

Force field parameters

45A3

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Changes with respect to 43A2 in bold

- Optimised for the aliphatics: J. Comput. Chem. 22, 1205-1218 (2001)

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} $= K_{b_n}^{harm} / 2b_{0_n}^2$	b_{0_n}		$K_{b_n}^{harm}$
	$10^6 \text{kJmol}^{-1} \text{nm}^{-4}$	nm		$\text{kcalmol}^{-1} \text{\AA}^{-2}$
ICBH[N] ICB[N]	CB[N]	BO[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	16.6	0.123	C – O	1200
5	13.4	0.125	C – OM	1000
6	12.0	0.132	CR1 – NR (6-ring)	1000
7	8.87	0.133	H – S	750
8	10.6	0.133	C – NT, NL	900
9	11.8	0.133	C, CR1 – N, NR, CR1, C (peptide, 5-ring)	1000
10	10.5	0.134	C – N, NZ, NE	900
11	11.7	0.134	C – NR (no H) (6-ring)	1000
12	10.2	0.136	C – OA	900
13	11.0	0.138	C – NR (heme)	1000
14	8.66	0.139	CH2 – C, CR1 (6-ring)	800
15	10.8	0.139	C, CR1 – CH2, C, CR1 (6-ring)	1000
16	8.54	0.140	C, CR1, CH2 – NR (6-ring)	800
17	8.18	0.143	CHn – OA	800
18	9.21	0.143	CHn – OM	900
19	6.10	0.1435	CHn – OA (sugar)	600
20	8.71	0.147	CHn – N, NT, NL, NZ, NE	900
21	5.73	0.148	CHn – NR (5-ring)	600
22	7.64	0.148	CHn – NR (6-ring)	800
23	8.60	0.148	O, OM – P	900
24	8.37	0.150	O – S	900
25	5.43	0.152	CHn – CHn (sugar)	600
26	7.15	0.153	C, CHn – C, CHn	800
27	4.84	0.161	OA – P	600
28	4.72	0.163	OA – SI	600
29	5.94	0.178	CH3 – S	900
30	5.62	0.183	CH2 – S	900
31	3.59	0.187	CH1 – SI	600
32	0.640	0.198	NR – FE	120
33	5.03	0.204	S – S	1000
34	0.628	0.200	NR (heme) – FE	120

35	23.2	0.100	HWat – OWat	1110
36	12.1	0.110	HChl – CChl	700
37	8.12	0.1758	CChl – CLChl	1200
38	8.04	0.153	ODmso – SDmso	900
39	4.95	0.195	SDmso – CDmso	900
40	8.10	0.176	CCL4 – CLCL4	1200
41	8.71	0.163299	HWat – HWat	1110
42	2.68	0.233839	HChl – CLChl	700
43	2.98	0.290283	CLChl – CLChl	1200
44	2.39	0.280412	ODmso – CDmso	900
45	2.19	0.292993	CDmso – CDmso	900
46	3.97	0.198842	HMet – CMet	750
47	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_{θ_n} $= g(K_{\theta_n}^{harm}, \theta_{n_0}, E_{k_n T})$	θ_{0_n}		$K_{\theta_n}^{harm}$
	kJmol ⁻¹	degree		kcalmol ⁻¹ rad ⁻²
ICTH[N] ICT[N]	CT[N]	(T0[N])		
1	420	90.0	NR(heme) – FE – NR(heme)	100
2	405	96.0	H – S – CH2	95
3	475	100.0	CH2 – S – CH3	110
4	420	103.0	OA – P – OA	95
5	490	104.0	CH2 – S – S	110
6	465	108.0	NR, C, CR1(5-ring)	100
7	285	109.5	CHn – CHn – CHn, NR(6-ring) (sugar)	60
8	320	109.5	CHn, OA – CHn – OA, NR(ring) (sugar)	68
9	380	109.5	H – NL, NT – H, CHn – OA – CHn(sugar)	80
10	425	109.5	H – NL – C, CHn H – NT – CHn	90
11	450	109.5	X – OA, SI – X	95
12	520	109.5	CH, C – CHn – C, CHn, OA, OM, N, NE	110
13	450	109.6	OM – P – OA	95
14	530	111.0	CHn – CHn – C, CHn, OA, NR, NT, NL	110
15	545	113.0	CHn – CH2 – S	110
16	50.0	115.0	NR(heme) – FE – NR (His)	10
17	460	115.0	H – N – CHn	90
18	610	115.0	CHn, C – C – OA, N, NT, NL	120
19	465	116.0	H – NE – CH2	90
20	620	116.0	CH2 – N – CH1	120
21	635	117.0	CH3 – N – C, CHn – C – OM	120
22	390	120.0	H – NT, NZ, NE – C	70
23	445	120.0	H – NT, NZ – H	80
24	505	120.0	H – N – CH3, H, HC – 6-ring, H – NT – CHn	90
25	530	120.0	P, SI – OA – CHn, P	95
26	560	120.0	N, C, CR1 (6-ring, no H)	100
27	670	120.0	NZ – C – NZ, NE	120
28	780	120.0	OM – P – OM	140
29	685	121.0	O – C – CHn, C CH3 – N –	120

			CHn	
30	700	122.0	CH1, CH2 – N – C	120
31	415	123.0	H – N – C	70
32	730	124.0	O – C – OA, N, NT, NL C – NE – CH2	120
33	375	125.0	FE – NR – CR1 (5-ring)	60
34	750	125.0	–	120
35	575	126.0	H, HC – 5-ring	90
36	640	126.0	X(noH) – 5-ring	100
37	770	126.0	OM – C – OM	120
38	760	132.0	5, 6 ring connnection	100
39	2215	155.0	SI – OA – SI	95
40	434	109.5	HWat – OWat – HWat	92
41	484	107.57	HChl – CChl – CLChl	105
42	632	111.30	CLChl – CChl – CLChl	131
43	469	97.4	CDmso – SDmso – CDmso	110
44	503	106.75	CDmso – SDmso – ODmso	110
45	443	108.53	HMet – OMet – CMet	95
46	618	109.5	CLCl4 – CCl4 – CLCl4	131

Table 2.5.4.1

GROMOS improper (harmonic) dihedral angle parameters

Improper dihedral-angle type code	Force constant	Ideal improper dihedral angle	Example of usage	
	K_{ξ_n}	ξ_{0_n}		K_{ξ_n}
	$\text{kJmol}^{-1} \text{degree}^{-2}$	degree		$\text{kcalmol}^{-1} \text{rad}^{-2}$
ICQH[N] ICQ[N]	CQ[N]	(Q0[N])		
1	0.0510	0.0	planar groups	40
2	0.102	35.26439	tetrahedral 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_{φ_n}	$\cos(\delta_n)$	m_n		K_{φ_n}
	kJmol^{-1}				kcalmol^{-1}
ICPH[N] ICP[N]	CP[N]	PD[N]	NP[N]		
1	5.86	-1.0	2	-C-C-	1.4
2	7.11	-1.0	2	-C-OA- (at ring)	1.7
3	16.7	-1.0	2	-C-OA- (carboxyl)	4.0
4	33.5	-1.0	2	-C-N, NT, NE, NZ,NR-	8.0
5	41.8	-1.0	2	-C-CR1- (6-ring)	10.0
6	0.0	+1.0	2	-CH1 (sugar)-NR(base)-	0.0
7	0.418	+1.0	2	O-CH1-CHn-no O	0.1
8	2.09	+1.0	2	O-CH1-CHn-O	0.5
9	3.14	+1.0	2	-OA-P-	0.75
10	16.7	+1.0	2	-S-S-	4.0
11	1.05	+1.0	3	-OA-P-	0.25
12	1.26	+1.0	3	-CHn-OA(no sugar)-	0.3
13	2.93	+1.0	3	-CH2-S-	0.7
14	3.77	+1.0	3	-C,CHn,SI- NT,NL,OA(sugar)-	0.9
15	4.18	+1.0	3	HC-C-S-	1.0
16	5.44	+1.0	3	HC-C-C-	1.3
17	5.92	+1.0	3	-CHn,SI-CHn-	1.4
18	0.0	+1.0	4	-NR-FE-	0.0
19	1.0	-1.0	6	-CHn-N,NE-	0.24
20	1.0	+1.0	6	-CHn-C,NR (ring), CR1-	0.24
21	3.77	+1.0	6	-CHn-NT-	0.9

Table 2.5.6.2.1

GROMOS 45A3/45B3 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, sugar or ester oxygen
4	OW	water oxygen
5	N	peptide nitrogen (NH)
6	NT	terminal nitrogen (NH ₂)
7	NL	terminal nitrogen (NH ₃)
8	NR	aromatic nitrogen
9	NZ	Arg NH (NH ₂)
10	NE	Arg NE (NH)
11	C	bare carbon
12	CH1	aliphatic or sugar CH-group
13	CH2	aliphatic or sugar CH ₂ -group
14	CH3	aliphatic CH ₃ -group
15	CH4	methane
16	CR1	aromatic CH-group
17	HC	hydrogen bound to carbon
18	H	hydrogen not bound to carbon
19	DUM	dummy atom
20	S	sulphur
21	CU1+	copper (charge 1+)
22	CU2+	copper (charge 2+)
23	FE	iron (heme)
24	ZN2+	zinc (charge 2+)
25	MG2+	magnesium (charge 2+)
26	CA2+	calcium (charge 2+)
27	P, SI	phosphor or silicon
28	AR	argon
29	F	fluor (non-ionic)
30	CL	chlorine (non-ionic)
31	BR	bromine (non-ionic)
32	CMet	CH ₃ -group in methanol (solvent)
33	OMet	oxygen in methanol (solvent)
34	NA+	sodium (charge 1+)
35	CL-	chloride (charge 1-)
36	CChl	carbon in chloroform (solvent)
37	CLChl	chloride in chloroform (solvent)
38	HChl	hydrogen in chloroform (solvent)
39	SDmso	sulphur in DMSO (solvent)
40	CDmso	CH ₃ -group in DMSO (solvent)
41	ODmso	oxygen in DMSO (solvent)
42	CCl4	carbon in carbontetrachloride (solvent)
43	CLCl4	chloride in carbontetrachloride (solvent)

44	CH2r	CH2-group in a ring
45	CH0	bare sp3 carbon, 4 bound heavy atoms

Table 2.5.6.2.2

GROMOS 45A3 normal van der Waals parameters

integer atom code	atom type	$(C6(I,I))^{1/6}$	$(C12(I,I))^{1/6}$		
		$[\text{kJmol}^{-1} \text{ nm}^6]^{1/6}$	$10^{-3}[\text{kJmol}^{-1} \text{ nm}^{12}]^{1/6}$		
I=IAC[N]	TYPE[N]		1	2	3
1	O	0.04756	0.8611	1.125	-
2	OM	0.04756	0.8611	1.841	3.068
3	OA	0.04756	1.125	1.227	-
4	OW	0.05116	1.623	1.623	-
5	N	0.04936	1.301	1.943	-
6	NT	0.04936	1.301	2.250	-
7	NL	0.04936	1.301	3.068	-
8	NR	0.04936	1.301	1.841	-
9	NZ	0.04936	1.301	2.148	-
10	NE	0.04936	1.301	1.984	-
11	C	0.04838	1.837	-	-
12	CH1	0.07790	9.850	-	-
13	CH2	0.08642	5.828	-	-
14	CH3	0.09805	5.162	-	-
15	CH4	0.1148	5.862	-	-
16	CR1	0.07425	3.888	-	-
17	HC	0.009200	0.1230	-	-
18	H	0.0	0.0	-	-
19	DUM	0.0	0.0	-	-
20	S	0.09992	3.616	-	-
21	CU1+	0.02045	0.07159	0.2250	-
22	CU2+	0.02045	0.07159	0.4091	-
23	FE	0.0	0.0	0.0	-
24	ZN2+	0.02045	0.09716	0.09716	-
25	MG2+	0.008080	0.05838	0.05838	-
26	CA2+	0.03170	0.7057	0.7057	-
27	P, SI	0.1214	4.711	-	-
28	AR	0.07915	3.138	-	-
29	F	0.03432	0.8722	1.227	-
30	CL	0.09362	3.911	-	-
31	BR	0.03434	8.092	-	-
32	CMet	0.09421	4.5665	-	-
33	OMet	0.04756	1.1250	1.2270	-
34	NA+	0.008489	0.1450	0.1450	-
35	CL-	0.1175	10.34	10.34	10.34
36	CChl	0.051292	2.0160	-	-
37	CLChl	0.091141	3.7101	-	-
38	HChl	0.0061400	0.065574	-	-
39	SDmso	0.10277	4.6366	-	-

40	CDmso	0.095139	4.6645	-	-
41	ODmso	0.047652	0.86686	1.1250	-
42	CCl4	0.051292	2.7568	-	-
43	CLCl4	0.087201	3.5732	-	-
44	CH2r	0.08564	5.297	-	-
45	CH0	0.04896	14.33	-	-

Table 2.5.6.2.3

GROMOS 43B1 (vacuo) normal 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
2	OM	0.04756	0.8611	1.125	1.125
7	NL	0.04936	1.301	1.943	-

Table 2.5.6.2.4

Selection of van der Waals (repulsive) $(C12(I,I))^{1/6}$ parameters

	J	1	2	3	4	5	6	7	8	9	10	21	22	23	24	25	26	27	29	30	31	33	34	35	41
I		O	OM	OA	OW	N	NT	NL	NR	NZ	NE	CU1+	CU2+	FE	ZN2+	MG2+	CA2+	P,SI	F	CL	BR	OMet	NA+	CL-	ODmso
1	O	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1
2	OM	1	1	2	2	2	2	3	2	3	3	3	3	3	3	3	3	3	1	1	1	2	3	1	1
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
4	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
5	N	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
6	NT	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
7	NL	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
8	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
9	NZ	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
10	NE	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
21	CU1+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
22	CU2+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
23	FE	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
24	ZN2+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
25	MG2+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
26	CA2+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
27	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
29	F	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1
30	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
31	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
33	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
34	NA+	2	2	2	2	1	1	1	2	1	1	1	1	1	1	1	1	1	2	2	2	2	1	2	2
35	CL-	1	1	2	2	2	2	3	2	3	3	3	3	3	3	3	3	3	1	1	1	2	3	1	1
41	ODmso	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	2	2	1	1

Table 2.5.6.2.5

GROMOS 45A3 normal van der Waals parameters for mixed atom type pairs (I,J)

integer atom code	atom type	integer atom code	atom type	C6(I,J)	C12(I,J)
I		J		$10^{-3} \text{kJmol}^{-1} \text{nm}^6$	$10^{-6} \text{kJmol}^{-1} \text{nm}^{12}$
36	CChl	37	CLChl	4.6754	7.4813
36	CChl	38	HChl	0.3622	0.1745
37	CLChl	38	HChl	0.6493	0.3266
39	SDmso	40	CDmso	9.7827	21.6523
39	SDmso	41	ODmso	5.2442	4.6094
40	CDmso	41	ODmso	4.9187	4.7597

Table 2.5.6.3.1

GROMOS 45A3/45B3 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
12	CH1	0.05396	1.933	-	-
13	CH2	0.06873	2.178	-	-
14	CH3	0.08278	2.456	-	-
16	CR1	0.07435	2.886	-	-
44	CH2r	0.06873	2.178	-	-
45	CH0	0.04838	1.837	-	-

Table 2.5.6.5.1

GROMOS 45A3 (45A3) atomic charges and charge group definitions for amino acid residues

atom name	charge in e	occurring in
N	-0.280	all residues
H	0.280	
C	0.380	all residues
O	-0.380	
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	-0.280	Argn (neutral)
HE	0.280	
CZ	0.150	Argn (neutral)
NH1	-0.548	
HH1	0.398	
NH2	-0.830	Argn (neutral)
HH21/22	0.415	
CG, CD	0.380	Asn, Gln
OD1, OE1	-0.380	
ND2, NE2, NZ	-0.830	Asn, Gln, Lys (neutral)
HD21/22, HE21/22, HZ1/2	0.415	
CG, CD	0.270 (0.720)	Asp, Glu (charge -1)
OD1/2, OE1/2	-0.635 (-0.360)	
CG, CD	0.530	Asph, Gluh
OD1, OE1	-0.380	
OD2, OE2	-0.548	
HD2, HE2	0.398	
CB	-0.100 (0.200)	Cys (charge -.5)
SG	-0.400 (-0.200)	
SG	-0.064	Cysh
HG	0.064	
CG	0.0	Hisa (proton at D1)
ND1	0.0	
HD1	0.190	
CD2	0.130	
CE1	0.260	
NE2	-0.580	
CG	0.130	Hisb (proton at E2)
ND1	-0.580	
CD2	0.0	
CE1	0.260	
NE2	0.0	
HE2	0.190	

CG	-0.050 (0.0)	Hish (charge +1)
ND1	0.380 (-0.300)	
HD1	0.300 (0.300)	
CD2	0.0 (0.0)	
CE1	-0.240 (0.0)	
NE2	0.310 (-0.300)	
HE2	0.300 (0.300)	
CG, CB, CB, CZ	0.150	Hyp, Ser, Thr, Tyr
OD1, OG, OG1, OH	-0.548	
HD1, HG, HG1, HH	0.398	
CE	0.127 (0.0)	Lysh (charge +1)
NZ	0.129 (-0.744)	
HZ1/2/3	0.248 (0.248)	
CG	-0.140	Trp
CD1	-0.100	
HD1	0.100	
CD2	0.0	
NE1	-0.050	
HE1	0.190	
CE2	0.0	
C	-0.100	all aromatic C-H groups in Phe, Tyr, Trp
H	0.100	

The charges for the 45B3 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 45A3 atomic charges for various solvents

atom name	charge in e	occurring in
OW	-0.82000	H ₂ O (SPC model)
HW1/2	0.41000	
OW	-0.84760	H ₂ O (SPC/E model)
HW1/2	0.42380	
CChl	0.17900	Chloroform
CLChl	-0.08700	
HChl	0.08200	
SDmso	0.13900	DMSO
CDmso	0.16000	
ODmso	-0.45900	
CMet	0.17600	Methanol
OMet	-0.57400	
HMet	0.39800	
CCl4	0.0	Carbontetrachloride
CLCl4	0.0	

Table 2.5.6.5.3

GROMOS 45A3 (45B3) 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, C6, C6, C6	0.200	
N3, N3	-0.360	dAde, dGua
C2, C2	0.360	
N1, N3	-0.360	dAde, dCyt
C6, C4	0.360	
N6, N2, N4	-0.830	dAde, dGua, dCyt
H61/62, H21/22, H41/42	0.415	
N7, N7	-0.360	dAde, dGua
C8, C8	0.360	
N1, N3, N3	-0.280	dGua, dThy, Ura
H1, H3, H3	0.280	
C6, C2, C2, C2	0.380	dGua, dCyt, dThy, Ura
O6, O2, O2, O2	-0.380	
C4, C4	0.380	dThy, Ura
O4, O4	-0.380	

Table 4.2.1

43A3 Solute building blocks

Name	Description (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 st member of S-S bridge)
CYS2	Cysteine (2 nd 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)
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 ₂ -)	
FMNS	flavin mononucleotide (semi-reduced, protonated at FN5; charge -1, OPOHO ₂ -)	
FMNR	flavin mononucleotide (reduced, protonated at FN5 and FN1; charge -1, OPOHO ₂ -)	
PFN	proflavin (protonated at FN5; charge +1)	
NADP	nicotinamide adenine dinucleotide (NAD ⁺ ; charge -1)	
NADH	nicotinamide adenine dinucleotide (NADH; charge -2)	
NDPH	nicotinamide adenine dinucleotide phosphate (NADPH; charge -3, OPOHO ₂ -)	
NDPP	nicotinamide adenine dinucleotide phosphate (NADP ⁺ ; charge -2, OPOHO ₂ -)	
NDPHN	nicotinamide adenine dinucleotide phosphate (NADPH; neutral, OPO(OH) ₂)	

sugars

GLCA	-D-glucopyranosyl (1-4 linkage; neutral)
GLCB	β-D-glucopyranosyl (1-2 linkage; neutral)
GALB	β-D-galactopyranosyl (1-3 linkage; neutral)

other molecules

HEME	heme group (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 ₄ ²⁻ 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>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, [95.12])
CH3OH	methanol (rigid)
CCL4	carbontetrachloride (rigid, [96.33])

Table 4.2.2

45A3 Solvent building blocks

Name	Description
H2O	water (SPC model, [81.4])
H2OE	water (SPC/E model, [87.5])
CHCL3	chloroform ([94.36])
DMSO	dimethylsulfoxide ([95.12])
CH3OH	methanol
CCL4	carbontetrachloride ([96.33])