H	1	0.000000E+00	0.000000E+00
CL	DUM	1	0.000000E+00	0.000000E+00
CL	S	1	9.354510E-03	1.414218E-05
CL	CU1+	1	1.914529E-03	8.799750E-07
CL	CU2+	1	1.914529E-03	1.599990E-06
CL	FE	1	0.000000E+00	0.000000E+00
CL	ZN2+	1	1.914529E-03	3.799928E-07

CL	MG2+	1	7.564496E-04	2.283242E-07
CL	CA2+	1	2.967754E-03	2.759993E-06
CL	P	1	1.136547E-02	1.842472E-05
CL	AR	1	7.410023E-03	1.227272E-05
CL	F	1	3.213038E-03	3.411174E-06
BR	O	1	7.909228E-03	8.092000E-06
BR	OM	1	7.909228E-03	6.968021E-06
BR	OA	1	7.909228E-03	9.928884E-06
BR	OE	1	7.909228E-03	8.901200E-06
BR	OW	1	8.507908E-03	1.313332E-05
BR	N	1	8.208568E-03	1.572276E-05
BR	NT	1	8.208568E-03	1.820700E-05
BR	NL	1	8.208568E-03	2.482626E-05
BR	NR	1	8.208568E-03	1.489737E-05
BR	NZ	1	8.208568E-03	1.738162E-05
BR	NE	1	8.208568E-03	1.605453E-05
BR	C	1	8.045594E-03	1.798042E-05
BR	CH0	1	8.142048E-03	1.159584E-04
BR	CH1	1	1.295477E-02	7.970620E-05
BR	CH2	1	1.437165E-02	4.716018E-05
BR	CH3	1	1.630571E-02	4.177090E-05
BR	CH4	1	1.909124E-02	4.743530E-05
BR	CH2r	1	1.424193E-02	4.286332E-05
BR	CR1	1	1.234778E-02	3.146170E-05
BR	HC	1	1.529960E-03	9.953160E-07
BR	H	1	0.000000E+00	0.000000E+00
BR	DUM	1	0.000000E+00	0.000000E+00
BR	S	1	1.661670E-02	2.926067E-05
BR	CU1+	1	3.400835E-03	1.820700E-06
BR	CU2+	1	3.400835E-03	3.310437E-06

BR	FE	1	0.000000E+00	0.000000E+00
BR	ZN2+	1	3.400835E-03	7.862187E-07
BR	MG2+	1	1.343704E-03	4.724110E-07
BR	CA2+	1	5.271710E-03	5.710524E-06
BR	P	1	2.018882E-02	3.812141E-05
BR	AR	1	1.316265E-02	2.539270E-05
BR	F	1	5.707416E-03	7.057842E-06
BR	CL	1	1.556901E-02	3.164781E-05
CMet	O	1	4.480628E-03	4.400000E-06
CMet	OM	1	4.480628E-03	3.788840E-06
CMet	OA	1	4.480628E-03	4.840000E-06
CMet	OE	1	4.480628E-03	4.840000E-06
CMet	OW	1	4.819784E-03	7.141200E-06
CMet	N	1	4.650206E-03	6.701200E-06
CMet	NT	1	4.650206E-03	6.701200E-06
CMet	NL	1	4.650206E-03	6.701200E-06
CMet	NR	1	4.650206E-03	6.701200E-06
CMet	NZ	1	4.650206E-03	6.701200E-06
CMet	NE	1	4.650206E-03	6.701200E-06
CMet	C	1	4.557880E-03	9.776800E-06
CMet	CH0	1	4.612522E-03	6.305200E-05
CMet	CH1	1	7.338959E-03	4.334000E-05
CMet	CH2	1	8.141628E-03	2.564320E-05
CMet	CH3	1	9.237291E-03	2.271280E-05
CMet	CH4	1	1.081531E-02	2.579280E-05
CMet	CH2r	1	8.068144E-03	2.330680E-05
CMet	CR1	1	6.995093E-03	1.710720E-05
CMet	HC	1	8.667320E-04	5.412000E-07
CMet	H	1	0.000000E+00	0.000000E+00
CMet	DUM	1	0.000000E+00	0.000000E+00

CMet	S	1	9.413463E-03	1.591040E-05
CMet	CU1+	1	1.926594E-03	3.149960E-07
CMet	CU2+	1	1.926594E-03	3.149960E-07
CMet	FE	1	0.000000E+00	0.000000E+00
CMet	ZN2+	1	1.926594E-03	4.275040E-07
CMet	MG2+	1	7.612168E-04	2.568720E-07
CMet	CA2+	1	2.986457E-03	3.105080E-06
CMet	P	1	1.143709E-02	2.072840E-05
CMet	AR	1	7.456722E-03	1.380720E-05
CMet	F	1	3.233287E-03	3.837680E-06
CMet	CL	1	8.819940E-03	1.720840E-05
CMet	BR	1	1.566712E-02	3.560480E-05
OMet	O	1	2.261954E-03	1.723250E-06
OMet	OM	1	2.261954E-03	2.807525E-06
OMet	OA	1	2.261954E-03	1.871175E-06
OMet	OE	1	2.261954E-03	1.871175E-06
OMet	OW	1	2.433170E-03	2.475075E-06
OMet	N	1	2.347562E-03	2.963075E-06
OMet	NT	1	2.347562E-03	3.431250E-06
OMet	NL	1	2.347562E-03	4.678700E-06
OMet	NR	1	2.347562E-03	2.807525E-06
OMet	NZ	1	2.347562E-03	3.275700E-06
OMet	NE	1	2.347562E-03	3.025600E-06
OMet	C	1	2.300953E-03	3.388550E-06
OMet	CH0	1	2.328538E-03	2.185325E-05
OMet	CH1	1	3.704924E-03	1.502125E-05
OMet	CH2	1	4.110135E-03	8.887700E-06
OMet	CH3	1	4.663258E-03	7.872050E-06
OMet	CH4	1	5.459888E-03	8.939550E-06
OMet	CH2r	1	4.073038E-03	8.077925E-06

OMet CR1 1 3.531330E-03 5.929200E-06

OMet HC 1 4.375520E-04 1.875750E-07

OMet H 1 0.000000E+00 0.000000E+00

OMet DUM 1 0.000000E+00 0.000000E+00

OMet S 1 4.752195E-03 5.514400E-06

OMet CU1+ 1 9.726020E-04 3.431250E-07

OMet CU2+ 1 9.726020E-04 6.238775E-07

OMet FE 1 0.000000E+00 0.000000E+00

OMet ZN2+ 1 9.726020E-04 1.481690E-07

OMet MG2+ 1 3.842848E-04 8.902950E-08

OMet CA2+ 1 1.507652E-03 1.076193E-06

OMet P 1 5.773784E-03 7.184275E-06

OMet AR 1 3.764374E-03 4.785450E-06

OMet F 1 1.632259E-03 1.871175E-06

OMet CL 1 4.452567E-03 5.964275E-06

OMet BR 1 7.909228E-03 1.234030E-05

OMet CMet 1 4.480628E-03 6.710000E-06

NA+ O 1 4.222948E-04 3.051000E-07

NA+ OM 1 4.222948E-04 8.283600E-07

NA+ OA 1 4.222948E-04 3.312900E-07

NA+ OE 1 4.222948E-04 3.312900E-07

NA+ OW 1 4.542599E-04 4.382100E-07

NA+ N 1 4.382773E-04 4.112100E-07

NA+ NT 1 4.382773E-04 4.112100E-07

NA+ NL 1 4.382773E-04 4.112100E-07

NA+ NR 1 4.382773E-04 4.970700E-07

NA+ NZ 1 4.382773E-04 4.112100E-07

NA+ NE 1 4.382773E-04 4.112100E-07

NA+ C 1 4.295757E-04 5.999400E-07

NA+ CH0 1 4.347256E-04 3.869100E-06

NA+ CH1 1 6.916897E-04 2.659500E-06

NA+ CH2 1 7.673405E-04 1.573560E-06

NA+ CH3 1 8.706056E-04 1.393740E-06

NA+ CH4 1 1.019332E-03 1.582740E-06

NA+ CH2r 1 7.604147E-04 1.430190E-06

NA+ CR1 1 6.592806E-04 1.049760E-06

NA+ HC 1 8.168864E-05 3.321000E-08

NA+ H 1 0.000000E+00 0.000000E+00

NA+ DUM 1 0.000000E+00 0.000000E+00

NA+ S 1 8.872097E-04 9.763200E-07

NA+ CU1+ 1 1.815796E-04 1.932930E-08

NA+ CU2+ 1 1.815796E-04 1.932930E-08

NA+ FE 1 0.000000E+00 0.000000E+00

NA+ ZN2+ 1 1.815796E-04 2.623320E-08

NA+ MG2+ 1 7.174394E-05 1.576260E-08

NA+ CA2+ 1 2.814706E-04 1.905390E-07

NA+ P 1 1.077935E-03 1.271970E-06

NA+ AR 1 7.027887E-04 8.472600E-07

NA+ F 1 3.047341E-04 3.312900E-07

NA+ CL 1 8.312707E-04 1.055970E-06

NA+ BR 1 1.476611E-03 2.184840E-06

NA+ CMet 1 8.365094E-04 1.188000E-06

NA+ OMet 1 4.222948E-04 4.117500E-07

CL- O 1 5.382841E-03 7.776000E-06

CL- OM 1 5.382841E-03 6.695914E-06

CL- OA 1 5.382841E-03 9.541152E-06

CL- OE 1 5.382841E-03 8.553600E-06

CL- OW 1 5.790289E-03 1.262045E-05

CL- N 1 5.586565E-03 1.510877E-05

CL- NT 1 5.586565E-03 1.749600E-05

CL-	NL	1	5.586565E-03	2.385677E-05
CL-	NR	1	5.586565E-03	1.431562E-05
CL-	NZ	1	5.586565E-03	1.670285E-05
CL-	NE	1	5.586565E-03	1.542758E-05
CL-	C	1	5.475648E-03	1.727827E-05
CL-	CH0	1	5.541293E-03	1.114301E-04
CL-	CH1	1	8.816722E-03	7.659360E-05
CL-	CH2	1	9.781016E-03	4.531853E-05
CL-	CH3	1	1.109730E-02	4.013971E-05
CL-	CH4	1	1.299306E-02	4.558291E-05
CL-	CH2r	1	9.692735E-03	4.118947E-05
CL-	CR1	1	8.403615E-03	3.023309E-05
CL-	HC	1	1.041256E-03	9.564480E-07
CL-	H	1	0.000000E+00	0.000000E+00
CL-	DUM	1	0.000000E+00	0.000000E+00
CL-	S	1	1.130895E-02	2.811802E-05
CL-	CU1+	1	2.314531E-03	1.749600E-06
CL-	CU2+	1	2.314531E-03	3.181162E-06
CL-	FE	1	0.000000E+00	0.000000E+00
CL-	ZN2+	1	2.314531E-03	7.555162E-07
CL-	MG2+	1	9.144944E-04	4.539629E-07
CL-	CA2+	1	3.587806E-03	5.487523E-06
CL-	P	1	1.374005E-02	3.663274E-05
CL-	AR	1	8.958197E-03	2.440109E-05
CL-	F	1	3.884338E-03	6.782227E-06
CL-	CL	1	1.059591E-02	3.041194E-05
CL-	BR	1	1.882183E-02	6.292339E-05
CL-	CMet	1	1.066269E-02	3.421440E-05
CL-	OMet	1	5.382841E-03	1.185840E-05
CL-	NA+	1	1.004948E-03	2.099520E-06

CChl	O	1	2.439448E-03	2.016000E-06
CChl	OM	1	2.439448E-03	1.735978E-06
CChl	OA	1	2.439448E-03	2.217600E-06
CChl	OE	1	2.439448E-03	2.217600E-06
CChl	OW	1	2.624099E-03	3.271968E-06
CChl	N	1	2.531773E-03	3.070368E-06
CChl	NT	1	2.531773E-03	3.070368E-06
CChl	NL	1	2.531773E-03	3.070368E-06
CChl	NR	1	2.531773E-03	3.070368E-06
CChl	NZ	1	2.531773E-03	3.070368E-06
CChl	NE	1	2.531773E-03	3.070368E-06
CChl	C	1	2.481507E-03	4.479552E-06
CChl	CH0	1	2.511256E-03	2.888928E-05
CChl	CH1	1	3.995647E-03	1.985760E-05
CChl	CH2	1	4.432655E-03	1.174925E-05
CChl	CH3	1	5.029181E-03	1.040659E-05
CChl	CH4	1	5.888322E-03	1.181779E-05
CChl	CH2r	1	4.392647E-03	1.067875E-05
CChl	CR1	1	3.808431E-03	7.838208E-06
CChl	HC	1	4.718864E-04	2.479680E-07
CChl	H	1	0.000000E+00	0.000000E+00
CChl	DUM	1	0.000000E+00	0.000000E+00
CChl	S	1	5.125097E-03	7.289856E-06
CChl	CU1+	1	1.048921E-03	1.443254E-07
CChl	CU2+	1	1.048921E-03	1.443254E-07
CChl	FE	1	0.000000E+00	0.000000E+00
CChl	ZN2+	1	1.048921E-03	1.958746E-07
CChl	MG2+	1	4.144394E-04	1.176941E-07
CChl	CA2+	1	1.625956E-03	1.422691E-06
CChl	P	1	6.226849E-03	9.497376E-06

CChl AR	1	4.059762E-03	6.326208E-06
CChl F	1	1.760341E-03	1.758355E-06
CChl CL	1	4.801957E-03	7.884576E-06
CChl BR	1	8.529860E-03	1.631347E-05
CChl CMet	1	4.832219E-03	8.870400E-06
CChl OMet	1	2.439448E-03	3.074400E-06
CChl NA+	1	4.554319E-04	5.443200E-07
CChl CL-	1	5.805229E-03	1.567642E-05
CLChlO	1	4.334666E-03	3.710100E-06
CLChlOM	1	4.334666E-03	3.194767E-06
CLChlOA	1	4.334666E-03	4.081110E-06
CLChlOE	1	4.334666E-03	4.081110E-06
CLChlOW	1	4.662774E-03	6.021492E-06
CLChlN	1	4.498720E-03	5.650482E-06
CLChlNT	1	4.498720E-03	5.650482E-06
CLChlNL	1	4.498720E-03	5.650482E-06
CLChlNR	1	4.498720E-03	5.650482E-06
CLChlNZ	1	4.498720E-03	5.650482E-06
CLChlNE	1	4.498720E-03	5.650482E-06
CLChlC	1	4.409402E-03	8.243842E-06
CLChlCH0	1	4.462263E-03	5.316573E-05
CLChlCH1	1	7.099884E-03	3.654449E-05
CLChlCH2	1	7.876405E-03	2.162246E-05
CLChlCH3	1	8.936375E-03	1.915154E-05
CLChlCH4	1	1.046299E-02	2.174861E-05
CLChlCH2r	1	7.805315E-03	1.965240E-05
CLChlCR1	1	6.767219E-03	1.442487E-05
CLChlHC	1	8.384972E-04	4.563423E-07
CLChlH	1	0.000000E+00	0.000000E+00
CLChlDUM	1	0.000000E+00	0.000000E+00

CLChl S 1 9.106809E-03 1.341572E-05

CLChl CU1+ 1 1.863833E-03 2.656061E-07

CLChl CU2+ 1 1.863833E-03 2.656061E-07

CLChl FE 1 0.000000E+00 0.000000E+00

CLChl ZN2+ 1 1.863833E-03 3.604733E-07

CLChl MG2+ 1 7.364193E-04 2.165956E-07

CLChl CA2+ 1 2.889170E-03 2.618218E-06

CLChl P 1 1.106452E-02 1.747828E-05

CLChl AR 1 7.213810E-03 1.164229E-05

CLChl F 1 3.127959E-03 3.235949E-06

CLChl CL 1 8.532620E-03 1.451020E-05

CLChl BR 1 1.515675E-02 3.002213E-05

CLChl CMet 1 8.586394E-03 1.632444E-05

CLChl OMet 1 4.334666E-03 5.657903E-06

CLChl NA+ 1 8.092592E-04 1.001727E-06

CLChl CL- 1 1.031534E-02 2.884974E-05

CLChl CChl 1 4.675400E-03 7.481300E-06

HChl O 1 2.920184E-04 6.557400E-08

HChl OM 1 2.920184E-04 5.646577E-08

HChl OA 1 2.920184E-04 7.213140E-08

HChl OE 1 2.920184E-04 7.213140E-08

HChl OW 1 3.141224E-04 1.064266E-07

HChl N 1 3.030704E-04 9.986920E-08

HChl NT 1 3.030704E-04 9.986920E-08

HChl NL 1 3.030704E-04 9.986920E-08

HChl NR 1 3.030704E-04 9.986920E-08

HChl NZ 1 3.030704E-04 9.986920E-08

HChl NE 1 3.030704E-04 9.986920E-08

HChl C 1 2.970532E-04 1.457054E-07

HChl CH0 1 3.006144E-04 9.396754E-07

HChl CH1 1 4.783060E-04 6.459039E-07

HChl CH2 1 5.306188E-04 3.821653E-07

HChl CH3 1 6.020270E-04 3.384930E-07

HChl CH4 1 7.048720E-04 3.843948E-07

HChl CH2r 1 5.258296E-04 3.473455E-07

HChl CR1 1 4.558950E-04 2.549517E-07

HChl HC 1 5.648800E-05 8.065602E-09

HChl H 1 0.000000E+00 0.000000E+00

HChl DUM 1 0.000000E+00 0.000000E+00

HChl S 1 6.135088E-04 2.371156E-07

HChl CU1+ 1 1.255630E-04 4.694443E-09

HChl CU2+ 1 1.255630E-04 4.694443E-09

HChl FE 1 0.000000E+00 0.000000E+00

HChl ZN2+ 1 1.255630E-04 6.371170E-09

HChl MG2+ 1 4.961120E-05 3.828210E-09

HChl CA2+ 1 1.946380E-04 4.627557E-08

HChl P 1 7.453960E-04 3.089191E-07

HChl AR 1 4.859810E-04 2.057712E-07

HChl F 1 2.107248E-04 5.719364E-08

HChl CL 1 5.748268E-04 2.564599E-07

HChl BR 1 1.021082E-03 5.306248E-07

HChl CMet 1 5.784494E-04 2.885256E-07

HChl OMet 1 2.920184E-04 1.000004E-07

HChl NA+ 1 5.451829E-05 1.770498E-08

HChl CL- 1 6.949252E-04 5.099034E-07

HChl CChl 1 3.622000E-04 1.745000E-07

HChl CLChl 1 6.493000E-04 3.266000E-07

SDmso O 1 4.887741E-03 4.636600E-06

SDmso OM 1 4.887741E-03 3.992576E-06

SDmso OA 1 4.887741E-03 5.100260E-06

SDmso	OE	1	4.887741E-03	5.100260E-06
SDmso	OW	1	5.257713E-03	7.525202E-06
SDmso	N	1	5.072727E-03	7.061542E-06
SDmso	NT	1	5.072727E-03	7.061542E-06
SDmso	NL	1	5.072727E-03	7.061542E-06
SDmso	NR	1	5.072727E-03	7.061542E-06
SDmso	NZ	1	5.072727E-03	7.061542E-06
SDmso	NE	1	5.072727E-03	7.061542E-06
SDmso	C	1	4.972013E-03	1.030253E-05
SDmso	CH0	1	5.031619E-03	6.644248E-05
SDmso	CH1	1	8.005783E-03	4.567051E-05
SDmso	CH2	1	8.881383E-03	2.702210E-05
SDmso	CH3	1	1.007660E-02	2.393413E-05
SDmso	CH4	1	1.179800E-02	2.717975E-05
SDmso	CH2r	1	8.801223E-03	2.456007E-05
SDmso	CR1	1	7.630672E-03	1.802710E-05
SDmso	HC	1	9.454840E-04	5.703018E-07
SDmso	H	1	0.000000E+00	0.000000E+00
SDmso	DUM	1	0.000000E+00	0.000000E+00
SDmso	S	1	1.026878E-02	1.676595E-05
SDmso	CU1+	1	2.101647E-03	3.319342E-07
SDmso	CU2+	1	2.101647E-03	3.319342E-07
SDmso	FE	1	0.000000E+00	0.000000E+00
SDmso	ZN2+	1	2.101647E-03	4.504921E-07
SDmso	MG2+	1	8.303816E-04	2.706847E-07
SDmso	CA2+	1	3.257809E-03	3.272049E-06
SDmso	P	1	1.247628E-02	2.184302E-05
SDmso	AR	1	8.134245E-03	1.454965E-05
SDmso	F	1	3.527066E-03	4.044043E-06
SDmso	CL	1	9.621327E-03	1.813374E-05

SDmso	BR	1	1.709065E-02	3.751937E-05
SDmso	CMet	1	9.681962E-03	2.040104E-05
SDmso	OMet	1	4.887741E-03	7.070815E-06
SDmso	NA+	1	9.125154E-04	1.251882E-06
SDmso	CL-	1	1.163151E-02	3.605420E-05
SDmso	CChl	1	5.271279E-03	9.347386E-06
SDmso	CLChl	1	9.366561E-03	1.720225E-05
SDmso	HChl	1	6.310078E-04	3.040404E-07
CDmso	O	1	4.663258E-03	5.162000E-06
CDmso	OM	1	4.663258E-03	4.444998E-06
CDmso	OA	1	4.663258E-03	5.678200E-06
CDmso	OE	1	4.663258E-03	5.678200E-06
CDmso	OW	1	5.016238E-03	8.377926E-06
CDmso	N	1	4.839748E-03	7.861726E-06
CDmso	NT	1	4.839748E-03	7.861726E-06
CDmso	NL	1	4.839748E-03	7.861726E-06
CDmso	NR	1	4.839748E-03	7.861726E-06
CDmso	NZ	1	4.839748E-03	7.861726E-06
CDmso	NE	1	4.839748E-03	7.861726E-06
CDmso	C	1	4.743659E-03	1.146996E-05
CDmso	CH0	1	4.800528E-03	7.397146E-05
CDmso	CH1	1	7.638095E-03	5.084570E-05
CDmso	CH2	1	8.473481E-03	3.008414E-05
CDmso	CH3	1	9.613802E-03	2.664624E-05
CDmso	CH4	1	1.125614E-02	3.025964E-05
CDmso	CH2r	1	8.397002E-03	2.734311E-05
CDmso	CR1	1	7.280212E-03	2.006986E-05
CDmso	HC	1	9.020600E-04	6.349260E-07
CDmso	H	1	0.000000E+00	0.000000E+00
CDmso	DUM	1	0.000000E+00	0.000000E+00

CDmso	S	1	9.797156E-03	1.866579E-05
CDmso	CU1+	1	2.005122E-03	3.695476E-07
CDmso	CU2+	1	2.005122E-03	3.695476E-07
CDmso	FE	1	0.000000E+00	0.000000E+00
CDmso	ZN2+	1	2.005122E-03	5.015399E-07
CDmso	MG2+	1	7.922440E-04	3.013576E-07
CDmso	CA2+	1	3.108185E-03	3.642823E-06
CDmso	P	1	1.190327E-02	2.431818E-05
CDmso	AR	1	7.760657E-03	1.619836E-05
CDmso	F	1	3.365076E-03	4.502296E-06
CDmso	CL	1	9.179441E-03	2.018858E-05
CDmso	BR	1	1.630571E-02	4.177090E-05
CDmso	CMet	1	9.237291E-03	2.271280E-05
CDmso	OMet	1	4.663258E-03	7.872050E-06
CDmso	NA+	1	8.706056E-04	1.393740E-06
CDmso	CL-	1	1.109730E-02	4.013971E-05
CDmso	CChl	1	5.029181E-03	1.040659E-05
CDmso	CLChl	1	8.936375E-03	1.915154E-05
CDmso	HChl	1	6.020270E-04	3.384930E-07
CDmso	SDmso	1	1.007660E-02	2.393413E-05
ODmso	O	1	2.266329E-03	8.668600E-07
ODmso	OM	1	2.266329E-03	7.464531E-07
ODmso	OA	1	2.266329E-03	1.380375E-06
ODmso	OE	1	2.266329E-03	9.535460E-07
ODmso	OW	1	2.437876E-03	1.825875E-06
ODmso	N	1	2.352103E-03	2.185875E-06
ODmso	NT	1	2.352103E-03	2.531250E-06
ODmso	NL	1	2.352103E-03	3.451500E-06
ODmso	NR	1	2.352103E-03	2.071125E-06
ODmso	NZ	1	2.352103E-03	2.416500E-06

ODmso	NE	1	2.352103E-03	2.232000E-06
ODmso	C	1	2.305404E-03	1.926163E-06
ODmso	CH0	1	2.333042E-03	1.242210E-05
ODmso	CH1	1	3.712091E-03	8.538571E-06
ODmso	CH2	1	4.118086E-03	5.052060E-06
ODmso	CH3	1	4.672279E-03	4.474731E-06
ODmso	CH4	1	5.470450E-03	5.081533E-06
ODmso	CH2r	1	4.080917E-03	4.591757E-06
ODmso	CR1	1	3.538161E-03	3.370352E-06
ODmso	HC	1	4.383984E-04	1.066238E-07
ODmso	H	1	0.000000E+00	0.000000E+00
ODmso	DUM	1	0.000000E+00	0.000000E+00
ODmso	S	1	4.761388E-03	3.134566E-06
ODmso	CU1+	1	9.744834E-04	2.531250E-07
ODmso	CU2+	1	9.744834E-04	4.602375E-07
ODmso	FE	1	0.000000E+00	0.000000E+00
ODmso	ZN2+	1	9.744834E-04	1.093050E-07
ODmso	MG2+	1	3.850282E-04	6.567750E-08
ODmso	CA2+	1	1.510568E-03	7.939125E-07
ODmso	P	1	5.784953E-03	5.299875E-06
ODmso	AR	1	3.771656E-03	2.720207E-06
ODmso	F	1	1.635417E-03	7.560753E-07
ODmso	CL	1	4.461180E-03	3.390289E-06
ODmso	BR	1	7.924528E-03	7.014631E-06
ODmso	CMet	1	4.489295E-03	3.814184E-06
ODmso	OMet	1	2.266329E-03	1.715625E-06
ODmso	NA+	1	4.231116E-04	3.037500E-07
ODmso	CL-	1	5.393253E-03	6.740703E-06
ODmso	CChl	1	2.444166E-03	1.747590E-06
ODmso	CLChl	1	4.343051E-03	3.216137E-06

ODmso HChl 1 2.925833E-04 5.684348E-08

ODmso SDmso 1 4.897196E-03 4.019283E-06

ODmso CDmso 1 4.672279E-03 4.474731E-06

CCl4 O 1 2.439448E-03 2.756800E-06

CCl4 OM 1 2.439448E-03 2.373880E-06

CCl4 OA 1 2.439448E-03 3.032480E-06

CCl4 OE 1 2.439448E-03 3.032480E-06

CCl4 OW 1 2.624099E-03 4.474286E-06

CCl4 N 1 2.531773E-03 4.198606E-06

CCl4 NT 1 2.531773E-03 4.198606E-06

CCl4 NL 1 2.531773E-03 4.198606E-06

CCl4 NR 1 2.531773E-03 4.198606E-06

CCl4 NZ 1 2.531773E-03 4.198606E-06

CCl4 NE 1 2.531773E-03 4.198606E-06

CCl4 C 1 2.481507E-03 6.125610E-06

CCl4 CH0 1 2.511256E-03 3.950494E-05

CCl4 CH1 1 3.995647E-03 2.715448E-05

CCl4 CH2 1 4.432655E-03 1.606663E-05

CCl4 CH3 1 5.029181E-03 1.423060E-05

CCl4 CH4 1 5.888322E-03 1.616036E-05

CCl4 CH2r 1 4.392647E-03 1.460277E-05

CCl4 CR1 1 3.808431E-03 1.071844E-05

CCl4 HC 1 4.718864E-04 3.390864E-07

CCl4 H 1 0.000000E+00 0.000000E+00

CCl4 DUM 1 0.000000E+00 0.000000E+00

CCl4 S 1 5.125097E-03 9.968589E-06

CCl4 CU1+ 1 1.048921E-03 1.973593E-07

CCl4 CU2+ 1 1.048921E-03 1.973593E-07

CCl4 FE 1 0.000000E+00 0.000000E+00

CCl4 ZN2+ 1 1.048921E-03 2.678507E-07

CCl4	MG2+	1	4.144394E-04	1.609420E-07
CCl4	CA2+	1	1.625956E-03	1.945474E-06
CCl4	P	1	6.226849E-03	1.298728E-05
CCl4	AR	1	4.059762E-03	8.650838E-06
CCl4	F	1	1.760341E-03	2.404481E-06
CCl4	CL	1	4.801957E-03	1.078184E-05
CCl4	BR	1	8.529860E-03	2.230803E-05
CCl4	CMet	1	4.832219E-03	1.212992E-05
CCl4	OMet	1	2.439448E-03	4.204120E-06
CCl4	NA+	1	4.554319E-04	7.443360E-07
CCl4	CL-	1	5.805229E-03	2.143688E-05
CCl4	CChl	1	2.630869E-03	5.557709E-06
CCl4	CLChl	1	4.674804E-03	1.022800E-05
CCl4	HChl	1	3.149329E-04	1.807744E-07
CCl4	SDmso	1	5.271279E-03	1.278218E-05
CCl4	CDmso	1	5.029181E-03	1.423060E-05
CCl4	ODmso	1	2.444166E-03	2.389760E-06
CLCl4	O	1	4.147280E-03	3.573200E-06
CLCl4	OM	1	4.147280E-03	3.076883E-06
CLCl4	OA	1	4.147280E-03	3.930520E-06
CLCl4	OE	1	4.147280E-03	3.930520E-06
CLCl4	OW	1	4.461203E-03	5.799304E-06
CLCl4	N	1	4.304241E-03	5.441984E-06
CLCl4	NT	1	4.304241E-03	5.441984E-06
CLCl4	NL	1	4.304241E-03	5.441984E-06
CLCl4	NR	1	4.304241E-03	5.441984E-06
CLCl4	NZ	1	4.304241E-03	5.441984E-06
CLCl4	NE	1	4.304241E-03	5.441984E-06
CLCl4	C	1	4.218784E-03	7.939650E-06
CLCl4	CH0	1	4.269361E-03	5.120396E-05

CLCl4 CH1 1 6.792958E-03 3.519602E-05

CLCl4 CH2 1 7.535910E-03 2.082461E-05

CLCl4 CH3 1 8.550058E-03 1.844486E-05

CLCl4 CH4 1 1.001067E-02 2.094610E-05

CLCl4 CH2r 1 7.467894E-03 1.892724E-05

CLCl4 CR1 1 6.474674E-03 1.389260E-05

CLCl4 HC 1 8.022492E-04 4.395036E-07

CLCl4 H 1 0.000000E+00 0.000000E+00

CLCl4 DUM 1 0.000000E+00 0.000000E+00

CLCl4 S 1 8.713124E-03 1.292069E-05

CLCl4 CU1+ 1 1.783260E-03 2.558054E-07

CLCl4 CU2+ 1 1.783260E-03 2.558054E-07

CLCl4 FE 1 0.000000E+00 0.000000E+00

CLCl4 ZN2+ 1 1.783260E-03 3.471721E-07

CLCl4 MG2+ 1 7.045841E-04 2.086034E-07

CLCl4 CA2+ 1 2.764272E-03 2.521607E-06

CLCl4 P 1 1.058620E-02 1.683335E-05

CLCl4 AR 1 6.901959E-03 1.121270E-05

CLCl4 F 1 2.992738E-03 3.116545E-06

CLCl4 CL 1 8.163758E-03 1.397479E-05

CLCl4 BR 1 1.450153E-02 2.891433E-05

CLCl4 CMet 1 8.215206E-03 1.572208E-05

CLCl4 OMet 1 4.147280E-03 5.449130E-06

CLCl4 NA+ 1 7.742751E-04 9.647640E-07

CLCl4 CL- 1 9.869409E-03 2.778520E-05

CLCl4 CChl 1 4.472714E-03 7.203571E-06

CLCl4 CLChl 1 7.947586E-03 1.325693E-05

CLCl4 HChl 1 5.354141E-04 2.343090E-07

CLCl4 SDmso 1 8.961647E-03 1.656750E-05

CLCl4 CDmso 1 8.550058E-03 1.844486E-05

CLCl4 ODmso 1 4.155302E-03 3.097464E-06

CLCl4 CCl4 1 4.472714E-03 9.850598E-06

FTFE O 1 1.632259E-03 1.000000E-06

FTFE OM 1 1.632259E-03 8.611000E-07

FTFE OA 1 1.632259E-03 1.227000E-06

FTFE OE 1 1.632259E-03 1.100000E-06

FTFE OW 1 1.755811E-03 1.623000E-06

FTFE N 1 1.694035E-03 1.943000E-06

FTFE NT 1 1.694035E-03 2.250000E-06

FTFE NL 1 1.694035E-03 3.068000E-06

FTFE NR 1 1.694035E-03 1.841000E-06

FTFE NZ 1 1.694035E-03 2.148000E-06

FTFE NE 1 1.694035E-03 1.984000E-06

FTFE C 1 1.660402E-03 2.222000E-06

FTFE CH0 1 1.680307E-03 1.433000E-05

FTFE CH1 1 2.673528E-03 9.850000E-06

FTFE CH2 1 2.965934E-03 5.828000E-06

FTFE CH3 1 3.365076E-03 5.162000E-06

FTFE CH4 1 3.939936E-03 5.862000E-06

FTFE CH2r 1 2.939165E-03 5.297000E-06

FTFE CR1 1 2.548260E-03 3.888000E-06

FTFE HC 1 3.157440E-04 1.230000E-07

FTFE H 1 0.000000E+00 0.000000E+00

FTFE DUM 1 0.000000E+00 0.000000E+00

FTFE S 1 3.429254E-03 3.616000E-06

FTFE CU1+ 1 7.018440E-04 2.250000E-07

FTFE CU2+ 1 7.018440E-04 4.091000E-07

FTFE FE 1 0.000000E+00 0.000000E+00

FTFE ZN2+ 1 7.018440E-04 9.716000E-08

FTFE MG2+ 1 2.773056E-04 5.838000E-08

FTFE CA2+ 1 1.087944E-03 7.057000E-07

FTFE P 1 4.166448E-03 4.711000E-06

FTFE AR 1 2.716428E-03 3.138000E-06

FTFE F 1 1.177862E-03 8.722000E-07

FTFE CL 1 3.213038E-03 3.911000E-06

FTFE BR 1 5.707416E-03 8.092000E-06

FTFE CMet 1 3.233287E-03 4.400000E-06

FTFE OMet 1 1.632259E-03 1.525000E-06

FTFE NA+ 1 3.047341E-04 2.700000E-07

FTFE CL- 1 3.884338E-03 7.776000E-06

FTFE CChl 1 1.760341E-03 2.016000E-06

FTFE CLChl 1 3.127959E-03 3.710100E-06

FTFE HChl 1 2.107248E-04 6.557400E-08

FTFE SDmso 1 3.527066E-03 4.636600E-06

FTFE CDmso 1 3.365076E-03 5.162000E-06

FTFE ODmso 1 1.635417E-03 8.668600E-07

FTFE CCl4 1 1.760341E-03 2.756800E-06

FTFE CLCl4 1 2.992738E-03 3.573200E-06

CTFE O 1 2.300953E-03 1.837000E-06

CTFE OM 1 2.300953E-03 1.581841E-06

CTFE OA 1 2.300953E-03 2.020700E-06

CTFE OE 1 2.300953E-03 2.020700E-06

CTFE OW 1 2.475121E-03 2.981451E-06

CTFE N 1 2.388037E-03 2.797751E-06

CTFE NT 1 2.388037E-03 2.797751E-06

CTFE NL 1 2.388037E-03 2.797751E-06

CTFE NR 1 2.388037E-03 2.797751E-06

CTFE NZ 1 2.388037E-03 2.797751E-06

CTFE NE 1 2.388037E-03 2.797751E-06

CTFE C 1 2.340624E-03 4.081814E-06

CTFE CH0 1 2.368685E-03 2.632421E-05

CTFE CH1 1 3.768802E-03 1.809445E-05

CTFE CH2 1 4.181000E-03 1.070604E-05

CTFE CH3 1 4.743659E-03 9.482594E-06

CTFE CH4 1 5.554024E-03 1.076849E-05

CTFE CH2r 1 4.143263E-03 9.730589E-06

CTFE CR1 1 3.592215E-03 7.142256E-06

CTFE HC 1 4.450960E-04 2.259510E-07

CTFE H 1 0.000000E+00 0.000000E+00

CTFE DUM 1 0.000000E+00 0.000000E+00

CTFE S 1 4.834130E-03 6.642592E-06

CTFE CU1+ 1 9.893710E-04 1.315108E-07

CTFE CU2+ 1 9.893710E-04 1.315108E-07

CTFE FE 1 0.000000E+00 0.000000E+00

CTFE ZN2+ 1 9.893710E-04 1.784829E-07

CTFE MG2+ 1 3.909104E-04 1.072441E-07

CTFE CA2+ 1 1.533646E-03 1.296371E-06

CTFE P 1 5.873332E-03 8.654107E-06

CTFE AR 1 3.829277E-03 5.764506E-06

CTFE F 1 1.660402E-03 1.602231E-06

CTFE CL 1 4.529336E-03 7.184507E-06

CTFE BR 1 8.045594E-03 1.486500E-05

CTFE CMet 1 4.557880E-03 8.082800E-06

CTFE OMet 1 2.300953E-03 2.801425E-06

CTFE NA+ 1 4.295757E-04 4.959900E-07

CTFE CL- 1 5.475648E-03 1.428451E-05

CTFE CChl 1 2.481507E-03 3.703392E-06

CTFE CLChl 1 4.409402E-03 6.815454E-06

CTFE HChl 1 2.970532E-04 1.204594E-07

CTFE SDmso 1 4.972013E-03 8.517434E-06

CTFE	CDmso	1	4.743659E-03	9.482594E-06
CTFE	ODmso	1	2.305404E-03	1.592422E-06
CTFE	CCl4	1	2.481507E-03	5.064242E-06
CTFE	CLCl4	1	4.218784E-03	6.563968E-06
CTFE	FTFE	1	1.660402E-03	1.837000E-06
CHTFE	O	1	4.008832E-03	5.077000E-06
CHTFE	OM	1	4.008832E-03	4.371805E-06
CHTFE	OA	1	4.008832E-03	5.584700E-06
CHTFE	OE	1	4.008832E-03	5.584700E-06
CHTFE	OW	1	4.312276E-03	8.239971E-06
CHTFE	N	1	4.160554E-03	7.732271E-06
CHTFE	NT	1	4.160554E-03	7.732271E-06
CHTFE	NL	1	4.160554E-03	7.732271E-06
CHTFE	NR	1	4.160554E-03	7.732271E-06
CHTFE	NZ	1	4.160554E-03	7.732271E-06
CHTFE	NE	1	4.160554E-03	7.732271E-06
CHTFE	C	1	4.077950E-03	1.128109E-05
CHTFE	CH0	1	4.126838E-03	7.275341E-05
CHTFE	CH1	1	6.566191E-03	5.000845E-05
CHTFE	CH2	1	7.284342E-03	2.958876E-05
CHTFE	CH3	1	8.264634E-03	2.620747E-05
CHTFE	CH4	1	9.676492E-03	2.976137E-05
CHTFE	CH2r	1	7.218596E-03	2.689287E-05
CHTFE	CR1	1	6.258533E-03	1.973938E-05
CHTFE	HC	1	7.754680E-04	6.244710E-07
CHTFE	H	1	0.000000E+00	0.000000E+00
CHTFE	DUM	1	0.000000E+00	0.000000E+00
CHTFE	S	1	8.422257E-03	1.835843E-05
CHTFE	CU1+	1	1.723731E-03	3.634624E-07
CHTFE	CU2+	1	1.723731E-03	3.634624E-07

CHTFE FE 1 0.000000E+00 0.000000E+00

CHTFE ZN2+ 1 1.723731E-03 4.932813E-07

CHTFE MG2+ 1 6.810632E-04 2.963953E-07

CHTFE CA2+ 1 2.671993E-03 3.582839E-06

CHTFE P 1 1.023281E-02 2.391775E-05

CHTFE AR 1 6.671553E-03 1.593163E-05

CHTFE F 1 2.892833E-03 4.428159E-06

CHTFE CL 1 7.891230E-03 1.985615E-05

CHTFE BR 1 1.401743E-02 4.108308E-05

CHTFE CMet 1 7.940961E-03 2.233880E-05

CHTFE OMet 1 4.008832E-03 7.742425E-06

CHTFE NA+ 1 7.484278E-04 1.370790E-06

CHTFE CL- 1 9.539942E-03 3.947875E-05

CHTFE CChl 1 4.323403E-03 1.023523E-05

CHTFE CLChl 1 7.682275E-03 1.883618E-05

CHTFE HChl 1 5.175406E-04 3.329192E-07

CHTFE SDmso 1 8.662483E-03 2.354002E-05

CHTFE CDmso 1 8.264634E-03 2.620747E-05

CHTFE ODmso 1 4.016587E-03 4.401048E-06

CHTFE CCl4 1 4.323403E-03 1.399627E-05

CHTFE CLCl4 1 7.350172E-03 1.814114E-05

CHTFE FTFE 1 2.892833E-03 5.077000E-06

CHTFE CTFE 1 4.077950E-03 9.326449E-06

OTFE O 1 2.261954E-03 1.227000E-06

OTFE OM 1 2.261954E-03 1.056570E-06

OTFE OA 1 2.261954E-03 1.505529E-06

OTFE OE 1 2.261954E-03 1.349700E-06

OTFE OW 1 2.433170E-03 1.991421E-06

OTFE N 1 2.347562E-03 1.868721E-06

OTFE NT 1 2.347562E-03 2.760750E-06

OTFE NL 1 2.347562E-03 1.868721E-06

OTFE NR 1 2.347562E-03 2.258907E-06

OTFE NZ 1 2.347562E-03 1.868721E-06

OTFE NE 1 2.347562E-03 1.868721E-06

OTFE C 1 2.300953E-03 2.726394E-06

OTFE CH0 1 2.328538E-03 1.758291E-05

OTFE CH1 1 3.704924E-03 1.208595E-05

OTFE CH2 1 4.110135E-03 7.150956E-06

OTFE CH3 1 4.663258E-03 6.333774E-06

OTFE CH4 1 5.459888E-03 7.192674E-06

OTFE CH2r 1 4.073038E-03 6.499419E-06

OTFE CR1 1 3.531330E-03 4.770576E-06

OTFE HC 1 4.375520E-04 1.509210E-07

OTFE H 1 0.000000E+00 0.000000E+00

OTFE DUM 1 0.000000E+00 0.000000E+00

OTFE S 1 4.752195E-03 4.436832E-06

OTFE CU1+ 1 9.726020E-04 8.784093E-08

OTFE CU2+ 1 9.726020E-04 8.784093E-08

OTFE FE 1 0.000000E+00 0.000000E+00

OTFE ZN2+ 1 9.726020E-04 1.192153E-07

OTFE MG2+ 1 3.842848E-04 7.163226E-08

OTFE CA2+ 1 1.507652E-03 8.658939E-07

OTFE P 1 5.773784E-03 5.780397E-06

OTFE AR 1 3.764374E-03 3.850326E-06

OTFE F 1 1.632259E-03 1.070189E-06

OTFE CL 1 4.452567E-03 4.798797E-06

OTFE BR 1 7.909228E-03 9.928884E-06

OTFE CMet 1 4.480628E-03 5.398800E-06

OTFE OMet 1 2.261954E-03 1.871175E-06

OTFE NA+ 1 4.222948E-04 3.312900E-07

OTFE	CL-	1	5.382841E-03	9.541152E-06
OTFE	CChl	1	2.439448E-03	2.473632E-06
OTFE	CLChl	1	4.334666E-03	4.552293E-06
OTFE	HChl	1	2.920184E-04	8.045930E-08
OTFE	SDmso	1	4.887741E-03	5.689108E-06
OTFE	CDmso	1	4.663258E-03	6.333774E-06
OTFE	ODmso	1	2.266329E-03	1.380375E-06
OTFE	CCl4	1	2.439448E-03	3.382594E-06
OTFE	CLCl4	1	4.147280E-03	4.384316E-06
OTFE	FTFE	1	1.632259E-03	1.227000E-06
OTFE	CTFE	1	2.300953E-03	2.253999E-06
OTFE	CHTFE	1	4.008832E-03	6.229479E-06
CUrea	O	1	3.324729E-03	3.686400E-06
CUrea	OM	1	3.324729E-03	3.174359E-06
CUrea	OA	1	3.324729E-03	4.055040E-06
CUrea	OE	1	3.324729E-03	4.055040E-06
CUrea	OW	1	3.576391E-03	5.983027E-06
CUrea	N	1	3.450560E-03	5.614387E-06
CUrea	NT	1	3.450560E-03	5.614387E-06
CUrea	NL	1	3.450560E-03	5.614387E-06
CUrea	NR	1	3.450560E-03	5.614387E-06
CUrea	NZ	1	3.450560E-03	5.614387E-06
CUrea	NE	1	3.450560E-03	5.614387E-06
CUrea	C	1	3.382052E-03	8.191181E-06
CUrea	CH0	1	3.422598E-03	5.282611E-05
CUrea	CH1	1	5.445677E-03	3.631104E-05
CUrea	CH2	1	6.041277E-03	2.148434E-05
CUrea	CH3	1	6.854283E-03	1.902920E-05
CUrea	CH4	1	8.025209E-03	2.160968E-05
CUrea	CH2r	1	5.986750E-03	1.952686E-05

CUrea	CR1	1	5.190520E-03	1.433272E-05
CUrea	HC	1	6.431352E-04	4.534272E-07
CUrea	H	1	0.000000E+00	0.000000E+00
CUrea	DUM	1	0.000000E+00	0.000000E+00
CUrea	S	1	6.985008E-03	1.333002E-05
CUrea	CU1+	1	1.429578E-03	2.639094E-07
CUrea	CU2+	1	1.429578E-03	2.639094E-07
CUrea	FE	1	0.000000E+00	0.000000E+00
CUrea	ZN2+	1	1.429578E-03	3.581706E-07
CUrea	MG2+	1	5.648405E-04	2.152120E-07
CUrea	CA2+	1	2.216020E-03	2.601492E-06
CUrea	P	1	8.486588E-03	1.736663E-05
CUrea	AR	1	5.533060E-03	1.156792E-05
CUrea	F	1	2.399174E-03	3.215278E-06
CUrea	CL	1	6.544600E-03	1.441751E-05
CUrea	BR	1	1.162537E-02	2.983035E-05
CUrea	CMet	1	6.585844E-03	1.622016E-05
CUrea	OMet	1	3.324729E-03	5.621760E-06
CUrea	NA+	1	6.207094E-04	9.953280E-07
CUrea	CL-	1	7.911961E-03	2.866545E-05
CUrea	CChl	1	3.585619E-03	7.431782E-06
CUrea	CLChl	1	6.371303E-03	1.367691E-05
CUrea	HChl	1	4.292228E-04	2.417320E-07
CUrea	SDmso	1	7.184240E-03	1.709236E-05
CUrea	CDmso	1	6.854283E-03	1.902920E-05
CUrea	ODmso	1	3.331161E-03	3.195593E-06
CUrea	CCl4	1	3.585619E-03	1.016267E-05
CUrea	CLCl4	1	6.095873E-03	1.317224E-05
CUrea	FTFE	1	2.399174E-03	3.686400E-06
CUrea	CTFE	1	3.382052E-03	6.771917E-06

CUrea	CHTFE	1	5.892377E-03	1.871585E-05
CUrea	OTFE	1	3.324729E-03	4.523213E-06
OUrea	O	1	2.312367E-03	1.260900E-06
OUrea	OM	1	2.312367E-03	1.085761E-06
OUrea	OA	1	2.312367E-03	1.547124E-06
OUrea	OE	1	2.312367E-03	1.386990E-06
OUrea	OW	1	2.487399E-03	2.046441E-06
OUrea	N	1	2.399883E-03	2.449929E-06
OUrea	NT	1	2.399883E-03	2.837025E-06
OUrea	NL	1	2.399883E-03	3.868441E-06
OUrea	NR	1	2.399883E-03	2.321317E-06
OUrea	NZ	1	2.399883E-03	2.708413E-06
OUrea	NE	1	2.399883E-03	2.501626E-06
OUrea	C	1	2.352236E-03	2.801720E-06
OUrea	CH0	1	2.380435E-03	1.806870E-05
OUrea	CH1	1	3.787498E-03	1.241986E-05
OUrea	CH2	1	4.201740E-03	7.348525E-06
OUrea	CH3	1	4.767191E-03	6.508766E-06
OUrea	CH4	1	5.581576E-03	7.391396E-06
OUrea	CH2r	1	4.163817E-03	6.678987E-06
OUrea	CR1	1	3.610035E-03	4.902379E-06
OUrea	HC	1	4.473040E-04	1.550907E-07
OUrea	H	1	0.000000E+00	0.000000E+00
OUrea	DUM	1	0.000000E+00	0.000000E+00
OUrea	S	1	4.858110E-03	4.559414E-06
OUrea	CU1+	1	9.942790E-04	2.837025E-07
OUrea	CU2+	1	9.942790E-04	5.158342E-07
OUrea	FE	1	0.000000E+00	0.000000E+00
OUrea	ZN2+	1	9.942790E-04	1.225090E-07
OUrea	MG2+	1	3.928496E-04	7.361134E-08

OUrea	CA2+	1	1.541254E-03	8.898171E-07
OUrea	P	1	5.902468E-03	5.940100E-06
OUrea	AR	1	3.848273E-03	3.956704E-06
OUrea	F	1	1.668638E-03	1.099757E-06
OUrea	CL	1	4.551804E-03	4.931380E-06
OUrea	BR	1	8.085506E-03	1.020320E-05
OUrea	CMet	1	4.580490E-03	5.547960E-06
OUrea	OMet	1	2.312367E-03	1.922873E-06
OUrea	NA+	1	4.317067E-04	3.404430E-07
OUrea	CL-	1	5.502812E-03	9.804758E-06
OUrea	CChl	1	2.493817E-03	2.541974E-06
OUrea	CLChl	1	4.431275E-03	4.678065E-06
OUrea	HChl	1	2.985268E-04	8.268226E-08
OUrea	SDmso	1	4.996677E-03	5.846289E-06
OUrea	CDmso	1	4.767191E-03	6.508766E-06
OUrea	ODmso	1	2.316840E-03	1.093024E-06
OUrea	CCl4	1	2.493817E-03	3.476049E-06
OUrea	CLCl4	1	4.239713E-03	4.505448E-06
OUrea	FTFE	1	1.668638E-03	1.260900E-06
OUrea	CTFE	1	2.352236E-03	2.316273E-06
OUrea	CHTFE	1	4.098180E-03	6.401589E-06
OUrea	OTFE	1	2.312367E-03	1.547124E-06
OUrea	CUrea	1	3.398830E-03	4.648182E-06
NUrea	O	1	2.753867E-03	2.246101E-06
NUrea	OM	1	2.753867E-03	3.659356E-06
NUrea	OA	1	2.753867E-03	2.438908E-06
NUrea	OE	1	2.753867E-03	2.438908E-06
NUrea	OW	1	2.962317E-03	3.226037E-06
NUrea	N	1	2.858092E-03	3.862101E-06
NUrea	NT	1	2.858092E-03	4.472325E-06

NUrea	NL	1	2.858092E-03	6.098264E-06
NUrea	NR	1	2.858092E-03	3.659356E-06
NUrea	NZ	1	2.858092E-03	4.269580E-06
NUrea	NE	1	2.858092E-03	3.943597E-06
NUrea	C	1	2.801347E-03	4.416669E-06
NUrea	CH0	1	2.834931E-03	2.848374E-05
NUrea	CH1	1	4.510644E-03	1.957884E-05
NUrea	CH2	1	5.003977E-03	1.158432E-05
NUrea	CH3	1	5.677389E-03	1.026051E-05
NUrea	CH4	1	6.647264E-03	1.165190E-05
NUrea	CH2r	1	4.958813E-03	1.052885E-05
NUrea	CR1	1	4.299298E-03	7.728178E-06
NUrea	HC	1	5.327076E-04	2.444871E-07
NUrea	H	1	0.000000E+00	0.000000E+00
NUrea	DUM	1	0.000000E+00	0.000000E+00
NUrea	S	1	5.785668E-03	7.187523E-06
NUrea	CU1+	1	1.184116E-03	1.422994E-07
NUrea	CU2+	1	1.184116E-03	1.422994E-07
NUrea	FE	1	0.000000E+00	0.000000E+00
NUrea	ZN2+	1	1.184116E-03	1.931249E-07
NUrea	MG2+	1	4.678562E-04	1.160419E-07
NUrea	CA2+	1	1.835525E-03	1.402720E-06
NUrea	P	1	7.029424E-03	9.364055E-06
NUrea	AR	1	4.583022E-03	6.237403E-06
NUrea	F	1	1.987231E-03	2.438908E-06
NUrea	CL	1	5.420879E-03	7.773895E-06
NUrea	BR	1	9.629269E-03	1.608447E-05
NUrea	CMet	1	5.455042E-03	8.745880E-06
NUrea	OMet	1	2.753867E-03	3.031242E-06
NUrea	NA+	1	5.141323E-04	5.366790E-07

NUrea	CL-	1	6.553462E-03	1.545636E-05
NUrea	CChl	1	2.969961E-03	4.007203E-06
NUrea	CLChl	1	5.277337E-03	7.374566E-06
NUrea	HChl	1	3.555244E-04	1.303414E-07
NUrea	SDmso	1	5.950691E-03	9.216170E-06
NUrea	CDmso	1	5.677389E-03	1.026051E-05
NUrea	ODmso	1	2.759194E-03	2.236162E-06
NUrea	CCl4	1	2.969961E-03	5.479691E-06
NUrea	CLCl4	1	5.049200E-03	7.102450E-06
NUrea	FTFE	1	1.987231E-03	1.987700E-06
NUrea	CTFE	1	2.801347E-03	3.651405E-06
NUrea	CHTFE	1	4.880644E-03	1.009155E-05
NUrea	OTFE	1	2.753867E-03	2.438908E-06
NUrea	CUrea	1	4.047767E-03	7.327457E-06
NUrea	OUrea	1	2.815244E-03	2.506291E-06
CH3p	O	1	4.663258E-03	5.162000E-06
CH3p	OM	1	4.663258E-03	1.583702E-05
CH3p	OA	1	4.663258E-03	5.678200E-06
CH3p	OE	1	4.663258E-03	5.678200E-06
CH3p	OW	1	5.016238E-03	8.377926E-06
CH3p	N	1	4.839748E-03	7.861726E-06
CH3p	NT	1	4.839748E-03	7.861726E-06
CH3p	NL	1	4.839748E-03	7.861726E-06
CH3p	NR	1	4.839748E-03	7.861726E-06
CH3p	NZ	1	4.839748E-03	7.861726E-06
CH3p	NE	1	4.839748E-03	7.861726E-06
CH3p	C	1	4.743659E-03	1.146996E-05
CH3p	CH0	1	4.800528E-03	7.397146E-05
CH3p	CH1	1	7.638095E-03	5.084570E-05
CH3p	CH2	1	8.473481E-03	3.008414E-05

CH3p CH3	1	9.613802E-03	2.664624E-05
CH3p CH4	1	1.125614E-02	3.025964E-05
CH3p CH2r	1	8.397002E-03	2.734311E-05
CH3p CR1	1	7.280212E-03	2.006986E-05
CH3p HC	1	9.020600E-04	6.349260E-07
CH3p H	1	0.000000E+00	0.000000E+00
CH3p DUM	1	0.000000E+00	0.000000E+00
CH3p S	1	9.797156E-03	1.866579E-05
CH3p CU1+	1	2.005122E-03	3.695476E-07
CH3p CU2+	1	2.005122E-03	3.695476E-07
CH3p FE	1	0.000000E+00	0.000000E+00
CH3p ZN2+	1	2.005122E-03	5.015399E-07
CH3p MG2+	1	7.922440E-04	3.013576E-07
CH3p CA2+	1	3.108185E-03	3.642823E-06
CH3p P	1	1.190327E-02	2.431818E-05
CH3p AR	1	7.760657E-03	1.619836E-05
CH3p F	1	3.365076E-03	4.502296E-06
CH3p CL	1	9.179441E-03	2.018858E-05
CH3p BR	1	1.630571E-02	4.177090E-05
CH3p CMet	1	9.237291E-03	2.271280E-05
CH3p OMet	1	4.663258E-03	7.872050E-06
CH3p NA+	1	8.706056E-04	1.393740E-06
CH3p CL-	1	1.109730E-02	4.013971E-05
CH3p CChl	1	5.029181E-03	1.040659E-05
CH3p CLChl	1	8.936375E-03	1.915154E-05
CH3p HChl	1	6.020270E-04	3.384930E-07
CH3p SDmso	1	1.007660E-02	2.393413E-05
CH3p CDmso	1	9.613802E-03	2.664624E-05
CH3p ODmso	1	4.672279E-03	4.474731E-06
CH3p CCl4	1	5.029181E-03	1.423060E-05

CH3p	CLCl4	1	8.550058E-03	1.844486E-05
CH3p	FTFE	1	3.365076E-03	5.162000E-06
CH3p	CTFE	1	4.743659E-03	9.482594E-06
CH3p	CHTFE	1	8.264634E-03	2.620747E-05
CH3p	OTFE	1	4.663258E-03	6.333774E-06
CH3p	CUrea	1	6.854283E-03	1.902920E-05
CH3p	OUrea	1	4.767191E-03	6.508766E-06
CH3p	NUrea	1	5.677389E-03	1.026051E-05
SI	O	1	5.773784E-03	5.323430E-06
SI	OM	1	5.773784E-03	1.445335E-05
SI	OA	1	5.773784E-03	5.780397E-06
SI	OE	1	5.773784E-03	5.780397E-06
SI	OW	1	6.210824E-03	7.645953E-06
SI	N	1	5.992304E-03	7.174853E-06
SI	NT	1	5.992304E-03	7.174853E-06
SI	NL	1	5.992304E-03	7.174853E-06
SI	NR	1	5.992304E-03	8.672951E-06
SI	NZ	1	5.992304E-03	7.174853E-06
SI	NE	1	5.992304E-03	7.174853E-06
SI	C	1	5.873332E-03	1.046784E-05
SI	CH0	1	5.943744E-03	6.750863E-05
SI	CH1	1	9.457060E-03	4.640335E-05
SI	CH2	1	1.049139E-02	2.745571E-05
SI	CH3	1	1.190327E-02	2.431818E-05
SI	CH4	1	1.393672E-02	2.761588E-05
SI	CH2r	1	1.039670E-02	2.495417E-05
SI	CR1	1	9.013950E-03	1.831637E-05
SI	HC	1	1.116880E-03	5.794530E-07
SI	H	1	0.000000E+00	0.000000E+00
SI	DUM	1	0.000000E+00	0.000000E+00

SI	S	1	1.213029E-02	1.703498E-05
SI	CU1+	1	2.482630E-03	3.372605E-07
SI	CU2+	1	2.482630E-03	3.372605E-07
SI	FE	1	0.000000E+00	0.000000E+00
SI	ZN2+	1	2.482630E-03	4.577208E-07
SI	MG2+	1	9.809120E-04	2.750282E-07
SI	CA2+	1	3.848380E-03	3.324553E-06
SI	P	1	1.473796E-02	2.2193521E-05
SI	AR	1	9.608810E-03	1.478312E-05
SI	F	1	4.166448E-03	5.780397E-06
SI	CL	1	1.136547E-02	1.842472E-05
SI	BR	1	2.018882E-02	3.812141E-05
SI	CMet	1	1.143709E-02	2.072840E-05
SI	OMet	1	5.773784E-03	7.184275E-06
SI	NA+	1	1.077935e-03	1.271970e-06
SI	CL-	1	1.374005e-02	3.663274e-05
SI	CChl	1	6.226849E-03	9.497376E-06
SI	CLChl	1	1.106452E-02	1.747828E-05
SI	HChl	1	7.453960E-04	3.089191E-07
SI	SDmso	1	1.247628E-02	2.184302E-05
SI	CDmso	1	1.190327E-02	2.431818E-05
SI	ODmso	1	5.784953E-03	5.299875E-06
SI	CCl4	1	6.226849E-03	1.298729E-05
SI	CLCl4	1	1.058620E-02	1.683335E-05
SI	FTFE	1	4.166448E-03	4.711000E-06
SI	CTFE	1	5.873332E-03	8.654107E-06
SI	CHTFE	1	1.023281E-02	2.391775E-05
SI	OTFE	1	5.773784E-03	5.780397E-06
SI	CUrea	1	8.486588E-03	1.736663E-05
SI	OUrea	1	5.902468E-03	5.940100E-06

SI	NUrea	1	7.029424E-03	9.364055E-06
SI	CH3p	1	1.190327E-02	2.431818E-05
CLCl4	I	1	0.0186172	4.352158e-05
CLCl4	CLOpt	1	0.00716348	1.026223e-05
CLCl4	B	1	0.004218736	7.93965e-06
CLCl4	SE	1	0.008713024	1.292069e-05
CLCl4	HS14	1	0	0
CLCl4	CLAro	1	0.00716348	1.026223e-05
CLCl4	BROpt	1	0.01612677	3.9198e-05
CLCl4	OEOpt	1	0.004846576	7.807442e-06
CLCl4	NOpt	1	0.00792648	1.929528e-05
CLCl4	CAro	1	0.004218736	7.543025e-06
CLCl4	CPos	1	0.003924	3.5732e-06
CLCl4	NPri	1	0.0090688	2.50124e-05
CLCl4	NTer	1	0.00810088	1.60794e-05
CLCl4	OAlc	1	0.003673736	3.93052e-06
CUrea	I	1	0.01492578	4.490035e-05
CUrea	CLOpt	1	0.005743107	1.058734e-05
CUrea	B	1	0.003382246	8.191181e-06
CUrea	SE	1	0.006985407	1.333002e-05
CUrea	HS14	1	0	0
CUrea	CLAro	1	0.005743107	1.058734e-05
CUrea	BROpt	1	0.01292916	4.043981e-05
CUrea	OEOpt	1	0.003885598	8.054784e-06
CUrea	NOpt	1	0.006354819	1.990656e-05
CUrea	CAro	1	0.003382246	7.78199e-06
CUrea	CPos	1	0.00314595	3.6864e-06
CUrea	NPri	1	0.00727064	2.58048e-05
CUrea	NTer	1	0.006494639	1.65888e-05
CUrea	OAlc	1	0.002945308	4.05504e-06

CU2+	I	1	0.004366075	8.719662e-07
CU2+	CLOpt	1	0.001679968	2.056065e-07
CU2+	B	1	0.000989371	1.59073e-07
CU2+	SE	1	0.002043364	2.588694e-07
CU2+	HS14	1	0	0
CU2+	CLAro	1	0.001679968	2.056065e-07
CU2+	BROpt	1	0.003782023	7.853423e-07
CU2+	OEOpt	1	0.001136611	1.564241e-07
CU2+	NOpt	1	0.001858905	3.86586e-07
CU2+	CAro	1	0.000989371	1.511265e-07
CU2+	CPos	1	0.00092025	7.159e-08
CU2+	NPri	1	0.0021268	5.0113e-07
CU2+	NTer	1	0.001899805	3.22155e-07
CU2+	OAlc	1	0.0008615585	7.8749e-08
ZN2+	I	1	0.004366075	1.183409e-06
ZN2+	CLOpt	1	0.001679968	2.790435e-07
ZN2+	B	1	0.000989371	2.158895e-07
ZN2+	SE	1	0.002043364	3.513306e-07
ZN2+	HS14	1	0	0
ZN2+	CLAro	1	0.001679968	2.790435e-07
ZN2+	BROpt	1	0.003782023	1.065845e-06
ZN2+	OEOpt	1	0.001136611	2.122946e-07
ZN2+	NOpt	1	0.001858905	5.24664e-07
ZN2+	CAro	1	0.000989371	2.051048e-07
ZN2+	CPos	1	0.00092025	9.716e-08
ZN2+	NPri	1	0.0021268	6.8012e-07
ZN2+	NTer	1	0.001899805	4.3722e-07
ZN2+	OAlc	1	0.0008615585	1.06876e-07
O	I	1	0.01015406	1.218e-05
O	CLOpt	1	0.003907054	2.872e-06

O	B	1	0.002300953	2.222e-06
O	SE	1	0.004752195	3.616e-06
O	HS14	1	0	0
O	CLAro	1	0.003907054	2.872e-06
O	BROpt	1	0.008795746	1.097e-05
O	OEOpt	1	0.002643385	2.185e-06
O	NOpt	1	0.004323204	5.4e-06
O	CAro	1	0.002300953	2.111e-06
O	CPos	1	0.0021402	1e-06
O	NPri	1	0.00494624	7e-06
O	NTer	1	0.004418324	4.5e-06
O	OAlc	1	0.002003703	1.1e-06
NR	I	1	0.01053836	1.855014e-05
NR	CLOpt	1	0.004054924	4.374056e-06
NR	B	1	0.002388037	3.384106e-06
NR	SE	1	0.004932051	5.507168e-06
NR	HS14	1	0	0
NR	CLAro	1	0.004054924	4.374056e-06
NR	BROpt	1	0.009128638	1.670731e-05
NR	OEOpt	1	0.002743429	3.327755e-06
NR	NOpt	1	0.004486824	8.2242e-06
NR	CAro	1	0.002388037	3.215053e-06
NR	CPos	1	0.0022212	1.523e-06
NR	NPri	1	0.00513344	1.0661e-05
NR	NTer	1	0.004585544	6.8535e-06
NR	OAlc	1	0.002079537	1.6753e-06
ODmso	I	1	0.01017327	1.055835e-05
ODmso	CLOpt	1	0.003914448	2.489622e-06
ODmso	B	1	0.002305307	1.926163e-06
ODmso	SE	1	0.004761188	3.134566e-06

ODmso	HS14	1	0	0
ODmso	CLAro	1	0.003914448	2.489622e-06
ODmso	BROpt	1	0.008812391	9.509454e-06
ODmso	OEOpt	1	0.002648387	1.894089e-06
ODmso	NOpt	1	0.004331385	4.681044e-06
ODmso	CAro	1	0.002305307	1.829941e-06
ODmso	CPos	1	0.00214425	8.6686e-07
ODmso	NPri	1	0.0049556	6.06802e-06
ODmso	NTer	1	0.004426685	3.90087e-06
ODmso	OAlc	1	0.002007495	9.53546e-07
HChl	I	1	0.00131089	7.986913e-07
HChl	CLOpt	1	0.000504401	1.883285e-07
HChl	B	1	0.0002970532	1.457054e-07
HChl	SE	1	0.0006135088	2.371156e-07
HChl	HS14	1	0	0
HChl	CLAro	1	0.000504401	1.883285e-07
HChl	BROpt	1	0.001135532	7.193468e-07
HChl	OEOpt	1	0.0003412612	1.432792e-07
HChl	NOpt	1	0.000558126	3.540996e-07
HChl	CAro	1	0.0002970532	1.384267e-07
HChl	CPos	1	0.0002763	6.5574e-08
HChl	NPri	1	0.00063856	4.59018e-07
HChl	NTer	1	0.000570406	2.95083e-07
HChl	OAlc	1	0.0002586782	7.21314e-08
CL-	I	1	0.02416393	9.471168e-05
CL-	CLOpt	1	0.009297737	2.233267e-05
CL-	B	1	0.005475648	1.727827e-05
CL-	SE	1	0.01130895	2.811802e-05
CL-	HS14	1	0	0
CL-	CLAro	1	0.009297737	2.233267e-05

CL-	BROpt 1	0.02093151	8.530272e-05
CL-	OEOpt 1	0.006290544	1.699056e-05
CL-	NOpt 1	0.01028806	4.19904e-05
CL-	CAro 1	0.005475648	1.641514e-05
CL-	CPos 1	0.0050931	7.776e-06
CL-	NPri 1	0.01177072	5.4432e-05
CL-	NTer 1	0.01051442	3.4992e-05
CL-	OAlc 1	0.004768273	8.5536e-06
CCl4	I 1	0.01095041	3.357782e-05
CCl4	CLOpt 1	0.004213474	7.91753e-06
CCl4	B 1	0.00248141	6.12561e-06
CCl4	SE 1	0.005124897	9.968589e-06
CCl4	HS14 1	0	0
CCl4	CLAro 1	0.004213474	7.91753e-06
CCl4	BROpt 1	0.009485573	3.02421e-05
CCl4	OEOpt 1	0.002850698	6.023608e-06
CCl4	NOpt 1	0.004662261	1.488672e-05
CCl4	CAro 1	0.00248141	5.819605e-06
CCl4	CPos 1	0.00230805	2.7568e-06
CCl4	NPri 1	0.00533416	1.92976e-05
CCl4	NTer 1	0.004764841	1.24056e-05
CCl4	OAlc 1	0.002160848	3.03248e-06
CChl	I 1	0.01095041	2.455488e-05
CChl	CLOpt 1	0.004213474	5.789952e-06
CChl	B 1	0.00248141	4.479552e-06
CChl	SE 1	0.005124897	7.289856e-06
CChl	HS14 1	0	0
CChl	CLAro 1	0.004213474	5.789952e-06
CChl	BROpt 1	0.009485573	2.211552e-05
CChl	OEOpt 1	0.002850698	4.40496e-06

CChl	NOpt	1	0.004662261	1.08864e-05
CChl	CAro	1	0.00248141	4.255776e-06
CChl	CPos	1	0.00230805	2.016e-06
CChl	NPri	1	0.00533416	1.4112e-05
CChl	NTer	1	0.004764841	9.072e-06
CChl	OAlc	1	0.002160848	2.2176e-06
OE	I	1	0.01015406	1.3398e-05
OE	CLOpt	1	0.003907054	3.1592e-06
OE	B	1	0.002300953	2.4442e-06
OE	SE	1	0.004752195	3.9776e-06
OE	HS14	1	0	0
OE	CLAro	1	0.003907054	3.1592e-06
OE	BROpt	1	0.008795746	1.2067e-05
OE	OEOpt	1	0.002643385	2.4035e-06
OE	NOpt	1	0.004323204	5.94e-06
OE	CAro	1	0.002300953	2.3221e-06
OE	CPos	1	0.0021402	1.1e-06
OE	NPri	1	0.00494624	7.7e-06
OE	NTer	1	0.004418324	4.95e-06
OE	OAlc	1	0.002003703	1.21e-06
C	I	1	0.01032913	2.706396e-05
C	CLOpt	1	0.003974417	6.381584e-06
C	B	1	0.002340624	4.937284e-06
C	SE	1	0.00483413	8.034752e-06
C	HS14	1	0	0
C	CLAro	1	0.003974417	6.381584e-06
C	BROpt	1	0.008947397	2.437534e-05
C	OEOpt	1	0.00268896	4.85507e-06
C	NOpt	1	0.004397742	1.19988e-05
C	CAro	1	0.002340624	4.690642e-06

C	CPos	1	0.0021771	2.222e-06
C	NPri	1	0.00503152	1.5554e-05
C	NTer	1	0.004494502	9.999e-06
C	OAlc	1	0.002038249	2.4442e-06
BR	I	1	0.03550505	9.856056e-05
BR	CLOpt	1	0.01366155	2.324022e-05
BR	B	1	0.008045594	1.798042e-05
BR	SE	1	0.0166167	2.926067e-05
BR	HS14	1	0	0
BR	CLAro	1	0.01366155	2.324022e-05
BR	BROpt	1	0.03075552	8.876924e-05
BR	OEOpt	1	0.009242954	1.768102e-05
BR	NOpt	1	0.01511667	4.36968e-05
BR	CAro	1	0.008045594	1.708221e-05
BR	CPos	1	0.0074835	8.092e-06
BR	NPri	1	0.0172952	5.6644e-05
BR	NTer	1	0.01544927	3.6414e-05
BR	OAlc	1	0.007006219	8.9012e-06
NUrea	I	1	0.01236165	2.421019e-05
NUrea	CLOpt	1	0.004756485	5.708674e-06
NUrea	B	1	0.002801202	4.416669e-06
NUrea	SE	1	0.005785368	7.187523e-06
NUrea	HS14	1	0	0
NUrea	CLAro	1	0.004756485	5.708674e-06
NUrea	BROpt	1	0.01070803	2.180507e-05
NUrea	OEOpt	1	0.003218082	4.343124e-06
NUrea	NOpt	1	0.00526311	1.073358e-05
NUrea	CAro	1	0.002801202	4.196035e-06
NUrea	CPos	1	0.0026055	1.9877e-06
NUrea	NPri	1	0.0060216	1.39139e-05

NUrea	NTer 1	0.00537891	8.94465e-06
NUrea	OAlc 1	0.002439327	2.18647e-06
NT	I 1	0.01053836	1.855014e-05
NT	CLOpt 1	0.004054924	4.374056e-06
NT	B 1	0.002388037	3.384106e-06
NT	SE 1	0.004932051	5.507168e-06
NT	HS14 1	0	0
NT	CLAro 1	0.004054924	4.374056e-06
NT	BROpt 1	0.009128638	1.670731e-05
NT	OEOpt 1	0.002743429	3.327755e-06
NT	NOpt 1	0.004486824	8.2242e-06
NT	CAro 1	0.002388037	3.215053e-06
NT	CPos 1	0.0022212	1.523e-06
NT	NPri 1	0.00513344	1.0661e-05
NT	NTer 1	0.004585544	6.8535e-06
NT	OAlc 1	0.002079537	1.6753e-06
CR1	I 1	0.01585237	4.735584e-05
CR1	CLOpt 1	0.006099637	1.116634e-05
CR1	B 1	0.003592215	8.639136e-06
CR1	SE 1	0.00741906	1.405901e-05
CR1	HS14 1	0	0
CR1	CLAro 1	0.006099637	1.116634e-05
CR1	BROpt 1	0.01373179	4.265136e-05
CR1	OEOpt 1	0.004126815	8.49528e-06
CR1	NOpt 1	0.006749325	2.09952e-05
CR1	CAro 1	0.003592215	8.207568e-06
CR1	CPos 1	0.00334125	3.888e-06
CR1	NPri 1	0.007722	2.7216e-05
CR1	NTer 1	0.006897825	1.7496e-05
CR1	OAlc 1	0.003128153	4.2768e-06

S	I	1	0.02133292	4.404288e-05
S	CLOpt	1	0.008208428	1.038515e-05
S	B	1	0.00483413	8.034752e-06
S	SE	1	0.009984006	1.307546e-05
S	HS14	1	0	0
S	CLAro	1	0.008208428	1.038515e-05
S	BROpt	1	0.0184792	3.966752e-05
S	OEOpt	1	0.005553554	7.90096e-06
S	NOpt	1	0.009082728	1.95264e-05
S	CAro	1	0.00483413	7.633376e-06
S	CPos	1	0.0044964	3.616e-06
S	NPri	1	0.01039168	2.5312e-05
S	NTer	1	0.009282568	1.6272e-05
S	OAlc	1	0.00420963	3.9776e-06
CH3p	I	1	0.02093367	6.287316e-05
CH3p	CLOpt	1	0.008054808	1.482526e-05
CH3p	B	1	0.004743659	1.146996e-05
CH3p	SE	1	0.009797156	1.866579e-05
CH3p	HS14	1	0	0
CH3p	CLAro	1	0.008054808	1.482526e-05
CH3p	BROpt	1	0.01813337	5.662714e-05
CH3p	OEOpt	1	0.005449619	1.127897e-05
CH3p	NOpt	1	0.008912745	2.78748e-05
CH3p	CAro	1	0.004743659	1.089698e-05
CH3p	CPos	1	0.00441225	5.162e-06
CH3p	NPri	1	0.0101972	3.6134e-05
CH3p	NTer	1	0.009108845	2.3229e-05
CH3p	OAlc	1	0.004130846	5.6782e-06
H	I	1	0	0
H	CLOpt	1	0	0

H	B	1	0	0
H	SE	1	0	0
H	HS14	1	0	0
H	CLAro	1	0	0
H	BROpt	1	0	0
H	OEOpt	1	0	0
H	NOpt	1	0	0
H	CAro	1	0	0
H	CPos	1	0	0
H	NPri	1	0	0
H	NTer	1	0	0
H	OAlc	1	0	0
CA2+	I	1	0.00676795	8.595426e-06
CA2+	CLOpt	1	0.002604155	2.02677e-06
CA2+	B	1	0.001533646	1.568065e-06
CA2+	SE	1	0.003167464	2.551811e-06
CA2+	HS14	1	0	0
CA2+	CLAro	1	0.002604155	2.02677e-06
CA2+	BROpt	1	0.005862598	7.741529e-06
CA2+	OEOpt	1	0.001761886	1.541954e-06
CA2+	NOpt	1	0.00288153	3.81078e-06
CA2+	CAro	1	0.001533646	1.489733e-06
CA2+	CPos	1	0.0014265	7.057e-07
CA2+	NPri	1	0.0032968	4.9399e-06
CA2+	NTer	1	0.00294493	3.17565e-06
CA2+	OAlc	1	0.001335521	7.7627e-07
F	I	1	0.00732732	1.06234e-05
F	CLOpt	1	0.002819388	2.504958e-06
F	B	1	0.001660402	1.938028e-06
F	SE	1	0.003429254	3.153875e-06

F	HS14	1	0	0
F	CLAro	1	0.002819388	2.504958e-06
F	BROpt	1	0.006347141	9.568034e-06
F	OEOpt	1	0.001907506	1.905757e-06
F	NOpt	1	0.003119688	4.70988e-06
F	CAro	1	0.001660402	1.841214e-06
F	CPos	1	0.0015444	8.722e-07
F	NPri	1	0.00356928	6.1054e-06
F	NTer	1	0.003188328	3.9249e-06
F	OAlc	1	0.001445902	9.5942e-07
N	I	1	0.01053836	1.855014e-05
N	CLOpt	1	0.004054924	4.374056e-06
N	B	1	0.002388037	3.384106e-06
N	SE	1	0.004932051	5.507168e-06
N	HS14	1	0	0
N	CLAro	1	0.004054924	4.374056e-06
N	BROpt	1	0.009128638	1.670731e-05
N	OEOpt	1	0.002743429	3.327755e-06
N	NOpt	1	0.004486824	8.2242e-06
N	CAro	1	0.002388037	3.215053e-06
N	CPos	1	0.0022212	1.523e-06
N	NPri	1	0.00513344	1.0661e-05
N	NTer	1	0.004585544	6.8535e-06
N	OAlc	1	0.002079537	1.6753e-06
CH0	I	1	0.01045296	0.0001745394
CH0	CLOpt	1	0.004022064	4.115576e-05
CH0	B	1	0.002368685	3.184126e-05
CH0	SE	1	0.004892083	5.181728e-05
CH0	HS14	1	0	0
CH0	CLAro	1	0.004022064	4.115576e-05

CH0	BROpt	1	0.009054662	0.0001572001
CH0	OEOpt	1	0.002721197	3.131105e-05
CH0	NOpt	1	0.004450464	7.7382e-05
CH0	CAro	1	0.002368685	3.025063e-05
CH0	CPos	1	0.0022032	1.433e-05
CH0	NPri	1	0.00509184	0.00010031
CH0	NTer	1	0.004548384	6.4485e-05
CH0	OAlc	1	0.002062685	1.5763e-05
CLChl	I	1	0.01945839	4.518902e-05
CLChl	CLOpt	1	0.007487151	1.065541e-05
CLChl	B	1	0.004409353	8.243842e-06
CLChl	SE	1	0.009106709	1.341572e-05
CLChl	HS14	1	0	0
CLChl	CLAro	1	0.007487151	1.065541e-05
CLChl	BROpt	1	0.01685543	4.06998e-05
CLChl	OEOpt	1	0.005065561	8.106569e-06
CLChl	NOpt	1	0.008284626	2.003454e-05
CLChl	CAro	1	0.004409353	7.832021e-06
CLChl	CPos	1	0.0041013	3.7101e-06
CLChl	NPri	1	0.00947856	2.59707e-05
CLChl	NTer	1	0.008466906	1.669545e-05
CLChl	OAlc	1	0.003839728	4.08111e-06
FTFE	I	1	0.00732732	1.218e-05
FTFE	CLOpt	1	0.002819388	2.872e-06
FTFE	B	1	0.001660402	2.222e-06
FTFE	SE	1	0.003429254	3.616e-06
FTFE	HS14	1	0	0
FTFE	CLAro	1	0.002819388	2.872e-06
FTFE	BROpt	1	0.006347141	1.097e-05
FTFE	OEOpt	1	0.001907506	2.185e-06

FTFE	NOpt	1	0.003119688	5.4e-06
FTFE	CAro	1	0.001660402	2.111e-06
FTFE	CPos	1	0.0015444	1e-06
FTFE	NPri	1	0.00356928	7e-06
FTFE	NTer	1	0.003188328	4.5e-06
FTFE	OAlc	1	0.001445902	1.1e-06
SI	I	1	0.0259189	5.737998e-05
SI	CLOpt	1	0.00997301	1.352999e-05
SI	B	1	0.005873332	1.046784e-05
SI	SE	1	0.01213029	1.703498e-05
SI	HS14	1	0	0
SI	CLAro	1	0.00997301	1.352999e-05
SI	BROpt	1	0.02245172	5.167967e-05
SI	OEOpt	1	0.006747412	1.029353e-05
SI	NOpt	1	0.01103526	2.54394e-05
SI	CAro	1	0.005873332	9.944921e-06
SI	CPos	1	0.005463	4.711e-06
SI	NPri	1	0.0126256	3.2977e-05
SI	NTer	1	0.01127806	2.11995e-05
SI	OAlc	1	0.005114582	5.1821e-06
CDmso	I	1	0.02093367	6.287316e-05
CDmso	CLOpt	1	0.008054808	1.482526e-05
CDmso	B	1	0.004743659	1.146996e-05
CDmso	SE	1	0.009797156	1.866579e-05
CDmso	HS14	1	0	0
CDmso	CLAro	1	0.008054808	1.482526e-05
CDmso	BROpt	1	0.01813337	5.662714e-05
CDmso	OEOpt	1	0.005449619	1.127897e-05
CDmso	NOpt	1	0.008912745	2.78748e-05
CDmso	CAro	1	0.004743659	1.089698e-05

CDmso	CPos	1	0.00441225	5.162e-06
CDmso	NPri	1	0.0101972	3.6134e-05
CDmso	NTer	1	0.009108845	2.3229e-05
CDmso	OAlc	1	0.004130846	5.6782e-06
CH4	I	1	0.0245098	7.139916e-05
CH4	CLOpt	1	0.00943082	1.683566e-05
CH4	B	1	0.005554024	1.302536e-05
CH4	SE	1	0.01147082	2.119699e-05
CH4	HS14	1	0	0
CH4	CLAro	1	0.00943082	1.683566e-05
CH4	BROpt	1	0.02123111	6.430614e-05
CH4	OEOpt	1	0.006380584	1.280847e-05
CH4	NOpt	1	0.01043532	3.16548e-05
CH4	CAro	1	0.005554024	1.237468e-05
CH4	CPos	1	0.005166	5.862e-06
CH4	NPri	1	0.0119392	4.1034e-05
CH4	NTer	1	0.01066492	2.6379e-05
CH4	OAlc	1	0.004836524	6.4482e-06
FE	I	1	0	0
FE	CLOpt	1	0	0
FE	B	1	0	0
FE	SE	1	0	0
FE	HS14	1	0	0
FE	CLAro	1	0	0
FE	BROpt	1	0	0
FE	OEOpt	1	0	0
FE	NOpt	1	0	0
FE	CAro	1	0	0
FE	CPos	1	0	0
FE	NPri	1	0	0

FE	NTer	1	0	0
FE	OAlc	1	0	0
CTFE	I	1	0.01032913	2.237466e-05
CTFE	CLOpt	1	0.003974417	5.275864e-06
CTFE	B	1	0.002340624	4.081814e-06
CTFE	SE	1	0.00483413	6.642592e-06
CTFE	HS14	1	0	0
CTFE	CLAro	1	0.003974417	5.275864e-06
CTFE	BROpt	1	0.008947397	2.015189e-05
CTFE	OEOpt	1	0.00268896	4.013845e-06
CTFE	NOpt	1	0.004397742	9.9198e-06
CTFE	CAro	1	0.002340624	3.877907e-06
CTFE	CPos	1	0.0021771	1.837e-06
CTFE	NPri	1	0.00503152	1.2859e-05
CTFE	NTer	1	0.004494502	8.2665e-06
CTFE	OAlc	1	0.002038249	2.0207e-06
OA	I	1	0.01015406	1.3398e-05
OA	CLOpt	1	0.003907054	3.1592e-06
OA	B	1	0.002300953	2.4442e-06
OA	SE	1	0.004752195	3.9776e-06
OA	HS14	1	0	0
OA	CLAro	1	0.003907054	3.1592e-06
OA	BROpt	1	0.008795746	1.2067e-05
OA	OEOpt	1	0.002643385	2.4035e-06
OA	NOpt	1	0.004323204	5.94e-06
OA	CAro	1	0.002300953	2.3221e-06
OA	CPos	1	0.0021402	1.1e-06
OA	NPri	1	0.00494624	7.7e-06
OA	NTer	1	0.004418324	4.95e-06
OA	OAlc	1	0.002003703	1.21e-06

OW	I	1	0.01092266	1.976814e-05
OW	CLOpt	1	0.004202794	4.661256e-06
OW	B	1	0.002475121	3.606306e-06
OW	SE	1	0.005111907	5.868768e-06
OW	HS14	1	0	0
OW	CLAro	1	0.004202794	4.661256e-06
OW	BROpt	1	0.00946153	1.780431e-05
OW	OEOpt	1	0.002843473	3.546255e-06
OW	NOpt	1	0.004650444	8.7642e-06
OW	CAro	1	0.002475121	3.426153e-06
OW	CPos	1	0.0023022	1.623e-06
OW	NPri	1	0.00532064	1.1361e-05
OW	NTer	1	0.004752764	7.3035e-06
OW	OAlc	1	0.002155371	1.7853e-06
CH2	I	1	0.01845067	7.098504e-05
CH2	CLOpt	1	0.007099403	1.673802e-05
CH2	B	1	0.004181	1.294982e-05
CH2	SE	1	0.008635086	2.107405e-05
CH2	HS14	1	0	0
CH2	CLAro	1	0.007099403	1.673802e-05
CH2	BROpt	1	0.01598251	6.393316e-05
CH2	OEOpt	1	0.004803224	1.273418e-05
CH2	NOpt	1	0.007855578	3.14712e-05
CH2	CAro	1	0.004181	1.230291e-05
CH2	CPos	1	0.0038889	5.828e-06
CH2	NPri	1	0.00898768	4.0796e-05
CH2	NTer	1	0.008028418	2.6226e-05
CH2	OAlc	1	0.003640875	6.4108e-06
SDmso	I	1	0.02194139	5.647379e-05
SDmso	CLOpt	1	0.008442556	1.331632e-05

SDmso	B	1	0.004972013	1.030253e-05
SDmso	SE	1	0.01026878	1.676595e-05
SDmso	HS14	1	0	0
SDmso	CLAro	1	0.008442556	1.331632e-05
SDmso	BROpt	1	0.01900628	5.08635e-05
SDmso	OEOpt	1	0.005711957	1.013097e-05
SDmso	NOpt	1	0.009341793	2.503764e-05
SDmso	CAro	1	0.004972013	9.787863e-06
SDmso	CPos	1	0.00462465	4.6366e-06
SDmso	NPri	1	0.01068808	3.24562e-05
SDmso	NTer	1	0.009547333	2.08647e-05
SDmso	OAlc	1	0.0043297	5.10026e-06
DUM	I	1	0	0
DUM	CLOpt	1	0	0
DUM	B	1	0	0
DUM	SE	1	0	0
DUM	HS14	1	0	0
DUM	CLAro	1	0	0
DUM	BROpt	1	0	0
DUM	OEOpt	1	0	0
DUM	NOpt	1	0	0
DUM	CAro	1	0	0
DUM	CPos	1	0	0
DUM	NPri	1	0	0
DUM	NTer	1	0	0
DUM	OAlc	1	0	0
CH1	I	1	0.01663165	0.000119973
CH1	CLOpt	1	0.006399485	2.82892e-05
CH1	B	1	0.003768802	2.18867e-05
CH1	SE	1	0.007783768	3.56176e-05

CH1	HS14	1	0	0
CH1	CLAro	1	0.006399485	2.82892e-05
CH1	BROpt	1	0.01440683	0.0001080545
CH1	OEOpt	1	0.004329682	2.152225e-05
CH1	NOpt	1	0.00708111	5.319e-05
CH1	CAro	1	0.003768802	2.079335e-05
CH1	CPos	1	0.0035055	9.85e-06
CH1	NPri	1	0.0081016	6.895e-05
CH1	NTer	1	0.00723691	4.4325e-05
CH1	OAlc	1	0.003281927	1.0835e-05
CHTFE	I	1	0.01799592	6.183786e-05
CHTFE	CLOpt	1	0.006924424	1.458114e-05
CHTFE	B	1	0.00407795	1.128109e-05
CHTFE	SE	1	0.008422257	1.835843e-05
CHTFE	HS14	1	0	0
CHTFE	CLAro	1	0.006924424	1.458114e-05
CHTFE	BROpt	1	0.01558859	5.569469e-05
CHTFE	OEOpt	1	0.004684838	1.109324e-05
CHTFE	NOpt	1	0.007661961	2.74158e-05
CHTFE	CAro	1	0.00407795	1.071755e-05
CHTFE	CPos	1	0.00379305	5.077e-06
CHTFE	NPri	1	0.00876616	3.5539e-05
CHTFE	NTer	1	0.007830541	2.28465e-05
CHTFE	OAlc	1	0.003551138	5.5847e-06
NL	I	1	0.01053836	1.855014e-05
NL	CLOpt	1	0.004054924	4.374056e-06
NL	B	1	0.002388037	3.384106e-06
NL	SE	1	0.004932051	5.507168e-06
NL	HS14	1	0	0
NL	CLAro	1	0.004054924	4.374056e-06

NL	BROpt 1	0.009128638	1.670731e-05
NL	OEOpt 1	0.002743429	3.327755e-06
NL	NOpt 1	0.004486824	8.2242e-06
NL	CAro 1	0.002388037	3.215053e-06
NL	CPos 1	0.0022212	1.523e-06
NL	NPri 1	0.00513344	1.0661e-05
NL	NTer 1	0.004585544	6.8535e-06
NL	OAlc 1	0.002079537	1.6753e-06
AR	I 1	0.01689853	3.822084e-05
AR	CLOpt 1	0.006502172	9.012336e-06
AR	B 1	0.003829277	6.972636e-06
AR	SE 1	0.007908668	1.134701e-05
AR	HS14 1	0	0
AR	CLAro 1	0.006502172	9.012336e-06
AR	BROpt 1	0.014638	3.442386e-05
AR	OEOpt 1	0.004399157	6.85653e-06
AR	NOpt 1	0.007194735	1.69452e-05
AR	CAro 1	0.003829277	6.624318e-06
AR	CPos 1	0.00356175	3.138e-06
AR	NPri 1	0.0082316	2.1966e-05
AR	NTer 1	0.007353035	1.4121e-05
AR	OAlc 1	0.003334589	3.4518e-06
CH2r	I 1	0.01828414	6.451746e-05
CH2r	CLOpt 1	0.007035326	1.521298e-05
CH2r	B 1	0.004143263	1.176993e-05
CH2r	SE 1	0.008557149	1.915395e-05
CH2r	HS14 1	0	0
CH2r	CLAro 1	0.007035326	1.521298e-05
CH2r	BROpt 1	0.01583826	5.810809e-05
CH2r	OEOpt 1	0.004759871	1.157394e-05

CH2r	NOpt 1	0.007784676	2.86038e-05
CH2r	CAro 1	0.004143263	1.118197e-05
CH2r	CPos 1	0.0038538	5.297e-06
CH2r	NPri 1	0.00890656	3.7079e-05
CH2r	NTer 1	0.007955956	2.38365e-05
CH2r	OAlc 1	0.003608013	5.8267e-06
NA+	I 1	0.00189588	3.2886e-06
NA+	CLOpt 1	0.000729492	7.7544e-07
NA+	B 1	0.0004296144	5.9994e-07
NA+	SE 1	0.0008872896	9.7632e-07
NA+	HS14 1	0	0
NA+	CLAro 1	0.000729492	7.7544e-07
NA+	BROpt 1	0.001642267	2.9619e-06
NA+	OEOpt 1	0.0004935504	5.8995e-07
NA+	NOpt 1	0.000807192	1.458e-06
NA+	CAro 1	0.0004296144	5.6997e-07
NA+	CPos 1	0.0003996	2.7e-07
NA+	NPri 1	0.00092352	1.89e-06
NA+	NTer 1	0.000824952	1.215e-06
NA+	OAlc 1	0.0003741144	2.97e-07
OTFE	I 1	0.01015406	1.494486e-05
OTFE	CLOpt 1	0.003907054	3.523944e-06
OTFE	B 1	0.002300953	2.726394e-06
OTFE	SE 1	0.004752195	4.436832e-06
OTFE	HS14 1	0	0
OTFE	CLAro 1	0.003907054	3.523944e-06
OTFE	BROpt 1	0.008795746	1.346019e-05
OTFE	OEOpt 1	0.002643385	2.680995e-06
OTFE	NOpt 1	0.004323204	6.6258e-06
OTFE	CAro 1	0.002300953	2.590197e-06

OTFE	CPos 1	0.0021402	1.227e-06
OTFE	NPri 1	0.00494624	8.589e-06
OTFE	NTer 1	0.004418324	5.5215e-06
OTFE	OAlc 1	0.002003703	1.3497e-06
OMet	I 1	0.01015406	1.85745e-05
OMet	CLOpt 1	0.003907054	4.3798e-06
OMet	B 1	0.002300953	3.38855e-06
OMet	SE 1	0.004752195	5.5144e-06
OMet	HS14 1	0	0
OMet	CLAro 1	0.003907054	4.3798e-06
OMet	BROpt 1	0.008795746	1.672925e-05
OMet	OEOpt 1	0.002643385	3.332125e-06
OMet	NOpt 1	0.004323204	8.235e-06
OMet	CAro 1	0.002300953	3.219275e-06
OMet	CPos 1	0.0021402	1.525e-06
OMet	NPri 1	0.00494624	1.0675e-05
OMet	NTer 1	0.004418324	6.8625e-06
OMet	OAlc 1	0.002003703	1.6775e-06
CU1+	I 1	0.004366075	8.719662e-07
CU1+	CLOpt 1	0.001679968	2.056065e-07
CU1+	B 1	0.000989371	1.59073e-07
CU1+	SE 1	0.002043364	2.588694e-07
CU1+	HS14 1	0	0
CU1+	CLAro 1	0.001679968	2.056065e-07
CU1+	BROpt 1	0.003782023	7.853423e-07
CU1+	OEOpt 1	0.001136611	1.564241e-07
CU1+	NOpt 1	0.001858905	3.86586e-07
CU1+	CAro 1	0.000989371	1.511265e-07
CU1+	CPos 1	0.00092025	7.159e-08
CU1+	NPri 1	0.0021268	5.0113e-07

CU1+	NTer	1	0.001899805	3.22155e-07
CU1+	OAlc	1	0.0008615585	7.8749e-08
OUrea	I	1	0.01038037	1.535776e-05
OUrea	CLOpt	1	0.003994133	3.621305e-06
OUrea	B	1	0.002352236	2.80172e-06
OUrea	SE	1	0.00485811	4.559414e-06
OUrea	HS14	1	0	0
OUrea	CLAro	1	0.003994133	3.621305e-06
OUrea	BROpt	1	0.008991783	1.383207e-05
OUrea	OEOpt	1	0.0027023	2.755066e-06
OUrea	NOpt	1	0.004419558	6.80886e-06
OUrea	CAro	1	0.002352236	2.66176e-06
OUrea	CPos	1	0.0021879	1.2609e-06
OUrea	NPri	1	0.00505648	8.8263e-06
OUrea	NTer	1	0.004516798	5.67405e-06
OUrea	OAlc	1	0.002048361	1.38699e-06
CMet	I	1	0.02011384	5.3592e-05
CMet	CLOpt	1	0.007739351	1.26368e-05
CMet	B	1	0.00455788	9.7768e-06
CMet	SE	1	0.009413463	1.59104e-05
CMet	HS14	1	0	0
CMet	CLAro	1	0.007739351	1.26368e-05
CMet	BROpt	1	0.0174232	4.8268e-05
CMet	OEOpt	1	0.005236192	9.614e-06
CMet	NOpt	1	0.008563689	2.376e-05
CMet	CAro	1	0.00455788	9.2884e-06
CMet	CPos	1	0.00423945	4.4e-06
CMet	NPri	1	0.00979784	3.08e-05
CMet	NTer	1	0.008752109	1.98e-05
CMet	OAlc	1	0.003969067	4.84e-06

NZ	I	1	0.01053836	1.855014e-05
NZ	CLOpt	1	0.004054924	4.374056e-06
NZ	B	1	0.002388037	3.384106e-06
NZ	SE	1	0.004932051	5.507168e-06
NZ	HS14	1	0	0
NZ	CLAro	1	0.004054924	4.374056e-06
NZ	BROpt	1	0.009128638	1.670731e-05
NZ	OEOpt	1	0.002743429	3.327755e-06
NZ	NOpt	1	0.004486824	8.2242e-06
NZ	CAro	1	0.002388037	3.215053e-06
NZ	CPos	1	0.0022212	1.523e-06
NZ	NPri	1	0.00513344	1.0661e-05
NZ	NTer	1	0.004585544	6.8535e-06
NZ	OAlc	1	0.002079537	1.6753e-06
CH3	I	1	0.02093367	6.287316e-05
CH3	CLOpt	1	0.008054808	1.482526e-05
CH3	B	1	0.004743659	1.146996e-05
CH3	SE	1	0.009797156	1.866579e-05
CH3	HS14	1	0	0
CH3	CLAro	1	0.008054808	1.482526e-05
CH3	BROpt	1	0.01813337	5.662714e-05
CH3	OEOpt	1	0.005449619	1.127897e-05
CH3	NOpt	1	0.008912745	2.78748e-05
CH3	CAro	1	0.004743659	1.089698e-05
CH3	CPos	1	0.00441225	5.162e-06
CH3	NPri	1	0.0101972	3.6134e-05
CH3	NTer	1	0.009108845	2.3229e-05
CH3	OAlc	1	0.004130846	5.6782e-06
P	I	1	0.0259189	5.737998e-05
P	CLOpt	1	0.00997301	1.352999e-05

P	B	1	0.005873332	1.046784e-05
P	SE	1	0.01213029	1.703498e-05
P	HS14	1	0	0
P	CLAro	1	0.00997301	1.352999e-05
P	BROpt	1	0.02245172	5.167967e-05
P	OEOpt	1	0.006747412	1.029353e-05
P	NOpt	1	0.01103526	2.54394e-05
P	CAro	1	0.005873332	9.944921e-06
P	CPos	1	0.005463	4.711e-06
P	NPri	1	0.0126256	3.2977e-05
P	NTer	1	0.01127806	2.11995e-05
P	OAlc	1	0.005114582	5.1821e-06
NE	I	1	0.01053836	1.855014e-05
NE	CLOpt	1	0.004054924	4.374056e-06
NE	B	1	0.002388037	3.384106e-06
NE	SE	1	0.004932051	5.507168e-06
NE	HS14	1	0	0
NE	CLAro	1	0.004054924	4.374056e-06
NE	BROpt	1	0.009128638	1.670731e-05
NE	OEOpt	1	0.002743429	3.327755e-06
NE	NOpt	1	0.004486824	8.2242e-06
NE	CAro	1	0.002388037	3.215053e-06
NE	CPos	1	0.0022212	1.523e-06
NE	NPri	1	0.00513344	1.0661e-05
NE	NTer	1	0.004585544	6.8535e-06
NE	OAlc	1	0.002079537	1.6753e-06
MG2+	I	1	0.00172508	7.110684e-07
MG2+	CLOpt	1	0.000663772	1.676674e-07
MG2+	B	1	0.0003909104	1.297204e-07
MG2+	SE	1	0.0008073536	2.111021e-07

MG2+	HS14	1	0	0
MG2+	CLAro	1	0.000663772	1.676674e-07
MG2+	BROpt	1	0.001494315	6.404286e-07
MG2+	OEOpt	1	0.0004490864	1.275603e-07
MG2+	NOpt	1	0.000734472	3.15252e-07
MG2+	CAro	1	0.0003909104	1.232402e-07
MG2+	CPos	1	0.0003636	5.838e-08
MG2+	NPri	1	0.00084032	4.0866e-07
MG2+	NTer	1	0.000750632	2.6271e-07
MG2+	OAlc	1	0.0003404104	6.4218e-08
CL	I	1	0.01998787	4.763598e-05
CL	CLOpt	1	0.007690883	1.123239e-05
CL	B	1	0.004529336	8.690242e-06
CL	SE	1	0.00935451	1.414218e-05
CL	HS14	1	0	0
CL	CLAro	1	0.007690883	1.123239e-05
CL	BROpt	1	0.01731408	4.290367e-05
CL	OEOpt	1	0.0052034	8.545535e-06
CL	NOpt	1	0.008510058	2.11194e-05
CL	CAro	1	0.004529336	8.256121e-06
CL	CPos	1	0.0042129	3.911e-06
CL	NPri	1	0.00973648	2.7377e-05
CL	NTer	1	0.008697298	1.75995e-05
CL	OAlc	1	0.003944211	4.3021e-06
OM	I	1	0.01015406	1.04882e-05
OM	CLOpt	1	0.003907054	2.473079e-06
OM	B	1	0.002300953	1.913364e-06
OM	SE	1	0.004752195	3.113738e-06
OM	HS14	1	0	0
OM	CLAro	1	0.003907054	2.473079e-06

OM	BROpt	1	0.008795746	9.446267e-06
OM	OEOpt	1	0.002643385	1.881503e-06
OM	NOpt	1	0.004323204	4.64994e-06
OM	CAro	1	0.002300953	1.817782e-06
OM	CPos	1	0.0021402	8.611e-07
OM	NPri	1	0.00494624	6.0277e-06
OM	NTer	1	0.004418324	3.87495e-06
OM	OAlc	1	0.002003703	9.4721e-07
HC	I	1	0.0019642	1.49814e-06
HC	CLOpt	1	0.00075578	3.53256e-07
HC	B	1	0.000445096	2.73306e-07
HC	SE	1	0.000919264	4.44768e-07
HC	HS14	1	0	0
HC	CLAro	1	0.00075578	3.53256e-07
HC	BROpt	1	0.001701448	1.34931e-06
HC	OEOpt	1	0.000511336	2.68755e-07
HC	NOpt	1	0.00083628	6.642e-07
HC	CAro	1	0.000445096	2.59653e-07
HC	CPos	1	0.000414	1.23e-07
HC	NPri	1	0.0009568	8.61e-07
HC	NTer	1	0.00085468	5.535e-07
HC	OAlc	1	0.000387596	1.353e-07
I	CLOpt	1	0.01753902	3.498096e-05
I	B	1	0.01032913	2.706396e-05
I	SE	1	0.02133292	4.404288e-05
I	HS14	1	0	0
I	CLAro	1	0.01753902	3.498096e-05
I	BROpt	1	0.03948469	0.0001336146
I	OEOpt	1	0.01186633	2.66133e-05
I	NOpt	1	0.01940715	6.5772e-05

	I	CAro	1	0.01032913	2.571198e-05
	I	CPos	1	0.0096075	1.218e-05
	I	NPri	1	0.022204	8.526e-05
	I	NTer	1	0.01983415	5.481e-05
	I	OAlc	1	0.008994755	1.3398e-05
CLOpt		I	1	0.01753902	3.498096e-05
CLOpt		B	1	0.003974417	6.381584e-06
CLOpt		SE	1	0.008208428	1.038515e-05
CLOpt		HS14	1	0	0
CLOpt		CLAro	1	0.006748622	8.248384e-06
CLOpt		BROpt	1	0.01519282	3.150584e-05
CLOpt		OEOpt	1	0.004565897	6.27532e-06
CLOpt		NOpt	1	0.007467435	1.55088e-05
CLOpt		CAro	1	0.003974417	6.062792e-06
CLOpt		CPos	1	0.00369675	2.872e-06
CLOpt		NPri	1	0.0085436	2.0104e-05
CLOpt		NTer	1	0.007631735	1.2924e-05
CLOpt		OAlc	1	0.00346098	3.1592e-06
	B	I	1	0.01032913	2.706396e-05
	B	CLOpt	1	0.003974417	6.381584e-06
	B	SE	1	0.00483413	8.034752e-06
	B	HS14	1	0	0
	B	CLAro	1	0.003974417	6.381584e-06
	B	BROpt	1	0.008947397	2.437534e-05
	B	OEOpt	1	0.00268896	4.85507e-06
	B	NOpt	1	0.004397742	1.19988e-05
	B	CAro	1	0.002340624	4.690642e-06
	B	CPos	1	0.0021771	2.222e-06
	B	NPri	1	0.00503152	1.5554e-05
	B	NTer	1	0.004494502	9.999e-06

B	OAlc 1	0.002038249	2.4442e-06
SE	I 1	0.02133292	4.404288e-05
SE	CLOpt 1	0.008208428	1.038515e-05
SE	B 1	0.00483413	8.034752e-06
SE	HS14 1	0	0
SE	CLAro 1	0.008208428	1.038515e-05
SE	BROpt 1	0.0184792	3.966752e-05
SE	OEOpt 1	0.005553554	7.90096e-06
SE	NOpt 1	0.009082728	1.95264e-05
SE	CAro 1	0.00483413	7.633376e-06
SE	CPos 1	0.0044964	3.616e-06
SE	NPri 1	0.01039168	2.5312e-05
SE	NTer 1	0.009282568	1.6272e-05
SE	OAlc 1	0.00420963	3.9776e-06
HS14	I 1	0	0
HS14	CLOpt 1	0	0
HS14	B 1	0	0
HS14	SE 1	0	0
HS14	CLAro 1	0	0
HS14	BROpt 1	0	0
HS14	OEOpt 1	0	0
HS14	NOpt 1	0	0
HS14	CAro 1	0	0
HS14	CPos 1	0	0
HS14	NPri 1	0	0
HS14	NTer 1	0	0
HS14	OAlc 1	0	0
CLAro	I 1	0.01753902	3.498096e-05
CLAro	CLOpt 1	0.006748622	8.248384e-06
CLAro	B 1	0.003974417	6.381584e-06

CLAro	SE	1	0.008208428	1.038515e-05
CLAro	HS14	1	0	0
CLAro	BROpt	1	0.01519282	3.150584e-05
CLAro	OEOpt	1	0.004565897	6.27532e-06
CLAro	NOpt	1	0.007467435	1.55088e-05
CLAro	CAro	1	0.003974417	6.062792e-06
CLAro	CPos	1	0.00369675	2.872e-06
CLAro	NPri	1	0.0085436	2.0104e-05
CLAro	NTer	1	0.007631735	1.2924e-05
CLAro	OAlc	1	0.00346098	3.1592e-06
BROpt	I	1	0.03948469	0.0001336146
BROpt	CLOpt	1	0.01519282	3.150584e-05
BROpt	B	1	0.008947397	2.437534e-05
BROpt	SE	1	0.0184792	3.966752e-05
BROpt	HS14	1	0	0
BROpt	CLAro	1	0.01519282	3.150584e-05
BROpt	OEOpt	1	0.01027897	2.396945e-05
BROpt	NOpt	1	0.01681105	5.9238e-05
BROpt	CAro	1	0.008947397	2.315767e-05
BROpt	CPos	1	0.0083223	1.097e-05
BROpt	NPri	1	0.01923376	7.679e-05
BROpt	NTer	1	0.01718093	4.9365e-05
BROpt	OAlc	1	0.007791522	1.2067e-05
OEOpt	I	1	0.01186633	2.66133e-05
OEOpt	CLOpt	1	0.004565897	6.27532e-06
OEOpt	B	1	0.00268896	4.85507e-06
OEOpt	SE	1	0.005553554	7.90096e-06
OEOpt	HS14	1	0	0
OEOpt	CLAro	1	0.004565897	6.27532e-06
OEOpt	BROpt	1	0.01027897	2.396945e-05

OEOpt	NOpt 1	0.005052222	1.1799e-05
OEOpt	CAro 1	0.00268896	4.612535e-06
OEOpt	CPos 1	0.0025011	2.185e-06
OEOpt	NPri 1	0.00578032	1.5295e-05
OEOpt	NTer 1	0.005163382	9.8325e-06
OEOpt	OAlc 1	0.002341585	2.4035e-06
NOpt	I 1	0.01940715	6.5772e-05
NOpt	CLOpt 1	0.007467435	1.55088e-05
NOpt	B 1	0.004397742	1.19988e-05
NOpt	SE 1	0.009082728	1.95264e-05
NOpt	HS14 1	0	0
NOpt	CLAro 1	0.007467435	1.55088e-05
NOpt	BROpt 1	0.01681105	5.9238e-05
NOpt	OEOpt 1	0.005052222	1.1799e-05
NOpt	CAro 1	0.004397742	1.13994e-05
NOpt	CPos 1	0.0040905	5.4e-06
NOpt	NPri 1	0.0094536	3.78e-05
NOpt	NTer 1	0.00844461	2.43e-05
NOpt	OAlc 1	0.003829617	5.94e-06
CAro	I 1	0.01032913	2.571198e-05
CAro	CLOpt 1	0.003974417	6.062792e-06
CAro	B 1	0.002340624	4.690642e-06
CAro	SE 1	0.00483413	7.633376e-06
CAro	HS14 1	0	0
CAro	CLAro 1	0.003974417	6.062792e-06
CAro	BROpt 1	0.008947397	2.315767e-05
CAro	OEOpt 1	0.00268896	4.612535e-06
CAro	NOpt 1	0.004397742	1.13994e-05
CAro	CPos 1	0.0021771	2.111e-06
CAro	NPri 1	0.00503152	1.4777e-05

CAro	NTer	1	0.004494502	9.4995e-06
CAro	OAlc	1	0.002038249	2.3221e-06
CPos	I	1	0.0096075	1.218e-05
CPos	CLOpt	1	0.00369675	2.872e-06
CPos	B	1	0.0021771	2.222e-06
CPos	SE	1	0.0044964	3.616e-06
CPos	HS14	1	0	0
CPos	CLAro	1	0.00369675	2.872e-06
CPos	BROpt	1	0.0083223	1.097e-05
CPos	OEOpt	1	0.0025011	2.185e-06
CPos	NOpt	1	0.0040905	5.4e-06
CPos	CAro	1	0.0021771	2.111e-06
CPos	NPri	1	0.00468	7e-06
CPos	NTer	1	0.0041805	4.5e-06
CPos	OAlc	1	0.00189585	1.1e-06
NPri	I	1	0.022204	8.526e-05
NPri	CLOpt	1	0.0085436	2.0104e-05
NPri	B	1	0.00503152	1.5554e-05
NPri	SE	1	0.01039168	2.5312e-05
NPri	HS14	1	0	0
NPri	CLAro	1	0.0085436	2.0104e-05
NPri	BROpt	1	0.01923376	7.679e-05
NPri	OEOpt	1	0.00578032	1.5295e-05
NPri	NOpt	1	0.0094536	3.78e-05
NPri	CAro	1	0.00503152	1.4777e-05
NPri	CPos	1	0.00468	7e-06
NPri	NTer	1	0.0096616	3.15e-05
NPri	OAlc	1	0.00438152	7.7e-06
NTer	I	1	0.01983415	5.481e-05
NTer	CLOpt	1	0.007631735	1.2924e-05

NTer B 1 0.004494502 9.999e-06

NTer SE 1 0.009282568 1.6272e-05

NTer HS14 1 0 0

NTer CLAro 1 0.007631735 1.2924e-05

NTer BROpt 1 0.01718093 4.9365e-05

NTer OEOpt 1 0.005163382 9.8325e-06

NTer NOpt 1 0.00844461 2.43e-05

NTer CAro 1 0.004494502 9.4995e-06

NTer CPos 1 0.0041805 4.5e-06

NTer NPri 1 0.0096616 3.15e-05

NTer OAlc 1 0.003913877 4.95e-06

OAlc I 1 0.008994755 1.3398e-05

OAlc CLOpt 1 0.00346098 3.1592e-06

OAlc B 1 0.002038249 2.4442e-06

OAlc SE 1 0.00420963 3.9776e-06

OAlc HS14 1 0 0

OAlc CLAro 1 0.00346098 3.1592e-06

OAlc BROpt 1 0.007791522 1.2067e-05

OAlc OEOpt 1 0.002341585 2.4035e-06

OAlc NOpt 1 0.003829617 5.94e-06

OAlc CAro 1 0.002038249 2.3221e-06

OAlc CPos 1 0.00189585 1.1e-06

OAlc NPri 1 0.00438152 7.7e-06

OAlc NTer 1 0.003913877 4.95e-06

[pairtypes]

; i j func c6 c12

O O 1 2.261954E-03 7.414932E-07

OM O 1 2.261954E-03 7.414932E-07

OM OM 1 2.261954E-03 7.414932E-07

OA	O	1	2.261954E-03	9.687375E-07
OA	OM	1	2.261954E-03	9.687375E-07
OA	OA	1	2.261954E-03	1.265625E-06
OE	O	1	2.261954E-03	9.687375E-07
OE	OM	1	2.261954E-03	9.687375E-07
OE	OA	1	2.261954E-03	1.265625E-06
OE	OE	1	2.261954E-03	1.265625E-06
OW	O	1	2.433170E-03	1.397565E-06
OW	OM	1	2.433170E-03	1.397565E-06
OW	OA	1	2.433170E-03	1.825875E-06
OW	OE	1	2.433170E-03	1.825875E-06
OW	OW	1	2.617346E-03	2.634129E-06
N	O	1	2.347562E-03	1.120291E-06
N	OM	1	2.347562E-03	1.120291E-06
N	OA	1	2.347562E-03	1.463625E-06
N	OE	1	2.347562E-03	1.463625E-06
N	OW	1	2.525258E-03	2.111523E-06
N	N	1	2.436410E-03	1.692601E-06
NT	O	1	2.347562E-03	1.120291E-06
NT	OM	1	2.347562E-03	1.120291E-06
NT	OA	1	2.347562E-03	1.463625E-06
NT	OE	1	2.347562E-03	1.463625E-06
NT	OW	1	2.525258E-03	2.111523E-06
NT	N	1	2.436410E-03	1.692601E-06
NT	NT	1	2.436410E-03	1.692601E-06
NL	O	1	2.347562E-03	1.120291E-06
NL	OM	1	2.347562E-03	1.120291E-06
NL	OA	1	2.347562E-03	1.463625E-06
NL	OE	1	2.347562E-03	1.463625E-06
NL	OW	1	2.525258E-03	2.111523E-06

NL	N	1	2.436410E-03	1.692601E-06
NL	NT	1	2.436410E-03	1.692601E-06
NL	NL	1	2.436410E-03	1.692601E-06
NR	O	1	2.347562E-03	1.120291E-06
NR	OM	1	2.347562E-03	1.120291E-06
NR	OA	1	2.347562E-03	1.463625E-06
NR	OE	1	2.347562E-03	1.463625E-06
NR	OW	1	2.525258E-03	2.111523E-06
NR	N	1	2.436410E-03	1.692601E-06
NR	NT	1	2.436410E-03	1.692601E-06
NR	NL	1	2.436410E-03	1.692601E-06
NR	NR	1	2.436410E-03	1.692601E-06
NZ	O	1	2.347562E-03	1.120291E-06
NZ	OM	1	2.347562E-03	1.120291E-06
NZ	OA	1	2.347562E-03	1.463625E-06
NZ	OE	1	2.347562E-03	1.463625E-06
NZ	OW	1	2.525258E-03	2.111523E-06
NZ	N	1	2.436410E-03	1.692601E-06
NZ	NT	1	2.436410E-03	1.692601E-06
NZ	NL	1	2.436410E-03	1.692601E-06
NZ	NR	1	2.436410E-03	1.692601E-06
NZ	NZ	1	2.436410E-03	1.692601E-06
NE	O	1	2.347562E-03	1.120291E-06
NE	OM	1	2.347562E-03	1.120291E-06
NE	OA	1	2.347562E-03	1.463625E-06
NE	OE	1	2.347562E-03	1.463625E-06
NE	OW	1	2.525258E-03	2.111523E-06
NE	N	1	2.436410E-03	1.692601E-06
NE	NT	1	2.436410E-03	1.692601E-06
NE	NL	1	2.436410E-03	1.692601E-06

NE	NR	1	2.436410E-03	1.692601E-06
NE	NZ	1	2.436410E-03	1.692601E-06
NE	NE	1	2.436410E-03	1.692601E-06
C	O	1	2.300953E-03	1.581841E-06
C	OM	1	2.300953E-03	1.581841E-06
C	OA	1	2.300953E-03	2.066625E-06
C	OE	1	2.300953E-03	2.066625E-06
C	OW	1	2.475121E-03	2.981451E-06
C	N	1	2.388037E-03	2.389937E-06
C	NT	1	2.388037E-03	2.389937E-06
C	NL	1	2.388037E-03	2.389937E-06
C	NR	1	2.388037E-03	2.389937E-06
C	NZ	1	2.388037E-03	2.389937E-06
C	NE	1	2.388037E-03	2.389937E-06
C	C	1	2.340624E-03	3.374569E-06
CH0	O	1	2.300953E-03	1.581841E-06
CH0	OM	1	2.300953E-03	1.581841E-06
CH0	OA	1	2.300953E-03	2.066625E-06
CH0	OE	1	2.300953E-03	2.066625E-06
CH0	OW	1	2.475121E-03	2.981451E-06
CH0	N	1	2.388037E-03	2.389937E-06
CH0	NT	1	2.388037E-03	2.389937E-06
CH0	NL	1	2.388037E-03	2.389937E-06
CH0	NR	1	2.388037E-03	2.389937E-06
CH0	NZ	1	2.388037E-03	2.389937E-06
CH0	NE	1	2.388037E-03	2.389937E-06
CH0	C	1	2.340624E-03	3.374569E-06
CH0	CH0	1	2.340624E-03	3.374569E-06
CH1	O	1	2.566338E-03	1.664506E-06
CH1	OM	1	2.566338E-03	1.664506E-06

CH1	OA	1	2.566338E-03	2.174625E-06
CH1	OE	1	2.566338E-03	2.174625E-06
CH1	OW	1	2.760594E-03	3.137259E-06
CH1	N	1	2.663466E-03	2.514833E-06
CH1	NT	1	2.663466E-03	2.514833E-06
CH1	NL	1	2.663466E-03	2.514833E-06
CH1	NR	1	2.663466E-03	2.514833E-06
CH1	NZ	1	2.663466E-03	2.514833E-06
CH1	NE	1	2.663466E-03	2.514833E-06
CH1	C	1	2.610585E-03	3.550921E-06
CH1	CH0	1	2.610585E-03	3.550921E-06
CH1	CH1	1	2.911682E-03	3.736489E-06
CH2	O	1	3.268799E-03	1.875128E-06
CH2	OM	1	3.268799E-03	1.875128E-06
CH2	OA	1	3.268799E-03	2.449796E-06
CH2	OE	1	3.268799E-03	2.449796E-06
CH2	OW	1	3.516227E-03	3.534239E-06
CH2	N	1	3.392513E-03	2.833053E-06
CH2	NT	1	3.392513E-03	2.833053E-06
CH2	NL	1	3.392513E-03	2.833053E-06
CH2	NR	1	3.392513E-03	2.833053E-06
CH2	NZ	1	3.392513E-03	2.833053E-06
CH2	NE	1	3.392513E-03	2.833053E-06
CH2	C	1	3.325157E-03	4.000245E-06
CH2	CH0	1	3.325157E-03	4.000245E-06
CH2	CH1	1	3.708671E-03	4.209294E-06
CH2	CH2	1	4.723813E-03	4.741926E-06
CH3	O	1	3.937017E-03	2.114674E-06
CH3	OM	1	3.937017E-03	2.114674E-06
CH3	OA	1	3.937017E-03	2.762755E-06

CH3	OE	1	3.937017E-03	2.762755E-06
CH3	OW	1	4.235025E-03	3.985734E-06
CH3	N	1	4.086021E-03	3.194972E-06
CH3	NT	1	4.086021E-03	3.194972E-06
CH3	NL	1	4.086021E-03	3.194972E-06
CH3	NR	1	4.086021E-03	3.194972E-06
CH3	NZ	1	4.086021E-03	3.194972E-06
CH3	NE	1	4.086021E-03	3.194972E-06
CH3	C	1	4.004896E-03	4.511272E-06
CH3	CH0	1	4.004896E-03	4.511272E-06
CH3	CH1	1	4.466809E-03	4.747027E-06
CH3	CH2	1	5.689469E-03	5.347702E-06
CH3	CH3	1	6.852528E-03	6.030865E-06
CH4	O	1	5.459888E-03	5.047768E-06
CH4	OM	1	5.459888E-03	5.047768E-06
CH4	OA	1	5.459888E-03	6.594750E-06
CH4	OE	1	5.459888E-03	6.594750E-06
CH4	OW	1	5.873168E-03	9.514026E-06
CH4	N	1	5.666528E-03	7.626462E-06
CH4	NT	1	5.666528E-03	7.626462E-06
CH4	NL	1	5.666528E-03	7.626462E-06
CH4	NR	1	5.666528E-03	7.626462E-06
CH4	NZ	1	5.666528E-03	7.626462E-06
CH4	NE	1	5.666528E-03	7.626462E-06
CH4	C	1	5.554024E-03	1.076849E-05
CH4	CH0	1	5.554024E-03	1.076849E-05
CH4	CH1	1	6.194608E-03	1.133125E-05
CH4	CH2	1	7.890204E-03	1.276507E-05
CH4	CH3	1	9.503144E-03	1.439579E-05
CH4	CH4	1	1.317904E-02	3.436304E-05

CH2r	O	1	3.268799E-03	1.875128E-06
CH2r	OM	1	3.268799E-03	1.875128E-06
CH2r	OA	1	3.268799E-03	2.449796E-06
CH2r	OE	1	3.268799E-03	2.449796E-06
CH2r	OW	1	3.516227E-03	3.534239E-06
CH2r	N	1	3.392513E-03	2.833053E-06
CH2r	NT	1	3.392513E-03	2.833053E-06
CH2r	NL	1	3.392513E-03	2.833053E-06
CH2r	NR	1	3.392513E-03	2.833053E-06
CH2r	NZ	1	3.392513E-03	2.833053E-06
CH2r	NE	1	3.392513E-03	2.833053E-06
CH2r	C	1	3.325157E-03	4.000245E-06
CH2r	CH0	1	3.325157E-03	4.000245E-06
CH2r	CH1	1	3.708671E-03	4.209294E-06
CH2r	CH2	1	4.723813E-03	4.741926E-06
CH2r	CH3	1	5.689469E-03	5.347702E-06
CH2r	CH4	1	7.890204E-03	1.276507E-05
CH2r	CH2r	1	4.723813E-03	4.741926E-06
CR1	O	1	3.536086E-03	2.485135E-06
CR1	OM	1	3.536086E-03	2.485135E-06
CR1	OA	1	3.536086E-03	3.246750E-06
CR1	OE	1	3.536086E-03	3.246750E-06
CR1	OW	1	3.803746E-03	4.683978E-06
CR1	N	1	3.669916E-03	3.754686E-06
CR1	NT	1	3.669916E-03	3.754686E-06
CR1	NL	1	3.669916E-03	3.754686E-06
CR1	NR	1	3.669916E-03	3.754686E-06
CR1	NZ	1	3.669916E-03	3.754686E-06
CR1	NE	1	3.669916E-03	3.754686E-06
CR1	C	1	3.597053E-03	5.301582E-06

CR1	CH0	1	3.597053E-03	5.301582E-06
CR1	CH1	1	4.011926E-03	5.578638E-06
CR1	CH2	1	5.110076E-03	6.284543E-06
CR1	CH3	1	6.154693E-03	7.087387E-06
CR1	CH4	1	8.535380E-03	1.691773E-05
CR1	CH2r	1	5.110076E-03	6.284543E-06
CR1	CR1	1	5.527922E-03	8.328996E-06
HC	O	1	4.375520E-04	1.059153E-07
HC	OM	1	4.375520E-04	1.059153E-07
HC	OA	1	4.375520E-04	1.383750E-07
HC	OE	1	4.375520E-04	1.383750E-07
HC	OW	1	4.706720E-04	1.996290E-07
HC	N	1	4.541120E-04	1.600230E-07
HC	NT	1	4.541120E-04	1.600230E-07
HC	NL	1	4.541120E-04	1.600230E-07
HC	NR	1	4.541120E-04	1.600230E-07
HC	NZ	1	4.541120E-04	1.600230E-07
HC	NE	1	4.541120E-04	1.600230E-07
HC	C	1	4.450960E-04	2.259510E-07
HC	CH0	1	4.450960E-04	2.259510E-07
HC	CH1	1	4.964320E-04	2.377590E-07
HC	CH2	1	6.323160E-04	2.678444E-07
HC	CH3	1	7.615760E-04	3.020612E-07
HC	CH4	1	1.056160E-03	7.210260E-07
HC	CH2r	1	6.323160E-04	2.678444E-07
HC	CR1	1	6.840200E-04	3.549780E-07
HC	HC	1	8.464000E-05	1.512900E-08
H	O	1	0.000000E+00	0.000000E+00
H	OM	1	0.000000E+00	0.000000E+00
H	OA	1	0.000000E+00	0.000000E+00

H OE 1 0.000000E+00 0.000000E+00

H OW 1 0.000000E+00 0.000000E+00

H N 1 0.000000E+00 0.000000E+00

H NT 1 0.000000E+00 0.000000E+00

H NL 1 0.000000E+00 0.000000E+00

H NR 1 0.000000E+00 0.000000E+00

H NZ 1 0.000000E+00 0.000000E+00

H NE 1 0.000000E+00 0.000000E+00

H C 1 0.000000E+00 0.000000E+00

H CH0 1 0.000000E+00 0.000000E+00

H CH1 1 0.000000E+00 0.000000E+00

H CH2 1 0.000000E+00 0.000000E+00

H CH3 1 0.000000E+00 0.000000E+00

H CH4 1 0.000000E+00 0.000000E+00

H CH2r 1 0.000000E+00 0.000000E+00

H CR1 1 0.000000E+00 0.000000E+00

H HC 1 0.000000E+00 0.000000E+00

H H 1 0.000000E+00 0.000000E+00

DUM O 1 0.000000E+00 0.000000E+00

DUM OM 1 0.000000E+00 0.000000E+00

DUM OA 1 0.000000E+00 0.000000E+00

DUM OE 1 0.000000E+00 0.000000E+00

DUM OW 1 0.000000E+00 0.000000E+00

DUM N 1 0.000000E+00 0.000000E+00

DUM NT 1 0.000000E+00 0.000000E+00

DUM NL 1 0.000000E+00 0.000000E+00

DUM NR 1 0.000000E+00 0.000000E+00

DUM NZ 1 0.000000E+00 0.000000E+00

DUM NE 1 0.000000E+00 0.000000E+00

DUM C 1 0.000000E+00 0.000000E+00

DUM	CH0	1	0.000000E+00	0.000000E+00
DUM	CH1	1	0.000000E+00	0.000000E+00
DUM	CH2	1	0.000000E+00	0.000000E+00
DUM	CH3	1	0.000000E+00	0.000000E+00
DUM	CH4	1	0.000000E+00	0.000000E+00
DUM	CH2r	1	0.000000E+00	0.000000E+00
DUM	CR1	1	0.000000E+00	0.000000E+00
DUM	HC	1	0.000000E+00	0.000000E+00
DUM	H	1	0.000000E+00	0.000000E+00
DUM	DUM	1	0.000000E+00	0.000000E+00
S	O	1	4.752195E-03	3.113738E-06
S	OM	1	4.752195E-03	3.113738E-06
S	OA	1	4.752195E-03	4.068000E-06
S	OE	1	4.752195E-03	4.068000E-06
S	OW	1	5.111907E-03	5.868768E-06
S	N	1	4.932051E-03	4.704416E-06
S	NT	1	4.932051E-03	4.704416E-06
S	NL	1	4.932051E-03	4.704416E-06
S	NR	1	4.932051E-03	4.704416E-06
S	NZ	1	4.932051E-03	4.704416E-06
S	NE	1	4.932051E-03	4.704416E-06
S	C	1	4.834130E-03	6.642592E-06
S	CH0	1	4.834130E-03	6.642592E-06
S	CH1	1	5.391683E-03	6.989728E-06
S	CH2	1	6.867502E-03	7.874189E-06
S	CH3	1	8.271378E-03	8.880108E-06
S	CH4	1	1.147082E-02	2.119699E-05
S	CH2r	1	6.867502E-03	7.874189E-06
S	CR1	1	7.429052E-03	1.043578E-05
S	HC	1	9.192640E-04	4.447680E-07

S	H	1	0.000000E+00	0.000000E+00
S	DUM	1	0.000000E+00	0.000000E+00
S	S	1	9.984006E-03	1.307546E-05
CU1+	O	1	9.726020E-04	6.164615E-08
CU1+	OM	1	9.726020E-04	6.164615E-08
CU1+	OA	1	9.726020E-04	8.053875E-08
CU1+	OE	1	9.726020E-04	8.053875E-08
CU1+	OW	1	1.046222E-03	1.161906E-07
CU1+	N	1	1.009412E-03	9.313859E-08
CU1+	NT	1	1.009412E-03	9.313859E-08
CU1+	NL	1	1.009412E-03	9.313859E-08
CU1+	NR	1	1.009412E-03	9.313859E-08
CU1+	NZ	1	1.009412E-03	9.313859E-08
CU1+	NE	1	1.009412E-03	9.313859E-08
CU1+	C	1	9.893710E-04	1.315108E-07
CU1+	CH0	1	9.893710E-04	1.315108E-07
CU1+	CH1	1	1.103482E-03	1.383835E-07
CU1+	CH2	1	1.405529E-03	1.558941E-07
CU1+	CH3	1	1.692851E-03	1.758094E-07
CU1+	CH4	1	2.347660E-03	4.196606E-07
CU1+	CH2r	1	1.405529E-03	1.558941E-07
CU1+	CR1	1	1.520457E-03	2.066087E-07
CU1+	HC	1	1.881400E-04	8.805570E-09
CU1+	H	1	0.000000E+00	0.000000E+00
CU1+	DUM	1	0.000000E+00	0.000000E+00
CU1+	S	1	2.043364E-03	2.588694E-07
CU1+	CU1+	1	4.182025E-04	5.125128E-09
CU2+	O	1	9.726020E-04	6.164615E-08
CU2+	OM	1	9.726020E-04	6.164615E-08
CU2+	OA	1	9.726020E-04	8.053875E-08

CU2+	OE	1	9.726020E-04	8.053875E-08
CU2+	OW	1	1.046222E-03	1.161906E-07
CU2+	N	1	1.009412E-03	9.313859E-08
CU2+	NT	1	1.009412E-03	9.313859E-08
CU2+	NL	1	1.009412E-03	9.313859E-08
CU2+	NR	1	1.009412E-03	9.313859E-08
CU2+	NZ	1	1.009412E-03	9.313859E-08
CU2+	NE	1	1.009412E-03	9.313859E-08
CU2+	C	1	9.893710E-04	1.315108E-07
CU2+	CH0	1	9.893710E-04	1.315108E-07
CU2+	CH1	1	1.103482E-03	1.383835E-07
CU2+	CH2	1	1.405529E-03	1.558941E-07
CU2+	CH3	1	1.692851E-03	1.758094E-07
CU2+	CH4	1	2.347660E-03	4.196606E-07
CU2+	CH2r	1	1.405529E-03	1.558941E-07
CU2+	CR1	1	1.520457E-03	2.066087E-07
CU2+	HC	1	1.881400E-04	8.805570E-09
CU2+	H	1	0.000000E+00	0.000000E+00
CU2+	DUM	1	0.000000E+00	0.000000E+00
CU2+	S	1	2.043364E-03	2.588694E-07
CU2+	CU1+	1	4.182025E-04	5.125128E-09
CU2+	CU2+	1	4.182025E-04	5.125128E-09
FE	O	1	0.000000E+00	0.000000E+00
FE	OM	1	0.000000E+00	0.000000E+00
FE	OA	1	0.000000E+00	0.000000E+00
FE	OE	1	0.000000E+00	0.000000E+00
FE	OW	1	0.000000E+00	0.000000E+00
FE	N	1	0.000000E+00	0.000000E+00
FE	NT	1	0.000000E+00	0.000000E+00
FE	NL	1	0.000000E+00	0.000000E+00

FE	NR	1	0.000000E+00	0.000000E+00
FE	NZ	1	0.000000E+00	0.000000E+00
FE	NE	1	0.000000E+00	0.000000E+00
FE	C	1	0.000000E+00	0.000000E+00
FE	CH0	1	0.000000E+00	0.000000E+00
FE	CH1	1	0.000000E+00	0.000000E+00
FE	CH2	1	0.000000E+00	0.000000E+00
FE	CH3	1	0.000000E+00	0.000000E+00
FE	CH4	1	0.000000E+00	0.000000E+00
FE	CH2r	1	0.000000E+00	0.000000E+00
FE	CR1	1	0.000000E+00	0.000000E+00
FE	HC	1	0.000000E+00	0.000000E+00
FE	H	1	0.000000E+00	0.000000E+00
FE	DUM	1	0.000000E+00	0.000000E+00
FE	S	1	0.000000E+00	0.000000E+00
FE	CU1+	1	0.000000E+00	0.000000E+00
FE	CU2+	1	0.000000E+00	0.000000E+00
FE	FE	1	0.000000E+00	0.000000E+00
ZN2+	O	1	9.726020E-04	8.366448E-08
ZN2+	OM	1	9.726020E-04	8.366448E-08
ZN2+	OA	1	9.726020E-04	1.093050E-07
ZN2+	OE	1	9.726020E-04	1.093050E-07
ZN2+	OW	1	1.046222E-03	1.576907E-07
ZN2+	N	1	1.009412E-03	1.264052E-07
ZN2+	NT	1	1.009412E-03	1.264052E-07
ZN2+	NL	1	1.009412E-03	1.264052E-07
ZN2+	NR	1	1.009412E-03	1.264052E-07
ZN2+	NZ	1	1.009412E-03	1.264052E-07
ZN2+	NE	1	1.009412E-03	1.264052E-07
ZN2+	C	1	9.893710E-04	1.784829E-07

ZN2+	CH0	1	9.893710E-04	1.784829E-07
ZN2+	CH1	1	1.103482E-03	1.878103E-07
ZN2+	CH2	1	1.405529E-03	2.115753E-07
ZN2+	CH3	1	1.692851E-03	2.386038E-07
ZN2+	CH4	1	2.347660E-03	5.695519E-07
ZN2+	CH2r	1	1.405529E-03	2.115753E-07
ZN2+	CR1	1	1.520457E-03	2.804038E-07
ZN2+	HC	1	1.881400E-04	1.195068E-08
ZN2+	H	1	0.000000E+00	0.000000E+00
ZN2+	DUM	1	0.000000E+00	0.000000E+00
ZN2+	S	1	2.043364E-03	3.513306E-07
ZN2+	CU1+	1	4.182025E-04	6.955684E-09
ZN2+	CU2+	1	4.182025E-04	6.955684E-09
ZN2+	FE	1	0.000000E+00	0.000000E+00
ZN2+	ZN2+	1	4.182025E-04	9.440066E-09
MG2+	O	1	3.842848E-04	5.027102E-08
MG2+	OM	1	3.842848E-04	5.027102E-08
MG2+	OA	1	3.842848E-04	6.567750E-08
MG2+	OE	1	3.842848E-04	6.567750E-08
MG2+	OW	1	4.133728E-04	9.475074E-08
MG2+	N	1	3.988288E-04	7.595238E-08
MG2+	NT	1	3.988288E-04	7.595238E-08
MG2+	NL	1	3.988288E-04	7.595238E-08
MG2+	NR	1	3.988288E-04	7.595238E-08
MG2+	NZ	1	3.988288E-04	7.595238E-08
MG2+	NE	1	3.988288E-04	7.595238E-08
MG2+	C	1	3.909104E-04	1.072441E-07
MG2+	CH0	1	3.909104E-04	1.072441E-07
MG2+	CH1	1	4.359968E-04	1.128485E-07
MG2+	CH2	1	5.553384E-04	1.271281E-07

MG2+ CH3 1 6.688624E-04 1.433686E-07

MG2+ CH4 1 9.275840E-04 3.422236E-07

MG2+ CH2r 1 5.553384E-04 1.271281E-07

MG2+ CR1 1 6.007480E-04 1.684847E-07

MG2+ HC 1 7.433600E-05 7.180740E-09

MG2+ H 1 0.000000E+00 0.000000E+00

MG2+ DUM 1 0.000000E+00 0.000000E+00

MG2+ S 1 8.073536E-04 2.111021E-07

MG2+ CU1+ 1 1.652360E-04 4.179424E-09

MG2+ CU2+ 1 1.652360E-04 4.179424E-09

MG2+ FE 1 0.000000E+00 0.000000E+00

MG2+ ZN2+ 1 1.652360E-04 5.672201E-09

MG2+ MG2+ 1 6.528640E-05 3.408224E-09

CA2+ O 1 1.507652E-03 6.076783E-07

CA2+ OM 1 1.507652E-03 6.076783E-07

CA2+ OA 1 1.507652E-03 7.939125E-07

CA2+ OE 1 1.507652E-03 7.939125E-07

CA2+ OW 1 1.621772E-03 1.145351E-06

CA2+ N 1 1.564712E-03 9.181157E-07

CA2+ NT 1 1.564712E-03 9.181157E-07

CA2+ NL 1 1.564712E-03 9.181157E-07

CA2+ NR 1 1.564712E-03 9.181157E-07

CA2+ NZ 1 1.564712E-03 9.181157E-07

CA2+ NE 1 1.564712E-03 9.181157E-07

CA2+ C 1 1.533646E-03 1.296371E-06

CA2+ CH0 1 1.533646E-03 1.296371E-06

CA2+ CH1 1 1.710532E-03 1.364118E-06

CA2+ CH2 1 2.178741E-03 1.536730E-06

CA2+ CH3 1 2.624126E-03 1.733045E-06

CA2+ CH4 1 3.639160E-03 4.136813E-06

CA2+	CH2r	1	2.178741E-03	1.536730E-06
CA2+	CR1	1	2.356895E-03	2.036650E-06
CA2+	HC	1	2.916400E-04	8.680110E-08
CA2+	H	1	0.000000E+00	0.000000E+00
CA2+	DUM	1	0.000000E+00	0.000000E+00
CA2+	S	1	3.167464E-03	2.551811E-06
CA2+	CU1+	1	6.482650E-04	5.052106E-08
CA2+	CU2+	1	6.482650E-04	5.052106E-08
CA2+	FE	1	0.000000E+00	0.000000E+00
CA2+	ZN2+	1	6.482650E-04	6.856581E-08
CA2+	MG2+	1	2.561360E-04	4.119877E-08
CA2+	CA2+	1	1.004890E-03	4.980125E-07
P	O	1	5.773784E-03	4.056642E-06
P	OM	1	5.773784E-03	4.056642E-06
P	OA	1	5.773784E-03	5.299875E-06
P	OE	1	5.773784E-03	5.299875E-06
P	OW	1	6.210824E-03	7.645953E-06
P	N	1	5.992304E-03	6.129011E-06
P	NT	1	5.992304E-03	6.129011E-06
P	NL	1	5.992304E-03	6.129011E-06
P	NR	1	5.992304E-03	6.129011E-06
P	NZ	1	5.992304E-03	6.129011E-06
P	NE	1	5.992304E-03	6.129011E-06
P	C	1	5.873332E-03	8.654107E-06
P	CH0	1	5.873332E-03	8.654107E-06
P	CH1	1	6.550744E-03	9.106363E-06
P	CH2	1	8.343822E-03	1.025866E-05
P	CH3	1	1.004949E-02	1.156919E-05
P	CH4	1	1.393672E-02	2.761588E-05
P	CH2r	1	8.343822E-03	1.025866E-05

P	CR1	1	9.026090E-03	1.359595E-05
P	HC	1	1.116880E-03	5.794530E-07
P	H	1	0.000000E+00	0.000000E+00
P	DUM	1	0.000000E+00	0.000000E+00
P	S	1	1.213029E-02	1.703498E-05
P	CU1+	1	2.482630E-03	3.372605E-07
P	CU2+	1	2.482630E-03	3.372605E-07
P	FE	1	0.000000E+00	0.000000E+00
P	ZN2+	1	2.482630E-03	4.577208E-07
P	MG2+	1	9.809120E-04	2.750282E-07
P	CA2+	1	3.848380E-03	3.324553E-06
P	P	1	1.473796E-02	2.219352E-05
AR	O	1	3.764374E-03	2.702132E-06
AR	OM	1	3.764374E-03	2.702132E-06
AR	OA	1	3.764374E-03	3.530250E-06
AR	OE	1	3.764374E-03	3.530250E-06
AR	OW	1	4.049314E-03	5.092974E-06
AR	N	1	3.906844E-03	4.082538E-06
AR	NT	1	3.906844E-03	4.082538E-06
AR	NL	1	3.906844E-03	4.082538E-06
AR	NR	1	3.906844E-03	4.082538E-06
AR	NZ	1	3.906844E-03	4.082538E-06
AR	NE	1	3.906844E-03	4.082538E-06
AR	C	1	3.829277E-03	5.764506E-06
AR	CH0	1	3.829277E-03	5.764506E-06
AR	CH1	1	4.270934E-03	6.065754E-06
AR	CH2	1	5.439979E-03	6.833298E-06
AR	CH3	1	6.552037E-03	7.706244E-06
AR	CH4	1	9.086420E-03	1.839496E-05
AR	CH2r	1	5.439979E-03	6.833298E-06

AR	CR1	1	5.884802E-03	9.056268E-06
AR	HC	1	7.281800E-04	3.859740E-07
AR	H	1	0.000000E+00	0.000000E+00
AR	DUM	1	0.000000E+00	0.000000E+00
AR	S	1	7.908668E-03	1.134701E-05
AR	CU1+	1	1.618617E-03	2.246494E-07
AR	CU2+	1	1.618617E-03	2.246494E-07
AR	FE	1	0.000000E+00	0.000000E+00
AR	ZN2+	1	1.618617E-03	3.048881E-07
AR	MG2+	1	6.395320E-04	1.831964E-07
AR	CA2+	1	2.509055E-03	2.214487E-06
AR	P	1	9.608810E-03	1.478312E-05
AR	AR	1	6.264723E-03	9.847044E-06
F	O	1	1.632259E-03	7.510514E-07
F	OM	1	1.632259E-03	7.510514E-07
F	OA	1	1.632259E-03	9.812250E-07
F	OE	1	1.632259E-03	9.812250E-07
F	OW	1	1.755811E-03	1.415581E-06
F	N	1	1.694035E-03	1.134732E-06
F	NT	1	1.694035E-03	1.134732E-06
F	NL	1	1.694035E-03	1.134732E-06
F	NR	1	1.694035E-03	1.134732E-06
F	NZ	1	1.694035E-03	1.134732E-06
F	NE	1	1.694035E-03	1.134732E-06
F	C	1	1.660402E-03	1.602231E-06
F	CH0	1	1.660402E-03	1.602231E-06
F	CH1	1	1.851907E-03	1.685963E-06
F	CH2	1	2.358814E-03	1.899300E-06
F	CH3	1	2.841010E-03	2.141933E-06
F	CH4	1	3.939936E-03	5.112836E-06

F	CH2r	1	2.358814E-03	1.899300E-06
F	CR1	1	2.551692E-03	2.517169E-06
F	HC	1	3.157440E-04	1.072806E-07
F	H	1	0.000000E+00	0.000000E+00
F	DUM	1	0.000000E+00	0.000000E+00
F	S	1	3.429254E-03	3.153875E-06
F	CU1+	1	7.018440E-04	6.244080E-08
F	CU2+	1	7.018440E-04	6.244080E-08
F	FE	1	0.000000E+00	0.000000E+00
F	ZN2+	1	7.018440E-04	8.474295E-08
F	MG2+	1	2.773056E-04	5.091904E-08
F	CA2+	1	1.087944E-03	6.155115E-07
F	P	1	4.166448E-03	4.108934E-06
F	AR	1	2.716428E-03	2.736964E-06
F	F	1	1.177862E-03	7.607328E-07
CL	O	1	4.452567E-03	3.367762E-06
CL	OM	1	4.452567E-03	3.367762E-06
CL	OA	1	4.452567E-03	4.399875E-06
CL	OE	1	4.452567E-03	4.399875E-06
CL	OW	1	4.789599E-03	6.347553E-06
CL	N	1	4.621083E-03	5.088211E-06
CL	NT	1	4.621083E-03	5.088211E-06
CL	NL	1	4.621083E-03	5.088211E-06
CL	NR	1	4.621083E-03	5.088211E-06
CL	NZ	1	4.621083E-03	5.088211E-06
CL	NE	1	4.621083E-03	5.088211E-06
CL	C	1	4.529336E-03	7.184507E-06
CL	CH0	1	4.529336E-03	7.184507E-06
CL	CH1	1	5.051735E-03	7.559963E-06
CL	CH2	1	6.434503E-03	8.516580E-06

CL	CH3	1	7.749864E-03	9.604563E-06
CL	CH4	1	1.074758E-02	2.292628E-05
CL	CH2r	1	6.434503E-03	8.516580E-06
CL	CR1	1	6.960647E-03	1.128715E-05
CL	HC	1	8.613040E-04	4.810530E-07
CL	H	1	0.000000E+00	0.000000E+00
CL	DUM	1	0.000000E+00	0.000000E+00
CL	S	1	9.354510E-03	1.414218E-05
CL	CU1+	1	1.914529E-03	2.799885E-07
CL	CU2+	1	1.914529E-03	2.799885E-07
CL	FE	1	0.000000E+00	0.000000E+00
CL	ZN2+	1	1.914529E-03	3.799928E-07
CL	MG2+	1	7.564496E-04	2.283242E-07
CL	CA2+	1	2.967754E-03	2.759993E-06
CL	P	1	1.136547E-02	1.842472E-05
CL	AR	1	7.410023E-03	1.227272E-05
CL	F	1	3.213038E-03	3.411174E-06
CL	CL	1	8.764704E-03	1.529592E-05
BR	O	1	7.909228E-03	6.968021E-06
BR	OM	1	7.909228E-03	6.968021E-06
BR	OA	1	7.909228E-03	9.103500E-06
BR	OE	1	7.909228E-03	9.103500E-06
BR	OW	1	8.507908E-03	1.313332E-05
BR	N	1	8.208568E-03	1.052769E-05
BR	NT	1	8.208568E-03	1.052769E-05
BR	NL	1	8.208568E-03	1.052769E-05
BR	NR	1	8.208568E-03	1.052769E-05
BR	NZ	1	8.208568E-03	1.052769E-05
BR	NE	1	8.208568E-03	1.052769E-05
BR	C	1	8.045594E-03	1.486500E-05

BR	CH0	1	8.045594E-03	1.486500E-05
BR	CH1	1	8.973548E-03	1.564184E-05
BR	CH2	1	1.142980E-02	1.762111E-05
BR	CH3	1	1.376631E-02	1.987219E-05
BR	CH4	1	1.909124E-02	4.743530E-05
BR	CH2r	1	1.142980E-02	1.762111E-05
BR	CR1	1	1.236441E-02	2.335351E-05
BR	HC	1	1.529960E-03	9.953160E-07
BR	H	1	0.000000E+00	0.000000E+00
BR	DUM	1	0.000000E+00	0.000000E+00
BR	S	1	1.661670E-02	2.926067E-05
BR	CU1+	1	3.400835E-03	5.793063E-07
BR	CU2+	1	3.400835E-03	5.793063E-07
BR	FE	1	0.000000E+00	0.000000E+00
BR	ZN2+	1	3.400835E-03	7.862187E-07
BR	MG2+	1	1.343704E-03	4.724110E-07
BR	CA2+	1	5.271710E-03	5.710524E-06
BR	P	1	2.018882E-02	3.812141E-05
BR	AR	1	1.316265E-02	2.539270E-05
BR	F	1	5.707416E-03	7.057842E-06
BR	CL	1	1.556901E-02	3.164781E-05
BR	BR	1	2.765569E-02	6.548046E-05
CMet	O	1	4.480628E-03	3.788840E-06
CMet	OM	1	4.480628E-03	3.788840E-06
CMet	OA	1	4.480628E-03	4.950000E-06
CMet	OE	1	4.480628E-03	4.950000E-06
CMet	OW	1	4.819784E-03	7.141200E-06
CMet	N	1	4.650206E-03	5.724400E-06
CMet	NT	1	4.650206E-03	5.724400E-06
CMet	NL	1	4.650206E-03	5.724400E-06

CMet	NR	1	4.650206E-03	5.724400E-06
CMet	NZ	1	4.650206E-03	5.724400E-06
CMet	NE	1	4.650206E-03	5.724400E-06
CMet	C	1	4.557880E-03	8.082800E-06
CMet	CH0	1	4.557880E-03	8.082800E-06
CMet	CH1	1	5.083572E-03	8.505200E-06
CMet	CH2	1	6.475053E-03	9.581424E-06
CMet	CH3	1	7.798704E-03	1.080544E-05
CMet	CH4	1	1.081531E-02	2.579280E-05
CMet	CH2r	1	6.475053E-03	9.581424E-06
CMet	CR1	1	7.004514E-03	1.269840E-05
CMet	HC	1	8.667320E-04	5.412000E-07
CMet	H	1	0.000000E+00	0.000000E+00
CMet	DUM	1	0.000000E+00	0.000000E+00
CMet	S	1	9.413463E-03	1.591040E-05
CMet	CU1+	1	1.926594E-03	3.149960E-07
CMet	CU2+	1	1.926594E-03	3.149960E-07
CMet	FE	1	0.000000E+00	0.000000E+00
CMet	ZN2+	1	1.926594E-03	4.275040E-07
CMet	MG2+	1	7.612168E-04	2.568720E-07
CMet	CA2+	1	2.986457E-03	3.105080E-06
CMet	P	1	1.143709E-02	2.072840E-05
CMet	AR	1	7.456722E-03	1.380720E-05
CMet	F	1	3.233287E-03	3.837680E-06
CMet	CL	1	8.819940E-03	1.720840E-05
CMet	BR	1	1.566712E-02	3.560480E-05
CMet	CMet	1	8.875524E-03	1.936000E-05
OMet	O	1	2.261954E-03	1.313178E-06
OMet	OM	1	2.261954E-03	1.313178E-06
OMet	OA	1	2.261954E-03	1.715625E-06

OMet	OE	1	2.261954E-03	1.715625E-06
OMet	OW	1	2.433170E-03	2.475075E-06
OMet	N	1	2.347562E-03	1.984025E-06
OMet	NT	1	2.347562E-03	1.984025E-06
OMet	NL	1	2.347562E-03	1.984025E-06
OMet	NR	1	2.347562E-03	1.984025E-06
OMet	NZ	1	2.347562E-03	1.984025E-06
OMet	NE	1	2.347562E-03	1.984025E-06
OMet	C	1	2.300953E-03	2.801425E-06
OMet	CH0	1	2.300953E-03	2.801425E-06
OMet	CH1	1	2.566338E-03	2.947825E-06
OMet	CH2	1	3.268799E-03	3.320835E-06
OMet	CH3	1	3.937017E-03	3.745068E-06
OMet	CH4	1	5.459888E-03	8.939550E-06
OMet	CH2r	1	3.268799E-03	3.320835E-06
OMet	CR1	1	3.536086E-03	4.401150E-06
OMet	HC	1	4.375520E-04	1.875750E-07
OMet	H	1	0.000000E+00	0.000000E+00
OMet	DUM	1	0.000000E+00	0.000000E+00
OMet	S	1	4.752195E-03	5.514400E-06
OMet	CU1+	1	9.726020E-04	1.091748E-07
OMet	CU2+	1	9.726020E-04	1.091748E-07
OMet	FE	1	0.000000E+00	0.000000E+00
OMet	ZN2+	1	9.726020E-04	1.481690E-07
OMet	MG2+	1	3.842848E-04	8.902950E-08
OMet	CA2+	1	1.507652E-03	1.076193E-06
OMet	P	1	5.773784E-03	7.184275E-06
OMet	AR	1	3.764374E-03	4.785450E-06
OMet	F	1	1.632259E-03	1.330105E-06
OMet	CL	1	4.452567E-03	5.964275E-06

OMet	BR	1	7.909228E-03	1.234030E-05
OMet	CMet	1	4.480628E-03	6.710000E-06
OMet	OMet	1	2.261954E-03	2.325625E-06
NA+	O	1	4.222948E-04	2.324970E-07
NA+	OM	1	4.222948E-04	2.324970E-07
NA+	OA	1	4.222948E-04	3.037500E-07
NA+	OE	1	4.222948E-04	3.037500E-07
NA+	OW	1	4.542599E-04	4.382100E-07
NA+	N	1	4.382773E-04	3.512700E-07
NA+	NT	1	4.382773E-04	3.512700E-07
NA+	NL	1	4.382773E-04	3.512700E-07
NA+	NR	1	4.382773E-04	3.512700E-07
NA+	NZ	1	4.382773E-04	3.512700E-07
NA+	NE	1	4.382773E-04	3.512700E-07
NA+	C	1	4.295757E-04	4.959900E-07
NA+	CH0	1	4.295757E-04	4.959900E-07
NA+	CH1	1	4.791216E-04	5.219100E-07
NA+	CH2	1	6.102674E-04	5.879510E-07
NA+	CH3	1	7.350202E-04	6.630611E-07
NA+	CH4	1	1.019332E-03	1.582740E-06
NA+	CH2r	1	6.102674E-04	5.879510E-07
NA+	CR1	1	6.601685E-04	7.792200E-07
NA+	HC	1	8.168864E-05	3.321000E-08
NA+	H	1	0.000000E+00	0.000000E+00
NA+	DUM	1	0.000000E+00	0.000000E+00
NA+	S	1	8.872097E-04	9.763200E-07
NA+	CU1+	1	1.815796E-04	1.932930E-08
NA+	CU2+	1	1.815796E-04	1.932930E-08
NA+	FE	1	0.000000E+00	0.000000E+00
NA+	ZN2+	1	1.815796E-04	2.623320E-08

NA+	MG2+	1	7.174394E-05	1.576260E-08
NA+	CA2+	1	2.814706E-04	1.905390E-07
NA+	P	1	1.077935E-03	1.271970E-06
NA+	AR	1	7.027887E-04	8.472600E-07
NA+	F	1	3.047341E-04	2.354940E-07
NA+	CL	1	8.312707E-04	1.055970E-06
NA+	BR	1	1.476611E-03	2.184840E-06
NA+	CMet	1	8.365094E-04	1.188000E-06
NA+	OMet	1	4.222948E-04	4.117500E-07
NA+	NA+	1	7.884019E-05	7.290000E-08
CL-	O	1	5.382841E-03	6.695914E-06
CL-	OM	1	5.382841E-03	6.695914E-06
CL-	OA	1	5.382841E-03	8.748000E-06
CL-	OE	1	5.382841E-03	8.748000E-06
CL-	OW	1	5.790289E-03	1.262045E-05
CL-	N	1	5.586565E-03	1.011658E-05
CL-	NT	1	5.586565E-03	1.011658E-05
CL-	NL	1	5.586565E-03	1.011658E-05
CL-	NR	1	5.586565E-03	1.011658E-05
CL-	NZ	1	5.586565E-03	1.011658E-05
CL-	NE	1	5.586565E-03	1.011658E-05
CL-	C	1	5.475648E-03	1.428451E-05
CL-	CH0	1	5.475648E-03	1.428451E-05
CL-	CH1	1	6.107193E-03	1.503101E-05
CL-	CH2	1	7.778861E-03	1.693299E-05
CL-	CH3	1	9.369040E-03	1.909616E-05
CL-	CH4	1	1.299306E-02	4.558291E-05
CL-	CH2r	1	7.778861E-03	1.693299E-05
CL-	CR1	1	8.414933E-03	2.244154E-05
CL-	HC	1	1.041256E-03	9.564480E-07

CL-	H	1	0.000000E+00	0.000000E+00
CL-	DUM	1	0.000000E+00	0.000000E+00
CL-	S	1	1.130895E-02	2.811802E-05
CL-	CU1+	1	2.314531E-03	5.566838E-07
CL-	CU2+	1	2.314531E-03	5.566838E-07
CL-	FE	1	0.000000E+00	0.000000E+00
CL-	ZN2+	1	2.314531E-03	7.555162E-07
CL-	MG2+	1	9.144944E-04	4.539629E-07
CL-	CA2+	1	3.587806E-03	5.487523E-06
CL-	P	1	1.374005E-02	3.663274E-05
CL-	AR	1	8.958197E-03	2.440109E-05
CL-	F	1	3.884338E-03	6.782227E-06
CL-	CL	1	1.059591E-02	3.041194E-05
CL-	BR	1	1.882183E-02	6.292339E-05
CL-	CMet	1	1.066269E-02	3.421440E-05
CL-	OMet	1	5.382841E-03	1.185840E-05
CL-	NA+	1	1.004948E-03	2.099520E-06
CL-	CL-	1	1.280971E-02	6.046618E-05
CChl	O	1	2.439448E-03	1.735978E-06
CChl	OM	1	2.439448E-03	1.735978E-06
CChl	OA	1	2.439448E-03	2.268000E-06
CChl	OE	1	2.439448E-03	2.268000E-06
CChl	OW	1	2.624099E-03	3.271968E-06
CChl	N	1	2.531773E-03	2.622816E-06
CChl	NT	1	2.531773E-03	2.622816E-06
CChl	NL	1	2.531773E-03	2.622816E-06
CChl	NR	1	2.531773E-03	2.622816E-06
CChl	NZ	1	2.531773E-03	2.622816E-06
CChl	NE	1	2.531773E-03	2.622816E-06
CChl	C	1	2.481507E-03	3.703392E-06

CChl	CH0	1	2.481507E-03	3.703392E-06
CChl	CH1	1	2.767716E-03	3.896928E-06
CChl	CH2	1	3.525299E-03	4.390034E-06
CChl	CH3	1	4.245952E-03	4.950857E-06
CChl	CH4	1	5.888322E-03	1.181779E-05
CChl	CH2r	1	3.525299E-03	4.390034E-06
CChl	CR1	1	3.813560E-03	5.818176E-06
CChl	HC	1	4.718864E-04	2.479680E-07
CChl	H	1	0.000000E+00	0.000000E+00
CChl	DUM	1	0.000000E+00	0.000000E+00
CChl	S	1	5.125097E-03	7.289856E-06
CChl	CU1+	1	1.048921E-03	1.443254E-07
CChl	CU2+	1	1.048921E-03	1.443254E-07
CChl	FE	1	0.000000E+00	0.000000E+00
CChl	ZN2+	1	1.048921E-03	1.958746E-07
CChl	MG2+	1	4.144394E-04	1.176941E-07
CChl	CA2+	1	1.625956E-03	1.422691E-06
CChl	P	1	6.226849E-03	9.497376E-06
CChl	AR	1	4.059762E-03	6.326208E-06
CChl	F	1	1.760341E-03	1.758355E-06
CChl	CL	1	4.801957E-03	7.884576E-06
CChl	BR	1	8.529860E-03	1.631347E-05
CChl	CMet	1	4.832219E-03	8.870400E-06
CChl	OMet	1	2.439448E-03	3.074400E-06
CChl	NA+	1	4.554319E-04	5.443200E-07
CChl	CL-	1	5.805229E-03	1.567642E-05
CChl	CChl	1	2.630869E-03	4.064256E-06
CLChl	O	1	4.334666E-03	3.194767E-06
CLChl	OM	1	4.334666E-03	3.194767E-06
CLChl	OA	1	4.334666E-03	4.173862E-06

CLChlOE	1	4.334666E-03	4.173862E-06
CLChlOW	1	4.662774E-03	6.021492E-06
CLChlN	1	4.498720E-03	4.826840E-06
CLChlNT	1	4.498720E-03	4.826840E-06
CLChlNL	1	4.498720E-03	4.826840E-06
CLChlNR	1	4.498720E-03	4.826840E-06
CLChlNZ	1	4.498720E-03	4.826840E-06
CLChlNE	1	4.498720E-03	4.826840E-06
CLChlC	1	4.409402E-03	6.815454E-06
CLChlCH0	1	4.409402E-03	6.815454E-06
CLChlCH1	1	4.917968E-03	7.171623E-06
CLChlCH2	1	6.264121E-03	8.079100E-06
CLChlCH3	1	7.544652E-03	9.111197E-06
CLChlCH4	1	1.046299E-02	2.174861E-05
CLChlCH2r	1	6.264121E-03	8.079100E-06
CLChlCR1	1	6.776333E-03	1.070735E-05
CLChlHC	1	8.384972E-04	4.563423E-07
CLChlH	1	0.000000E+00	0.000000E+00
CLChlDUM	1	0.000000E+00	0.000000E+00
CLChlS	1	9.106809E-03	1.341572E-05
CLChlCU1+	1	1.863833E-03	2.656061E-07
CLChlCU2+	1	1.863833E-03	2.656061E-07
CLChlFE	1	0.000000E+00	0.000000E+00
CLChlZN2+	1	1.863833E-03	3.604733E-07
CLChlMG2+	1	7.364193E-04	2.165956E-07
CLChlCA2+	1	2.889170E-03	2.618218E-06
CLChlP	1	1.106452E-02	1.747828E-05
CLChlAR	1	7.213810E-03	1.164229E-05
CLChlF	1	3.127959E-03	3.235949E-06
CLChlCL	1	8.532620E-03	1.451020E-05

CLChl	BR	1	1.515675E-02 3.002213E-05
CLChl	CMet	1	8.586394E-03 1.632444E-05
CLChl	OMet	1	4.334666E-03 5.657903E-06
CLChl	NA+	1	8.092592E-04 1.001727E-06
CLChl	CL-	1	1.031534E-02 2.884974E-05
CLChl	CChl	1	4.675400E-03 7.481300E-06
CLChl	CLChl	1	8.306682E-03 1.376484E-05
HChl	O	1	2.920184E-04 5.646577E-08
HChl	OM	1	2.920184E-04 5.646577E-08
HChl	OA	1	2.920184E-04 7.377075E-08
HChl	OE	1	2.920184E-04 7.377075E-08
HChl	OW	1	3.141224E-04 1.064266E-07
HChl	N	1	3.030704E-04 8.531177E-08
HChl	NT	1	3.030704E-04 8.531177E-08
HChl	NL	1	3.030704E-04 8.531177E-08
HChl	NR	1	3.030704E-04 8.531177E-08
HChl	NZ	1	3.030704E-04 8.531177E-08
HChl	NE	1	3.030704E-04 8.531177E-08
HChl	C	1	2.970532E-04 1.204594E-07
HChl	CH0	1	2.970532E-04 1.204594E-07
HChl	CH1	1	3.313144E-04 1.267545E-07
HChl	CH2	1	4.220022E-04 1.427937E-07
HChl	CH3	1	5.082692E-04 1.610354E-07
HChl	CH4	1	7.048720E-04 3.843948E-07
HChl	CH2r	1	4.220022E-04 1.427937E-07
HChl	CR1	1	4.565090E-04 1.892466E-07
HChl	HC	1	5.648800E-05 8.065602E-09
HChl	H	1	0.000000E+00 0.000000E+00
HChl	DUM	1	0.000000E+00 0.000000E+00
HChl	S	1	6.135088E-04 2.371156E-07

HChl	CU1+	1	1.255630E-04	4.694443E-09
HChl	CU2+	1	1.255630E-04	4.694443E-09
HChl	FE	1	0.000000E+00	0.000000E+00
HChl	ZN2+	1	1.255630E-04	6.371170E-09
HChl	MG2+	1	4.961120E-05	3.828210E-09
HChl	CA2+	1	1.946380E-04	4.627557E-08
HChl	P	1	7.453960E-04	3.089191E-07
HChl	AR	1	4.859810E-04	2.057712E-07
HChl	F	1	2.107248E-04	5.719364E-08
HChl	CL	1	5.748268E-04	2.564599E-07
HChl	BR	1	1.021082E-03	5.306248E-07
HChl	CMet	1	5.784494E-04	2.885256E-07
HChl	OMet	1	2.920184E-04	1.000004E-07
HChl	NA+	1	5.451829E-05	1.770498E-08
HChl	CL-	1	6.949252E-04	5.099034E-07
HChl	CChl	1	3.622000E-04	1.745000E-07
HChl	CLChl	1	6.493000E-04	3.266000E-07
HChl	HChl	1	3.769960E-05	4.299949E-09
SDmso	O	1	4.887741E-03	3.992576E-06
SDmso	OM	1	4.887741E-03	3.992576E-06
SDmso	OA	1	4.887741E-03	5.216175E-06
SDmso	OE	1	4.887741E-03	5.216175E-06
SDmso	OW	1	5.257713E-03	7.525202E-06
SDmso	N	1	5.072727E-03	6.032217E-06
SDmso	NT	1	5.072727E-03	6.032217E-06
SDmso	NL	1	5.072727E-03	6.032217E-06
SDmso	NR	1	5.072727E-03	6.032217E-06
SDmso	NZ	1	5.072727E-03	6.032217E-06
SDmso	NE	1	5.072727E-03	6.032217E-06
SDmso	C	1	4.972013E-03	8.517434E-06

SDmso CH0 1 4.972013E-03 8.517434E-06

SDmso CH1 1 5.545469E-03 8.962548E-06

SDmso CH2 1 7.063382E-03 1.009664E-05

SDmso CH3 1 8.507301E-03 1.138648E-05

SDmso CH4 1 1.179800E-02 2.717975E-05

SDmso CH2r 1 7.063382E-03 1.009664E-05

SDmso CR1 1 7.640949E-03 1.338123E-05

SDmso HC 1 9.454840E-04 5.703018E-07

SDmso H 1 0.000000E+00 0.000000E+00

SDmso DUM 1 0.000000E+00 0.000000E+00

SDmso S 1 1.026878E-02 1.676595E-05

SDmso CU1+ 1 2.101647E-03 3.319342E-07

SDmso CU2+ 1 2.101647E-03 3.319342E-07

SDmso FE 1 0.000000E+00 0.000000E+00

SDmso ZN2+ 1 2.101647E-03 4.504921E-07

SDmso MG2+ 1 8.303816E-04 2.706847E-07

SDmso CA2+ 1 3.257809E-03 3.272049E-06

SDmso P 1 1.247628E-02 2.184302E-05

SDmso AR 1 8.134245E-03 1.454965E-05

SDmso F 1 3.527066E-03 4.044043E-06

SDmso CL 1 9.621327E-03 1.813374E-05

SDmso BR 1 1.709065E-02 3.751937E-05

SDmso CMet 1 9.681962E-03 2.040104E-05

SDmso OMet 1 4.887741E-03 7.070815E-06

SDmso NA+ 1 9.125154E-04 1.251882E-06

SDmso CL- 1 1.163151E-02 3.605420E-05

SDmso CChl 1 5.271279E-03 9.347386E-06

SDmso CLChl 1 9.366561E-03 1.720225E-05

SDmso HChl 1 6.310078E-04 3.040404E-07

SDmso SDmso 1 1.056167E-02 2.149806E-05

CDmso	O	1	4.663258E-03	4.444998E-06
CDmso	OM	1	4.663258E-03	4.444998E-06
CDmso	OA	1	4.663258E-03	5.807250E-06
CDmso	OE	1	4.663258E-03	5.807250E-06
CDmso	OW	1	5.016238E-03	8.377926E-06
CDmso	N	1	4.839748E-03	6.715762E-06
CDmso	NT	1	4.839748E-03	6.715762E-06
CDmso	NL	1	4.839748E-03	6.715762E-06
CDmso	NR	1	4.839748E-03	6.715762E-06
CDmso	NZ	1	4.839748E-03	6.715762E-06
CDmso	NE	1	4.839748E-03	6.715762E-06
CDmso	C	1	4.743659E-03	9.482594E-06
CDmso	CH0	1	4.743659E-03	9.482594E-06
CDmso	CH1	1	5.290778E-03	9.978146E-06
CDmso	CH2	1	6.738976E-03	1.124075E-05
CDmso	CH3	1	8.116579E-03	1.267675E-05
CDmso	CH4	1	1.125614E-02	3.025964E-05
CDmso	CH2r	1	6.738976E-03	1.124075E-05
CDmso	CR1	1	7.290017E-03	1.489753E-05
CDmso	HC	1	9.020600E-04	6.349260E-07
CDmso	H	1	0.000000E+00	0.000000E+00
CDmso	DUM	1	0.000000E+00	0.000000E+00
CDmso	S	1	9.797156E-03	1.866579E-05
CDmso	CU1+	1	2.005122E-03	3.695476E-07
CDmso	CU2+	1	2.005122E-03	3.695476E-07
CDmso	FE	1	0.000000E+00	0.000000E+00
CDmso	ZN2+	1	2.005122E-03	5.015399E-07
CDmso	MG2+	1	7.922440E-04	3.013576E-07
CDmso	CA2+	1	3.108185E-03	3.642823E-06
CDmso	P	1	1.190327E-02	2.431818E-05

CDmso	AR	1	7.760657E-03	1.619836E-05
CDmso	F	1	3.365076E-03	4.502296E-06
CDmso	CL	1	9.179441E-03	2.018858E-05
CDmso	BR	1	1.630571E-02	4.177090E-05
CDmso	CMet	1	9.237291E-03	2.271280E-05
CDmso	OMet	1	4.663258E-03	7.872050E-06
CDmso	NA+	1	8.706056E-04	1.393740E-06
CDmso	CL-	1	1.109730E-02	4.013971E-05
CDmso	CChl	1	5.029181E-03	1.040659E-05
CDmso	CLChl	1	8.936375E-03	1.915154E-05
CDmso	HChl	1	6.020270E-04	3.384930E-07
CDmso	SDmso	1	1.007660E-02	2.393413E-05
CDmso	CDmso	1	9.613802E-03	2.664624E-05
ODmso	O	1	2.266329E-03	7.464531E-07
ODmso	OM	1	2.266329E-03	7.464531E-07
ODmso	OA	1	2.266329E-03	9.752175E-07
ODmso	OE	1	2.266329E-03	9.752175E-07
ODmso	OW	1	2.437876E-03	1.406914E-06
ODmso	N	1	2.352103E-03	1.127785E-06
ODmso	NT	1	2.352103E-03	1.127785E-06
ODmso	NL	1	2.352103E-03	1.127785E-06
ODmso	NR	1	2.352103E-03	1.127785E-06
ODmso	NZ	1	2.352103E-03	1.127785E-06
ODmso	NE	1	2.352103E-03	1.127785E-06
ODmso	C	1	2.305404E-03	1.592422E-06
ODmso	CH0	1	2.305404E-03	1.592422E-06
ODmso	CH1	1	2.571302E-03	1.675640E-06
ODmso	CH2	1	3.275122E-03	1.887671E-06
ODmso	CH3	1	3.944633E-03	2.128819E-06
ODmso	CH4	1	5.470450E-03	5.081533E-06

ODmso CH2r 1 3.275122E-03 1.887671E-06

ODmso CR1 1 3.542926E-03 2.501758E-06

ODmso HC 1 4.383984E-04 1.066238E-07

ODmso H 1 0.000000E+00 0.000000E+00

ODmso DUM 1 0.000000E+00 0.000000E+00

ODmso S 1 4.761388E-03 3.134566E-06

ODmso CU1+ 1 9.744834E-04 6.205851E-08

ODmso CU2+ 1 9.744834E-04 6.205851E-08

ODmso FE 1 0.000000E+00 0.000000E+00

ODmso ZN2+ 1 9.744834E-04 8.422412E-08

ODmso MG2+ 1 3.850282E-04 5.060729E-08

ODmso CA2+ 1 1.510568E-03 6.117431E-07

ODmso P 1 5.784953E-03 4.083777E-06

ODmso AR 1 3.771656E-03 2.720207E-06

ODmso F 1 1.635417E-03 7.560753E-07

ODmso CL 1 4.461180E-03 3.390289E-06

ODmso BR 1 7.924528E-03 7.014631E-06

ODmso CMet 1 4.489295E-03 3.814184E-06

ODmso OMet 1 2.266329E-03 1.321962E-06

ODmso NA+ 1 4.231116E-04 2.340522E-07

ODmso CL- 1 5.393253E-03 6.740703E-06

ODmso CChl 1 2.444166E-03 1.747590E-06

ODmso CLChl 1 4.343051E-03 3.216137E-06

ODmso HChl 1 2.925833E-04 5.684348E-08

ODmso SDmso 1 4.897196E-03 4.019283E-06

ODmso CDmso 1 4.672279E-03 4.474731E-06

ODmso ODmso 1 2.270713E-03 7.514463E-07

CCl4 O 1 2.439448E-03 2.373880E-06

CCl4 OM 1 2.439448E-03 2.373880E-06

CCl4 OA 1 2.439448E-03 3.101400E-06

CCl4 OE 1 2.439448E-03 3.101400E-06

CCl4 OW 1 2.624099E-03 4.474286E-06

CCl4 N 1 2.531773E-03 3.586597E-06

CCl4 NT 1 2.531773E-03 3.586597E-06

CCl4 NL 1 2.531773E-03 3.586597E-06

CCl4 NR 1 2.531773E-03 3.586597E-06

CCl4 NZ 1 2.531773E-03 3.586597E-06

CCl4 NE 1 2.531773E-03 3.586597E-06

CCl4 C 1 2.481507E-03 5.064242E-06

CCl4 CH0 1 2.481507E-03 5.064242E-06

CCl4 CH1 1 2.767716E-03 5.328894E-06

CCl4 CH2 1 3.525299E-03 6.003198E-06

CCl4 CH3 1 4.245952E-03 6.770100E-06

CCl4 CH4 1 5.888322E-03 1.616036E-05

CCl4 CH2r 1 3.525299E-03 6.003198E-06

CCl4 CR1 1 3.813560E-03 7.956125E-06

CCl4 HC 1 4.718864E-04 3.390864E-07

CCl4 H 1 0.000000E+00 0.000000E+00

CCl4 DUM 1 0.000000E+00 0.000000E+00

CCl4 S 1 5.125097E-03 9.968589E-06

CCl4 CU1+ 1 1.048921E-03 1.973593E-07

CCl4 CU2+ 1 1.048921E-03 1.973593E-07

CCl4 FE 1 0.000000E+00 0.000000E+00

CCl4 ZN2+ 1 1.048921E-03 2.678507E-07

CCl4 MG2+ 1 4.144394E-04 1.609420E-07

CCl4 CA2+ 1 1.625956E-03 1.945474E-06

CCl4 P 1 6.226849E-03 1.298728E-05

CCl4 AR 1 4.059762E-03 8.650838E-06

CCl4 F 1 1.760341E-03 2.404481E-06

CCl4 CL 1 4.801957E-03 1.078184E-05

CCl4	BR	1	8.529860E-03	2.230803E-05
CCl4	CMet	1	4.832219E-03	1.212992E-05
CCl4	OMet	1	2.439448E-03	4.204120E-06
CCl4	NA+	1	4.554319E-04	7.443360E-07
CCl4	CL-	1	5.805229E-03	2.143688E-05
CCl4	CChl	1	2.630869E-03	5.557709E-06
CCl4	CLChl	1	4.674804E-03	1.022800E-05
CCl4	HChl	1	3.149329E-04	1.807744E-07
CCl4	SDmso	1	5.271279E-03	1.278218E-05
CCl4	CDmso	1	5.029181E-03	1.423060E-05
CCl4	ODmso	1	2.444166E-03	2.389760E-06
CCl4	CCl4	1	2.630869E-03	7.599946E-06
CLCl4	O	1	4.147280E-03	3.076883E-06
CLCl4	OM	1	4.147280E-03	3.076883E-06
CLCl4	OA	1	4.147280E-03	4.019850E-06
CLCl4	OE	1	4.147280E-03	4.019850E-06
CLCl4	OW	1	4.461203E-03	5.799304E-06
CLCl4	N	1	4.304241E-03	4.648733E-06
CLCl4	NT	1	4.304241E-03	4.648733E-06
CLCl4	NL	1	4.304241E-03	4.648733E-06
CLCl4	NR	1	4.304241E-03	4.648733E-06
CLCl4	NZ	1	4.304241E-03	4.648733E-06
CLCl4	NE	1	4.304241E-03	4.648733E-06
CLCl4	C	1	4.218784E-03	6.563968E-06
CLCl4	CH0	1	4.218784E-03	6.563968E-06
CLCl4	CH1	1	4.705366E-03	6.906996E-06
CLCl4	CH2	1	5.993325E-03	7.780987E-06
CLCl4	CH3	1	7.218499E-03	8.775000E-06
CLCl4	CH4	1	1.001067E-02	2.094610E-05
CLCl4	CH2r	1	5.993325E-03	7.780987E-06

CLCl4 CR1 1 6.483394E-03 1.031226E-05

CLCl4 HC 1 8.022492E-04 4.395036E-07

CLCl4 H 1 0.000000E+00 0.000000E+00

CLCl4 DUM 1 0.000000E+00 0.000000E+00

CLCl4 S 1 8.713124E-03 1.292069E-05

CLCl4 CU1+ 1 1.783260E-03 2.558054E-07

CLCl4 CU2+ 1 1.783260E-03 2.558054E-07

CLCl4 FE 1 0.000000E+00 0.000000E+00

CLCl4 ZN2+ 1 1.783260E-03 3.471721E-07

CLCl4 MG2+ 1 7.045841E-04 2.086034E-07

CLCl4 CA2+ 1 2.764272E-03 2.521607E-06

CLCl4 P 1 1.058620E-02 1.683335E-05

CLCl4 AR 1 6.901959E-03 1.121270E-05

CLCl4 F 1 2.992738E-03 3.116545E-06

CLCl4 CL 1 8.163758E-03 1.397479E-05

CLCl4 BR 1 1.450153E-02 2.891433E-05

CLCl4 CMet 1 8.215206E-03 1.572208E-05

CLCl4 OMet 1 4.147280E-03 5.449130E-06

CLCl4 NA+ 1 7.742751E-04 9.647640E-07

CLCl4 CL- 1 9.869409E-03 2.778520E-05

CLCl4 CChl 1 4.472714E-03 7.203571E-06

CLCl4 CLChl 1 7.947586E-03 1.325693E-05

CLCl4 HChl 1 5.354141E-04 2.343090E-07

CLCl4 SDmso 1 8.961647E-03 1.656750E-05

CLCl4 CDmso 1 8.550058E-03 1.844486E-05

CLCl4 ODmso 1 4.155302E-03 3.097464E-06

CLCl4 CCl4 1 4.472714E-03 9.850598E-06

CLCl4 CLCl4 1 7.604014E-03 1.276776E-05

FTFE O 1 1.632259E-03 8.611000E-07

FTFE OM 1 1.632259E-03 8.611000E-07

FTFE OA 1 1.632259E-03 1.125000E-06

FTFE OE 1 1.632259E-03 1.125000E-06

FTFE OW 1 1.755811E-03 1.623000E-06

FTFE N 1 1.694035E-03 1.301000E-06

FTFE NT 1 1.694035E-03 1.301000E-06

FTFE NL 1 1.694035E-03 1.301000E-06

FTFE NR 1 1.694035E-03 1.301000E-06

FTFE NZ 1 1.694035E-03 1.301000E-06

FTFE NE 1 1.694035E-03 1.301000E-06

FTFE C 1 1.660402E-03 1.837000E-06

FTFE CH0 1 1.660402E-03 1.837000E-06

FTFE CH1 1 1.851907E-03 1.933000E-06

FTFE CH2 1 2.358814E-03 2.177596E-06

FTFE CH3 1 2.841010E-03 2.455782E-06

FTFE CH4 1 3.939936E-03 5.862000E-06

FTFE CH2r 1 2.358814E-03 2.177596E-06

FTFE CR1 1 2.551692E-03 2.886000E-06

FTFE HC 1 3.157440E-04 1.230000E-07

FTFE H 1 0.000000E+00 0.000000E+00

FTFE DUM 1 0.000000E+00 0.000000E+00

FTFE S 1 3.429254E-03 3.616000E-06

FTFE CU1+ 1 7.018440E-04 7.159000E-08

FTFE CU2+ 1 7.018440E-04 7.159000E-08

FTFE FE 1 0.000000E+00 0.000000E+00

FTFE ZN2+ 1 7.018440E-04 9.716000E-08

FTFE MG2+ 1 2.773056E-04 5.838000E-08

FTFE CA2+ 1 1.087944E-03 7.057000E-07

FTFE P 1 4.166448E-03 4.711000E-06

FTFE AR 1 2.716428E-03 3.138000E-06

FTFE F 1 1.177862E-03 8.722000E-07

FTFE CL 1 3.213038E-03 3.911000E-06

FTFE BR 1 5.707416E-03 8.092000E-06

FTFE CMet 1 3.233287E-03 4.400000E-06

FTFE OMet 1 1.632259E-03 1.525000E-06

FTFE NA+ 1 3.047341E-04 2.700000E-07

FTFE CL- 1 3.884338E-03 7.776000E-06

FTFE CChl 1 1.760341E-03 2.016000E-06

FTFE CLChl 1 3.127959E-03 3.710100E-06

FTFE HChl 1 2.107248E-04 6.557400E-08

FTFE SDmso 1 3.527066E-03 4.636600E-06

FTFE CDmso 1 3.365076E-03 5.162000E-06

FTFE ODmso 1 1.635417E-03 8.668600E-07

FTFE CCl4 1 1.760341E-03 2.756800E-06

FTFE CLCl4 1 2.992738E-03 3.573200E-06

FTFE FTFE 1 1.177862E-03 1.000000E-06

CTFE O 1 2.300953E-03 1.581841E-06

CTFE OM 1 2.300953E-03 1.581841E-06

CTFE OA 1 2.300953E-03 2.066625E-06

CTFE OE 1 2.300953E-03 2.066625E-06

CTFE OW 1 2.475121E-03 2.981451E-06

CTFE N 1 2.388037E-03 2.389937E-06

CTFE NT 1 2.388037E-03 2.389937E-06

CTFE NL 1 2.388037E-03 2.389937E-06

CTFE NR 1 2.388037E-03 2.389937E-06

CTFE NZ 1 2.388037E-03 2.389937E-06

CTFE NE 1 2.388037E-03 2.389937E-06

CTFE C 1 2.340624E-03 3.374569E-06

CTFE CH0 1 2.340624E-03 3.374569E-06

CTFE CH1 1 2.610585E-03 3.550921E-06

CTFE CH2 1 3.325157E-03 4.000245E-06

CTFE CH3 1 4.004896E-03 4.511272E-06

CTFE CH4 1 5.554024E-03 1.076849E-05

CTFE CH2r 1 3.325157E-03 4.000245E-06

CTFE CR1 1 3.597053E-03 5.301582E-06

CTFE HC 1 4.450960E-04 2.259510E-07

CTFE H 1 0.000000E+00 0.000000E+00

CTFE DUM 1 0.000000E+00 0.000000E+00

CTFE S 1 4.834130E-03 6.642592E-06

CTFE CU1+ 1 9.893710E-04 1.315108E-07

CTFE CU2+ 1 9.893710E-04 1.315108E-07

CTFE FE 1 0.000000E+00 0.000000E+00

CTFE ZN2+ 1 9.893710E-04 1.784829E-07

CTFE MG2+ 1 3.909104E-04 1.072441E-07

CTFE CA2+ 1 1.533646E-03 1.296371E-06

CTFE P 1 5.873332E-03 8.654107E-06

CTFE AR 1 3.829277E-03 5.764506E-06

CTFE F 1 1.660402E-03 1.602231E-06

CTFE CL 1 4.529336E-03 7.184507E-06

CTFE BR 1 8.045594E-03 1.486500E-05

CTFE CMet 1 4.557880E-03 8.082800E-06

CTFE OMet 1 2.300953E-03 2.801425E-06

CTFE NA+ 1 4.295757E-04 4.959900E-07

CTFE CL- 1 5.475648E-03 1.428451E-05

CTFE CChl 1 2.481507E-03 3.703392E-06

CTFE CLChl 1 4.409402E-03 6.815454E-06

CTFE HChl 1 2.970532E-04 1.204594E-07

CTFE SDmso 1 4.972013E-03 8.517434E-06

CTFE CDmso 1 4.743659E-03 9.482594E-06

CTFE ODmso 1 2.305404E-03 1.592422E-06

CTFE CCl4 1 2.481507E-03 5.064242E-06

CTFE	CLCl4	1	4.218784E-03	6.563968E-06
CTFE	FTFE	1	1.660402E-03	1.837000E-06
CTFE	CTFE	1	2.340624E-03	3.374569E-06
CHTFE	O	1	4.008832E-03	4.371805E-06
CHTFE	OM	1	4.008832E-03	4.371805E-06
CHTFE	OA	1	4.008832E-03	5.711625E-06
CHTFE	OE	1	4.008832E-03	5.711625E-06
CHTFE	OW	1	4.312276E-03	8.239971E-06
CHTFE	N	1	4.160554E-03	6.605177E-06
CHTFE	NT	1	4.160554E-03	6.605177E-06
CHTFE	NL	1	4.160554E-03	6.605177E-06
CHTFE	NR	1	4.160554E-03	6.605177E-06
CHTFE	NZ	1	4.160554E-03	6.605177E-06
CHTFE	NE	1	4.160554E-03	6.605177E-06
CHTFE	C	1	4.077950E-03	9.326449E-06
CHTFE	CH0	1	4.077950E-03	9.326449E-06
CHTFE	CH1	1	4.548288E-03	9.813841E-06
CHTFE	CH2	1	5.793252E-03	1.105566E-05
CHTFE	CH3	1	6.977526E-03	1.246801E-05
CHTFE	CH4	1	9.676492E-03	2.976137E-05
CHTFE	CH2r	1	5.793252E-03	1.105566E-05
CHTFE	CR1	1	6.266962E-03	1.465222E-05
CHTFE	HC	1	7.754680E-04	6.244710E-07
CHTFE	H	1	0.000000E+00	0.000000E+00
CHTFE	DUM	1	0.000000E+00	0.000000E+00
CHTFE	S	1	8.422257E-03	1.835843E-05
CHTFE	CU1+	1	1.723731E-03	3.634624E-07
CHTFE	CU2+	1	1.723731E-03	3.634624E-07
CHTFE	FE	1	0.000000E+00	0.000000E+00
CHTFE	ZN2+	1	1.723731E-03	4.932813E-07

CHTFE MG2+ 1 6.810632E-04 2.963953E-07

CHTFE CA2+ 1 2.671993E-03 3.582839E-06

CHTFE P 1 1.023281E-02 2.391775E-05

CHTFE AR 1 6.671553E-03 1.593163E-05

CHTFE F 1 2.892833E-03 4.428159E-06

CHTFE CL 1 7.891230E-03 1.985615E-05

CHTFE BR 1 1.401743E-02 4.108308E-05

CHTFE CMet 1 7.940961E-03 2.233880E-05

CHTFE OMet 1 4.008832E-03 7.742425E-06

CHTFE NA+ 1 7.484278E-04 1.370790E-06

CHTFE CL- 1 9.539942E-03 3.947875E-05

CHTFE CChl 1 4.323403E-03 1.023523E-05

CHTFE CLChl 1 7.682275E-03 1.883618E-05

CHTFE HChl 1 5.175406E-04 3.329192E-07

CHTFE SDmso 1 8.662483E-03 2.354002E-05

CHTFE CDmso 1 8.264634E-03 2.620747E-05

CHTFE ODmso 1 4.016587E-03 4.401048E-06

CHTFE CCl4 1 4.323403E-03 1.399627E-05

CHTFE CLCl4 1 7.350172E-03 1.814114E-05

CHTFE FTFE 1 2.892833E-03 5.077000E-06

CHTFE CTFE 1 4.077950E-03 9.326449E-06

CHTFE CHTFE 1 7.104804E-03 2.577593E-05

OTFE O 1 2.261954E-03 1.056570E-06

OTFE OM 1 2.261954E-03 1.056570E-06

OTFE OA 1 2.261954E-03 1.380375E-06

OTFE OE 1 2.261954E-03 1.380375E-06

OTFE OW 1 2.433170E-03 1.991421E-06

OTFE N 1 2.347562E-03 1.596327E-06

OTFE NT 1 2.347562E-03 1.596327E-06

OTFE NL 1 2.347562E-03 1.596327E-06

OTFE NR 1 2.347562E-03 1.596327E-06

OTFE NZ 1 2.347562E-03 1.596327E-06

OTFE NE 1 2.347562E-03 1.596327E-06

OTFE C 1 2.300953E-03 2.253999E-06

OTFE CH0 1 2.300953E-03 2.253999E-06

OTFE CH1 1 2.566338E-03 2.371791E-06

OTFE CH2 1 3.268799E-03 2.671911E-06

OTFE CH3 1 3.937017E-03 3.013245E-06

OTFE CH4 1 5.459888E-03 7.192674E-06

OTFE CH2r 1 3.268799E-03 2.671911E-06

OTFE CR1 1 3.536086E-03 3.541122E-06

OTFE HC 1 4.375520E-04 1.509210E-07

OTFE H 1 0.000000E+00 0.000000E+00

OTFE DUM 1 0.000000E+00 0.000000E+00

OTFE S 1 4.752195E-03 4.436832E-06

OTFE CU1+ 1 9.726020E-04 8.784093E-08

OTFE CU2+ 1 9.726020E-04 8.784093E-08

OTFE FE 1 0.000000E+00 0.000000E+00

OTFE ZN2+ 1 9.726020E-04 1.192153E-07

OTFE MG2+ 1 3.842848E-04 7.163226E-08

OTFE CA2+ 1 1.507652E-03 8.658939E-07

OTFE P 1 5.773784E-03 5.780397E-06

OTFE AR 1 3.764374E-03 3.850326E-06

OTFE F 1 1.632259E-03 1.070189E-06

OTFE CL 1 4.452567E-03 4.798797E-06

OTFE BR 1 7.909228E-03 9.928884E-06

OTFE CMet 1 4.480628E-03 5.398800E-06

OTFE OMet 1 2.261954E-03 1.871175E-06

OTFE NA+ 1 4.222948E-04 3.312900E-07

OTFE CL- 1 5.382841E-03 9.541152E-06

OTFE CChl 1 2.439448E-03 2.473632E-06

OTFE CLChl 1 4.334666E-03 4.552293E-06

OTFE HChl 1 2.920184E-04 8.045930E-08

OTFE SDmso 1 4.887741E-03 5.689108E-06

OTFE CDmso 1 4.663258E-03 6.333774E-06

OTFE ODmso 1 2.266329E-03 1.063637E-06

OTFE CCl4 1 2.439448E-03 3.382594E-06

OTFE CLCl4 1 4.147280E-03 4.384316E-06

OTFE FTFE 1 1.632259E-03 1.227000E-06

OTFE CTFE 1 2.300953E-03 2.253999E-06

OTFE CHTFE 1 4.008832E-03 6.229479E-06

OTFE OTFE 1 2.261954E-03 1.505529E-06

CUrea O 1 3.324729E-03 3.174359E-06

CUrea OM 1 3.324729E-03 3.174359E-06

CUrea OA 1 3.324729E-03 4.147200E-06

CUrea OE 1 3.324729E-03 4.147200E-06

CUrea OW 1 3.576391E-03 5.983027E-06

CUrea N 1 3.450560E-03 4.796006E-06

CUrea NT 1 3.450560E-03 4.796006E-06

CUrea NL 1 3.450560E-03 4.796006E-06

CUrea NR 1 3.450560E-03 4.796006E-06

CUrea NZ 1 3.450560E-03 4.796006E-06

CUrea NE 1 3.450560E-03 4.796006E-06

CUrea C 1 3.382052E-03 6.771917E-06

CUrea CH0 1 3.382052E-03 6.771917E-06

CUrea CH1 1 3.772128E-03 7.125811E-06

CUrea CH2 1 4.804639E-03 8.027491E-06

CUrea CH3 1 5.786819E-03 9.052995E-06

CUrea CH4 1 8.025209E-03 2.160968E-05

CUrea CH2r 1 4.804639E-03 8.027491E-06

CUrea	CR1	1	5.197511E-03	1.063895E-05
CUrea	HC	1	6.431352E-04	4.534272E-07
CUrea	H	1	0.000000E+00	0.000000E+00
CUrea	DUM	1	0.000000E+00	0.000000E+00
CUrea	S	1	6.985008E-03	1.333002E-05
CUrea	CU1+	1	1.429578E-03	2.639094E-07
CUrea	CU2+	1	1.429578E-03	2.639094E-07
CUrea	FE	1	0.000000E+00	0.000000E+00
CUrea	ZN2+	1	1.429578E-03	3.581706E-07
CUrea	MG2+	1	5.648405E-04	2.152120E-07
CUrea	CA2+	1	2.216020E-03	2.601492E-06
CUrea	P	1	8.486588E-03	1.736663E-05
CUrea	AR	1	5.533060E-03	1.156792E-05
CUrea	F	1	2.399174E-03	3.215278E-06
CUrea	CL	1	6.544600E-03	1.441751E-05
CUrea	BR	1	1.162537E-02	2.983035E-05
CUrea	CMet	1	6.585844E-03	1.622016E-05
CUrea	OMet	1	3.324729E-03	5.621760E-06
CUrea	NA+	1	6.207094E-04	9.953280E-07
CUrea	CL-	1	7.911961E-03	2.866545E-05
CUrea	CChl	1	3.585619E-03	7.431782E-06
CUrea	CLChl	1	6.371303E-03	1.367691E-05
CUrea	HChl	1	4.292228E-04	2.417320E-07
CUrea	SDmso	1	7.184240E-03	1.709236E-05
CUrea	CDmso	1	6.854283E-03	1.902920E-05
CUrea	ODmso	1	3.331161E-03	3.195593E-06
CUrea	CCl4	1	3.585619E-03	1.016267E-05
CUrea	CLCl4	1	6.095873E-03	1.317224E-05
CUrea	FTFE	1	2.399174E-03	3.686400E-06
CUrea	CTFE	1	3.382052E-03	6.771917E-06

CUrea	CHTFE	1	5.892377E-03	1.871585E-05
CUrea	OTFE	1	3.324729E-03	4.523213E-06
CUrea	CUrea	1	4.886849E-03	1.358954E-05
OUrea	O	1	2.312367E-03	1.085761E-06
OUrea	OM	1	2.312367E-03	1.085761E-06
OUrea	OA	1	2.312367E-03	1.418512E-06
OUrea	OE	1	2.312367E-03	1.418512E-06
OUrea	OW	1	2.487399E-03	2.046441E-06
OUrea	N	1	2.399883E-03	1.640431E-06
OUrea	NT	1	2.399883E-03	1.640431E-06
OUrea	NL	1	2.399883E-03	1.640431E-06
OUrea	NR	1	2.399883E-03	1.640431E-06
OUrea	NZ	1	2.399883E-03	1.640431E-06
OUrea	NE	1	2.399883E-03	1.640431E-06
OUrea	C	1	2.352236E-03	2.316273E-06
OUrea	CH0	1	2.352236E-03	2.316273E-06
OUrea	CH1	1	2.623535E-03	2.437320E-06
OUrea	CH2	1	3.341653E-03	2.745731E-06
OUrea	CH3	1	4.024764E-03	3.096496E-06
OUrea	CH4	1	5.581576E-03	7.391396E-06
OUrea	CH2r	1	3.341653E-03	2.745731E-06
OUrea	CR1	1	3.614897E-03	3.638957E-06
OUrea	HC	1	4.473040E-04	1.550907E-07
OUrea	H	1	0.000000E+00	0.000000E+00
OUrea	DUM	1	0.000000E+00	0.000000E+00
OUrea	S	1	4.858110E-03	4.559414E-06
OUrea	CU1+	1	9.942790E-04	9.026783E-08
OUrea	CU2+	1	9.942790E-04	9.026783E-08
OUrea	FE	1	0.000000E+00	0.000000E+00
OUrea	ZN2+	1	9.942790E-04	1.225090E-07

OUrea	MG2+	1	3.928496E-04	7.361134E-08
OUrea	CA2+	1	1.541254E-03	8.898171E-07
OUrea	P	1	5.902468E-03	5.940100E-06
OUrea	AR	1	3.848273E-03	3.956704E-06
OUrea	F	1	1.668638E-03	1.099757E-06
OUrea	CL	1	4.551804E-03	4.931380E-06
OUrea	BR	1	8.085506E-03	1.020320E-05
OUrea	CMet	1	4.580490E-03	5.547960E-06
OUrea	OMet	1	2.312367E-03	1.922873E-06
OUrea	NA+	1	4.317067E-04	3.404430E-07
OUrea	CL-	1	5.502812E-03	9.804758E-06
OUrea	CChl	1	2.493817E-03	2.541974E-06
OUrea	CLChl	1	4.431275E-03	4.678065E-06
OUrea	HChl	1	2.985268E-04	8.268226E-08
OUrea	SDmso	1	4.996677E-03	5.846289E-06
OUrea	CDmso	1	4.767191E-03	6.508766E-06
OUrea	ODmso	1	2.316840E-03	1.093024E-06
OUrea	CCl4	1	2.493817E-03	3.476049E-06
OUrea	CLCl4	1	4.239713E-03	4.505448E-06
OUrea	FTFE	1	1.668638E-03	1.260900E-06
OUrea	CTFE	1	2.352236E-03	2.316273E-06
OUrea	CHTFE	1	4.098180E-03	6.401589E-06
OUrea	OTFE	1	2.312367E-03	1.547124E-06
OUrea	CUrea	1	3.398830E-03	4.648182E-06
OUrea	OUrea	1	2.363904E-03	1.589869E-06
NUrea	O	1	2.753867E-03	1.711608E-06
NUrea	OM	1	2.753867E-03	1.711608E-06
NUrea	OA	1	2.753867E-03	2.236162E-06
NUrea	OE	1	2.753867E-03	2.236162E-06
NUrea	OW	1	2.962317E-03	3.226037E-06

NUrea	N	1	2.858092E-03	2.585998E-06
NUrea	NT	1	2.858092E-03	2.585998E-06
NUrea	NL	1	2.858092E-03	2.585998E-06
NUrea	NR	1	2.858092E-03	2.585998E-06
NUrea	NZ	1	2.858092E-03	2.585998E-06
NUrea	NE	1	2.858092E-03	2.585998E-06
NUrea	C	1	2.801347E-03	3.651405E-06
NUrea	CH0	1	2.801347E-03	3.651405E-06
NUrea	CH1	1	3.124446E-03	3.842224E-06
NUrea	CH2	1	3.979673E-03	4.328408E-06
NUrea	CH3	1	4.793210E-03	4.881358E-06
NUrea	CH4	1	6.647264E-03	1.165190E-05
NUrea	CH2r	1	3.979673E-03	4.328408E-06
NUrea	CR1	1	4.305088E-03	5.736502E-06
NUrea	HC	1	5.327076E-04	2.444871E-07
NUrea	H	1	0.000000E+00	0.000000E+00
NUrea	DUM	1	0.000000E+00	0.000000E+00
NUrea	S	1	5.785668E-03	7.187523E-06
NUrea	CU1+	1	1.184116E-03	1.422994E-07
NUrea	CU2+	1	1.184116E-03	1.422994E-07
NUrea	FE	1	0.000000E+00	0.000000E+00
NUrea	ZN2+	1	1.184116E-03	1.931249E-07
NUrea	MG2+	1	4.678562E-04	1.160419E-07
NUrea	CA2+	1	1.835525E-03	1.402720E-06
NUrea	P	1	7.029424E-03	9.364055E-06
NUrea	AR	1	4.583022E-03	6.237403E-06
NUrea	F	1	1.987231E-03	1.733672E-06
NUrea	CL	1	5.420879E-03	7.773895E-06
NUrea	BR	1	9.629269E-03	1.608447E-05
NUrea	CMet	1	5.455042E-03	8.745880E-06

NUrea	OMet	1	2.753867E-03	3.031242E-06
NUrea	NA+	1	5.141323E-04	5.366790E-07
NUrea	CL-	1	6.553462E-03	1.545636E-05
NUrea	CChl	1	2.969961E-03	4.007203E-06
NUrea	CLChl	1	5.277337E-03	7.374566E-06
NUrea	HChl	1	3.555244E-04	1.303414E-07
NUrea	SDmso	1	5.950691E-03	9.216170E-06
NUrea	CDmso	1	5.677389E-03	1.026051E-05
NUrea	ODmso	1	2.759194E-03	1.723058E-06
NUrea	CCl4	1	2.969961E-03	5.479691E-06
NUrea	CLCl4	1	5.049200E-03	7.102450E-06
NUrea	FTFE	1	1.987231E-03	1.987700E-06
NUrea	CTFE	1	2.801347E-03	3.651405E-06
NUrea	CHTFE	1	4.880644E-03	1.009155E-05
NUrea	OTFE	1	2.753867E-03	2.438908E-06
NUrea	CUrea	1	4.047767E-03	7.327457E-06
NUrea	OUrea	1	2.815244E-03	2.506291E-06
NUrea	NUrea	1	3.352757E-03	3.950951E-06
CH3p	O	1	3.937017E-03	2.114674E-06
CH3p	OM	1	3.937017E-03	2.114674E-06
CH3p	OA	1	3.937017E-03	2.762755E-06
CH3p	OE	1	3.937017E-03	2.762755E-06
CH3p	OW	1	4.235025E-03	3.985734E-06
CH3p	N	1	4.086021E-03	3.194972E-06
CH3p	NT	1	4.086021E-03	3.194972E-06
CH3p	NL	1	4.086021E-03	3.194972E-06
CH3p	NR	1	4.086021E-03	3.194972E-06
CH3p	NZ	1	4.086021E-03	3.194972E-06
CH3p	NE	1	4.086021E-03	3.194972E-06
CH3p	C	1	4.004896E-03	4.511272E-06

CH3p CH0	1	4.004896E-03	4.511272E-06
CH3p CH1	1	4.466809E-03	4.747027E-06
CH3p CH2	1	5.689469E-03	5.347702E-06
CH3p CH3	1	6.852528E-03	6.030865E-06
CH3p CH4	1	9.503144E-03	1.439579E-05
CH3p CH2r	1	5.689469E-03	5.347702E-06
CH3p CR1	1	6.154693E-03	7.087387E-06
CH3p HC	1	7.615760E-04	3.020612E-07
CH3p H	1	0.000000E+00	0.000000E+00
CH3p DUM	1	0.000000E+00	0.000000E+00
CH3p S	1	8.271378E-03	8.880108E-06
CH3p CU1+	1	1.692851E-03	1.758094E-07
CH3p CU2+	1	1.692851E-03	1.758094E-07
CH3p FE	1	0.000000E+00	0.000000E+00
CH3p ZN2+	1	1.692851E-03	2.386038E-07
CH3p MG2+	1	6.688624E-04	1.433686E-07
CH3p CA2+	1	2.624126E-03	1.733045E-06
CH3p P	1	1.004949E-02	1.156919E-05
CH3p AR	1	6.552037E-03	7.706244E-06
CH3p F	1	2.841010E-03	2.141933E-06
CH3p CL	1	7.749864E-03	9.604563E-06
CH3p BR	1	1.376631E-02	1.987219E-05
CH3p CMet	1	7.798704E-03	1.080544E-05
CH3p OMet	1	3.937017E-03	3.745068E-06
CH3p NA+	1	7.350202E-04	6.630611E-07
CH3p CL-	1	9.369040E-03	1.909616E-05
CH3p CChl	1	4.245952E-03	4.950857E-06
CH3p CLChl	1	7.544652E-03	9.111197E-06
CH3p HChl	1	5.082692E-04	1.610354E-07
CH3p SDmso	1	8.507301E-03	1.138648E-05

CH3p	CDmso	1	8.116579E-03	1.267675E-05
CH3p	ODmso	1	3.944633E-03	2.128819E-06
CH3p	CCl4	1	4.245952E-03	6.770100E-06
CH3p	CLCl4	1	7.218499E-03	8.775000E-06
CH3p	FTFE	1	2.841010E-03	2.455782E-06
CH3p	CTFE	1	4.004896E-03	4.511272E-06
CH3p	CHTFE	1	6.977526E-03	1.246801E-05
CH3p	OTFE	1	3.937017E-03	3.013245E-06
CH3p	CUrea	1	5.786819E-03	9.052995E-06
CH3p	OUrea	1	4.024764E-03	3.096496E-06
CH3p	NUrea	1	4.793210E-03	4.881358E-06
CH3p	CH3p	1	6.852528E-03	6.030865E-06
Sl	O	1	5.773784E-03	4.056642E-06
Sl	OM	1	5.773784E-03	4.056642E-06
Sl	OA	1	5.773784E-03	5.299875E-06
Sl	OE	1	5.773784E-03	5.299875E-06
Sl	OW	1	6.210824E-03	7.645953E-06
Sl	N	1	5.992304E-03	6.129011E-06
Sl	NT	1	5.992304E-03	6.129011E-06
Sl	NL	1	5.992304E-03	6.129011E-06
Sl	NR	1	5.992304E-03	6.129011E-06
Sl	NZ	1	5.992304E-03	6.129011E-06
Sl	NE	1	5.992304E-03	6.129011E-06
Sl	C	1	5.873332E-03	8.654107E-06
Sl	CH0	1	5.873332E-03	8.654107E-06
Sl	CH1	1	6.550744E-03	9.106363E-06
Sl	CH2	1	8.343822E-03	1.025866E-05
Sl	CH3	1	1.004949E-02	1.156919E-05
Sl	CH4	1	1.393672E-02	2.761588E-05
Sl	CH2r	1	8.343822E-03	1.025866E-05

SI CR1 1 9.026090E-03 1.359595E-05

SI HC 1 1.116880E-03 5.794530E-07

SI H 1 0.000000E+00 0.000000E+00

SI DUM 1 0.000000E+00 0.000000E+00

SI S 1 1.213029E-02 1.703498E-05

SI CU1+ 1 2.482630E-03 3.372605E-07

SI CU2+ 1 2.482630E-03 3.372605E-07

SI FE 1 0.000000E+00 0.000000E+00

SI ZN2+ 1 2.482630E-03 4.577208E-07

SI MG2+ 1 9.809120E-04 2.750282E-07

SI CA2+ 1 3.848380E-03 3.324553E-06

SI P 1 1.473796E-02 2.219352E-05

SI AR 1 9.608810E-03 1.478312E-05

SI F 1 4.166448E-03 4.108934E-06

SI CL 1 1.136547E-02 1.842472E-05

SI BR 1 2.018882E-02 3.812141E-05

SI CMet 1 1.143709E-02 2.072840E-05

SI OMet 1 5.773784E-03 7.184275E-06

SI NA+ 1 1.077935e-03 1.271970e-06

SI CL- 1 1.374005e-02 3.663274e-05

SI CChl 1 6.226849E-03 9.497376E-06

SI CLChl 1 1.106452E-02 1.747828E-05

SI HChl 1 7.453960E-04 3.089191E-07

SI SDmso 1 1.247628E-02 2.184302E-05

SI CDmso 1 1.190327E-02 2.431818E-05

SI ODmso 1 5.784953E-03 4.083778E-06

SI CCl4 1 6.226849E-03 1.298729E-05

SI CLCl4 1 1.058620E-02 1.683335E-05

SI FTFE 1 4.166448E-03 4.711000E-06

SI CTFE 1 5.873332E-03 8.654107E-06

SI	CHTFE	1	1.023281E-02	2.391775E-05
SI	OTFE	1	5.773784E-03	5.780397E-06
SI	CUrea	1	8.486588E-03	1.736663E-05
SI	OUrea	1	5.902468E-03	5.940100E-06
SI	NUrea	1	7.029424E-03	9.364055E-06
SI	CH3p	1	1.004949E-02	1.156919E-05
SI	SI	1	1.473796E-02	2.219352E-05
CLCl4	I	1	0.0186172	4.352158e-05
CLCl4	CLOpt	1	0.00716348	1.026223e-05
CLCl4	B	1	0.004218736	7.93965e-06
CLCl4	SE	1	0.008713024	1.292069e-05
CLCl4	HS14	1	0.00080224	4.395036e-07
CLCl4	CLAro	1	0.00716348	1.026223e-05
CLCl4	BROpt	1	0.01612677	3.9198e-05
CLCl4	OEOpt	1	0.004846576	7.807442e-06
CLCl4	NOpt	1	0.00792648	1.929528e-05
CLCl4	CAro	1	0.004218736	7.543025e-06
CLCl4	CPos	1	0.003924	3.5732e-06
CLCl4	NPri	1	0.0090688	2.50124e-05
CLCl4	NTer	1	0.00810088	1.60794e-05
CLCl4	OAlc	1	0.003673736	4.484723e-06
CUrea	I	1	0.01492578	4.490035e-05
CUrea	CLOpt	1	0.005743107	1.058734e-05
CUrea	B	1	0.003382246	8.191181e-06
CUrea	SE	1	0.006985407	1.333002e-05
CUrea	HS14	1	0.000643172	4.534272e-07
CUrea	CLAro	1	0.005743107	1.058734e-05
CUrea	BROpt	1	0.01292916	4.043981e-05
CUrea	OEOpt	1	0.003885598	8.054784e-06
CUrea	NOpt	1	0.006354819	1.990656e-05

CUrea	CAro 1	0.003382246	7.78199e-06
CUrea	CPos 1	0.00314595	3.6864e-06
CUrea	NPri 1	0.00727064	2.58048e-05
CUrea	NTer 1	0.006494639	1.65888e-05
CUrea	OAlc 1	0.002945308	4.626801e-06
CU2+	I 1	0.004366075	8.719662e-07
CU2+	CLOpt 1	0.001679968	2.056065e-07
CU2+	B 1	0.000989371	1.59073e-07
CU2+	SE 1	0.002043364	2.588694e-07
CU2+	HS14 1	0.00018814	8.80557e-09
CU2+	CLAro 1	0.001679968	2.056065e-07
CU2+	BROpt 1	0.003782023	7.853423e-07
CU2+	OEOpt 1	0.001136611	1.564241e-07
CU2+	NOpt 1	0.001858905	3.86586e-07
CU2+	CAro 1	0.000989371	1.511265e-07
CU2+	CPos 1	0.00092025	7.159e-08
CU2+	NPri 1	0.0021268	5.0113e-07
CU2+	NTer 1	0.001899805	3.22155e-07
CU2+	OAlc 1	0.0008615585	8.985261e-08
ZN2+	I 1	0.004366075	1.183409e-06
ZN2+	CLOpt 1	0.001679968	2.790435e-07
ZN2+	B 1	0.000989371	2.158895e-07
ZN2+	SE 1	0.002043364	3.513306e-07
ZN2+	HS14 1	0.00018814	1.195068e-08
ZN2+	CLAro 1	0.001679968	2.790435e-07
ZN2+	BROpt 1	0.003782023	1.065845e-06
ZN2+	OEOpt 1	0.001136611	2.122946e-07
ZN2+	NOpt 1	0.001858905	5.24664e-07
ZN2+	CAro 1	0.000989371	2.051048e-07
ZN2+	CPos 1	0.00092025	9.716e-08

ZN2+	NPri 1	0.0021268	6.8012e-07
ZN2+	NTer 1	0.001899805	4.3722e-07
ZN2+	OAlc 1	0.0008615585	1.219455e-07
O	I 1	0.01015406	1.04882e-05
O	CLOpt 1	0.003907054	2.473079e-06
O	B 1	0.002300953	1.913364e-06
O	SE 1	0.004752195	3.113738e-06
O	HS14 1	0.000437552	1.059153e-07
O	CLAro 1	0.003907054	2.473079e-06
O	BROpt 1	0.008795746	9.446267e-06
O	OEOpt 1	0.002643385	1.881503e-06
O	NOpt 1	0.004323204	4.64994e-06
O	CAro 1	0.002300953	1.817782e-06
O	CPos 1	0.0021402	8.611e-07
O	NPri 1	0.00494624	6.0277e-06
O	NTer 1	0.004418324	3.87495e-06
O	OAlc 1	0.002003703	1.080767e-06
NR	I 1	0.01053836	1.584618e-05
NR	CLOpt 1	0.004054924	3.736472e-06
NR	B 1	0.002388037	2.890822e-06
NR	SE 1	0.004932051	4.704416e-06
NR	HS14 1	0.000454112	1.60023e-07
NR	CLAro 1	0.004054924	3.736472e-06
NR	BROpt 1	0.009128638	1.427197e-05
NR	OEOpt 1	0.002743429	2.842685e-06
NR	NOpt 1	0.004486824	7.0254e-06
NR	CAro 1	0.002388037	2.746411e-06
NR	CPos 1	0.0022212	1.301e-06
NR	NPri 1	0.00513344	9.107e-06
NR	NTer 1	0.004585544	5.8545e-06

NR	OAlc 1	0.002079537	1.632885e-06
ODmso	I 1	0.01017327	1.055835e-05
ODmso	CLOpt 1	0.003914448	2.489622e-06
ODmso	B 1	0.002305307	1.926163e-06
ODmso	SE 1	0.004761188	3.134566e-06
ODmso	HS14 1	0.00043838	1.066238e-07
ODmso	CLAro 1	0.003914448	2.489622e-06
ODmso	BROpt 1	0.008812391	9.509454e-06
ODmso	OEOpt 1	0.002648387	1.894089e-06
ODmso	NOpt 1	0.004331385	4.681044e-06
ODmso	CAro 1	0.002305307	1.829941e-06
ODmso	CPos 1	0.00214425	8.6686e-07
ODmso	NPri 1	0.0049556	6.06802e-06
ODmso	NTer 1	0.004426685	3.90087e-06
ODmso	OAlc 1	0.002007495	1.087996e-06
HChl	I 1	0.00131089	7.986913e-07
HChl	CLOpt 1	0.000504401	1.883285e-07
HChl	B 1	0.0002970532	1.457054e-07
HChl	SE 1	0.0006135088	2.371156e-07
HChl	HS14 1	5.6488e-05	8.065602e-09
HChl	CLAro 1	0.000504401	1.883285e-07
HChl	BROpt 1	0.001135532	7.193468e-07
HChl	OEOpt 1	0.0003412612	1.432792e-07
HChl	NOpt 1	0.000558126	3.540996e-07
HChl	CAro 1	0.0002970532	1.384267e-07
HChl	CPos 1	0.0002763	6.5574e-08
HChl	NPri 1	0.00063856	4.59018e-07
HChl	NTer 1	0.000570406	2.95083e-07
HChl	OAlc 1	0.0002586782	8.230193e-08
CL-	I 1	0.02416393	9.471168e-05

CL-	CLOpt 1	0.009297737	2.233267e-05
CL-	B 1	0.005475648	1.727827e-05
CL-	SE 1	0.01130895	2.811802e-05
CL-	HS14 1	0.001041256	9.56448e-07
CL-	CLAro 1	0.009297737	2.233267e-05
CL-	BROpt 1	0.02093151	8.530272e-05
CL-	OEOpt 1	0.006290544	1.699056e-05
CL-	NOpt 1	0.01028806	4.19904e-05
CL-	CAro 1	0.005475648	1.641514e-05
CL-	CPos 1	0.0050931	7.776e-06
CL-	NPri 1	0.01177072	5.4432e-05
CL-	NTer 1	0.01051442	3.4992e-05
CL-	OAlc 1	0.004768273	9.759658e-06
CCl4	I 1	0.01095041	3.357782e-05
CCl4	CLOpt 1	0.004213474	7.91753e-06
CCl4	B 1	0.00248141	6.12561e-06
CCl4	SE 1	0.005124897	9.968589e-06
CCl4	HS14 1	0.000471868	3.390864e-07
CCl4	CLAro 1	0.004213474	7.91753e-06
CCl4	BROpt 1	0.009485573	3.02421e-05
CCl4	OEOpt 1	0.002850698	6.023608e-06
CCl4	NOpt 1	0.004662261	1.488672e-05
CCl4	CAro 1	0.00248141	5.819605e-06
CCl4	CPos 1	0.00230805	2.7568e-06
CCl4	NPri 1	0.00533416	1.92976e-05
CCl4	NTer 1	0.004764841	1.24056e-05
CCl4	OAlc 1	0.002160848	3.46006e-06
CChl	I 1	0.01095041	2.455488e-05
CChl	CLOpt 1	0.004213474	5.789952e-06
CChl	B 1	0.00248141	4.479552e-06

CChl	SE	1	0.005124897	7.289856e-06
CChl	HS14	1	0.000471868	2.47968e-07
CChl	CLAro	1	0.004213474	5.789952e-06
CChl	BROpt	1	0.009485573	2.211552e-05
CChl	OEOpt	1	0.002850698	4.40496e-06
CChl	NOpt	1	0.004662261	1.08864e-05
CChl	CAro	1	0.00248141	4.255776e-06
CChl	CPos	1	0.00230805	2.016e-06
CChl	NPri	1	0.00533416	1.4112e-05
CChl	NTer	1	0.004764841	9.072e-06
CChl	OAlc	1	0.002160848	2.530282e-06
OE	I	1	0.01015406	1.37025e-05
OE	CLOpt	1	0.003907054	3.231e-06
OE	B	1	0.002300953	2.49975e-06
OE	SE	1	0.004752195	4.068e-06
OE	HS14	1	0.000437552	1.38375e-07
OE	CLAro	1	0.003907054	3.231e-06
OE	BROpt	1	0.008795746	1.234125e-05
OE	OEOpt	1	0.002643385	2.458125e-06
OE	NOpt	1	0.004323204	6.075e-06
OE	CAro	1	0.002300953	2.374875e-06
OE	CPos	1	0.0021402	1.125e-06
OE	NPri	1	0.00494624	7.875e-06
OE	NTer	1	0.004418324	5.0625e-06
OE	OAlc	1	0.002003703	1.411987e-06
C	I	1	0.01032913	2.237466e-05
C	CLOpt	1	0.003974417	5.275864e-06
C	B	1	0.002340624	4.081814e-06
C	SE	1	0.00483413	6.642592e-06
C	HS14	1	0.000445096	2.25951e-07

C	CLAro	1	0.003974417	5.275864e-06
C	BROpt	1	0.008947397	2.015189e-05
C	OEOpt	1	0.00268896	4.013845e-06
C	NOpt	1	0.004397742	9.9198e-06
C	CAro	1	0.002340624	3.877907e-06
C	CPos	1	0.0021771	1.837e-06
C	NPri	1	0.00503152	1.2859e-05
C	NTer	1	0.004494502	8.2665e-06
C	OAlc	1	0.002038249	2.305619e-06
BR	I	1	0.03550505	9.856056e-05
BR	CLOpt	1	0.01366155	2.324022e-05
BR	B	1	0.008045594	1.798042e-05
BR	SE	1	0.0166167	2.926067e-05
BR	HS14	1	0.00152996	9.95316e-07
BR	CLAro	1	0.01366155	2.324022e-05
BR	BROpt	1	0.03075552	8.876924e-05
BR	OEOpt	1	0.009242954	1.768102e-05
BR	NOpt	1	0.01511667	4.36968e-05
BR	CAro	1	0.008045594	1.708221e-05
BR	CPos	1	0.0074835	8.092e-06
BR	NPri	1	0.0172952	5.6644e-05
BR	NTer	1	0.01544927	3.6414e-05
BR	OAlc	1	0.007006219	1.015627e-05
NUrea	I	1	0.01236165	2.421019e-05
NUrea	CLOpt	1	0.004756485	5.708674e-06
NUrea	B	1	0.002801202	4.416669e-06
NUrea	SE	1	0.005785368	7.187523e-06
NUrea	HS14	1	0.00053268	2.444871e-07
NUrea	CLAro	1	0.004756485	5.708674e-06
NUrea	BROpt	1	0.01070803	2.180507e-05

NUrea	OEOpt 1	0.003218082	4.343124e-06
NUrea	NOpt 1	0.00526311	1.073358e-05
NUrea	CAro 1	0.002801202	4.196035e-06
NUrea	CPos 1	0.0026055	1.9877e-06
NUrea	NPri 1	0.0060216	1.39139e-05
NUrea	NTer 1	0.00537891	8.94465e-06
NUrea	OAlc 1	0.002439327	2.494762e-06
NT	I 1	0.01053836	1.584618e-05
NT	CLOpt 1	0.004054924	3.736472e-06
NT	B 1	0.002388037	2.890822e-06
NT	SE 1	0.004932051	4.704416e-06
NT	HS14 1	0.000454112	1.60023e-07
NT	CLAro 1	0.004054924	3.736472e-06
NT	BROpt 1	0.009128638	1.427197e-05
NT	OEOpt 1	0.002743429	2.842685e-06
NT	NOpt 1	0.004486824	7.0254e-06
NT	CAro 1	0.002388037	2.746411e-06
NT	CPos 1	0.0022212	1.301e-06
NT	NPri 1	0.00513344	9.107e-06
NT	NTer 1	0.004585544	5.8545e-06
NT	OAlc 1	0.002079537	1.632885e-06
CR1	I 1	0.01587372	3.515148e-05
CR1	CLOpt 1	0.006107853	8.288592e-06
CR1	B 1	0.003597053	6.412692e-06
CR1	SE 1	0.007429052	1.043578e-05
CR1	HS14 1	0.00068402	3.54978e-07
CR1	CLAro 1	0.006107853	8.288592e-06
CR1	BROpt 1	0.01375029	3.165942e-05
CR1	OEOpt 1	0.004132373	6.30591e-06
CR1	NOpt 1	0.006758415	1.55844e-05

CR1	CAro 1	0.003597053	6.092346e-06
CR1	CPos 1	0.00334575	2.886e-06
CR1	NPri 1	0.0077324	2.0202e-05
CR1	NTer 1	0.006907115	1.2987e-05
CR1	OAlc 1	0.003132365	3.622219e-06
S	I 1	0.02133292	4.404288e-05
S	CLOpt 1	0.008208428	1.038515e-05
S	B 1	0.00483413	8.034752e-06
S	SE 1	0.009984006	1.307546e-05
S	HS14 1	0.000919264	4.44768e-07
S	CLAro 1	0.008208428	1.038515e-05
S	BROpt 1	0.0184792	3.966752e-05
S	OEOpt 1	0.005553554	7.90096e-06
S	NOpt 1	0.009082728	1.95264e-05
S	CAro 1	0.00483413	7.633376e-06
S	CPos 1	0.0044964	3.616e-06
S	NPri 1	0.01039168	2.5312e-05
S	NTer 1	0.009282568	1.6272e-05
S	OAlc 1	0.00420963	4.538442e-06
CH3p	I 1	0.01767353	2.991164e-05
CH3p	CLOpt 1	0.006800377	7.053058e-06
CH3p	B 1	0.004004896	5.456788e-06
CH3p	SE 1	0.008271378	8.880173e-06
CH3p	HS14 1	0.000761576	3.020634e-07
CH3p	CLAro 1	0.006800377	7.053058e-06
CH3p	BROpt 1	0.01530933	2.694013e-05
CH3p	OEOpt 1	0.004600912	5.365923e-06
CH3p	NOpt 1	0.007524702	1.326132e-05
CH3p	CAro 1	0.004004896	5.184194e-06
CH3p	CPos 1	0.0037251	2.4558e-06

CH3p	NPri 1	0.00860912	1.71906e-05
CH3p	NTer 1	0.007690262	1.10511e-05
CH3p	OAlc 1	0.003487521	3.082275e-06
H	I 1	0	0
H	CLOpt 1	0	0
H	B 1	0	0
H	SE 1	0	0
H	HS14 1	0	0
H	CLAro 1	0	0
H	BROpt 1	0	0
H	OEOpt 1	0	0
H	NOpt 1	0	0
H	CAro 1	0	0
H	CPos 1	0	0
H	NPri 1	0	0
H	NTer 1	0	0
H	OAlc 1	0	0
CA2+	I 1	0.00676795	8.595426e-06
CA2+	CLOpt 1	0.002604155	2.02677e-06
CA2+	B 1	0.001533646	1.568065e-06
CA2+	SE 1	0.003167464	2.551811e-06
CA2+	HS14 1	0.00029164	8.68011e-08
CA2+	CLAro 1	0.002604155	2.02677e-06
CA2+	BROpt 1	0.005862598	7.741529e-06
CA2+	OEOpt 1	0.001761886	1.541954e-06
CA2+	NOpt 1	0.00288153	3.81078e-06
CA2+	CAro 1	0.001533646	1.489733e-06
CA2+	CPos 1	0.0014265	7.057e-07
CA2+	NPri 1	0.0032968	4.9399e-06
CA2+	NTer 1	0.00294493	3.17565e-06

CA2+	OAlc 1	0.001335521	8.857241e-07
F	I 1	0.00732732	1.06234e-05
F	CLOpt 1	0.002819388	2.504958e-06
F	B 1	0.001660402	1.938028e-06
F	SE 1	0.003429254	3.153875e-06
F	HS14 1	0.000315744	1.072806e-07
F	CLAro 1	0.002819388	2.504958e-06
F	BROpt 1	0.006347141	9.568034e-06
F	OEOpt 1	0.001907506	1.905757e-06
F	NOpt 1	0.003119688	4.70988e-06
F	CAro 1	0.001660402	1.841214e-06
F	CPos 1	0.0015444	8.722e-07
F	NPri 1	0.00356928	6.1054e-06
F	NTer 1	0.003188328	3.9249e-06
F	OAlc 1	0.001445902	1.094698e-06
N	I 1	0.01053836	1.584618e-05
N	CLOpt 1	0.004054924	3.736472e-06
N	B 1	0.002388037	2.890822e-06
N	SE 1	0.004932051	4.704416e-06
N	HS14 1	0.000454112	1.60023e-07
N	CLAro 1	0.004054924	3.736472e-06
N	BROpt 1	0.009128638	1.427197e-05
N	OEOpt 1	0.002743429	2.842685e-06
N	NOpt 1	0.004486824	7.0254e-06
N	CAro 1	0.002388037	2.746411e-06
N	CPos 1	0.0022212	1.301e-06
N	NPri 1	0.00513344	9.107e-06
N	NTer 1	0.004585544	5.8545e-06
N	OAlc 1	0.002079537	1.632885e-06
CH0	I 1	0.01032913	2.237466e-05

CH0	CLOpt	1	0.003974417	5.275864e-06
CH0	B	1	0.002340624	4.081814e-06
CH0	SE	1	0.00483413	6.642592e-06
CH0	HS14	1	0.000445096	2.25951e-07
CH0	CLAro	1	0.003974417	5.275864e-06
CH0	BROpt	1	0.008947397	2.015189e-05
CH0	OEOpt	1	0.00268896	4.013845e-06
CH0	NOpt	1	0.004397742	9.9198e-06
CH0	CAro	1	0.002340624	3.877907e-06
CH0	CPos	1	0.0021771	1.837e-06
CH0	NPri	1	0.00503152	1.2859e-05
CH0	NTer	1	0.004494502	8.2665e-06
CH0	OAlc	1	0.002038249	2.305619e-06
CLChl	I	1	0.01945839	4.518902e-05
CLChl	CLOpt	1	0.007487151	1.065541e-05
CLChl	B	1	0.004409353	8.243842e-06
CLChl	SE	1	0.009106709	1.341572e-05
CLChl	HS14	1	0.000838488	4.563423e-07
CLChl	CLAro	1	0.007487151	1.065541e-05
CLChl	BROpt	1	0.01685543	4.06998e-05
CLChl	OEOpt	1	0.005065561	8.106569e-06
CLChl	NOpt	1	0.008284626	2.003454e-05
CLChl	CAro	1	0.004409353	7.832021e-06
CLChl	CPos	1	0.0041013	3.7101e-06
CLChl	NPri	1	0.00947856	2.59707e-05
CLChl	NTer	1	0.008466906	1.669545e-05
CLChl	OAlc	1	0.003839728	4.656547e-06
FTFE	I	1	0.00732732	1.218e-05
FTFE	CLOpt	1	0.002819388	2.872e-06
FTFE	B	1	0.001660402	2.222e-06

FTFE	SE	1	0.003429254	3.616e-06
FTFE	HS14	1	0.000315744	1.23e-07
FTFE	CLAro	1	0.002819388	2.872e-06
FTFE	BROpt	1	0.006347141	1.097e-05
FTFE	OEOpt	1	0.001907506	2.185e-06
FTFE	NOpt	1	0.003119688	5.4e-06
FTFE	CAro	1	0.001660402	2.111e-06
FTFE	CPos	1	0.0015444	1e-06
FTFE	NPri	1	0.00356928	7e-06
FTFE	NTer	1	0.003188328	4.5e-06
FTFE	OAlc	1	0.001445902	1.2551e-06
SI	I	1	0.0259189	5.737998e-05
SI	CLOpt	1	0.00997301	1.352999e-05
SI	B	1	0.005873332	1.046784e-05
SI	SE	1	0.01213029	1.703498e-05
SI	HS14	1	0.00111688	5.79453e-07
SI	CLAro	1	0.00997301	1.352999e-05
SI	BROpt	1	0.02245172	5.167967e-05
SI	OEOpt	1	0.006747412	1.029353e-05
SI	NOpt	1	0.01103526	2.54394e-05
SI	CAro	1	0.005873332	9.944921e-06
SI	CPos	1	0.005463	4.711e-06
SI	NPri	1	0.0126256	3.2977e-05
SI	NTer	1	0.01127806	2.11995e-05
SI	OAlc	1	0.005114582	5.912776e-06
CDmso	I	1	0.02093367	6.287316e-05
CDmso	CLOpt	1	0.008054808	1.482526e-05
CDmso	B	1	0.004743659	1.146996e-05
CDmso	SE	1	0.009797156	1.866579e-05
CDmso	HS14	1	0.00090206	6.34926e-07

CDmso	CLAro	1	0.008054808	1.482526e-05
CDmso	BROpt	1	0.01813337	5.662714e-05
CDmso	OEOpt	1	0.005449619	1.127897e-05
CDmso	NOpt	1	0.008912745	2.78748e-05
CDmso	CAro	1	0.004743659	1.089698e-05
CDmso	CPos	1	0.00441225	5.162e-06
CDmso	NPri	1	0.0101972	3.6134e-05
CDmso	NTer	1	0.009108845	2.3229e-05
CDmso	OAlc	1	0.004130846	6.478826e-06
CH4	I	1	0.0245098	7.139916e-05
CH4	CLOpt	1	0.00943082	1.683566e-05
CH4	B	1	0.005554024	1.302536e-05
CH4	SE	1	0.01147082	2.119699e-05
CH4	HS14	1	0.00105616	7.21026e-07
CH4	CLAro	1	0.00943082	1.683566e-05
CH4	BROpt	1	0.02123111	6.430614e-05
CH4	OEOpt	1	0.006380584	1.280847e-05
CH4	NOpt	1	0.01043532	3.16548e-05
CH4	CAro	1	0.005554024	1.237468e-05
CH4	CPos	1	0.005166	5.862e-06
CH4	NPri	1	0.0119392	4.1034e-05
CH4	NTer	1	0.01066492	2.6379e-05
CH4	OAlc	1	0.004836524	7.357396e-06
FE	I	1	0	0
FE	CLOpt	1	0	0
FE	B	1	0	0
FE	SE	1	0	0
FE	HS14	1	0	0
FE	CLAro	1	0	0
FE	BROpt	1	0	0

FE	OEOpt	1	0	0
FE	NOpt	1	0	0
FE	CAro	1	0	0
FE	CPos	1	0	0
FE	NPri	1	0	0
FE	NTer	1	0	0
FE	OAlc	1	0	0
CTFE	I	1	0.01032913	2.237466e-05
CTFE	CLOpt	1	0.003974417	5.275864e-06
CTFE	B	1	0.002340624	4.081814e-06
CTFE	SE	1	0.00483413	6.642592e-06
CTFE	HS14	1	0.000445096	2.25951e-07
CTFE	CLAro	1	0.003974417	5.275864e-06
CTFE	BROpt	1	0.008947397	2.015189e-05
CTFE	OEOpt	1	0.00268896	4.013845e-06
CTFE	NOpt	1	0.004397742	9.9198e-06
CTFE	CAro	1	0.002340624	3.877907e-06
CTFE	CPos	1	0.0021771	1.837e-06
CTFE	NPri	1	0.00503152	1.2859e-05
CTFE	NTer	1	0.004494502	8.2665e-06
CTFE	OAlc	1	0.002038249	2.305619e-06
OA	I	1	0.01015406	1.37025e-05
OA	CLOpt	1	0.003907054	3.231e-06
OA	B	1	0.002300953	2.49975e-06
OA	SE	1	0.004752195	4.068e-06
OA	HS14	1	0.000437552	1.38375e-07
OA	CLAro	1	0.003907054	3.231e-06
OA	BROpt	1	0.008795746	1.234125e-05
OA	OEOpt	1	0.002643385	2.458125e-06
OA	NOpt	1	0.004323204	6.075e-06

OA	CAro	1	0.002300953	2.374875e-06
OA	CPos	1	0.0021402	1.125e-06
OA	NPri	1	0.00494624	7.875e-06
OA	NTer	1	0.004418324	5.0625e-06
OA	OAlc	1	0.002003703	1.411987e-06
OW	I	1	0.01092266	1.976814e-05
OW	CLOpt	1	0.004202794	4.661256e-06
OW	B	1	0.002475121	3.606306e-06
OW	SE	1	0.005111907	5.868768e-06
OW	HS14	1	0.000470672	1.99629e-07
OW	CLAro	1	0.004202794	4.661256e-06
OW	BROpt	1	0.00946153	1.780431e-05
OW	OEOpt	1	0.002843473	3.546255e-06
OW	NOpt	1	0.004650444	8.7642e-06
OW	CAro	1	0.002475121	3.426153e-06
OW	CPos	1	0.0023022	1.623e-06
OW	NPri	1	0.00532064	1.1361e-05
OW	NTer	1	0.004752764	7.3035e-06
OW	OAlc	1	0.002155371	2.037027e-06
CH2	I	1	0.01467385	2.652317e-05
CH2	CLOpt	1	0.00564617	6.254067e-06
CH2	B	1	0.003325157	4.838627e-06
CH2	SE	1	0.006867502	7.874202e-06
CH2	HS14	1	0.000632316	2.678448e-07
CH2	CLAro	1	0.00564617	6.254067e-06
CH2	BROpt	1	0.01271093	2.388827e-05
CH2	OEOpt	1	0.003820013	4.758056e-06
CH2	NOpt	1	0.006247557	1.175904e-05
CH2	CAro	1	0.003325157	4.596914e-06
CH2	CPos	1	0.00309285	2.1776e-06

CH2	NPri 1	0.00714792	1.52432e-05
CH2	NTer 1	0.006385017	9.7992e-06
CH2	OAlc 1	0.002895595	2.733106e-06
SDmso	I 1	0.02194139	5.647379e-05
SDmso	CLOpt 1	0.008442556	1.331632e-05
SDmso	B 1	0.004972013	1.030253e-05
SDmso	SE 1	0.01026878	1.676595e-05
SDmso	HS14 1	0.000945484	5.703018e-07
SDmso	CLAro 1	0.008442556	1.331632e-05
SDmso	BROpt 1	0.01900628	5.08635e-05
SDmso	OEOpt 1	0.005711957	1.013097e-05
SDmso	NOpt 1	0.009341793	2.503764e-05
SDmso	CAro 1	0.004972013	9.787863e-06
SDmso	CPos 1	0.00462465	4.6366e-06
SDmso	NPri 1	0.01068808	3.24562e-05
SDmso	NTer 1	0.009547333	2.08647e-05
SDmso	OAlc 1	0.0043297	5.819397e-06
DUM	I 1	0	0
DUM	CLOpt 1	0	0
DUM	B 1	0	0
DUM	SE 1	0	0
DUM	HS14 1	0	0
DUM	CLAro 1	0	0
DUM	BROpt 1	0	0
DUM	OEOpt 1	0	0
DUM	NOpt 1	0	0
DUM	CAro 1	0	0
DUM	CPos 1	0	0
DUM	NPri 1	0	0
DUM	NTer 1	0	0

DUM	OAlc	1	0	0
CH1	I	1	0.01152046	2.354394e-05
CH1	CLOpt	1	0.004432814	5.551576e-06
CH1	B	1	0.002610585	4.295126e-06
CH1	SE	1	0.005391683	6.989728e-06
CH1	HS14	1	0.000496432	2.37759e-07
CH1	CLAro	1	0.004432814	5.551576e-06
CH1	BROpt	1	0.009979362	2.120501e-05
CH1	OEOpt	1	0.002999097	4.223605e-06
CH1	NOpt	1	0.004904964	1.04382e-05
CH1	CAro	1	0.002610585	4.080563e-06
CH1	CPos	1	0.0024282	1.933e-06
CH1	NPri	1	0.00561184	1.3531e-05
CH1	NTer	1	0.005012884	8.6985e-06
CH1	OAlc	1	0.002273335	2.426108e-06
CHTFE	I	1	0.01799592	6.183786e-05
CHTFE	CLOpt	1	0.006924424	1.458114e-05
CHTFE	B	1	0.00407795	1.128109e-05
CHTFE	SE	1	0.008422257	1.835843e-05
CHTFE	HS14	1	0.000775468	6.24471e-07
CHTFE	CLAro	1	0.006924424	1.458114e-05
CHTFE	BROpt	1	0.01558859	5.569469e-05
CHTFE	OEOpt	1	0.004684838	1.109324e-05
CHTFE	NOpt	1	0.007661961	2.74158e-05
CHTFE	CAro	1	0.00407795	1.071755e-05
CHTFE	CPos	1	0.00379305	5.077e-06
CHTFE	NPri	1	0.00876616	3.5539e-05
CHTFE	NTer	1	0.007830541	2.28465e-05
CHTFE	OAlc	1	0.003551138	6.372143e-06
NL	I	1	0.01053836	1.584618e-05

NL	CLOpt	1	0.004054924	3.736472e-06
NL	B	1	0.002388037	2.890822e-06
NL	SE	1	0.004932051	4.704416e-06
NL	HS14	1	0.000454112	1.60023e-07
NL	CLAro	1	0.004054924	3.736472e-06
NL	BROpt	1	0.009128638	1.427197e-05
NL	OEOpt	1	0.002743429	2.842685e-06
NL	NOpt	1	0.004486824	7.0254e-06
NL	CAro	1	0.002388037	2.746411e-06
NL	CPos	1	0.0022212	1.301e-06
NL	NPri	1	0.00513344	9.107e-06
NL	NTer	1	0.004585544	5.8545e-06
NL	OAlc	1	0.002079537	1.632885e-06
AR	I	1	0.01689853	3.822084e-05
AR	CLOpt	1	0.006502172	9.012336e-06
AR	B	1	0.003829277	6.972636e-06
AR	SE	1	0.007908668	1.134701e-05
AR	HS14	1	0.00072818	3.85974e-07
AR	CLAro	1	0.006502172	9.012336e-06
AR	BROpt	1	0.014638	3.442386e-05
AR	OEOpt	1	0.004399157	6.85653e-06
AR	NOpt	1	0.007194735	1.69452e-05
AR	CAro	1	0.003829277	6.624318e-06
AR	CPos	1	0.00356175	3.138e-06
AR	NPri	1	0.0082316	2.1966e-05
AR	NTer	1	0.007353035	1.4121e-05
AR	OAlc	1	0.003334589	3.938504e-06
CH2r	I	1	0.01467385	2.652317e-05
CH2r	CLOpt	1	0.00564617	6.254067e-06
CH2r	B	1	0.003325157	4.838627e-06

CH2r	SE	1	0.006867502	7.874202e-06
CH2r	HS14	1	0.000632316	2.678448e-07
CH2r	CLAro	1	0.00564617	6.254067e-06
CH2r	BROpt	1	0.01271093	2.388827e-05
CH2r	OEOpt	1	0.003820013	4.758056e-06
CH2r	NOpt	1	0.006247557	1.175904e-05
CH2r	CAro	1	0.003325157	4.596914e-06
CH2r	CPos	1	0.00309285	2.1776e-06
CH2r	NPri	1	0.00714792	1.52432e-05
CH2r	NTer	1	0.006385017	9.7992e-06
CH2r	OAlc	1	0.002895595	2.733106e-06
NA+	I	1	0.00189588	3.2886e-06
NA+	CLOpt	1	0.000729492	7.7544e-07
NA+	B	1	0.0004296144	5.9994e-07
NA+	SE	1	0.0008872896	9.7632e-07
NA+	HS14	1	8.1696e-05	3.321e-08
NA+	CLAro	1	0.000729492	7.7544e-07
NA+	BROpt	1	0.001642267	2.9619e-06
NA+	OEOpt	1	0.0004935504	5.8995e-07
NA+	NOpt	1	0.000807192	1.458e-06
NA+	CAro	1	0.0004296144	5.6997e-07
NA+	CPos	1	0.0003996	2.7e-07
NA+	NPri	1	0.00092352	1.89e-06
NA+	NTer	1	0.000824952	1.215e-06
NA+	OAlc	1	0.0003741144	3.38877e-07
OTFE	I	1	0.01015406	1.494486e-05
OTFE	CLOpt	1	0.003907054	3.523944e-06
OTFE	B	1	0.002300953	2.726394e-06
OTFE	SE	1	0.004752195	4.436832e-06
OTFE	HS14	1	0.000437552	1.50921e-07

OTFE	CLAro 1	0.003907054	3.523944e-06
OTFE	BROpt 1	0.008795746	1.346019e-05
OTFE	OEOpt 1	0.002643385	2.680995e-06
OTFE	NOpt 1	0.004323204	6.6258e-06
OTFE	CAro 1	0.002300953	2.590197e-06
OTFE	CPos 1	0.0021402	1.227e-06
OTFE	NPri 1	0.00494624	8.589e-06
OTFE	NTer 1	0.004418324	5.5215e-06
OTFE	OAlc 1	0.002003703	1.540008e-06
OMet	I 1	0.01015406	1.85745e-05
OMet	CLOpt 1	0.003907054	4.3798e-06
OMet	B 1	0.002300953	3.38855e-06
OMet	SE 1	0.004752195	5.5144e-06
OMet	HS14 1	0.000437552	1.87575e-07
OMet	CLAro 1	0.003907054	4.3798e-06
OMet	BROpt 1	0.008795746	1.672925e-05
OMet	OEOpt 1	0.002643385	3.332125e-06
OMet	NOpt 1	0.004323204	8.235e-06
OMet	CAro 1	0.002300953	3.219275e-06
OMet	CPos 1	0.0021402	1.525e-06
OMet	NPri 1	0.00494624	1.0675e-05
OMet	NTer 1	0.004418324	6.8625e-06
OMet	OAlc 1	0.002003703	1.914028e-06
CU1+	I 1	0.004366075	8.719662e-07
CU1+	CLOpt 1	0.001679968	2.056065e-07
CU1+	B 1	0.000989371	1.59073e-07
CU1+	SE 1	0.002043364	2.588694e-07
CU1+	HS14 1	0.00018814	8.80557e-09
CU1+	CLAro 1	0.001679968	2.056065e-07
CU1+	BROpt 1	0.003782023	7.853423e-07

CU1+	OEOpt 1	0.001136611	1.564241e-07
CU1+	NOpt 1	0.001858905	3.86586e-07
CU1+	CAro 1	0.000989371	1.511265e-07
CU1+	CPos 1	0.00092025	7.159e-08
CU1+	NPri 1	0.0021268	5.0113e-07
CU1+	NTer 1	0.001899805	3.22155e-07
CU1+	OAlc 1	0.0008615585	8.985261e-08
OUrea	I 1	0.01038037	1.535776e-05
OUrea	CLOpt 1	0.003994133	3.621305e-06
OUrea	B 1	0.002352236	2.80172e-06
OUrea	SE 1	0.00485811	4.559414e-06
OUrea	HS14 1	0.000447304	1.550907e-07
OUrea	CLAro 1	0.003994133	3.621305e-06
OUrea	BROpt 1	0.008991783	1.383207e-05
OUrea	OEOpt 1	0.0027023	2.755066e-06
OUrea	NOpt 1	0.004419558	6.80886e-06
OUrea	CAro 1	0.002352236	2.66176e-06
OUrea	CPos 1	0.0021879	1.2609e-06
OUrea	NPri 1	0.00505648	8.8263e-06
OUrea	NTer 1	0.004516798	5.67405e-06
OUrea	OAlc 1	0.002048361	1.582556e-06
CMet	I 1	0.02011384	5.3592e-05
CMet	CLOpt 1	0.007739351	1.26368e-05
CMet	B 1	0.00455788	9.7768e-06
CMet	SE 1	0.009413463	1.59104e-05
CMet	HS14 1	0.000866732	5.412e-07
CMet	CLAro 1	0.007739351	1.26368e-05
CMet	BROpt 1	0.0174232	4.8268e-05
CMet	OEOpt 1	0.005236192	9.614e-06
CMet	NOpt 1	0.008563689	2.376e-05

CMet	CAro	1	0.00455788	9.2884e-06
CMet	CPos	1	0.00423945	4.4e-06
CMet	NPri	1	0.00979784	3.08e-05
CMet	NTer	1	0.008752109	1.98e-05
CMet	OAlc	1	0.003969067	5.52244e-06
NZ	I	1	0.01053836	1.584618e-05
NZ	CLOpt	1	0.004054924	3.736472e-06
NZ	B	1	0.002388037	2.890822e-06
NZ	SE	1	0.004932051	4.704416e-06
NZ	HS14	1	0.000454112	1.60023e-07
NZ	CLAro	1	0.004054924	3.736472e-06
NZ	BROpt	1	0.009128638	1.427197e-05
NZ	OEOpt	1	0.002743429	2.842685e-06
NZ	NOpt	1	0.004486824	7.0254e-06
NZ	CAro	1	0.002388037	2.746411e-06
NZ	CPos	1	0.0022212	1.301e-06
NZ	NPri	1	0.00513344	9.107e-06
NZ	NTer	1	0.004585544	5.8545e-06
NZ	OAlc	1	0.002079537	1.632885e-06
CH3	I	1	0.01767353	2.991164e-05
CH3	CLOpt	1	0.006800377	7.053058e-06
CH3	B	1	0.004004896	5.456788e-06
CH3	SE	1	0.008271378	8.880173e-06
CH3	HS14	1	0.000761576	3.020634e-07
CH3	CLAro	1	0.006800377	7.053058e-06
CH3	BROpt	1	0.01530933	2.694013e-05
CH3	OEOpt	1	0.004600912	5.365923e-06
CH3	NOpt	1	0.007524702	1.326132e-05
CH3	CAro	1	0.004004896	5.184194e-06
CH3	CPos	1	0.0037251	2.4558e-06

CH3	NPri 1	0.00860912	1.71906e-05
CH3	NTer 1	0.007690262	1.10511e-05
CH3	OAlc 1	0.003487521	3.082275e-06
P	I 1	0.0259189	5.737998e-05
P	CLOpt 1	0.00997301	1.352999e-05
P	B 1	0.005873332	1.046784e-05
P	SE 1	0.01213029	1.703498e-05
P	HS14 1	0.00111688	5.79453e-07
P	CLAro 1	0.00997301	1.352999e-05
P	BROpt 1	0.02245172	5.167967e-05
P	OEOpt 1	0.006747412	1.029353e-05
P	NOpt 1	0.01103526	2.54394e-05
P	CAro 1	0.005873332	9.944921e-06
P	CPos 1	0.005463	4.711e-06
P	NPri 1	0.0126256	3.2977e-05
P	NTer 1	0.01127806	2.11995e-05
P	OAlc 1	0.005114582	5.912776e-06
NE	I 1	0.01053836	1.584618e-05
NE	CLOpt 1	0.004054924	3.736472e-06
NE	B 1	0.002388037	2.890822e-06
NE	SE 1	0.004932051	4.704416e-06
NE	HS14 1	0.000454112	1.60023e-07
NE	CLAro 1	0.004054924	3.736472e-06
NE	BROpt 1	0.009128638	1.427197e-05
NE	OEOpt 1	0.002743429	2.842685e-06
NE	NOpt 1	0.004486824	7.0254e-06
NE	CAro 1	0.002388037	2.746411e-06
NE	CPos 1	0.0022212	1.301e-06
NE	NPri 1	0.00513344	9.107e-06
NE	NTer 1	0.004585544	5.8545e-06

NE	OAlc 1	0.002079537	1.632885e-06
MG2+	I 1	0.00172508	7.110684e-07
MG2+	CLOpt 1	0.000663772	1.676674e-07
MG2+	B 1	0.0003909104	1.297204e-07
MG2+	SE 1	0.0008073536	2.111021e-07
MG2+	HS14 1	7.4336e-05	7.18074e-09
MG2+	CLAro 1	0.000663772	1.676674e-07
MG2+	BROpt 1	0.001494315	6.404286e-07
MG2+	OEOpt 1	0.0004490864	1.275603e-07
MG2+	NOpt 1	0.000734472	3.15252e-07
MG2+	CAro 1	0.0003909104	1.232402e-07
MG2+	CPos 1	0.0003636	5.838e-08
MG2+	NPri 1	0.00084032	4.0866e-07
MG2+	NTer 1	0.000750632	2.6271e-07
MG2+	OAlc 1	0.0003404104	7.327274e-08
CL	I 1	0.01998787	4.763598e-05
CL	CLOpt 1	0.007690883	1.123239e-05
CL	B 1	0.004529336	8.690242e-06
CL	SE 1	0.00935451	1.414218e-05
CL	HS14 1	0.000861304	4.81053e-07
CL	CLAro 1	0.007690883	1.123239e-05
CL	BROpt 1	0.01731408	4.290367e-05
CL	OEOpt 1	0.0052034	8.545535e-06
CL	NOpt 1	0.008510058	2.11194e-05
CL	CAro 1	0.004529336	8.256121e-06
CL	CPos 1	0.0042129	3.911e-06
CL	NPri 1	0.00973648	2.7377e-05
CL	NTer 1	0.008697298	1.75995e-05
CL	OAlc 1	0.003944211	4.908696e-06
OM	I 1	0.01015406	1.04882e-05

OM	CLOpt 1	0.003907054	2.473079e-06
OM	B 1	0.002300953	1.913364e-06
OM	SE 1	0.004752195	3.113738e-06
OM	HS14 1	0.000437552	1.059153e-07
OM	CLAro 1	0.003907054	2.473079e-06
OM	BROpt 1	0.008795746	9.446267e-06
OM	OEOpt 1	0.002643385	1.881503e-06
OM	NOpt 1	0.004323204	4.64994e-06
OM	CAro 1	0.002300953	1.817782e-06
OM	CPos 1	0.0021402	8.611e-07
OM	NPri 1	0.00494624	6.0277e-06
OM	NTer 1	0.004418324	3.87495e-06
OM	OAlc 1	0.002003703	1.080767e-06
HC	I 1	0.0019642	1.49814e-06
HC	CLOpt 1	0.00075578	3.53256e-07
HC	B 1	0.000445096	2.73306e-07
HC	SE 1	0.000919264	4.44768e-07
HC	HS14 1	8.464e-05	1.5129e-08
HC	CLAro 1	0.00075578	3.53256e-07
HC	BROpt 1	0.001701448	1.34931e-06
HC	OEOpt 1	0.000511336	2.68755e-07
HC	NOpt 1	0.00083628	6.642e-07
HC	CAro 1	0.000445096	2.59653e-07
HC	CPos 1	0.000414	1.23e-07
HC	NPri 1	0.0009568	8.61e-07
HC	NTer 1	0.00085468	5.535e-07
HC	OAlc 1	0.000387596	1.543773e-07
I	I 1	0.04558225	0.0001483524
I	CLOpt 1	0.01753902	3.498096e-05
I	B 1	0.01032913	2.706396e-05

I	SE	1	0.02133292	4.404288e-05
I	HS14	1	0.0019642	1.49814e-06
I	CLAro	1	0.01753902	3.498096e-05
I	BROpt	1	0.03948469	0.0001336146
I	OEOpt	1	0.01186633	2.66133e-05
I	NOpt	1	0.01940715	6.5772e-05
I	CAro	1	0.01032913	2.571198e-05
I	CPos	1	0.0096075	1.218e-05
I	NPri	1	0.022204	8.526e-05
I	NTer	1	0.01983415	5.481e-05
I	OAlc	1	0.008994755	1.528712e-05
CLOpt	I	1	0.01753902	3.498096e-05
CLOpt	CLOpt	1	0.006748622	8.248384e-06
CLOpt	B	1	0.003974417	6.381584e-06
CLOpt	SE	1	0.008208428	1.038515e-05
CLOpt	HS14	1	0.00075578	3.53256e-07
CLOpt	CLAro	1	0.006748622	8.248384e-06
CLOpt	BROpt	1	0.01519282	3.150584e-05
CLOpt	OEOpt	1	0.004565897	6.27532e-06
CLOpt	NOpt	1	0.007467435	1.55088e-05
CLOpt	CAro	1	0.003974417	6.062792e-06
CLOpt	CPos	1	0.00369675	2.872e-06
CLOpt	NPri	1	0.0085436	2.0104e-05
CLOpt	NTer	1	0.007631735	1.2924e-05
CLOpt	OAlc	1	0.00346098	3.604647e-06
B	I	1	0.01032913	2.706396e-05
B	CLOpt	1	0.003974417	6.381584e-06
B	B	1	0.002340624	4.937284e-06
B	SE	1	0.00483413	8.034752e-06
B	HS14	1	0.000445096	2.73306e-07

B	CLAro	1	0.003974417	6.381584e-06
B	BROpt	1	0.008947397	2.437534e-05
B	OEOpt	1	0.00268896	4.85507e-06
B	NOpt	1	0.004397742	1.19988e-05
B	CAro	1	0.002340624	4.690642e-06
B	CPos	1	0.0021771	2.222e-06
B	NPri	1	0.00503152	1.5554e-05
B	NTer	1	0.004494502	9.999e-06
B	OAlc	1	0.002038249	2.788832e-06
SE	I	1	0.02133292	4.404288e-05
SE	CLOpt	1	0.008208428	1.038515e-05
SE	B	1	0.00483413	8.034752e-06
SE	SE	1	0.009984006	1.307546e-05
SE	HS14	1	0.000919264	4.44768e-07
SE	CLAro	1	0.008208428	1.038515e-05
SE	BROpt	1	0.0184792	3.966752e-05
SE	OEOpt	1	0.005553554	7.90096e-06
SE	NOpt	1	0.009082728	1.95264e-05
SE	CAro	1	0.00483413	7.633376e-06
SE	CPos	1	0.0044964	3.616e-06
SE	NPri	1	0.01039168	2.5312e-05
SE	NTer	1	0.009282568	1.6272e-05
SE	OAlc	1	0.00420963	4.538442e-06
HS14	I	1	0.0019642	1.49814e-06
HS14	CLOpt	1	0.00075578	3.53256e-07
HS14	B	1	0.000445096	2.73306e-07
HS14	SE	1	0.000919264	4.44768e-07
HS14	HS14	1	8.464e-05	1.5129e-08
HS14	CLAro	1	0.00075578	3.53256e-07
HS14	BROpt	1	0.001701448	1.34931e-06

HS14	OEOpt 1	0.000511336	2.68755e-07
HS14	NOpt 1	0.00083628	6.642e-07
HS14	CAro 1	0.000445096	2.59653e-07
HS14	CPos 1	0.000414	1.23e-07
HS14	NPri 1	0.0009568	8.61e-07
HS14	NTer 1	0.00085468	5.535e-07
HS14	OAlc 1	0.000387596	1.543773e-07
CLAro	I 1	0.01753902	3.498096e-05
CLAro	CLOpt 1	0.006748622	8.248384e-06
CLAro	B 1	0.003974417	6.381584e-06
CLAro	SE 1	0.008208428	1.038515e-05
CLAro	HS14 1	0.00075578	3.53256e-07
CLAro	CLAro 1	0.006748622	8.248384e-06
CLAro	BROpt 1	0.01519282	3.150584e-05
CLAro	OEOpt 1	0.004565897	6.27532e-06
CLAro	NOpt 1	0.007467435	1.55088e-05
CLAro	CAro 1	0.003974417	6.062792e-06
CLAro	CPos 1	0.00369675	2.872e-06
CLAro	NPri 1	0.0085436	2.0104e-05
CLAro	NTer 1	0.007631735	1.2924e-05
CLAro	OAlc 1	0.00346098	3.604647e-06
BROpt	I 1	0.03948469	0.0001336146
BROpt	CLOpt 1	0.01519282	3.150584e-05
BROpt	B 1	0.008947397	2.437534e-05
BROpt	SE 1	0.0184792	3.966752e-05
BROpt	HS14 1	0.001701448	1.34931e-06
BROpt	CLAro 1	0.01519282	3.150584e-05
BROpt	BROpt 1	0.0342028	0.0001203409
BROpt	OEOpt 1	0.01027897	2.396945e-05
BROpt	NOpt 1	0.01681105	5.9238e-05

BROpt	CAro 1	0.008947397	2.315767e-05
BROpt	CPos 1	0.0083223	1.097e-05
BROpt	NPri 1	0.01923376	7.679e-05
BROpt	NTer 1	0.01718093	4.9365e-05
BROpt	OAlc 1	0.007791522	1.376845e-05
OEOpt	I 1	0.01186633	2.66133e-05
OEOpt	CLOpt 1	0.004565897	6.27532e-06
OEOpt	B 1	0.00268896	4.85507e-06
OEOpt	SE 1	0.005553554	7.90096e-06
OEOpt	HS14 1	0.000511336	2.68755e-07
OEOpt	CLAro 1	0.004565897	6.27532e-06
OEOpt	BROpt 1	0.01027897	2.396945e-05
OEOpt	OEOpt 1	0.003089136	4.774225e-06
OEOpt	NOpt 1	0.005052222	1.1799e-05
OEOpt	CAro 1	0.00268896	4.612535e-06
OEOpt	CPos 1	0.0025011	2.185e-06
OEOpt	NPri 1	0.00578032	1.5295e-05
OEOpt	NTer 1	0.005163382	9.8325e-06
OEOpt	OAlc 1	0.002341585	2.742393e-06
NOpt	I 1	0.01940715	6.5772e-05
NOpt	CLOpt 1	0.007467435	1.55088e-05
NOpt	B 1	0.004397742	1.19988e-05
NOpt	SE 1	0.009082728	1.95264e-05
NOpt	HS14 1	0.00083628	6.642e-07
NOpt	CLAro 1	0.007467435	1.55088e-05
NOpt	BROpt 1	0.01681105	5.9238e-05
NOpt	OEOpt 1	0.005052222	1.1799e-05
NOpt	NOpt 1	0.00826281	2.916e-05
NOpt	CAro 1	0.004397742	1.13994e-05
NOpt	CPos 1	0.0040905	5.4e-06

NOpt	NPri 1	0.0094536	3.78e-05
NOpt	NTer 1	0.00844461	2.43e-05
NOpt	OAlc 1	0.003829617	6.77754e-06
CAro	I 1	0.01032913	2.571198e-05
CAro	CLOpt 1	0.003974417	6.062792e-06
CAro	B 1	0.002340624	4.690642e-06
CAro	SE 1	0.00483413	7.633376e-06
CAro	HS14 1	0.000445096	2.59653e-07
CAro	CLAro 1	0.003974417	6.062792e-06
CAro	BROpt 1	0.008947397	2.315767e-05
CAro	OEOpt 1	0.00268896	4.612535e-06
CAro	NOpt 1	0.004397742	1.13994e-05
CAro	CAro 1	0.002340624	4.456321e-06
CAro	CPos 1	0.0021771	2.111e-06
CAro	NPri 1	0.00503152	1.4777e-05
CAro	NTer 1	0.004494502	9.4995e-06
CAro	OAlc 1	0.002038249	2.649516e-06
CPos	I 1	0.0096075	1.218e-05
CPos	CLOpt 1	0.00369675	2.872e-06
CPos	B 1	0.0021771	2.222e-06
CPos	SE 1	0.0044964	3.616e-06
CPos	HS14 1	0.000414	1.23e-07
CPos	CLAro 1	0.00369675	2.872e-06
CPos	BROpt 1	0.0083223	1.097e-05
CPos	OEOpt 1	0.0025011	2.185e-06
CPos	NOpt 1	0.0040905	5.4e-06
CPos	CAro 1	0.0021771	2.111e-06
CPos	CPos 1	0.002025	1e-06
CPos	NPri 1	0.00468	7e-06
CPos	NTer 1	0.0041805	4.5e-06

CPos	OAlc	1	0.00189585	1.2551e-06
NPri	I	1	0.022204	8.526e-05
NPri	CLOpt	1	0.0085436	2.0104e-05
NPri	B	1	0.00503152	1.5554e-05
NPri	SE	1	0.01039168	2.5312e-05
NPri	HS14	1	0.0009568	8.61e-07
NPri	CLAro	1	0.0085436	2.0104e-05
NPri	BROpt	1	0.01923376	7.679e-05
NPri	OEOpt	1	0.00578032	1.5295e-05
NPri	NOpt	1	0.0094536	3.78e-05
NPri	CAro	1	0.00503152	1.4777e-05
NPri	CPos	1	0.00468	7e-06
NPri	NPri	1	0.010816	4.9e-05
NPri	NTer	1	0.0096616	3.15e-05
NPri	OAlc	1	0.00438152	8.7857e-06
NTer	I	1	0.01983415	5.481e-05
NTer	CLOpt	1	0.007631735	1.2924e-05
NTer	B	1	0.004494502	9.999e-06
NTer	SE	1	0.009282568	1.6272e-05
NTer	HS14	1	0.00085468	5.535e-07
NTer	CLAro	1	0.007631735	1.2924e-05
NTer	BROpt	1	0.01718093	4.9365e-05
NTer	OEOpt	1	0.005163382	9.8325e-06
NTer	NOpt	1	0.00844461	2.43e-05
NTer	CAro	1	0.004494502	9.4995e-06
NTer	CPos	1	0.0041805	4.5e-06
NTer	NPri	1	0.0096616	3.15e-05
NTer	NTer	1	0.00863041	2.025e-05
NTer	OAlc	1	0.003913877	5.64795e-06
OAlc	I	1	0.008994755	1.528712e-05

OAlc	CLOpt 1	0.00346098	3.604647e-06
OAlc	B 1	0.002038249	2.788832e-06
OAlc	SE 1	0.00420963	4.538442e-06
OAlc	HS14 1	0.000387596	1.543773e-07
OAlc	CLAro 1	0.00346098	3.604647e-06
OAlc	BROpt 1	0.007791522	1.376845e-05
OAlc	OEOpt 1	0.002341585	2.742393e-06
OAlc	NOpt 1	0.003829617	6.77754e-06
OAlc	CAro 1	0.002038249	2.649516e-06
OAlc	CPos 1	0.00189585	1.2551e-06
OAlc	NPri 1	0.00438152	8.7857e-06
OAlc	NTer 1	0.003913877	5.64795e-06
OAlc	OAlc 1	0.001774937	1.575276e-06