Supporting Information
to the paper "Character of localization and microenvironment of the solvatochromic Reichardt's betaine dye in SDS and CTAB micelles: MD simulation study"

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Table S1. Average numbers of surfactant C and H within 0.4 nm of different parts of the dye molecule.

| system | Py *p*-Ph | Py *o*-Ph | Ph *o*-Ph | Δ Py *o*-Ph | Δ Ph *o*-Ph | O |
|---|---|---|---|---|---|---|
| $^{+}$D$^{-}$ in SDS | 26.3 ± 1.2 | 21.3 ± 1.0 | 14.9 ± 0.4 | 17.1 ± 3 | 15.3 ± 0.9 | 2.4 ± 0.05 |
| $^{+}$D$^{-}$ in CTAB | 26.4 ± 0.8 | 23.2 ± 0.5 | 17.9 ± 0.6 | 15.1 ± 1.2 | 21.5 ± 1.2 | 3.9 ± 0.10 |
| $^{+}$DH in SDS | 16.4 ± 0.01 | 21.2 ± 0.2 | 22.2 ± 0.5 | 15.8 ± 1.0 | 16.1 ± 1.0 | 8.3 ± 0.3 |
| $^{+}$DH in CTAB | 18.5 ± 1.1 | 19.8 ± 0.5 | 20.7 ± 1.0 | 14.8 ± 1.5 | 14.8 ± 2 | 7.1 ± 0.8 |

Table S2. Maximum numbers of surfactant C and H atoms found within 0.4 nm of different parts of the dye molecule (averaged over 10 ps intervals).

| system | Py *p*-Ph | Py *o*-Ph | Ph *o*-Ph | O |
|---|---|---|---|---|
| $^{+}$D$^{-}$ in SDS | 49.2 | 46.7 | 44.6 | 10.9 |
| $^{+}$D$^{-}$ in CTAB | 48.4 | 49.7 | 46.1 | 12.9 |
| $^{+}$DH in SDS | 44.7 | 47.9 | 48.8 | 17.7 |
| $^{+}$DH in CTAB | 48.2 | 47.3 | 49.0 | 17.1 |

Table S3. Average numbers of surfactant C and H atoms within 0.4 nm of different parts of $^{+}$D$^{-}$ in SDS solution for runs starting from the different initial configurations.

| initial configurations | Py *p*-Ph | Py *o*-Ph | Ph *o*-Ph | Δ Py *o*-Ph | Δ Ph *o*-Ph | O |
|---|---|---|---|---|---|---|
| dye in bulk water | 25.7 ± 1.6 | 21.4 ± 0.4 | 15.1 ± 0.5 | 17.3 ± 0.9 | 15.9 ± 0.3 | 2.5 ± 0.09 |
| dye in micelle core | 26.3 ± 1.2 | 21.3 ± 1.0 | 14.9 ± 0.4 | 17.1 ± 3 | 15.3 ± 0.9 | 2.4 ± 0.05 |

Table S4. Average numbers of various atoms in microenvironment of $^{+}$D$^{-}$ and its O atom on SDS micelles for runs starting from the different initial configurations.

| initial configurations | micelle core | water | headgroups | counterions | total |
|---|---|---|---|---|---|
| the dye molecule | | | | | |
| dye in bulk water | 119.1 ± 1.6 | 89.5 ± 0.4 | 8.6 ± 0.3 | 0.37 ± 0.02 | 217.6 ± 2.3 |
| dye in micelle core | 120 ± 5 | 89 ± 5 | 8.4 ± 0.7 | 0.37 ± 0.03 | 218 ± 11 |
| the O atom | | | | | |
| dye in bulk water | 2.5 ± 0.18 | 10.3 ± 0.17 | 0.028 ± 0.006 | 0.082 ± 0.006 | 12.8 ± 0.4 |
| dye in micelle core | 2.6 ± 0.17 | 10.29 ± 0.04 | 0.032 ± 0.007 | 0.10 ± 0.02 | 13.0 ± 0.3 |

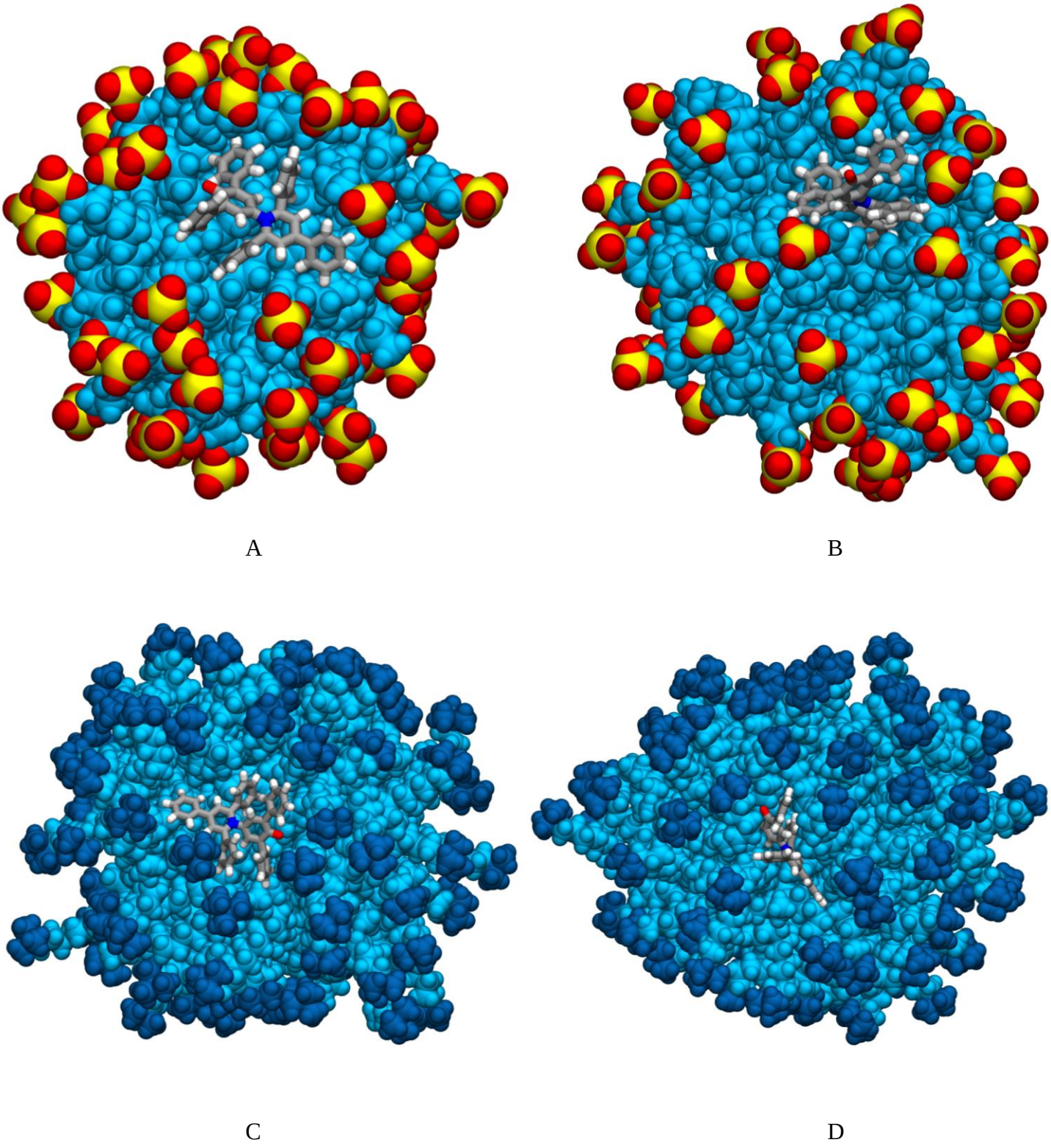


Figure S1. Snapshots from MD trajectories showing typical localizations and orientations of the neutral form of RD on SDS (A, B) and CTAB (C, D) micelles.

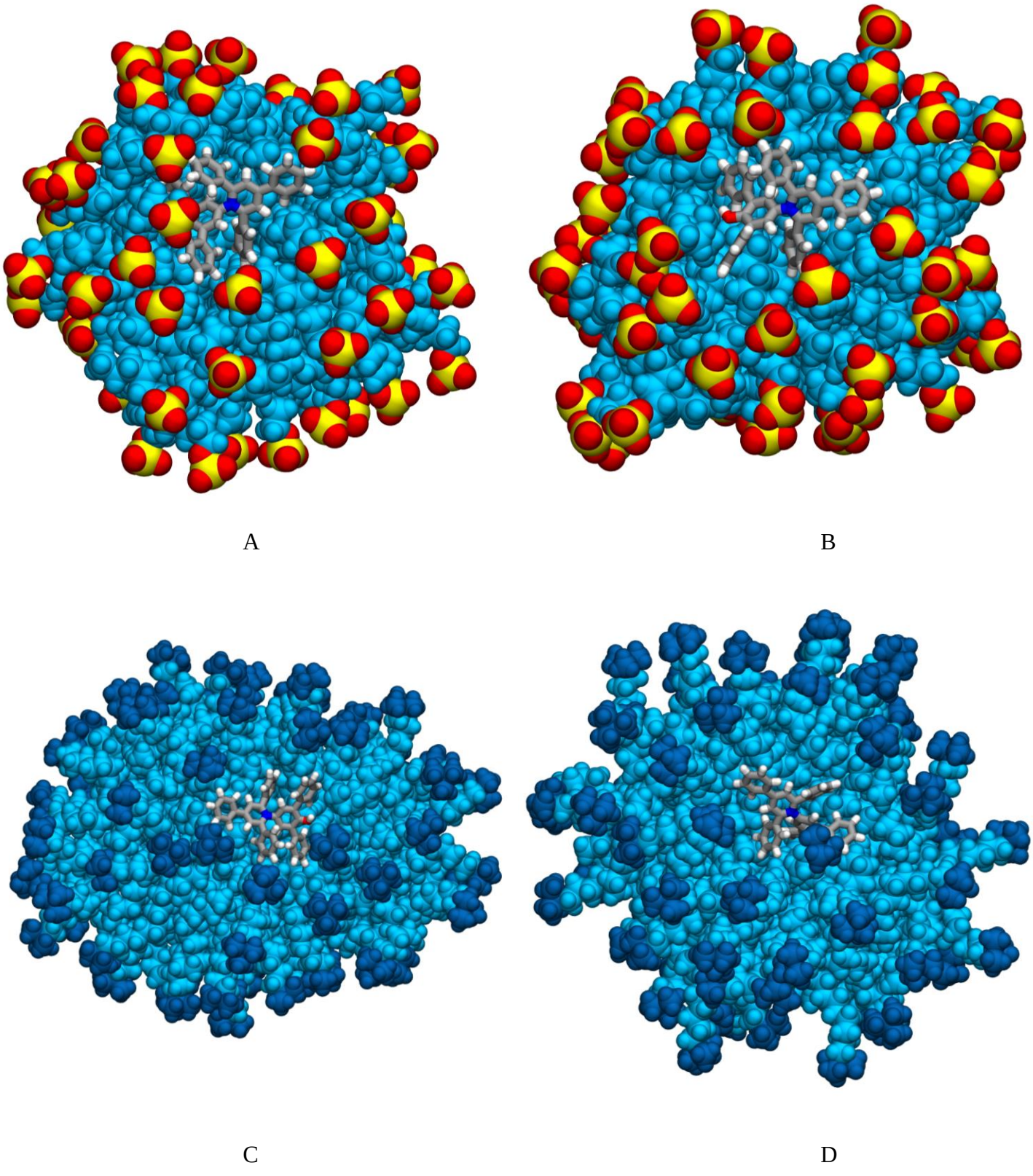


Figure S2. Snapshots from MD trajectories showing typical localizations and orientations of the protonated form of RD on SDS (A, B) and CTAB (C, D) micelles.

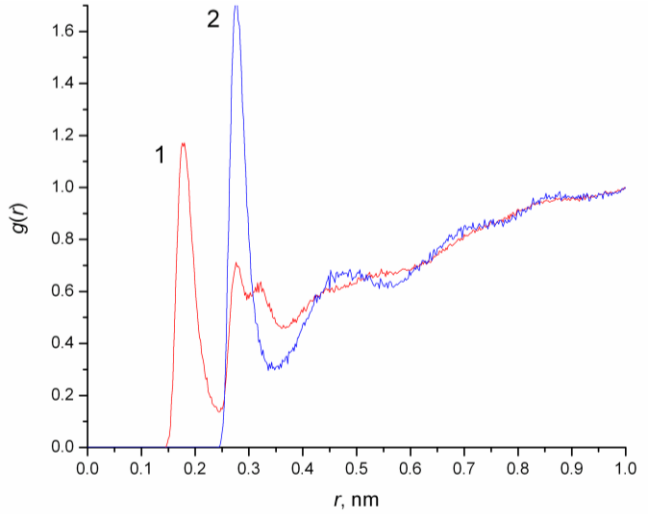


Figure S3. Radial distribution functions between the $^{+}D^{-}$ O atom and either both water O and H atoms (red curve, 1) or water O atoms only (blue curve, 2) in pure water solution.

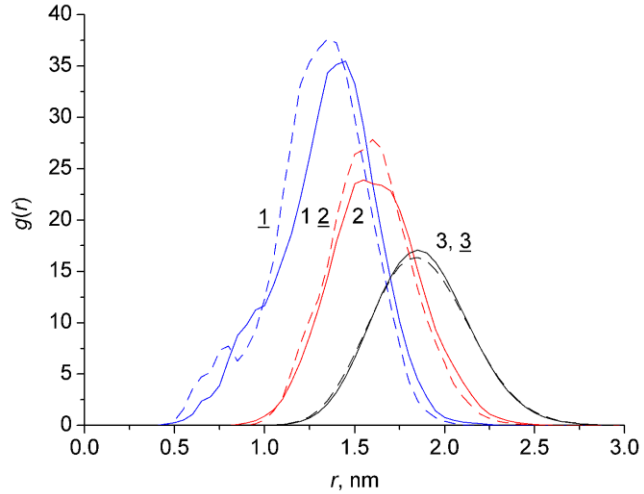


Figure S4. Radial distribution functions micelle COM — RD N (blue curves, 1) and micelle COM — RD O (red curves, 2) in comparison with RDFs micelle COM — surfactant S (N) (black curves, 3). Solid lines are for the runs starting from the initial configurations with the solubilized dye, dashed lines with underlined numbers are for the runs starting from the initial configurations with the dye placed in bulk water.

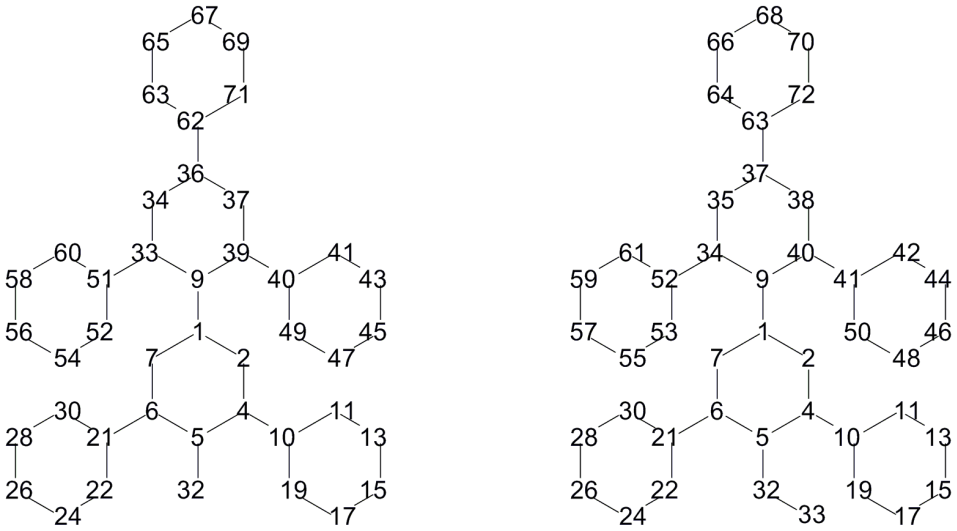

Figure S5. Scheme of numeration of atoms in potential models of the neutral and protonated forms of the RD. Hydrogen atoms in rings are not shown, they always follow the carbon atoms they are bonded to.

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******* File C-C_long_dihs.itp *******

; Krzysztof Murzyn, Maciej Bratek, and Marta Pasenkiewicz-Gierula
; Refined OPLS All-Atom Force Field Parameters for n-Pentadecane,
; Methyl Acetate, and Dimethyl Phosphate
; J. Phys. Chem. B 2013, 117, 16388-16396

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******* File Ph-Ph_params.itp *******

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C!     NC     C!      1   117.000    585.760

; Markus K. Dahlgren, Patric Schyman, Julian Tirado-Rives, and William L. Jorgensen
; Characterization of Biaryl Torsional Energetics and its Treatment in OPLS All-Atom Force Fields
; J. Chem. Inf. Model., 2013, 53 (5), 1191-1199

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******* File CTA.itp *******
; V.S. Farafonov, A.V. Lebed. Kharkov Univ. Bull., Chem. Ser. 2016,
; 27, 25-30. http://chembull.univer.kharkov.ua/archiv/2016_2/03.pdf

[ moleculetype ]
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54  53  56  58     HC_CT_CT_HC_long
54  53  56  59     3
55  53  56  57     HC_CT_CT_HC_long
55  53  56  58     HC_CT_CT_HC_long
55  53  56  59     3
57  56  59  60     HC_CT_CT_HC_long
57  56  59  62     HC_CT_CT_HC_long
57  56  59  61     HC_CT_CT_HC_long
53  56  59  60     3
53  56  59  62     3
53  56  59  61     3
58  56  59  60     HC_CT_CT_HC_long
58  56  59  62     HC_CT_CT_HC_long
58  56  59  61     HC_CT_CT_HC_long
 1  14  17  20     3
 1  14  17  18     3
 1  14  17  19     3
23  20  17  14     CT_CT_CT_CT_long
17  20  23  26     CT_CT_CT_CT_long
29  26  23  20     CT_CT_CT_CT_long
23  26  29  32     CT_CT_CT_CT_long
35  32  29  26     CT_CT_CT_CT_long
29  32  35  38     CT_CT_CT_CT_long
41  38  35  32     CT_CT_CT_CT_long
35  38  41  44     CT_CT_CT_CT_long
47  44  41  38     CT_CT_CT_CT_long
41  44  47  50     CT_CT_CT_CT_long
44  47  50  53     CT_CT_CT_CT_long
47  50  53  56     CT_CT_CT_CT_long
50  53  56  59     CT_CT_CT_CT_long
```

******* File RD.itp *******

```
[ moleculetype ]
  RD    3

[ atoms ]
   1  opls_916   1  RD    C1     1    0.0249
   2  opls_145   1  RD    C2     2   -0.1793
   3  opls_146   1  RD    H2     2    0.0461
   4  opls_145B  1  RD    C3     3   -0.1221
   5  opls_166   1  RD    C4     4    0.4152
   6  opls_145B  1  RD    C5     5   -0.1221
   7  opls_145   1  RD    C6     6   -0.1793
   8  opls_146   1  RD    H6     6    0.0461
   9  opls_520   1  RD    N      7    0.1992
  10  opls_145B  1  RD    C7     8    0.1032
  11  opls_145   1  RD    C8     9   -0.1197
  12  opls_146   1  RD    H8     9    0.1044
  13  opls_145   1  RD    C9    10   -0.1337
  14  opls_146   1  RD    H9    10    0.0974
  15  opls_145   1  RD    C10   11   -0.1122
  16  opls_146   1  RD    H10   11    0.0937
  17  opls_145   1  RD    C11   12   -0.1337
  18  opls_146   1  RD    H11   12    0.0974
  19  opls_145   1  RD    C12   13   -0.1197
  20  opls_146   1  RD    H12   13    0.1044
  21  opls_145B  1  RD    C13   14    0.1032
  22  opls_145   1  RD    C14   15   -0.1197
  23  opls_146   1  RD    H14   15    0.1044
  24  opls_145   1  RD    C15   16   -0.1337
  25  opls_146   1  RD    H15   16    0.0974
  26  opls_145   1  RD    C16   17   -0.1122
  27  opls_146   1  RD    H16   17    0.0937
  28  opls_145   1  RD    C17   18   -0.1337
  29  opls_146   1  RD    H17   18    0.0974
  30  opls_145   1  RD    C18   19   -0.1197
  31  opls_146   1  RD    H18   19    0.1044
  32  opls_167   1  RD    O     20   -0.566
  33  opls_145B  1  RD    C19   21    0.0877
  34  opls_145   1  RD    C20   22   -0.1749
  35  opls_146   1  RD    H20   22    0.0768
  36  opls_145B  1  RD    C21   23    0.1031
  37  opls_145   1  RD    C22   24   -0.1749
  38  opls_146   1  RD    H21   24    0.0768
  39  opls_145B  1  RD    C23   25    0.0877
  40  opls_145B  1  RD    C24   26    0.1156
  41  opls_145   1  RD    C25   27   -0.1208
  42  opls_146   1  RD    H25   27    0.1065
  43  opls_145   1  RD    C26   28   -0.1219
  44  opls_146   1  RD    H26   28    0.1216
  45  opls_145   1  RD    C27   29   -0.0776
  46  opls_146   1  RD    H27   29    0.1165
  47  opls_145   1  RD    C28   30   -0.1219
```

```
 48  opls_146   1  RD    H28   30    0.1216
 49  opls_145   1  RD    C29   31   -0.1208
 50  opls_146   1  RD    H29   31    0.1065
 51  opls_145B  1  RD    C30   32    0.1156
 52  opls_145   1  RD    C31   33   -0.1208
 53  opls_146   1  RD    H31   33    0.1065
 54  opls_145   1  RD    C32   34   -0.1219
 55  opls_146   1  RD    H32   34    0.1216
 56  opls_145   1  RD    C33   35   -0.0776
 57  opls_146   1  RD    H33   35    0.1165
 58  opls_145   1  RD    C34   36   -0.1219
 59  opls_146   1  RD    H34   36    0.1216
 60  opls_145   1  RD    C35   37   -0.1208
 61  opls_146   1  RD    H35   37    0.1065
 62  opls_145B  1  RD    C36   38    0.0969
 63  opls_145   1  RD    C37   39   -0.1311
 64  opls_146   1  RD    H37   39    0.1291
 65  opls_145   1  RD    C38   40   -0.1146
 66  opls_146   1  RD    H38   40    0.1169
 67  opls_145   1  RD    C39   41   -0.0679
 68  opls_146   1  RD    H39   41    0.1118
 69  opls_145   1  RD    C40   42   -0.1146
 70  opls_146   1  RD    H40   42    0.1169
 71  opls_145   1  RD    C41   43   -0.1311
 72  opls_146   1  RD    H41   43    0.1291

[ bonds ]
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 29  28  1
 15  16  1
 26  27  1
 19  20  1
 17  18  1
 64  63  1
 22  23  1
 24  25  1
 66  65  1
 45  46  1
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 67  68  1
 69  70  1
 56  57  1
 41  42  1
 43  44  1
 60  61  1
 58  59  1
 60  58  1
 11  13  1
```

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 49  40  1
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 28  26  1
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 52  51  1
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 26  24  1
 19  17  1
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 45  43  1
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 5   6   1
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 6   7   1
 7   1   1
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 36  34  1
 3   2   1
 7   8   1
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 9   39  1
 9   33  1
 39  37  1
 33  34  1
 39  40  1
 33  51  1

[ angles ]
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```

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| 4 | 10 | 11 | 1 |
| 4 | 10 | 19 | 1 |
| 6 | 21 | 30 | 1 |
| 6 | 21 | 22 | 1 |
| 34 | 36 | 37 | 1 |
| 36 | 62 | 63 | 1 |
| 36 | 62 | 71 | 1 |
| 2 | 1 | 9 | 1 |
| 7 | 1 | 9 | 1 |
| 17 | 19 | 20 | 1 |
| 3 | 2 | 4 | 1 |
| 1 | 2 | 3 | 1 |
| 6 | 7 | 8 | 1 |
| 1 | 7 | 8 | 1 |
| 12 | 11 | 13 | 1 |
| 10 | 11 | 12 | 1 |
| 11 | 13 | 14 | 1 |
| 14 | 13 | 15 | 1 |
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| 24 | 26 | 27 | 1 |
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| 28 | 30 | 31 | 1 |
| 21 | 30 | 31 | 1 |
| 35 | 34 | 36 | 1 |
| 36 | 37 | 38 | 1 |
| 40 | 41 | 42 | 1 |
| 42 | 41 | 43 | 1 |
| 44 | 43 | 45 | 1 |
| 41 | 43 | 44 | 1 |
| 46 | 45 | 47 | 1 |
| 43 | 45 | 46 | 1 |
| 48 | 47 | 49 | 1 |
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| 52 | 54 | 55 | 1 |
| 55 | 54 | 56 | 1 |
| 54 | 56 | 57 | 1 |
| 57 | 56 | 58 | 1 |
| 56 | 58 | 59 | 1 |

| | | | | | |
|---|---|---|---|---|---|
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| 51 | 60 | 61 | 1 | | |
| 58 | 60 | 61 | 1 | | |
| 62 | 63 | 64 | 1 | | |
| 64 | 63 | 65 | 1 | | |
| 63 | 65 | 66 | 1 | | |
| 66 | 65 | 67 | 1 | | |
| 65 | 67 | 68 | 1 | | |
| 68 | 67 | 69 | 1 | | |
| 70 | 69 | 71 | 1 | | |
| 67 | 69 | 70 | 1 | | |
| 62 | 71 | 72 | 1 | | |
| 69 | 71 | 72 | 1 | | |
| 5 | 4 | 10 | 1 | | |
| 2 | 4 | 10 | 1 | | |
| 7 | 6 | 21 | 1 | | |
| 33 | 34 | 36 | 1 | | |
| 37 | 36 | 62 | 1 | | |
| 34 | 36 | 62 | 1 | | |
| 36 | 37 | 39 | 1 | | |
| 2 | 4 | 5 | 1 | | |
| 5 | 6 | 7 | 1 | | |
| 4 | 5 | 32 | 1 | 120.000 | 585.760 |
| 6 | 5 | 32 | 1 | 120.000 | 585.760 |
| 4 | 5 | 6 | 1 | 120.000 | 527.184 |
| 5 | 6 | 21 | 1 | | |
| 1 | 9 | 39 | 1 | | |
| 1 | 9 | 33 | 1 | | |
| 33 | 9 | 39 | 1 | | |
| 11 | 10 | 19 | 1 | | |
| 10 | 11 | 13 | 1 | | |
| 11 | 13 | 15 | 1 | | |
| 13 | 15 | 17 | 1 | | |
| 15 | 17 | 19 | 1 | | |
| 10 | 19 | 17 | 1 | | |
| 22 | 21 | 30 | 1 | | |
| 21 | 22 | 24 | 1 | | |
| 22 | 24 | 26 | 1 | | |
| 24 | 26 | 28 | 1 | | |
| 26 | 28 | 30 | 1 | | |
| 21 | 30 | 28 | 1 | | |
| 41 | 40 | 49 | 1 | | |
| 40 | 41 | 43 | 1 | | |
| 41 | 43 | 45 | 1 | | |
| 43 | 45 | 47 | 1 | | |
| 45 | 47 | 49 | 1 | | |
| 40 | 49 | 47 | 1 | | |
| 52 | 51 | 60 | 1 | | |
| 51 | 52 | 54 | 1 | | |
| 52 | 54 | 56 | 1 | | |
| 54 | 56 | 58 | 1 | | |
| 56 | 58 | 60 | 1 | | |
| 51 | 60 | 58 | 1 | | |
| 63 | 62 | 71 | 1 | | |

```
 62   63   65    1
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 65   67   69    1
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 9    39   40    1
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 39   40   49    1
 39   40   41    1
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 33   51   60    1

[ dihedrals ]
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 10   11   13   14    3
 10   11   13   15    3
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 12   11   10   19    3
 13   11   10   4     3
 13   11   10   19    3
 14   13   15   16    3
 14   13   15   17    3
 11   13   15   16    3
 11   13   15   17    3
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 50   49   47   45    3
 40   49   47   48    3
 40   49   47   45    3
 50   49   40   39    3
 50   49   40   41    3
 47   49   40   39    3
 47   49   40   41    3
 48   47   45   46    3
 48   47   45   43    3
 49   47   45   46    3
 49   47   45   43    3
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 31   30   28   26    3
 21   30   28   29    3
 21   30   28   26    3
 31   30   21   6     3
 31   30   21   22    3
 28   30   21   6     3
 28   30   21   22    3
 29   28   26   27    3
 29   28   26   24    3
 30   28   26   27    3
```

| | | | | |
|---|---|---|---|---|
| 30 | 28 | 26 | 24 | 3 |
| 53 | 52 | 54 | 55 | 3 |
| 53 | 52 | 54 | 56 | 3 |
| 51 | 52 | 54 | 55 | 3 |
| 51 | 52 | 54 | 56 | 3 |
| 53 | 52 | 51 | 33 | 3 |
| 53 | 52 | 51 | 60 | 3 |
| 54 | 52 | 51 | 33 | 3 |
| 54 | 52 | 51 | 60 | 3 |
| 55 | 54 | 56 | 57 | 3 |
| 55 | 54 | 56 | 58 | 3 |
| 52 | 54 | 56 | 57 | 3 |
| 52 | 54 | 56 | 58 | 3 |
| 11 | 10 | 19 | 17 | 3 |
| 11 | 10 | 19 | 20 | 3 |
| 4 | 10 | 19 | 17 | 3 |
| 4 | 10 | 19 | 20 | 3 |
| 13 | 15 | 17 | 19 | 3 |
| 13 | 15 | 17 | 18 | 3 |
| 16 | 15 | 17 | 19 | 3 |
| 16 | 15 | 17 | 18 | 3 |
| 30 | 21 | 22 | 24 | 3 |
| 30 | 21 | 22 | 23 | 3 |
| 6 | 21 | 22 | 24 | 3 |
| 6 | 21 | 22 | 23 | 3 |
| 28 | 26 | 24 | 22 | 3 |
| 28 | 26 | 24 | 25 | 3 |
| 27 | 26 | 24 | 22 | 3 |
| 27 | 26 | 24 | 25 | 3 |
| 10 | 19 | 17 | 15 | 3 |
| 10 | 19 | 17 | 18 | 3 |
| 20 | 19 | 17 | 15 | 3 |
| 20 | 19 | 17 | 18 | 3 |
| 9 | 39 | 40 | 49 | 3 |
| 9 | 39 | 40 | 41 | 3 |
| 37 | 39 | 40 | 49 | 3 |
| 37 | 39 | 40 | 41 | 3 |
| 21 | 22 | 24 | 26 | 3 |
| 21 | 22 | 24 | 25 | 3 |
| 23 | 22 | 24 | 26 | 3 |
| 23 | 22 | 24 | 25 | 3 |
| 49 | 40 | 41 | 43 | 3 |
| 49 | 40 | 41 | 42 | 3 |
| 39 | 40 | 41 | 43 | 3 |
| 39 | 40 | 41 | 42 | 3 |
| 64 | 63 | 62 | 36 | 3 |
| 64 | 63 | 62 | 71 | 3 |
| 65 | 63 | 62 | 36 | 3 |
| 65 | 63 | 62 | 71 | 3 |
| 64 | 63 | 65 | 66 | 3 |
| 64 | 63 | 65 | 67 | 3 |
| 62 | 63 | 65 | 66 | 3 |
| 62 | 63 | 65 | 67 | 3 |
| 9 | 33 | 51 | 52 | 3 |

| | | | | |
|---|---|---|---|---|
| 9 | 33 | 51 | 60 | 3 |
| 34 | 33 | 51 | 52 | 3 |
| 34 | 33 | 51 | 60 | 3 |
| 36 | 62 | 71 | 72 | 3 |
| 36 | 62 | 71 | 69 | 3 |
| 63 | 62 | 71 | 72 | 3 |
| 63 | 62 | 71 | 69 | 3 |
| 63 | 65 | 67 | 69 | 3 |
| 63 | 65 | 67 | 68 | 3 |
| 66 | 65 | 67 | 69 | 3 |
| 66 | 65 | 67 | 68 | 3 |
| 47 | 45 | 43 | 41 | 3 |
| 47 | 45 | 43 | 44 | 3 |
| 46 | 45 | 43 | 41 | 3 |
| 46 | 45 | 43 | 44 | 3 |
| 62 | 71 | 69 | 67 | 3 |
| 62 | 71 | 69 | 70 | 3 |
| 72 | 71 | 69 | 67 | 3 |
| 72 | 71 | 69 | 70 | 3 |
| 52 | 51 | 60 | 58 | 3 |
| 52 | 51 | 60 | 61 | 3 |
| 33 | 51 | 60 | 58 | 3 |
| 33 | 51 | 60 | 61 | 3 |
| 65 | 67 | 69 | 71 | 3 |
| 65 | 67 | 69 | 70 | 3 |
| 68 | 67 | 69 | 71 | 3 |
| 68 | 67 | 69 | 70 | 3 |
| 54 | 56 | 58 | 60 | 3 |
| 54 | 56 | 58 | 59 | 3 |
| 57 | 56 | 58 | 60 | 3 |
| 57 | 56 | 58 | 59 | 3 |
| 40 | 41 | 43 | 45 | 3 |
| 40 | 41 | 43 | 44 | 3 |
| 42 | 41 | 43 | 45 | 3 |
| 42 | 41 | 43 | 44 | 3 |
| 51 | 60 | 58 | 56 | 3 |
| 51 | 60 | 58 | 59 | 3 |
| 61 | 60 | 58 | 56 | 3 |
| 61 | 60 | 58 | 59 | 3 |
| 51 | 33 | 34 | 35 | 3 |
| 11 | 10 | 4 | 5 | 3 |
| 19 | 10 | 4 | 5 | 3 |
| 32 | 5 | 4 | 10 | 3 |
| 6 | 5 | 4 | 10 | 3 |
| 6 | 5 | 4 | 2 | 3 |
| 32 | 5 | 6 | 21 | 3 |
| 4 | 5 | 6 | 21 | 3 |
| 4 | 5 | 6 | 7 | 3 |
| 30 | 21 | 6 | 5 | 3 |
| 22 | 21 | 6 | 5 | 3 |
| 2 | 1 | 9 | 39 | 3 |
| 2 | 1 | 9 | 33 | 3 |
| 7 | 1 | 9 | 39 | 3 |
| 7 | 1 | 9 | 33 | 3 |

```
1   9   39  37    3
1   9   39  40    3
33  9   39  37    3
33  9   39  40    3
1   9   33  34    3
1   9   33  51    3
39  9   33  34    3
39  9   33  51    3
9   39  37  38    3
9   39  37  36    3
40  39  37  38    3
40  39  37  36    3
9   33  34  36    3
9   33  34  35    3
51  33  34  36    3
11  10  4   2     3
19  10  4   2     3
30  21  6   7     3
22  21  6   7     3
37  36  62  63    3
37  36  62  71    3
34  36  62  63    3
34  36  62  71    3
32  5   4   2     3
32  5   6   7     3
10  4   2   3     3
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4   2   1   7     3
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3   2   1   7     3
3   2   1   9     3
5   6   7   1     3
5   6   7   8     3
21  6   7   1     3
21  6   7   8     3
6   7   1   2     3
6   7   1   9     3
8   7   1   2     3
8   7   1   9     3
39  37  36  34    3
39  37  36  62    3
38  37  36  34    3
38  37  36  62    3
37  36  34  33    3
37  36  34  35    3
62  36  34  33    3
62  36  34  35    3
4   6   5   32    4   improper_O_C_X_Y
```

```
******* File RDH.itp *******

[ moleculetype ]
  RDH    3

[ atoms ]
   1  opls_916   1  RD    C1     1    0.0289
   2  opls_145   1  RD    C2     2   -0.1710
   3  opls_146   1  RD    H2     2    0.0970
   4  opls_145B  1  RD    C3     3   -0.0410
   5  opls_166   1  RD    C4     4    0.2523
   6  opls_145B  1  RD    C5     5   -0.0410
   7  opls_145   1  RD    C6     6   -0.1710
   8  opls_146   1  RD    H6     6    0.0970
   9  opls_520   1  RD    N      7    0.1769
  10  opls_145B  1  RD    C7     8    0.1010
  11  opls_145   1  RD    C8     9   -0.1223
  12  opls_146   1  RD    H8     9    0.1040
  13  opls_145   1  RD    C9    10   -0.1159
  14  opls_146   1  RD    H9    10    0.1231
  15  opls_145   1  RD    C10   11   -0.0888
  16  opls_146   1  RD    H10   11    0.1172
  17  opls_145   1  RD    C11   12   -0.1159
  18  opls_146   1  RD    H11   12    0.1231
  19  opls_145   1  RD    C12   13   -0.1223
  20  opls_146   1  RD    H12   13    0.1040
  21  opls_145B  1  RD    C13   14    0.1010
  22  opls_145   1  RD    C14   15   -0.1223
  23  opls_146   1  RD    H14   15    0.1040
  24  opls_145   1  RD    C15   16   -0.1159
  25  opls_146   1  RD    H15   16    0.1231
  26  opls_145   1  RD    C16   17   -0.0888
  27  opls_146   1  RD    H16   17    0.1172
  28  opls_145   1  RD    C17   18   -0.1159
  29  opls_146   1  RD    H17   18    0.1231
  30  opls_145   1  RD    C18   19   -0.1223
  31  opls_146   1  RD    H18   19    0.1040
  32  opls_167   1  RD    O     20   -0.5019
  33  opls_168   1  RD    HO    20    0.3723
  34  opls_145B  1  RD    C19   21    0.0899
  35  opls_145   1  RD    C20   22   -0.1677
  36  opls_146   1  RD    H20   22    0.0978
  37  opls_145B  1  RD    C21   23    0.1300
  38  opls_145   1  RD    C22   24   -0.1677
  39  opls_146   1  RD    H21   24    0.0978
  40  opls_145B  1  RD    C23   25    0.0899
  41  opls_145B  1  RD    C24   26    0.1096
  42  opls_145   1  RD    C25   27   -0.1264
  43  opls_146   1  RD    H25   27    0.1126
  44  opls_145   1  RD    C26   28   -0.1212
  45  opls_146   1  RD    H26   28    0.1328
  46  opls_145   1  RD    C27   29   -0.0637
  47  opls_146   1  RD    H27   29    0.1255
  48  opls_145   1  RD    C28   30   -0.1212
```

```
 49  opls_146   1  RD    H28   30    0.1328
 50  opls_145   1  RD    C29   31   -0.1264
 51  opls_146   1  RD    H29   31    0.1126
 52  opls_145B  1  RD    C30   32    0.1096
 53  opls_145   1  RD    C31   33   -0.1264
 54  opls_146   1  RD    H31   33    0.1126
 55  opls_145   1  RD    C32   34   -0.1212
 56  opls_146   1  RD    H32   34    0.1328
 57  opls_145   1  RD    C33   35   -0.0637
 58  opls_146   1  RD    H33   35    0.1255
 59  opls_145   1  RD    C34   36   -0.1212
 60  opls_146   1  RD    H34   36    0.1328
 61  opls_145   1  RD    C35   37   -0.1264
 62  opls_146   1  RD    H35   37    0.1126
 63  opls_145B  1  RD    C36   38    0.0701
 64  opls_145   1  RD    C37   39   -0.1256
 65  opls_146   1  RD    H37   39    0.1315
 66  opls_145   1  RD    C38   40   -0.1145
 67  opls_146   1  RD    H38   40    0.1274
 68  opls_145   1  RD    C39   41   -0.0466
 69  opls_146   1  RD    H39   41    0.1220
 70  opls_145   1  RD    C40   42   -0.1145
 71  opls_146   1  RD    H40   42    0.1274
 72  opls_145   1  RD    C41   43   -0.1256
 73  opls_146   1  RD    H41   43    0.1315

[ bonds ]
 51  50  1
 49  48  1
 54  53  1
 12  11  1
 56  55  1
 14  13  1
 31  30  1
 29  28  1
 15  16  1
 26  27  1
 19  20  1
 17  18  1
 65  64  1
 22  23  1
 24  25  1
 67  66  1
 46  47  1
 72  73  1
 68  69  1
 70  71  1
 57  58  1
 42  43  1
 44  45  1
 61  62  1
 59  60  1
 61  59  1
 11  13  1
```

```
 11  10  1
 13  15  1
 50  48  1
 50  41  1
 48  46  1
 30  28  1
 30  21  1
 28  26  1
 53  55  1
 53  52  1
 55  57  1
 10  19  1
 15  17  1
 21  22  1
 26  24  1
 19  17  1
 22  24  1
 41  42  1
 64  63  1
 64  66  1
 63  72  1
 66  68  1
 46  44  1
 72  70  1
 52  61  1
 68  70  1
 57  59  1
 42  44  1
 32  5   1
 32  33  1
 10  4   1
 21  6   1
 37  63  1
 5   4   1
 5   6   1
 4   2   1
 2   1   1
 6   7   1
 7   1   1
 38  37  1
 37  35  1
 3   2   1
 7   8   1
 38  39  1
 35  36  1
 1   9   1
 9   40  1
 9   34  1
 40  38  1
 34  35  1
 40  41  1
 34  52  1

[ angles ]
```

2 1 7 1
1 2 4 1
1 7 6 1
4 10 11 1
4 10 19 1
6 21 30 1
6 21 22 1
35 37 38 1
37 63 64 1
37 63 72 1
2 1 9 1
7 1 9 1
17 19 20 1
3 2 4 1
1 2 3 1
6 7 8 1
1 7 8 1
12 11 13 1
10 11 12 1
11 13 14 1
14 13 15 1
13 15 16 1
16 15 17 1
15 17 18 1
18 17 19 1
10 19 20 1
21 22 23 1
23 22 24 1
25 24 26 1
22 24 25 1
27 26 28 1
24 26 27 1
29 28 30 1
26 28 29 1
28 30 31 1
21 30 31 1
36 35 37 1
37 38 39 1
41 42 43 1
43 42 44 1
45 44 46 1
42 44 45 1
47 46 48 1
44 46 47 1
49 48 50 1
46 48 49 1
48 50 51 1
41 50 51 1
54 53 55 1
52 53 54 1
53 55 56 1
56 55 57 1
55 57 58 1
58 57 59 1

| | | | | | |
|---|---|---|---|---|---|
| 57 | 59 | 60 | 1 | | |
| 60 | 59 | 61 | 1 | | |
| 52 | 61 | 62 | 1 | | |
| 59 | 61 | 62 | 1 | | |
| 63 | 64 | 65 | 1 | | |
| 65 | 64 | 66 | 1 | | |
| 64 | 66 | 67 | 1 | | |
| 67 | 66 | 68 | 1 | | |
| 66 | 68 | 69 | 1 | | |
| 69 | 68 | 70 | 1 | | |
| 71 | 70 | 72 | 1 | | |
| 68 | 70 | 71 | 1 | | |
| 63 | 72 | 73 | 1 | | |
| 70 | 72 | 73 | 1 | | |
| 5 | 4 | 10 | 1 | | |
| 2 | 4 | 10 | 1 | | |
| 7 | 6 | 21 | 1 | | |
| 34 | 35 | 37 | 1 | | |
| 38 | 37 | 63 | 1 | | |
| 35 | 37 | 63 | 1 | | |
| 37 | 38 | 40 | 1 | | |
| 2 | 4 | 5 | 1 | | |
| 5 | 6 | 7 | 1 | | |
| 4 | 5 | 32 | 1 | 120.000 | 585.760 |
| 6 | 5 | 32 | 1 | 120.000 | 585.760 |
| 4 | 5 | 6 | 1 | 120.000 | 527.184 |
| 5 | 32 | 33 | 1 | | |
| 5 | 6 | 21 | 1 | | |
| 1 | 9 | 40 | 1 | | |
| 1 | 9 | 34 | 1 | | |
| 34 | 9 | 40 | 1 | | |
| 11 | 10 | 19 | 1 | | |
| 10 | 11 | 13 | 1 | | |
| 11 | 13 | 15 | 1 | | |
| 13 | 15 | 17 | 1 | | |
| 15 | 17 | 19 | 1 | | |
| 10 | 19 | 17 | 1 | | |
| 22 | 21 | 30 | 1 | | |
| 21 | 22 | 24 | 1 | | |
| 22 | 24 | 26 | 1 | | |
| 24 | 26 | 28 | 1 | | |
| 26 | 28 | 30 | 1 | | |
| 21 | 30 | 28 | 1 | | |
| 42 | 41 | 50 | 1 | | |
| 41 | 42 | 44 | 1 | | |
| 42 | 44 | 46 | 1 | | |
| 44 | 46 | 48 | 1 | | |
| 46 | 48 | 50 | 1 | | |
| 41 | 50 | 48 | 1 | | |
| 53 | 52 | 61 | 1 | | |
| 52 | 53 | 55 | 1 | | |
| 53 | 55 | 57 | 1 | | |
| 55 | 57 | 59 | 1 | | |
| 57 | 59 | 61 | 1 | | |

```
 52  61  59    1
 64  63  72    1
 63  64  66    1
 64  66  68    1
 66  68  70    1
 68  70  72    1
 63  72  70    1
 9   34  35    1
 9   34  52    1
 35  34  52    1
 34  35  36    1
 39  38  40    1
 9   40  38    1
 9   40  41    1
 38  40  41    1
 40  41  50    1
 40  41  42    1
 34  52  53    1
 34  52  61    1

[ dihedrals ]
 12  11  13  14    3
 12  11  13  15    3
 10  11  13  14    3
 10  11  13  15    3
 12  11  10  4     3
 12  11  10  19    3
 13  11  10  4     3
 13  11  10  19    3
 14  13  15  16    3
 14  13  15  17    3
 11  13  15  16    3
 11  13  15  17    3
 51  50  48  49    3
 51  50  48  46    3
 41  50  48  49    3
 41  50  48  46    3
 51  50  41  40    3
 51  50  41  42    3
 48  50  41  40    3
 48  50  41  42    3
 49  48  46  47    3
 49  48  46  44    3
 50  48  46  47    3
 50  48  46  44    3
 31  30  28  29    3
 31  30  28  26    3
 21  30  28  29    3
 21  30  28  26    3
 31  30  21  6     3
 31  30  21  22    3
 28  30  21  6     3
 28  30  21  22    3
 29  28  26  27    3
```

| | | | | |
|---|---|---|---|---|
| 29 | 28 | 26 | 24 | 3 |
| 30 | 28 | 26 | 27 | 3 |
| 30 | 28 | 26 | 24 | 3 |
| 54 | 53 | 55 | 56 | 3 |
| 54 | 53 | 55 | 57 | 3 |
| 52 | 53 | 55 | 56 | 3 |
| 52 | 53 | 55 | 57 | 3 |
| 54 | 53 | 52 | 34 | 3 |
| 54 | 53 | 52 | 61 | 3 |
| 55 | 53 | 52 | 34 | 3 |
| 55 | 53 | 52 | 61 | 3 |
| 56 | 55 | 57 | 58 | 3 |
| 56 | 55 | 57 | 59 | 3 |
| 53 | 55 | 57 | 58 | 3 |
| 53 | 55 | 57 | 59 | 3 |
| 11 | 10 | 19 | 17 | 3 |
| 11 | 10 | 19 | 20 | 3 |
| 4 | 10 | 19 | 17 | 3 |
| 4 | 10 | 19 | 20 | 3 |
| 13 | 15 | 17 | 19 | 3 |
| 13 | 15 | 17 | 18 | 3 |
| 16 | 15 | 17 | 19 | 3 |
| 16 | 15 | 17 | 18 | 3 |
| 30 | 21 | 22 | 24 | 3 |
| 30 | 21 | 22 | 23 | 3 |
| 6 | 21 | 22 | 24 | 3 |
| 6 | 21 | 22 | 23 | 3 |
| 28 | 26 | 24 | 22 | 3 |
| 28 | 26 | 24 | 25 | 3 |
| 27 | 26 | 24 | 22 | 3 |
| 27 | 26 | 24 | 25 | 3 |
| 10 | 19 | 17 | 15 | 3 |
| 10 | 19 | 17 | 18 | 3 |
| 20 | 19 | 17 | 15 | 3 |
| 20 | 19 | 17 | 18 | 3 |
| 9 | 40 | 41 | 50 | 3 |
| 9 | 40 | 41 | 42 | 3 |
| 38 | 40 | 41 | 50 | 3 |
| 38 | 40 | 41 | 42 | 3 |
| 21 | 22 | 24 | 26 | 3 |
| 21 | 22 | 24 | 25 | 3 |
| 23 | 22 | 24 | 26 | 3 |
| 23 | 22 | 24 | 25 | 3 |
| 50 | 41 | 42 | 44 | 3 |
| 50 | 41 | 42 | 43 | 3 |
| 40 | 41 | 42 | 44 | 3 |
| 40 | 41 | 42 | 43 | 3 |
| 65 | 64 | 63 | 37 | 3 |
| 65 | 64 | 63 | 72 | 3 |
| 66 | 64 | 63 | 37 | 3 |
| 66 | 64 | 63 | 72 | 3 |
| 65 | 64 | 66 | 67 | 3 |
| 65 | 64 | 66 | 68 | 3 |
| 63 | 64 | 66 | 67 | 3 |

| | | | | |
|---|---|---|---|---|
| 63 | 64 | 66 | 68 | 3 |
| 9 | 34 | 52 | 53 | 3 |
| 9 | 34 | 52 | 61 | 3 |
| 35 | 34 | 52 | 53 | 3 |
| 35 | 34 | 52 | 61 | 3 |
| 37 | 63 | 72 | 73 | 3 |
| 37 | 63 | 72 | 70 | 3 |
| 64 | 63 | 72 | 73 | 3 |
| 64 | 63 | 72 | 70 | 3 |
| 64 | 66 | 68 | 70 | 3 |
| 64 | 66 | 68 | 69 | 3 |
| 67 | 66 | 68 | 70 | 3 |
| 67 | 66 | 68 | 69 | 3 |
| 48 | 46 | 44 | 42 | 3 |
| 48 | 46 | 44 | 45 | 3 |
| 47 | 46 | 44 | 42 | 3 |
| 47 | 46 | 44 | 45 | 3 |
| 63 | 72 | 70 | 68 | 3 |
| 63 | 72 | 70 | 71 | 3 |
| 73 | 72 | 70 | 68 | 3 |
| 73 | 72 | 70 | 71 | 3 |
| 53 | 52 | 61 | 59 | 3 |
| 53 | 52 | 61 | 62 | 3 |
| 34 | 52 | 61 | 59 | 3 |
| 34 | 52 | 61 | 62 | 3 |
| 66 | 68 | 70 | 72 | 3 |
| 66 | 68 | 70 | 71 | 3 |
| 69 | 68 | 70 | 72 | 3 |
| 69 | 68 | 70 | 71 | 3 |
| 55 | 57 | 59 | 61 | 3 |
| 55 | 57 | 59 | 60 | 3 |
| 58 | 57 | 59 | 61 | 3 |
| 58 | 57 | 59 | 60 | 3 |
| 41 | 42 | 44 | 46 | 3 |
| 41 | 42 | 44 | 45 | 3 |
| 43 | 42 | 44 | 46 | 3 |
| 43 | 42 | 44 | 45 | 3 |
| 52 | 61 | 59 | 57 | 3 |
| 52 | 61 | 59 | 60 | 3 |
| 62 | 61 | 59 | 57 | 3 |
| 62 | 61 | 59 | 60 | 3 |
| 52 | 34 | 35 | 36 | 3 |
| 11 | 10 | 4 | 5 | 3 |
| 19 | 10 | 4 | 5 | 3 |
| 32 | 5 | 4 | 10 | 3 |
| 6 | 5 | 32 | 33 | 3 |
| 4 | 5 | 32 | 33 | 3 |
| 6 | 5 | 4 | 10 | 3 |
| 6 | 5 | 4 | 2 | 3 |
| 32 | 5 | 6 | 21 | 3 |
| 4 | 5 | 6 | 21 | 3 |
| 4 | 5 | 6 | 7 | 3 |
| 30 | 21 | 6 | 5 | 3 |
| 22 | 21 | 6 | 5 | 3 |

```
2   1   9   40    3
2   1   9   34    3
7   1   9   40    3
7   1   9   34    3
1   9   40  38    3
1   9   40  41    3
34  9   40  38    3
34  9   40  41    3
1   9   34  35    3
1   9   34  52    3
40  9   34  35    3
40  9   34  52    3
9   40  38  39    3
9   40  38  37    3
41  40  38  39    3
41  40  38  37    3
9   34  35  37    3
9   34  35  36    3
52  34  35  37    3
11  10  4   2     3
19  10  4   2     3
30  21  6   7     3
22  21  6   7     3
38  37  63  64    3
38  37  63  72    3
35  37  63  64    3
35  37  63  72    3
32  5   4   2     3
32  5   6   7     3
10  4   2   3     3
10  4   2   1     3
5   4   2   3     3
5   4   2   1     3
4   2   1   7     3
4   2   1   9     3
3   2   1   7     3
3   2   1   9     3
5   6   7   1     3
5   6   7   8     3
21  6   7   1     3
21  6   7   8     3
6   7   1   2     3
6   7   1   9     3
8   7   1   2     3
8   7   1   9     3
40  38  37  35    3
40  38  37  63    3
39  38  37  35    3
39  38  37  63    3
38  37  35  34    3
38  37  35  36    3
63  37  35  34    3
63  37  35  36    3
4   6   5   32    4   improper_O_C_X_Y
```

```
******* File topol_CTAB_neu.top *******

#include "oplsaa.ff/forcefield.itp"
#include "C-C_params.itp"
#include "Ph-Ph_params.itp"
#include "CTA.itp"
#include "oplsaa.ff/ions.itp"
#include "oplsaa.ff/spc.itp"
#include "RD.itp"

[ system ]
; Name
RD in CTAB micelle

[ molecules ]
; Compound   #mols
CTA    80
BR     80
RD     1
SOL    28571


******* File topol_SDS_prot.top *******

#include "oplsaa.ff/forcefield.itp"
#include "C-C_params.itp"
#include "Ph-Ph_params.itp"
#include "DS.itp"
; DS.itp is provided in the Supporting information to
; V.S. Farafonov, A.V. Lebed. Jour. Chem. Theor. Comput. 2017, 13, 2742-2750
#include "oplsaa.ff/ions.itp"
#include "oplsaa.ff/spc.itp"
#include "RDH.itp"

[ system ]
; Name
RDH in SDS micelle

[ molecules ]
; Compound       #mols
DS              60
Na              60
RDH             1
CL              1
SOL             16123
```