Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Theoretical-computational modeling of photo-induced charge separation spectrum and charge recombination kinetics in solution.

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SUPPLEMENTARY INFORMATION

1. Gromacs format topologies

BENZENE

```
[ moleculetype ]
; Name nrexcl
benzene  3

[ atoms ]
;   nr       type  resnr resid  atom  cgnr    charge      mass
     1         C      1  DRG       C     1   -0.110   12.0110
     2         C      1  DRG       C     1   -0.110   12.0110
     3         C      1  DRG       C     1   -0.110   12.0110
     4         C      1  DRG       C     1   -0.110   12.0110
     5         C      1  DRG       C     1   -0.110   12.0110
     6         C      1  DRG       C     1   -0.110   12.0110
     7         HC     1  DRG       H     1    0.110    1.0080
     8         HC     1  DRG       H     1    0.110    1.0080
     9         HC     1  DRG       H     1    0.110    1.0080
    10         HC     1  DRG       H     1    0.110    1.0080
    11         HC     1  DRG       H     1    0.110    1.0080
    12         HC     1  DRG       H     1    0.110    1.0080

[ bonds ]
; ai   aj   fu    c0, c1, ...
   1    2    2    0.139   10800000.0
   2    3    2    0.139   10800000.0
   3    4    2    0.139   10800000.0
   4    5    2    0.139   10800000.0
   5    6    2    0.139   10800000.0
   6    1    2    0.139   10800000.0
   1    7    2    0.108   12300000.0
   2    8    2    0.108   12300000.0
   3    9    2    0.108   12300000.0
   4   10    2    0.108   12300000.0
```

```
   5  11   2    0.108   12300000.0
   6  12   2    0.108   12300000.0

[ pairs ]
; ai   aj  fu    c0, c1, ...
   1   9   1
   1   4   1
   1  11   1
   2  10   1
   2   5   1
   2  12   1
   3  11   1
   3   6   1
   3   7   1
   4   8   1
   4  12   1
   5   9   1
   5   7   1
   6  10   1
   6   8   1
   7   8   1
   8   9   1
   9  10   1
  10  11   1
  11  12   1
  12   7   1

[ angles ]
; ai   aj  ak  fu    c0, c1, ...
   6   1   7   2      120.000   505.0
   6   1   2   2      120.000   505.0
   7   1   2   2      120.000   505.0
   1   2   3   2      120.000   505.0
   1   2   8   2      120.000   505.0
   8   2   3   2      120.000   505.0
   2   3   9   2      120.000   505.0
   2   3   4   2      120.000   505.0
   9   3   4   2      120.000   505.0
   3   4  10   2      120.000   505.0
   3   4   5   2      120.000   505.0
  10   4   5   2      120.000   505.0
   4   5  11   2      120.000   505.0
   4   5   6   2      120.000   505.0
   6   5  11   2      120.000   505.0
   5   6  12   2      120.000   505.0
   5   6   1   2      120.000   505.0
```

```
   1   6  12   2      120.000   505.0

[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
   4   3   2   1   2   0.0  167.423
   4   5   6   1   2   0.0  167.423
   3   2   1   6   2   0.0  167.423
   3   4   5   6   2   0.0  167.423
   2   1   6   5   2   0.0  167.423
   2   3   4   5   2   0.0  167.423
   3   4   2   9   2   0.0  167.423
   2   1   3   8   2   0.0  167.423
   5   4   6  11   2   0.0  167.423
   6   1   5  12   2   0.0  167.423
   1   6   2   7   2   0.0  167.423
   4   5   3  10   2   0.0  167.423
```

INDENE

```
[ moleculetype ]
; Name nrexcl
indene  3

[ atoms ]
;   nr      type  resnr resid  atom  cgnr    charge     mass
     1        C      1  DRG       C     1  -0.222    12.0110
     2        C      1  DRG       C     1   0.198    12.0110
     3        C      1  DRG       C     1   0.101    12.0110
     4        C      1  DRG       C     1  -0.223    12.0110
     5        C      1  DRG       C     1  -0.114    12.0110
     6        C      1  DRG       C     1  -0.153    12.0110
     7        HC     1  DRG       H     1   0.138     1.0080
     8        C      1  DRG       C     1  -0.328    12.0110
     9        C      1  DRG       C     1  -0.165    12.0110
    10        HC     1  DRG       H     1   0.132     1.0080
    11        HC     1  DRG       H     1   0.120     1.0080
    12        HC     1  DRG       H     1   0.128     1.0080
    13        C      1  DRG       C     1  -0.066    12.0110
    14        HC     1  DRG       H     1   0.167     1.0080
    15        HC     1  DRG       H     1   0.104     1.0080
    16        HC     1  DRG       H     1   0.092     1.0080
    17        HC     1  DRG       H     1   0.092     1.0080

[ bonds ]
; ai  aj  fu    c0, c1, ...
   1   2   2    0.139  10800000.0
```

```
   2    3    2     0.139   10800000.0
   3    4    2     0.139   10800000.0
   4    5    2     0.139   10800000.0
   5    6    2     0.139   10800000.0
   6    1    2     0.139   10800000.0
   1    7    2     0.108   12300000.0
   2    8    2     0.147   11800000.0
   3    9    2     0.151   11800000.0
   4   10    2     0.108   12300000.0
   5   11    2     0.108   12300000.0
   6   12    2     0.108   12300000.0
   8   13    2     0.134   11800000.0
  13    9    2     0.151   11800000.0
   8   14    2     0.108   12300000.0
  13   15    2     0.108   12300000.0
   9   16    2     0.110   12300000.0
   9   17    2     0.110   12300000.0

[ pairs ]
; ai   aj   fu     c0, c1, ...
   1    9    1
   1    4    1
   1   11    1
   2   10    1
   2    5    1
   2   12    1
   3   11    1
   3    6    1
   3    7    1
   4    8    1
   4   12    1
   5    9    1
   5    7    1
   6   10    1
   6    8    1
   7    8    1
   8    9    1
   9   10    1
  10   11    1
  11   12    1
  12    7    1
  13    3    1
  13    1    1
  13    4    1
  14   15    1
  14    7    1
```

```
  14   3   1
  14   9   1
  15   2   1
  15   3   1
  15  16   1
  15  17   1
  16   8   1
  16   4   1
  16   2   1
  17   8   1
  17   4   1
  17   2   1

[ angles ]
; ai  aj  ak  fu    c0, c1, ...
   6   1   7   2      120.000   505.0
   6   1   2   2      120.000   505.0
   7   1   2   2      120.000   505.0
   1   2   3   2      120.000   560.0
   1   2   8   2      131.000   760.0
   8   2   3   2      108.000   465.0
   2   3   9   2      109.000   465.0
   2   3   4   2      120.000   560.0
   9   3   4   2      131.000   760.0
   3   4  10   2      120.000   505.0
   3   4   5   2      120.000   505.0
  10   4   5   2      120.000   505.0
   4   5  11   2      120.000   505.0
   4   5   6   2      120.000   505.0
   6   5  11   2      120.000   505.0
   5   6  12   2      120.000   505.0
   5   6   1   2      120.000   505.0
   1   6  12   2      120.000   505.0
   2   8  14   2      124.000   575.0
   2   8  13   2      110.000   465.0
  14   8  13   2      126.000   575.0
   8  13  15   2      126.000   575.0
   8  13   9   2      110.000   465.0
   9  13  15   2      123.000   575.0
  13   9  17   2      112.000   425.0
  13   9  16   2      112.000   425.0
  13   9   3   2      103.000   465.0
  16   9  17   2      106.000   380.0
   3   9  16   2      112.000   425.0
   3   9  17   2      112.000   425.0
```

```
[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
   4   3   2   1   2    0.0  167.423
   4   5   6   1   2    0.0  167.423
   3   2   1   6   2    0.0  167.423
   3   4   5   6   2    0.0  167.423
   2   1   6   5   2    0.0  167.423
   2   3   4   5   2    0.0  167.423
   3   4   2   9   2    0.0  167.423
   2   1   3   8   2    0.0  167.423
   5   4   6  11   2    0.0  167.423
   6   1   5  12   2    0.0  167.423
   1   6   2   7   2    0.0  167.423
   4   5   3  10   2    0.0  167.423
   3   2   8  13   2    0.0  167.423
   2   8  13   9   2    0.0  167.423
   8  13   9   3   2    0.0  167.423
   8   2  13  14   2    0.0  167.423
  13   9   8  15   2    0.0  167.423
   2   3   9  17   2  120.0  167.423
   2   3   9  16   2  240.0  167.423
```

TCNE

```
[ moleculetype ]
; Name nrexcl
tetracianoetilene 3

[ atoms ]
;   nr       type  resnr resid  atom  cgnr    charge      mass
     1          C      1  TCNE      C     1    -0.082   12.0110
     2          C      1  TCNE      C     1    -0.082   12.0110
     3          C      1  TCNE      C     1     0.379   12.0110
     4          C      1  TCNE      C     1     0.379   12.0110
     5          C      1  TCNE      C     1     0.379   12.0110
     6          C      1  TCNE      C     1     0.379   12.0110
     7         NR      1  TCNE      N     1    -0.338   14.0070
     8         NR      1  TCNE      N     1    -0.338   14.0070
     9         NR      1  TCNE      N     1    -0.338   14.0070
    10         NR      1  TCNE      N     1    -0.338   14.0070

[ bonds ]
; ai  aj  fu    c0, c1, ...
   1   2   2    0.134  10800000.0
   2   3   2    0.143   5730000.0
   2   4   2    0.143   5730000.0
   1   5   2    0.143   5730000.0
```

```
   1    6    2     0.143    5730000.0
   3    7    2     0.115   42000000.0
   4    8    2     0.115   42000000.0
   5    9    2     0.115   42000000.0
   6   10    2     0.115   42000000.0
   5    4    2     0.284   42000000.0
   3    6    2     0.284   42000000.0

[ pairs ]
; ai   aj   fu    c0, c1, ...
   1    7    1
   1    8    1
   2    9    1
   2   10    1
   3    8    1
   3    5    1
   3    6    1
   4    7    1
   4    5    1
   4    6    1
   5   10    1
   6    9    1
  8    7    1
   9   10    1

[ angles ]
; ai   aj   ak   fu    c0, c1, ...
   1    6    3    2       58.2     960.0
   1    6   10    2      180.0     960.0
  10    6    3    2      121.8     960.0
   1    5    4    2       58.2     960.0
   1    5    9    2      180.0     960.0
   9    5    4    2      121.8     960.0
   2    4    5    2       58.2     960.0
   2    4    8    2      180.0     960.0
   8    4    5    2      121.8     960.0
   2    3    6    2       58.2     960.0
   2    3    7    2      180.0     960.0
   7    3    6    2      121.8     960.0
  6    1    2    2      120.000    560.0
   6    1    5    2      120.000    560.0
   5    1    2    2      120.000    560.0
   1    2    3    2      120.000    560.0
   1    2    4    2      120.000    560.0
   3    2    4    2      120.000    560.0
```

```
[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
   6   1   2   3   2    0.0 600.0
   5   1   2   4   2    0.0 600.0
   6   2   5   1   2    gi_1
   3   1   4   2   2    gi_1
```

BENZENE RADICAL CATION

```
[ moleculetype ]
; Name nrexcl
benzene  3

[ atoms ]
;   nr       type  resnr resid  atom  cgnr    charge      mass
     1          C      1  DRG       C     1    0.003   12.0110
     2          C      1  DRG       C     1    0.003   12.0110
     3          C      1  DRG       C     1    0.003   12.0110
     4          C      1  DRG       C     1    0.003   12.0110
     5          C      1  DRG       C     1    0.003   12.0110
     6          C      1  DRG       C     1    0.003   12.0110
     7         HC      1  DRG       H     1    0.163    1.0080
     8         HC      1  DRG       H     1    0.163    1.0080
     9         HC      1  DRG       H     1    0.163    1.0080
    10         HC      1  DRG       H     1    0.163    1.0080
    11         HC      1  DRG       H     1    0.163    1.0080
    12         HC      1  DRG       H     1    0.164    1.0080

[ bonds ]
; ai  aj  fu    c0, c1, ...
   1   2   2    0.139  10800000.0
   2   3   2    0.139  10800000.0
   3   4   2    0.139  10800000.0
   4   5   2    0.139  10800000.0
   5   6   2    0.139  10800000.0
   6   1   2    0.139  10800000.0
   1   7   2    0.108  12300000.0
   2   8   2    0.108  12300000.0
   3   9   2    0.108  12300000.0
   4  10   2    0.108  12300000.0
   5  11   2    0.108  12300000.0
   6  12   2    0.108  12300000.0

[ pairs ]
; ai  aj  fu    c0, c1, ...
```

```
   1   9   1
   1   4   1
   1  11   1
   2  10   1
   2   5   1
   2  12   1
   3  11   1
   3   6   1
   3   7   1
   4   8   1
   4  12   1
   5   9   1
   5   7   1
   6  10   1
   6   8   1
   7   8   1
   8   9   1
   9  10   1
  10  11   1
  11  12   1
  12   7   1

[ angles ]
; ai  aj  ak  fu    c0, c1, ...
   6   1   7   2      120.000   505.0
   6   1   2   2      120.000   505.0
   7   1   2   2      120.000   505.0
   1   2   3   2      120.000   505.0
   1   2   8   2      120.000   505.0
   8   2   3   2      120.000   505.0
   2   3   9   2      120.000   505.0
   2   3   4   2      120.000   505.0
   9   3   4   2      120.000   505.0
   3   4  10   2      120.000   505.0
   3   4   5   2      120.000   505.0
  10   4   5   2      120.000   505.0
   4   5  11   2      120.000   505.0
   4   5   6   2      120.000   505.0
   6   5  11   2      120.000   505.0
   5   6  12   2      120.000   505.0
   5   6   1   2      120.000   505.0
   1   6  12   2      120.000   505.0

[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
   4   3   2   1   2   0.0  167.423
```

```
   4    5    6    1    2    0.0   167.423
   3    2    1    6    2    0.0   167.423
   3    4    5    6    2    0.0   167.423
   2    1    6    5    2    0.0   167.423
   2    3    4    5    2    0.0   167.423
   3    4    2    9    2    0.0   167.423
   2    1    3    8    2    0.0   167.423
   5    4    6   11    2    0.0   167.423
   6    1    5   12    2    0.0   167.423
   1    6    2    7    2    0.0   167.423
   4    5    3   10    2    0.0   167.423
```

INDENE RADICAL CATION

```
[ moleculetype ]
; Name nrexcl
indene  3

[ atoms ]
;   nr       type  resnr resid  atom  cgnr    charge      mass
     1          C      1  DRG       C     1  -0.153    12.0110
     2          C      1  DRG       C     1   0.249    12.0110
     3          C      1  DRG       C     1   0.233    12.0110
     4          C      1  DRG       C     1  -0.290    12.0110
     5          C      1  DRG       C     1   0.100    12.0110
     6          C      1  DRG       C     1  -0.156    12.0110
     7         HC      1  DRG       H     1   0.192     1.0080
     8          C      1  DRG       C     1  -0.285    12.0110
     9          C      1  DRG       C     1  -0.356    12.0110
    10         HC      1  DRG       H     1   0.207     1.0080
    11         HC      1  DRG       H     1   0.153     1.0080
    12         HC      1  DRG       H     1   0.185     1.0080
    13          C      1  DRG       C     1   0.180    12.0110
    14         HC      1  DRG       H     1   0.221     1.0080
    15         HC      1  DRG       H     1   0.146     1.0080
    16         HC      1  DRG       H     1   0.187     1.0080
    17         HC      1  DRG       H     1   0.187     1.0080

[ bonds ]
; ai  aj  fu    c0, c1, ...
   1   2   2    0.139  10800000.0
   2   3   2    0.139  10800000.0
   3   4   2    0.139  10800000.0
   4   5   2    0.139  10800000.0
   5   6   2    0.139  10800000.0
   6   1   2    0.139  10800000.0
```

```
   1    7    2     0.108   12300000.0
   2    8    2     0.147   11800000.0
   3    9    2     0.151   11800000.0
   4   10    2     0.108   12300000.0
   5   11    2     0.108   12300000.0
   6   12    2     0.108   12300000.0
   8   13    2     0.134   11800000.0
  13    9    2     0.151   11800000.0
   8   14    2     0.108   12300000.0
  13   15    2     0.108   12300000.0
   9   16    2     0.110   12300000.0
   9   17    2     0.110   12300000.0

[ pairs ]
; ai   aj   fu     c0, c1, ...
   1    9    1
   1    4    1
   1   11    1
   2   10    1
   2    5    1
   2   12    1
   3   11    1
   3    6    1
   3    7    1
   4    8    1
   4   12    1
   5    9    1
   5    7    1
   6   10    1
   6    8    1
   7    8    1
   8    9    1
   9   10    1
  10   11    1
  11   12    1
  12    7    1
  13    3    1
  13    1    1
  13    4    1
  14   15    1
  14    7    1
  14    3    1
  14    9    1
  15    2    1
  15    3    1
  15   16    1
```

```
  15  17   1
  16   8   1
  16   4   1
  16   2   1
  17   8   1
  17   4   1
  17   2   1

[ angles ]
; ai  aj  ak  fu    c0, c1, ...
   6   1   7   2      120.000   505.0
   6   1   2   2      120.000   505.0
   7   1   2   2      120.000   505.0
   1   2   3   2      120.000   560.0
   1   2   8   2      131.000   760.0
   8   2   3   2      108.000   465.0
   2   3   9   2      109.000   465.0
   2   3   4   2      120.000   560.0
   9   3   4   2      131.000   760.0
   3   4  10   2      120.000   505.0
   3   4   5   2      120.000   505.0
  10   4   5   2      120.000   505.0
   4   5  11   2      120.000   505.0
   4   5   6   2      120.000   505.0
   6   5  11   2      120.000   505.0
   5   6  12   2      120.000   505.0
   5   6   1   2      120.000   505.0
   1   6  12   2      120.000   505.0
   2   8  14   2      124.000   575.0
   2   8  13   2      110.000   465.0
  14   8  13   2      126.000   575.0
   8  13  15   2      126.000   575.0
   8  13   9   2      110.000   465.0
   9  13  15   2      123.000   575.0
  13   9  17   2      112.000   425.0
  13   9  16   2      112.000   425.0
  13   9   3   2      103.000   465.0
  16   9  17   2      106.000   380.0
   3   9  16   2      112.000   425.0
   3   9  17   2      112.000   425.0

[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
   4   3   2   1   2    0.0  167.423
   4   5   6   1   2    0.0  167.423
   3   2   1   6   2    0.0  167.423
```

```
   3    4    5    6    2     0.0   167.423
   2    1    6    5    2     0.0   167.423
   2    3    4    5    2     0.0   167.423
   3    4    2    9    2     0.0   167.423
   2    1    3    8    2     0.0   167.423
   5    4    6   11    2     0.0   167.423
   6    1    5   12    2     0.0   167.423
   1    6    2    7    2     0.0   167.423
   4    5    3   10    2     0.0   167.423
   3    2    8   13    2     0.0   167.423
   2    8   13    9    2     0.0   167.423
   8   13    9    3    2     0.0   167.423
   8    2   13   14    2     0.0   167.423
  13    9    8   15    2     0.0   167.423
   2    3    9   17    2   120.0   167.423
   2    3    9   16    2   240.0   167.423

TCNE RADICAL ANION
[ moleculetype ]
; Name nrexcl
tetracianoetilene 3

[ atoms ]
;   nr       type  resnr resid  atom  cgnr    charge      mass
     1          C      1  TCNE      C     1    -0.310   12.0110
     2          C      1  TCNE      C     1    -0.310   12.0110
     3          C      1  TCNE      C     1     0.443   12.0110
     4          C      1  TCNE      C     1     0.443   12.0110
     5          C      1  TCNE      C     1     0.443   12.0110
     6          C      1  TCNE      C     1     0.443   12.0110
     7         NR      1  TCNE      N     1    -0.538   14.0070
     8         NR      1  TCNE      N     1    -0.538   14.0070
     9         NR      1  TCNE      N     1    -0.538   14.0070
    10         NR      1  TCNE      N     1    -0.538   14.0070

[ bonds ]
; ai  aj  fu    c0, c1, ...
   1    2    2     0.134  10800000.0
   2    3    2     0.143   5730000.0
   2    4    2     0.143   5730000.0
   1    5    2     0.143   5730000.0
   1    6    2     0.143   5730000.0
   3    7    2     0.115  42000000.0
   4    8    2     0.115  42000000.0
   5    9    2     0.115  42000000.0
   6   10    2     0.115  42000000.0
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   5   4   2    0.284  42000000.0
   3   6   2    0.284  42000000.0

[ pairs ]
; ai  aj  fu    c0, c1, ...
   1   7   1
   1   8   1
   2   9   1
   2  10   1
   3   8   1
   3   5   1
   3   6   1
   4   7   1
   4   5   1
   4   6   1
   5  10   1
   6   9   1
  8   7   1
   9  10   1

[ angles ]
; ai  aj  ak  fu    c0, c1, ...
   1   6   3   2       58.2     960.0
   1   6  10   2      180.0     960.0
  10   6   3   2      121.8     960.0
   1   5   4   2       58.2     960.0
   1   5   9   2      180.0     960.0
   9   5   4   2      121.8     960.0
   2   4   5   2       58.2     960.0
   2   4   8   2      180.0     960.0
   8   4   5   2      121.8     960.0
   2   3   6   2       58.2     960.0
   2   3   7   2      180.0     960.0
   7   3   6   2      121.8     960.0
  6   1   2   2      120.000   560.0
   6   1   5   2      120.000   560.0
   5   1   2   2      120.000   560.0
   1   2   3   2      120.000   560.0
   1   2   4   2      120.000   560.0
   3   2   4   2      120.000   560.0

[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
   6   1   2   3   2    0.0 600.0
   5   1   2   4   2    0.0 600.0
   6   2   5   1   2    gi_1
```

3 1 4 2 2 gi_1

2. Locally Relaxed Structures (see Table 1 of the text)

Bz-TCNE

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C	-2.6576030847	-0.1771341780	-0.4812274083
C	-2.3717027409	1.0943261510	0.0104132775
C	1.4258106453	0.2452060189	0.1511399939
C	0.8990009194	-0.1864228004	-1.0167192545
C	0.8307912440	-1.5781783361	-1.3311153945
C	0.4188366206	0.7281858753	-2.0032847156
C	1.5516003060	1.6389067522	0.4547756542
C	1.9622265565	-0.6635152199	1.1146978469
H	-1.4751041137	2.1953291805	1.6232753288
H	-0.7897707506	0.1749328633	2.8666992534
H	-1.2638349690	-2.0702788473	1.9608301812
H	-2.4757655967	-2.3054309633	-0.1949141520
H	-3.1966959191	-0.2793251656	-1.4149392015

H	-2.6786597728	1.9737358350	-0.5388283392
N	0.7895260663	-2.6920783440	-1.5996740212
N	0.0499419602	1.4495098606	-2.8147521257
N	1.6838476062	2.7482672444	0.7130783544
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C	3.0230170656	-0.7888899280	0.2531179056
C	2.3012829430	-1.3884963885	-0.7724924245
C	1.5851163435	-0.6129696371	-1.6775184662
C	1.5823996666	0.7730319842	-1.5561997127
C	2.3083248399	1.3653828790	-0.5261507265
C	3.0284712774	0.5921204653	0.3799795385
C	-1.2932420984	-0.6222414469	0.5914212901
C	-1.5160194958	0.6413151924	0.1711593443
C	-1.0769502456	1.7712026200	0.9268872563
C	-2.2020141308	0.9019812305	-1.0530434910
C	-1.7501642046	-1.7600211556	-0.1402517476
C	-0.5994121580	-0.8908370249	1.8147019966
H	3.5784325247	-1.4009677258	0.9535797840
H	2.2976675194	-2.4676960423	-0.8685022166
H	1.0326404798	-1.0906766903	-2.4779689603
H	1.0376692487	1.3856825245	-2.2649850722
H	2.3177219918	2.4445119903	-0.4308232155

H	3.5748397029	1.0688623697	1.1852451743
N	-0.7414317036	2.6875823877	1.5282081860
N	-2.7504402535	1.1184409416	-2.0362590113
N	-2.1025306152	-2.6940412402	-0.7041705342
N	-0.0521743964	-1.1218559096	2.7955663031

C	3.4014728568	-0.7595842708	0.3243717984
C	3.2228749795	-1.1229451669	-1.0034641364
C	2.5626210480	-0.2670519268	-1.8735561529
C	2.0872865979	0.9513208505	-1.4136488697
C	2.2664414994	1.3209487666	-0.0875621976
C	2.9221145425	0.4593435461	0.7822544682
C	-1.2285039760	0.2774770254	0.7282137455
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C	-2.1147764773	-1.8290664927	-0.0931309993
C	-2.9579833365	0.2792451231	-0.9740431951
C	-1.1917236547	1.7070131737	0.7213583631
C	-0.3711365803	-0.4009373906	1.6450111569
H	3.9188070584	-1.4258306648	1.0034711911
H	3.6035145161	-2.0714440667	-1.3627190283
H	2.4300186613	-0.5409024661	-2.9130753223
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H	1.9055232650	2.2816392051	0.2633762081

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N	-3.6827111336	0.8160946484	-1.6821198016
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C	-2.0971377361	-1.3612404761	-0.2299683997
C	-1.8260030485	-0.7215613627	-1.4325984800
C	-1.8499414822	0.6664645248	-1.5082000857
C	-2.1613646485	1.4112800757	-0.3794765415
C	1.1856541324	0.3846710324	0.7079112455
C	1.3731437308	-0.4125148138	-0.3660224143
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C	0.9254741426	-0.1566868906	2.0071467084
C	1.2672599603	1.8058277397	0.6075480618
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H	-2.6060925509	-1.1108601301	1.8406589216
H	-2.0712448400	-2.4427663279	-0.1741420256
H	-1.5975729469	-1.3058951341	-2.3163029167
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C	-2.5977556472	-0.0241446753	-0.8800790804
C	-2.5642875372	1.2374332366	-0.2995858182
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C	1.0953765869	-0.2401972311	-0.8478747330
C	1.5001065253	0.1072537243	0.3922164396
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C	1.7691225982	1.4648031349	0.7418306146
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C	0.0575069976	-0.4498083591	1.8206961197
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Ind-TCNE

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C	1.7160613859	0.0285284239	0.9712464192
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C	1.6592399421	-0.9212967196	0.4557922390
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C	3.1629280556	0.9330143258	0.0136096337
C	1.2934635985	1.2211154055	1.5400052462
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