LJ parameters of the 103 atoms and six molecules implemented in the mcmgs code

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TABLE I. LJ parameters of the 103 atoms and six molecules implemented in the code. σ is in Å and ϵ in eV. Part I.

	σ	ϵ	Source		σ	ϵ	Source
Ac	3.099	0.001431	[1]	Mg	2.691	0.004813	[1]
Ag	2.644	0.345000	[2]	Mn	2.587	0.047219	[3]
Al	2.574	0.507220	[4]	Mo	2.489	0.151000	[5]
Am	3.012	0.000607	[1]	N_2	3.663	0.008352	[6]
Ar	3.420	0.010368	[7]	N	3.310	0.003214	[8]
As	3.769	0.013398	[1]	Na	3.143	0.001220	[9]
At	4.232	0.012314	[1]	Nb	2.820	0.002558	[1]
Au	2.934	0.001691	[1]	Nd	3.185	0.000434	[1]
B	3.453	0.004116	[10]	Ne	2.780	0.003008	[7]
Ba	3.299	0.015783	[1]	Ni	2.239	0.660920	[4]
Be	2.446	0.003686	[1]	No	2.894	0.000477	[1]
Bi	3.050	0.059000	[11]	Np	3.050	0.000824	[1]
Bk	2.975	0.000564	[1]	O_2	3.297	0.004540	[12]
Br	3.519	0.016043	[13]	O	3.033	0.004150	[13]
C	3.400	0.003744	[14]	Os	2.780	0.001604	[1]
Ca	3.028	0.010320	[1]	P	3.656	0.019100	[5]
Cd	2.700	0.000259	[15]	Pa	3.050	0.000954	[1]
Ce	3.168	0.000564	[1]	Pb	3.000	0.008291	[15]
Cf	2.952	0.000564	[1]	Pd	2.583	0.002081	[1]
CH_4	3.730	0.012748	[16]	Pm	3.160	0.000390	[1]
Cl	3.350	0.014951	[17]	Po	4.195	0.014092	[1]
Cm	2.963	0.000564	[1]	Pr	3.213	0.000434	[1]
CO_2	3.832	0.019868	[6]	Pt	2.454	0.003469	[1]
Co	2.499	0.051859	[3]	Pu	3.050	0.000694	[1]
Cr	2.281	0.673220	[4]	Ra	3.276	0.017517	[1]

TABLE II. LJ parameters of the 103 atoms and six molecules implemented in the code. σ is in Å and ϵ in eV. Part II.

	σ	ϵ	Source		σ	ϵ	Source
Cs	3.501	0.006415	[9]	Rb	3.362	0.005106	[9]
Cu	2.297	0.520310	[4]	Re	2.632	0.002862	[1]
Dy	3.054	0.000304	[1]	Rh	2.609	0.002298	[1]
Er	3.021	0.000304	[1]	Rn	4.530	0.023458	[18]
Es	2.939	0.000520	[1]	Ru	2.640	0.002428	[1]
Eu	3.112	0.000347	[1]	S	3.590	0.014916	[13]
F	3.217	0.005419	[9]	Sb	3.938	0.019469	[1]
Fe	2.645	0.030265	[3]	Sc	2.936	0.000824	[1]
Fm	2.927	0.000520	[1]	Se	3.746	0.012618	[1]
Fr	4.365	0.002168	[1]	Si	2.574	0.059400	[5]
Ga	3.905	0.017994	[1]	Sm	3.136	0.000347	[1]
Gd	3.001	0.000390	[1]	Sn	3.913	0.024585	[1]
Ge	3.813	0.016433	[1]	Sr	3.244	0.010190	[1]
H_2	2.970	0.002870	[19]	Ta	2.824	0.003512	[1]
H	2.846	0.000659	[13]	Tb	3.074	0.000304	[1]
H_2O	2.725	0.030655	[20]	Tc	2.671	0.002081	[1]
He	2.640	0.000939	[21]	Te	3.982	0.017257	[1]
Hf	2.798	0.003122	[1]	Th	3.025	0.001127	[1]
Hg	2.969	0.064630	[22]	Ti	2.556	0.039761	[3]
Ho	3.037	0.000304	[1]	Tl	3.873	0.029485	[1]
I	3.909	0.007829	[9]	Tm	3.006	0.000260	[1]
In	2.810	0.052290	[23]	U	3.025	0.000954	[1]
Ir	2.530	0.003165	[1]	V	2.391	0.871730	[4]
K	3.262	0.003965	[9]	W	2.734	0.002905	[1]
Kr	3.660	0.015110	[7]	Xe	4.080	0.019519	[7]

TABLE III. LJ parameters of the 103 atoms and six molecules implemented in the code. σ is in Å and ϵ in eV. Part III.

	σ	ϵ	Source		σ	ϵ	Source
La	3.138	0.000737	[1]	Y	2.980	0.003122	[1]
Li	2.051	0.013225	[24]	Yb	2.989	0.009886	[1]
Lr	2.883	0.000477	[1]	Zn	0.998	0.008291	[25]
Lu	3.243	0.001778	[1]	Zr	2.910	0.735981	[26]
Md	2.917	0.000477	[1]				
C-H_2	3.190	0.002628	[19]				

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