

TABLES

Symbol	Label	Config.	Bonds	Comment
C.1	1	Linear	2	sp carbon
C.2	3	Trigonal	3	sp ² carbon
C.3	3	Tetrahedral	4	sp ³ carbon
C.ar	4	Trigonal	3	aromatic
H	5	Linear	1	
O.2	6	Trigonal	1	sp ² oxygen
O.3	7	Tetrahedral	2	sp ³ oxygen

TABLE I. Atom types.

Bond type	Label
Single	1
Double	2
Triple	3
Aromatic	4

TABLE II. Bond types.

Atom <i>i</i>	Atom <i>j</i>	Bond type	$d_{i,j}^0$	$k_{i,j}^0$
1	1	1	0.138000E+01	0.350000E+03
1	2	1	0.144000E+01	0.670000E+03
1	3	1	0.145800E+01	0.320000E+03
1	4	1	0.144000E+01	0.670000E+03
1	5	1	0.105600E+01	0.350000E+03
2	2	1	0.147000E+01	0.350000E+03
2	3	1	0.150100E+01	0.319500E+03
2	4	1	0.151000E+01	0.670000E+03
2	5	1	0.109557E+01	0.346000E+03
2	7	1	0.136522E+01	0.349920E+03
3	3	1	0.153816E+01	0.316800E+03
3	4	1	0.152217E+01	0.320000E+03
3	5	1	0.110225E+01	0.331200E+03
3	7	1	0.143000E+01	0.309450E+03
4	4	1	0.148000E+01	0.500000E+03
4	5	1	0.109234E+01	0.384000E+03
4	7	1	0.140849E+01	0.350000E+03
5	7	1	0.992045E+00	0.503750E+03
7	7	1	0.148000E+01	0.310000E+03
1	2	2	0.144000E+01	0.670000E+03
2	2	2	0.133500E+01	0.670000E+03
6	2	2	0.120746E+01	0.777600E+03
1	1	3	0.120400E+01	0.700000E+03
4	4	4	0.139746E+01	0.400000E+03

TABLE III. Bond stretching parameters. Distances are in Å and the force constants are in kcal/mol. The parameters not listed are equal to those reported in Ref. [18].

Atom <i>i</i>	Atom <i>j</i>	Atom <i>k</i>	θ^0	k^0
1	2	5	0.120328E+03	0.240000E-01
1	2	6	0.122022E+03	0.600000E-01
2	7	4	0.109937E+03	0.200000E-01
2	7	5	0.105901E+03	0.200000E-01
3	3	3	0.110319E+03	0.240000E-01
3	3	4	0.108843E+03	0.240000E-01
3	3	5	0.111074E+03	0.160000E-01
3	4	4	0.122230E+03	0.240000E-01
4	3	4	0.110207E+03	0.180000E-01
4	4	3	0.122230E+03	0.240000E-01
4	4	4	0.119475E+03	0.240000E-01
4	4	5	0.119653E+03	0.180000E-01
4	4	7	0.118536E+03	0.420000E-01
4	7	2	0.109937E+03	0.200000E-01
5	3	5	0.108619E+03	0.240000E-01
5	4	4	0.119653E+03	0.180000E-01
5	7	2	0.105901E+03	0.200000E-01
6	2	7	0.126152E+03	0.300000E-01
7	2	7	0.113752E+03	0.240000E-01

TABLE IV. Bond bending parameters. Angles are in degrees and the force constants are in kcal/mol. The parameters not listed are equal to those reported in Ref. [18].

Atom i	k^0
2	0.130000E+03
4	0.130000E+03

TABLE V. Out of planarity energy parameters. The force constants are in kcal/mol. The parameters not listed are equal to those reported in Ref. [18].

Atom i	Atom j	Atom k	Atom l	Bond Type	k^0	s
2	7	4	4	1	0.150000E+01	-.200000E+01
3	3	4	4	1	0.420000E+00	0.200000E+01
4	4	3	3	1	0.420000E+00	0.200000E+01
4	4	7	2	1	0.150000E+01	-.200000E+01

TABLE VI. Bond torsion parameters. Angles are in degrees and the force constants are in kcal/mol. The parameters not listed are equal to those reported in Ref. [18]

Atom i	Atom j	$\sigma_{i,j}$	$k_{i,j}^0$
5	5	0.420000D-01	0.264000D+01
5	6	0.697997D-01	0.292000D+01

TABLE VII. Lennard-Jones parameters. Distances are in Å and the force constants are in kcal/mol. The parameters not listed are equal to those reported in Ref. [18].

Atom i	Atom j	$\sigma_{i,j}^{(1,4)}$	$k_{i,j}^{(1,4)}$
2	4	0.167189D+00	0.340000D+01
4	2	0.167189D+00	0.340000D+01
4	7	0.473697D+01	0.242000D+01
5	5	0.861962D-02	0.300000D+01
5	6	0.000000D+00	0.288000D+01
6	5	0.000000D+00	0.288000D+01
7	4	0.473697D+01	0.242000D+01

TABLE VIII. Parameters for the 1-4 interactions. Distances are in Å and the force constants are in kcal/mol. The parameters not listed are equal to those reported in Ref. [18].