

Supplementary_Material

Study of antiradical mechanisms with dihydroxybenzenes using the reaction force
and reaction electronic flux

Cristina Ortega-Moo, Rocío Durán, Bárbara Herrera, Soledad Gutiérrez-Oliva,
Alejandro Toro-Labbé and Rubicelia Vargas

Transition State Structures

Phenol-H M05-2X/6-311++g(d,p) SCRF=(SMD,Solvent=Water)

16

O	-1.24107200	0.74175100	1.21798700
H	-2.06427900	0.36960200	0.55966800
C	2.37059500	-0.31415500	-0.43810100
C	1.85813700	0.97037900	-0.64822600
C	0.63946400	1.32713800	-0.10874200
C	-0.08104300	0.39435200	0.66682900
C	0.44152000	-0.90141200	0.87406200
C	1.66030700	-1.24553400	0.32141500
H	3.32405400	-0.58736400	-0.86796500
H	2.41719100	1.68298600	-1.23821700
H	0.21706900	2.31146100	-0.25825600
H	-0.13138100	-1.60006100	1.46906200
H	2.06375000	-2.23634100	0.47672300
O	-2.72369700	-0.14260700	-0.39726700
O	-1.73540200	-0.57770300	-1.21922900
H	-1.55891400	-1.49641100	-0.95635400

ortho-H M05-2X/6-311++g(d,p) SCRF=(SMD,Solvent=Water)

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C	-1.59960500	1.11454400	0.42650400
C	-0.37900000	0.98198100	-0.22440100
C	0.02740200	-0.27662700	-0.73340300
C	-0.81305100	-1.39019400	-0.57761400
C	-2.02545100	-1.24988600	0.06118500
O	1.19832500	-0.34887400	-1.37357400
H	1.98710500	-0.42533200	-0.63177900
C	-2.41293100	0.00260300	0.56482700
O	2.63263800	-0.48419300	0.52937400
H	-2.67873900	-2.10219300	0.18043800
O	0.43539000	2.04979000	-0.36006100
H	1.21313200	1.78562600	-0.87402200
H	-1.89201000	2.08184900	0.81007700
O	1.60276100	-0.53772900	1.40293700
H	1.47839500	0.37085900	1.72601000
H	-3.36384200	0.10368200	1.06916200
H	-0.48112800	-2.34097200	-0.97188500

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meta-H M05-2X/6-311++g(d,p) SCRF=(SMD,Solvent=Water)

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C	-0.87758000	1.79625000	-0.13362100
C	0.28782900	1.25612200	-0.65148100
C	0.40176000	-0.14792500	-0.78458600
C	-0.65214100	-0.98935600	-0.38872900
C	-1.80384600	-0.42513900	0.11493600
O	1.50795800	-0.67368800	-1.30091500
H	2.31518500	-0.62014000	-0.53236300
C	-1.92434400	0.96835200	0.24925700
O	2.97014900	-0.48779500	0.55245800
H	-0.55280700	-2.06100300	-0.48981700
H	-0.97830400	2.86668500	-0.02460500
O	2.05725100	0.10326700	1.36650000
H	2.19108600	1.06010800	1.26295200
H	1.11634800	1.87729900	-0.96269900
H	-2.83977700	1.38165600	0.65247400
O	-2.82056600	-1.25605600	0.48588900
H	-3.56014800	-0.74024800	0.82794100

Phenol-CH3 M05-2X/6-311++g(d,p) SCRF=(SMD,Solvent=Water)

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C	-1.32478100	-0.90171700	0.81035500
C	-0.02221000	-0.62663500	1.17153200
C	0.62359700	0.51350300	0.65191700
C	-0.06631700	1.35552000	-0.24200600
C	-1.36876600	1.06555400	-0.59081300
O	1.86917300	0.81398200	1.03283500
H	2.56746100	0.29179800	0.37235500
C	-2.01892300	-0.06541800	-0.07626300
O	3.08311200	-0.44025900	-0.58000400
H	-1.90194900	1.71522900	-1.27252000
H	0.44374800	2.22490800	-0.63408000
H	-1.82365900	-1.77272500	1.21474900
C	-3.42228500	-0.39094900	-0.48635500
H	-3.96401700	-0.87041400	0.32784400
H	-3.95636700	0.50535100	-0.79682000
O	1.97312900	-0.84282700	-1.24319300
H	1.72118600	-1.69292500	-0.84616000
H	0.52090900	-1.26252600	1.85788100
H	-3.41251100	-1.08502300	-1.33055700

ortho-CH3 M05-2X/6-311++g(d,p) SCRF=(SMD,Solvent=Water)

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C	-1.26993000	1.07203000	0.05527000
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C	0.03324600	0.93341500	-0.40651300
C	0.52991000	-0.33569400	-0.77815500
C	-0.31158500	-1.45397100	-0.68278700
C	-1.60381600	-1.30532100	-0.23476800
O	1.78649800	-0.42032400	-1.24247900
H	2.45285500	-0.45746300	-0.40888100
C	-2.09735800	-0.03913700	0.14258500
O	2.94429300	-0.43040100	0.86482600
H	-2.25611300	-2.16598300	-0.16631100
H	0.08188000	-2.41876400	-0.97273400
O	0.83832100	2.01762800	-0.48523800
H	1.68272700	1.75056600	-0.87726400
H	-1.62485100	2.05317800	0.34113700
C	-3.51205100	0.09258700	0.62274100
H	-3.70594000	-0.60962900	1.43435400
H	-3.71599800	1.10240800	0.97189500
O	1.80591100	-0.35247000	1.58356100
H	1.68154000	0.59022700	1.78760900
H	-4.20679100	-0.14345000	-0.18539500

meta-CH3 M05-2X/6-311++g(d,p) SCRF=(SMD,Solvent=Water)

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C	0.77047200	-1.46069400	-0.52304400
C	-0.49600300	-1.03347000	-0.88019600
C	-0.82605900	0.33328800	-0.75823800
C	0.12571800	1.24447400	-0.27495500
C	1.38304800	0.79350400	0.06116200
O	-2.03296000	0.76641800	-1.12665300
H	-2.76402800	0.43535000	-0.38353900
C	1.73338900	-0.57154300	-0.04841300
O	-3.33866600	-0.02435200	0.69921600
H	-0.12840300	2.29080600	-0.17923100
H	1.03006600	-2.50709400	-0.61050800
C	3.10211200	-1.03356300	0.34455700
H	3.30188800	-0.81210200	1.39608200
H	3.19693800	-2.10599000	0.19383800
O	-2.27863400	-0.52441100	1.38103900
H	-2.21318300	-1.45875600	1.12321300
H	3.87116900	-0.53456000	-0.25077500
H	-1.24205500	-1.72092000	-1.25530200
O	2.28211100	1.71673600	0.51526600
H	3.13673300	1.30616100	0.69003600

Phenol-COH M05-2X/6-311++g(d,p) SCRF=(SMD,Solvent=Water)

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O	-2.24476000	0.64569000	1.05514300
H	-2.90344000	0.07484500	0.30374300
C	1.66961900	0.20635600	-0.05716900

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C	0.93678900	1.30185100	-0.52786100
C	-0.38503700	1.45248000	-0.16811800
C	-0.98685500	0.49842000	0.68408900
C	-0.23726700	-0.60978000	1.15255500
C	1.08034800	-0.74807500	0.78431000
H	1.41574100	2.02274200	-1.17779800
H	-0.98092500	2.28394800	-0.51731000
H	-0.72632600	-1.32599400	1.79828300
H	1.66706200	-1.58645000	1.13272400
O	-3.29290000	-0.60837900	-0.63600500
O	-2.13895600	-0.90622000	-1.28263100
H	-1.85081600	-1.76186000	-0.92296000
C	3.07731000	0.07571400	-0.47087400
H	3.45169000	0.86700700	-1.13374400
O	3.80131400	-0.83559600	-0.11957500

ortho-COH M05-2X/6-311++g(d,p) SCRF=(SMD,Solvent=Water)

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C	-0.89522200	1.20096300	-0.00325700
C	0.41941700	0.98564500	-0.39842100
C	0.83692900	-0.31093800	-0.79985300
C	-0.08737200	-1.37464200	-0.79796700
C	-1.38515000	-1.15414400	-0.41396800
O	2.09296900	-0.46947700	-1.18943800
H	2.73306300	-0.55386800	-0.28372100
C	-1.78349400	0.13694400	-0.01284600
O	3.14693500	-0.58674800	0.93140700
H	-2.10714300	-1.95808600	-0.41046800
H	0.25900000	-2.34997700	-1.10999200
O	1.30278100	1.99904100	-0.38684500
H	2.15084400	1.68479400	-0.73586100
H	-1.21001400	2.18929500	0.30562600
C	-3.16921300	0.39454500	0.41917600
H	-3.39336600	1.43388100	0.69339400
O	1.98981200	-0.49770200	1.62728400
H	1.90309400	0.43847700	1.87600900
O	-4.02635300	-0.46446000	0.48107000

meta-COH M05-2X/6-311++g(d,p) SCRF=(SMD,Solvent=Water)

19

C	0.51987500	-1.40336800	-0.62033900
C	-0.77197500	-1.02228200	-0.92048300
C	-1.13779300	0.33817100	-0.76487400
C	-0.19809800	1.27764800	-0.30201500
C	1.08936800	0.88211100	-0.01439800
O	-2.36208900	0.72626000	-1.05832200
H	-3.06016000	0.39815500	-0.19544400
C	1.46473200	-0.47964100	-0.16806100

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O	-3.51239200	-0.03856900	0.84968800
H	-0.49841900	2.31049700	-0.18415500
H	0.81998500	-2.43656400	-0.73517800
C	2.80614100	-1.00903500	0.11805700
H	2.90587400	-2.08564000	-0.07850800
O	-2.45090900	-0.69951700	1.38013500
H	-2.53273300	-1.61641200	1.06845700
O	3.75612000	-0.37388200	0.53339500
H	-1.50872700	-1.72592700	-1.28104000
O	2.01951800	1.76149300	0.41755700
H	1.63869600	2.64798500	0.45891600