```
; penglb.itp
;
; b3lyp/6-31g(d) resp chearge.

#if defined WILLIAMS
; model W, Williams IV buckingham potential.
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ fudgeQQ
2               2               no              0.5     0.8333

[ atomtypes ]
;name            mass     charge  ptype   a             b           c
ha        ha      1.0080  0.0000  A     0.11104e+05   3.74000e+01   0.11422e-03
ca        ca     12.0100  0.0000  A     3.49908e+05   3.60000e+01   2.37651e-03

[ nonbond_params ]
; ai    aj      funct                   a             b           c
ha      ha      2                     0.11104e+05   3.74000e+01   0.11422e-03
ca      ca      2                     3.49908e+05   3.60000e+01   2.37651e-03
ca      ha      2                     0.36677e+05   3.67000e+01   0.52300e-03

[ pairtypes ]
; ai    aj      funct                     sigma       epsilon
ha      ha      1                       2.59964e-01  0.31380e-01
ca      ca      1                       3.39967e-01  1.79912e-01
ca      ha      1                       2.99966e-01  0.75137e-01
#elif defined YOKOI
; model Y, Yokoi95 buckingham potential.
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ fudgeQQ
2               2               no              0.5     0.8333

[ atomtypes ]
;name            mass     charge  ptype   a             b           c
ha        ha      1.0080  0.0000  A     0.34548e+05   4.09162e+01   0.16543e-03
ca        ca     12.0100  0.0000  A     5.91346e+07   5.25427e+01   1.89560e-03
```

```
[ nonbond_params ]
; ai    aj      funct                   a             b           c
ha      ha      2                   0.34548e+05   4.09162e+01   0.16543e-03
ca      ca      2                   5.91346e+07   5.25427e+01   1.89560e-03
ca      ha      2                   1.01672e+06   4.60820e+01   0.57773e-03

[ pairtypes ]
; ai    aj      funct                     sigma      epsilon
ha      ha      1                       2.59964e-01  0.31380e-01
ca      ca      1                       3.39967e-01  1.79912e-01
ca      ha      1                       2.99966e-01  0.75137e-01
#else
; model G, Genaral Amber Force Field (GAFF).

[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ fudgeQQ
1               2               yes             0.5     0.8333

[ atomtypes ]
;name  bond_type    mass    charge   ptype  sigma      epsilon
ha            ha      1.0080  0.0000  A   2.59964e-01  6.27600e-02
ca            ca     12.0100  0.0000  A   3.39967e-01  3.59824e-01
n1            n1     14.0100  0.0000  A   3.25000e-01  7.11280e-01
sio2          sio2   20.0300  0.0000  A   3.00000e-01  8.00000e-01 ; for surface
#endif

[ moleculetype ]
; Name            nrexcl
pentc             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
     1         ca      1    MOL     C0      1   -0.22144  12.0100
     2         ca      1    MOL     C1      1   -0.10233  12.0100
     3         ca      1    MOL     C2      2   -0.10233  12.0100
```

```
     4          ca       1    MOL      C3       2   -0.22144   12.0100
     5          ca       1    MOL      C4       3    0.16215   12.0100
     6          ca       1    MOL      C5       4    0.16215   12.0100
     7          ca       1    MOL      C6       3   -0.30138   12.0100
     8          ca       1    MOL      C7       5    0.12039   12.0100
     9          ca       1    MOL      C8       6    0.12039   12.0100
    10          ca       1    MOL      C9       4   -0.30138   12.0100
    11          ca       1    MOL     C10       6   -0.24767   12.0100
    12          ha       1    MOL      H0       1    0.13263    1.0080
    13          ha       1    MOL      H1       1    0.11701    1.0080
    14          ha       1    MOL      H2       2    0.11701    1.0080
    15          ha       1    MOL      H3       2    0.13263    1.0080
    16          ha       1    MOL      H4       3    0.14777    1.0080
    17          ha       1    MOL      H5       4    0.14777    1.0080
    18          ha       1    MOL      H6       6    0.13807    1.0080
    19          ca       1    MOL     C11       9   -0.22144   12.0100
    20          ca       1    MOL     C12       9   -0.10233   12.0100
    21          ca       1    MOL     C13      10   -0.10233   12.0100
    22          ca       1    MOL     C14      10   -0.22144   12.0100
    23          ca       1    MOL     C15       7    0.16215   12.0100
    24          ca       1    MOL     C16       8    0.16215   12.0100
    25          ca       1    MOL     C17       7   -0.30138   12.0100
    26          ca       1    MOL     C18       6    0.12039   12.0100
    27          ca       1    MOL     C19       5    0.12039   12.0100
    28          ca       1    MOL     C20       8   -0.30138   12.0100
    29          ca       1    MOL     C21       5   -0.24767   12.0100
    30          ha       1    MOL      H7       9    0.13263    1.0080
    31          ha       1    MOL      H8       9    0.11701    1.0080
    32          ha       1    MOL      H9      10    0.11701    1.0080
    33          ha       1    MOL     H10      10    0.13263    1.0080
    34          ha       1    MOL     H11       7    0.14777    1.0080
    35          ha       1    MOL     H12       8    0.14777    1.0080
    36          ha       1    MOL     H13       5    0.13807    1.0080

[ bonds ]
;  ai    aj funct   r   k
```

| | | | | |
|---|---|---|---|---|
| 1 | 12 | 1 | 1.0870e-01 | 2.8811e+05 |
| 2 | 13 | 1 | 1.0870e-01 | 2.8811e+05 |
| 3 | 14 | 1 | 1.0870e-01 | 2.8811e+05 |
| 4 | 15 | 1 | 1.0870e-01 | 2.8811e+05 |
| 7 | 16 | 1 | 1.0870e-01 | 2.8811e+05 |
| 10 | 17 | 1 | 1.0870e-01 | 2.8811e+05 |
| 11 | 18 | 1 | 1.0870e-01 | 2.8811e+05 |
| 19 | 30 | 1 | 1.0870e-01 | 2.8811e+05 |
| 20 | 31 | 1 | 1.0870e-01 | 2.8811e+05 |
| 21 | 32 | 1 | 1.0870e-01 | 2.8811e+05 |
| 22 | 33 | 1 | 1.0870e-01 | 2.8811e+05 |
| 25 | 34 | 1 | 1.0870e-01 | 2.8811e+05 |
| 28 | 35 | 1 | 1.0870e-01 | 2.8811e+05 |
| 29 | 36 | 1 | 1.0870e-01 | 2.8811e+05 |
| 1 | 2 | 1 | 1.3870e-01 | 4.0033e+05 |
| 1 | 6 | 1 | 1.3870e-01 | 4.0033e+05 |
| 2 | 3 | 1 | 1.3870e-01 | 4.0033e+05 |
| 3 | 4 | 1 | 1.3870e-01 | 4.0033e+05 |
| 4 | 5 | 1 | 1.3870e-01 | 4.0033e+05 |
| 5 | 6 | 1 | 1.3870e-01 | 4.0033e+05 |
| 5 | 7 | 1 | 1.3870e-01 | 4.0033e+05 |
| 6 | 10 | 1 | 1.3870e-01 | 4.0033e+05 |
| 7 | 8 | 1 | 1.3870e-01 | 4.0033e+05 |
| 8 | 9 | 1 | 1.3870e-01 | 4.0033e+05 |
| 8 | 29 | 1 | 1.3870e-01 | 4.0033e+05 |
| 9 | 10 | 1 | 1.3870e-01 | 4.0033e+05 |
| 9 | 11 | 1 | 1.3870e-01 | 4.0033e+05 |
| 11 | 26 | 1 | 1.3870e-01 | 4.0033e+05 |
| 19 | 20 | 1 | 1.3870e-01 | 4.0033e+05 |
| 19 | 24 | 1 | 1.3870e-01 | 4.0033e+05 |
| 20 | 21 | 1 | 1.3870e-01 | 4.0033e+05 |
| 21 | 22 | 1 | 1.3870e-01 | 4.0033e+05 |
| 22 | 23 | 1 | 1.3870e-01 | 4.0033e+05 |
| 23 | 24 | 1 | 1.3870e-01 | 4.0033e+05 |
| 23 | 25 | 1 | 1.3870e-01 | 4.0033e+05 |
| 24 | 28 | 1 | 1.3870e-01 | 4.0033e+05 |

```
   25     26      1   1.3870e-01   4.0033e+05
   26     27      1   1.3870e-01   4.0033e+05
   27     28      1   1.3870e-01   4.0033e+05
   27     29      1   1.3870e-01   4.0033e+05

[ pairs ]
;  ai    aj funct
    1     14       1
    1     17       1
    2     15       1
   12      3       1
    4     13       1
    4     16       1
    5     14       1
   12      5       1
    5     17       1
    6     13       1
    6     15       1
    6     16       1
    7     15       1
    7     36       1
    8     17       1
    8     18       1
    9     16       1
    9     36       1
   12     10       1
   10     18       1
   11     17       1
   11     34       1
   12     13       1
   13     14       1
   14     15       1
   16     29       1
   18     25       1
   18     27       1
   19     32       1
```

| | | |
|---|---|---|
| 19 | 35 | 1 |
| 20 | 33 | 1 |
| 21 | 30 | 1 |
| 22 | 31 | 1 |
| 22 | 34 | 1 |
| 23 | 32 | 1 |
| 23 | 30 | 1 |
| 23 | 35 | 1 |
| 24 | 31 | 1 |
| 24 | 33 | 1 |
| 24 | 34 | 1 |
| 25 | 33 | 1 |
| 26 | 35 | 1 |
| 26 | 36 | 1 |
| 27 | 34 | 1 |
| 28 | 30 | 1 |
| 28 | 36 | 1 |
| 29 | 35 | 1 |
| 30 | 31 | 1 |
| 31 | 32 | 1 |
| 32 | 33 | 1 |
| 1 | 4 | 1 |
| 1 | 7 | 1 |
| 1 | 9 | 1 |
| 2 | 5 | 1 |
| 2 | 10 | 1 |
| 6 | 3 | 1 |
| 3 | 7 | 1 |
| 4 | 10 | 1 |
| 4 | 8 | 1 |
| 5 | 9 | 1 |
| 5 | 29 | 1 |
| 6 | 8 | 1 |
| 6 | 11 | 1 |
| 7 | 10 | 1 |
| 7 | 11 | 1 |

```
     7     27      1
     8     26      1
     8     28      1
     9     27      1
     9     25      1
    10     29      1
    10     26      1
    11     29      1
    11     23      1
    11     28      1
    19     22      1
    19     25      1
    19     27      1
    20     23      1
    20     28      1
    21     24      1
    21     25      1
    22     28      1
    22     26      1
    23     27      1
    24     26      1
    24     29      1
    25     28      1
    25     29      1

[ angles ]
;  ai    aj    ak funct  theta   cth
     1     2    13     1  1.2001e+02  4.0585e+02
     2     1    12     1  1.2001e+02  4.0585e+02
     2     3    14     1  1.2001e+02  4.0585e+02
     3     2    13     1  1.2001e+02  4.0585e+02
     3     4    15     1  1.2001e+02  4.0585e+02
     4     3    14     1  1.2001e+02  4.0585e+02
     5     4    15     1  1.2001e+02  4.0585e+02
     5     7    16     1  1.2001e+02  4.0585e+02
     6     1    12     1  1.2001e+02  4.0585e+02
```

| | | | | | |
|---|---|---|---|---|---|
| 6 | 10 | 17 | 1 | 1.2001e+02 | 4.0585e+02 |
| 8 | 7 | 16 | 1 | 1.2001e+02 | 4.0585e+02 |
| 8 | 29 | 36 | 1 | 1.2001e+02 | 4.0585e+02 |
| 9 | 10 | 17 | 1 | 1.2001e+02 | 4.0585e+02 |
| 9 | 11 | 18 | 1 | 1.2001e+02 | 4.0585e+02 |
| 18 | 11 | 26 | 1 | 1.2001e+02 | 4.0585e+02 |
| 19 | 20 | 31 | 1 | 1.2001e+02 | 4.0585e+02 |
| 20 | 19 | 30 | 1 | 1.2001e+02 | 4.0585e+02 |
| 20 | 21 | 32 | 1 | 1.2001e+02 | 4.0585e+02 |
| 21 | 20 | 31 | 1 | 1.2001e+02 | 4.0585e+02 |
| 21 | 22 | 33 | 1 | 1.2001e+02 | 4.0585e+02 |
| 22 | 21 | 32 | 1 | 1.2001e+02 | 4.0585e+02 |
| 23 | 22 | 33 | 1 | 1.2001e+02 | 4.0585e+02 |
| 23 | 25 | 34 | 1 | 1.2001e+02 | 4.0585e+02 |
| 24 | 19 | 30 | 1 | 1.2001e+02 | 4.0585e+02 |
| 24 | 28 | 35 | 1 | 1.2001e+02 | 4.0585e+02 |
| 26 | 25 | 34 | 1 | 1.2001e+02 | 4.0585e+02 |
| 27 | 28 | 35 | 1 | 1.2001e+02 | 4.0585e+02 |
| 27 | 29 | 36 | 1 | 1.2001e+02 | 4.0585e+02 |
| 1 | 2 | 3 | 1 | 1.1997e+02 | 5.6233e+02 |
| 1 | 6 | 5 | 1 | 1.1997e+02 | 5.6233e+02 |
| 1 | 6 | 10 | 1 | 1.1997e+02 | 5.6233e+02 |
| 2 | 1 | 6 | 1 | 1.1997e+02 | 5.6233e+02 |
| 2 | 3 | 4 | 1 | 1.1997e+02 | 5.6233e+02 |
| 3 | 4 | 5 | 1 | 1.1997e+02 | 5.6233e+02 |
| 4 | 5 | 6 | 1 | 1.1997e+02 | 5.6233e+02 |
| 4 | 5 | 7 | 1 | 1.1997e+02 | 5.6233e+02 |
| 5 | 6 | 10 | 1 | 1.1997e+02 | 5.6233e+02 |
| 5 | 7 | 8 | 1 | 1.1997e+02 | 5.6233e+02 |
| 6 | 5 | 7 | 1 | 1.1997e+02 | 5.6233e+02 |
| 6 | 10 | 9 | 1 | 1.1997e+02 | 5.6233e+02 |
| 7 | 8 | 9 | 1 | 1.1997e+02 | 5.6233e+02 |
| 7 | 8 | 29 | 1 | 1.1997e+02 | 5.6233e+02 |
| 8 | 9 | 10 | 1 | 1.1997e+02 | 5.6233e+02 |
| 8 | 9 | 11 | 1 | 1.1997e+02 | 5.6233e+02 |
| 8 | 29 | 27 | 1 | 1.1997e+02 | 5.6233e+02 |

```
    9      8     29      1   1.1997e+02   5.6233e+02
    9     11     26      1   1.1997e+02   5.6233e+02
   10      9     11      1   1.1997e+02   5.6233e+02
   11     26     25      1   1.1997e+02   5.6233e+02
   11     26     27      1   1.1997e+02   5.6233e+02
   19     20     21      1   1.1997e+02   5.6233e+02
   19     24     23      1   1.1997e+02   5.6233e+02
   19     24     28      1   1.1997e+02   5.6233e+02
   20     19     24      1   1.1997e+02   5.6233e+02
   20     21     22      1   1.1997e+02   5.6233e+02
   21     22     23      1   1.1997e+02   5.6233e+02
   22     23     24      1   1.1997e+02   5.6233e+02
   22     23     25      1   1.1997e+02   5.6233e+02
   23     24     28      1   1.1997e+02   5.6233e+02
   23     25     26      1   1.1997e+02   5.6233e+02
   24     23     25      1   1.1997e+02   5.6233e+02
   24     28     27      1   1.1997e+02   5.6233e+02
   25     26     27      1   1.1997e+02   5.6233e+02
   26     27     28      1   1.1997e+02   5.6233e+02
   26     27     29      1   1.1997e+02   5.6233e+02
   28     27     29      1   1.1997e+02   5.6233e+02

[ dihedrals ]
;i  j   k  l     func   C0  ...  C5
    1     2     3     14      3     30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
    1     6     10    17      3     30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
    2     3     4     15      3     30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
    12    1     2     3       3     30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
    4     3     2     13      3     30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
    4     5     7     16      3     30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
```

5 4 3 14 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
12 1 6 5 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
5 6 10 17 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
6 1 2 13 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
6 5 4 15 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
6 5 7 16 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
7 5 4 15 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
7 8 29 36 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
8 9 10 17 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
8 9 11 18 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
9 8 7 16 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
9 8 29 36 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
12 1 6 10 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
10 9 11 18 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
11 9 10 17 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
11 26 25 34 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
12 1 2 13 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
13 2 3 14 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;

14 3 4 15 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
16 7 8 29 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
18 11 26 25 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
18 11 26 27 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
19 20 21 32 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
19 24 28 35 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
20 21 22 33 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
21 20 19 30 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
22 21 20 31 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
22 23 25 34 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
23 22 21 32 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
23 24 19 30 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
23 24 28 35 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
24 19 20 31 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
24 23 22 33 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
24 23 25 34 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
25 23 22 33 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
26 27 28 35 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;

26 27 29 36 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
27 26 25 34 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
28 24 19 30 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
28 27 29 36 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
29 27 28 35 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
30 19 20 31 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
31 20 21 32 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
32 21 22 33 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
12 1 6 2 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
1 3 2 13 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
2 4 3 14 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
3 5 4 15 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
5 8 7 16 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
6 9 10 17 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
9 26 11 18 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
20 24 19 30 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
19 21 20 31 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
20 22 21 32 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;

21 23 22 33 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
23 26 25 34 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
24 27 28 35 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
8 27 29 36 3 9.20480 0.00000 -9.20480 0.00000
0.00000 0.00000 ;
1 2 3 4 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
1 6 5 4 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
1 6 5 7 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
1 6 10 9 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
2 1 6 5 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
2 1 6 10 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
2 3 4 5 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
6 1 2 3 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
3 4 5 6 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
3 4 5 7 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
4 5 6 10 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
4 5 7 8 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
5 6 10 9 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
5 7 8 9 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;

5 7 8 29 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
6 5 7 8 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
6 10 9 8 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
6 10 9 11 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
7 5 6 10 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
7 8 9 10 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
7 8 9 11 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
7 8 29 27 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
8 9 11 26 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
8 29 27 26 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
8 29 27 28 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
9 8 29 27 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
9 11 26 25 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
9 11 26 27 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
10 9 8 29 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
10 9 11 26 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
11 9 8 29 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
11 26 25 23 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;

11 26 27 28 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
11 26 27 29 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
19 20 21 22 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
19 24 23 22 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
19 24 23 25 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
19 24 28 27 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
20 19 24 23 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
20 19 24 28 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
20 21 22 23 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
21 20 19 24 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
21 22 23 24 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
21 22 23 25 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
22 23 24 28 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
22 23 25 26 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
23 24 28 27 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
23 25 26 27 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
24 23 25 26 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;
24 28 27 26 3 30.33400 0.00000 -30.33400 0.00000
0.00000 0.00000 ;

```
    24    28    27    29      3      30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
    25    23    24    28      3      30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
    25    26    27    28      3      30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
    25    26    27    29      3      30.33400      0.00000    -30.33400      0.00000
0.00000      0.00000      ;
    4     6     5     7       3       9.20480      0.00000     -9.20480      0.00000
0.00000      0.00000      ;
    1     5     6     10      3       9.20480      0.00000     -9.20480      0.00000
0.00000      0.00000      ;
    7     9     8     29      3       9.20480      0.00000     -9.20480      0.00000
0.00000      0.00000      ;
    8     10    9     11      3       9.20480      0.00000     -9.20480      0.00000
0.00000      0.00000      ;
    22    24    23    25      3       9.20480      0.00000     -9.20480      0.00000
0.00000      0.00000      ;
    19    23    24    28      3       9.20480      0.00000     -9.20480      0.00000
0.00000      0.00000      ;
    11    25    26    27      3       9.20480      0.00000     -9.20480      0.00000
0.00000      0.00000      ;
    26    28    27    29      3       9.20480      0.00000     -9.20480      0.00000
0.00000      0.00000      ;

#ifdef N2MOL
; n2m.itp

[ moleculetype ]
;name            nrexcl
 n2m              3

[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       typeB    chargeB
     1   n1     1   GAS    N1    1       0.00000     14.01000 ; qtot 0.000
     2   n1     1   GAS    N2    2       0.00000     14.01000 ; qtot 0.000
```

```
[ bonds ]
;   ai     aj funct   r             k
     1      2   1    1.1240e-01    1.0223e+06 ;     N1 - N2
#endif

; end of itp
```