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27  1

MASS      1 HGA2        1.00800 H ! nonpolar, aliphatic H
MASS      2 HGA3        1.00800 H ! nonpolar, aliphatic H
MASS      3 HGR61    1.00800 H ! aromatic H
MASS      4 HGA4     1.00800 H ! alkene H
MASS      5 CG2R61A  12.01100 C ! aromatic C (see notes for convention)
MASS      6 CG2R61B  12.01100 C ! aromatic C (see notes for convention)
MASS      7 CG2R61C  12.01100 C ! aromatic C (see notes for convention)
MASS      8 CG2R61D  12.01100 C ! aromatic C (see notes for convention)
MASS      9 CG321    12.01100 C ! aliphatic sp3 C for CH2
MASS     10 CG331    12.01100 C ! aliphatic sp3 C for CH3
MASS     11 CG2DC1A  12.01100 C ! alkene C (adjacent to central ring)
MASS     12 CG2DC1B  12.01100 C ! alkene C (adjacent to central ring)
MASS     13 CG2DC1C  12.01100 C ! alkene C (adjacent to central ring)
MASS     14 CG2DC1D  12.01100 C ! alkene C (adjacent to peripheral ring)
MASS     15 OG301    15.99940 O ! ether O
MASS     16 CG2R61   12.01100 C ! aromatic C (graphite)

AUTO ANGLES DIHE

RESI BEN    0.00
ATOM C1   CG2R61  -0.12
ATOM H1   HGR61    0.12 !      H5  H4
ATOM C2  CG2R61  -0.12 !        |    |
ATOM H2  HGR61    0.12 !      C5--C4
ATOM C3  CG2R61  -0.12 !      /       \
ATOM H3  HGR61    0.12 ! H6--C6      C3--H3
ATOM C4  CG2R61  -0.12 !      \       /
ATOM H4  HGR61    0.12 !      C1--C2
ATOM C5  CG2R61  -0.12 !        |    |
ATOM H5  HGR61    0.12 !      H1  H2
ATOM C6   CG2R61  -0.12 !
ATOM H6   HGR61    0.12
BOND C5 C6 C1 C6 C4 C5
BOND C2 C1 C3 C4 C3 C2
BOND C6 H6 C5 H5 C1 H1 C4 H4
BOND C2 H2 C3 H3


RESI     TSB 0
ATOM    CR01    CG2R61A 0.00
ATOM    CR02    CG2R61B -0.15
ATOM    CR03    CG2R61A 0.00
ATOM    CR04    CG2R61C -0.15
ATOM    CR05    CG2R61A 0.00
ATOM    CR06    CG2R61D -0.15
ATOM    HR02    HGR61   0.15
ATOM    HR04    HGR61   0.15
ATOM    HR06    HGR61   0.15
ATOM    CR11    CG2R61A 0.00
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ATOM      CR12      CG2R61B  -0.23
ATOM      CR13      CG2R61B  0.45
ATOM      CR14      CG2R61D  -0.30
ATOM      CR15      CG2R61C  0.45
ATOM      CR16      CG2R61C  -0.23
ATOM      HR12      HGR61    0.16
ATOM      HR14      HGR61    0.16
ATOM      HR16      HGR61    0.16
ATOM      CR21      CG2R61A  0.00
ATOM      CR22      CG2R61B  -0.23
ATOM      CR23      CG2R61B  0.45
ATOM      CR24      CG2R61D  -0.30
ATOM      CR25      CG2R61C  0.45
ATOM      CR26      CG2R61C  -0.23
ATOM      HR22      HGR61    0.16
ATOM      HR24      HGR61    0.16
ATOM      HR26      HGR61    0.16
ATOM      CR31      CG2R61A  0.00
ATOM      CR32      CG2R61B  -0.23
ATOM      CR33      CG2R61B  0.45
ATOM      CR34      CG2R61D  -0.30
ATOM      CR35      CG2R61C  0.45
ATOM      CR36      CG2R61C  -0.23
ATOM      HR32      HGR61    0.16
ATOM      HR34      HGR61    0.16
ATOM      HR36      HGR61    0.16
ATOM      CL11      CG2DC1A  -0.13
ATOM      CL12      CG2DC1D  -0.13
ATOM      HL11      HGA4     0.14
ATOM      HL12      HGA4     0.14
ATOM      CL21      CG2DC1B  -0.13
ATOM      CL22      CG2DC1D  -0.13
ATOM      HL21      HGA4     0.14
ATOM      HL22      HGA4     0.14
ATOM      CL31      CG2DC1C  -0.13
ATOM      CL32      CG2DC1D  -0.13
ATOM      HL31      HGA4     0.14
ATOM      HL32      HGA4     0.14
ATOM      O13       OG301    -0.69
ATOM      CA1       CG321    0.10
ATOM      HA1       HGA2     0.11
ATOM      HA21      HGA2     0.11
ATOM      CA2       CG321    -0.20
ATOM      HA2       HGA2     0.11
ATOM      HA22      HGA2     0.11
ATOM      CA3       CG321    -0.20
ATOM      HA3       HGA2     0.11
ATOM      HA23      HGA2     0.11
ATOM      CA4       CG321    -0.20
ATOM      HA4       HGA2     0.11
ATOM      HA24      HGA2     0.11
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ATOM      CA5      CG321     -0.21
ATOM      HA5      HGA2       0.11
ATOM      HA25     HGA2       0.11
ATOM      CA6      CG331     -0.33
ATOM      HA6      HGA3       0.11
ATOM      HA26     HGA3       0.11
ATOM      HA27     HGA3       0.11
ATOM      O15      OG301     -0.69
ATOM      CB1      CG321      0.10
ATOM      HB1      HGA2       0.11
ATOM      HB21     HGA2       0.11
ATOM      CB2      CG321     -0.20
ATOM      HB2      HGA2       0.11
ATOM      HB22     HGA2       0.11
ATOM      CB3      CG321     -0.20
ATOM      HB3      HGA2       0.11
ATOM      HB23     HGA2       0.11
ATOM      CB4      CG321     -0.20
ATOM      HB4      HGA2       0.11
ATOM      HB24     HGA2       0.11
ATOM      CB5      CG321     -0.21
ATOM      HB5      HGA2       0.11
ATOM      HB25     HGA2       0.11
ATOM      CB6      CG331     -0.33
ATOM      HB6      HGA3       0.11
ATOM      HB26     HGA3       0.11
ATOM      HB27     HGA3       0.11
ATOM      O23      OG301     -0.69
ATOM      CC1      CG321      0.10
ATOM      HC1      HGA2       0.11
ATOM      HC21     HGA2       0.11
ATOM      CC2      CG321     -0.20
ATOM      HC2      HGA2       0.11
ATOM      HC22     HGA2       0.11
ATOM      CC3      CG321     -0.20
ATOM      HC3      HGA2       0.11
ATOM      HC23     HGA2       0.11
ATOM      CC4      CG321     -0.20
ATOM      HC4      HGA2       0.11
ATOM      HC24     HGA2       0.11
ATOM      CC5      CG321     -0.21
ATOM      HC5      HGA2       0.11
ATOM      HC25     HGA2       0.11
ATOM      CC6      CG331     -0.33
ATOM      HC6      HGA3       0.11
ATOM      HC26     HGA3       0.11
ATOM      HC27     HGA3       0.11
ATOM      O25      OG301     -0.69
ATOM      CD1      CG321      0.10
ATOM      HD1      HGA2       0.11
ATOM      HD21     HGA2       0.11
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ATOM     CD2     CG321    -0.20
ATOM     HD2     HGA2      0.11
ATOM     HD22    HGA2      0.11
ATOM     CD3     CG321    -0.20
ATOM     HD3     HGA2      0.11
ATOM     HD23    HGA2      0.11
ATOM     CD4     CG321    -0.20
ATOM     HD4     HGA2      0.11
ATOM     HD24    HGA2      0.11
ATOM     CD5     CG321    -0.21
ATOM     HD5     HGA2      0.11
ATOM     HD25    HGA2      0.11
ATOM     CD6     CG331    -0.33
ATOM     HD6     HGA3      0.11
ATOM     HD26    HGA3      0.11
ATOM     HD27    HGA3      0.11
ATOM     O33     OG301    -0.69
ATOM     CE1     CG321     0.10
ATOM     HE1     HGA2      0.11
ATOM     HE21    HGA2      0.11
ATOM     CE2     CG321    -0.20
ATOM     HE2     HGA2      0.11
ATOM     HE22    HGA2      0.11
ATOM     CE3     CG321    -0.20
ATOM     HE3     HGA2      0.11
ATOM     HE23    HGA2      0.11
ATOM     CE4     CG321    -0.20
ATOM     HE4     HGA2      0.11
ATOM     HE24    HGA2      0.11
ATOM     CE5     CG321    -0.21
ATOM     HE5     HGA2      0.11
ATOM     HE25    HGA2      0.11
ATOM     CE6     CG331    -0.33
ATOM     HE6     HGA3      0.11
ATOM     HE26    HGA3      0.11
ATOM     HE27    HGA3      0.11
ATOM     O35     OG301    -0.69
ATOM     CF1     CG321     0.10
ATOM     HF1     HGA2      0.11
ATOM     HF21    HGA2      0.11
ATOM     CF2     CG321    -0.20
ATOM     HF2     HGA2      0.11
ATOM     HF22    HGA2      0.11
ATOM     CF3     CG321    -0.20
ATOM     HF3     HGA2      0.11
ATOM     HF23    HGA2      0.11
ATOM     CF4     CG321    -0.20
ATOM     HF4     HGA2      0.11
ATOM     HF24    HGA2      0.11
ATOM     CF5     CG321    -0.21
ATOM     HF5     HGA2      0.11
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ATOM     HF25    HGA2     0.11
ATOM      CF6    CG331   -0.33
ATOM      HF6    HGA3     0.11
ATOM     HF26    HGA3     0.11
ATOM     HF27    HGA3     0.11


BOND CR01   CR02         CR01   CR06        CR01   CL11
BOND CR02   CR03         CR02   HR02
BOND CR03   CR04         CR03   CL31
BOND CR04   CR05         CR04   HR04
BOND CR05   CR06         CR05   CL21
BOND CR06   HR06
BOND CR11   CR12         CR11   CR16        CR11   CL12
BOND CR12   CR13         CR12   HR12
BOND CR13   CR14         CR13   O13
BOND CR14   CR15         CR14   HR14
BOND CR15   CR16         CR15   O15
BOND CR16   HR16
BOND CR21   CR22         CR21   CR26        CR21   CL22
BOND CR22   CR23         CR22   HR22
BOND CR23   CR24         CR23   O23
BOND CR24   CR25         CR24   HR24
BOND CR25   CR26         CR25   O25
BOND CR26   HR26
BOND CR31   CR32         CR31   CR36        CR31   CL32
BOND CR32   CR33         CR32   HR32
BOND CR33   CR34         CR33   O33
BOND CR34   CR35         CR34   HR34
BOND CR35   CR36         CR35   O35
BOND CR36   HR36
BOND CL11   CL12         CL11   HL11
BOND CL12   HL12
BOND CL21   CL22         CL21   HL21
BOND CL22   HL22
BOND CL31   CL32         CL31   HL31
BOND CL32   HL32
BOND O13    CA1
BOND CA1    HA1          CA1    HA21        CA1    CA2
BOND CA2    HA2          CA2    HA22        CA2    CA3
BOND CA3    HA3          CA3    HA23        CA3    CA4
BOND CA4    HA4          CA4    HA24        CA4    CA5
BOND CA5    HA5          CA5    HA25        CA5    CA6
BOND CA6    HA6          CA6    HA26        CA6    HA27
BOND O15    CB1
BOND CB1    HB1          CB1    HB21        CB1    CB2
BOND CB2    HB2          CB2    HB22        CB2    CB3
BOND CB3    HB3          CB3    HB23        CB3    CB4
BOND CB4    HB4          CB4    HB24        CB4    CB5
BOND CB5    HB5          CB5    HB25        CB5    CB6
BOND CB6    HB6          CB6    HB26        CB6    HB27
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BOND 023   CC1
BOND CC1   HC1        CC1   HC21        CC1   CC2
BOND CC2   HC2        CC2   HC22        CC2   CC3
BOND CC3   HC3        CC3   HC23        CC3   CC4
BOND CC4   HC4        CC4   HC24        CC4   CC5
BOND CC5   HC5        CC5   HC25        CC5   CC6
BOND CC6   HC6        CC6   HC26        CC6   HC27
BOND 025   CD1
BOND CD1   HD1        CD1   HD21        CD1   CD2
BOND CD2   HD2        CD2   HD22        CD2   CD3
BOND CD3   HD3        CD3   HD23        CD3   CD4
BOND CD4   HD4        CD4   HD24        CD4   CD5
BOND CD5   HD5        CD5   HD25        CD5   CD6
BOND CD6   HD6        CD6   HD26        CD6   HD27
BOND 033   CE1
BOND CE1   HE1        CE1   HE21        CE1   CE2
BOND CE2   HE2        CE2   HE22        CE2   CE3
BOND CE3   HE3        CE3   HE23        CE3   CE4
BOND CE4   HE4        CE4   HE24        CE4   CE5
BOND CE5   HE5        CE5   HE25        CE5   CE6
BOND CE6   HE6        CE6   HE26        CE6   HE27
BOND 035   CF1
BOND CF1   HF1        CF1   HF21        CF1   CF2
BOND CF2   HF2        CF2   HF22        CF2   CF3
BOND CF3   HF3        CF3   HF23        CF3   CF4
BOND CF4   HF4        CF4   HF24        CF4   CF5
BOND CF5   HF5        CF5   HF25        CF5   CF6
BOND CF6   HF6        CF6   HF26        CF6   HF27
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