Inorganics **2019**, *7*

Supplementary Materials: Computational characterization of single electron transfer steps in water oxidation

Adiran de Aguirre, Ignacio Funes-Ardoiz and Feliu Maseras

Cartesian Coordinates and Energies (in hartrees)

1c

E = -1255.43774291

G_{corr} = 0.180434

N	-1.47506000	-0.66765000	-2.23531000
N	-1.09191000	-1.90762000	-0.02735000
N	-0.56407000	0.15034000	1.31839000
N	-1.35940000	1.83710000	-0.43857000
C	-0.70508000	-2.19279000	1.25025000
C	-0.41322000	-1.00549000	2.02915000
C	-0.57638000	-3.47218000	1.83339000
C	-0.03941000	-1.12488000	3.38747000
C	-0.19994000	-3.55657000	3.16096000
H	-0.77906000	-4.35784000	1.24712000
C	0.06075000	-2.39021000	3.93398000
H	0.17047000	-0.24072000	3.97287000
H	-0.10066000	-4.53242000	3.62657000
H	0.35472000	-2.49978000	4.97345000
C	-0.39038000	1.45198000	1.71977000
C	-0.84285000	2.43418000	0.63429000
C	-1.53688000	-2.74158000	-1.01505000
C	-1.31555000	0.11776000	-3.45266000
H	-0.80123000	-0.47612000	-4.21603000
H	-2.28567000	0.43665000	-3.85120000
H	-0.71204000	0.99844000	-3.23608000
C	-1.92051000	2.65888000	-1.50075000
H	-1.13793000	3.07637000	-2.14648000
H	-2.59784000	2.05674000	-2.10502000
H	-2.48718000	3.48997000	-1.06645000
C	-1.70662000	-1.98025000	-2.33283000
O	-1.76627000	-3.94582000	-0.91103000
O	-1.99477000	-2.60255000	-3.37763000
O	0.04085000	1.82217000	2.80919000
O	-0.75247000	3.66595000	0.84320000
Cu	-0.96668000	-0.07480000	-0.50090000
H	1.55527000	0.67895000	-0.36818000
O	1.19690000	0.04640000	-1.01374000

-OH

E = -75.9476898532

G_{corr} = -0.00776

O	-4.35016100	2.28678800	0.00000000
H	-4.67435600	3.20228700	0.00000000

MT_A-1d-S

E = -1255.62933375

G_{corr} = 0.180469

N	-1.52074500	-0.66363600	-2.23638300
N	-1.05746900	-1.90545000	-0.04789000
N	-0.60529500	0.16209800	1.33432400
N	-1.35149600	1.83750200	-0.45225200
C	-0.68062900	-2.19320200	1.27603700
C	-0.42144300	-1.03582600	2.04849700
C	-0.54405300	-3.46578800	1.84289600
C	-0.04395200	-1.15719400	3.39167500
C	-0.15989200	-3.57765600	3.18528100
H	-0.73508800	-4.34795400	1.24636800
C	0.08555000	-2.43498200	3.95178600
H	0.15316800	-0.27269400	3.98225100
H	-0.05233600	-4.56501000	3.62620200
H	0.38817200	-2.52938400	4.99119600
C	-0.48525100	1.42843800	1.74948900
C	-0.88972900	2.42110100	0.65323500
C	-1.53798600	-2.72258500	-0.99300900
C	-1.37564900	0.10090100	-3.46942800
H	-0.89350700	-0.51231500	-4.23901200
H	-2.34598000	0.43789200	-3.85384100
H	-0.74755600	0.97090000	-3.28113300
C	-1.81723200	2.67654500	-1.54658600
H	-0.98539200	3.03082700	-2.16891500
H	-2.51286600	2.11326800	-2.16778000
H	-2.34289800	3.55113200	-1.14785100
C	-1.74666600	-1.97650900	-2.31501000
O	-1.77036800	-3.94447100	-0.89073200
O	-2.05374500	-2.61209900	-3.35236800
O	-0.11630200	1.82117400	2.87547000
O	-0.80448400	3.65580700	0.86958200
Cu	-0.99186400	-0.06996200	-0.49259100
H	1.52982300	0.74659000	-0.33407000
O	1.29306200	0.18515000	-1.09065000

·OH

E = -75.7419532424

G_{corr} = -0.008698

O	-4.34786300	2.28030000	0.00000000
H	-4.67665400	3.20877500	0.00000000

MECP_A(S-T)

E (S) = -1255.62429553

G_{corr} (S) = 0.175936

E (T) = -1255.6242964

G_{corr} (T) = 0.175936

N	-1.47000900	-0.72871000	-2.30361600
N	-1.02034700	-1.92995500	-0.04764000
N	-0.57966600	0.15760300	1.35067600
N	-1.31573400	1.89852200	-0.42637500
C	-0.67252700	-2.20197400	1.26174300
C	-0.42561300	-1.02398100	2.05079000
C	-0.54520800	-3.47619700	1.85007100
C	-0.08613900	-1.15566100	3.41276400
C	-0.19591100	-3.57840200	3.19294200
H	-0.71983700	-4.36299400	1.25564900
C	0.02716900	-2.42508200	3.97047400
H	0.09072500	-0.27204500	4.01105800
H	-0.09360000	-4.56186500	3.64360300
H	0.30125200	-2.52303700	5.01711000
C	-0.48121500	1.43180000	1.78694300
C	-0.87024000	2.44652700	0.69833400
C	-1.45777000	-2.76820400	-1.01108600
C	-1.48225000	0.01705700	-3.55424800
H	-1.00350900	-0.55802300	-4.35611000
H	-2.50603600	0.25824300	-3.87162900
H	-0.93121800	0.94881200	-3.42092000
C	-1.75654500	2.79019100	-1.48891400
H	-0.90630700	3.23498400	-2.02544400
H	-2.36176900	2.22932900	-2.20138400
H	-2.36418900	3.60810800	-1.08364900
C	-1.68240500	-2.04021700	-2.34781200
O	-1.66929300	-3.99117900	-0.90582600
O	-2.01246800	-2.71604700	-3.36148400
O	-0.14044200	1.81321800	2.92245300
O	-0.77396600	3.67964200	0.95530200
Cu	-0.91496000	-0.05144400	-0.54333700
H	1.57792600	0.79734000	-0.38289800
O	1.30200200	0.20625000	-1.10275100

MT_A-1d-T

E = -1255.62878018

G_{corr} = 0.174743

N	-1.43518500	-0.79819900	-2.36877400
N	-0.97112900	-1.94722300	-0.05706000
N	-0.56353200	0.15647700	1.35923800
N	-1.29199600	1.96195600	-0.40052100
C	-0.65776300	-2.20659200	1.23737800
C	-0.41373500	-1.00482100	2.04394800
C	-0.54583200	-3.48300800	1.84729000
C	-0.08574700	-1.15052100	3.41806900

C	-0.21659300	-3.57685700	3.18551100
H	-0.71397000	-4.37114400	1.25344900
C	0.00826500	-2.41300700	3.97014400
H	0.09502300	-0.26848100	4.01685600
H	-0.12445000	-4.55544700	3.64816900
H	0.26451700	-2.52149400	5.02026600
C	-0.48623300	1.43746000	1.82147400
C	-0.88177900	2.47620800	0.74996800
C	-1.41606800	-2.80672500	-1.01579700
C	-1.56126000	-0.08974400	-3.63436800
H	-1.06648200	-0.63220200	-4.45086300
H	-2.61470200	0.04985000	-3.91674200
H	-1.09674500	0.89353700	-3.53676600
C	-1.71436900	2.90166100	-1.43007900
H	-0.85386400	3.40981900	-1.88949400
H	-2.24888000	2.36099600	-2.21334700
H	-2.37867800	3.67541000	-1.02324400
C	-1.64511500	-2.10724400	-2.37340000
O	-1.65171200	-4.01920200	-0.88394400
O	-1.99561500	-2.82323000	-3.36007200
O	-0.16112000	1.80255100	2.96279500
O	-0.80944300	3.70455900	1.06185900
Cu	-0.84455700	-0.02240200	-0.60842900
H	1.59791400	0.85195000	-0.37802400
O	1.34073600	0.26772000	-1.11070100

MT_B-1c

E = -1179.48229854

G_{corr} = 0.172624

N	-1.43549600	-0.66014400	-2.23462500
N	-1.04827700	-1.90397000	-0.03361000
N	-0.54115000	0.15073300	1.32359700
N	-1.30314200	1.81529900	-0.46427900
C	-0.69415000	-2.19102100	1.25230400
C	-0.40902300	-1.00300900	2.03926900
C	-0.59179700	-3.47165200	1.83863200
C	-0.05852200	-1.12134200	3.40261300
C	-0.23962900	-3.55417000	3.17132600
H	-0.79638600	-4.35643400	1.25244800
C	0.02105600	-2.38679600	3.94939900
H	0.14551600	-0.23740000	3.99059000
H	-0.16168100	-4.52897600	3.64273700
H	0.29071500	-2.50036500	4.99485400
C	-0.34474700	1.45158500	1.71361800
C	-0.79330800	2.42193100	0.61756100
C	-1.45209100	-2.74769700	-1.03796900
C	-1.37804900	0.14576700	-3.44927800
H	-0.90202600	-0.43531100	-4.24594200
H	-2.37769900	0.44358200	-3.78479500
H	-0.77674700	1.03496000	-3.26755900
C	-1.91114800	2.63637300	-1.50511200

H	-1.15729500	3.05997000	-2.17843300
H	-2.61370400	2.03498000	-2.07896400
H	-2.46240200	3.45952700	-1.03910900
C	-1.65059700	-1.97822100	-2.34520500
O	-1.61925300	-3.95921000	-0.94725100
O	-1.93506200	-2.59510300	-3.38943900
O	0.10687000	1.82825700	2.78967800
O	-0.71456300	3.65012300	0.80855700
Cu	-1.08848500	-0.07500500	-0.45890200

[HO----OH]-2

E = -151.895544104

G_{corr} = -0.005036

O	-4.76875800	2.26113000	0.00000000
H	-4.30449800	3.11439600	0.00000000
O	-1.34045600	2.43002300	0.00000000
H	-2.29297200	2.22898000	0.00000000

MT_B-1d-S

E = -1179.68067257

G_{corr} = 0.173762

N	-1.46697400	-0.65029900	-2.24051500
N	-1.06465800	-1.89893100	-0.04342300
N	-0.55216000	0.16338400	1.31759600
N	-1.29261100	1.82726400	-0.48199300
C	-0.69084400	-2.18808600	1.28261700
C	-0.41463400	-1.03171300	2.04918300
C	-0.57801700	-3.45947900	1.85643900
C	-0.05835800	-1.14735800	3.39769000
C	-0.21197700	-3.56680500	3.20413800
H	-0.78460800	-4.34204400	1.26593400
C	0.04225800	-2.42330400	3.96706800
H	0.14540900	-0.26143600	3.98422700
H	-0.13144600	-4.55238800	3.65447600
H	0.32575400	-2.51624400	5.01187700
C	-0.37679500	1.43380200	1.70884800
C	-0.80763900	2.41956100	0.61359400
C	-1.46315800	-2.72560500	-1.02137800
C	-1.38302400	0.14255000	-3.46290500
H	-0.90039100	-0.44410100	-4.25195500
H	-2.37305800	0.45117600	-3.81867800
H	-0.77853100	1.02988100	-3.27940100
C	-1.89179000	2.65655400	-1.52164600
H	-1.13526500	3.08050900	-2.19287000
H	-2.59162100	2.06005700	-2.10495500
H	-2.44536700	3.48208100	-1.06185500
C	-1.66350400	-1.96837600	-2.34029100
O	-1.63638900	-3.95556400	-0.94355300
O	-1.93646200	-2.59833700	-3.38694600
O	0.05361100	1.83114700	2.80677100

O	-0.73076600	3.65226100	0.81675200
Cu	-1.09925500	-0.07289700	-0.45813800

[HO--OH]-1

E = -151.7136811

G_{corr} = -0.00417

O	-4.16169600	2.27559200	0.30172300
H	-4.06259200	3.08136200	-0.23413200
O	-1.94126000	2.16134200	-0.13233900
H	-1.86811400	2.15090400	0.83795600

MECP_B(S-T)

E (S) = -1179.67542523

G_{corr} (S) = 0.167424

E (T) = -1179.67542158

G_{corr} (T) = 0.165361

N	-1.39313000	-0.71006300	-2.31431700
N	-1.02300200	-1.91331600	-0.04194400
N	-0.59388700	0.17012800	1.36310800
N	-1.25392900	1.89830100	-0.45497600
C	-0.68778400	-2.18673500	1.26983800
C	-0.44518800	-1.00977700	2.06385300
C	-0.56338100	-3.46195800	1.85462200
C	-0.10327200	-1.14190300	3.42419900
C	-0.21145700	-3.56493300	3.19522200
H	-0.74872700	-4.34490200	1.25882200
C	0.01564200	-2.41259000	3.97548700
H	0.07542900	-0.25783400	4.02056500
H	-0.11435500	-4.54808800	3.64664900
H	0.29414000	-2.51672200	5.01995700
C	-0.44527500	1.44740300	1.77981400
C	-0.84366300	2.45535300	0.68600700
C	-1.38350100	-2.76153400	-1.03121000
C	-1.48895400	0.04193000	-3.55894100
H	-0.98134500	-0.48993600	-4.37216700
H	-2.53521600	0.19586100	-3.85447100
H	-1.01103800	1.01295300	-3.43289400
C	-1.77328600	2.77165200	-1.49737800
H	-0.96409100	3.23236200	-2.07944600
H	-2.40491100	2.19084200	-2.16920400
H	-2.37783700	3.57437000	-1.06044200
C	-1.58918800	-2.02835200	-2.36873800
O	-1.54509000	-3.99028000	-0.94370000
O	-1.89342900	-2.69984700	-3.38836300
O	-0.05803500	1.83273200	2.89541100
O	-0.79147300	3.68481400	0.94543100
Cu	-1.05303800	-0.04267100	-0.50408500

MT_B-1d-T

E = -1179.67947276

G_{corr} = 0.167824

N	-1.45804300	-0.76888900	-2.35799700
N	-0.98079000	-1.93404400	-0.05245400
N	-0.62339600	0.16695600	1.37931300
N	-1.25726500	1.97490100	-0.41610500
C	-0.66839000	-2.19644100	1.24181800
C	-0.45537000	-0.99473400	2.05833100
C	-0.53255900	-3.47405500	1.84398800
C	-0.12496300	-1.13889300	3.43098300
C	-0.20613200	-3.56675100	3.18240400
H	-0.68672400	-4.36233400	1.24734900
C	-0.00531800	-2.40218900	3.97473500
H	0.02924100	-0.25582900	4.03561800
H	-0.10047700	-4.54535600	3.64183300
H	0.24747500	-2.51237800	5.02537300
C	-0.47899200	1.44841300	1.82352400
C	-0.84187700	2.48720700	0.74069300
C	-1.28651700	-2.81072700	-1.05236800
C	-1.66381900	-0.06170400	-3.61524200
H	-1.12567900	-0.54753700	-4.43894000
H	-2.72839500	-0.02752400	-3.88662900
H	-1.29849900	0.96088400	-3.51665800
C	-1.65476300	2.92088900	-1.45192800
H	-0.77975100	3.32106700	-1.98320000
H	-2.29230600	2.41295500	-2.17709800
H	-2.20761900	3.76835900	-1.02964900
C	-1.56573800	-2.09518900	-2.39182000
O	-1.35556000	-4.04520200	-0.97083000
O	-1.85654400	-2.80613200	-3.39511800
O	-0.10480600	1.81350400	2.94703300
O	-0.73477100	3.71080400	1.03601800
Cu	-1.09392200	-0.01277100	-0.54627100

MT_B-1e

E = -1179.85392232

G_{corr} = 0.168181

N	-1.46274200	-0.75525700	-2.36789900
N	-0.99456600	-1.93552000	-0.06210500
N	-0.63621400	0.18125300	1.38135600
N	-1.26692000	1.98167700	-0.43030400
C	-0.66908600	-2.19693200	1.27354200
C	-0.45709700	-1.02196700	2.07151400
C	-0.52944000	-3.46264900	1.86480500
C	-0.11094300	-1.16274600	3.42490000
C	-0.18428200	-3.57965900	3.21818100
H	-0.69070300	-4.34949200	1.26591500
C	0.02410800	-2.43661200	3.99367700
H	0.05238500	-0.27750300	4.02577600
H	-0.07942500	-4.56808900	3.65893000
H	0.29284300	-2.52711500	5.04333100

C	-0.52311200	1.43031900	1.82535300
C	-0.86246400	2.47937000	0.73364300
C	-1.29311500	-2.79210100	-1.03612900
C	-1.66391600	-0.05807200	-3.63144300
H	-1.11343700	-0.53966000	-4.45068700
H	-2.72530600	-0.02961600	-3.91869100
H	-1.30736400	0.96876700	-3.53738800
C	-1.63595800	2.93381300	-1.47085500
H	-0.75161600	3.32938200	-1.99172900
H	-2.26752200	2.43379700	-2.20777400
H	-2.19062000	3.78743600	-1.06149100
C	-1.57086900	-2.07921700	-2.38629500
O	-1.36778100	-4.04986300	-0.97768400
O	-1.86294600	-2.79443200	-3.39460300
O	-0.19520500	1.82521400	2.97783700
O	-0.74830900	3.70937900	1.02844400
Cu	-1.10064800	-0.01664200	-0.53541400

HOOH

E = -151.561812656

G_{corr} = 0.003801

O	-3.75801300	2.16432900	0.20474500
H	-4.00153800	3.07414800	-0.05659700
O	-2.34282200	2.12870300	-0.12221100
H	-1.93129000	2.30202000	0.74727000