Supplementary Material (ESI) for New Journal of Chemistry

Quantification of substituent effects using molecular electrostatic potentials: additive nature and proximity effects

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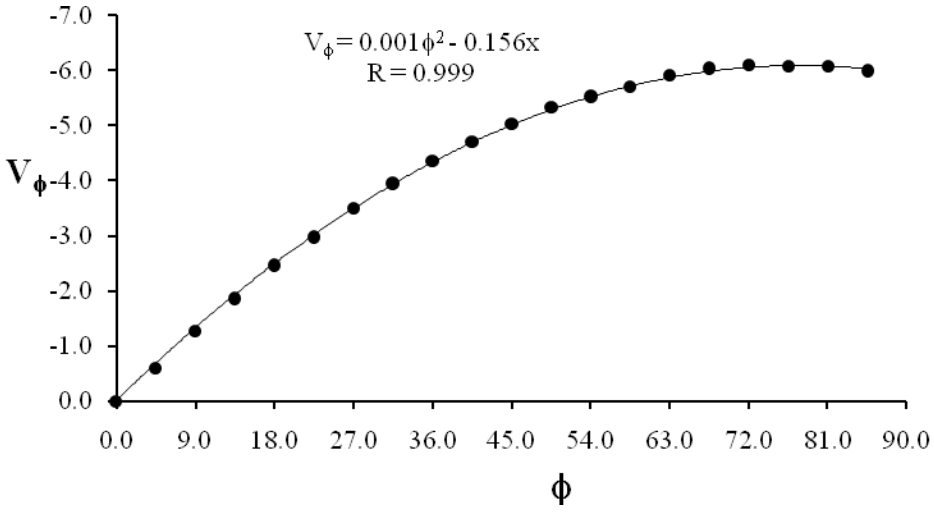

Fig. S1 Dependence of V_ϕ with ϕ in the unsubstituted benzoic acid.

Table S1 ϕ (in degrees) and V_ϕ (kcal/mol) are reported by modelling the free benzoic acid.

ϕ	V_ϕ[a]
0.0	0.00
4.5	-0.59
9.0	-1.27
13.5	-1.86
18.0	-2.46
22.5	-2.97
27.0	-3.50
31.5	-3.95
36.0	-4.35
40.5	-4.69
45.0	-5.02
49.5	-5.33
54.0	-5.52
58.5	-5.69
63.0	-5.90
67.5	-6.03
72.0	-6.08
76.5	-6.07
81.0	-6.07
85.5	-5.98
90.0	-6.04

[a] V_ϕ = -24.08 kcal/mol for ϕ = 0

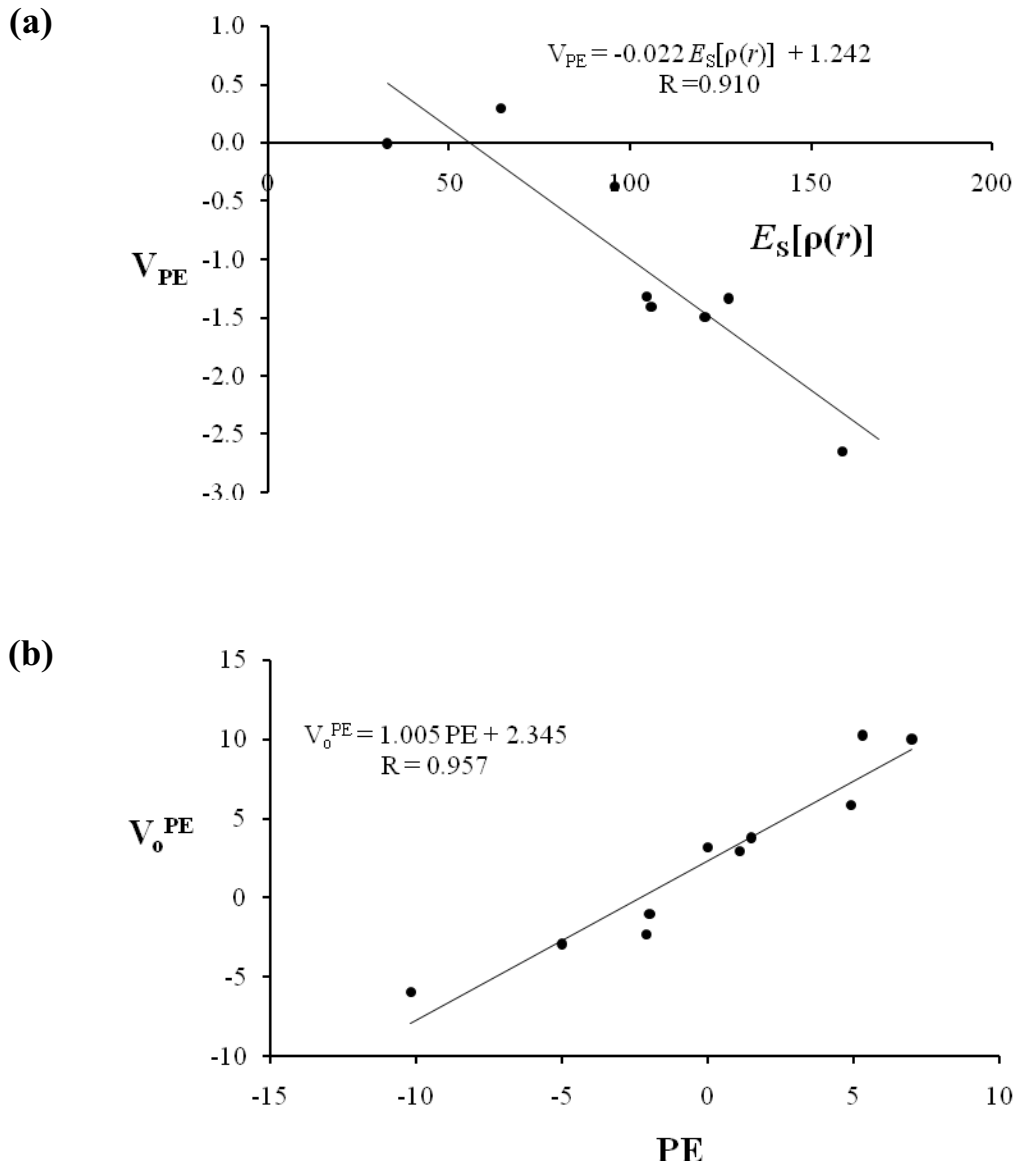

Fig. S2 (a) Plot of $E_S[\rho(r)]$ vs V_{PE} [the hydrogen bonded substituents NH_2 and OH are excluded in correlation] (b) Plot of V_o^E with PE values derived by Exner (PE represents polar effect and the values are taken from Ref.60).

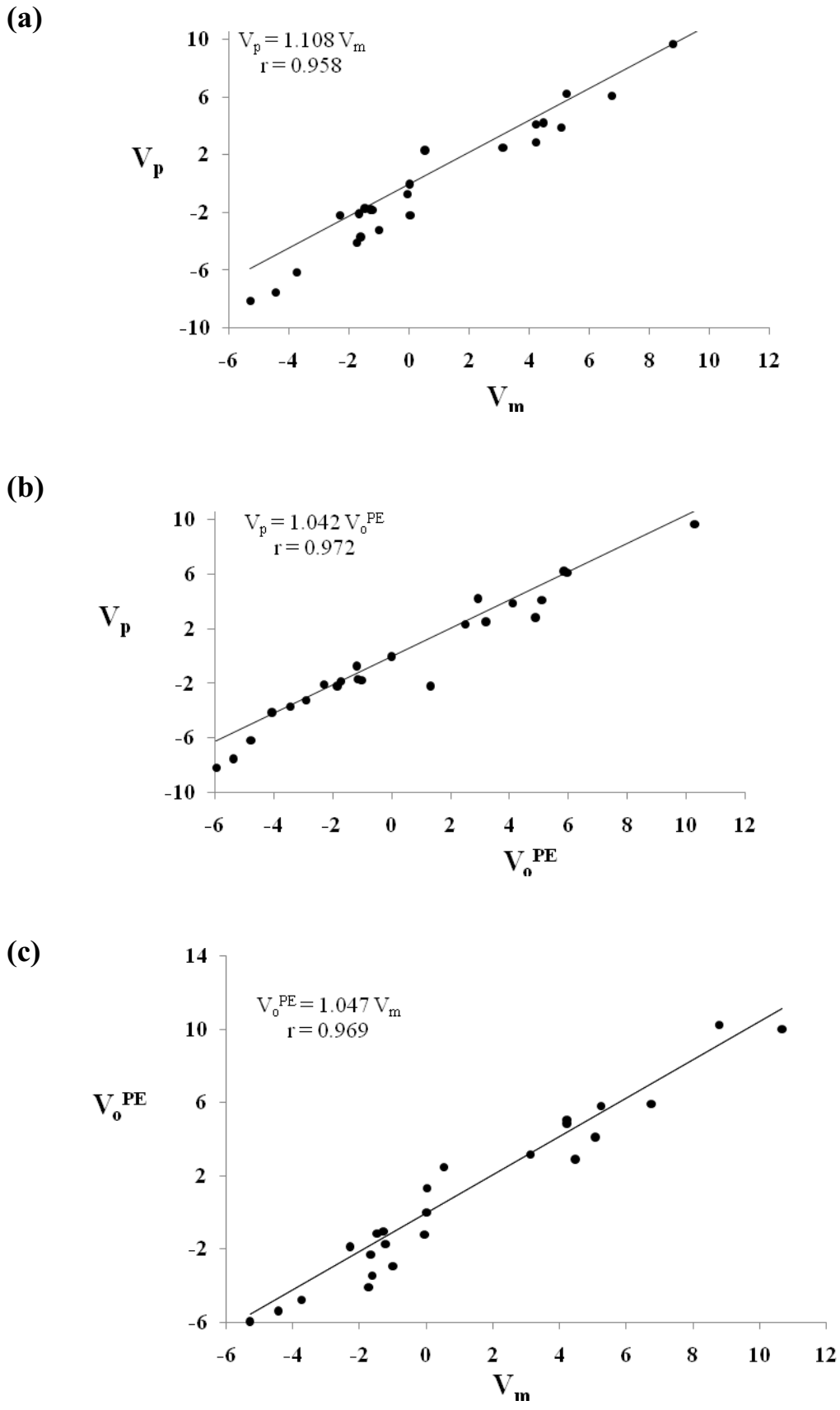

Fig. S3 Inter relationships between electronic effects of ortho, meta and para substituent effects. (a) Plot of V_p vs V_m (b) Plot of V_p vs V_o^{PE} (c) plot of V_o^{PE} vs V_m.

Table S2 B3LYP/6-31G(d,p) optimized geometry of benzoic acid

Benzoic acid molecule E_{scf} = -420.8354491a.u.

6	0.511811000	1.222115000	-0.000147000
6	1.903315000	1.187028000	-0.000243000
6	2.570147000	-0.041018000	-0.000044000
6	1.843664000	-1.233975000	0.000212000
6	0.450507000	-1.204121000	0.000312000
6	-0.219988000	0.026941000	0.000071000
6	-1.703666000	0.120873000	0.000095000
8	-2.314944000	-1.091282000	-0.000724000
8	-2.335512000	1.159029000	0.000489000
1	-0.030154000	2.161640000	-0.000532000
1	2.468783000	2.113940000	-0.000379000
1	3.656028000	-0.068327000	-0.000119000
1	2.363355000	-2.187371000	0.000202000
1	-0.121064000	-2.125092000	0.000704000
1	-3.268041000	-0.903820000	0.000473000

Table S3 B3LYP/6-31G(d,p) optimized geometries of ortho substituted benzoic acids. SCF energy (in a.u.) is also provided

O-CH_3 E_{scf} = -460.1532948				O-CH_2CH_3 E_{scf} = -460.1532948			
6	-0.534855000	0.976764000	-0.000288000	6	0.364574000	0.792484000	-0.284615000
6	-1.933162000	0.888854000	-0.000082000	6	1.726328000	1.125197000	-0.250125000
6	-2.597617000	-0.336059000	0.000019000	6	2.716121000	0.179759000	0.006311000
6	-1.867693000	-1.524363000	0.000112000	6	2.363724000	-1.151271000	0.230138000
6	-0.478706000	-1.468586000	0.000132000	6	1.023008000	-1.514003000	0.193705000
6	0.197679000	-0.236508000	-0.000049000	6	0.016836000	-0.562219000	-0.053625000
6	1.684644000	-0.229612000	0.000105000	6	-1.400599000	-1.017865000	-0.070515000
8	2.221808000	-1.480443000	-0.000368000	8	-1.520586000	-2.371653000	0.000794000
8	2.400888000	0.754490000	0.000365000	8	-2.391371000	-0.313079000	-0.135290000
1	-2.510748000	1.809061000	0.000024000	1	2.010267000	2.158178000	-0.433241000
1	-3.683672000	-0.360236000	-0.000071000	1	3.759576000	0.481397000	0.025717000
1	-2.374304000	-2.484425000	0.000345000	1	3.125101000	-1.899508000	0.427186000
1	0.102086000	-2.382866000	0.000426000	1	0.735970000	-2.544865000	0.360371000
1	3.183225000	-1.343360000	-0.000260000	1	-2.476855000	-2.541524000	-0.002304000
6	0.106829000	2.343027000	-0.000030000	6	-0.631007000	1.905158000	-0.548684000
1	0.751017000	2.484650000	0.871630000	1	-0.113988000	2.691876000	-1.110521000
1	0.751720000	2.484776000	-0.871173000	1	-1.452072000	1.541520000	-1.168013000
1	-0.663598000	3.118925000	-0.000408000	6	-1.212752000	2.509440000	0.742052000
				1	-1.779543000	1.757876000	1.295542000
				1	-0.419969000	2.897304000	1.390376000
				1	-1.890232000	3.335518000	0.503003000
O-$CH(CH_3)_2$ E_{scf} = -538.7823509				O-$C(CH_3)_3$ E_{scf} = -578.0872517			
6	0.517537000	0.385525000	-0.067459000	6	-0.275191000	0.610113000	0.009202000
6	0.786613000	1.759266000	0.021827000	6	-0.150620000	2.009360000	0.034032000
6	-0.223587000	2.710749000	0.142609000	6	1.076567000	2.669476000	0.077390000
6	-1.558957000	2.311523000	0.165060000	6	2.259001000	1.939204000	0.075237000
6	-1.860387000	0.958690000	0.073077000	6	2.181822000	0.552648000	0.041161000
6	-0.845114000	-0.009876000	-0.029783000	6	0.947259000	-0.122055000	0.030399000
6	-1.257449000	-1.441297000	-0.074136000	6	1.065967000	-1.612350000	0.107836000
8	-2.573704000	-1.598920000	-0.382399000	8	2.114183000	-2.075651000	-0.624707000
8	-0.554712000	-2.411497000	0.144170000	8	0.385367000	-2.377614000	0.763119000
1	1.816908000	2.096154000	-0.006355000	1	-1.043240000	2.619260000	0.012303000
1	0.035012000	3.763504000	0.214432000	1	1.098171000	3.755308000	0.102041000
1	-2.355702000	3.043538000	0.252783000	1	3.224832000	2.434041000	0.097482000
1	-2.892618000	0.630983000	0.087714000	1	3.091212000	-0.036323000	0.035419000
1	-2.729323000	-2.557099000	-0.345620000	1	2.148149000	-3.030922000	-0.446865000
6	1.679278000	-0.599975000	-0.185734000	6	-1.695061000	-0.011990000	-0.068422000
1	1.303119000	-1.496102000	-0.681535000	6	-2.092626000	-0.593071000	1.311439000
6	2.853053000	-0.064943000	-1.024157000	6	-1.774416000	-1.102630000	-1.164830000
1	2.520286000	0.307069000	-1.998468000	1	-1.469879000	-0.700146000	-2.137038000
1	3.397141000	0.742143000	-0.521688000	1	-1.165172000	-1.976009000	-0.940198000
1	3.572433000	-0.871322000	-1.199666000	1	-2.809351000	-1.448734000	-1.257831000
6	2.159920000	-1.033075000	1.214521000	1	-1.409778000	-1.381442000	1.624312000
1	2.530453000	-0.173813000	1.785332000	1	-3.106224000	-1.007390000	1.259608000
1	1.348764000	-1.501852000	1.775695000	1	-2.092409000	0.195242000	2.072243000
1	2.975416000	-1.759385000	1.128263000	6	-2.761328000	1.045350000	-0.440582000
				1	-2.889822000	1.805995000	0.335480000
				1	-2.534086000	1.548813000	-1.386187000
				1	-3.727050000	0.544101000	-0.555237000

O-C_6H_5 E_{scf} = -651.8889278			
6	-0.481072000	-0.661683000	0.017916000
6	-0.932019000	-1.988832000	0.110491000
6	-2.288092000	-2.300471000	0.174998000
6	-3.238794000	-1.279347000	0.168706000
6	-2.817207000	0.041921000	0.073319000
6	-1.454922000	0.363811000	-0.026747000
6	-1.168867000	1.817370000	-0.228189000
8	-0.050124000	2.064518000	-0.946627000
8	-1.896845000	2.712914000	0.154756000
1	-0.193633000	-2.782932000	0.163275000
1	-2.599042000	-3.338590000	0.248309000
1	-4.297486000	-1.510131000	0.233985000
1	-3.533816000	0.855695000	0.056128000
1	0.008642000	3.032515000	-1.014572000
6	0.990535000	-0.425225000	0.048985000
6	1.833135000	-1.083411000	-0.858370000
6	1.569795000	0.394107000	1.030156000
6	3.216582000	-0.915283000	-0.797260000
6	2.951773000	0.557071000	1.095506000
6	3.780623000	-0.095132000	0.180160000
1	1.397091000	-1.715259000	-1.626677000
1	0.931647000	0.891941000	1.754570000
1	3.852746000	-1.424697000	-1.515344000
1	3.382908000	1.189547000	1.866230000
1	4.857870000	0.033071000	0.231036000

O-F E_{scf} = -520.0609513			
6	0.551044000	0.954486000	-0.000219000
6	1.941438000	0.907860000	-0.000255000
6	2.582993000	-0.328374000	-0.000027000
6	1.835274000	-1.508944000	0.000220000
6	0.446024000	-1.446670000	0.000224000
6	-0.228957000	-0.213113000	0.000014000
6	-1.714290000	-0.146049000	0.000071000
8	-2.279957000	-1.384811000	0.000006000
8	-2.388341000	0.861496000	0.000462000
1	2.492562000	1.841589000	-0.000469000
1	3.668073000	-0.367701000	-0.000041000
1	2.333942000	-2.472519000	0.000406000
1	-0.143324000	-2.355606000	0.000386000
1	-3.238657000	-1.228495000	0.000173000
9	-0.027486000	2.161565000	-0.000485000

O-Cl E_{scf} = -880.4192247			
6	0.539227000	0.717011000	-0.006734000
6	1.935973000	0.720232000	-0.005507000
6	2.642714000	-0.478812000	0.019641000
6	1.956671000	-1.693447000	0.037371000
6	0.567277000	-1.695260000	0.029921000
6	-0.173664000	-0.498797000	0.011505000
6	-1.664750000	-0.572526000	0.032257000
8	-2.111908000	-1.840988000	-0.182142000
8	-2.434149000	0.343843000	0.220903000
1	2.457459000	1.670219000	-0.025514000
1	3.728322000	-0.458922000	0.023527000
1	2.499633000	-2.632768000	0.056099000
1	0.024729000	-2.632155000	0.042306000
1	-3.079768000	-1.781499000	-0.125963000
17	-0.240154000	2.283640000	-0.058309000

O-Br E_{scf} = -2991.9290605			
6	0.106659000	-0.639925000	-0.000003000
6	-0.200061000	-2.002274000	0.000077000
6	-1.525864000	-2.427036000	0.000104000
6	-2.558343000	-1.489029000	0.000036000
6	-2.251953000	-0.133944000	-0.000057000
6	-0.920577000	0.324269000	-0.000068000
6	-0.667841000	1.795985000	-0.000098000
8	-1.826756000	2.511288000	-0.000204000
8	0.410457000	2.349047000	0.000455000
1	0.609989000	-2.722044000	0.000115000
1	-1.745887000	-3.490373000	0.000175000
1	-3.594957000	-1.809916000	0.000058000
1	-3.046409000	0.601372000	-0.000117000
1	-1.549563000	3.442023000	0.000015000
35	1.964717000	-0.213486000	-0.000063000

O- OCH_3 E_{scf} = -535.3530417			
6	-0.742762000	-0.282528000	0.000073000
6	-1.880500000	0.539692000	-0.000161000
6	-1.752223000	1.926704000	-0.000476000
6	-0.492987000	2.524821000	-0.000484000
6	0.638288000	1.716108000	-0.000283000
6	0.546014000	0.315468000	-0.000103000
6	1.786949000	-0.503513000	-0.000455000
8	2.911728000	0.273917000	0.002873000
8	1.869720000	-1.713862000	-0.003380000
1	-2.869320000	0.099244000	-0.000086000
1	-2.649001000	2.539903000	-0.000692000
1	-0.393108000	3.605085000	-0.000657000
1	1.625066000	2.162065000	-0.000332000
1	3.647956000	-0.359012000	0.001856000

O- OCH_2CH_3 E_{scf} =-574.6753906			
6	-0.248949000	-0.527736000	0.000025000
6	-0.175993000	-1.930294000	-0.000023000
6	1.058091000	-2.575829000	-0.000233000
6	2.244577000	-1.843722000	-0.000378000
6	2.180378000	-0.454694000	-0.000319000
6	0.954120000	0.228811000	-0.000140000
6	0.940600000	1.715245000	-0.000206000
8	2.204060000	2.238085000	0.000455000
8	-0.030399000	2.442982000	-0.000744000
1	-1.083048000	-2.520786000	0.000116000
1	1.085636000	-3.661904000	-0.000274000
1	3.205671000	-2.346976000	-0.000538000
1	3.091262000	0.131024000	-0.000429000
1	2.072037000	3.199957000	0.000273000

8	-0.811879000	-1.632623000	0.000585000	8	-1.419382000	0.146241000	0.000291000
6	-2.086355000	-2.259415000	0.001132000	6	-2.652757000	-0.576367000	0.000380000
1	-2.665996000	-1.999422000	0.895576000	1	-2.708007000	-1.220454000	0.888947000
1	-2.666257000	-2.000494000	-0.893450000	1	-2.708221000	-1.220308000	-0.888278000
1	-1.884438000	-3.330843000	0.001691000	6	-3.771864000	0.448762000	0.000597000
				1	-3.708277000	1.086421000	-0.884781000
				1	-3.708082000	1.086266000	0.886073000
				1	-4.742417000	-0.056763000	0.000663000
O- $OCH(CH_3)_2$ E_{scf} = -613.9946837				O- $CONH_2$ E_{scf} = -589.5357441			
6	0.049217000	0.449466000	-0.112011000	6	-0.630834000	0.427648000	-0.028354000
6	0.131956000	1.850579000	-0.188057000	6	-0.887030000	1.806405000	-0.069602000
6	-1.019553000	2.632863000	-0.169896000	6	0.131288000	2.749444000	-0.154858000
6	-2.280497000	2.045276000	-0.072850000	6	1.460794000	2.332028000	-0.158493000
6	-2.372326000	0.660839000	0.007351000	6	1.746970000	0.975241000	-0.076358000
6	-1.231975000	-0.158708000	-0.006742000	6	0.725590000	0.006384000	-0.029054000
6	-1.389850000	-1.633611000	0.095198000	6	1.190851000	-1.412133000	0.012319000
8	-2.705826000	-2.006742000	0.100354000	8	2.390880000	-1.542032000	0.621620000
8	-0.511335000	-2.467126000	0.173551000	8	0.636887000	-2.393185000	-0.459397000
1	1.096314000	2.336142000	-0.261239000	1	-1.923950000	2.115653000	-0.016165000
1	-0.923185000	3.713349000	-0.230544000	1	-0.114518000	3.805926000	-0.205594000
1	-3.177015000	2.655943000	-0.057106000	1	2.269880000	3.053597000	-0.213626000
1	-3.341731000	0.184606000	0.085388000	1	2.625677000	-2.482317000	0.544414000
1	-2.685710000	-2.974049000	0.180928000	1	2.777751000	0.643962000	-0.054232000
8	1.123367000	-0.367036000	-0.152806000	6	-1.914939000	-0.392910000	0.110185000
6	2.469559000	0.147877000	-0.214622000	8	-2.883899000	0.117040000	0.667470000
1	2.500742000	0.990748000	-0.917434000	7	-1.968653000	-1.616022000	-0.466216000
6	3.307420000	-0.994905000	-0.775374000	1	-2.818636000	-2.136800000	-0.307295000
1	2.946939000	-1.285789000	-1.765201000	1	-1.122724000	-2.095089000	-0.756245000
1	3.243661000	-1.867034000	-0.118609000				
1	4.355554000	-0.691625000	-0.858270000				
6	2.932053000	0.593907000	1.171703000				
1	3.955296000	0.980118000	1.124290000				
1	2.289871000	1.378749000	1.579673000				
1	2.913597000	-0.255428000	1.861129000				
O-OH E_{scf} = -496.0682445				O- NH_2 E_{scf} = -476.2013253			
6	0.506423000	0.982331000	0.000020000	6	-0.528762000	0.988350000	-0.010809000
6	1.911259000	0.965893000	-0.000039000	6	-1.941339000	0.906491000	0.006747000
6	2.593934000	-0.240745000	-0.000060000	6	-2.587873000	-0.316389000	0.013919000
6	1.904202000	-1.464463000	-0.000022000	6	-1.861740000	-1.517997000	0.004209000
6	0.519606000	-1.461560000	0.000019000	6	-0.478833000	-1.461611000	-0.007464000
6	-0.199434000	-0.249641000	0.000026000	6	0.211185000	-0.232475000	-0.011472000
6	-1.663001000	-0.217783000	-0.000020000	6	1.678122000	-0.203922000	0.003729000
8	-2.259158000	-1.426902000	0.000144000	8	2.254191000	-1.433490000	-0.012664000
8	-2.338896000	0.813978000	-0.000286000	8	2.381747000	0.802705000	0.033887000
1	2.433035000	1.916625000	-0.000037000	1	-2.515613000	1.829338000	0.008750000
1	3.680298000	-0.235570000	-0.000094000	1	-3.674204000	-0.340123000	0.026612000
1	2.450660000	-2.401511000	-0.000040000	1	-2.374692000	-2.473625000	0.008116000
1	-0.035379000	-2.392861000	0.000021000	1	3.210724000	-1.267023000	0.005110000
1	-3.215458000	-1.254330000	0.000047000	1	0.105307000	-2.374464000	-0.009429000
8	-0.110608000	2.173585000	0.000142000	7	0.083774000	2.204835000	-0.051869000
1	-1.081794000	1.998165000	0.000552000	1	1.090575000	2.228949000	0.047641000
				1	-0.460569000	3.034698000	0.113352000
O- $NHCH_3$ E_{scf} = -515.5109166				O- $N(CH3)_2$ E_{scf} = -554.7995971			
6	-0.754142000	-0.221753000	-0.000012000	6	-0.520615000	0.521469000	-0.006991000
6	-1.827609000	0.703740000	-0.000048000	6	-0.573578000	1.934651000	-0.070101000
6	-1.594377000	2.069196000	0.000001000	6	0.574674000	2.711415000	-0.020549000

6	-0.290842000	2.585415000	0.000037000	6	1.834597000	2.118610000	0.103610000
6	0.774574000	1.700315000	-0.000017000	6	1.917387000	0.734787000	0.128153000
6	0.578835000	0.306326000	-0.000033000	6	0.774364000	-0.083755000	0.036953000
6	1.734127000	-0.596116000	-0.000035000	6	0.985421000	-1.530128000	-0.207583000
8	2.934661000	0.038720000	0.000134000	8	2.231958000	-1.951339000	0.159242000
8	1.694414000	-1.825530000	-0.000109000	8	0.203298000	-2.306139000	-0.726902000
1	-2.846591000	0.335375000	-0.000235000	1	-1.536840000	2.428501000	-0.107544000
1	-2.443880000	2.747144000	-0.000029000	1	0.481310000	3.793637000	-0.052756000
1	-0.118878000	3.656278000	0.000038000	1	2.732294000	2.725100000	0.160528000
1	1.792629000	2.071684000	-0.000013000	1	2.885592000	0.251465000	0.176695000
1	3.597202000	-0.671136000	0.000030000	1	2.273317000	-2.878675000	-0.126145000
7	-0.983006000	-1.562938000	-0.000121000	7	-1.695236000	-0.211224000	0.019020000
1	-0.153520000	-2.145470000	0.000037000	6	-2.940445000	0.391698000	-0.421516000
6	-2.294611000	-2.167493000	0.000135000	1	-2.777288000	1.001322000	-1.313042000
1	-2.174846000	-3.252418000	0.000459000	1	-3.639307000	-0.406159000	-0.689213000
1	-2.879620000	-1.891813000	0.888350000	1	-3.421954000	1.016556000	0.349320000
1	-2.879792000	-1.892382000	-0.888157000	6	-1.865203000	-1.366852000	0.892374000
				1	-1.976715000	-2.296523000	0.326919000
				1	-1.004428000	-1.473732000	1.553808000
				1	-2.750988000	-1.214479000	1.523468000
O- NHOH E_{scf} = -551.3593161				O- NO_2 E_{scf} = -625.318279			
6	-0.720203000	-0.332986000	0.079864000	6	-0.536263000	0.558586000	-0.014561000
6	-1.917674000	0.406379000	0.035692000	6	-1.918864000	0.704721000	-0.008630000
6	-1.890627000	1.791524000	-0.019672000	6	-2.724854000	-0.432970000	0.006262000
6	-0.676953000	2.491940000	-0.032386000	6	-2.140092000	-1.698670000	0.015508000
6	0.509759000	1.777219000	-0.006731000	6	-0.750696000	-1.829500000	0.024914000
6	0.518480000	0.370118000	0.039593000	6	0.076517000	-0.701525000	0.019130000
6	1.792406000	-0.363576000	-0.003814000	6	1.553854000	-0.877020000	0.207956000
8	2.887499000	0.435872000	-0.009242000	8	2.038378000	-1.882082000	-0.556477000
8	1.917306000	-1.583508000	-0.046006000	8	2.224501000	-0.257353000	0.999437000
1	-2.855535000	-0.133419000	0.034705000	1	-2.339971000	1.702377000	-0.030814000
1	-2.830139000	2.336287000	-0.053774000	1	-3.804679000	-0.326470000	0.001237000
1	-0.664423000	3.575969000	-0.070165000	1	-2.763119000	-2.587333000	0.021441000
1	1.461645000	2.294219000	-0.033872000	1	-0.292958000	-2.811842000	0.052935000
1	3.646940000	-0.167805000	-0.055198000	1	2.981235000	-1.960077000	-0.330274000
7	-0.749645000	-1.710759000	0.237147000	7	0.265262000	1.788898000	-0.155527000
1	0.082328000	-2.186126000	-0.107948000	8	1.284726000	1.722329000	-0.836006000
8	-1.927266000	-2.332596000	-0.253062000	8	-0.171974000	2.807022000	0.376881000
1	-2.304742000	-2.745674000	0.537439000				
O- CF_3 E_{scf} = -757.8595559				O- CHO E_{scf} = -534.1511824			
6	0.190427000	-0.637568000	0.007008000	6	0.730680000	0.435791000	-0.000361000
6	-0.044997000	-2.013623000	0.021483000	6	1.965737000	-0.225763000	-0.000020000
6	-1.342800000	-2.524243000	0.048889000	6	2.045131000	-1.614171000	0.000440000
6	-2.428892000	-1.654608000	0.050385000	6	0.873559000	-2.372102000	0.000442000
6	-2.208465000	-0.279474000	0.030786000	6	-0.365130000	-1.735947000	0.000108000
6	-0.910434000	0.250152000	0.018952000	6	-0.460047000	-0.335300000	-0.000204000
6	-0.753811000	1.738411000	0.063151000	6	-1.820245000	0.284563000	-0.000088000
8	-1.892066000	2.379643000	-0.313925000	8	-2.812371000	-0.641740000	-0.001564000
8	0.234944000	2.345766000	0.407355000	8	-2.078355000	1.472945000	0.002504000
1	0.799938000	-2.689785000	0.003079000	1	2.858392000	0.390539000	-0.000179000
1	-1.496825000	-3.598724000	0.061667000	1	3.014553000	-2.103451000	0.000728000
1	-3.443850000	-2.039071000	0.066406000	1	0.920855000	-3.456743000	0.000723000
1	-3.047391000	0.405082000	0.032673000	1	-1.274257000	-2.323781000	0.000178000
1	-1.697954000	3.326731000	-0.216797000	1	-3.640442000	-0.133637000	-0.000557000
6	1.639333000	-0.178678000	-0.044985000	6	0.791777000	1.937533000	-0.001453000
9	2.467705000	-1.232842000	-0.263094000	8	1.855601000	2.532306000	0.000107000
9	1.858448000	0.689547000	-1.050491000	1	-0.166873000	2.471367000	-0.002444000
9	2.040614000	0.386659000	1.105976000				

O- CN E_{scf} = -513.0684712

6	-0.432328000	0.825973000	0.000001000
6	-1.826579000	0.994903000	0.000000000
6	-2.673522000	-0.110007000	-0.000008000
6	-2.139073000	-1.398709000	-0.000012000
6	-0.757695000	-1.578334000	-0.000011000
6	0.110103000	-0.479839000	-0.000007000
6	1.587300000	-0.680255000	-0.000016000
8	1.933505000	-1.992068000	0.000089000
8	2.412299000	0.207109000	-0.000113000
1	-2.231585000	2.000768000	0.000007000
1	-3.748837000	0.037672000	-0.000009000
1	-2.795514000	-2.263024000	-0.000018000
1	-0.335662000	-2.575728000	-0.000013000
1	2.904970000	-2.007655000	0.000068000
6	0.360744000	2.024255000	0.000020000
7	0.866644000	3.071389000	0.000052000

O- $COCH_3$ E_{scf} = -573.4732232

6	-0.000113000	-0.746295000	-0.035493000
6	0.893564000	-1.822523000	-0.025290000
6	2.269192000	-1.611621000	0.059436000
6	2.775981000	-0.312480000	0.115197000
6	1.902540000	0.770126000	0.073940000
6	0.516727000	0.565369000	-0.001759000
6	-0.408610000	1.720045000	-0.130238000
8	0.205284000	2.919874000	0.013202000
8	-1.601928000	1.634477000	-0.352771000
1	0.498120000	-2.831717000	-0.082083000
1	2.944602000	-2.461920000	0.075000000
1	3.846449000	-0.143366000	0.176215000
1	2.284096000	1.784236000	0.085200000
1	-0.487774000	3.588008000	-0.117949000
6	-1.477144000	-1.098581000	-0.092802000
8	-1.898928000	-1.735084000	-1.039310000
6	-2.325228000	-0.821930000	1.132710000
1	-2.154068000	-1.635450000	1.849986000
1	-2.069044000	0.118708000	1.619817000
1	-3.379249000	-0.825305000	0.850640000

O-CH_2F E_{scf} = -559.3787832

6	-0.711912000	-0.291054000	-0.000049000
6	-1.860431000	0.505414000	-0.000055000
6	-1.772619000	1.896805000	-0.000078000
6	-0.526684000	2.524217000	-0.000076000
6	0.627418000	1.748856000	-0.000002000
6	0.550620000	0.346794000	0.000036000
6	1.793919000	-0.461080000	0.000222000
8	2.925273000	0.287662000	-0.000131000
8	1.842762000	-1.679245000	-0.000107000
1	-2.826928000	0.017457000	-0.000039000
1	-2.681942000	2.491001000	-0.000085000
1	-0.454345000	3.607244000	-0.000078000
1	1.603661000	2.218560000	0.000053000
1	3.658649000	-0.349234000	-0.000319000
6	-0.870990000	-1.796735000	0.000089000
1	-0.403338000	-2.245763000	-0.880893000
1	-0.403218000	-2.245668000	0.881062000
9	-2.223638000	-2.133359000	0.000187000

Table S4 B3LYP/6-31G(d,p) optimized geometries of meta substituted benzoic acids. SCF energy (in a.u.) is also provided

m- CH_3, E_{scf} = -460.1562306				m- CH_2CH_3, E_{scf} = -499.4708889			
6	-0.463954000	-0.818830000	-0.005945000	6	0.079358000	-0.717285000	0.000056000
6	-1.794821000	-0.397866000	-0.007246000	6	1.372846000	-0.182215000	0.000104000
6	-2.051605000	0.981932000	-0.006718000	6	1.504183000	1.212170000	-0.000107000
6	-1.011030000	1.910526000	-0.000441000	6	0.380537000	2.044648000	-0.000325000
6	0.314468000	1.480159000	0.003676000	6	-0.899578000	1.501823000	-0.000339000
6	0.588028000	0.107003000	0.000395000	6	-1.049370000	0.107198000	-0.000147000
6	1.976432000	-0.424029000	-0.000221000	6	-2.384675000	-0.546389000	-0.000170000
8	2.921248000	0.551669000	0.006585000	8	-3.412589000	0.341350000	-0.000235000
8	2.272833000	-1.602867000	-0.005655000	8	-2.575000000	-1.746977000	-0.000120000
1	-0.216519000	-1.875700000	-0.011385000	1	-0.073257000	-1.792674000	0.000191000
1	-3.081390000	1.331243000	-0.013230000	1	2.491461000	1.662277000	-0.000111000
1	-1.234865000	2.973146000	-0.001934000	1	0.511015000	3.122788000	-0.000488000
1	1.130114000	2.193580000	0.006248000	1	-1.775453000	2.139849000	-0.000500000
1	3.774634000	0.087705000	0.005789000	1	-4.221340000	-0.196670000	-0.000251000
6	-2.929687000	-1.394732000	0.008824000	6	2.562388000	-1.129165000	0.000320000
1	-3.380834000	-1.464782000	1.006053000	1	2.475068000	-1.790468000	0.872614000
1	-3.725255000	-1.105831000	-0.685567000	1	2.475533000	-1.790247000	-0.872188000
1	-2.585516000	-2.394755000	-0.267357000	6	3.948482000	-0.481705000	0.000765000
				1	4.103515000	0.143515000	0.886303000
				1	4.103852000	0.144010000	-0.884366000
				1	4.725281000	-1.251841000	0.000702000
m- $CH(CH_3)_2$, E_{scf} = -538.7884214				m- $C(CH_3)_3$, E_{scf} = -578.1017962			
6	-0.139271000	-0.613338000	-0.000020000	6	-0.294500000	-0.463800000	-0.000029000
6	1.098865000	0.031599000	0.000144000	6	0.891719000	0.274135000	-0.000069000
6	1.108416000	1.435984000	0.000151000	6	0.777182000	1.676535000	-0.000085000
6	-0.079138000	2.167462000	-0.000018000	6	-0.463558000	2.311211000	-0.000029000
6	-1.309178000	1.512309000	-0.000192000	6	-1.637614000	1.560865000	0.000017000
6	-1.338066000	0.112751000	-0.000190000	6	-1.548274000	0.165459000	0.000014000
6	-2.612208000	-0.652694000	-0.000378000	6	-2.754101000	-0.703760000	-0.000011000
8	-3.712995000	0.143110000	-0.000428000	8	-3.917552000	-0.002518000	-0.000011000
8	-2.698357000	-1.865215000	-0.000491000	8	-2.739759000	-1.919426000	-0.000013000
1	-0.197795000	-1.697471000	-0.000029000	1	-0.286718000	-1.546366000	-0.000060000
1	2.056616000	1.967215000	0.000295000	1	1.674274000	2.288811000	-0.000099000
1	-0.044823000	3.252911000	-0.000016000	1	-0.513653000	3.396060000	-0.000035000
1	-2.237051000	2.072121000	-0.000320000	1	-2.608036000	2.043042000	0.000019000
1	-4.472238000	-0.462769000	-0.000573000	1	-4.623370000	-0.669819000	-0.000025000
6	2.393441000	-0.771318000	0.000369000	6	2.283812000	-0.383654000	-0.000018000
1	2.110230000	-1.831621000	0.000418000	6	3.060548000	0.059083000	1.262693000
6	3.224655000	-0.513984000	1.270847000	6	3.061306000	0.059943000	-1.261922000
6	3.224995000	-0.514195000	-1.269930000	1	2.538092000	-0.247560000	-2.173115000
1	2.646969000	-0.732150000	-2.173085000	1	3.191486000	1.145521000	-1.301542000
1	3.552678000	0.529702000	-1.327164000	1	4.058121000	-0.394528000	-1.272957000
1	4.121401000	-1.143451000	-1.278512000	1	3.190671000	1.144644000	1.303018000
1	3.552301000	0.529931000	1.327997000	1	4.057334000	-0.395450000	1.274092000
1	4.121070000	-1.143224000	1.279764000	1	2.536698000	-0.248976000	2.173329000
1	2.646395000	-0.731804000	2.173883000	6	2.201051000	-1.921360000	-0.000601000
				1	1.683518000	-2.302138000	0.885622000
				1	1.683886000	-2.301550000	-0.887288000
				1	3.210763000	-2.344088000	-0.000528000
m- C_6H_5, E_{scf} = -651.8988713				m- F, E_{scf} = -520.0662222			

6	0.778710000	-0.358755000	0.057690000	6	0.148282000	1.503180000	0.000192000
6	-0.271948000	0.556363000	-0.086628000	6	-1.208758000	1.816976000	0.000315000
6	0.054902000	1.909953000	-0.283828000	6	-2.168420000	0.802857000	0.000188000
6	1.382841000	2.331910000	-0.331646000	6	-1.740747000	-0.521087000	-0.000063000
6	2.419703000	1.412720000	-0.187600000	6	-0.396630000	-0.866147000	-0.000198000
6	2.112730000	0.059628000	0.006792000	6	0.554402000	0.162422000	-0.000077000
6	3.167685000	-0.975390000	0.174743000	6	2.015086000	-0.124123000	-0.000237000
8	4.425518000	-0.467301000	0.119367000	8	2.294807000	-1.451222000	-0.000046000
8	2.960660000	-2.160735000	0.344515000	8	2.886640000	0.721604000	0.000107000
1	0.579097000	-1.409810000	0.234846000	1	0.907640000	2.276557000	0.000275000
1	-0.742081000	2.633975000	-0.423880000	1	-1.526408000	2.854853000	0.000515000
1	1.608765000	3.381804000	-0.491920000	1	-3.231098000	1.019555000	0.000276000
1	3.454577000	1.731758000	-0.225094000	1	-0.101947000	-1.907950000	-0.000397000
1	5.019608000	-1.226534000	0.238591000	1	3.263979000	-1.517097000	0.000104000
6	-1.688053000	0.109564000	-0.032299000	9	-2.664782000	-1.503716000	-0.000220000
6	-2.671366000	0.901753000	0.583428000				
6	-2.078762000	-1.116502000	-0.595842000				
6	-3.999924000	0.483183000	0.632944000				
6	-3.406956000	-1.535676000	-0.545175000				
6	-4.373523000	-0.737468000	0.068662000				
1	-2.386867000	1.840044000	1.050332000				
1	-1.339646000	-1.733936000	-1.097201000				
1	-4.742405000	1.107600000	1.121445000				
1	-3.688264000	-2.484200000	-0.993315000				
1	-5.408440000	-1.064103000	0.107688000				
m- Cl, E_{scf} = -880.4286437				m- Br, E_{scf} = -2991.9374814			
6	0.827704000	1.580417000	0.000333000	6	1.648786000	1.576407000	0.000451000
6	-0.432471000	2.171350000	0.000337000	6	0.486328000	2.341966000	0.000390000
6	-1.584017000	1.381533000	0.000128000	6	-0.766226000	1.724290000	0.000167000
6	-1.454979000	-0.007745000	-0.000072000	6	-0.837353000	0.331727000	0.000009000
6	-0.205159000	-0.619937000	-0.000057000	6	0.311301000	-0.452572000	0.000078000
6	0.941760000	0.184799000	0.000151000	6	1.562326000	0.178648000	0.000304000
6	2.309825000	-0.403452000	0.000162000	6	2.831040000	-0.600271000	0.000367000
8	2.305150000	-1.759198000	-0.000038000	8	2.630355000	-1.941217000	-0.000034000
8	3.338712000	0.241283000	-0.000070000	8	3.942233000	-0.110715000	-0.000053000
1	1.733246000	2.176304000	0.000477000	1	2.630399000	2.036573000	0.000596000
1	-0.526901000	3.252649000	0.000498000	1	0.547545000	3.425654000	0.000512000
1	-2.569761000	1.833150000	0.000120000	1	-1.675724000	2.314091000	0.000113000
1	-0.119407000	-1.698995000	-0.000197000	1	0.243241000	-1.532618000	-0.000031000
1	3.238477000	-2.028873000	-0.000211000	1	3.514966000	-2.342788000	-0.000302000
17	-2.901325000	-1.006629000	-0.000336000	35	-2.550238000	-0.516761000	-0.000308000
m- OCH_3, E_{scf} = -535.3610865				m- OCH_2CH_3, E_{scf} = -574.6832523			
6	0.346787000	-0.498102000	0.000140000	6	-0.009354000	-0.319632000	0.000007000
6	1.521846000	0.253887000	0.000208000	6	0.994523000	0.650039000	0.000100000
6	1.450428000	1.656987000	0.000039000	6	0.644817000	2.011058000	0.000010000
6	0.215243000	2.294120000	-0.000199000	6	-0.692226000	2.390582000	-0.000169000
6	-0.968571000	1.552596000	-0.000275000	6	-1.705655000	1.429300000	-0.000263000
6	-0.894422000	0.156917000	-0.000101000	6	-1.355773000	0.076074000	-0.000175000
6	-2.109885000	-0.700092000	-0.000163000	6	-2.376374000	-1.005593000	-0.000266000
8	-3.265923000	0.010921000	-0.000579000	8	-3.650967000	-0.539110000	-0.000431000
8	-2.104842000	-1.916057000	-0.000147000	8	-2.129663000	-2.196343000	-0.000197000
1	0.349957000	-1.580409000	0.000267000	1	0.207466000	-1.379851000	0.000071000
1	2.377885000	2.220196000	0.000099000	1	1.441815000	2.747434000	0.000085000
1	0.174068000	3.379097000	-0.000330000	1	-0.947587000	3.445923000	-0.000237000
1	-1.933680000	2.043944000	-0.000465000	1	-2.748972000	1.719881000	-0.000402000
1	-3.978414000	-0.649279000	-0.000700000	1	-4.217542000	-1.328097000	-0.000474000
8	2.779078000	-0.272996000	0.000438000	8	2.330336000	0.383053000	0.000283000

6	2.911930000	-1.687790000	0.000601000	6	2.755984000	-0.982039000	0.000379000
1	2.459601000	-2.135874000	0.893992000	1	2.360940000	-1.495049000	-0.887246000
1	2.459833000	-2.136055000	-0.892817000	1	2.360717000	-1.494992000	0.887940000
1	3.984119000	-1.887702000	0.000761000	6	4.273708000	-0.987028000	0.000571000
				1	4.661337000	-0.478130000	0.887349000
				1	4.661562000	-0.478192000	-0.886143000
				1	4.644708000	-2.016295000	0.000655000
m- $OCH(CH_3)_2$, E_{scf} = -614.0026931				m- $CONH_2$, E_{scf} = -589.5427289			
6	0.232382000	-0.209639000	-0.090063000	6	-0.020016000	-0.520482000	-0.035364000
6	-0.700557000	0.827484000	-0.023767000	6	-1.219050000	0.193963000	0.002194000
6	-0.248199000	2.152557000	0.103517000	6	-1.178891000	1.594607000	0.055919000
6	1.112571000	2.430719000	0.156952000	6	0.040229000	2.266880000	0.095314000
6	2.053302000	1.401081000	0.087013000	6	1.236850000	1.550942000	0.070146000
6	1.603603000	0.083369000	-0.036243000	6	1.207246000	0.152200000	0.000228000
6	2.541799000	-1.067975000	-0.111825000	6	2.445586000	-0.670342000	-0.042215000
8	3.847053000	-0.698877000	-0.061792000	8	3.579200000	0.073061000	-0.017415000
8	2.208950000	-2.233631000	-0.209024000	8	2.469282000	-1.884505000	-0.091535000
1	-0.056891000	-1.248223000	-0.180908000	1	0.003695000	-1.601560000	-0.121118000
1	-0.988423000	2.944358000	0.154213000	1	-2.121669000	2.130804000	0.062782000
1	1.443371000	3.460438000	0.253444000	1	0.060092000	3.351184000	0.143099000
1	3.114883000	1.610905000	0.129009000	1	2.190255000	2.065688000	0.098914000
1	4.353859000	-1.525570000	-0.118387000	1	4.313489000	-0.562330000	-0.047735000
8	-2.053201000	0.678576000	-0.085819000	6	-2.577565000	-0.454400000	-0.036485000
6	-2.643856000	-0.633651000	-0.192485000	8	-3.587035000	0.189587000	-0.295043000
1	-2.051429000	-1.232109000	-0.896856000	7	-2.619529000	-1.801279000	0.210382000
6	-4.032372000	-0.409591000	-0.779070000	1	-3.540848000	-2.207327000	0.280509000
1	-3.964878000	0.084724000	-1.751695000	1	-1.866217000	-2.272856000	0.684400000
1	-4.630157000	0.220128000	-0.112929000				
1	-4.549115000	-1.365241000	-0.908631000				
6	-2.684018000	-1.316259000	1.174090000				
1	-3.133219000	-2.310865000	1.088665000				
1	-1.683221000	-1.431914000	1.597579000				
1	-3.285127000	-0.723748000	1.870855000				
m- OH, E_{scf} = -496.0560253				m- NH_2, E_{scf} = -476.1942831			
6	-0.453049000	-0.858381000	-0.000128000	6	0.453109000	-0.843244000	-0.009438000
6	-1.791389000	-0.468357000	-0.000170000	6	1.797873000	-0.449038000	-0.009429000
6	-2.122262000	0.893342000	-0.000030000	6	2.091606000	0.927153000	-0.001161000
6	-1.111664000	1.851258000	0.000148000	6	1.068566000	1.872141000	0.005959000
6	0.231903000	1.474014000	0.000190000	6	-0.268980000	1.479894000	0.004593000
6	0.556272000	0.112454000	0.000052000	6	-0.568267000	0.111010000	-0.002996000
6	1.962911000	-0.370235000	0.000092000	6	-1.967950000	-0.391733000	0.001332000
8	2.872901000	0.635711000	0.000209000	8	-2.893274000	0.602091000	-0.001546000
8	2.296240000	-1.539460000	0.000012000	8	-2.289394000	-1.564412000	0.007566000
1	-0.167433000	-1.906630000	-0.000227000	1	0.180632000	-1.894033000	-0.016776000
1	-3.169652000	1.176331000	-0.000063000	1	3.129608000	1.250758000	-0.004878000
1	-1.376434000	2.904228000	0.000258000	1	1.321714000	2.928246000	0.014177000
1	1.019042000	2.217780000	0.000325000	1	-1.066703000	2.211995000	0.011298000
1	3.742363000	0.202527000	0.000225000	1	-3.755043000	0.153972000	0.001268000
8	-2.821876000	-1.363529000	-0.000349000	7	2.819035000	-1.395971000	-0.074519000
1	-2.462333000	-2.260578000	-0.000419000	1	2.569439000	-2.321403000	0.245644000
				1	3.712713000	-1.096270000	0.289586000
m- $NHCH_3$, E_{scf} = -515.5031016				m- $N(CH_3)_2$, E_{scf} = -554.8093315			
6	-0.339039000	-0.474408000	-0.042824000	6	-0.054446000	-0.511191000	-0.001998000
6	-1.517504000	0.287296000	-0.050023000	6	1.173789000	0.181493000	-0.003089000
6	-1.401448000	1.693454000	-0.011027000	6	1.123241000	1.596302000	-0.001351000

6	-0.155273000	2.307096000	0.028336000	6	-0.095337000	2.269884000	0.000138000
6	1.016754000	1.548910000	0.027875000	6	-1.304825000	1.579346000	0.000481000
6	0.911685000	0.154258000	-0.008927000	6	-1.268986000	0.179230000	-0.000506000
6	2.110687000	-0.725603000	-0.005581000	6	-2.510267000	-0.640016000	0.000347000
8	3.280728000	-0.036530000	0.030306000	8	-3.644624000	0.107506000	0.001898000
8	2.087083000	-1.941275000	-0.031593000	8	-2.548931000	-1.855770000	-0.000265000
1	-0.363120000	-1.556708000	-0.063816000	1	-0.096142000	-1.592143000	-0.002247000
1	-2.304378000	2.299853000	-0.017079000	1	2.039150000	2.174440000	-0.001222000
1	-0.097734000	3.391234000	0.059162000	1	-0.094206000	3.356180000	0.001250000
1	1.989841000	2.022721000	0.057524000	1	-2.252098000	2.103545000	0.001766000
1	3.978597000	-0.712058000	0.027875000	1	-4.375263000	-0.532421000	0.002255000
7	-2.773650000	-0.296764000	-0.127620000	7	2.379873000	-0.496949000	-0.006192000
1	-3.529504000	0.296171000	0.181532000	6	3.628416000	0.241104000	0.004026000
6	-2.973268000	-1.715334000	0.098888000	1	3.731923000	0.888325000	-0.878282000
1	-4.042812000	-1.930600000	0.050501000	1	3.728202000	0.873742000	0.897574000
1	-2.482631000	-2.303405000	-0.684053000	1	4.461369000	-0.462590000	-0.000409000
1	-2.590769000	-2.061428000	1.071698000	6	2.395043000	-1.948956000	0.001839000
				1	3.428662000	-2.296359000	-0.004329000
				1	1.905157000	-2.361653000	0.894569000
				1	1.892815000	-2.369477000	-0.879961000
m- NHOH, E_{scf} = -551.3537398				m- NO_2, E_{scf} = -625.3325257			
6	-0.340396000	-0.504152000	0.061843000	6	-0.031891000	-0.565456000	-0.000032000
6	-1.526236000	0.232183000	0.065852000	6	-1.228186000	0.140177000	-0.000141000
6	-1.468245000	1.634610000	0.016312000	6	-1.270729000	1.534184000	-0.000013000
6	-0.238010000	2.285095000	-0.028945000	6	-0.068984000	2.238996000	0.000227000
6	0.951371000	1.557377000	-0.031632000	6	1.147125000	1.555259000	0.000332000
6	0.891046000	0.158920000	0.012553000	6	1.167255000	0.153398000	0.000208000
6	2.118220000	-0.682615000	0.008979000	6	2.438956000	-0.624977000	0.000337000
8	3.263138000	0.044880000	-0.058648000	8	3.538120000	0.167029000	0.000242000
8	2.133196000	-1.896612000	0.061643000	8	2.504623000	-1.835975000	0.000101000
1	-0.363076000	-1.585429000	0.079991000	1	-0.023734000	-1.647855000	-0.000125000
1	-2.389439000	2.212391000	0.019276000	1	-2.230346000	2.035580000	-0.000104000
1	-0.209774000	3.369819000	-0.068239000	1	-0.081699000	3.323846000	0.000331000
1	1.910548000	2.058638000	-0.070438000	1	2.083520000	2.100689000	0.000516000
1	3.984701000	-0.605333000	-0.052415000	1	4.301883000	-0.433687000	0.000165000
7	-2.788592000	-0.389071000	0.205130000	7	-2.498513000	-0.609354000	-0.000397000
1	-3.503805000	0.101591000	-0.326581000	8	-3.541941000	0.042867000	-0.000396000
8	-2.800394000	-1.732419000	-0.274227000	8	-2.435966000	-1.836744000	-0.000386000
1	-3.003032000	-2.243490000	0.522585000				
m- CF_3, E_{scf} = -757.8701384				m- CHO, E_{scf} = -534.1585679			
6	-0.276297000	-0.453271000	-0.023944000	6	0.195023000	-0.736237000	0.000103000
6	0.903467000	0.289896000	-0.033066000	6	1.479550000	-0.190206000	0.000148000
6	0.859140000	1.687303000	-0.022408000	6	1.647193000	1.204180000	-0.000032000
6	-0.371259000	2.343813000	-0.001764000	6	0.534777000	2.039052000	-0.000252000
6	-1.553346000	1.608398000	0.008666000	6	-0.751318000	1.492421000	-0.000305000
6	-1.509015000	0.208582000	-0.002943000	6	-0.925259000	0.101878000	-0.000131000
6	-2.801912000	-0.530226000	0.002358000	6	-2.270982000	-0.533933000	-0.000176000
8	-2.642027000	-1.875760000	-0.012514000	8	-3.283032000	0.367848000	-0.000416000
8	-3.896600000	-0.005216000	0.018807000	8	-2.468112000	-1.732196000	-0.000059000
1	-0.241434000	-1.535342000	-0.040346000	1	0.044051000	-1.811955000	0.000241000
1	1.784213000	2.253349000	-0.039510000	1	2.656987000	1.602062000	0.000005000
1	-0.405356000	3.428466000	0.002243000	1	0.661790000	3.117087000	-0.000386000
1	-2.522037000	2.095855000	0.022704000	1	-1.622189000	2.137961000	-0.000477000
1	-3.537854000	-2.251666000	-0.007422000	1	-4.103547000	-0.152457000	-0.000445000
6	2.235123000	-0.413240000	0.000189000	6	2.662848000	-1.084032000	0.000380000
9	2.170807000	-1.641128000	-0.557363000	8	3.814732000	-0.695863000	0.000783000

9	3.184558000	0.286402000	-0.660474000
9	2.679756000	-0.577538000	1.267777000

1	2.423219000	-2.169747000	0.000197000

m- CN, E_{scf} = -513.0749293

6	-0.312965000	-0.641897000	-0.000166000
6	-1.575465000	-0.032316000	-0.000177000
6	-1.683239000	1.369596000	0.000035000
6	-0.531773000	2.153014000	0.000253000
6	0.724380000	1.550141000	0.000262000
6	0.835815000	0.153671000	0.000049000
6	2.204754000	-0.435667000	0.000059000
8	2.195667000	-1.789373000	0.000073000
8	3.231507000	0.211617000	0.000408000
1	-0.229461000	-1.721790000	-0.000328000
1	-2.665795000	1.829150000	0.000026000
1	-0.615493000	3.234856000	0.000415000
1	1.633433000	2.141375000	0.000426000
1	3.126992000	-2.066794000	0.000239000
6	-2.760885000	-0.841101000	-0.000403000
7	-3.724401000	-1.492485000	-0.000586000

m- $COCH_3$, E_{scf} = -573.4848152

6	0.030483000	-0.498438000	0.000026000
6	1.217919000	0.238174000	0.000009000
6	1.151708000	1.641466000	-0.000008000
6	-0.077890000	2.292702000	-0.000007000
6	-1.261674000	1.553380000	0.000004000
6	-1.208402000	0.153633000	0.000020000
6	-2.433990000	-0.689630000	-0.000009000
8	-3.578783000	0.037251000	0.000023000
8	-2.438801000	-1.904614000	-0.000054000
1	0.031549000	-1.582384000	0.000082000
1	2.084709000	2.194969000	-0.000037000
1	-0.118719000	3.377520000	0.000010000
1	-2.224112000	2.052036000	0.000008000
1	-4.303611000	-0.609632000	-0.000007000
6	2.574768000	-0.407725000	0.000023000
8	3.583649000	0.280181000	-0.000035000
6	2.664437000	-1.922606000	0.000034000
1	2.170882000	-2.345547000	0.881784000
1	2.170655000	-2.345370000	-0.881703000
1	3.715967000	-2.209875000	-0.000157000

m-CH_2F, E_{scf} = -559.37796

6	0.346197000	-0.487518000	0.000280000
6	1.524030000	0.255243000	0.000254000
6	1.452088000	1.654697000	0.000010000
6	0.217213000	2.301256000	-0.000170000
6	-0.962817000	1.558437000	-0.000154000
6	-0.896566000	0.160239000	0.000061000
6	-2.119117000	-0.687770000	0.000089000
8	-3.268131000	0.036249000	-0.000335000
8	-2.124584000	-1.902313000	0.000434000
1	0.378628000	-1.569990000	0.000416000
1	2.366823000	2.243684000	-0.000069000
1	0.174662000	3.386115000	-0.000372000
1	-1.927338000	2.052228000	-0.000336000
1	-3.987867000	-0.616117000	-0.000255000
6	2.872215000	-0.426420000	0.000714000
1	3.452175000	-0.138441000	-0.886212000
1	3.450433000	-0.140692000	0.889512000
9	2.737193000	-1.806362000	-0.001109000

Table S5 B3LYP/6-31G(d,p) optimized geometries of para substituted benzoic acids. SCF energy (in a.u.) is also provided

p-CH_3 E_{scf} = -460.156802

6	-0.023138000	1.228246000	-0.003994000
6	-1.412957000	1.202507000	-0.010366000
6	-2.112985000	-0.013480000	-0.010579000
6	-1.375000000	-1.205683000	-0.010640000
6	0.016849000	-1.190831000	-0.004367000
6	0.703788000	0.030456000	-0.000362000
6	2.185606000	0.110879000	0.003135000
8	2.786653000	-1.107850000	0.004830000
8	2.828973000	1.142472000	0.005092000
1	-1.967193000	2.137418000	-0.017047000
1	-1.899793000	-2.157440000	-0.017478000
1	0.574968000	-2.120132000	-0.006364000
1	3.740987000	-0.927038000	0.007510000
1	0.521500000	2.166305000	-0.005448000
6	-3.621802000	-0.036888000	0.015323000
1	-3.995888000	-0.016002000	1.046575000
1	-4.044756000	0.830139000	-0.500387000
1	-4.016999000	-0.941469000	-0.455641000

p- CH_2CH_3, E_{scf} = -499.4714995

6	-0.312737000	-1.130341000	-0.000009000
6	1.070460000	-0.964584000	-0.000027000
6	1.642841000	0.314124000	-0.000043000
6	0.781305000	1.424531000	-0.000035000
6	-0.599056000	1.269976000	-0.000017000
6	-1.158815000	-0.016808000	-0.000006000
6	-2.624376000	-0.248465000	0.000009000
8	-3.346478000	0.903053000	0.000032000
8	-3.159891000	-1.340009000	-0.000004000
1	1.705556000	-1.843786000	-0.000028000
1	1.206260000	2.425506000	-0.000042000
1	-1.248996000	2.137555000	-0.000011000
1	-4.277246000	0.625408000	0.000029000
1	-0.756469000	-2.120201000	0.000000000
6	3.143686000	0.548245000	-0.000089000
1	3.393219000	1.167289000	-0.872513000
1	3.393223000	1.167639000	0.872082000
6	4.029958000	-0.698929000	0.000154000
1	3.855114000	-1.319050000	-0.884929000
1	3.855075000	-1.318729000	0.885454000
1	5.085617000	-0.412484000	0.000121000

p- $CH(CH_3)_2$, E_{scf} = -538.7888479

6	0.678008000	-1.157515000	-0.000158000
6	-0.705827000	-1.033187000	-0.000103000
6	-1.319792000	0.230470000	0.000068000
6	-0.495938000	1.364288000	0.000184000
6	0.892293000	1.251619000	0.000129000
6	1.489913000	-0.014718000	-0.000043000
6	2.962299000	-0.201430000	-0.000107000
8	3.649247000	0.971001000	0.000036000
8	3.529953000	-1.276586000	-0.000212000
1	-1.317654000	-1.930754000	-0.000194000
1	-0.950916000	2.351445000	0.000320000
1	1.514829000	2.139073000	0.000219000
1	4.588070000	0.721950000	0.000007000
1	1.154202000	-2.132128000	-0.000288000
6	-2.834859000	0.373450000	0.000121000
1	-3.056397000	1.448631000	0.000290000
6	-3.465397000	-0.228289000	1.270346000
6	-3.465432000	-0.227895000	-1.270276000
1	-3.044076000	0.222089000	-2.174299000
1	-3.297041000	-1.308774000	-1.325337000
1	-4.547615000	-0.059722000	-1.277897000
1	-3.297006000	-1.309184000	1.325070000
1	-4.547579000	-0.060118000	1.278045000
1	-3.044018000	0.221416000	2.174499000

p- $C(CH_3)_3$, E_{scf} = -578.1020706

6	1.045357000	-1.218962000	-0.000014000
6	-0.342448000	-1.187930000	-0.000014000
6	-1.052901000	0.027529000	-0.000013000
6	-0.303053000	1.212744000	-0.000028000
6	1.091156000	1.193321000	-0.000027000
6	1.778387000	-0.024467000	-0.000013000
6	3.259819000	-0.108007000	0.000006000
8	3.863767000	1.109251000	0.000018000
8	3.900655000	-1.141220000	0.000014000
1	-0.883140000	-2.129246000	-0.000023000
1	-0.803845000	2.173456000	-0.000054000
1	1.647531000	2.123821000	-0.000038000
1	4.817661000	0.926081000	0.000032000
1	1.584482000	-2.160267000	-0.000013000
6	-2.591838000	0.014985000	0.000005000
6	-3.097649000	-0.722534000	1.262882000
6	-3.097677000	-0.722577000	-1.262835000
1	-2.758652000	-0.218441000	-2.173546000
1	-2.743141000	-1.756471000	-1.301700000
1	-4.192959000	-0.745558000	-1.274970000
1	-2.743087000	-1.756414000	1.301793000
1	-4.192931000	-0.745527000	1.275013000
1	-2.758628000	-0.218337000	2.173560000
6	-3.191499000	1.433832000	-0.000001000
1	-2.895249000	2.002858000	-0.887198000
1	-4.284079000	1.369326000	-0.000006000
1	-2.895259000	2.002860000	0.887197000

p- C_6H_5, E_{scf} = -651.8995199

6	-1.663402000	1.191914000	-0.321353000
6	-0.274485000	1.180526000	-0.319307000
6	0.439785000	0.010269000	-0.002954000
6	-0.292059000	-1.148798000	0.311102000
6	-1.682667000	-1.143446000	0.309349000
6	-2.380526000	0.029868000	-0.007360000
6	-3.863334000	0.095125000	-0.025205000
8	-4.453083000	-1.085805000	0.295737000
8	-4.514486000	1.085718000	-0.294514000
1	0.268473000	2.080102000	-0.591321000
1	0.237456000	-2.055790000	0.585069000
1	-2.232787000	-2.042712000	0.561676000
1	-5.409192000	-0.920423000	0.250940000
1	-2.215696000	2.090882000	-0.572992000
6	1.923884000	-0.000511000	-0.000343000
6	2.638110000	-1.120070000	-0.460038000
6	2.652060000	1.109025000	0.461769000
6	4.031654000	-1.129349000	-0.458481000
6	4.045595000	1.098688000	0.465242000
6	4.741440000	-0.020268000	0.004684000
1	2.095790000	-1.977564000	-0.846782000
1	2.120448000	1.974269000	0.846063000
1	4.563821000	-2.001393000	-0.827284000
1	4.588591000	1.963320000	0.835682000
1	5.827323000	-0.027832000	0.006536000

p- F, E_{scf} = -520.0676569

6	-0.068487000	1.230713000	-0.000038000
6	-1.458595000	1.216052000	-0.000071000
6	-2.108891000	-0.015006000	-0.000040000
6	-1.418032000	-1.223209000	0.000022000
6	-0.026592000	-1.195600000	0.000055000
6	0.655763000	0.029857000	0.000026000
6	2.137729000	0.112325000	0.000061000
8	2.737765000	-1.105709000	0.000075000
8	2.777132000	1.145840000	-0.000008000
1	-2.041551000	2.130202000	-0.000120000
1	-1.971457000	-2.155561000	0.000043000
1	0.535524000	-2.122029000	0.000104000
1	3.692674000	-0.927803000	0.000057000
1	0.479185000	2.166606000	-0.000061000
9	-3.454546000	-0.038138000	-0.000072000

p- Cl, E_{scf} = -880.4295115

6	0.372284000	1.232641000	-0.000044000
6	-1.018361000	1.223338000	-0.000060000
6	-1.685767000	-0.003049000	-0.000027000
6	-0.988224000	-1.211886000	0.000021000
6	0.403850000	-1.190471000	0.000037000
6	1.091476000	0.030403000	0.000004000
6	2.575697000	0.106846000	0.000017000
8	3.169220000	-1.113176000	0.000108000
8	3.216911000	1.138653000	0.000020000
1	-1.582253000	2.149100000	-0.000098000
1	-1.529841000	-2.150894000	0.000046000
1	0.959738000	-2.120766000	0.000075000
1	4.125459000	-0.942038000	0.000136000
1	0.921508000	2.167753000	-0.000070000
17	-3.440553000	-0.025524000	-0.000047000

p- Br, E_{scf} = -2991.9382305

6	1.062152000	1.235471000	-0.000011000
6	-0.328840000	1.229359000	-0.000046000
6	-0.998697000	0.005184000	-0.000018000
6	-0.305296000	-1.205183000	0.000044000
6	1.087125000	-1.188103000	0.000080000
6	1.777814000	0.031109000	0.000053000
6	3.262343000	0.103417000	0.000091000
8	3.852414000	-1.118299000	0.000107000
8	3.906435000	1.133409000	0.000024000
1	-0.888871000	2.157268000	-0.000095000
1	-0.848100000	-2.143302000	0.000064000
1	1.640364000	-2.120042000	0.000129000
1	4.809143000	-0.949866000	0.000093000
1	1.613697000	2.169287000	-0.000032000
35	-2.906761000	-0.014336000	-0.000067000

p-OCH_3, E_{scf} = -535.3627273

6	-0.280358000	-1.136857000	-0.000027000
6	1.104497000	-0.999246000	0.000000000
6	1.669140000	0.285111000	0.000011000
6	0.835959000	1.417001000	-0.000007000
6	-0.541019000	1.267176000	-0.000033000
6	-1.116879000	-0.015456000	-0.000045000
6	-2.580342000	-0.233873000	-0.000078000
8	-3.293212000	0.924529000	0.000012000
8	-3.127799000	-1.320570000	-0.000024000
1	1.729180000	-1.883997000	0.000010000
1	1.298285000	2.398240000	0.000001000
1	-1.181824000	2.141349000	-0.000045000

p-OCH_2CH_3, E_{scf} = -574.6849756

6	-0.787772000	-1.141332000	0.000011000
6	0.597704000	-1.011381000	0.000000000
6	1.170390000	0.270064000	-0.000042000
6	0.341949000	1.405926000	-0.000075000
6	-1.035771000	1.263790000	-0.000065000
6	-1.618693000	-0.015661000	-0.000022000
6	-3.083051000	-0.226206000	-0.000013000
8	-3.789977000	0.936059000	0.000049000
8	-3.636775000	-1.309823000	0.000082000
1	1.217223000	-1.899557000	0.000023000
1	0.809327000	2.384806000	-0.000108000
1	-1.671715000	2.141533000	-0.000089000

1	-4.225862000	0.653710000	0.000043000
1	-0.735555000	-2.121482000	-0.000038000
8	3.004032000	0.539838000	0.000036000
6	3.905880000	-0.558897000	0.000096000
1	3.782187000	-1.181993000	0.894279000
1	3.782294000	-1.182003000	-0.894095000
1	4.905868000	-0.123948000	0.000153000

1	-4.723919000	0.669780000	0.000107000
1	-1.248158000	-2.123569000	0.000041000
8	2.505580000	0.517552000	-0.000056000
6	3.418161000	-0.584181000	0.000021000
1	3.247433000	-1.207575000	-0.888253000
1	3.247367000	-1.207507000	0.888329000
6	4.823390000	-0.011078000	0.000050000
1	4.987905000	0.606952000	0.886833000
1	4.987963000	0.606897000	-0.886761000
1	5.558109000	-0.821711000	0.000098000

p-$OCH(CH_3)_2$, E_{scf} = -614.0045326

6	1.055006000	-1.069650000	-0.257719000
6	-0.324068000	-0.886012000	-0.258169000
6	-0.852344000	0.395617000	-0.030907000
6	0.020923000	1.474066000	0.199628000
6	1.392176000	1.278868000	0.198897000
6	1.928209000	-0.000058000	-0.030969000
6	3.382336000	-0.267829000	-0.041292000
8	4.132695000	0.843671000	0.188506000
8	3.894968000	-1.355099000	-0.231569000
1	-0.971183000	-1.736511000	-0.432285000
1	-0.409274000	2.454685000	0.372531000
1	2.058943000	2.115021000	0.375815000
1	5.055326000	0.542154000	0.157699000
1	1.477542000	-2.053511000	-0.431913000
8	-2.172823000	0.711453000	-0.024179000
6	-3.182825000	-0.302820000	-0.216110000
1	-2.850050000	-0.987501000	-1.006685000
6	-4.422581000	0.441490000	-0.696041000
1	-4.214136000	0.980610000	-1.623745000
1	-4.747986000	1.164797000	0.057798000
1	-5.240760000	-0.261876000	-0.877483000
6	-3.420104000	-1.069631000	1.083911000
1	-3.766294000	-0.385026000	1.864303000
1	-4.183339000	-1.840502000	0.936970000
1	-2.507886000	-1.556774000	1.437546000

p-$CONH_2$, E_{scf} = -589.5417298

6	0.676276000	1.224580000	-0.121586000
6	-0.714128000	1.196639000	-0.129560000
6	-1.397452000	-0.023750000	-0.021812000
6	-0.666981000	-1.215085000	0.073283000
6	0.723163000	-1.191040000	0.088248000
6	1.401818000	0.032335000	-0.005755000
6	2.887631000	0.121196000	0.003891000
8	3.490513000	-1.088339000	0.113107000
8	3.520315000	1.155240000	-0.075222000
1	1.220729000	2.158171000	-0.210990000
1	-1.262960000	2.124952000	-0.254911000
1	-1.214373000	-2.149204000	0.132457000
1	1.287718000	-2.112524000	0.169974000
1	4.445501000	-0.909995000	0.108121000
6	-2.898983000	-0.133905000	-0.027768000
8	-3.466067000	-1.184773000	-0.297321000
7	-3.593188000	1.014431000	0.261634000
1	-3.158944000	1.761455000	0.780311000
1	-4.591504000	0.903280000	0.365447000

p-OH, E_{scf} = -496.0578549

6	-0.063050000	1.222751000	0.000176000
6	-1.451454000	1.198434000	0.000219000
6	-2.125145000	-0.031024000	0.000063000
6	-1.400880000	-1.230868000	-0.000133000
6	-0.013392000	-1.196987000	-0.000172000
6	0.671242000	0.029203000	-0.000018000
6	2.148252000	0.118860000	-0.000058000
8	2.757502000	-1.096746000	-0.000212000
8	2.786968000	1.154411000	0.000047000
1	0.476550000	2.163578000	0.000292000
1	-2.016484000	2.127912000	0.000375000
1	-1.943753000	-2.169760000	-0.000255000
1	0.550180000	-2.122867000	-0.000322000
1	3.710393000	-0.909024000	-0.000224000
8	-3.482755000	-0.122401000	0.000094000
1	-3.864039000	0.765839000	0.000230000

p-NH_2, E_{scf} = -476.1975078

6	-0.046683000	1.226414000	-0.004107000
6	-1.431662000	1.209703000	-0.005871000
6	-2.130557000	-0.014565000	-0.006393000
6	-1.391974000	-1.214539000	-0.004948000
6	-0.005349000	-1.189244000	-0.003461000
6	0.688752000	0.030914000	-0.002331000
6	2.161877000	0.112267000	0.002970000
8	2.767631000	-1.108020000	0.003625000
8	2.810618000	1.142845000	0.006703000
1	0.495447000	2.166059000	-0.001464000
1	-1.988653000	2.143051000	-0.010279000
1	-1.918468000	-2.165454000	-0.008745000
1	0.551209000	-2.119626000	-0.000417000
1	3.720246000	-0.919761000	0.006462000
7	-3.513550000	-0.037154000	-0.058328000
1	-3.992174000	0.799448000	0.241543000
1	-3.965175000	-0.887944000	0.243421000

p-$NHCH_3$, E_{scf} = -515.5065603

p-$N(CH_3)_2$, E_{scf} = -554.8128738

6	0.534333000	1.311715000	0.002646000	6	-0.753368000	-1.228706000	-0.005116000
6	-0.841782000	1.434823000	-0.014919000	6	0.631109000	-1.222658000	-0.012404000
6	-1.669674000	0.287986000	-0.041311000	6	1.351855000	-0.001258000	-0.021877000
6	-1.055714000	-0.982886000	-0.044237000	6	0.603100000	1.202585000	-0.012403000
6	0.328709000	-1.093883000	-0.029618000	6	-0.782863000	1.179986000	-0.005182000
6	1.145187000	0.045371000	-0.005496000	6	-1.487267000	-0.033316000	-0.002771000
6	2.617409000	-0.025084000	0.014410000	6	-2.959061000	-0.107087000	0.005433000
8	3.096597000	-1.301009000	0.003027000	8	-3.559736000	1.116692000	0.007362000
8	3.369092000	0.933301000	0.038814000	8	-3.614859000	-1.133865000	0.009803000
1	1.168906000	2.191340000	0.023798000	1	-1.296796000	-2.167783000	0.000803000
1	-1.300576000	2.420685000	-0.012123000	1	1.158439000	-2.168150000	-0.009941000
1	-1.662321000	-1.881088000	-0.058549000	1	1.108771000	2.159840000	-0.009973000
1	0.786916000	-2.076611000	-0.032742000	1	-1.331980000	2.114987000	0.000636000
1	4.063071000	-1.208894000	0.017730000	1	-4.512814000	0.931201000	0.012624000
7	-3.037044000	0.437340000	-0.086083000	7	2.730558000	0.014654000	-0.042104000
1	-3.385095000	1.360651000	0.119832000	6	3.475552000	-1.231808000	0.022511000
6	-3.967168000	-0.658657000	0.089900000	1	3.230630000	-1.891148000	-0.819516000
1	-3.834190000	-1.184781000	1.046888000	1	4.542818000	-1.014199000	-0.025705000
1	-4.984604000	-0.264673000	0.052528000	1	3.282925000	-1.784965000	0.952656000
1	-3.866106000	-1.392649000	-0.717760000	6	3.446623000	1.277695000	0.022933000
				1	4.518671000	1.084582000	-0.023432000
				1	3.188096000	1.930884000	-0.819936000
				1	3.240025000	1.826952000	0.952453000
p-NHOH, E_{scf} = -551.3524436				p-NO_2, E_{scf} = -625.3324734			
6	-0.275560000	-1.139645000	-0.088273000	6	-0.642209000	1.237511000	-0.000130000
6	1.105772000	-1.006115000	-0.132595000	6	0.747856000	1.230011000	-0.000218000
6	1.682401000	0.275358000	-0.102906000	6	1.404525000	0.000471000	-0.000074000
6	0.851212000	1.410251000	-0.033411000	6	0.720522000	-1.213240000	0.000146000
6	-0.526491000	1.263508000	0.003073000	6	-0.670974000	-1.193044000	0.000221000
6	-1.108438000	-0.014971000	-0.019172000	6	-1.354692000	0.030719000	0.000086000
6	-2.571226000	-0.225664000	0.029238000	6	-2.845124000	0.105682000	0.000177000
8	-3.277142000	0.936139000	0.089414000	8	-3.432976000	-1.113559000	0.000181000
8	-3.124513000	-1.309262000	0.018894000	8	-3.480409000	1.139267000	0.000054000
1	-0.735081000	-2.122071000	-0.109923000	1	-1.195909000	2.169542000	-0.000225000
1	1.746297000	-1.876330000	-0.207593000	1	1.326999000	2.144317000	-0.000394000
1	1.294455000	2.402451000	-0.011328000	1	1.279867000	-2.139802000	0.000254000
1	-1.162583000	2.139406000	0.058730000	1	-1.229451000	-2.121320000	0.000380000
1	-4.210672000	0.669619000	0.115234000	1	-4.391184000	-0.951886000	0.000145000
7	3.063306000	0.450243000	-0.198910000	7	2.880581000	-0.016886000	-0.000159000
1	3.414972000	1.300293000	0.232456000	8	3.436970000	-1.113829000	-0.000008000
8	3.859711000	-0.646654000	0.178038000	8	3.462189000	1.066708000	-0.000263000
1	3.598995000	-0.883191000	1.088301000				
p-CF_3, E_{scf} = -757.8698076				p-CHO, E_{scf} = -534.1577662			
6	-1.007128000	-1.235852000	-0.016464000	6	-0.410212000	1.299096000	-0.000177000
6	0.382866000	-1.222586000	-0.032459000	6	0.977844000	1.380746000	-0.000237000
6	1.064163000	-0.001332000	-0.039968000	6	1.751223000	0.212325000	-0.000070000
6	0.356791000	1.203465000	-0.033197000	6	1.125585000	-1.043345000	0.000148000
6	-1.035241000	1.189808000	-0.017643000	6	-0.260575000	-1.129131000	0.000194000
6	-1.721663000	-0.031090000	-0.007770000	6	-1.032817000	0.044080000	0.000035000
6	-3.209481000	-0.105007000	0.008408000	6	-2.523103000	0.011482000	0.000088000
8	-3.799586000	1.115162000	0.014885000	8	-3.025140000	-1.247072000	0.000225000
8	-3.849594000	-1.136580000	0.015818000	8	-3.234900000	0.995173000	0.000015000
1	-1.559674000	-2.168752000	-0.013120000	1	-1.031236000	2.187926000	-0.000294000
1	0.940500000	-2.152429000	-0.046714000	1	1.468986000	2.350650000	-0.000410000
1	0.895130000	2.144357000	-0.047811000	1	1.747516000	-1.932446000	0.000278000
1	-1.591756000	2.119469000	-0.015605000	1	-0.754037000	-2.093922000	0.000355000
1	-4.756706000	0.948475000	0.025876000	1	-3.991803000	-1.149013000	0.000255000

6	2.570496000	0.012354000	0.003546000
9	3.099847000	-1.045484000	-0.648500000
9	3.080023000	1.132280000	-0.553594000
9	3.026922000	-0.039946000	1.275987000

p-CN, E_{scf} = -513.0748827

6	-0.248739000	1.234161000	-0.000336000
6	1.139634000	1.223475000	-0.000234000
6	1.826474000	-0.003677000	-0.000030000
6	1.110348000	-1.213037000	0.000068000
6	-0.279595000	-1.193735000	-0.000041000
6	-0.963650000	0.029266000	-0.000254000
6	-2.452166000	0.105567000	-0.000392000
8	-3.041961000	-1.113692000	0.000417000
8	-3.087863000	1.139468000	0.000240000
1	-0.801439000	2.166962000	-0.000480000
1	1.700048000	2.151819000	-0.000313000
1	1.648694000	-2.154378000	0.000236000
1	-0.838362000	-2.121990000	0.000020000
1	-3.999509000	-0.948839000	0.000868000
6	3.261033000	-0.022014000	0.000083000
7	4.424161000	-0.037118000	0.000176000

p-CH_2F, E_{scf} = -559.3766323

6	-0.398409000	1.234357000	-0.100903000
6	0.986011000	1.214568000	-0.229598000
6	1.678542000	-0.001003000	-0.304231000
6	0.956643000	-1.199271000	-0.240555000
6	-0.429380000	-1.189900000	-0.111443000
6	-1.113311000	0.031150000	-0.041435000
6	-2.593188000	0.105641000	0.091744000
8	-3.184656000	-1.114571000	0.140176000
8	-3.233457000	1.136146000	0.153231000
1	1.537548000	2.149713000	-0.275062000
1	1.486097000	-2.146676000	-0.294648000
1	-0.984662000	-2.119467000	-0.066167000
1	-4.136727000	-0.942601000	0.228022000
1	-0.946729000	2.168385000	-0.046175000
6	3.181613000	-0.019458000	-0.395685000
1	3.530405000	-0.912071000	-0.927258000
1	3.552687000	0.869376000	-0.918388000
9	3.743905000	-0.032861000	0.882782000

6	3.231992000	0.307674000	-0.000121000
8	3.981455000	-0.648993000	-0.000160000
1	3.629634000	1.346387000	0.000015000

p-$COCH_3$, E_{scf} = -573.4838249

6	0.669019000	1.221679000	-0.000104000
6	-0.721077000	1.172309000	-0.000119000
6	-1.386810000	-0.063195000	-0.000063000
6	-0.633806000	-1.247522000	0.000054000
6	0.754663000	-1.203306000	0.000062000
6	1.413106000	0.035597000	-0.000017000
6	2.898267000	0.146882000	0.000009000
8	3.519635000	-1.057872000	0.000168000
8	3.513814000	1.193965000	-0.000116000
1	1.198834000	2.167848000	-0.000142000
1	-1.283645000	2.099801000	-0.000160000
1	-1.166339000	-2.192187000	0.000125000
1	1.334837000	-2.118742000	0.000143000
1	4.472020000	-0.865809000	0.000148000
6	-2.886296000	-0.179244000	-0.000041000
8	-3.419008000	-1.277712000	-0.000280000
6	-3.721085000	1.088406000	0.000306000
1	-3.506032000	1.700852000	-0.882171000
1	-4.775235000	0.811043000	0.000366000
1	-3.505864000	1.700514000	0.882990000