

Supplementary Information
for
Analysis of the gas phase acidity of substituted benzoic acids using density functional concepts

Jorge A. Amador-Balderas¹, Michael-Adán Martínez-Sánchez², Ramsés E. Ramírez^{1*}, Francisco Méndez^{2,3,4*} and Francisco J. Meléndez⁵

- 1 Departamento de Fisicomatemáticas, Facultad de Ciencias Químicas, Av. San Claudio y 14 Sur, Col. San Manuel, Benemérita Universidad Autónoma de Puebla, C.P. 72570, Puebla, Pue., México.
- 2 Departamento de Química, División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Iztapalapa, A.P. 55-534, México, D.F., 09340 México.
- 3 LE STUDIUM GUEST RESEARCH FELLOW, Loire Valley Institute for Advanced Studies, 45000 Orléans & Tours, France.
- 4 Conditions Extrêmes et Matériaux: Haute Température et Irradiation (CEMHTI), UPR3079 CNRS, CEMHTI 1, Avenue de la Recherche Scientifique, 45071 Orléans, France.
- 5 Departamento de Fisicoquímica, Facultad de Ciencias Químicas, Av. San Claudio y 14 Sur, Col. San Manuel, Benemérita Universidad Autónoma de Puebla, C.P. 72570, Puebla, Pue., México.

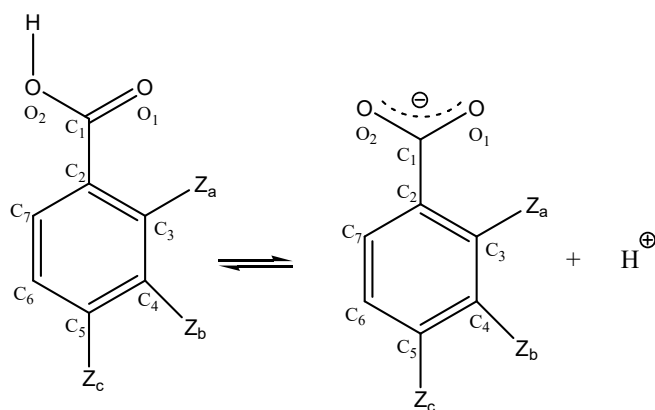
*fm@xanum.uam.mx and ramses.ramirez@correo.buap.mx

Table of contents

Computed Cartesian Coordinates and Energies of Substituted Benzoic Acids.....	2S
Computed Hirshfeld Atomic Charges	18S
Electronegativity and Global Softness	24S
Condensed Fukui Function Calculated Using Hirshfeld Atomic Charges.....	25S
Absolute gas phase acidities for 1a–6c calculated at the M062X/6-311++G(2d,2p) and MP2/6-311++G(2d,2p) levels of theory	29S

All data were obtained at the B3LYP/6-311++G(2d,2p) level of theory.

Computed Cartesian Coordinates and Energies of substituted benzoic acids (in Hartrees)
--



Benzoic acid

Benzoate anion

1 $Z_a=Z_b=Z_c=H$	
1a $Z_a=CH_3, Z_b=Z_c=H$	4a $Z_a=CF_3, Z_b=Z_c=H$
1b $Z_b=CH_3, Z_a=Z_c=H$	4b $Z_b=CF_3, Z_a=Z_c=H$
1c $Z_c=CH_3, Z_a=Z_b=H$	4c $Z_c=CF_3, Z_a=Z_b=H$
2a $Z_a=OCH_3, Z_b=Z_c=H$	5a $Z_a=NO_2, Z_b=Z_c=H$
2b $Z_b=OCH_3, Z_a=Z_c=H$	5b $Z_b=NO_2, Z_a=Z_c=H$
2c $Z_c=OCH_3, Z_a=Z_b=H$	5c $Z_c=NO_2, Z_a=Z_b=H$
3a $Z_a=NH_2, Z_b=Z_c=H$	6a $Z_a=SO_2CF_3, Z_b=Z_c=H$
3b $Z_b=NH_2, Z_a=Z_c=H$	6b $Z_b=SO_2CF_3, Z_a=Z_c=H$
3c $Z_c=NH_2, Z_a=Z_b=H$	6c $Z_c=SO_2CF_3, Z_a=Z_b=H$

Acid 1a

Sum of electronic and thermal Free energies = -460.179703 a.u.

E (RB3LYP) = -460.28867884 a.u.

Sum of electronic and thermal Enthalpies = -460.135976 a.u.

C	-0.19857600	-0.23298600	-0.00002900
C	0.47075300	-1.46460600	-0.00002200
C	1.85454300	-1.52820900	0.00000000
C	2.58818500	-0.34764000	0.00001800
C	1.93218900	0.87646600	0.00001300
C	0.53863200	0.97248300	-0.00000800
H	-0.10961200	-2.37364800	-0.00003700
H	2.35371700	-2.48688700	0.00000400
H	3.66950700	-0.37737200	0.00003600
H	2.51294300	1.78917700	0.00002700
C	-1.68385000	-0.22121800	-0.00005600
O	-2.39178800	0.75969300	0.00003400
O	-2.22793100	-1.46983700	0.00002700
H	-3.18597700	-1.33918600	0.00008100
C	-0.08824100	2.34252900	-0.00001100

H	-0.72668900	2.49139000	-0.86946000
H	-0.72670900	2.49138500	0.86942300
H	0.68875700	3.10536200	0.00000000

Acid 1b

Sum of electronic and thermal Free energies = -460.184648 a.u.

E (RB3LYP) = -460.29222707 a.u.

Sum of electronic and thermal Enthalpies = -460.139662 a.u.

C	-0.58532600	0.10378600	-0.00001200
C	-0.31393900	1.47215500	0.00000600
C	1.00713500	1.90360000	-0.00000500
C	2.04548100	0.98031900	-0.00002600
C	1.79145300	-0.39588000	-0.00002800
C	0.46619600	-0.81720900	-0.00003100
H	-1.12516100	2.18358100	0.00001100
H	1.22773700	2.96215100	-0.00001000
H	3.07004700	1.33113200	-0.00005000
H	0.22482100	-1.87090700	-0.00005900
C	-1.97278400	-0.42532500	-0.00002900
O	-2.26934500	-1.59677100	-0.00002800
O	-2.91848100	0.54986000	0.00005700
H	-3.77319900	0.09736400	0.00007300
C	2.92766100	-1.38764200	0.00004800
H	3.56165100	-1.26038300	0.87923500
H	2.55842500	-2.41151000	-0.00104100
H	3.56303200	-1.25897300	-0.87792500

Acid 1c

Sum of electronic and thermal Free energies = -460.185856 a.u.

E (RB3LYP) = -460.29288638 a.u.

Sum of electronic and thermal Enthalpies = -460.140338 a.u.

C	0.70140900	0.03388800	-0.00034300
C	0.01781900	-1.18363600	-0.00442800
C	-1.37022600	-1.20207400	-0.00975000
C	-2.10846700	-0.01638600	-0.00938100
C	-1.41211400	1.19698200	-0.00938000
C	-0.02715900	1.22603300	-0.00386300
H	0.57272300	-2.10950500	-0.00641500
H	-1.88882200	-2.15192600	-0.01705800
H	-1.96452500	2.12771700	-0.01643100
H	0.50892700	2.16392500	-0.00527400
C	2.18122000	0.11337800	0.00293500
O	2.82230000	1.13814800	0.00461600
O	2.78426500	-1.10478000	0.00466300
H	3.73616900	-0.93422700	0.00729000
C	-3.61444500	-0.04001300	0.01407000
H	-4.03361200	0.77779000	-0.57155100
H	-4.00448000	-0.97757100	-0.37949700
H	-3.98712300	0.06782500	1.03554600

Acid 2a

Sum of electronic and thermal Free energies = -535.404842 a.u.

E (RB3LYP) = -535.51534497 a.u.

Sum of electronic and thermal Enthalpies = -535.357000 a.u.

C	0.64820300	1.70568200	-0.00004400
---	------------	------------	-------------

C	-0.47280900	2.52045200	-0.00002100
C	-1.73233100	1.93394500	0.00003900
C	-1.87012100	0.55259400	0.00002700
C	-0.74295100	-0.27689200	-0.00005600
C	0.54704400	0.30974500	-0.00004900
H	1.63253100	2.14585300	-0.00004800
H	-0.36480100	3.59526200	-0.00005700
H	-2.62048300	2.55150500	0.00009800
H	-2.85800600	0.12148200	0.00009700
C	1.78087700	-0.51572500	-0.00000400
O	1.85361000	-1.71961600	-0.00003200
O	2.91367400	0.25122700	0.00010700
H	3.64848700	-0.37681800	0.00012700
O	-0.82654300	-1.62193500	-0.00015100
C	-2.10729800	-2.23948600	0.00009600
H	-1.91176700	-3.30722200	0.00007400
H	-2.67761600	-1.97467000	0.89273300
H	-2.67795500	-1.97469900	-0.89233400

Acid 2b

Sum of electronic and thermal Free energies = -535.410485 a.u.

E (RB3LYP) = -535.52247645 a.u.

Sum of electronic and thermal Enthalpies = -535.364174 a.u.

C	-0.83616700	1.49314600	-0.00000200
C	0.44545800	2.01848200	-0.00001000
C	1.56419100	1.18617300	-0.00000800
C	1.39381500	-0.19944400	0.00000100
C	0.10708100	-0.73695800	0.00000600
C	-1.00056400	0.10281400	0.00000500
H	-1.69856500	2.14044900	-0.00000200
H	0.58756200	3.09035500	-0.00001700
H	2.55026300	1.62390100	-0.00001400
H	-0.02673800	-1.80826200	0.00001000
C	-2.34523000	-0.53196800	0.00001000
O	-2.55166300	-1.72186700	-0.00002600
O	-3.36052300	0.36978000	0.00001800
H	-4.17920100	-0.14511500	0.00000100
O	2.41304700	-1.10325800	0.00000400
C	3.74871800	-0.61795400	0.00000500
H	4.38358200	-1.49873700	0.00001400
H	3.95620100	-0.02279700	-0.89212600
H	3.95619500	-0.02278300	0.89212800

Acid 2c

Sum of electronic and thermal Free energies = -535.413393 a.u.

E (RB3LYP) = -535.52549207 a.u.

Sum of electronic and thermal Enthalpies = -535.367086 a.u.

C	0.54058600	1.25960600	0.00000100
C	-0.83136700	1.41244800	0.00000000
C	-1.66434700	0.28671600	-0.00001200
C	-1.10332900	-0.99391000	-0.00002500
C	0.27707500	-1.13470800	-0.00002200
C	1.11390100	-0.01962500	-0.00000900
H	1.17798200	2.13063500	0.00001100
H	-1.28602600	2.39249800	0.00000900
H	-1.72618600	-1.87433100	-0.00003900

H	0.72346800	-2.11853800	-0.00003100
C	2.57512600	-0.23606300	-0.00000500
O	3.12165900	-1.31549200	0.00002400
O	3.28938200	0.92204400	0.00000500
H	4.22082000	0.66253500	0.00002700
O	-2.99708300	0.54055600	-0.00001800
C	-3.90278300	-0.55793100	0.00003600
H	-3.77723600	-1.17415500	0.89227600
H	-4.89633100	-0.12054600	0.00008200
H	-3.77732500	-1.17417000	-0.89220700

Acid 3a

Sum of electronic and thermal Free energies = -476.248501 a.u.

E (RB3LYP) = -476.34729293 a.u.

Sum of electronic and thermal Enthalpies = -476.205831 a.u.

C	0.21226700	-0.22907200	-0.01037500
C	-0.47144200	-1.45783900	-0.00699000
C	-1.84903600	-1.52015300	0.00426400
C	-2.57903100	-0.32565400	0.01416800
C	-1.93903300	0.89487900	0.00660100
C	-0.53143900	0.98300700	-0.01059400
H	0.11114400	-2.36606700	-0.00917200
H	-2.35520300	-2.47415900	0.00799200
H	-3.66053200	-0.35463000	0.02638800
H	-2.51569500	1.81086500	0.00743000
C	1.67682600	-0.19716400	0.00421000
O	2.37165800	0.80624600	0.03625600
O	2.25728800	-1.42509700	-0.01459700
H	3.21107400	-1.26774000	0.00269400
N	0.06813700	2.20588600	-0.05608200
H	-0.48319000	3.02458400	0.12173800
H	1.06920400	2.24872200	0.05452400

Acid 3b

Sum of electronic and thermal Free energies = -476.243215 a.u.

E (RB3LYP) = -476.34147946 a.u.

Sum of electronic and thermal Enthalpies = -476.200014 a.u.

C	-0.56589000	0.10773300	-0.00182000
C	-0.26862400	1.47235500	0.00500900
C	1.06386400	1.86695600	0.00595400
C	2.08502500	0.92689800	-0.00132600
C	1.79383900	-0.44423400	-0.00761400
C	0.45546900	-0.84039400	-0.00823200
H	-1.06243100	2.20194100	0.01070600
H	1.31275000	2.91923700	0.01239000
H	3.11777000	1.25202200	-0.00690300
H	0.19003700	-1.88854700	-0.01651400
C	-1.96458200	-0.39383200	0.00133000
O	-2.28471500	-1.55944500	0.00740100
O	-2.89084800	0.59889600	-0.00247300
H	-3.75386800	0.16252500	0.00000300
N	2.81763500	-1.39000600	-0.07504600
H	3.70925800	-1.09122200	0.28530500
H	2.57293800	-2.31440400	0.24110700

Acid 3c

Sum of electronic and thermal Free energies = -476.246443 a.u.

E (RB3LYP) = -476.34478458 a.u.

Sum of electronic and thermal Enthalpies = -476.203329 a.u.

C	0.68645400	0.03483600	-0.00163800
C	-0.00430300	-1.18213300	-0.00283100
C	-1.38666800	-1.21010400	-0.00486000
C	-2.12440500	-0.01629800	-0.00503300
C	-1.43021200	1.20453300	-0.00562300
C	-0.04965100	1.22491800	-0.00331900
H	0.54930000	-2.10891000	-0.00082100
H	-1.90751100	-2.15889300	-0.00979400
H	-1.98530200	2.13370900	-0.01107300
H	0.48412600	2.16425900	-0.00153600
C	2.15759300	0.11452300	0.00279300
O	2.80451500	1.13810300	0.00596300
O	2.76451000	-1.10554000	0.00338100
H	3.71503100	-0.92913700	0.00584900
N	-3.50784500	-0.04082100	-0.05900700
H	-3.95826900	-0.88931200	0.23985400
H	-3.98751100	0.79186700	0.23888700

Acid 4a

Sum of electronic and thermal Free energies = -758.021258 a.u.

E (RB3LYP) = -758.10565905 a.u.

Sum of electronic and thermal Enthalpies = -757.975232 a.u.

C	-0.92277600	0.20889400	-0.00011300
C	-2.18613500	-0.38987100	-0.00010000
C	-2.33646500	-1.76955800	-0.00001500
C	-1.21179400	-2.57831100	0.00007100
C	0.05377900	-2.00225600	0.00006300
C	0.22031800	-0.62090700	-0.00003400
H	-3.05815500	0.24330500	-0.00015400
H	-3.32656200	-2.20299700	-0.00000700
H	-1.30814200	-3.65496500	0.00014400
H	0.92530200	-2.63594000	0.00012400
C	-0.84984200	1.70364600	-0.00017300
O	0.15120300	2.36961900	0.00021400
O	-2.08330000	2.27879800	0.00014100
H	-1.92927900	3.23359300	0.00038400
C	1.65045700	-0.10069600	-0.00004700
F	1.93490500	0.62786800	1.09159000
F	1.93502100	0.62751800	-1.09188600
F	2.53544700	-1.13049400	0.00015900

Acid 4b

Sum of electronic and thermal Free energies = -758.034600 a.u.

E (RB3LYP) = -758.11796778 a.u.

Sum of electronic and thermal Enthalpies = -757.987517 a.u.

C	-1.49964500	0.15274900	-0.00006200
C	-1.56180400	1.54593500	-0.00009200
C	-0.38890100	2.29298100	-0.00016000
C	0.84305500	1.65486100	-0.00018900
C	0.90350500	0.26026600	-0.00017700

C	-0.26044800	-0.49156100	-0.00011400
H	-2.52215300	2.03816200	-0.00006600
H	-0.43639000	3.37250700	-0.00019700
H	1.75597600	2.23352300	-0.00025000
H	-0.22967800	-1.57006500	-0.00010600
C	-2.72210600	-0.69545700	0.00004800
O	-2.72148800	-1.90187800	0.00004600
O	-3.86882200	0.02774600	0.00011100
H	-4.59633600	-0.60991200	0.00017600
C	2.25618800	-0.39925800	0.00002300
F	2.98325800	-0.04159000	1.08423400
F	2.17967500	-1.74140600	-0.00188100
F	2.98506700	-0.03858800	-1.08196000

Acid 4c

Sum of electronic and thermal Free energies = -758.037065 a.u.

E (RB3LYP) = -758.11787879 a.u.

Sum of electronic and thermal Enthalpies = -757.986438 a.u.

C	-1.71882800	-0.03202900	-0.00445200
C	-1.04079500	1.18685100	-0.00984700
C	0.34810000	1.21009600	-0.01856000
C	1.05833200	0.01466800	-0.02321000
C	0.38576100	-1.20716900	-0.01780900
C	-0.99860000	-1.22895100	-0.00885700
H	-1.59690900	2.11140200	-0.00852900
H	0.87494000	2.15195800	-0.02611000
H	0.94359300	-2.13227000	-0.02579600
H	-1.53908500	-2.16375900	-0.00673600
C	-3.20532400	-0.11067900	0.00442900
O	-3.83802900	-1.13809500	0.00787100
O	-3.80123300	1.10643200	0.00887500
H	-4.75545400	0.94700000	0.01493100
C	2.56382300	0.01657200	0.00029300
F	3.04101100	-0.33391600	1.21754400
F	3.08048900	-0.86426200	-0.88323800
F	3.08207900	1.22515800	-0.29137900

Acid 5a

Sum of electronic and thermal Free energies = -625.435630 a.u.

E (RB3LYP) = -625.51653385 a.u.

Sum of electronic and thermal Enthalpies = -625.388516 a.u.

C	-0.05614600	-0.73068800	-0.00114400
C	-1.05768400	-1.69911400	0.01470000
C	-2.39950200	-1.33708100	0.02959900
C	-2.76034000	0.00542100	0.03088600
C	-1.77797800	0.98692500	0.00499300
C	-0.44400600	0.61025100	-0.02232600
H	-0.76754900	-2.73959200	0.02336500
H	-3.16055500	-2.10426000	0.04322400
H	-3.80219400	0.29179200	0.04062400
H	-2.02815100	2.03633800	-0.01279500
C	1.36108300	-1.21474400	0.05926100
O	1.78756500	-2.11545900	-0.61403500
O	2.07368200	-0.59571800	1.02094200

H	2.97663800	-0.94312300	0.98123700
N	0.55496800	1.68621900	-0.16856500
O	0.31651400	2.75399700	0.37950100
O	1.53529800	1.44836800	-0.86034800

Acid 5b

Sum of electronic and thermal Free energies = -625.447520 a.u.

E (RB3LYP) = -625.52859207 a.u.

Sum of electronic and thermal Enthalpies = -625.400382 a.u.

C	-1.16422000	0.15156400	-0.00006000
C	-1.14567400	1.54864300	-0.00003100
C	0.06526800	2.23208200	0.00000200
C	1.26400000	1.53160700	0.00000800
C	1.22457800	0.14234000	-0.00001900
C	0.03315000	-0.56171100	-0.00005100
H	-2.07751300	2.09297700	-0.00003800
H	0.07605400	3.31235300	0.00002300
H	2.21715100	2.03614900	0.00003400
H	0.02784100	-1.63992800	-0.00007100
C	-2.43438000	-0.62679000	-0.00010600
O	-2.49955900	-1.83027000	0.00003200
O	-3.53505100	0.16304600	0.00008500
H	-4.30095500	-0.42806500	0.00019200
N	2.49845500	-0.60770300	-0.00001200
O	2.43747000	-1.82912900	0.00000900
O	3.53612800	0.04310600	0.00005900

Acid 5c

Sum of electronic and thermal Free energies = -625.447559 a.u.

E (RB3LYP) = -625.52860492 a.u.

Sum of electronic and thermal Enthalpies = -625.400350 a.u.

C	-1.35212800	0.03427000	-0.00001300
C	-0.67091100	-1.18533700	-0.00000700
C	0.71612400	-1.20690700	0.00001100
C	1.40062100	0.00036900	0.00002300
C	0.74582900	1.22518900	0.00001800
C	-0.63969300	1.23558000	0.00000100
H	-1.22500800	-2.11086400	-0.00001800
H	1.26707100	-2.13363400	0.00001500
H	1.31914900	2.13823800	0.00002800
H	-1.18529000	2.16726000	-0.00000400
C	-2.84136900	0.10738200	-0.00003500
O	-3.47447900	1.13366200	0.00000300
O	-3.43012000	-1.11151700	0.00001000
H	-4.38582800	-0.96002300	0.00003200
N	2.87999700	-0.01850500	0.00004400
O	3.45965500	1.05945300	-0.00003100
O	3.43233000	-1.11093800	-0.00002400

Acid 6a

Sum of electronic and thermal Free energies = -1306.667309 a.u.

E (RB3LYP) = -1306.75303312 a.u.

Sum of electronic and thermal Enthalpies = -1306.608470 a.u.

C	-1.62402400	0.24727500	-0.09513900
C	-2.85615900	-0.28560700	-0.46975600

C	-3.05745400	-1.66035600	-0.49762600
C	-2.03468800	-2.52754100	-0.13214000
C	-0.80817500	-2.01469000	0.26518400
C	-0.60548600	-0.63662600	0.27528200
H	-3.65886600	0.38408300	-0.74360300
H	-4.01911800	-2.05195500	-0.79828200
H	-2.19235000	-3.59633000	-0.14260700
H	-0.01269100	-2.66841000	0.58859200
C	-1.46888600	1.74337200	-0.17615400
O	-0.89923000	2.31336900	-1.06559100
O	-2.13602200	2.36506000	0.81431700
H	-2.00622400	3.31784900	0.69289200
S	0.97761600	-0.06347900	0.88749900
O	0.86729800	1.31557500	1.30269300
O	1.54042100	-1.08643700	1.73981200
C	2.08127300	-0.07561800	-0.65374000
F	1.62161500	0.75229900	-1.58163300
F	2.13153500	-1.31352100	-1.15756200
F	3.30343300	0.29773900	-0.28550200

Acid 6b

Sum of electronic and thermal Free energies = -1306.681221 a.u.

E (RB3LYP) = -1306.76757891 a.u.

Sum of electronic and thermal Enthalpies = -1306.622730 a.u.

C	-2.32544700	0.12346000	0.00618000
C	-2.53018700	1.45711300	0.36818400
C	-1.47356400	2.36071100	0.35345300
C	-0.20286400	1.94141400	-0.01750800
C	-0.01159500	0.60750300	-0.37171000
C	-1.05402900	-0.30794900	-0.36887500
H	-3.51821800	1.78272800	0.65563800
H	-1.64047700	3.39240900	0.62721400
H	0.62728700	2.63108200	-0.04885200
H	-0.89919400	-1.33517800	-0.66257400
C	-3.42891200	-0.87792500	-0.00035500
O	-3.29683100	-2.03733800	-0.30101600
O	-4.61934000	-0.35078100	0.37240900
H	-5.26567000	-1.07009200	0.33749500
S	1.61617400	0.06995100	-0.86666500
O	1.50799600	-1.12372300	-1.67217300
O	2.39527200	1.22002600	-1.26629200
C	2.36930100	-0.49677000	0.77507500
F	1.63845000	-1.47882200	1.30542400
F	2.41321500	0.52247600	1.63744400
F	3.60216800	-0.93598500	0.54909100

Acid 6c

Sum of electronic and thermal Free energies = -1306.681348 a.u.

E (RB3LYP) = -1306.76737261 a.u.

Sum of electronic and thermal Enthalpies = -1306.622545 a.u.

C	-2.62132300	0.03488500	-0.02955200
C	-1.95067500	-1.18212200	-0.16925300
C	-0.58455800	-1.19640000	-0.41382800
C	0.09183100	0.01485700	-0.51530200
C	-0.56169400	1.23718200	-0.38459200
C	-1.92613600	1.24087000	-0.14000000

H	-2.49631500	-2.10941700	-0.09073800
H	-0.05188900	-2.12661800	-0.54042000
H	-0.01152300	2.15996600	-0.48876200
H	-2.46834300	2.16882800	-0.03632500
C	-4.08926400	0.10035800	0.23237400
O	-4.71309300	1.12384100	0.36080000
O	-4.66524900	-1.12099200	0.31401800
H	-5.60693300	-0.97614200	0.48354200
S	1.84519400	0.00108700	-0.85338700
O	2.21071600	-1.26817600	-1.43949400
O	2.23387400	1.27038200	-1.42393900
C	2.59254900	-0.01671300	0.88622100
F	2.21516200	1.07023900	1.56258900
F	2.18828500	-1.10117400	1.55136700
F	3.91628100	-0.03261600	0.77931000

Anion 1a

Sum of electronic and thermal Free energies = -459.640560 a.u.

E (RB3LYP) = -459.734719833 a.u.

Sum of electronic and thermal Enthalpies = -459.596284 a.u.

C	-0.23425000	-0.27442900	-0.01127400
C	0.51670900	-1.44928300	-0.10234600
C	1.90670300	-1.43564300	-0.13595000
C	2.57998700	-0.22160200	-0.04191400
C	1.84546700	0.95447400	0.07519100
C	0.44610700	0.95640700	0.07801200
H	-0.03204300	-2.38073200	-0.13005200
H	2.46017700	-2.36349800	-0.22164800
H	3.66288700	-0.18777800	-0.05204800
H	2.36895900	1.90047000	0.16390100
C	-1.77769500	-0.39971200	-0.02415900
O	-2.39605100	0.52883200	-0.59678400
O	-2.23282300	-1.43034400	0.52169700
C	-0.28137900	2.27398200	0.19192300
H	-0.86332300	2.47186500	-0.70652000
H	-1.00426000	2.25959500	1.00761300
H	0.42869800	3.08701100	0.36255200

Anion 1b

Sum of electronic and thermal Free energies = -459.645067 a.u.

E (RB3LYP) = -459.738075705 a.u.

Sum of electronic and thermal Enthalpies = -459.599636 a.u.

C	-0.64581200	0.11792600	0.00031200
C	-0.33874600	1.48020500	0.00340400
C	0.98513900	1.90498800	-0.00252500
C	2.02275000	0.97293400	-0.00843900
C	1.74075400	-0.39420000	-0.00773300
C	0.40363700	-0.79921700	-0.00665500
H	-1.16401100	2.17872000	0.00619300
H	1.21713500	2.96409400	-0.00589900
H	3.05368700	1.30994100	-0.01649800
H	0.13632600	-1.84864400	-0.01335900
C	-2.11998900	-0.36611700	0.00065800
O	-2.27812600	-1.60919900	-0.01146000

O	-2.98304000	0.54213200	0.01329700
C	2.85409500	-1.41680600	0.01270500
H	2.97765900	-1.85281900	1.00826200
H	2.64800500	-2.24077400	-0.67257500
H	3.80955300	-0.97224900	-0.27118100

Anion 1c

Sum of electronic and thermal Free energies = -459.644568 a.u.

E (RB3LYP) = -459.737899720 a.u.

Sum of electronic and thermal Enthalpies = -459.599439 a.u.

C	-0.76346800	-0.00001100	-0.00001600
C	-0.04340800	1.19461100	-0.00481000
C	1.34882700	1.19612300	-0.01107800
C	2.07068700	-0.00000800	-0.01095400
C	1.34883800	-1.19612600	-0.01138000
C	-0.04341100	-1.19461900	-0.00506400
H	-0.60944600	2.11626900	-0.00745800
H	1.88560600	2.13952600	-0.01919500
H	1.88559900	-2.13953800	-0.01975300
H	-0.60941300	-2.11629800	-0.00782700
C	-2.31325700	-0.00000200	0.00416900
O	-2.85067100	-1.13215100	0.00623500
O	-2.85064800	1.13216800	0.00557700
C	3.58108700	0.00001000	0.01802000
H	3.98906800	-0.88211300	-0.47860800
H	3.98902600	0.88245300	-0.47806900
H	3.96473900	-0.00029900	1.04309500

Anion 2a

Sum of electronic and thermal Free energies = -534.862083 a.u.

E (RB3LYP) = -534.958256800 a.u.

Sum of electronic and thermal Enthalpies = -534.814279 a.u.

C	-0.05787500	-1.85353900	0.00007900
C	1.28660300	-2.22791700	0.00020300
C	2.26859400	-1.24784300	0.00013200
C	1.90239900	0.10034300	0.00000100
C	0.55383300	0.45716600	-0.00002700
C	-0.45493200	-0.52020800	0.00001200
H	-0.82748600	-2.61515500	-0.00006100
H	1.55960900	-3.27609600	0.00031900
H	3.31772700	-1.51607000	0.00017200
H	2.67478700	0.85565700	-0.00013500
C	-1.95339000	-0.15633200	0.00008800
O	-2.46789000	-0.05040300	-1.13342300
O	-2.46732600	-0.04838500	1.13363500
O	0.12354400	1.76167500	-0.00021600
C	1.08642000	2.78624400	-0.00034400
H	0.53053900	3.72145100	-0.00045100
H	1.72415100	2.74992100	0.89003000
H	1.72413800	2.74970200	-0.89072100

Anion 2b

Sum of electronic and thermal Free energies = -534.868580 a.u.

E (RB3LYP) = -534.968511685 a.u.

Sum of electronic and thermal Enthalpies = -534.822220 a.u.

C	0.87195100	1.49404200	-0.00001900
C	-0.40957400	2.02198100	0.00001200
C	-1.53197200	1.18657800	0.00001700
C	-1.33749500	-0.19330600	-0.00000900
C	-0.04822600	-0.72410400	-0.00003900
C	1.06499500	0.10748200	-0.00004500
H	1.75130400	2.12207900	-0.00002600
H	-0.55686800	3.09598500	0.00003200
H	-2.52166900	1.61866100	0.00004200
H	0.10790800	-1.79363600	-0.00005800
C	2.49650700	-0.49558600	-0.00008400
O	2.55336700	-1.74633000	0.00005600
O	3.42786000	0.34233400	0.00005200
O	-2.37131800	-1.11491600	-0.00000600
C	-3.69163000	-0.62304000	0.00002000
H	-4.34189800	-1.49568900	0.00001500
H	-3.90268600	-0.02020400	0.88958100
H	-3.90271100	-0.02017500	-0.88951500

Anion 2c

Sum of electronic and thermal Free energies = -534.871058 a.u.

E (RB3LYP) = -534.969171878 a.u.

Sum of electronic and thermal Enthalpies = -534.824836 a.u.

C	0.57717900	1.27058900	0.00001200
C	-0.80313900	1.41708500	0.00000300
C	-1.62210100	0.28733800	-0.00000800
C	-1.04772400	-0.98181100	-0.00000900
C	0.34405800	-1.10395200	0.00000200
C	1.17819100	0.00845500	0.00001200
H	1.23116800	2.13202600	0.00001900
H	-1.26726100	2.39518200	0.00000400
H	-1.65998500	-1.87223800	-0.00001800
H	0.81414400	-2.07803400	0.00000300
C	2.71838200	-0.14492700	0.00002600
O	3.14280300	-1.32457600	-0.00000800
O	3.36436900	0.92934100	-0.00001900
O	-2.98602000	0.52771500	-0.00001900
C	-3.84735900	-0.58954200	0.00001100
H	-3.70574400	-1.21175600	0.88921500
H	-4.86068900	-0.19263700	0.00002000
H	-3.70577300	-1.21178500	-0.88917700

Anion 3a

Sum of electronic and thermal Free energies = -475.710976 a.u.

E (RB3LYP) = -475.796308280 a.u.

Sum of electronic and thermal Enthalpies = -475.668973 a.u.

C	0.23826800	-0.26465900	-0.02854200
C	-0.51458600	-1.43698800	0.00260000
C	-1.90649900	-1.43417400	0.03643600

C	-2.57678500	-0.21206800	0.03794200
C	-1.85822900	0.97354200	-0.00634900
C	-0.45176200	0.97351500	-0.04519400
H	0.04594200	-2.36193700	0.00923000
H	-2.45870900	-2.36517000	0.06550600
H	-3.65993000	-0.18035600	0.06797500
H	-2.38037500	1.92440400	-0.02484700
C	1.77961300	-0.37481800	0.00784500
O	2.42045500	0.70936000	0.16080500
O	2.25544300	-1.52168600	-0.09663500
N	0.24664200	2.16840200	-0.14608900
H	-0.18459600	2.95544500	0.31079100
H	1.24387100	2.00131000	0.05218300

Anion 3b

Sum of electronic and thermal Free energies = -475.701596 a.u.

E (RB3LYP) = -475.785945371 a.u.

Sum of electronic and thermal Enthalpies = -475.658400 a.u.

C	-0.62839200	0.12674000	-0.00865500
C	-0.29045500	1.48225800	0.00542800
C	1.04522400	1.86824600	0.00871400
C	2.06303400	0.91568400	-0.00529300
C	1.73651500	-0.44216300	-0.01761200
C	0.39316400	-0.81917200	-0.02085300
H	-1.09580200	2.20263600	0.01655100
H	1.30687100	2.92035300	0.02125600
H	3.10318900	1.22250900	-0.01393400
H	0.10067500	-1.86238500	-0.02750400
C	-2.11209000	-0.32997300	0.00233700
O	-2.29258100	-1.57054600	0.01225800
O	-2.95853100	0.59311600	0.00234600
N	2.76111300	-1.42595800	-0.08147000
H	3.58747600	-1.16375200	0.43640000
H	2.43669600	-2.32794000	0.23629100

Anion 3c

Sum of electronic and thermal Free energies = -475.700607 a.u.

E (RB3LYP) = -475.784932367 a.u.

Sum of electronic and thermal Enthalpies = -475.657388 a.u.

C	-0.74670700	-0.00004100	-0.00644200
C	-0.02410900	1.19265500	-0.01042600
C	1.36774300	1.20047500	-0.01477700
C	2.08120300	0.00000200	-0.01341000
C	1.36775400	-1.20046000	-0.01483000
C	-0.02410000	-1.19267300	-0.01045900
H	-0.58846100	2.11534900	-0.00674700
H	1.90865200	2.14159600	-0.02102900
H	1.90870300	-2.14156500	-0.02115100
H	-0.58848100	-2.11537400	-0.00680100
C	-2.29374600	-0.00002400	0.00709300
O	-2.83314500	-1.13198700	0.01249500
O	-2.83299800	1.13205200	0.01240600
N	3.50209500	-0.00002600	-0.06840500
H	3.90296100	0.82340500	0.35729400

H	3.90287500	-0.82335700	0.35755700
---	------------	-------------	------------

Anion 4a

Sum of electronic and thermal Free energies = -757.491786 a.u.

E (RB3LYP) = -757.56221838 a.u.

Sum of electronic and thermal Enthalpies = -757.445872 a.u.

C	-0.92259600	0.34063500	0.00000600
C	-2.22487900	-0.17016900	0.00000700
C	-2.49742700	-1.53005100	0.00000900
C	-1.44532300	-2.43801700	0.00000500
C	-0.14113800	-1.96404200	0.00000100
C	0.13615500	-0.59082700	0.00000300
H	-3.01160000	0.57080700	0.00000600
H	-3.52289100	-1.88011500	0.00001100
H	-1.63014700	-3.50472800	0.00000500
H	0.67454500	-2.66937000	-0.00000400
C	-0.79842100	1.90746000	0.00000800
O	0.35662300	2.36634800	0.00004400
O	-1.89773400	2.50649700	-0.00004500
C	1.60622800	-0.20487100	-0.00000400
F	1.99705900	0.46916000	1.09312700
F	1.99702800	0.46923000	-1.09310200
F	2.39962200	-1.33839700	-0.00005000

Anion 4b

Sum of electronic and thermal Free energies = -757.507749 a.u.

E (RB3LYP) = -757.57729204 a.u.

Sum of electronic and thermal Enthalpies = -757.460822 a.u.

C	-1.56451500	0.14157300	-0.00013600
C	-1.60907400	1.53339700	-0.00013700
C	-0.43806300	2.28994600	-0.00017300
C	0.79918600	1.66109100	-0.00019900
C	0.85273200	0.26436900	-0.00022100
C	-0.31844300	-0.48752700	-0.00018400
H	-2.58642700	1.99624300	-0.00011200
H	-0.48806300	3.37188600	-0.00018700
H	1.71244500	2.24093900	-0.00023700
H	-0.30660000	-1.56737200	-0.00019300
C	-2.87134600	-0.69697700	-0.00006900
O	-2.70598000	-1.93691300	0.00021900
O	-3.92929500	-0.02884500	0.00026500
C	2.19785900	-0.38832900	0.00000500
F	2.95068400	-0.03518600	1.08346100
F	2.14801800	-1.73495900	-0.00188400
F	2.95250200	-0.03217600	-1.08118300

Anion 4c

Sum of electronic and thermal Free energies = -757.511382 a.u.

E (RB3LYP) = -757.57814467 a.u.

Sum of electronic and thermal Enthalpies = -757.460686 a.u.

C	-1.78620500	0.00172700	-0.00489900
C	-1.07644100	1.20244200	-0.01221300

C	0.31334900	1.21613800	-0.02514500
C	1.01758300	0.01207700	-0.03491900
C	0.32088600	-1.19842000	-0.02619600
C	-1.06727200	-1.19535600	-0.01264200
H	-1.64992800	2.11884100	-0.00919200
H	0.85135000	2.15386100	-0.03407800
H	0.86574300	-2.13320300	-0.03653200
H	-1.63479200	-2.11544500	-0.00980300
C	-3.33865500	-0.00402700	0.00849800
O	-3.86460700	-1.13940000	0.01358100
O	-3.87323500	1.12722300	0.01293100
C	2.50902300	0.00319100	-0.00052300
F	3.01208600	-0.21946000	1.25023200
F	3.05173300	-0.96958300	-0.78018400
F	3.06026600	1.17201200	-0.41163300

Anion 5a

Sum of electronic and thermal Free energies = -624.912727 a.u.

E (RB3LYP) = -624.978913573 a.u.

Sum of electronic and thermal Enthalpies = -624.864800 a.u.

C	0.04492200	-0.73265800	0.00065900
C	-0.93484800	-1.73545300	0.02887100
C	-2.28951800	-1.44300000	0.02996400
C	-2.72431800	-0.11644000	-0.01056600
C	-1.78440600	0.89973800	-0.04643000
C	-0.42728500	0.58072500	-0.04759700
H	-0.59475700	-2.76170400	0.04439800
H	-3.01387200	-2.24785700	0.05863100
H	-3.77975300	0.12013600	-0.02150000
H	-2.07842000	1.93776100	-0.08268700
C	1.52150900	-1.17168600	0.13877900
O	1.91546600	-1.94214600	-0.75772800
O	2.07920700	-0.75421500	1.17100200
N	0.50269600	1.71826700	-0.13557400
O	0.15954500	2.77601800	0.40418700
O	1.53473100	1.57489800	-0.76894800

Anion 5b

Sum of electronic and thermal Free energies = -624.926774 a.u.

E (RB3LYP) = -624.994053664 a.u.

Sum of electronic and thermal Enthalpies = -624.879700 a.u.

C	-1.22781300	0.14186300	-0.00001400
C	-1.19026500	1.53594600	-0.00001400
C	0.02091000	2.22815600	0.00000800
C	1.22230100	1.53548100	0.00002500
C	1.17684700	0.14184000	0.00002200
C	-0.02436400	-0.55972100	0.00000500
H	-2.14101500	2.05128400	-0.00003600
H	0.03023900	3.31079600	0.00001200
H	2.17466100	2.04059400	0.00004200
H	-0.05418800	-1.63788500	0.00000900
C	-2.58553800	-0.61351500	-0.00003700
O	-2.49731500	-1.85944100	0.00007000

O	-3.59579000	0.12447900	-0.00003200
N	2.44567600	-0.59581400	0.00003700
O	2.41087700	-1.82289500	-0.00005900
O	3.49699100	0.05105900	-0.00001100

Anion 5c

Sum of electronic and thermal Free energies = -624.928978 a.u.

E (RB3LYP) = -624.996264165 a.u.

Sum of electronic and thermal Enthalpies = -624.881797 a.u.

C	-1.41610900	0.00010900	0.00001100
C	-0.70326600	1.20301400	-0.00000800
C	0.68263900	1.21595900	-0.00001800
C	1.36561900	0.00000800	-0.00000100
C	0.68259100	-1.21595900	0.00002000
C	-0.70326200	-1.20288500	0.00002300
H	-1.27669100	2.11904600	-0.00001200
H	1.24241900	2.13820300	-0.00003400
H	1.24235400	-2.13821300	0.00003200
H	-1.27671600	-2.11892100	0.00003400
C	-2.96878900	-0.00009200	0.00002100
O	-3.49584100	-1.13400900	-0.00007100
O	-3.49579800	1.13396300	0.00004300
N	2.82401200	-0.00001800	-0.00000700
O	3.41232200	-1.08359600	0.00001500
O	3.41231800	1.08352800	-0.00001900

Anion 6a

Sum of electronic and thermal Free energies = -1306.149160 a.u.

E (RB3LYP) = -1306.22362698 a.u.

Sum of electronic and thermal Enthalpies = -1306.092783 a.u.

C	-1.60675600	0.52274300	0.02706000
C	-2.94925000	0.32828000	-0.30353400
C	-3.47092300	-0.93841500	-0.52647700
C	-2.65418900	-2.05900200	-0.40174500
C	-1.32117900	-1.89882800	-0.04837900
C	-0.80845800	-0.61700200	0.16186000
H	-3.55656600	1.21941800	-0.37816100
H	-4.51310000	-1.05495800	-0.79749500
H	-3.04843200	-3.05239300	-0.57054900
H	-0.67583700	-2.75317800	0.07871400
C	-1.07786300	1.97039300	0.14105600
O	0.15481700	2.06731200	-0.03635300
O	-1.93842900	2.84552800	0.35067900
S	0.90419500	-0.59731400	0.76733500
O	1.07658600	0.19876000	1.96007500
O	1.31591700	-1.99812600	0.80996300
C	2.04633400	0.10068400	-0.62321500
F	2.65361800	1.21442600	-0.26104700
F	1.39534900	0.25971400	-1.77361400
F	3.00763300	-0.82555900	-0.83695600

Anion 6b

Sum of electronic and thermal Free energies = -1306.164266 a.u.

E (RB3LYP) = -1306.23684066 a.u.

Sum of electronic and thermal Enthalpies = -1306.105936 a.u

C	-2.37872800	0.09249100	0.00900100
C	-2.57854100	1.41717900	0.39610000
C	-1.53553200	2.34270400	0.39623800
C	-0.25983600	1.95580700	0.01245700
C	-0.06457000	0.62759000	-0.37464700
C	-1.10205100	-0.30410300	-0.38296200
H	-3.58174800	1.69149400	0.69283100
H	-1.71499300	3.36808900	0.69328000
H	0.56348300	2.65342500	-0.00563800
H	-0.95804900	-1.32898500	-0.69240600
C	-3.55622000	-0.92285800	0.01509200
O	-3.25532000	-2.07773100	-0.35123300
O	-4.65136600	-0.44944600	0.38863300
S	1.56058000	0.13236800	-0.85468700
O	1.52681900	-1.02013100	-1.72971400
O	2.37558000	1.29351000	-1.16488700
C	2.31106100	-0.52738800	0.75418900
F	1.62197000	-1.56966800	1.21990200
F	2.33507100	0.42496400	1.69604600
F	3.56993900	-0.91752400	0.51646500

Anion 6c

Sum of electronic and thermal Free energies = -1306.166269 a.u.

E (RB3LYP) = -1306.23880257 a.u.

Sum of electronic and thermal Enthalpies = -1306.107801 a.u.

C	2.68064700	0.00013400	-0.02291400
C	1.98447200	1.20483000	-0.15462900
C	0.62213000	1.22011800	-0.41132000
C	-0.05008900	0.00173800	-0.54106000
C	0.62190200	-1.21750700	-0.41756500
C	1.98415800	-1.20380500	-0.16073500
H	2.55158200	2.11910700	-0.05137500
H	0.08129100	2.14811500	-0.52536400
H	0.08084600	-2.14477100	-0.53643200
H	2.55101700	-2.11873800	-0.06207300
C	4.20722700	-0.00091200	0.26823600
O	4.72241400	-1.13546700	0.36451000
O	4.72239500	1.13304600	0.36975600
S	-1.77800300	0.00269000	-0.85363200
O	-2.20453100	1.26950900	-1.41625600
O	-2.20452600	-1.26061100	-1.42415900
C	-2.54550400	-0.00273100	0.87719300
F	-2.17881900	-1.09074200	1.56281600
F	-2.17862100	1.08079600	1.56973000
F	-3.87948800	-0.00225100	0.76293300

Computed Hirshfeld atomic charges									
Substituted benzoic acids with N electrons									
Atoms	1a	1b	1c	2a	2b	2c	3a	3b	3c
C ₁	0.2158	0.2153	0.2136	0.2097	0.2171	0.2101	0.2083	0.2162	0.2069
C ₂	-0.0189	-0.0167	-0.0206	-0.0285	-0.0143	-0.0299	-0.0406	-0.0169	-0.0352
C ₃	0.0240	-0.0329	-0.0268	0.0939	-0.0404	-0.0242	0.0725	-0.0505	-0.0259
C ₄	-0.0465	0.0078	-0.0455	-0.0685	0.0777	-0.0655	-0.0667	0.0533	-0.0636
C ₅	-0.0315	-0.0359	0.0168	-0.0311	-0.0576	0.0869	-0.0322	-0.0540	0.0630
C ₆	-0.0471	-0.0422	-0.0471	-0.0584	-0.0414	-0.0562	-0.0676	-0.0425	-0.0655
C ₇	-0.0341	-0.0375	-0.0327	-0.0316	-0.0494	-0.0304	-0.0349	-0.0535	-0.0319
C ₈	-0.0985	-0.0929	-0.0922	-0.0037	-0.0076	-0.0056			
O ₁	-0.2792	-0.2936	-0.2954	-0.2918	-0.2913	-0.3006	-0.2873	-0.2953	-0.3045
O ₂	-0.1832	-0.1824	-0.1838	-0.1893	-0.1814	-0.1859	-0.1819	-0.1816	-0.1810
O ₃				-0.1174	-0.1367	-0.1320			
N ₁							-0.1705	-0.1927	-0.1810
H ₁	0.1822	0.1840	0.1835	0.1793	0.1844	0.1824	0.1823	0.1836	0.1804
H ₂	0.0462	0.0489	0.0488	0.0451	0.0566	0.0507	0.0435	0.0470	0.0492
H ₃	0.0514	0.0489	0.0468	0.0516	0.0467	0.0537	0.0506	0.0458	0.0444
H ₄	0.0495	0.0493	0.0480	0.0477	0.0501	0.0468	0.0444	0.0494	0.0453
H ₅	0.0462	0.0482	0.0528	0.0476	0.0464	0.0537	0.0465	0.0449	0.0532
H ₆	0.0436	0.0436	0.0442	0.0576	0.0548	0.0453	0.1285	0.1221	0.1272
H ₇	0.0436	0.0442	0.0432	0.0438	0.0420	0.0553	0.1051	0.1244	0.1274
H ₈	0.0365	0.0436	0.0463	0.0438	0.0430	0.0453			

Atoms	4a	4b	4c	5a	5b	5c	6a	6b	6c
C ₁	0.2169	0.2188	0.2195	0.2196	0.2203	0.2214	0.2196	0.2210	0.2224
C ₂	-0.0060	-0.0088	-0.0057	0.0028	-0.0059	0.0005	0.0107	-0.0037	0.0040
C ₃	-0.0092	-0.0204	-0.0246	0.0468	-0.0117	-0.0159	-0.0276	-0.0080	-0.0135
C ₄	-0.0354	-0.0226	-0.0334	-0.0250	0.0417	-0.0238	-0.0204	-0.0290	-0.0193
C ₅	-0.0232	-0.0217	-0.0158	-0.0237	-0.0161	0.0478	-0.0250	-0.0117	-0.0231
C ₆	-0.0295	-0.0317	-0.0305	-0.0217	-0.0284	-0.0250	-0.0153	-0.0257	-0.0205
C ₇	-0.0265	-0.0207	-0.0186	-0.0198	-0.0143	-0.0220	-0.0248	-0.0105	-0.0196
C ₈	0.2294	0.2291	0.2295				0.2102	0.2088	0.2090
O ₁	-0.2706	-0.2836	-0.2840	-0.2784	-0.2787	-0.2795	-0.2717	-0.2766	-0.2774
O ₂	-0.1782	-0.1779	-0.1769	-0.1781	-0.1762	-0.1742	-0.1733	-0.1752	-0.1729
O ₃				-0.1956	-0.1911	-0.1933	-0.2884	-0.2918	-0.2946
O ₄				-0.1903	-0.1974	-0.1942	-0.2952	-0.2962	-0.2941
N ₁				0.2257	0.2262	0.2268			
S ₁							0.4569	0.4575	0.4580
F ₁	-0.0903	-0.0980	-0.0983				-0.0599	-0.0690	-0.0703
F ₂	-0.0903	-0.0813	-0.0922				-0.0733	-0.0723	-0.0708
F ₃	-0.0919	-0.0980	-0.0850				-0.0605	-0.0587	-0.0585
H ₁	0.1875	0.1888	0.1891	0.1939	0.1908	0.1913	0.1942	0.1918	0.1924
H ₂	0.0512	0.0566	0.0548	0.0611	0.0620	0.0575	0.0611	0.0648	0.0586
H ₃	0.0581	0.0592	0.0551	0.0605	0.0610	0.0602	0.0609	0.0643	0.0635
H ₄	0.0571	0.0572	0.0582	0.0603	0.0602	0.0609	0.0615	0.0616	0.0642
H ₅	0.0509	0.0548	0.0588	0.0616	0.0575	0.0614	0.0605	0.0587	0.0625

Substituted benzoic acids with N+1 electrons

Atoms	1a	1b	1c	2a	2b	2c	3a	3b	3c
C ₁	0.1143	0.1155	0.1171	0.1154	0.1120	0.1416	0.1056	0.1128	0.1572
C ₂	-0.0810	-0.0812	-0.0819	-0.0912	-0.0802	-0.0682	-0.0890	-0.0804	-0.0677
C ₃	-0.0287	-0.0911	-0.0991	0.0486	-0.1196	-0.0740	0.0292	-0.1225	-0.0704
C ₄	-0.1014	-0.0384	-0.1002	-0.1290	0.0343	-0.0971	-0.1356	0.0092	-0.1021
C ₅	-0.1422	-0.1409	-0.0676	-0.1431	-0.1523	0.0367	-0.1407	-0.1517	0.0166
C ₆	-0.1059	-0.1020	-0.0991	-0.1128	-0.1061	-0.0920	-0.1192	-0.1063	-0.0982
C ₇	-0.1036	-0.1053	-0.0890	-0.1103	-0.1021	-0.0713	-0.1145	-0.1093	-0.0634
C ₈	-0.1196	-0.1167	-0.1262	-0.0242	-0.0266	-0.0899			
O ₁	-0.3932	-0.4095	-0.4077	-0.4053	-0.4101	-0.3789	-0.3985	-0.4116	-0.3665
O ₂	-0.2377	-0.2368	-0.2362	-0.2389	-0.2396	-0.2246	-0.2362	-0.2387	-0.2178
O ₃				-0.1366	-0.1600	-0.1608			
N ₁							-0.2105	-0.2250	-0.2066
H ₁	0.1365	0.1389	0.1397	0.1354	0.1379	0.1502	0.1373	0.1373	0.1528
H ₂	0.0086	0.0136	0.0087	0.0088	0.0143	0.0236	0.0002	0.0053	0.0219
H ₃	-0.0088	-0.0096	0.0067	-0.0085	-0.0020	0.0239	-0.0099	-0.0106	-0.0178
H ₄	0.0077	0.0081	0.0073	0.0074	0.0068	0.0125	0.0042	0.0060	-0.0096
H ₅	0.0056	0.0076	0.0137	0.0042	0.0105	0.0225	0.0025	0.0078	0.0274
H ₆	0.0199	0.0125	0.0043	0.0345	0.0309	-0.0446	0.0936	0.0888	-0.0819
H ₇	0.0199	0.0224	0.0095	0.0229	0.0259	-0.0909	0.0814	0.0883	-0.0742
H ₈	0.0094	0.0125	-0.0001	0.0229	0.0259	-0.0187			

Atoms	4a	4b	4c	5a	5b	5c	6a	6b	6c
C ₁	0.1256	0.1245	0.1272	0.1949	0.1860	0.1667	0.2035	0.1530	0.1485
C ₂	-0.0779	-0.0787	-0.0774	-0.0453	-0.0509	-0.0640	-0.0521	-0.0659	-0.0678
C ₃	-0.0750	-0.0708	-0.0933	0.0085	-0.0411	-0.0712	-0.0970	-0.0374	-0.0774
C ₄	-0.0834	-0.0750	-0.0940	-0.0693	0.0032	-0.0766	-0.0819	-0.0790	-0.0791
C ₅	-0.1300	-0.1334	-0.1030	-0.0835	-0.0917	0.0028	-0.0937	-0.1179	-0.0903
C ₆	-0.1023	-0.0911	-0.0915	-0.1050	-0.0769	-0.0746	-0.1265	-0.0778	-0.0772
C ₇	-0.0851	-0.1012	-0.0814	-0.0605	-0.1069	-0.0646	-0.0735	-0.1098	-0.0708
C ₈	0.2073	0.2099	0.1995				0.1827	0.1906	0.1874
O ₁	-0.3784	-0.3985	-0.3962	-0.3400	-0.3364	-0.3576	-0.3192	-0.3696	-0.3732
O ₂	-0.2300	-0.2296	-0.2289	-0.1961	-0.2014	-0.2094	-0.1960	-0.2140	-0.2171
O ₃				-0.3548	-0.3395	-0.3333	-0.3403	-0.3350	-0.3423
O ₄				-0.3403	-0.3411	-0.3342	-0.3509	-0.3369	-0.3418
N ₁				0.1321	0.1388	0.1454			
S ₁							0.3834	0.4127	0.4001
F ₁	-0.1182	-0.1245	-0.1356				-0.0784	-0.0825	-0.0859
F ₂	-0.1182	-0.1052	-0.1256				-0.0932	-0.0864	-0.0864
F ₃	-0.1224	-0.1245	-0.1144				-0.1009	-0.0906	-0.0934
H ₁	0.1438	0.1446	0.1453	0.1622	0.1621	0.1584	0.1613	0.1548	0.1541
H ₂	0.0177	0.0248	0.0145	0.0311	0.0390	0.0255	0.0262	0.0418	0.0240
H ₃	0.0008	0.0029	0.0160	0.0211	0.0205	0.0279	0.0177	0.0158	0.0298
H ₄	0.0111	0.0157	0.0185	0.0137	0.0244	0.0289	0.0029	0.0240	0.0309
H ₅	0.0146	0.0102	0.0202	0.0308	0.0118	0.0298	0.0260	0.0096	0.0281

Substituted benzoic acids with N-1 electrons

Atoms	1a	1b	1c	2a	2b	2c	3a	3b	3c
C₁	0.2332	0.2314	0.2420	0.2285	0.2305	0.2373	0.2331	0.2304	0.2351
C₂	0.0386	0.0427	0.1003	0.0404	0.0294	0.0776	0.0248	0.0303	0.0710
C₃	0.1342	0.0413	0.0356	0.1654	0.0419	0.0332	0.1264	0.0255	0.0224
C₄	0.0395	0.1285	0.0216	0.0063	0.1578	-0.0002	0.0157	0.1249	0.0102
C₅	0.0292	0.0344	0.1285	0.0283	0.0054	0.1616	0.0185	0.0158	0.1284
C₆	0.0970	0.0292	0.0340	0.0692	0.0298	0.0295	0.0552	0.0180	0.0128
C₇	0.0386	0.0990	0.0245	0.0217	0.0705	0.0161	0.0243	0.0631	0.0172
C₈	-0.0587	-0.0521	-0.0536	0.0305	0.0285	0.0284			
O₁	-0.2259	-0.2371	-0.2038	-0.2375	-0.2431	-0.2195	-0.2363	-0.2469	-0.2248
O₂	-0.1575	-0.1577	-0.1518	-0.1616	-0.1596	-0.1555	-0.1486	-0.1588	-0.1585
O₃				0.0009	-0.0085	-0.0137			
N₁							-0.0134	-0.0267	-0.0285
H₁	0.2108	0.2135	0.2151	0.2079	0.2114	0.2123	0.2123	0.2109	0.2106
H₂	0.0900	0.0872	0.0861	0.0817	0.0942	0.0847	0.0838	0.0824	0.0834
H₃	0.0940	0.0905	0.0898	0.0917	0.0822	0.0956	0.0892	0.0845	0.0843
H₄	0.1054	0.0940	0.0885	0.0999	0.0925	0.0822	0.0965	0.0901	0.0842
H₅	0.0856	0.0981	0.0898	0.0823	0.0933	0.0885	0.0824	0.0915	0.0867
H₆	0.0895	0.0912	0.0813	0.0896	0.0882	0.0774	0.1849	0.1819	0.1825
H₇	0.0895	0.0747	0.0762	0.0773	0.0777	0.0874	0.1513	0.1828	0.1829
H₈	0.0670	0.0912	0.0960	0.0773	0.0777	0.0774			

Atoms	4a	4b	4c	5a	5b	5c	6a	6b	6c
C ₁	0.2315	0.2492	0.2521	0.2566	0.2543	0.2409	0.2630	0.2568	0.2401
C ₂	0.0320	0.1084	0.1063	0.0771	0.0755	0.0503	0.0842	0.0787	0.0476
C ₃	0.1074	0.0687	0.0701	0.0977	0.0793	0.1207	0.0006	0.0716	0.1188
C ₄	0.0768	0.0197	0.0159	0.0175	0.0715	0.0570	0.0521	-0.0024	0.0670
C ₅	0.0264	0.1110	0.0955	0.0787	0.0781	0.0923	0.0885	0.0835	0.0142
C ₆	0.1076	0.0736	0.0604	0.0512	0.0827	0.1051	0.0308	0.0727	0.1049
C ₇	0.0831	0.0271	0.0251	0.0212	0.0263	0.0526	0.0474	0.0273	0.0590
C ₈	0.2468	0.2407	0.2471				0.2197	0.2249	0.2216
O ₁	-0.2169	-0.1799	-0.1724	-0.1306	-0.1643	-0.2093	-0.1037	-0.1572	-0.2126
O ₂	-0.1515	-0.1434	-0.1391	-0.1294	-0.1336	-0.1444	-0.1119	-0.1309	-0.1445
O ₃				-0.0979	-0.1134	-0.1234	-0.2613	-0.2495	-0.2387
O ₄				-0.1037	-0.1163	-0.1148	-0.2558	-0.2365	-0.2504
N ₁				0.2457	0.2438	0.2417			
S ₁							0.4707	0.4822	0.4801
F ₁	-0.0516	-0.0704	-0.0570				-0.0548	-0.0535	-0.0563
F ₂	-0.0516	-0.0566	-0.0561				-0.0597	-0.0547	-0.0566
F ₃	-0.0598	-0.0704	-0.0529				-0.0346	-0.0283	-0.0297
H ₁	0.2166	0.2208	0.2226	0.2271	0.2227	0.2200	0.2297	0.2236	0.2201
H ₂	0.0969	0.0943	0.0969	0.0926	0.0955	0.0966	0.0954	0.0954	0.0972
H ₃	0.0993	0.1097	0.0917	0.1047	0.1004	0.1058	0.1070	0.1016	0.1069
H ₄	0.1117	0.1063	0.1011	0.1000	0.1075	0.1002	0.0973	0.1051	0.1030
H ₅	0.0950	0.0910	0.0926	0.0913	0.0899	0.1086	0.0953	0.0895	0.1082

Electronegativity and Global Softness						
---------------------------------------	--	--	--	--	--	--

Electronegativity (eV)

Benzoic acids	1	2	3	4	5	6
a	4.5337	4.1803	3.8855	5.1136	5.5469	5.4444
b	4.5534	4.2241	3.9573	5.1959	5.6893	5.5630
c	4.5168	4.1790	3.8947	5.2949	5.8478	5.7976

Global softness (eV⁻¹)

Benzoic acids	1	2	3	4	5	6
a	0.1149	0.1227	0.1307	0.1158	0.1239	0.1213
b	0.1151	0.1240	0.1313	0.1120	0.1195	0.1158
c	0.1144	0.1206	0.1261	0.1142	0.1254	0.1208

Condensed Fukui function calculated using Hirshfeld charge

Electrophilic attack

Atoms	1a	1b	1c	2a	2b	2c	3a	3b	3c
C ₁	0.017	0.016	0.028	0.019	0.013	0.027	0.025	0.014	0.028
C ₂	0.058	0.059	0.121	0.069	0.044	0.110	0.065	0.047	0.110
C ₃	0.110	0.074	0.062	0.071	0.082	0.057	0.054	0.076	0.049
C ₄	0.086	0.121	0.067	0.075	0.080	0.065	0.082	0.072	0.074
C ₅	0.061	0.070	0.112	0.059	0.063	0.075	0.051	0.070	0.066
C ₆	0.144	0.071	0.081	0.130	0.071	0.086	0.123	0.061	0.079
C ₇	0.073	0.136	0.057	0.053	0.120	0.046	0.059	0.120	0.050
C ₈	0.040	0.041	0.039	0.034	0.036	0.034			
O ₁	0.053	0.056	0.092	0.054	0.048	0.081	0.051	0.048	0.080
O ₂	0.026	0.025	0.032	0.028	0.022	0.030	0.033	0.023	0.023
O ₃				0.118	0.128	0.118			
N ₁							0.157	0.166	0.154
H ₁	0.029	0.029	0.032	0.029	0.027	0.030	0.030	0.027	0.030
H ₂	0.044	0.038	0.037	0.037	0.038	0.034	0.040	0.035	0.035
H ₃	0.043	0.042	0.043	0.040	0.036	0.042	0.039	0.039	0.040
H ₄	0.056	0.045	0.040	0.052	0.042	0.035	0.052	0.041	0.039
H ₅	0.039	0.050	0.037	0.035	0.047	0.035	0.036	0.047	0.034
H ₆	0.046	0.048	0.037	0.032	0.033	0.032	0.056	0.060	0.056
H ₇	0.046	0.031	0.033	0.033	0.033	0.032	0.046	0.058	0.056
H ₈	0.030	0.048	0.050	0.033	0.035	0.032			

Atoms	4a	4b	4c	5a	5b	5c	6a	6b	6c
C ₁	0.091	0.094	0.092	0.037	0.034	0.020	0.043	0.036	0.018
C ₂	0.072	0.070	0.072	0.074	0.081	0.050	0.073	0.082	0.044
C ₃	0.066	0.050	0.069	0.051	0.091	0.137	0.028	0.080	0.132
C ₄	0.048	0.052	0.061	0.043	0.030	0.081	0.073	0.027	0.086
C ₅	0.107	0.112	0.087	0.102	0.094	0.044	0.114	0.095	0.037
C ₆	0.073	0.059	0.061	0.073	0.111	0.130	0.046	0.098	0.125
C ₇	0.059	0.080	0.063	0.041	0.041	0.074	0.072	0.038	0.079
C ₈	0.022	0.019	0.030				0.010	0.016	0.013
O ₁	0.108	0.115	0.112	0.148	0.114	0.070	0.168	0.119	0.065
O ₂	0.052	0.052	0.052	0.049	0.043	0.030	0.061	0.044	0.028
O ₃				0.098	0.078	0.070	0.027	0.042	0.056
O ₄				0.087	0.081	0.079	0.039	0.060	0.044
N ₁				0.020	0.018	0.015			
S ₁							0.014	0.025	0.022
F ₁	0.028	0.027	0.037				0.018	0.013	0.016
F ₂	0.028	0.024	0.033				0.020	0.014	0.016
F ₃	0.030	0.027	0.029				0.040	0.032	0.035
H ₁	0.029	0.032	0.033	0.033	0.032	0.029	0.035	0.032	0.028
H ₂	0.046	0.038	0.042	0.031	0.034	0.039	0.034	0.031	0.039
H ₃	0.041	0.050	0.037	0.044	0.039	0.046	0.046	0.037	0.043
H ₄	0.055	0.049	0.043	0.040	0.047	0.039	0.036	0.044	0.039
H ₅	0.044	0.036	0.034	0.030	0.032	0.047	0.035	0.031	0.046

Nucleophilic attack

Atoms	1a	1b	1c	2a	2b	2c	3a	3b	3c
C₁	0.102	0.100	0.097	0.094	0.105	0.069	0.103	0.103	0.049
C₂	0.062	0.065	0.061	0.063	0.066	0.038	0.048	0.063	0.032
C₃	0.053	0.058	0.072	0.045	0.079	0.050	0.043	0.072	0.044
C₄	0.055	0.046	0.055	0.061	0.043	0.032	0.069	0.044	0.038
C₅	0.111	0.105	0.084	0.112	0.095	0.050	0.108	0.098	0.046
C₆	0.059	0.060	0.052	0.054	0.065	0.036	0.052	0.064	0.032
C₇	0.069	0.068	0.056	0.079	0.053	0.041	0.080	0.056	0.031
C₈	0.021	0.024	0.034	0.021	0.019	0.084			
O₁	0.114	0.116	0.112	0.113	0.119	0.078	0.111	0.116	0.062
O₂	0.054	0.054	0.052	0.050	0.058	0.039	0.054	0.057	0.036
O₃				0.019	0.023	0.029			
N₁							0.040	0.032	0.025
H₁	0.046	0.045	0.044	0.044	0.047	0.032	0.045	0.046	0.027
H₂	0.038	0.035	0.039	0.036	0.042	0.027	0.043	0.042	0.027
H₃	0.060	0.059	0.041	0.060	0.049	0.030	0.061	0.056	0.062
H₄	0.042	0.041	0.040	0.040	0.043	0.034	0.040	0.043	0.054
H₅	0.041	0.041	0.040	0.043	0.036	0.031	0.044	0.037	0.026
H₆	0.024	0.031	0.040	0.023	0.024	0.090	0.035	0.033	0.207
H₇	0.024	0.022	0.034	0.021	0.016	0.146	0.024	0.036	0.200
H₈	0.027	0.031	0.046	0.021	0.017	0.064			

Atoms	4a	4b	4c	5a	5b	5c	6a	6b	6c
C₁	0.091	0.094	0.092	0.025	0.034	0.055	0.016	0.068	0.074
C₂	0.072	0.070	0.072	0.048	0.045	0.064	0.063	0.062	0.072
C₃	0.066	0.050	0.069	0.038	0.029	0.055	0.069	0.029	0.064
C₄	0.048	0.052	0.061	0.044	0.038	0.053	0.061	0.050	0.060
C₅	0.107	0.112	0.087	0.060	0.076	0.045	0.069	0.106	0.067
C₆	0.073	0.059	0.061	0.083	0.049	0.050	0.111	0.052	0.057
C₇	0.059	0.080	0.063	0.041	0.093	0.043	0.049	0.099	0.051
C₈	0.022	0.019	0.030				0.028	0.018	0.022
O₁	0.108	0.115	0.112	0.062	0.058	0.078	0.047	0.093	0.096
O₂	0.052	0.052	0.052	0.018	0.025	0.035	0.023	0.039	0.044
O₃				0.159	0.148	0.140	0.052	0.043	0.048
O₄				0.150	0.144	0.140	0.056	0.041	0.048
N₁				0.094	0.087	0.081			
S₁							0.074	0.045	0.058
F₁	0.028	0.027	0.037				0.018	0.013	0.016
F₂	0.028	0.024	0.033				0.020	0.014	0.016
F₃	0.030	0.027	0.029				0.040	0.032	0.035
H₁	0.044	0.044	0.044	0.032	0.029	0.033	0.033	0.037	0.038
H₂	0.033	0.032	0.040	0.030	0.023	0.032	0.035	0.023	0.035
H₃	0.057	0.056	0.039	0.039	0.041	0.032	0.043	0.049	0.034
H₄	0.046	0.042	0.040	0.047	0.036	0.032	0.059	0.038	0.033
H₅	0.036	0.045	0.039	0.031	0.046	0.032	0.035	0.049	0.034

Absolute gas phase acidities for **1a–6c** calculated at the M062X/6-311++G(2d,2p) level of theory. The values are reported in kcal/mol. $\Delta_{\text{acid}}G^\circ = G^\circ(\text{anion}) + G^\circ(\text{H}^+) - G^\circ(\text{acid})$. The experimental values are given in parentheses and were obtained from <http://webbook.nist.gov/chemistry/>

	1	2	3	4	5	6
a	338.58 (332.46 ± 2.01)	342.80 (332.46 ± 2.01)	337.03 (330.31 ± 2.01)	332.39 (-----)	329.73 (324.33 ± 2.01)	322.5 (-----)
b	339.47 (333.65 ± 2.01)	339.43 (332.46 ± 2.01)	340.47 (334.61 ± 2.01)	331.50 (325.29 ± 2.01)	327.77 (322.18 ± 2.01)	324.86 (-----)
c	339.96 (333.89 ± 2.01)	340.74 (333.89 ± 2.01)	342.81 (336.28 ± 2.01)	330.78 (325.29 ± 2.01)	326.63 (320.98 ± 2.01)	323.50 (-----)

Absolute gas phase acidities for **1a–6c** calculated at the MP2/6-311++G(2d,2p) level of theory. The values are reported in kcal/mol. $\Delta_{\text{acid}}G^\circ = G^\circ(\text{anion}) + G^\circ(\text{H}^+) - G^\circ(\text{acid})$. The experimental values are given in parentheses and were obtained from <http://webbook.nist.gov/chemistry/>

	1	2	3	4	5	6
a	331.64 (332.46 ± 2.01)	332.50 (332.46 ± 2.01)	328.23 (330.31 ± 2.01)	324.61 (-----)	321.63 (324.33 ± 2.01)	320.09 (-----)
b	331.70 (333.65 ± 2.01)	332.46 (332.46 ± 2.01)	333.98 (334.61 ± 2.01)	323.31 (325.29 ± 2.01)	319.79 (322.18 ± 2.01)	317.42 (-----)
c	332.95 (333.89 ± 2.01)	332.26 (333.89 ± 2.01)	333.88 (336.28 ± 2.01)	323.29 (325.29 ± 2.01)	319.77 (320.98 ± 2.01)	316.82 (-----)