

Accurate Redox Potentials of Transition Metal Complexes Calculated Using Density Functional Theory and Electrostatics

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ABBREVIATIONS

TMC	transition metal complexes
DFT	density functional theory
LSDA	local spin density approximation
RMSD	root mean square deviation
MAD	mean absolute deviation
IUPAC	International Union of Pure and Applied Chemistry
ESP	electrostatic potential
RESP	restrained electrostatic potential
vdW	van der Waals
SHE	standard hydrogen electrode
W	water
AN	acetonitrile
DMF	dimethylformamide
HS	high spin
LS	low spin
ET	electron transfer
bRC	bacterial reaction center
PSII	photosystem II