

## Force field parameters

# 53A6

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### Changes with respect to 53A5 in bold ( [A404] )

- New charges for the polar groups in the amino acid sidechains

Table 2.4.1

**GROMOS mass atom type codes, masses and names**

| mass atom type code | mass in a.m.u. | mass atom name |
|---------------------|----------------|----------------|
| N                   | ATMAS[N]       | ATMASN[N]      |
| 1                   | 1.008          | H              |
| 3                   | 13.019         | CH1            |
| 4                   | 14.027         | CH2            |
| 5                   | 15.035         | CH3            |
| 6                   | 16.043         | CH4            |
| 12                  | 12.011         | C              |
| 14                  | 14.0067        | N              |
| 16                  | 15.9994        | O              |
| 19                  | 18.9984        | F              |
| 23                  | 22.9898        | NA             |
| 24                  | 24.305         | MG             |
| 28                  | 28.08          | SI             |
| 31                  | 30.9738        | P              |
| 32                  | 32.06          | S              |
| 35                  | 35.453         | CL             |
| 39                  | 39.948         | AR             |
| 40                  | 40.08          | CA             |
| 56                  | 55.847         | FE             |
| 63                  | 63.546         | CU             |
| 65                  | 65.37          | ZN             |
| 80                  | 79.904         | BR             |

Table 2.5.2.1

## GROMOS bond-stretching parameters

| Bond-type code    | Force constant                               | Ideal bond length | Examples of usage in terms of nonbonded atom types |                                       |
|-------------------|----------------------------------------------|-------------------|----------------------------------------------------|---------------------------------------|
|                   | $K_{b_n}$<br>$= K_{b_n}^{harm} / 2b_{0_n}^2$ | $b_{0_n}$         |                                                    | $K_{b_n}^{harm}$                      |
|                   | $10^6 \text{kJmol}^{-1} \text{nm}^{-4}$      | nm                |                                                    | $\text{kcalmol}^{-1} \text{\AA}^{-2}$ |
| ICBH[N]<br>ICB[N] | CB[N]                                        | B0[N]             |                                                    |                                       |
| 1                 | 15.7                                         | 0.100             | H – OA                                             | 750                                   |
| 2                 | 18.7                                         | 0.100             | H – N (all)                                        | 895                                   |
| 3                 | 12.3                                         | 0.109             | HC – C                                             | 700                                   |
| 4                 | 37.0                                         | 0.112             | C – O (CO bound to heme)                           | 2220                                  |
| 5                 | 16.6                                         | 0.123             | C – O                                              | 1200                                  |
| 6                 | 13.4                                         | 0.125             | C – OM                                             | 1000                                  |
| 7                 | 12.0                                         | 0.132             | CR1 – NR (6-ring)                                  | 1000                                  |
| 8                 | 8.87                                         | 0.133             | H – S                                              | 750                                   |
| 9                 | 10.6                                         | 0.133             | C – NT, NL                                         | 900                                   |
| 10                | 11.8                                         | 0.133             | C, CR1 – N, NR, CR1, C (peptide, 5-ring)           | 1000                                  |
| 11                | 10.5                                         | 0.134             | C – N, NZ, NE                                      | 900                                   |
| 12                | 11.7                                         | 0.134             | C – NR (no H) (6-ring)                             | 1000                                  |
| 13                | 10.2                                         | 0.136             | C – OA, FTfe – CTfe                                | 900                                   |
| 14                | 11.0                                         | 0.138             | C – NR (heme)                                      | 1000                                  |
| 15                | 8.66                                         | 0.139             | CH2 – C, CR1 (6-ring)                              | 800                                   |
| 16                | 10.8                                         | 0.139             | C, CR1 – CH2, C, CR1 (6-ring)                      | 1000                                  |
| 17                | 8.54                                         | 0.140             | C, CR1, CH2 – NR (6-ring)                          | 800                                   |
| 18                | 8.18                                         | 0.143             | CHn – OA                                           | 800                                   |
| 19                | 9.21                                         | 0.143             | CHn – OM                                           | 900                                   |
| 20                | 6.10                                         | 0.1435            | CHn – OA (sugar)                                   | 600                                   |
| 21                | 8.71                                         | 0.147             | CHn – N, NT, NL, NZ, NE                            | 900                                   |
| 22                | 5.73                                         | 0.148             | CHn – NR (5-ring)                                  | 600                                   |
| 23                | 7.64                                         | 0.148             | CHn – NR (6-ring)                                  | 800                                   |
| 24                | 8.60                                         | 0.148             | O, OM – P                                          | 900                                   |
| 25                | 8.37                                         | 0.150             | O – S                                              | 900                                   |
| 26                | 5.43                                         | 0.152             | CHn – CHn (sugar)                                  | 600                                   |
| 27                | 7.15                                         | 0.153             | C, CHn – C, CHn                                    | 800                                   |
| 28                | 4.84                                         | 0.161             | OA – P                                             | 600                                   |
| 29                | 4.72                                         | 0.163             | OA – SI                                            | 600                                   |
| 30                | 2.72                                         | 0.178             | FE – C (CO bound to heme)                          | 412                                   |
| 31                | 5.94                                         | 0.178             | CH3 – S                                            | 900                                   |
| 32                | 5.62                                         | 0.183             | CH2 – S                                            | 900                                   |
| 33                | 3.59                                         | 0.187             | CH1 – SI                                           | 600                                   |
| 34                | 0.640                                        | 0.198             | NR (His) – FE (43A1)                               | 120                                   |

|    |       |          |                |      |
|----|-------|----------|----------------|------|
| 35 | 0.628 | 0.200    | NR (heme) – FE | 120  |
| 36 | 5.03  | 0.204    | S – S          | 1000 |
| 37 | 0.540 | 0.221    | NR (His) – FE  | 126  |
| 38 | 23.2  | 0.100    | HWat – OWat    | 1110 |
| 39 | 12.1  | 0.110    | HChl – CChl    | 700  |
| 40 | 8.12  | 0.1758   | CChl – CLChl   | 1200 |
| 41 | 8.04  | 0.153    | ODmso – SDmso  | 900  |
| 42 | 4.95  | 0.193799 | SDmso – CDmso  | 890  |
| 43 | 8.10  | 0.176    | CCl4 – CLCl4   | 1200 |
| 44 | 13.1  | 0.1265   | CUrea – OUrea  | 1000 |
| 45 | 10.3  | 0.135    | CUrea – NUrea  | 900  |
| 46 | 8.71  | 0.163299 | HWat – HWat    | 1110 |
| 47 | 2.68  | 0.233839 | HChl – CLChl   | 700  |
| 48 | 2.98  | 0.290283 | CLChl – CLChl  | 1200 |
| 49 | 2.39  | 0.279388 | ODmso – CDmso  | 890  |
| 50 | 2.19  | 0.291189 | CDmso – CDmso  | 890  |
| 51 | 3.97  | 0.2077   | HMet – CMet    | 820  |
| 52 | 3.04  | 0.287407 | 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 nonbonded atom types |                                   |
|----------------------|-----------------------------------------------------------------------|------------------|---------------------------------------------------|-----------------------------------|
|                      | $K_{\theta_n}$<br>$= g(K_{\theta_n}^{harm}, \theta_{n_0}, E_{k_r T})$ | $\theta_{0_n}$   |                                                   | $K_{\theta_n}^{harm}$             |
|                      | $\text{kJmol}^{-1}$                                                   | degree           |                                                   | $\text{kcalmol}^{-1}\text{rad}^2$ |
| ICTH[N]<br>ICT[N]    | CT[N]                                                                 | (T0[N])          |                                                   |                                   |
| 1                    | 380                                                                   | 90.0             | NR (heme) – FE – C (CO bound to heme)             | 90                                |
| 2                    | 420                                                                   | 90.0             | NR(heme) – FE – NR(heme), NR (His)                | 100                               |
| 3                    | 405                                                                   | 96.0             | H – S – CH2                                       | 95                                |
| 4                    | 475                                                                   | 100.0            | CH2 – S – CH3                                     | 110                               |
| 5                    | 420                                                                   | 103.0            | OA – P – OA                                       | 95                                |
| 6                    | 490                                                                   | 104.0            | CH2 – S – S                                       | 110                               |
| 7                    | 465                                                                   | 108.0            | NR, C, CR1(5-ring)                                | 100                               |
| 8                    | 285                                                                   | 109.5            | CHn – CHn – CHn, NR(6-ring) (sugar)               | 60                                |
| 9                    | 320                                                                   | 109.5            | CHn, OA – CHn – OA, NR(ring) (sugar)              | 68                                |
| 10                   | 380                                                                   | 109.5            | H – NL, NT – H, CHn – OA – CHn(sugar)             | 80                                |
| 11                   | 425                                                                   | 109.5            | H – NL – C, CHn      H – NT – CHn                 | 90                                |
| 12                   | 450                                                                   | 109.5            | X – OA, SI – X                                    | 95                                |
| 13                   | 520                                                                   | 109.5            | CH, C – CHn – C, CHn, OA, OM, N, NE               | 110                               |
| 14                   | 450                                                                   | 109.6            | OM – P – OA                                       | 95                                |
| 15                   | 530                                                                   | 111.0            | CHn – CHn – C, CHn, OA, NR, NT, NL                | 110                               |
| 16                   | 545                                                                   | 113.0            | CHn – CH2 – S                                     | 110                               |
| 17                   | 50.0                                                                  | 115.0            | NR(heme) – FE – NR (His) (43A1)                   | 10                                |
| 18                   | 460                                                                   | 115.0            | H – N – CHn                                       | 90                                |
| 19                   | 610                                                                   | 115.0            | CHn, C – C – OA, N, NT, NL                        | 120                               |
| 20                   | 465                                                                   | 116.0            | H – NE – CH2                                      | 90                                |
| 21                   | 620                                                                   | 116.0            | CH2 – N – CH1                                     | 120                               |
| 22                   | 635                                                                   | 117.0            | CH3 – N – C, CHn – C – OM                         | 120                               |
| 23                   | 390                                                                   | 120.0            | H – NT, NZ, NE – C                                | 70                                |
| 24                   | 445                                                                   | 120.0            | H – NT, NZ – H                                    | 80                                |
| 25                   | 505                                                                   | 120.0            | H – N – CH3, H, HC – 6-ring, H – NT – CHn         | 90                                |
| 26                   | 530                                                                   | 120.0            | P, SI – OA – CHn, P                               | 95                                |
| 27                   | 560                                                                   | 120.0            | N, C, CR1 (6-ring, no H)                          | 100                               |
| 28                   | 670                                                                   | 120.0            | NZ – C – NZ, NE                                   | 120                               |

|    |       |        |                                                                     |     |
|----|-------|--------|---------------------------------------------------------------------|-----|
| 29 | 780   | 120.0  | OM – P – OM                                                         | 140 |
| 30 | 685   | 121.0  | O – C – CH <sub>n</sub> , C – CH <sub>3</sub> – N – CH <sub>n</sub> | 120 |
| 31 | 700   | 122.0  | CH <sub>1</sub> , CH <sub>2</sub> – N – C                           | 120 |
| 32 | 415   | 123.0  | H – N – C                                                           | 70  |
| 33 | 730   | 124.0  | O – C – OA, N, NT, NL C – NE – CH <sub>2</sub>                      | 120 |
| 34 | 375   | 125.0  | FE – NR – CR1 (5-ring)                                              | 60  |
| 35 | 750   | 125.0  | –                                                                   | 120 |
| 36 | 575   | 126.0  | H, HC – 5-ring                                                      | 90  |
| 37 | 640   | 126.0  | X(noH) – 5-ring                                                     | 100 |
| 38 | 770   | 126.0  | OM – C – OM                                                         | 120 |
| 39 | 760   | 132.0  | 5, 6 ring connection                                                | 100 |
| 40 | 2215  | 155.0  | SI – OA – SI                                                        | 95  |
| 41 | 91350 | 180.0  | Fe – C – O (CO bound to heme)                                       | 57  |
| 42 | 434   | 109.5  | HWat – OWat – HWat                                                  | 92  |
| 43 | 484   | 107.57 | HChl – CChl – CLChl                                                 | 105 |
| 44 | 632   | 111.30 | CLChl – CChl – CLChl                                                | 131 |
| 45 | 469   | 97.4   | CDmso – SDmso – CDmso                                               | 110 |
| 46 | 503   | 106.75 | CDmso – SDmso – ODmso                                               | 110 |
| 47 | 443   | 108.53 | HMet – OMet – CMet                                                  | 95  |
| 48 | 618   | 109.5  | CLCl4 – CCl4 – CLCl4                                                | 131 |
| 49 | 507   | 107.6  | FTfe – CTfe – FTfe                                                  | 110 |
| 50 | 448   | 109.5  | HTfe – OTfe – CHTfe                                                 | 95  |
| 51 | 524   | 110.3  | OTfe – CHTfe – CTfe                                                 | 110 |
| 52 | 531   | 111.4  | CHTfe – CTfe – FTfe                                                 | 110 |
| 53 | 636   | 117.2  | NUrea – CUrea – NUrea                                               | 120 |
| 54 | 690   | 121.4  | OUrea – CUrea – NUrea                                               | 120 |

Table 2.5.4.1

**GROMOS improper (harmonic) dihedral angle parameters**

| Improper<br>dihedral-angle<br>type code | Force constant                         | Ideal improper<br>dihedral angle | Example of usage       |                                       |
|-----------------------------------------|----------------------------------------|----------------------------------|------------------------|---------------------------------------|
|                                         | $K_{\xi_n}$                            | $\xi_{0_n}$                      |                        | $K_{\xi_n}$                           |
|                                         | $\text{kJmol}^{-1} \text{degree}^{-2}$ | degree                           |                        | $\text{kcalmol}^{-1} \text{rad}^{-2}$ |
| ICQH[N]<br>ICQ[N]                       | CQ[N]                                  | (Q0[N])                          |                        |                                       |
| 1                                       | 0.0510                                 | 0.0                              | planar groups          | 40                                    |
| 2                                       | 0.102                                  | 35.26439                         | tetrahedral<br>centres | 80                                    |
| 3                                       | 0.204                                  | 0.0                              | heme iron              | 160                                   |

Table 2.5.5.1

## GROMOS (trigonometric) dihedral torsional angle parameters

| Dihedral-angle type code | Force constant      | Phase shift      | Multiplicity | Example of usage in terms of nonbonded atom types                    |                       |
|--------------------------|---------------------|------------------|--------------|----------------------------------------------------------------------|-----------------------|
|                          | $K_{\phi_n}$        | $\cos(\delta_n)$ | $m_n$        |                                                                      | $K_{\phi_n}$          |
|                          | $\text{kJmol}^{-1}$ |                  |              |                                                                      | $\text{kcalmol}^{-1}$ |
| ICPH[N]<br>ICP[N]        | CP[N]               | PD[N]            | NP[N]        |                                                                      |                       |
| 1                        | 2.67                | -1.0             | 1            | CHn – CHn – CHn – OA<br>(sugar)<br>C4 – C5 – C6 – O6 <sup>a</sup>    | 0.6                   |
| 2                        | 3.41                | -1.0             | 1            | OA – CHn – OA – CHn, H<br>( $\beta$ sugar)<br>O5 – C1 – O1 – C1',H1  | 0.8                   |
| 3                        | 4.97                | -1.0             | 1            | OA – CHn – CHn – OA<br>(sugar)<br>C4 – C5 – C6 – O6 <sup>a</sup>     | 1.2                   |
| 4                        | 5.86                | -1.0             | 1            | N – CHn – CHn – OA (lipid)                                           | 1.4                   |
| 5                        | 9.35                | -1.0             | 1            | OA – CHn – CHn – OA<br>(sugar)<br>O5 – C5 – C6 – O6 <sup>b</sup>     | 2.2                   |
| 6                        | 9.45                | -1.0             | 1            | OA – CHn – OA – CHn, H<br>( $\alpha$ sugar)<br>O5 – C1 – O1 – C1',H1 | 2.3                   |
| 7                        | 2.79                | +1.0             | 1            | P – O5* – C5* – C4* (dna)                                            | 0.7                   |
| 8                        | 5.35                | +1.0             | 1            | O5* – C5* – C4* – O4* (dna)                                          | 1.3                   |
| 9                        | 1.53                | -1.0             | 2            | C1 – C2 – CAB – CBB<br>(heme)                                        | 0.4                   |
| 10                       | 5.86                | -1.0             | 2            | –C–C–                                                                | 1.4                   |
| 11                       | 7.11                | -1.0             | 2            | –C–OA– (at ring)                                                     | 1.7                   |
| 12                       | 16.7                | -1.0             | 2            | –C–OA– (carboxyl)                                                    | 4.0                   |
| 13                       | 24.0                | -1.0             | 2            | CHn – OA – C – CHn (ester lipid)                                     | 5.7                   |
| 14                       | 33.5                | -1.0             | 2            | –C–N, NT, NE, NZ,NR–                                                 | 8.0                   |
| 15                       | 41.8                | -1.0             | 2            | –C–CR1– (6-ring)                                                     | 10.0                  |
| 16                       | 0.0                 | +1.0             | 2            | –CH1 (sugar)–NR(base)–                                               | 0.0                   |
| 17                       | 0.418               | +1.0             | 2            | O–CH1–CHn–no O                                                       | 0.1                   |
| 18                       | 2.09                | +1.0             | 2            | O–CH1–CHn–O                                                          | 0.5                   |
| 19                       | 3.14                | +1.0             | 2            | –OA–P–                                                               | 0.75                  |
| 20                       | 5.09                | +1.0             | 2            | CHn – O – P – O (dna, phosphodiester)                                | 1.2                   |
| 21                       | 16.7                | +1.0             | 2            | –S–S–                                                                | 4.0                   |
| 22                       | 1.05                | +1.0             | 3            | –OA–P–                                                               | 0.25                  |
| 23                       | 1.26                | +1.0             | 3            | –CHn–OA(no sugar)–                                                   | 0.3                   |
| 24                       | 1.30                | +1.0             | 3            | HTfe – OTfe – CHTfe – CTfe                                           | 0.3                   |
| 25                       | 2.53                | +1.0             | 3            | O5* – C5* – C4* – O4* (dna)                                          | 0.6                   |
| 26                       | 2.93                | +1.0             | 3            | –CH2–S–                                                              | 0.7                   |

|    |      |      |   |                                                               |      |
|----|------|------|---|---------------------------------------------------------------|------|
| 27 | 3.19 | +1.0 | 3 | CHn – O – P – O (dna, phosphodiester)                         | 0.8  |
| 28 | 3.65 | +1.0 | 3 | OA – CHn – OA – CHn, H (α sugar)<br>O5 – C1 – O1 – C1',H1     | 0.9  |
| 29 | 3.77 | +1.0 | 3 | –C,CHn,SI–<br>NT,NL,OA(sugar)–                                | 0.9  |
| 30 | 3.90 | +1.0 | 3 | CHn – CHn – OA – H (sugar)                                    | 0.9  |
| 31 | 4.18 | +1.0 | 3 | HC–C–S–                                                       | 1.0  |
| 32 | 4.69 | +1.0 | 3 | OA – CHn – OA – CHn, H (β sugar)<br>O5 – C1 – O1 – C1',H1     | 1.1  |
| 33 | 5.44 | +1.0 | 3 | HC–C–C–                                                       | 1.3  |
| 34 | 5.92 | +1.0 | 3 | –CHn,SI–CHn–                                                  | 1.4  |
| 35 | 7.69 | +1.0 | 3 | OA – CHn – CHn – OA (sugar)<br>C4 – C5 – C6 – O6 <sup>a</sup> | 1.8  |
| 36 | 8.62 | +1.0 | 3 | N – CHn – CHn – OA (lipid)                                    | 2.1  |
| 37 | 9.50 | +1.0 | 3 | OA – CHn – CHn – OA (sugar)<br>O5 – C5 – C6 – O6 <sup>b</sup> | 2.3  |
| 38 | 0.0  | +1.0 | 4 | –NR–FE–                                                       | 0.0  |
| 39 | 1.0  | -1.0 | 6 | –CHn–N,NE–                                                    | 0.24 |
| 40 | 1.0  | +1.0 | 6 | –CHn–C,NR (ring), CR1–                                        | 0.24 |
| 41 | 3.77 | +1.0 | 6 | –CHn–NT–                                                      | 0.9  |

- a) To be used if – C5 – C6 – O6 and adjacent – C4 – O4 – are axial and the other equatorial, as in galactose  
b) To be used if – C5 – C6 – O6 and adjacent – Cn – On – Hn are both simultaneously axial or equatorial, as in glucose

Table 2.5.6.2.1

**GROMOS 53A6/53B6 non-bonded atom types and integer atom codes**

| integer atom code | atom type | description                                      |
|-------------------|-----------|--------------------------------------------------|
| IAC[N]            | TYPE[N]   |                                                  |
| 1                 | O         | carbonyl oxygen (C=O)                            |
| 2                 | OM        | carboxyl oxygen (CO)                             |
| 3                 | OA        | hydroxyl or sugar oxygen                         |
| 4                 | OE        | ether or ester oxygen                            |
| 5                 | OW        | water oxygen                                     |
| 6                 | N         | peptide nitrogen (NH)                            |
| 7                 | NT        | terminal nitrogen (NH <sub>2</sub> )             |
| 8                 | NL        | terminal nitrogen (NH <sub>3</sub> )             |
| 9                 | NR        | aromatic nitrogen                                |
| 10                | NZ        | Arg NH (NH <sub>2</sub> )                        |
| 11                | NE        | Arg NE (NH)                                      |
| 12                | C         | bare carbon                                      |
| 13                | CH0       | bare sp <sup>3</sup> carbon, 4 bound heavy atoms |
| 14                | CH1       | aliphatic or sugar CH-group                      |
| 15                | CH2       | aliphatic or sugar CH <sub>2</sub> -group        |
| 16                | CH3       | aliphatic CH <sub>3</sub> -group                 |
| 17                | CH4       | methane                                          |
| 18                | CH2r      | CH <sub>2</sub> -group in a ring                 |
| 19                | CR1       | aromatic CH-group                                |
| 20                | HC        | hydrogen bound to carbon                         |
| 21                | H         | hydrogen not bound to carbon                     |
| 22                | DUM       | dummy atom                                       |
| 23                | S         | sulphur                                          |
| 24                | CU1+      | copper (charge 1+)                               |
| 25                | CU2+      | copper (charge 2+)                               |
| 26                | FE        | iron (heme)                                      |
| 27                | ZN2+      | zinc (charge 2+)                                 |
| 28                | MG2+      | magnesium (charge 2+)                            |
| 29                | CA2+      | calcium (charge 2+)                              |
| 30                | P, SI     | phosphor or silicon                              |
| 31                | AR        | argon                                            |
| 32                | F         | fluor (non-ionic)                                |
| 33                | CL        | chlorine (non-ionic)                             |
| 34                | BR        | bromine (non-ionic)                              |
| 35                | CMet      | CH <sub>3</sub> -group in methanol (solvent)     |
| 36                | OMet      | oxygen in methanol (solvent)                     |
| 37                | NA+       | sodium (charge 1+)                               |
| 38                | CL-       | chloride (charge 1-)                             |
| 39                | CChl      | carbon in chloroform (solvent)                   |
| 40                | CLChl     | chloride in chloroform (solvent)                 |
| 41                | HChl      | hydrogen in chloroform (solvent)                 |
| 42                | SDmso     | sulphur in DMSO (solvent)                        |
| 43                | CDmso     | CH <sub>3</sub> -group in DMSO (solvent)         |

|    |       |                                           |
|----|-------|-------------------------------------------|
| 44 | ODmso | oxygen in DMSO (solvent)                  |
| 45 | CCl4  | carbon in carbontetrachloride (solvent)   |
| 46 | CLCl4 | chloride in carbontetrachloride (solvent) |
| 47 | FTfe  | fluor in trifluoroethanol                 |
| 48 | CTfe  | carbon in trifluoroethanol                |
| 49 | CHTfe | CH2-group in trifluoroethanol             |
| 50 | OTfe  | oxygen in trifluoroethanol                |
| 51 | CUrea | carbon in urea                            |
| 52 | OUrea | oxygen in urea                            |
| 53 | NUrea | nitrogen in urea                          |

Table 2.5.6.2.2

**GROMOS 53A6 normal van der Waals parameters**

| integer atom<br>code | atom type | $(C6(I,I))^{1/2}$         | $(C12(I,I))^{1/2}$                  |         |       |
|----------------------|-----------|---------------------------|-------------------------------------|---------|-------|
|                      |           | $[kJmol^{-1} nm^6]^{1/2}$ | $10^{-3}[kJmol^{-1} nm^{12}]^{1/2}$ |         |       |
| I=IAC[N]             | TYPE[N]   |                           | 1                                   | 2       | 3     |
| 1                    | O         | 0.04756                   | 1.000                               | 1.130   | -     |
| 2                    | OM        | 0.04756                   | 0.8611                              | 1.841   | 3.068 |
| 3                    | OA        | 0.04756                   | 1.100                               | 1.227   | -     |
| 4                    | OE        | 0.04756                   | 1.100                               | 1.227   | -     |
| 5                    | OW        | 0.05116                   | 1.623                               | 1.623   | -     |
| 6                    | N         | 0.04936                   | 1.523                               | 1.943   | -     |
| 7                    | NT        | 0.04936                   | 1.523                               | 2.250   | -     |
| 8                    | NL        | 0.04936                   | 1.523                               | 3.068   | -     |
| 9                    | NR        | 0.04936                   | 1.523                               | 1.841   | -     |
| 10                   | NZ        | 0.04936                   | 1.523                               | 2.148   | -     |
| 11                   | NE        | 0.04936                   | 1.523                               | 1.984   | -     |
| 12                   | C         | 0.04838                   | 2.222                               | -       | -     |
| 13                   | CH0       | 0.04896                   | 14.33                               | -       | -     |
| 14                   | CH1       | 0.07790                   | 9.850                               | -       | -     |
| 15                   | CH2       | 0.08642                   | 5.828                               | -       | -     |
| 16                   | CH3       | 0.09805                   | 5.162                               | -       | -     |
| 17                   | CH4       | 0.1148                    | 5.862                               | -       | -     |
| 18                   | CH2r      | 0.08564                   | 5.297                               | -       | -     |
| 19                   | CR1       | 0.07425                   | 3.888                               | -       | -     |
| 20                   | HC        | 0.009200                  | 0.1230                              | -       | -     |
| 21                   | H         | 0.0                       | 0.0                                 | -       | -     |
| 22                   | DUM       | 0.0                       | 0.0                                 | -       | -     |
| 23                   | S         | 0.09992                   | 3.616                               | -       | -     |
| 24                   | CU1+      | 0.02045                   | 0.07159                             | 0.2250  | -     |
| 25                   | CU2+      | 0.02045                   | 0.07159                             | 0.4091  | -     |
| 26                   | FE        | 0.0                       | 0.0                                 | 0.0     | -     |
| 27                   | ZN2+      | 0.02045                   | 0.09716                             | 0.09716 | -     |
| 28                   | MG2+      | 0.008080                  | 0.05838                             | 0.05838 | -     |
| 29                   | CA2+      | 0.03170                   | 0.7057                              | 0.7057  | -     |
| 30                   | P, SI     | 0.1214                    | 4.711                               | 4.711   | -     |
| 31                   | AR        | 0.07915                   | 3.138                               | -       | -     |
| 32                   | F         | 0.03432                   | 0.8722                              | 1.227   | -     |
| 33                   | CL        | 0.09362                   | 3.911                               | -       | -     |
| 34                   | BR        | 0.16630                   | 8.092                               | -       | -     |
| 35                   | CMet      | 0.09421                   | 4.400                               | -       | -     |
| 36                   | OMet      | 0.04756                   | 1.525                               | 1.525   | -     |
| 37                   | NA+       | 0.008489                  | 0.1450                              | 0.1450  | -     |
| 38                   | CL-       | 0.1175                    | 10.34                               | 10.34   | 10.34 |
| 39                   | CChl      | 0.051292                  | 2.0160                              | -       | -     |

|    |       |           |          |        |   |
|----|-------|-----------|----------|--------|---|
| 40 | CLChl | 0.091141  | 3.7101   | -      | - |
| 41 | HChl  | 0.0061400 | 0.065574 | -      | - |
| 42 | SDmso | 0.10277   | 4.6366   | -      | - |
| 43 | CDmso | 0.098050  | 5.1620   | -      | - |
| 44 | ODmso | 0.047652  | 0.86686  | 1.1250 | - |
| 45 | CCl4  | 0.051292  | 2.7568   | -      | - |
| 46 | CLCl4 | 0.087201  | 3.5732   | -      | - |
| 47 | FTfe  | 0.034320  | 1.0000   | 1.0000 | - |
| 48 | CTfe  | 0.048380  | 1.8370   | -      | - |
| 49 | CHTfe | 0.084290  | 5.0770   | -      | - |
| 50 | OTfe  | 0.047560  | 1.2270   | 1.2270 | - |
| 51 | CUrea | 0.069906  | 3.6864   | -      | - |
| 52 | OUrea | 0.048620  | 1.2609   | 1.2609 | - |
| 53 | NUrea | 0.057903  | 1.9877   | 1.9877 | - |

Table 2.5.6.2.3

**GROMOS 53B6 (vacuo) normal van der Waals parameters**

| integer atom code | atom type | $(C6(I,I))^{1/2}$        | $(C12(I,I))^{1/2}$                 |               |               |
|-------------------|-----------|--------------------------|------------------------------------|---------------|---------------|
|                   |           | $[kJmol^{-1}nm^6]^{1/2}$ | $10^{-3}[kJmol^{-1}nm^{12}]^{1/2}$ |               |               |
| I=IAC[N]          | TYPE[N]   |                          | <b>1</b>                           | <b>2</b>      | <b>3</b>      |
| 2                 | OM        | 0.04756 (23.25)          | 0.8611 (421.0)                     | 1.125 (550.0) | 1.125 (550.0) |
| 8                 | NL        | 0.04936 (24.13)          | 1.523 (636.0)                      | 1.943 (950.0) | -             |

Table 2.5.6.2.4

Selection of van der Waals (repulsive)  $(C12(I,I))^{\frac{1}{2}}$  parameters

|    | J     | 1 | 2  | 3  | 4  | 5  | 6 | 7  | 8  | 9  | 10 | 11 | 24   | 25   | 26 | 27   | 28   | 29   | 30   | 32 | 33 | 34 | 36   | 37  | 38  | 44    | 47   | 50   | 52    | 53    |
|----|-------|---|----|----|----|----|---|----|----|----|----|----|------|------|----|------|------|------|------|----|----|----|------|-----|-----|-------|------|------|-------|-------|
| I  |       | O | OM | OA | OE | OW | N | NT | NL | NR | NZ | NE | CU1+ | CU2+ | FE | ZN2+ | MG2+ | CA2+ | P,SI | F  | CL | BR | OMet | NA+ | CL- | ODmso | FTfe | OTfe | OUrea | NUrea |
| 1  | O     | 1 | 1  | 2  | 1  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 1  | 1  | 1  | 2    | 2   | 1   | 1     | 1    | 1    | 1     | 2     |
| 2  | OM    | 1 | 1  | 2  | 1  | 2  | 2 | 2  | 3  | 2  | 3  | 3  | 3    | 3    | 3  | 3    | 3    | 3    | 3    | 1  | 1  | 1  | 2    | 3   | 1   | 1     | 1    | 1    | 1     | 2     |
| 3  | OA    | 2 | 2  | 2  | 2  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 2  | 2  | 2  | 2    | 2   | 2   | 2     | 2    | 2    | 2     | 2     |
| 4  | OE    | 1 | 1  | 2  | 1  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 1  | 1  | 1  | 2    | 2   | 1   | 1     | 1    | 1    | 1     | 2     |
| 5  | OW    | 2 | 2  | 2  | 2  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 2  | 2  | 2  | 2    | 2   | 2   | 2     | 2    | 2    | 2     | 2     |
| 6  | N     | 2 | 2  | 2  | 2  | 2  | 1 | 2  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 2     |
| 7  | NT    | 2 | 2  | 2  | 2  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 2    | 2     | 2     |
| 8  | NL    | 2 | 2  | 2  | 2  | 2  | 1 | 2  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 2     |
| 9  | NR    | 2 | 2  | 2  | 2  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 2  | 2  | 2  | 2    | 2   | 2   | 2     | 2    | 2    | 2     | 2     |
| 10 | NZ    | 2 | 2  | 2  | 2  | 2  | 1 | 2  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 2     |
| 11 | NE    | 2 | 2  | 2  | 2  | 2  | 1 | 2  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 2     |
| 24 | CU1+  | 2 | 2  | 2  | 2  | 2  | 1 | 1  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 1     |
| 25 | CU2+  | 2 | 2  | 2  | 2  | 2  | 1 | 1  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 1     |
| 26 | FE    | 2 | 2  | 2  | 2  | 2  | 1 | 1  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 1     |
| 27 | ZN2+  | 2 | 2  | 2  | 2  | 2  | 1 | 1  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 1     |
| 28 | MG2+  | 2 | 2  | 2  | 2  | 2  | 1 | 1  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 1     |
| 29 | CA2+  | 2 | 2  | 2  | 2  | 2  | 1 | 1  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 1     |
| 30 | P,SI  | 1 | 1  | 1  | 1  | 1  | 1 | 1  | 1  | 1  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 1  | 1  | 1  | 1    | 1   | 1   | 1     | 1    | 1    | 1     | 1     |
| 32 | F     | 1 | 1  | 2  | 1  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 1  | 1  | 1  | 1    | 2   | 1   | 1     | 1    | 1    | 1     | 2     |
| 33 | CL    | 1 | 1  | 1  | 1  | 1  | 1 | 1  | 1  | 1  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 1  | 1  | 1  | 1    | 1   | 1   | 1     | 1    | 1    | 1     | 1     |
| 34 | BR    | 1 | 1  | 1  | 1  | 1  | 1 | 1  | 1  | 1  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 1  | 1  | 1  | 1    | 1   | 1   | 1     | 1    | 1    | 1     | 1     |
| 36 | OMet  | 2 | 2  | 2  | 2  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 2  | 2  | 2  | 2    | 2   | 2   | 2     | 2    | 2    | 2     | 2     |
| 37 | NA+   | 2 | 2  | 2  | 2  | 2  | 1 | 1  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 1    | 2     | 1     |
| 38 | CL-   | 1 | 1  | 2  | 1  | 2  | 2 | 2  | 3  | 2  | 3  | 3  | 3    | 3    | 3  | 3    | 3    | 3    | 3    | 1  | 1  | 1  | 2    | 3   | 1   | 1     | 1    | 1    | 1     | 2     |
| 44 | ODmso | 1 | 1  | 2  | 1  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 1  | 1  | 1  | 2    | 2   | 1   | 1     | 1    | 2    | 1     | 2     |
| 47 | FTfe  | 1 | 1  | 2  | 1  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 1  | 1  | 1  | 2    | 2   | 1   | 1     | 1    | 1    | 1     | 2     |
| 50 | OTfe  | 1 | 1  | 2  | 1  | 2  | 1 | 2  | 1  | 2  | 1  | 1  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 1  | 1  | 1  | 2    | 1   | 1   | 2     | 1    | 2    | 2     | 2     |
| 52 | OUrea | 1 | 1  | 2  | 1  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 2    | 2    | 2  | 2    | 2    | 2    | 2    | 1  | 1  | 1  | 2    | 2   | 1   | 1     | 1    | 2    | 1     | 2     |
| 53 | NUrea | 2 | 2  | 2  | 2  | 2  | 2 | 2  | 2  | 2  | 2  | 2  | 1    | 1    | 1  | 1    | 1    | 1    | 1    | 2  | 2  | 2  | 2    | 1   | 2   | 2     | 2    | 2    | 2     | 2     |

Table 2.5.6.2.5

**GROMOS 53A6 normal van der Waals parameters for mixed atom type pairs (I,J)**

| integer atom<br>code | atom type | integer atom<br>code | atom type | C6(I,J)                                 | C12(I,J)                                   |
|----------------------|-----------|----------------------|-----------|-----------------------------------------|--------------------------------------------|
| I                    |           | J                    |           | $10^{-3} \text{kJmol}^{-1} \text{nm}^6$ | $10^{-6} \text{kJmol}^{-1} \text{nm}^{12}$ |
| 39                   | CChl      | 40                   | CLChl     | 4.6754                                  | 7.4813                                     |
| 39                   | CChl      | 41                   | HChl      | 0.3622                                  | 0.1745                                     |
| 40                   | CLChl     | 41                   | HChl      | 0.6493                                  | 0.3266                                     |

Table 2.5.6.3.1

**GROMOS 53A6/53B6 third-neighbour van der Waals parameters**

| integer atom code | atom type | $(C6(I,I))^{1/2}$                      | $(C12(I,I))^{1/2}$                               |   |   |
|-------------------|-----------|----------------------------------------|--------------------------------------------------|---|---|
|                   |           | $[\text{kJmol}^{-1}\text{nm}^6]^{1/2}$ | $10^{-3}[\text{kJmol}^{-1}\text{nm}^{12}]^{1/2}$ |   |   |
| I=IAC[N]          | TYPE[N]   |                                        | 1                                                | 2 | 3 |
| 1                 | O         | 0.04756                                | 0.8611                                           | - | - |
| 3                 | OA        | 0.04756                                | 1.125                                            | - | - |
| 4                 | OE        | 0.04756                                | 1.125                                            | - | - |
| 6                 | N         | 0.04936                                | 1.301                                            | - | - |
| 7                 | NT        | 0.04936                                | 1.301                                            | - | - |
| 8                 | NL        | 0.04936                                | 1.301                                            | - | - |
| 9                 | NR        | 0.04936                                | 1.301                                            | - | - |
| 10                | NZ        | 0.04936                                | 1.301                                            | - | - |
| 11                | NE        | 0.04936                                | 1.301                                            | - | - |
| 12                | C         | 0.04838                                | 1.837                                            | - | - |
| 13                | CH0       | 0.04838                                | 1.837                                            | - | - |
| 14                | CH1       | 0.05396                                | 1.933                                            | - | - |
| 15                | CH2       | 0.06873                                | 2.178                                            | - | - |
| 16                | CH3       | 0.08278                                | 2.456                                            | - | - |
| 18                | CH2r      | 0.06873                                | 2.178                                            | - | - |
| 19                | CR1       | 0.07435                                | 2.886                                            | - | - |

Table 2.5.6.5.1

**GROMOS 53A6 (53B6) atomic charges and charge group definitions for amino acid residues**

| atom name               | charge in $e$   | occurring in         |
|-------------------------|-----------------|----------------------|
| N                       | -0.310          | all residues         |
| H                       | 0.310           |                      |
| C                       | 0.450           | all residues         |
| O                       | -0.450          |                      |
| CD                      | 0.090 (0.0)     | Arg (charge +1)      |
| NE                      | -0.110 (-0.240) |                      |
| HE                      | 0.240 (0.240)   |                      |
| CZ                      | 0.340 (0.0)     |                      |
| NH1/2                   | -0.260 (-0.480) |                      |
| HH11/12/21/22           | 0.240 (0.240)   |                      |
| NE                      | -0.310          | Argn (neutral)       |
| HE                      | 0.310           |                      |
| CZ                      | <b>0.266</b>    | Argn (neutral)       |
| NH1                     | <b>-0.674</b>   |                      |
| HH1                     | <b>0.408</b>    |                      |
| NH2                     | <b>-0.880</b>   | Argn (neutral)       |
| HH21/22                 | <b>0.440</b>    |                      |
| CG, CD                  | <b>0.290</b>    | Asn, Gln             |
| OD1, OE1                | <b>-0.450</b>   |                      |
| ND2, NE2, NZ            | <b>-0.720</b>   | Asn, Gln             |
| HD21/22, HE21/22, HZ1/2 | <b>0.440</b>    |                      |
| CG, CD                  | 0.270 (0.720)   | Asp, Glu (charge -1) |
| OD1/2, OE1/2            | -0.635 (-0.360) |                      |
| CG, CD                  | <b>0.330</b>    | Asph, Gluh           |
| OD1, OE1                | <b>-0.450</b>   |                      |
| OD2, OE2                | <b>-0.288</b>   |                      |
| HD2, HE2                | <b>0.408</b>    |                      |
| CB                      | -0.100 (0.200)  | Cys (charge -.5)     |
| SG                      | -0.400 (-0.200) |                      |
| CB                      | 0.150           | Cysh                 |
| SG                      | -0.370          |                      |
| HG                      | 0.220           |                      |
| CG                      | <b>0.0</b>      | Hisa (proton at D1)  |
| ND1                     | <b>-0.050</b>   |                      |
| HD1                     | <b>0.310</b>    |                      |
| CD2                     | <b>0.0</b>      |                      |
| HD2                     | <b>0.140</b>    |                      |
| CE1                     | <b>0.0</b>      |                      |
| HE1                     | <b>0.140</b>    |                      |
| NE2                     | <b>-0.540</b>   |                      |
| CG                      | <b>0.0</b>      | Hisb (proton at E2)  |
| ND1                     | <b>-0.540</b>   |                      |
| CD2                     | <b>0.0</b>      |                      |

|              |                 |                                                                  |
|--------------|-----------------|------------------------------------------------------------------|
| HD2          | <b>0.140</b>    |                                                                  |
| CE1          | <b>0.0</b>      |                                                                  |
| HE1          | <b>0.140</b>    |                                                                  |
| NE2          | <b>-0.050</b>   |                                                                  |
| HE2          | <b>0.310</b>    |                                                                  |
| CG           | -0.050 (0.0)    | Hish (charge +1)                                                 |
| ND1          | 0.380 (-0.300)  |                                                                  |
| HD1          | 0.300 (0.300)   |                                                                  |
| CD2          | -0.100 (-0.100) |                                                                  |
| HD2          | 0.100 (0.100)   |                                                                  |
| CE1          | -0.340 (-0.100) |                                                                  |
| HE1          | 0.100 (0.100)   |                                                                  |
| NE2          | 0.310 (-0.300)  |                                                                  |
| HE2          | 0.300 (0.300)   |                                                                  |
| CG, CB, CB   | <b>0.266</b>    | Hyp, Ser, Thr                                                    |
| OD1, OG, OG1 | <b>-0.674</b>   |                                                                  |
| HD1, HG, HG1 | <b>0.408</b>    |                                                                  |
| CE           | 0.127 (0.0)     | Lysh (charge +1)                                                 |
| NZ           | 0.129 (-0.744)  |                                                                  |
| HZ1/2/3      | 0.248 (0.248)   |                                                                  |
| CE           | <b>-0.240</b>   | Lys (neutral)                                                    |
| NZ           | <b>-0.640</b>   |                                                                  |
| HZ1/2        | <b>0.440</b>    |                                                                  |
| CG /CE       | <b>0.241</b>    | Met                                                              |
| SD           | <b>-0.482</b>   |                                                                  |
| CG           | <b>-0.210</b>   | Trp                                                              |
| CD1          | <b>-0.140</b>   |                                                                  |
| HD1          | <b>0.140</b>    |                                                                  |
| CD2          | <b>0.0</b>      |                                                                  |
| NE1          | <b>-0.100</b>   |                                                                  |
| HE1          | <b>0.310</b>    |                                                                  |
| CE2          | <b>0.0</b>      |                                                                  |
| CZ           | <b>0.203</b>    | Tyr                                                              |
| OH           | <b>-0.611</b>   |                                                                  |
| HH           | <b>0.408</b>    |                                                                  |
| C            | <b>-0.140</b>   | all aromatic C-H groups in Phe, Tyr, Trp                         |
| H            | <b>0.140</b>    |                                                                  |
| C            | <b>0.0</b>      | aromatic C connected to an aliphatic CH <sub>n</sub> in Phe, Tyr |
| CH2          | <b>0.0</b>      | aliphatic CH <sub>n</sub> connected to aromatic C in Phe, Tyr    |

The charges for the 53B6 force field are given between parentheses. The atoms that are not listed have zero partial charge and form single atom or multiple atom charge groups.

Table 2.5.6.2

## GROMOS 53A6 atomic charges for various (co)solvents

| atom name | charge in $e$ | occurring in                   |
|-----------|---------------|--------------------------------|
| OW        | -0.82000      | H <sub>2</sub> O (SPC model)   |
| HW1/2     | 0.41000       |                                |
|           |               |                                |
| OW        | -0.84760      | H <sub>2</sub> O (SPC/E model) |
| HW1/2     | 0.42380       |                                |
|           |               |                                |
| OW        | -0.68850      | H <sub>2</sub> O (SPC/L model) |
| HW1/2     | 0.34425       |                                |
|           |               |                                |
| CChl      | 0.17900       | Chloroform                     |
| CLChl     | -0.08700      |                                |
| HChl      | 0.08200       |                                |
|           |               |                                |
| SDmso     | 0.12753       | DMSO                           |
| CDmso     | 0.16000       |                                |
| ODmso     | -0.44753      |                                |
|           |               |                                |
| CMet      | 0.26600       | Methanol                       |
| OMet      | -0.67400      |                                |
| HMet      | 0.40800       |                                |
|           |               |                                |
| CCl4      | 0.0           | Carbontetrachloride            |
| CLCl4     | 0.0           |                                |
|           |               |                                |
| FTFE      | -0.17000      | 2,2,2-Trifluoroethanol         |
| CTFE      | 0.45200       |                                |
| CHTFE     | 0.27300       |                                |
| OTFE      | -0.62500      |                                |
| HTFE      | 0.41000       |                                |
|           |               |                                |
| CUrea     | 0.14200       | Urea                           |
| OUrea     | -0.39000      |                                |
| NUrea     | -0.54200      |                                |
| HUrea     | 0.33300       |                                |

Table 2.5.6.5.3

**GROMOS 53A6 (53B6) atomic charges and charge group definitions for nucleotides**

| atom name              | charge in $e$   | occurring in                             |
|------------------------|-----------------|------------------------------------------|
| O3/5*                  | -0.360 (-0.360) | all nucleotides                          |
| P                      | 0.990 (1.440)   |                                          |
| O1/2P                  | -0.635 (-0.360) |                                          |
| C4*                    | 0.160           | all nucleotides                          |
| O4*                    | -0.360          |                                          |
| C1*                    | 0.200           |                                          |
| N9, N9, N1, N1, N1     | -0.200          | dAde, dGua, dCyt, dThy, Ura              |
| C4, C4                 | 0.200           | dAde, dGua                               |
| C6, C6, C6             | 0.100           | dCyt, dThy, Ura                          |
| H6, H6, H6             | 0.100           | dCyt, dThy, Ura                          |
| N1, N3, N7, N3, N7, N3 | -0.540          | dAde, dAde, dAde, dGua, dGua, dGua, dCyt |
| C2, C8, C8             | 0.440           | dAde, dAde, dGua                         |
| H2, H8, H8             | 0.100           | dAde, dAde, dGua                         |
| C6, C2, C4             | 0.540           | dAde, dGua, dCyt                         |
| N6, N2, N4             | -0.830          | dAde, dGua, dCyt                         |
| H61/62, H21/22, H41/42 | 0.415           | dAde, dGua, dCyt                         |
| N1, N3, N3             | -0.310          | dGua, dThy, Ura                          |
| H1, H3, H3             | 0.310           | dGua, dThy, Ura                          |
| C6, C2, C2, C4, C2, C4 | 0.450           | dGua, dCyt, dThy, dThy, Ura, Ura         |
| O6, O2, O2, O4, O2, O4 | -0.450          | dGua, dCyt, dThy, dThy, Ura, Ura         |
| C5, C5                 | -0.100          | dCyt, Ura                                |
| H5, H5                 | 0.100           | dCyt, Ura                                |

Table 2.5.6.5.4

**GROMOS 53A6 (53B6) atomic charges and charge group definitions for lipids**

| atom name          | charge in $e$   | occurring in |
|--------------------|-----------------|--------------|
| C32, C33, C34, C35 | 0.250 (0.000)   | dppc         |
| N                  | 0.0             | dppc         |
| C31                | 0.0             | dppc         |
| O31, O32           | -0.360 (-0.360) | dppc         |
| O33, O34           | -0.635 (-0.360) | dppc         |
| P                  | 0.990 (1.440)   | dppc         |
| C3                 | 0.0             | dppc         |
| C1, C2             | 0.160           | dppc         |
| O11, O21           | -0.360          | dppc         |
| O12, O22           | -0.380          | dppc         |
| C11, C21           | 0.580           | dppc         |
| C12, ..., C22, ... | 0.0             | dppc         |

Table 2.5.6.5.5

**GROMOS 53A6 (53B6) atomic charges and charge group definitions for carbohydrates**

| atom name      | charge in $e$ | occurring in                                                  |
|----------------|---------------|---------------------------------------------------------------|
| C1, C2, C3, C6 | 0.232         | glucopyranose, polyuronate,<br>terminal – CHn – On – Hn group |
| O2, O3, O6     | -0.642        | glucopyranose, polyuronate,<br>terminal – CHn – On – Hn group |
| HO2, HO3, HO6  | 0.410         | glucopyranose, polyuronate,<br>terminal – CHn – On – Hn group |
| C5             | 0.376         | glucopyranose, polyuronate                                    |
| O5             | -0.480        | glucopyranose, polyuronate                                    |
| O1             | -0.360        | glucopyranose, polyuronate                                    |
| C4             | 0.232         | glucopyranose, polyuronate                                    |
| C6             | 0.360         | polyuronate                                                   |
| O61, O62       | -0.680        | polyuronate                                                   |
| C1             | 0.232         | terminal – C1 – O1 – CM group                                 |
| O1             | -0.360        | terminal – C1 – O1 – CM group                                 |
| CM (methyl)    | 0.232         | terminal – C1 – O1 – CM group                                 |

Table 4.2.1

## 53A6 Solute building blocks

---

| <b>Name</b>                                                     | <b>Description</b> (charges in <i>e</i> )        |
|-----------------------------------------------------------------|--------------------------------------------------|
| <i>amino acids and analogues</i> (L if not indicated otherwise) |                                                  |
| ALA                                                             | Alanine                                          |
| ARG                                                             | Arginine (protonated; charge +1)                 |
| ARGN                                                            | Arginine (deprotonated; neutral)                 |
| ASN                                                             | Asparagine                                       |
| ASN1                                                            | Asparagine (coordinated with ZN)                 |
| ASP                                                             | Aspartic acid (deprotonated; charge -1)          |
| ASPH                                                            | Aspartic acid (protonated; neutral)              |
| CYS                                                             | Cysteine (deprotonated; charge -1/2)             |
| CYSH                                                            | Cysteine (protonated; neutral)                   |
| CYS1                                                            | Cysteine (1 <sup>st</sup> member of S-S bridge)  |
| CYS2                                                            | Cysteine (2 <sup>nd</sup> member of S-S bridge)  |
| GLN                                                             | Glutamine                                        |
| GLU                                                             | Glutamic acid (deprotonated; charge -1)          |
| GLUH                                                            | Glutamic acid (protonated; neutral)              |
| GLY                                                             | Glycine                                          |
| HISA                                                            | Histidine (protonated at ND1; neutral)           |
| HISB                                                            | Histidine (protonated at NE2; neutral)           |
| HISH                                                            | Histidine (protonated at ND1 and NE2; charge +1) |
| HIS1                                                            | Histidine (coupled to HEME at NE2; neutral)      |
| HIS2                                                            | Histidine (coupled to HEMC at NE2; neutral)      |
| HYP                                                             | Hydroxyproline                                   |
| ILE                                                             | Isoleucine                                       |
| LEU                                                             | Leucine                                          |
| LYS                                                             | Lysine (deprotonated; neutral)                   |
| LYSH                                                            | Lysine (protonated; charge +1)                   |
| MET                                                             | Methionine                                       |
| PHE                                                             | Phenylalanine                                    |
| PRO                                                             | Proline                                          |
| SER                                                             | Serine                                           |
| THR                                                             | Threonine                                        |
| TRP                                                             | Tryptophan                                       |
| TYR                                                             | Tyrosine                                         |
| VAL                                                             | Valine                                           |
| DALA                                                            | D-Alanine                                        |
| ABU                                                             | L-2-amino-butanoic acid                          |
| MEBMT                                                           | (4R)-4-[(E)-2-butanyl]-4, N-dimethyl-L-threonine |
| MELEU                                                           | N-methyl-L-leucine                               |
| MEVAL                                                           | N-methyl-L-valine                                |

SAR                      Sarcosine or N-methylglycine

*nucleotides*

|       |                                                                                                   |                  |
|-------|---------------------------------------------------------------------------------------------------|------------------|
| DADE  | 2'-deoxyadenosine 5'-phosphoric acid                                                              |                  |
| DGUA  | 2'-deoxyguanosine 5'-phosphoric acid                                                              | (DNA; charge -1) |
| DCYT  | 2'-deoxycytidine 5'-phosphoric acid                                                               |                  |
| DTHY  | 2'-deoxythymidine 5'-phosphoric acid                                                              |                  |
| ADE   | adenosine 5'-phosphoric acid                                                                      |                  |
| GUA   | guanosine 5'-phosphoric acid                                                                      | (RNA; charge -1) |
| CYT   | cytidine 5'-phosphoric acid                                                                       |                  |
| URA   | uridine 5'-phosphoric acid                                                                        |                  |
| FMNO  | flavin mononucleotide (oxydized, deprotonated at FN5 and FN1; charge -1, OPOHO <sub>2</sub> -)    |                  |
| FMNS  | flavin mononucleotide (semi-reduced, protonated at FN5; charge -1, OPOHO <sub>2</sub> - )         |                  |
| FMNR  | flavin mononucleotide (reduced, protonated at FN5 and FN1; charge -1, OPOHO <sub>2</sub> - )      |                  |
| PFN   | proflavin (protonated at FN5; charge +1)                                                          |                  |
| NADP  | nicotinamide adenine dinucleotide (NAD <sup>+</sup> ; charge -1)                                  |                  |
| NADH  | nicotinamide adenine dinucleotide (NADH; charge -2)                                               |                  |
| NDPH  | nicotinamide adenine dinucleotide phosphate (NADPH; charge -3, OPOHO <sub>2</sub> -)              |                  |
| NDPP  | nicotinamide adenine dinucleotide phosphate (NADP <sup>+</sup> ; charge -2, OPOHO <sub>2</sub> -) |                  |
| NDPHN | nicotinamide adenine dinucleotide phosphate (NADPH; neutral, OPO(OH) <sub>2</sub> )               |                  |

*sugars*

|      |                                             |
|------|---------------------------------------------|
| GLCA | α -D-glucopyranosyl (1-4 linkage; neutral)  |
| GLCB | β-D-glucopyranosyl (1-4 linkage; neutral)   |
| GALA | α-D-galactopyranosyl (1-4 linkage; neutral) |
| GALB | β-D-galactopyranosyl (1-4 linkage; neutral) |
| MANA | α-D-mannoopyranosyl (1-4 linkage; neutral)  |
| MANB | β-D-mannoopyranosyl (1-4 linkage; neutral)  |
| TRH  | trehalose                                   |
| UGLB | β-D-glucuronan (1-4 linkage; neutral)       |
| UMNB | β-D-mannuronan (1-4 linkage; neutral)       |
| UGAA | α-D-galacturonan (1-4 linkage; neutral)     |
| UGUA | α-L-guluronan (1-4 linkage; neutral)        |

*lipids*

|      |                                          |
|------|------------------------------------------|
| DPPC | Dipalmitoylphosphatidylcholine (neutral) |
|------|------------------------------------------|

*other molecules*

|                     |                                                                  |             |
|---------------------|------------------------------------------------------------------|-------------|
| HEME                | heme group (charge -2, acidic groups deprotonated)               |             |
| HEMC                | heme group with bound CO (charge -2, acidic groups deprotonated) |             |
| CYT*                | 3',5'-O-(tetra isopropyl-1,3-disiloxanediyl) cytidine (neutral)  |             |
| MTXH                | methotrexate (protonated at N1; charge -2)                       |             |
| FOL                 | folate (charge -2)                                               |             |
| DHF                 | 7,8-dihydrofolate (charge -2)                                    |             |
| THF                 | 5,6,7,8-tetrahydrofolate (charge -2)                             |             |
| TMP                 | trimethoprim (deprotonated at N1; neutral)                       |             |
| TMPH                | trimethoprim (protonated at N1; neutral)                         |             |
| TMPHP               | trimethoprim (protonated at N1; charge +1)                       |             |
| PDG                 | 3-phospho-D-glycerate (charge -2)                                |             |
| ATP                 | adenosine 5'-triphosphate (ATP; charge -3)                       |             |
| PMB                 | p-methylbenzyl alcoholate (charge -1)                            |             |
| PMBH                | p-methylbenzyl alcohol (neutral)                                 |             |
| BA                  | benzoic acid                                                     |             |
| RTOL                | retinol (neutral)                                                |             |
| TEMP                | tetramethyl pyrrolinyl (nitroxide spin label; neutral)           |             |
| ETH                 | ethyl alcoholate (charge -1)                                     |             |
| ETHH                | ethyl alcohol (neutral)                                          |             |
| CH4                 | methane (united atom)                                            |             |
| AR                  | argon                                                            |             |
| <i>ions</i>         |                                                                  |             |
| SO42-               | SO <sub>4</sub> <sup>2-</sup> ion                                | (charge -2) |
| ZN2+                | zinc ion                                                         | (charge +2) |
| NA+                 | sodium ion                                                       | (charge +1) |
| CL-                 | chlorine ion                                                     | (charge -1) |
| CA2+                | calcium ion                                                      | (charge +2) |
| MG2+                | magnesium ion                                                    | (charge +2) |
| CU1+                | copper ion                                                       | (charge +1) |
| CU2+                | copper ion                                                       | (charge +2) |
| <i>(co)solvents</i> |                                                                  |             |
| H2O                 | water (SPC model, rigid, [81.4] )                                |             |
| H2OE                | water (SPC/E model, rigid, [87.5] )                              |             |
| CHCL3               | chloroform (rigid, [94.36] )                                     |             |
| DMSO                | dimethylsulfoxide (rigid, [04.6] )                               |             |
| CH3OH               | methanol (rigid ) [00.9]                                         |             |
| CCL4                | carbontetrachloride (rigid, [96.33] )                            |             |

|      |                                            |
|------|--------------------------------------------|
| TFE  | 2,2,2-trifluoroethanol (flexible, [00.34]) |
| UREA | Urea (flexible, [04.5])                    |

Table 4.2.2

**53A6 Solvent building blocks**


---

| <b>Name</b> | <b>Description</b>                       |
|-------------|------------------------------------------|
| H2O         | water (SPC model, [81.4])                |
| H2OE        | water (SPC/E model, [87.5])              |
| H2OL        | water (SPC/L model [02.18]) <sup>*</sup> |
| CHCL3       | chloroform ( [94.36] )                   |
| DMSO        | dimethylsulfoxide ( [04.6] )             |
| CH3OH       | methanol [00.9]                          |
| CCL4        | carbontetrachloride ( [96.33] )          |

<sup>\*</sup>) There is no building block for SPC/L in the 53A5 force field, because it requires an additional atom type. We suggest to use atom type 22 (DUM) for the hydrogens with van der Waals parameters  $C6(22,22)^{1/2} = 0.53 \text{ [kJ mol}^{-1} \text{ nm}^{6*1/2}]$  and  $C12(22,22)^{1/2} = 0$ . The constraints should be set to  $r_{OH} = 0.11 \text{ nm}$  and  $r_{HH} = 0.173952 \text{ nm}$ .

Table 4.2.3

## 53A6 End group building blocks

---

| Name                         | Description                        |             |
|------------------------------|------------------------------------|-------------|
| <i>proteins and peptides</i> |                                    |             |
| NH3+                         | N-terminus                         | (charge +1) |
| NH2                          | N-terminus                         | (neutral)   |
| NPRO                         | N-terminus for proline             | (charge +1) |
| COO-                         | O-terminus                         | (charge -1) |
| COOH                         | O-terminus                         | (neutral)   |
| <i>nucleic acids</i>         |                                    |             |
| D5OH                         | 5'-terminal of DNA                 | (neutral)   |
| D3OH                         | 3'-terminal of DNA                 | (neutral)   |
| <i>sugars</i>                |                                    |             |
| C1OH                         | -C1-O1-H1 group for carbohydrates  | (neutral)   |
| C1OC                         | -C1-O1-CH3 group for carbohydrates | (neutral)   |
| COHT                         | -Cn-On-Hon group for carbohydrates | (neutral)   |