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SUPPLEMENTARY MATERIAL TO

Consistent force field for metalloporphyrins

LJUBICA ANDJELKOVIĆ[1], SONJA GRUBIŠIĆ[1#], IVANA DJORDJEVIĆ[1], MATIJA ZLATAR[1], SVETOZAR NIKETIĆ[1#] and MAJA GRUDEN-PAVLOVIĆ[2*#]

[1]*Center for Chemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11001 Belgrade and* [2]*Faculty of Chemistry, University of Belgrade, Studentski Trg 12–16, 11001 Belgrade, Serbia*

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CFF PARAMETERS FOR METALLOPORPHYRINS

TABLE S-I. Bond stretching parameters

Bond	k_r / kcal mol^{-1} Å^{-2}	r_0 / Å	Bond	k_r / kcal mol^{-1} Å^{-2}	r_0 / Å
Ni–N	359.50	1.940	C_β–Cl	487.48	1.720
Tb–N	359.50	2.360	C_β–Br	355.86	1.881
N–C_α	1594.74	1.375	C_p–C_p	1380.48	1.394
C_α–C_β	1380.48	1.337	C_p–H	661.80	1.084
C_β–H	661.00	1.101	C_p–C_m	632.72	1.497
C_{sp3}–C_{sp3}	633.72	1.523	C_m–C_α	1409.24	1.370
C_{sp3}–H	661.48	1.113	C_β–C_{sp3}	1409.29	1.470

TABLE S-II. Angle bending parameters

Angle	k_θ / kcal mol^{-1} rad^{-2}	θ_0 / *rad*	Angle	k_θ / kcal mol^{-1} rad^{-2}	θ_0 / *rad*
N–M–N(cis)	5.00	1.571	C_{sp3}–C_{sp3}–H	20.84	1.902
N–M–N(trans)	30.32	3.146	H–C_{sp3}–H	46.08	1.902
M–N–C_α	129.60	2.182	C_α–N– C_α	61.92	1.832
C_α–C_β–H	129.60	2.182	C_p–C_p–H	51.84	2.094
C_β–C_β–H	129.60	2.182	C_p–C_p–C_m	61.92	2.094
N–C_α–C_β	129.60	2.182	C_α–C_m–C_α	61.92	2.120
C_α–C_β–C_β	129.60	2.182	N–C_α–C_m	61.92	2.175
C_m–C_α–C_β	129.60	2.182	C_α–C_β–Cl	134.00	2.094
C_β–C_β–Cl	129.60	2.182	C_p–C_p–C_p	61.92	2.094
C_α–C_m–C_p	129.60	2.182	C_β–C_β–Br	109.90	2.094
C_α–C_β–Br	109.90	2.094	C_β–C_β–C_{sp3}	134.00	2.094
C_{sp3}–C_{sp3}–C_{sp3}	61.92	2.094	C_β–C_{sp3}–C_{sp3}	80.80	1.902

* Corresponding author. E-mail: gmaja@chem.bg.ac.rs
# Serbian Chemical Society member.

TABLE S-III. Torsion angle parameters

Angle	k_Φ / kcal mol^{-1}	n	Angle	k_Φ / kcal mol^{-1}	n
C_m–C_α–N–M	1.57	–2.0	C_β–C_β–C_α–C_m	10.00	–2.0
C_α–C_β–C_β–C_α	3.00	–2.0	H–C_β–C_β–H	3.00	–2.0
H–C_β–C_β–C_α	3.00	–2.0	C_p–C_m–C_α–C_β	10.00	–2.0
C_p–C_p–C_m–C_α	0.50	–2.0	C_p–C_p–C_p–C_p	7.50	–2.0
C_m–C_p–C_p–H	7.50	–2.0	H–C_p–C_p–H	7.50	–2.0
Cl–C_β–C_β–Cl	3.00	–2.0	Cl–C_β–C_β–C_α	3.00	–2.0
Cl–C_β–C_β–H[a]	3.00	–2.0	H–C_β–C_β–C_α	3.00	–2.0
C_α–N–C_α–C_m	3.00	–2.0	H–C_{sp3}–C_{sp3}–C_m	0.50	3.0
H–C_{sp3}–C_{sp3}–C_{sp3}	0.00	0.0	Cl–C_β–C_β–Cl[a]	3.00	–2.0
H–C_{sp3}–C_{sp3}–C_β	0.50	3.0	H–C_{sp3}–C_β–C_β	0.24	6.0

[a]If the substituent is Br, the torsion angle parameters are the same

TABLE S-IV. Out-of-plane bending parameters

Conformation	k_ω / kcal mol^{-1}
N–C_β–C_m.C_α	10
C_α–H–C_α.C_m	90
C_β–H–C_α.C_β	10
C_α– C_p–C_α.C_m	90
C_α–C_{sp3}–C_α.C_m	90
C_β–X–C_α.C_β	10

TABLE S-V. Van der Waals parameters (all types of C atoms in C–Br)

Bond	ε / kcal mol^{-1}	r^* / Å	Bond	ε / kcal mol^{-1}	r^* / Å
M–C_β	0.130	3.24	M–H	0.134	2.70
M–C_m	0.130	3.24	M–Cl	0.115	3.28
M–C_p	0.130	3.24	N–H	0.051	3.32
N–C_β	0.049	3.76	N–C_α	0.049	3.76
M–C_m	0.049	3.76	H–H	0.047	3.00
C_α–C_β	0.044	3.88	C_α–C_α	0.044	3.88
C_β–C_β	0.044	3.88	C_m–H	0.046	3.34
C_m–C_α	0.046	3.88	C_m–C_β	0.046	3.88
C_p–C_p	0.044	3.88	N–Cl	0.115	3.85
H–C_β	0.046	3.34	H–C_α	0.046	3.34
Cl–C_β	0.103	3.97	Cl–C_α	0.103	3.97
Cl–Cl	0.240	4.00	H–Cl	0.106	3.53
Cl–C_m	0.103	3.97	N–N	0.055	3.64
H–C_p	0.046	3.34	C_p–C_p	0.044	3.88
C_p–C_m	0.044	3.88	C_p–C_α	0.044	3.88
C_p–C_β	0.044	3.88	C_p–N	0.049	3.74
C_p–Cl	0.103	3.97	C[a]–Br	0.119	4.12
Br–Br	0.320	4.36	M–Br	0.349	3.38
N–Br	0.133	4.00	H–Br	0.122	3.68
C_{sp3}–H	0.046	3.34	C_{sp3}–C_{sp3}	0.044	3.88
C_{sp3}–C_m	0.044	3.88	C_{sp3}–C_β	0.044	3.88
C_{sp3}–M	0.131	3.10	C_{sp3}–N	0.049	3.72

TABLE S-VI. Electrostatic parameters

Species	*Esu*
M	0.543
Cl	–0.315
C_α	0.285
C_p	–0.080
Br	0.032
N	–0.665
C_m	0.334
C_β	0.285
H	0.285
H[a]	0.070

[a]This value was used for CFF calculation of Br-substituted TPP molecules