Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information to

On Non-Additivity of the Substituent Effect in *ortho*-, *meta*-, and *para*-Homo-Disubstituted Benzenes

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XYZ Coordinates of all studied structures

[1.1] b3lyp/aug-cc-pvdz: *mono*

[1.2] b3lyp/aug-cc-pvdz: *ortho*
[1.3] b3lyp/aug-cc-pvdz: *meta*
[1.4] b3lyp/aug-cc-pvdz: para

[2.1] b3lyp/6-31G(d,p): *mono*
[2.2] b3lyp/6-31G(d,p): *ortho*
[2.3] b3lyp/6-31G(d,p): *meta*
[2.4] b3lyp/6-31G(d,p): para

[3.1] b3lyp/6-311++G(d,p): *mono*
[3.2] b3lyp/6-311++G(d,p): ortho
[3.3] b3lyp/6-311++G(d,p): *meta*
[3.4] b3lyp/6-311++G(d,p): *para*

[1.1] b3lyp/aug-cc-pvdz: *mono*

b3lyp/aug-cc-pvdz: C_6H_6
[total energy (hartree): -232.274590777]

C	0.00063400	0.00005300	-0.00203200
C	0.00056500	0.00049300	1.39712600
C	1.21221900	-0.00004900	2.09679900
C	2.42395600	-0.00104800	1.39724100
C	2.42402600	-0.00149500	-0.00190500
C	1.21235800	-0.00093900	-0.70158400
H	3.36859600	-0.00148200	1.94272700
H	3.36872000	-0.00227400	-0.54729700
H	-0.94414000	0.00127300	1.94249800
H	-0.94401600	0.00048600	-0.54749800
H	1.21242400	-0.00128400	-1.79240200
H	1.21217700	0.00029700	3.18761700

b3lyp/aug-cc-pvdz: C_6H_5-BF_2
[total energy (hartree): -456.374290097]

C	-0.03396100	0.00006100	-0.02349600
C	-0.01650000	0.00045800	1.38598800
C	1.19080900	-0.00008300	2.08651800
C	2.40191100	-0.00103500	1.38486900
C	2.40539700	-0.00144400	-0.01484300
C	1.19603900	-0.00089700	-0.71206800
H	3.34633800	-0.00146400	1.93084900
H	3.35082100	-0.00218900	-0.55818900
H	-0.95959200	0.00120500	1.93331000
H	1.20088200	-0.00121300	-1.80252900
H	1.19142900	0.00023300	3.17694500
B	-1.37117700	0.00067000	-0.79237100
F	-2.55556900	0.00156500	-0.15964300
F	-1.42401400	0.00034700	-2.13382700

b3lyp/aug-cc-pvdz: C_6H_5-BH_2
[total energy (hartree): -257.716265765]

C	-0.04032200	0.00006500	-0.02513800
C	-0.00919800	0.00046100	1.39044800
C	1.19696100	-0.00007800	2.09178300
C	2.40768500	-0.00103600	1.38779000
C	2.41158800	-0.00145100	-0.01271400
C	1.20099400	-0.00090500	-0.70638100
H	3.35273100	-0.00146300	1.93326100
H	3.35791100	-0.00220100	-0.55499600
H	-0.95207100	0.00121100	1.93988000
H	1.20504300	-0.00122700	-1.79764000
H	1.20079500	0.00024000	3.18245600
B	-1.37281400	0.00067000	-0.79409800
H	-1.37780700	0.00031800	-1.99626400
H	-2.41618900	0.00149700	-0.19688300

b3lyp/aug-cc-pvdz: C_6H_5-Br
[total energy (hartree): -2805.83068174]

C	0.00300300	0.00004300	0.00034800
C	-0.00621300	0.00053700	1.39939500
C	1.21215300	0.00001000	2.08100600
C	2.43067500	-0.00101000	1.39965100
C	2.42175800	-0.00150500	0.00061100
C	1.21245000	-0.00096700	-0.70124700
H	3.36992900	-0.00142000	1.95011100

H	3.36944900	-0.00230400	-0.53892900
H	-0.94559100	0.00132900	1.94964300
H	-0.94458300	0.00046300	-0.53938100
H	1.21257800	-0.00134500	-1.79127300
Br	1.21197300	0.00068200	4.00135500

b3lyp/aug-cc-pvdz: C_6H_5-CHO
[total energy (hartree): -345.616374444]

C	-0.01141300	0.00005700	-0.01251100
C	-0.00779900	0.00047000	1.39056500
C	1.20070600	-0.00008100	2.09131500
C	2.40879900	-0.00104600	1.38690600
C	2.41075700	-0.00146100	-0.01585200
C	1.20624500	-0.00091200	-0.71561400
H	3.35430900	-0.00148300	1.93070500
H	3.35698800	-0.00221800	-0.55768400
H	-0.95630600	0.00123100	1.93118000
H	1.18374700	-0.00121500	-1.80504200
H	1.20249000	0.00023900	3.18148800
C	-1.30495200	0.00065800	-0.73725300
O	-1.42430600	0.00037800	-1.94764900
H	-2.20798000	0.00142100	-0.08095500

b3lyp/aug-cc-pvdz: C_6H_5-Cl
[total energy (hartree): -691.894835506]

C	0.00295200	0.00004400	0.00045800
C	-0.00619000	0.00053400	1.39901000
C	1.21216800	0.00001300	2.08024400
C	2.43066100	-0.00101100	1.39923800
C	2.42178500	-0.00150700	0.00068900
C	1.21242900	-0.00095800	-0.70138100
H	3.36720600	-0.00142400	1.95435400
H	3.36925700	-0.00230600	-0.53910100
H	-0.94284000	0.00131900	1.95394800
H	-0.94442300	0.00046300	-0.53950400
H	1.21254200	-0.00133300	-1.79137500
Cl	1.21202200	0.00059200	3.84471100

b3lyp/aug-cc-pvdz: C_6H_5-CN
[total energy (hartree): -324.528901811]

C	-0.01287000	0.00005500	-0.00947500
C	-0.01456600	0.00050400	1.39714400
C	1.19681800	-0.00004600	2.08880100
C	2.40776100	-0.00103800	1.38782200
C	2.40908500	-0.00148500	-0.01135600
C	1.20432000	-0.00094300	-0.71449300
H	3.35200500	-0.00146800	1.93291200
H	3.35221800	-0.00226200	-0.55775600
H	-0.96150600	0.00128200	1.93504300
H	1.19646700	-0.00128400	-1.80350400
H	1.19537000	0.00030000	3.17877200
C	-1.25771600	0.00062500	-0.72802700
N	-2.26524500	0.00108800	-1.30945800

b3lyp/aug-cc-pvdz: C_6H_5-COOH (conformer no 1)
[total energy (hartree): -420.884274537]

C	-0.03466300	0.00003600	0.02487300
C	-0.00902700	0.00043300	1.42887700
C	1.21406800	-0.00009800	2.10246200
C	2.41248800	-0.00102200	1.38061700
C	2.38901300	-0.00141900	-0.01916700

C	1.16999000	-0.00089200	-0.69658900
H	3.36641700	-0.00143800	1.90943600
H	3.32307300	-0.00214100	-0.58136400
H	-0.94327400	0.00115800	1.98649200
H	1.13105300	-0.00118400	-1.78474300
H	1.23282300	0.00020900	3.19251800
C	-1.31066100	0.00057700	-0.74105400
O	-1.39693600	0.00025800	-1.95259100
O	-2.41441200	0.00149800	0.05610500
H	-3.17941300	0.00178600	-0.54078200

b3lyp/aug-cc-pvdz: C_6H_5-COOH (conformer no 2)
[total energy (hartree): -420.874160135]

C	0.00018300	0.00044500	-0.00023400
C	0.00000000	0.00001400	1.40410200
C	1.20349200	-0.00045700	2.10864200
C	2.42150500	0.01427500	1.41912400
C	2.43137700	0.02974900	0.02141000
C	1.22610700	0.01948700	-0.68517100
H	3.36225500	0.01876300	1.97049200
H	3.37699600	0.05574300	-0.52007600
H	-0.95640100	-0.00010500	1.92429300
H	1.26519500	0.06109400	-1.77548400
H	1.19321800	-0.00888200	3.19874800
C	-1.33306600	0.00411200	-0.69064900
O	-2.36874700	0.27718800	-0.13187400
O	-1.35521000	-0.32290000	-2.01368900
H	-0.48107400	-0.60700500	-2.31246000

b3lyp/aug-cc-pvdz: C_6H_5-F
[total energy (hartree): -331.525650093]

C	0.00165700	0.00005200	0.00005500
C	-0.00849400	0.00051600	1.39894500
C	1.21221600	-0.00005800	2.06566800
C	2.43300500	-0.00104400	1.39908500
C	2.42301700	-0.00148700	0.00019800
C	1.21237600	-0.00095600	-0.70087300
H	3.36191700	-0.00145000	1.96771600
H	3.36905100	-0.00226900	-0.54196000
H	-0.93747100	0.00130400	1.96746400
H	-0.94431300	0.00048300	-0.54220800
H	1.21244200	-0.00131300	-1.79073200
F	1.21213900	0.00041300	3.42793300

b3lyp/aug-cc-pvdz: C_6H_5-Li
[total energy (hartree): -239.168460538]

C	0.00260600	0.00004200	-0.00562400
C	0.01700400	0.00053600	1.39671700
C	1.20792100	0.00004400	2.16810300
C	2.39893400	-0.00098500	1.39685100
C	2.41349400	-0.00149700	-0.00548600
C	1.20808900	-0.00098100	-0.71489000
H	-0.94733700	0.00046300	-0.54615100
H	-0.95740200	0.00134800	1.90061500
H	3.37328400	-0.00142700	1.90086200
H	3.36349600	-0.00229900	-0.54591000
H	1.20815500	-0.00136600	-1.80650000
Li	1.20801600	0.00073000	4.13311400

b3lyp/aug-cc-pvdz: C_6H_5-$N(CH_3)_2$
[total energy (hartree): -366.255327479]

C	-0.00003600	0.00007300	-0.00006500
C	-0.00004700	0.00119700	1.41603300
C	1.25746200	0.00190200	2.06729800
C	2.44452500	0.02549900	1.33424600
C	2.43242700	0.04018800	-0.06348800
C	1.19690600	0.02352900	-0.71706100
H	-0.93549800	-0.02025900	-0.55312600
H	1.31810000	-0.01525100	3.15235200
H	3.39458500	0.02847500	1.87070800
H	1.15755500	0.02418700	-1.80740600
N	-1.18933300	0.01943300	2.14025100
C	-1.15027600	-0.24366400	3.56908300
H	-0.53918200	0.50644800	4.09005300
C	-2.44266100	-0.22637200	1.44688100
H	-3.26722700	-0.14545200	2.16241600
H	-2.61053200	0.52552800	0.66350700
H	-2.16614200	-0.17708100	3.97150500
H	-2.48585600	-1.22715100	0.97739000
H	-0.74511600	-1.24427400	3.81023400
H	3.36323900	0.05594900	-0.62965200

b3lyp/aug-cc-pvdz: C_6H_5-NH_2
[total energy (hartree): -287.643774693]

C	-0.00002800	0.00008200	0.00002600
C	0.00005900	0.00003200	1.40685300
C	2.42963300	-0.00011600	-0.03371500
C	1.20335000	-0.00021500	-0.70724200
H	-0.94936800	0.00550100	-0.53893900
H	1.18033000	-0.00115000	-1.79798100
N	-1.20314000	0.06467300	2.12042600
H	-2.01965100	-0.27466500	1.62871900
H	-1.16408000	-0.27783400	3.07162900
C	2.43219600	-0.00028800	1.36535500
H	3.36689800	-0.00058800	-0.58947000
C	1.23436700	0.00009900	2.08195400
H	3.37817400	-0.00118400	1.90884300
H	1.25161400	0.00584900	3.17345400

b3lyp/aug-cc-pvdz: C_6H_5-OCH_3
[total energy (hartree): -346.812567360]

C	0.01599800	0.00017500	-0.11776400
C	-0.07153000	0.00066100	1.28131000
C	1.10445700	0.00003600	2.04452000
C	2.35481500	-0.00105200	1.40407400
C	2.42396600	-0.00152200	0.01324100
C	1.25425100	-0.00091700	-0.75981200
H	-1.05075800	0.00152800	1.75414300
H	-0.90302800	0.00066800	-0.70529600
O	1.13964900	0.00043400	3.41280700
H	3.25632900	-0.00152100	2.01618100
H	3.40006500	-0.00237900	-0.47360900
C	-0.09666500	0.00136600	4.11662500
H	-0.68941100	-0.89755900	3.88592600
H	0.16530300	0.00142400	5.17928000
H	-0.68827800	0.90094400	3.88555600
H	1.31196100	-0.00128700	-1.84805000

b3lyp/aug-cc-pvdz: C_6H_5-OH
[total energy (hartree): -307.511948646]

C	-0.00000200	0.00005400	-0.00316400
C	-0.01344000	0.00054700	1.39531500

C	1.19663300	0.00001700	2.10000400
C	2.41489700	-0.00100400	1.41003300
C	2.41401800	-0.00148800	0.01419100
C	1.21062100	-0.00096200	-0.70145800
H	3.34519800	-0.00141000	1.97716500
H	3.36514100	-0.00228700	-0.51970900
H	-0.96221900	0.00134700	1.93657300
H	-0.94560900	0.00047500	-0.54666000
H	1.21728800	-0.00134000	-1.79112100
O	1.25172500	0.00044900	3.47188200
H	0.35623500	0.00114900	3.83145700

b3lyp/aug-cc-pvdz: C_6H_5-SH
[total energy (hartree): -630.485327456]

C	-0.01943400	-0.00001200	-0.00864000
C	-0.01604300	0.00044000	1.39370600
C	1.19671300	-0.00006600	2.08846000
C	2.41228800	-0.00101300	1.39765800
C	2.40553000	-0.00145600	-0.00089100
C	1.19903600	-0.00096400	-0.70496600
H	3.35552800	-0.00140700	1.94372300
H	3.34619600	-0.00220000	-0.55286100
H	-0.95545700	0.00118400	1.94687400
H	1.20543800	-0.00131500	-1.79548300
H	1.18687900	0.00028800	3.17913600
S	-1.52789200	0.00058000	-0.97587500
H	-2.39381700	0.00146000	0.06637900

b3lyp/aug-cc-pvdz: C_6H_5-tBu
[total energy (hartree): -389.542763370]

C	0.03530300	0.00000600	-0.01750800
C	0.04310800	0.00054900	1.39017100
C	1.23523600	0.00007100	2.11617500
C	2.46565700	-0.00098400	1.45028600
C	2.47992400	-0.00154900	0.05515300
C	1.27959000	-0.00105700	-0.66687700
H	3.39922400	-0.00136400	2.01373500
H	3.42950800	-0.00238300	-0.48173700
H	-0.89852000	0.00136700	1.93892400
H	1.33358300	-0.00152000	-1.75334800
H	1.20361600	0.00051900	3.20661600
C	-1.30438300	0.00058100	-0.77635000
C	-2.11274700	-1.26058900	-0.39286700
C	-2.11115900	1.26304400	-0.39377000
C	-1.10789100	-0.00009500	-2.30297900
H	-1.56144800	-2.17357900	-0.65604400
H	-2.32706700	-1.29516400	0.68282800
H	-3.07335000	-1.27392800	-0.92759000
H	-1.55862300	2.17515100	-0.65741000
H	-3.07165000	1.27730600	-0.92866600
H	-2.32562400	1.29855800	0.68186600
H	-2.08721900	0.00032900	-2.80029800
H	-0.56212600	0.88975800	-2.64480100
H	-0.56323900	-0.89088000	-2.64414700

[1.2] b3lyp/aug-cc-pvdz: *ortho*

b3lyp/aug-cc-pvdz: BF_2-C_6H_4-BF_2, *ortho*
[total energy (hartree): -680.463606276]

C	-0.00007200	0.00019400	0.00044600
C	-0.00043200	-0.00026600	1.40697200
C	1.24652600	-0.00062700	2.09456700

C	2.43564300	0.03745400	1.34440200
C	2.41498800	0.05136100	-0.05381400
C	1.19354300	0.02399400	-0.72793400
H	3.39409000	0.04493900	1.86357200
H	1.16725600	0.02727300	-1.81806200
B	-1.38453600	0.12253800	2.10483500
F	-1.55346400	0.67191200	3.31161200
F	-2.50615700	-0.25074200	1.46982300
H	-0.95022500	-0.00645100	-0.53385200
B	1.39920700	-0.16262900	3.63363800
F	2.52803500	0.21803500	4.25139200
F	0.48284300	-0.75382600	4.40639700
H	3.35087900	0.07775300	-0.61284200

b3lyp/aug-cc-pvdz: BH_2-C_6H_4-BH_2, *ortho* (conformer no 1)
[total energy (hartree): -283.144749654]

C	-0.00652300	-0.00005100	-0.00932800
C	0.01536000	0.00054100	1.39243500
C	1.22680900	0.00009600	2.09318800
C	2.44817400	-0.00098700	1.40032100
C	2.43773300	-0.00158600	-0.02630700
C	1.19852200	-0.00109500	-0.70804400
H	1.19528100	-0.00153900	-1.79974700
H	1.20529400	0.00059300	3.18473200
B	3.79023000	-0.00267000	-0.73970600
H	3.91233000	-0.00318900	-1.93376800
H	4.79083300	-0.00299900	-0.05209600
H	-0.95828400	0.00032500	-0.54116500
B	3.84399200	-0.00158100	2.11082700
H	4.37374200	-1.03432600	2.42256000
H	4.37497200	1.03073700	2.42188500
H	-0.92495300	0.00137900	1.94661200

b3lyp/aug-cc-pvdz: BH_2-C_6H_4-BH_2, *ortho* (conformer no 2)
[total energy (hartree): -283.150699259]

C	-0.00001700	-0.00035800	0.00002500
C	0.00006300	-0.00057400	1.39924400
C	1.19675100	-0.00036100	2.14807200
C	2.44799300	0.00009400	1.43645000
C	2.41627600	0.00030100	0.02517800
C	1.21378700	0.00008000	-0.69029000
H	-0.95343300	-0.00091900	1.92908600
H	1.22428000	0.00024900	-1.78121900
B	3.84469800	0.00037900	2.10989700
H	4.81315700	0.00075400	1.39722500
H	3.99853800	0.00024500	3.29506600
H	3.35906500	0.00064600	-0.52354200
H	-0.94295100	-0.00053600	-0.54872600
B	1.06164200	-0.00064800	3.69274400
H	2.00173700	-0.00052300	4.43061500
H	-0.04584200	-0.00101500	4.16094700

b3lyp/aug-cc-pvdz: Br-C_6H_4-Br, *ortho*
[total energy (hartree): -5379.38066992]

C	0.00313600	0.00001400	0.00313500
C	0.00281400	0.00052400	1.39853000
C	1.21273300	0.00005500	2.10328600
C	2.42680200	-0.00094600	1.40247100
C	2.42184400	-0.00145400	0.00246500
C	1.21363000	-0.00096300	-0.69551000
H	3.36989500	-0.00223000	-0.53234600

Br	1.13775900	0.00080400	4.01144000
H	-0.93490900	0.00129600	1.95162300
H	-0.94513700	0.00039700	-0.53408400
Br	4.11738500	-0.00166600	2.29104100
H	1.22323300	-0.00136000	-1.78533500

b3lyp/aug-cc-pvdz: CHO-C_6H_4-CHO, *ortho* (conformer no 1)
[total energy (hartree): -458.948439464]

C	-0.03240600	-0.00000100	-0.00916100
C	-0.03266100	-0.00000100	1.41017200
C	1.19370300	0.00000000	2.09777000
C	2.39951300	0.00000000	1.40223200
C	2.39976600	0.00000000	-0.00034200
C	1.19420700	-0.00000100	-0.69631500
H	1.17407400	-0.00000100	-1.78508800
H	1.17317600	0.00000000	3.18653600
C	-1.27826100	-0.00000200	-0.83099500
O	-1.27340900	0.00000300	-2.04775000
H	-2.24640300	0.00000100	-0.29059200
H	3.34345200	0.00000000	-0.54646400
C	-1.27881400	-0.00000200	2.23155300
H	-2.24675700	0.00000000	1.69079600
O	-1.27440600	0.00000100	3.44831000
H	3.34300300	0.00000100	1.94869400

b3lyp/aug-cc-pvdz: CHO-C_6H_4-CHO, *ortho* (conformer no 2)
[total energy (hartree): -458.949475435]

C	0.03340000	-0.00000100	0.01372500
C	0.05601900	0.00000100	1.41131300
C	1.28204700	0.00000100	2.07809100
C	2.49743900	0.00000000	1.37323400
C	2.47076600	-0.00000100	-0.04784900
C	1.23183600	-0.00000100	-0.70305900
H	1.23186100	-0.00000100	-1.79229500
H	1.30416800	0.00000200	3.16897900
C	3.70484900	0.00000600	-0.90344500
O	3.64317100	-0.00000700	-2.12016500
H	4.67398100	0.00002200	-0.37680700
H	-0.91834300	-0.00000200	-0.51825700
C	3.72416000	-0.00000500	2.21865400
H	3.49870900	0.00001600	3.31136400
O	4.87951000	-0.00003100	1.84118200
H	-0.87501500	0.00000100	1.97825400

b3lyp/aug-cc-pvdz: CHO-C_6H_4-CHO, *ortho* (conformer no 3)
[total energy (hartree): -458.937308742]

C	0.04094600	0.00000100	0.06237200
C	0.05930100	0.00000100	1.45995800
C	1.25366400	0.00000000	2.19735000
C	2.48958900	-0.00000100	1.48355600
C	2.44829200	-0.00000200	0.08062900
C	1.24722100	-0.00000100	-0.63416300
H	-0.88632800	0.00000200	2.00428900
H	1.25926900	-0.00000100	-1.72410100
C	3.88411600	-0.00000400	2.03898500
H	4.64649100	0.00000600	1.22079300
O	4.23955200	0.00000300	3.19291500
H	3.39256500	-0.00000300	-0.46599800
C	1.03758800	0.00000000	3.68281800
H	-0.05223700	-0.00000300	3.93377700
O	1.85913400	-0.00000100	4.56772400

H	-0.90893700	0.00000200	-0.47227300

b3lyp/aug-cc-pvdz: Cl-C_6H_4-Cl, *ortho*
[total energy (hartree): -1151.50949792]

C	-0.00508800	0.00009500	-0.00482000
C	-0.00513900	0.00056500	1.39745000
C	1.20761700	-0.00000100	2.09404400
C	2.41560700	-0.00104100	1.39540300
C	2.41565500	-0.00151700	-0.00259500
C	1.20771800	-0.00094400	-0.70132700
H	3.35530400	-0.00233000	-0.55458800
H	1.19123600	-0.00129500	-1.78983900
Cl	-1.50124400	0.00080700	-0.91586500
H	1.19105400	0.00038100	3.18255600
Cl	-1.50136100	0.00189700	2.30838600
H	3.35521500	-0.00147900	1.94746300

b3lyp/aug-cc-pvdz: CN-C_6H_4-CN, *ortho*
[total energy (hartree): -416.775488845]

C	-0.01642000	0.00015300	0.02108800
C	-0.02747800	0.00073600	1.42497900
C	1.19890600	0.00017300	2.13354500
C	2.40955300	-0.00096200	1.42259600
C	2.40517800	-0.00153000	0.02776900
C	1.19407500	-0.00097200	-0.67194500
H	3.34776700	-0.00139300	1.97464200
H	1.19086400	-0.00141400	-1.76157300
C	-1.28486700	0.00190400	2.11774900
N	-2.31837000	0.00285100	2.64996600
H	-0.96332200	0.00059600	-0.51589800
C	1.22685600	0.00074200	3.56885500
N	1.28205700	0.00117800	4.73003100
H	3.35070800	-0.00241300	-0.51378700

b3lyp/aug-cc-pvdz: COOH-C_6H_4-COOH, *ortho* (conformer no 1)
[total energy (hartree): -609.479192394]

C	0.00000600	0.00020200	0.00007800
C	0.00009000	0.00041800	1.39585500
C	1.20488800	0.00014000	2.11179900
C	2.42806200	0.03223600	1.40904600
C	2.41697200	0.01369300	0.00776400
C	1.21153600	-0.00406100	-0.69569200
H	-0.93647000	-0.01526300	1.95109500
H	1.22016200	-0.01259100	-1.78565900
C	3.77259500	0.16447900	2.05396400
O	4.78121900	-0.37373200	1.65171300
O	3.76990100	1.02944900	3.09828100
H	4.67697200	1.05355300	3.44432200
H	3.36839900	0.02975800	-0.52158000
C	1.08528000	-0.11324500	3.59978000
O	0.22689900	0.42929500	4.26128700
O	1.99320200	-0.96660100	4.13471800
H	1.83564600	-0.97879700	5.09290900
H	-0.94577300	-0.00513600	-0.54182800

b3lyp/aug-cc-pvdz: COOH-C_6H_4-COOH, *ortho* (conformer no 2)
[total energy (hartree): -609.479660238]

C	-0.00019400	-0.00183800	-0.00019500
C	-0.00029100	-0.00140600	1.39698200
C	1.20389900	0.00041800	2.10903600
C	2.42672200	-0.03050800	1.40660100

C	2.41581000	-0.02501100	0.00367100
C	1.20960500	-0.00705100	-0.69827500
H	-0.93994300	0.00432400	1.94774600
H	1.21575800	-0.00789500	-1.78818400
C	3.71425700	-0.18500800	2.14326200
O	3.82275400	-0.62030300	3.26969200
O	4.79318600	0.18119500	1.40144300
H	5.57453300	0.00864500	1.95081600
H	3.36109000	-0.05611800	-0.53358800
C	1.09681000	0.06253400	3.60650500
O	0.45122900	-0.71494900	4.27258400
O	1.71055100	1.15278400	4.12238000
H	1.61372200	1.10092800	5.08760700
H	-0.94672200	0.00216400	-0.54105800

b3lyp/aug-cc-pvdz: COOH-C_6H_4-COOH, *ortho* (conformer no 3)
[total energy (hartree): -609.478928669]

C	0.00115400	0.00736500	-0.00067700
C	-0.00028300	0.00586900	1.40952000
C	1.21767500	0.00332900	2.10051000
C	2.42940300	-0.02327600	1.40475000
C	2.42984200	-0.04885700	0.00924500
C	1.21902200	-0.03407700	-0.68919900
H	1.21536800	-0.03541000	-1.77775800
H	1.21107200	0.00145600	3.18876800
C	-1.26347200	0.19845700	-0.78125200
O	-2.12050700	1.01108500	-0.51908900
O	-1.31208200	-0.59740700	-1.88000800
H	-2.13716200	-0.38004500	-2.34430900
H	3.37121600	-0.07462600	-0.53983800
C	-1.27793000	-0.13404500	2.17504100
O	-2.22098500	-0.80957400	1.82918000
O	-1.24868300	0.53665600	3.35587800
H	-2.09504600	0.35727900	3.79694600
H	3.37025400	-0.03142400	1.95512600

b3lyp/aug-cc-pvdz: F-C_6H_4-F, *ortho*
[total energy (hartree): -430.769442148]

C	0.00054500	0.00004700	-0.00082700
C	-0.00659600	0.00051300	1.39816300
C	1.20413200	-0.00002600	2.08103900
C	2.41204700	-0.00100500	1.38360900
C	2.42630200	-0.00147800	-0.00630600
C	1.21132300	-0.00095700	-0.69984600
H	3.38426900	-0.00225600	-0.52495700
F	1.22338200	0.00042100	3.43304100
H	-0.93493800	0.00129100	1.96815000
H	-0.94492100	0.00046400	-0.54229900
H	1.21538300	-0.00132400	-1.78937200
F	3.57334800	-0.00151500	2.07613600

b3lyp/aug-cc-pvdz: $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *ortho* (conformer no 1)
[total energy (hartree): -500.228429784]

C	0.00060300	0.00194200	-0.00044000
C	-0.00031400	-0.00152400	1.39805500
C	1.18807100	-0.00216100	2.14667300
C	2.40985400	0.01985100	0.03899500
C	1.21295800	-0.00507900	-0.68396700
H	1.23855600	-0.01195800	-1.77384000
C	2.43500600	0.04337600	1.44304100
N	3.66513700	0.08772400	2.15191700

C	3.86791400	1.26966800	2.99389800
C	4.86881800	-0.26781000	1.41815300
H	4.10321000	2.16665400	2.38871200
H	2.96904100	1.46384600	3.58455700
H	4.70733100	1.08608100	3.67861400
H	5.68853800	-0.39768300	2.13730300
H	4.72356100	-1.21580400	0.88634500
H	5.18697000	0.50144100	0.68563500
H	3.34698000	0.05276000	-0.51190900
H	-0.95637700	-0.03583200	1.91527600
N	1.15829400	-0.02492400	3.56663400
C	-0.09599600	0.32862800	4.21105300
C	1.78608800	-1.19045200	4.19449400
H	-0.48470300	1.26677600	3.79692500
H	-0.87991000	-0.44979900	4.11557000
H	0.09336600	0.47677900	5.28261000
H	1.15406000	-2.09483400	4.10048700
H	2.75704100	-1.38410100	3.73142400
H	1.93919900	-0.98664300	5.26321900
H	-0.94509400	-0.00804900	-0.54274500

b3lyp/aug-cc-pvdz: $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *ortho* (conformer no 2)
[total energy (hartree): -500.218353540]

C	-0.00207200	-0.00043400	-0.00305600
C	-0.00097000	-0.00014500	1.40143100
C	1.23238400	0.00014100	2.09127300
C	2.41019900	-0.00016600	-0.05085100
C	1.18903400	-0.00044500	-0.73055500
H	-0.95446700	-0.00065700	-0.53476600
H	1.16370500	-0.00066900	-1.82095900
N	-1.24173900	-0.00014400	2.14136700
C	-2.03448800	-1.21212700	1.94271200
H	-1.41319300	-2.09560700	2.13187700
C	-2.03485800	1.21149700	1.94210600
H	-2.86902800	1.21730500	2.65773000
H	-1.41384800	2.09526300	2.13087300
H	-2.86863200	-1.21785600	2.65836600
H	-2.46072400	1.29891500	0.92202100
H	-2.46035600	-1.30016300	0.92268200
C	2.42196300	0.00012300	1.34495600
H	3.36248700	0.00034900	1.89525900
N	1.36196100	0.00046400	3.52385200
C	0.91300800	-1.21695700	4.19259100
C	0.91265100	1.21804600	4.19205600
H	-0.18745900	-1.30437300	4.25494100
H	1.30916400	-2.09270800	3.66365700
H	1.31737500	-1.22912600	5.21548100
H	1.31694400	1.23073900	5.21496900
H	1.30862500	2.09367800	3.66278800
H	-0.18784300	1.30520400	4.25428600
H	3.34957800	-0.00017000	-0.60480500

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *ortho* (conformer no 1)
[total energy (hartree): -343.012365163]

C	-0.00011100	-0.00009500	-0.00001100
C	0.00006300	0.00008000	1.39641900
C	1.21511600	0.00019700	2.09010100
C	2.43441800	-0.04256500	-0.00927000
C	1.21450300	-0.02575500	-0.69398600
H	1.21924600	0.01841700	3.18185000
H	1.21799300	-0.04404000	-1.78573700

C	2.43495000	-0.00864600	1.40508900
N	3.67903200	-0.04831700	2.07085900
H	3.60600900	0.12651700	3.06631000
H	4.36993600	0.57177600	1.65611700
H	-0.93929700	0.01073300	1.94921400
N	3.67890000	-0.02911800	-0.67535400
H	4.35662000	-0.66380900	-0.26094200
H	3.60191800	-0.20221200	-1.67081400
H	-0.93962200	0.00916300	-0.55257500

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *ortho* (conformer no 2)
[total energy (hartree): -343.007948301]

C	0.00004400	-0.00000600	0.00003200
C	0.00001200	0.00014000	1.39703500
C	1.21943100	0.00017000	2.08163900
C	2.43829100	-0.05891700	-0.01852700
C	1.21007100	-0.03209600	-0.69682600
H	1.22920300	0.02569100	3.17342500
H	1.21053400	-0.06381000	-1.78790400
C	2.43935600	-0.01808100	1.39680000
N	3.68435000	-0.05899700	2.08110900
H	3.56633900	-0.02466100	3.08787700
H	4.31421300	0.69279400	1.80801800
H	-0.93720800	0.01431300	1.95289300
N	3.63738000	-0.18534000	-0.72321800
H	3.67512400	0.19909300	-1.65549300
H	4.50028300	-0.12295500	-0.20625100
H	-0.94006100	0.01344600	-0.55186700

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *ortho* (conformer no 3)
[total energy (hartree): -342.994139418]

C	0.00006300	0.00000100	-0.01590000
C	0.01181100	0.00000100	1.38554000
C	1.21295800	0.00000000	2.09826900
C	2.42912600	0.00000000	0.01194000
C	1.22782700	0.00000100	-0.71239200
H	1.19923000	-0.00000100	3.18869200
C	2.42886300	-0.00000100	1.40888900
H	3.37488000	0.00000000	-0.53346500
N	-1.27905500	0.00000200	-0.68090400
H	-1.33453700	0.80280500	-1.30670400
H	-1.33454500	-0.80281200	-1.30669100
H	-0.94686400	0.00000100	1.90353200
H	3.37325600	-0.00000100	1.95425700
N	1.20194400	0.00000100	-2.15716800
H	1.68522600	0.81516700	-2.52869500
H	1.68522800	-0.81516300	-2.52869500

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *ortho* (conformer no 4)
[total energy (hartree): -342.987421112]

C	0.01712200	0.00000200	0.00557700
C	-0.01220200	0.00000000	1.41185000
C	1.21056800	-0.00000300	2.11788600
C	2.42851200	-0.00000200	-0.00536700
C	1.21779500	0.00000100	-0.70448600
H	-0.93198400	0.00000400	-0.53352600
H	1.20860000	0.00000200	-1.79503300
N	-1.25901100	0.00000200	2.13244000
H	-1.81644900	0.81717800	1.89486200
H	-1.81644700	-0.81717700	1.89487100
C	2.41383900	-0.00000300	1.38944400

H	3.35518200	-0.00000500	1.94202100
N	1.20987900	-0.00000700	3.55802400
H	1.69481900	-0.81715100	3.92146900
H	1.69477500	0.81716100	3.92147500
H	3.37760200	-0.00000300	-0.54260300

b3lyp/aug-cc-pvdz: OCH_3-C_6H_4-OCH_3, *ortho* (conformer no 1)
[total energy (hartree): -461.342377640]

C	0.00079700	0.00257900	-0.00009600
C	-0.00008700	-0.00054400	1.40127100
C	1.20096100	-0.00158900	2.10824000
C	2.41213900	-0.01054200	1.40521000
C	2.43079800	-0.01262300	0.01173200
C	1.21075100	0.00398800	-0.70548900
H	-0.95166200	0.00315100	1.93318900
H	-0.94758100	0.01417200	-0.53200900
H	3.36820900	-0.00430600	1.92857100
O	1.31254300	0.03361500	-2.06892400
C	0.11093600	0.09808100	-2.82875500
H	-0.51717300	-0.79073200	-2.66253500
H	-0.46428600	1.00538100	-2.58875800
H	0.42406900	0.13218000	-3.87685700
O	3.64264200	0.05325500	-0.63815800
C	4.03199700	-1.13154200	-1.34509000
H	4.12595300	-1.97976700	-0.64897400
H	3.31344700	-1.37691400	-2.13780000
H	5.00974200	-0.91207300	-1.78784600
H	1.20245700	0.00299200	3.19800600

b3lyp/aug-cc-pvdz: OCH_3-C_6H_4-OCH_3, *ortho* (conformer no 2)
[total energy (hartree): -461.339793846]

C	-0.00033000	-0.00076800	0.00014100
C	-0.00089500	-0.00028200	1.39796400
C	1.22474900	0.00028300	2.09476500
C	2.42536100	0.03940200	1.37999200
C	2.41883600	0.05384200	-0.01797000
C	1.20432600	0.02311200	-0.70904100
H	-0.95963700	-0.01803600	-0.51700000
H	1.19152100	0.02472800	-1.79909900
H	3.35995400	0.05577400	1.94060800
O	-1.20615900	-0.05645900	2.06680800
C	-1.57463400	1.15221100	2.74977700
H	-1.71062800	1.97181100	2.02782100
H	-2.52746200	0.94133200	3.24749300
H	-0.81748200	1.43373300	3.49362400
O	1.26599300	0.01907200	3.47360100
C	0.89150000	-1.21515700	4.10568300
H	-0.13102500	-1.50729100	3.83169300
H	1.59451800	-2.01484400	3.82695900
H	0.95194400	-1.03432100	5.18444000
H	3.36189600	0.08224900	-0.56408000

b3lyp/aug-cc-pvdz: OCH_3-C_6H_4-OCH_3, *ortho* (conformer no 3)
[total energy (hartree): -461.345106160]

C	-0.00004700	0.00043300	-0.00007300
C	-0.00007300	0.00085000	1.40449900
C	1.20249600	0.00103000	2.11281600
C	2.43232100	0.00079300	1.40270500
C	2.41998400	0.00037300	0.00704900
C	1.20339000	0.00019100	-0.69501600
H	-0.94854300	0.00103100	1.93616500

H	-0.94882700	0.00030500	-0.53626300
O	1.30785000	0.00144000	3.47380800
C	0.10630200	0.00167400	4.23320600
H	-0.49646700	-0.89752700	4.03022100
H	0.41861500	0.00197200	5.28215600
H	-0.49644500	0.90077400	4.02970900
H	3.35433700	0.00016800	-0.54912000
O	3.55811700	0.00100900	2.17457900
C	4.81656100	0.00074800	1.51394700
H	5.56875900	0.00098500	2.30894000
H	4.94206600	-0.89858200	0.89060600
H	4.94213300	0.89966000	0.89001600
H	1.21329700	-0.00013300	-1.78477400

b3lyp/aug-cc-pvdz: OH-C_6H_4-OH, *ortho* (conformer no 1)
[total energy (hartree): -382.749486444]

C	-0.01494600	0.00010000	0.01671500
C	-0.00701900	0.00044700	1.41011200
C	1.21185400	-0.00012300	2.10000800
C	2.41329100	-0.00103700	1.38728700
C	2.40365600	-0.00138500	-0.01193200
C	1.19232600	-0.00081900	-0.70320900
H	-0.95252700	0.00116800	1.95689200
H	3.36487500	-0.00148800	1.91852800
O	1.19169300	-0.00116500	-2.07060200
H	0.27301800	-0.00068300	-2.37481400
H	3.33034500	-0.00210000	-0.58515000
O	-1.16122600	0.00061100	-0.75416500
H	-1.94116600	0.00126400	-0.18733000
H	1.21508000	0.00014900	3.18958200

b3lyp/aug-cc-pvdz: OH-C_6H_4-OH, *ortho* (conformer no 2)
[total energy (hartree): -382.743554958]

C	-0.00420400	0.00001100	-0.00725900
C	0.00286700	0.00051200	1.39281800
C	1.20559500	0.00006700	2.10233800
C	2.42565500	-0.00090400	1.39793600
C	2.41273500	-0.00139600	0.00161000
C	1.20378700	-0.00093900	-0.70467400
H	-0.93946400	0.00126300	1.94542800
H	-0.95288100	0.00037500	-0.54326000
H	1.21398800	-0.00133200	-1.79424700
O	1.27293300	0.00051400	3.47087600
H	0.37791100	0.00116900	3.83129900
O	3.57695300	-0.00131500	2.14084300
H	4.33702500	-0.00199900	1.54648000
H	3.36245400	-0.00215000	-0.53820800

b3lyp/aug-cc-pvdz: SH-C_6H_4-SH, *ortho* (conformer no 1)
[total energy (hartree): -1028.69326366]

C	0.00002300	-0.00125400	-0.00002100
C	-0.00000800	-0.00093000	1.40331200
C	1.23046000	0.00044600	2.09357300
C	2.42802400	0.00141500	1.36198900
C	2.41588200	0.00105900	-0.03247700
C	1.19638400	-0.00026200	-0.71659800
H	3.38075300	0.00249500	1.89185000
H	1.17321500	-0.00053700	-1.80623500
S	-1.52424900	-0.00228800	2.34712400
H	-2.35552600	-0.00257100	1.27740600
H	-0.94878000	-0.00233100	-0.53691000

S	1.21936600	0.00097200	3.88624400
H	2.56552500	0.00147000	4.03843800
H	3.35783100	0.00183900	-0.58073800

b3lyp/aug-cc-pvdz: SH-C_6H_4-SH, *ortho* (conformer no 2)
[total energy (hartree): -1028.69433115]

C	0.00006600	-0.00067900	-0.00042300
C	-0.00030700	-0.00044400	1.40229700
C	1.22740600	0.00028500	2.09690400
C	2.42695500	-0.02319800	1.36793100
C	2.41391200	-0.01792700	-0.02710600
C	1.19768300	0.00159200	-0.71626500
H	3.38028700	-0.03034200	1.89644500
H	1.17900600	0.00361900	-1.80593700
S	-1.59118900	0.07328100	2.23293700
H	-1.30341700	-0.80426800	3.22997000
H	-0.95368900	-0.01451200	-0.52786100
S	1.21370600	0.04134700	3.88750400
H	2.54588800	-0.15960200	4.04141100
H	3.35737400	-0.02799400	-0.57319800

b3lyp/aug-cc-pvdz: SH-C_6H_4-SH, *ortho* (conformer no 3)
[total energy (hartree): -1028.69464706]

C	0.00070800	0.00184500	0.00321600
C	0.00336900	0.00624300	1.40682800
C	1.23682000	0.00605000	2.09521000
C	2.43216800	-0.03380700	1.36015100
C	2.41585000	-0.05302200	-0.03490800
C	1.19602900	-0.02246500	-0.71628800
H	3.38229100	-0.02931400	1.89432800
H	1.17091600	-0.02998500	-1.80600600
S	-1.59150400	0.08431000	2.22604500
H	-1.29054300	-0.76076200	3.24687100
H	-0.95342300	-0.00258600	-0.52358700
S	1.37821300	-0.01521600	3.88306200
H	0.32862400	0.80986000	4.13627900
H	3.35611300	-0.07954200	-0.58577400

b3lyp/aug-cc-pvdz: tBu-C_6H_4-tBu, *ortho* (conformer no 1)
[total energy (hartree): -546.772418743]

C	-0.00317400	0.01219500	0.00125700
C	-0.00177000	-0.01215700	1.44644200
C	1.26465000	-0.03258000	2.07442800
C	2.48848600	0.01977900	1.41383100
C	2.48533400	0.10917900	0.03038100
C	1.25954600	0.09823400	-0.62852100
H	1.30352400	0.15632200	-1.70896600
H	1.31325900	-0.08925600	3.15475900
C	-1.20806500	0.00011800	-1.00816800
C	-2.31156200	-1.03016000	-0.67368800
C	-1.78701600	1.42990200	-1.15933000
C	-0.75906000	-0.41501400	-2.43935300
H	-1.89122200	-2.04502400	-0.65110400
H	-2.82473000	-0.85785200	0.26938300
H	-3.07536300	-1.00567100	-1.46270800
H	-1.00731900	2.10924900	-1.52912000
H	-2.60685300	1.42788400	-1.89268500
H	-2.16946600	1.84606900	-0.22574100
H	-1.65491500	-0.53449100	-3.06238500
H	-0.13471400	0.33925100	-2.93232300
H	-0.22030500	-1.37168100	-2.43989800

H	3.41176500	0.17577500	-0.54055000
C	-1.20371700	-0.06603600	2.45913600
C	-0.77594900	0.38738700	3.88548600
C	-2.37182800	0.88990600	2.12267500
C	-1.69199400	-1.52804800	2.62096900
H	-0.10641300	-0.32379000	4.38306100
H	-0.29436700	1.37408200	3.87555700
H	-1.67481300	0.45956500	4.51137300
H	-2.01456700	1.92785600	2.07853500
H	-2.88771100	0.67030200	1.19052700
H	-3.12228100	0.83296500	2.92279000
H	-2.51191800	-1.57196300	3.35294700
H	-2.04569700	-1.97452500	1.68966800
H	-0.87194300	-2.15447600	2.99678800
H	3.41790300	0.00086500	1.98348500

[1.3] b3lyp/aug-cc-pvdz: *meta*

b3lyp/aug-cc-pvdz: BF_2-C_6H_4-BF_2, *meta*
[total energy (hartree): -680.472682001]

C	-0.01789300	0.00004100	-0.03337100
C	0.00272300	0.00048500	1.37642300
C	1.20982800	-0.00012000	2.07850900
C	2.41674700	-0.00118400	1.37610600
C	2.43699500	-0.00165600	-0.03369400
C	1.20946100	-0.00102800	-0.71991100
H	3.35983400	-0.00166200	1.92374400
H	-0.94022000	0.00132000	1.92430900
H	1.20931400	-0.00137700	-1.81041300
H	1.20997200	0.00023400	3.16863400
B	-1.35871400	0.00072400	-0.80095100
B	3.77762000	-0.00283900	-0.80161700
F	4.95645400	-0.00344300	-0.16130100
F	3.83060800	-0.00331900	-2.14057000
F	-2.53738700	0.00174300	-0.16034000
F	-1.41203800	0.00033700	-2.13989100

b3lyp/aug-cc-pvdz: BH_2-C_6H_4-BH_2, *meta*
[total energy (hartree): -283.157528302]

C	-0.03074600	0.00004000	-0.03108400
C	0.00394000	0.00052300	1.38545300
C	1.20982600	-0.00005500	2.09001500
C	2.41553200	-0.00113700	1.38514300
C	2.44985300	-0.00166900	-0.03140300
C	1.20946700	-0.00105500	-0.70651500
H	3.35868500	-0.00159200	1.93491900
H	-0.93907100	0.00137500	1.93547000
H	1.20932600	-0.00144300	-1.79841500
H	1.20996700	0.00033500	3.18064900
B	-1.36404200	0.00069100	-0.80127900
H	-2.40701100	0.00163000	-0.20440700
H	-1.36592200	0.00026600	-2.00244300
B	3.78295000	-0.00286400	-0.80194100
H	3.78451900	-0.00328000	-2.00310600
H	4.82607400	-0.00338100	-0.20534000

b3lyp/aug-cc-pvdz: Br-C_6H_4-Br, *meta*
[total energy (hartree): -5379.38527544]

C	0.01446800	0.00004300	0.00693300
C	-0.01037500	0.00054700	1.40341100
C	1.21148800	0.00000000	2.08021400
C	2.43023300	-0.00101500	1.39972000

C	2.41775500	-0.00149500	0.00177400
C	1.21330300	-0.00097300	-0.70797500
H	3.36948700	-0.00142500	1.94904500
H	3.36197400	-0.00229200	-0.54345700
H	1.20721000	-0.00134400	-1.79588100
Br	1.20464800	0.00068500	3.99687400
Br	-1.64842100	0.00078400	-0.94633900
H	-0.95167100	0.00134300	1.94700800

b3lyp/aug-cc-pvdz: CHO-C_6H_4-CHO, *meta* (conformer no 1)
[total energy (hartree): -458.954796761]

C	0.00248000	0.00000000	-0.04174900
C	0.00823300	0.00000000	1.36397100
C	1.21364800	0.00000000	2.06896600
C	2.41906300	0.00000000	1.36397100
C	2.42481600	0.00000000	-0.04174900
C	1.21364800	0.00000000	-0.74498500
H	3.36791200	0.00000000	1.90387300
H	-0.94061600	0.00000000	1.90387300
H	1.21364800	0.00000000	-1.83437000
H	1.21364800	0.00000000	3.15872700
C	-1.29734200	0.00000000	-0.76483900
O	-1.41492000	0.00000100	-1.97307600
C	3.72463800	0.00000000	-0.76483900
O	3.84221600	-0.00000100	-1.97307600
H	-2.19862500	-0.00000100	-0.10654900
H	4.62592100	0.00000100	-0.10654900

b3lyp/aug-cc-pvdz: CHO-C_6H_4-CHO, *meta* (conformer no 2)
[total energy (hartree): -458.956326191]

C	-0.01612300	0.00000100	0.00782400
C	0.01064700	0.00000100	1.41707400
C	1.22803200	0.00000100	2.09328100
C	2.42621800	0.00000100	1.36766600
C	2.41015000	0.00000100	-0.03403800
C	1.18039600	0.00000100	-0.71226200
H	3.38307800	0.00000100	1.89325500
H	-0.93567500	0.00000100	1.95752200
H	1.17935200	0.00000000	-1.80333700
H	1.24972000	0.00000000	3.18300300
C	-1.31125000	0.00000000	-0.72187200
O	-2.40145500	-0.00000500	-0.18542800
C	3.69052500	0.00000000	-0.78594500
O	3.77700100	0.00000300	-1.99802400
H	-1.22335800	0.00000200	-1.83331100
H	4.60795000	-0.00000500	-0.15120800

b3lyp/aug-cc-pvdz: CHO-C_6H_4-CHO, *meta* (conformer no 3)
[total energy (hartree): -458.956177648]

C	-0.00212500	0.00000000	0.01322000
C	0.00342000	0.00000000	1.41870300
C	1.21364800	0.00000000	2.11588300
C	2.42387600	0.00000000	1.41870300
C	2.42942100	0.00000000	0.01322000
C	1.21364800	0.00000000	-0.68232500
H	3.37804500	0.00000000	1.94528500
H	-0.95074900	0.00000000	1.94528500
H	1.21364800	0.00000000	-1.77531700
H	1.21364800	0.00000000	3.20597300
C	-1.28150400	0.00000000	-0.74076500
O	-2.38339800	0.00000200	-0.22904700

C	3.70880000	0.00000000	-0.74076500
O	4.81069400	0.00000000	-0.22904700
H	-1.17148200	-0.00000200	-1.85110300
H	3.59877800	0.00000000	-1.85110300

b3lyp/aug-cc-pvdz: Cl-C_6H_4-Cl, *meta*
[total energy (hartree): -1151.51355205]

C	0.01517300	0.00004200	0.00722100
C	-0.00985500	0.00054000	1.40308800
C	1.21146200	0.00001300	2.07949500
C	2.43038400	-0.00101300	1.39948000
C	2.41755400	-0.00150200	0.00187300
C	1.21363700	-0.00096000	-0.70814800
H	3.36698800	-0.00142700	1.95327100
H	3.36167500	-0.00230100	-0.54322000
H	1.20246300	-0.00132700	-1.79607200
Cl	1.20447800	0.00059300	3.83996700
Cl	-1.51269800	0.00072400	-0.86735300
H	-0.95126700	0.00132600	1.94671600

b3lyp/aug-cc-pvdz: CN-C_6H_4-CN, *meta*
[total energy (hartree): -416.778494758]

C	-0.00110700	0.00003700	-0.01783000
C	-0.00094200	0.00053400	1.38889800
C	1.20997900	-0.00004500	2.08183200
C	2.42077000	-0.00111300	1.38867000
C	2.42067100	-0.00161100	-0.01805600
C	1.20971500	-0.00103700	-0.72592100
H	3.36736500	-0.00156900	1.92657300
H	-0.94743700	0.00137200	1.92697600
H	1.20961400	-0.00141900	-1.81379200
H	1.21008200	0.00033800	3.17127500
C	-1.24701900	0.00063900	-0.73521300
N	-2.25719600	0.00113200	-1.31062000
C	3.66644500	-0.00271700	-0.73567700
N	4.67651100	-0.00361600	-1.31128000

b3lyp/aug-cc-pvdz: COOH-C_6H_4-COOH, *meta* (conformer no 1)
[total energy (hartree): -609.491737615]

C	-0.00000200	-0.00014300	-0.00001400
C	0.00000300	-0.00009900	1.40476500
C	1.20924000	-0.00013400	2.10271200
C	2.42060700	-0.00021200	1.40846700
C	2.42489000	-0.00025600	0.00369700
C	1.21351500	-0.00022000	-0.69776800
H	3.36383300	-0.00023900	1.95071000
H	-0.94487200	-0.00003700	1.94412800
H	1.21519300	-0.00025100	-1.78573400
H	1.20757000	-0.00010000	3.19253000
C	-1.26470900	-0.00011000	-0.78959600
O	-1.32817000	-0.00014200	-2.00059800
O	-2.37780100	-0.00003800	-0.00680300
H	-3.13709200	-0.00002100	-0.61118700
C	3.69200000	-0.00034100	-0.78202800
O	3.75914200	-0.00037600	-1.99283200
O	4.80270100	-0.00037600	0.00415300
H	5.56383200	-0.00043100	-0.59791200

b3lyp/aug-cc-pvdz: COOH-C_6H_4-COOH, *meta* (conformer no 2)
[total energy (hartree): -609.492513744]

C	-0.00001100	0.00024400	-0.00001800

C	0.00001000	0.00022000	1.40390400
C	1.20716200	0.00044300	2.10414600
C	2.41761200	0.00067600	1.40961900
C	2.42424500	0.00070000	0.00571300
C	1.21378100	0.00049100	-0.70018600
H	3.36958000	0.00084100	1.93825300
H	-0.95443600	0.00002300	1.92805400
H	1.21635100	0.00051400	-1.78637100
H	1.20458200	0.00043500	3.19388300
C	-1.31508900	0.00000200	-0.70102600
O	-2.39475400	-0.00023000	-0.14628200
O	-1.19766200	0.00007200	-2.05492000
H	-2.10109900	-0.00009200	-2.40927500
C	3.74263800	0.00095900	-0.68905000
O	4.81965200	0.00114400	-0.12917200
O	3.63166900	0.00097600	-2.04348700
H	4.53679300	0.00115900	-2.39350800

b3lyp/aug-cc-pvdz: COOH-C_6H_4-COOH, *meta* (conformer no 3)
[total energy (hartree): -609.492331859]

C	0.00001100	-0.00011800	-0.00002500
C	0.00000500	-0.00005300	1.40481400
C	1.20634400	-0.00034500	2.10434300
C	2.41919000	-0.00069800	1.41038100
C	2.42446900	-0.00076100	0.00661400
C	1.21282200	-0.00047500	-0.69801300
H	3.36213100	-0.00092700	1.95319200
H	-0.95434800	0.00022900	1.92911200
H	1.23197700	-0.00054000	-1.78496600
H	1.20386700	-0.00029500	3.19411500
C	-1.31574900	0.00020200	-0.70105800
O	-2.39452900	0.00055700	-0.14419700
O	-1.19839700	0.00010500	-2.05366100
H	-2.10128200	0.00035500	-2.40945000
C	3.69063400	-0.00114000	-0.77945100
O	3.75612900	-0.00120600	-1.99098600
O	4.80231500	-0.00138200	0.00439800
H	5.56271300	-0.00160900	-0.59859400

b3lyp/aug-cc-pvdz: F-C_6H_4-F, *meta*
[total energy (hartree): -430.775462120]

C	0.02679200	0.00004200	0.01376300
C	-0.01279500	0.00052400	1.40484800
C	1.21162600	-0.00005500	2.06624700
C	2.43268000	-0.00104400	1.39933700
C	2.41922900	-0.00148500	0.00085200
C	1.21490000	-0.00095800	-0.71022500
H	3.36193100	-0.00145400	1.96588200
H	3.36310500	-0.00226700	-0.54401700
H	1.18915500	-0.00129700	-1.79824400
F	1.20575900	0.00041200	3.42456500
F	-1.15252300	0.00057600	-0.66025200
H	-0.95481300	0.00131200	1.94854600

b3lyp/aug-cc-pvdz: Li-C_6H_4-Li, *meta*
[total energy (hartree): -246.053438115]

C	-0.05054200	0.00005000	-0.04373800
C	0.03052400	0.00050400	1.37708900
C	1.22021700	0.00003200	2.15813400
C	2.41750500	-0.00098600	1.39927800
C	2.42030000	-0.00149600	-0.00213400

C	1.20547700	-0.00099000	-0.70084600
H	3.39138700	-0.00141700	1.90576400
H	3.36898600	-0.00229800	-0.54969700
H	1.25404300	-0.00141700	-1.79746500
Li	1.17892900	0.00075300	4.11755900
Li	-1.76868000	0.00090900	-0.98644200
H	-0.92597900	0.00129600	1.92922200

b3lyp/aug-cc-pvdz: $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *meta* (conformer no 1)
[total energy (hartree): -500.235451247]

C	-0.00002300	0.00013800	-0.00024400
C	0.00008100	0.00005900	1.41429600
C	1.24137400	0.00050400	2.08739100
C	2.44253500	0.04426700	-0.02324400
C	1.21482200	0.02914500	-0.68279500
H	-0.92592400	-0.01542500	-0.56689800
H	1.25193600	-0.01039700	3.16960300
H	1.20434100	0.04030700	-1.77383600
N	-1.19492300	0.02126600	2.13331300
C	-1.16979300	-0.23615700	3.56242700
H	-0.58141100	0.52791300	4.09049000
C	-2.44350600	-0.22327600	1.43105800
H	-3.27370100	-0.13444000	2.13929500
H	-2.60120700	0.52476000	0.64219000
H	-2.19206400	-0.18961500	3.95130800
H	-2.48759200	-1.22611600	0.96630600
H	-0.74769400	-1.22772500	3.81252900
C	2.46947800	0.01499500	1.39075300
N	3.67810700	-0.02121300	2.08594300
C	3.68075600	0.20526100	3.52059800
C	4.91289700	0.23874800	1.36508200
H	4.71024900	0.14886400	3.88853800
H	3.26521000	1.19169900	3.80024000
H	3.10129700	-0.56933600	4.04314700
H	5.75661800	0.13526700	2.05509000
H	5.05538700	-0.49229300	0.55762100
H	4.94796200	1.25125400	0.92100000
H	3.35747500	0.07154900	-0.60698100

b3lyp/aug-cc-pvdz: $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *meta* (conformer no 2)
[total energy (hartree): -500.235486579]

C	0.00020600	0.00673700	0.00036200
C	0.00001300	0.00274600	1.41490900
C	1.24129100	0.00085500	2.08822400
C	2.44288000	-0.03209300	-0.02240300
C	1.21532900	-0.01048000	-0.68204900
H	-0.92541600	0.03188500	-0.56639700
H	1.25193900	0.02657200	3.17014900
H	1.20532000	0.00016600	-1.77309600
N	-1.19528700	-0.01268700	2.13332900
C	-2.44223800	0.24380700	1.43248900
H	-2.60480700	-0.49864000	0.63935800
C	-1.16950200	0.23299700	3.56425300
H	-2.19116200	0.17910900	3.95386500
H	-0.57750900	-0.53369300	4.08439200
H	-3.27298200	0.15625300	2.14026200
H	-0.75077800	1.22378500	3.82317400
H	-2.47994300	1.24957000	0.97357000
C	2.46918000	-0.03681900	1.39190100
N	3.67668000	-0.09157100	2.08771500
C	3.68584900	0.15422500	3.51895300

C	4.91748200	0.12738300	1.36356100
H	3.30719500	1.15904200	3.78545500
H	3.07682800	-0.59141800	4.04980100
H	4.71197200	0.06385400	3.88963700
H	5.75834000	0.01352700	2.05544700
H	5.04216200	-0.61875900	0.56705600
H	4.97730400	1.13204700	0.90458400
H	3.35819800	-0.03653900	-0.60615100

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *meta* (conformer no 1)
[total energy (hartree): -343.012998409]

C	0.00000200	0.00004100	0.00002900
C	-0.00000300	-0.00010300	1.40711900
C	1.22244300	-0.00010000	2.09664300
C	2.43560500	-0.00458400	-0.00536300
C	1.21629300	-0.00227600	-0.68414800
H	-0.94334700	-0.00506900	-0.54704600
H	1.22483200	-0.01613300	3.18886900
H	1.21387600	-0.00053400	-1.77520400
N	-1.20700200	-0.06250100	2.11538700
H	-1.17512100	0.28762100	3.06405100
H	-2.01836400	0.27519300	1.61424500
C	2.44181700	-0.00474600	1.40171200
N	3.65168700	-0.07175200	2.10465000
H	3.62531500	0.27848400	3.05343800
H	4.46211700	0.26283600	1.59993100
H	3.37649500	-0.01330100	-0.55660900

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *meta* (conformer no 2)
[total energy (hartree): -343.013124827]

C	0.00008000	0.00004800	0.00007800
C	-0.00001100	0.00006300	1.40712300
C	1.22230300	-0.00008100	2.09664300
C	2.43562400	-0.00026100	-0.00510200
C	1.21640100	-0.00012000	-0.68409000
H	-0.94320600	0.00670500	-0.54711500
H	1.22463300	-0.00008400	3.18897300
H	1.21407100	-0.00013600	-1.77514200
N	-1.20688700	0.06462800	2.11620900
H	-2.01857100	-0.26821400	1.61215100
H	-1.17578200	-0.29694300	3.06077800
C	2.44166900	-0.00023600	1.40193000
N	3.65155000	-0.06475200	2.10589600
H	3.62443500	0.29687300	3.05056500
H	4.46107800	0.26808300	1.59838100
H	3.37657900	-0.00693100	-0.55629300

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *meta* (conformer no 3)
[total energy (hartree): -342.994530368]

C	0.00002700	0.00000000	0.00004600
C	-0.00003700	0.00000000	1.40356500
C	1.22280800	0.00000000	2.08354800
C	2.42602900	0.00000000	-0.01288500
C	1.20821800	0.00000000	-0.70114500
H	-0.94877100	0.00000000	-0.53896800
H	1.21197400	0.00000000	3.17403100
H	1.20226900	0.00000000	-1.79187900
N	-1.21401700	0.00000000	2.18780900
H	-1.78400300	0.81559900	1.97185000
H	-1.78400300	-0.81559900	1.97185000
C	2.44094800	0.00000000	1.38600000

N	3.72034600	0.00000000	2.05785600
H	3.81063400	-0.81515900	2.66133700
H	3.81063400	0.81515900	2.66133700
H	3.37496800	0.00000000	-0.54797000

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *meta* (conformer no 4)
[total energy (hartree): -342.994083520]

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40260200
C	1.22252500	0.00000000	2.08551100
C	2.42427200	0.00000000	-0.01204200
C	1.20867800	0.00000000	-0.70222900
H	-0.94828600	0.00000000	-0.53985100
H	1.22793300	0.00000000	3.17423300
H	1.20325900	0.00000000	-1.79304500
N	-1.21510300	0.00000000	2.18456300
H	-1.78469900	0.81590900	1.96914300
H	-1.78469900	-0.81590900	1.96914300
C	2.43820600	0.00000000	1.39049100
N	3.66101700	0.00000000	2.16034200
H	4.22844500	0.81590900	1.93927400
H	4.22844500	-0.81590900	1.93927400
H	3.36714900	0.00000000	-0.56128700

b3lyp/aug-cc-pvdz: OCH_3-C_6H_4-OCH_3, *meta* (conformer no 1)
[total energy (hartree): -461.351048189]

C	0.00006800	0.00007700	0.00013300
C	0.00005800	0.00030000	1.39724900
C	1.23446200	0.00053100	2.06903600
C	2.43218100	0.00053800	1.34776000
C	2.40871800	0.00031100	-0.05019300
C	1.18464400	0.00007700	-0.74071200
H	-0.94290900	0.00029300	1.93683800
H	-0.95389200	-0.00010500	-0.52846100
O	1.37009100	0.00076300	3.43081000
C	0.18867900	0.00077200	4.22373700
H	-0.41849300	-0.89854300	4.03744500
H	0.52896900	0.00096500	5.26391900
H	-0.41866500	0.89991400	4.03716900
H	1.14186600	-0.00010000	-1.82627300
H	3.38421600	0.00072100	1.87538000
O	3.63532700	0.00033900	-0.65672000
C	3.68235400	0.00012600	-2.07882900
H	4.74494300	0.00019900	-2.34090700
H	3.20293400	-0.89913500	-2.49562300
H	3.20274100	0.89915600	-2.49589800

b3lyp/aug-cc-pvdz: OCH_3-C_6H_4-OCH_3, *meta* (conformer no 2)
[total energy (hartree): -461.350487335]

C	0.00006800	0.00007700	0.00013300
C	0.00005800	0.00030000	1.39724900
C	1.23446200	0.00053100	2.06903600
C	2.43218100	0.00053800	1.34776000
C	2.40871800	0.00031100	-0.05019300
C	1.18464400	0.00007700	-0.74071200
H	-0.94290900	0.00029300	1.93683800
H	-0.95389200	-0.00010500	-0.52846100
O	1.37009100	0.00076300	3.43081000
C	0.18867900	0.00077200	4.22373700
H	-0.41849300	-0.89854300	4.03744500
H	0.52896900	0.00096500	5.26391900

H	-0.41866500	0.89991400	4.03716900
H	1.14186600	-0.00010000	-1.82627300
H	3.38421600	0.00072100	1.87538000
O	3.63532700	0.00033900	-0.65672000
C	3.68235400	0.00012600	-2.07882900
H	4.74494300	0.00019900	-2.34090700
H	3.20293400	-0.89913500	-2.49562300
H	3.20274100	0.89915600	-2.49589800

b3lyp/aug-cc-pvdz: OCH_3-C_6H_4-OCH_3, *meta* (conformer no 3)
[total energy (hartree): -461.349985460]

C	0.04692400	-0.00347300	0.02658500
C	0.02973500	0.01262400	1.42171000
C	1.24555500	0.01398700	2.11676100
C	2.46811100	-0.00053300	1.42523500
C	2.45652900	-0.01663600	0.02073800
C	1.24694500	-0.01814200	-0.68523000
H	-0.90299900	0.02413000	1.98274000
H	-0.89744800	-0.00459300	-0.51901600
O	1.15112000	0.03012700	3.48288500
C	2.34947300	0.03163100	4.24768000
H	2.95776300	0.92565800	4.03876900
H	2.03364900	0.04509200	5.29550500
H	2.94721400	-0.87384800	4.05865500
H	1.26698200	-0.03066800	-1.77349000
H	3.40651700	0.00059700	1.96804300
O	3.59245000	-0.03171300	-0.74390000
C	4.85381600	-0.03082700	-0.08842300
H	5.60347700	-0.04470500	-0.88570800
H	4.98807800	0.87572500	0.52239400
H	4.97796700	-0.92371700	0.54425200

b3lyp/aug-cc-pvdz: OH-C_6H_4-OH, *meta* (conformer no 1)
[total energy (hartree): -382.749670437]

C	0.00511900	0.00003500	0.01378900
C	0.00124700	0.00057700	1.40796200
C	1.22739000	0.00003400	2.08657800
C	2.43604100	-0.00103100	1.38420400
C	2.41515700	-0.00156000	-0.01479500
C	1.20166400	-0.00103000	-0.71180400
H	-0.92634900	0.00141400	1.97741800
H	-0.94388800	0.00045700	-0.52342100
H	1.19055300	-0.00144000	-1.80286400
O	1.18464900	0.00059100	3.45705700
H	2.08281900	0.00013500	3.80999400
O	3.63250800	-0.00259800	-0.64793600
H	3.49712100	-0.00285600	-1.60336500
H	3.39581400	-0.00146400	1.90254200

b3lyp/aug-cc-pvdz: OH-C_6H_4-OH, *meta* (conformer no 2)
[total energy (hartree): -382.748554064]

C	0.02573200	0.00004200	0.01495200
C	0.00593100	0.00058900	1.41147000
C	1.22177200	0.00003500	2.10251100
C	2.43854000	-0.00104400	1.40814400
C	2.43157600	-0.00157800	0.00729400
C	1.22530400	-0.00103600	-0.70035500
H	-0.92758300	0.00143300	1.97118400
H	-0.91867500	0.00047200	-0.53041000
H	1.24347700	-0.00146300	-1.78864800
O	1.16742900	0.00059600	3.47354000

H	2.06102000	0.00011600	3.83721100
O	3.59165200	-0.00265000	-0.72542800
H	4.35374200	-0.00296000	-0.13381800
H	3.38526200	-0.00147500	1.95487600

b3lyp/aug-cc-pvdz: OH-C_6H_4-OH, *meta* (conformer no 3)
[total energy (hartree): -382.749622315]

C	-0.00637500	0.00005500	-0.00349800
C	-0.02008000	0.00055800	1.39305400
C	1.20032900	0.00000100	2.08383400
C	2.41515100	-0.00104300	1.39456900
C	2.40457800	-0.00153000	-0.00211600
C	1.19619700	-0.00098500	-0.71373600
H	-0.96477800	0.00138000	1.93901900
H	-0.95073900	0.00048900	-0.54869400
H	1.19663400	-0.00136600	-1.80485000
O	1.26751100	0.00044000	3.45362700
H	0.37450300	0.00116200	3.81912000
O	3.62450500	-0.00255000	-0.62869300
H	3.49492100	-0.00277600	-1.58488100
H	3.35761700	-0.00147400	1.93873800

b3lyp/aug-cc-pvdz: SH-C_6H_4-SH, *meta* (conformer no 1)
[total energy (hartree): -1028.69564091]

C	-0.00362400	0.00008400	-0.02211100
C	-0.00575500	0.00053700	1.38056200
C	1.21005000	-0.00006400	2.06691300
C	2.42566800	-0.00109400	1.38022600
C	2.42315000	-0.00154100	-0.02244300
C	1.20966500	-0.00095900	-0.72355100
H	3.36659800	-0.00155000	1.92975000
H	-0.94653500	0.00135500	1.93034100
H	1.20951700	-0.00131600	-1.81315400
H	1.21020300	0.00028500	3.15744100
S	4.01059900	-0.00288600	-0.85138500
H	3.53808600	-0.00297100	-2.12137100
S	-1.59130400	0.00087300	-0.85061100
H	-1.11915300	0.00028000	-2.12073100

b3lyp/aug-cc-pvdz: SH-C_6H_4-SH, *meta* (conformer no 2)
[total energy (hartree): -1028.69577493]

C	-0.00743100	-0.00002600	-0.01509900
C	-0.01231800	0.00046000	1.38653400
C	1.20371300	-0.00006600	2.07426200
C	2.42014300	-0.00105500	1.38999400
C	2.42009400	-0.00153200	-0.01325100
C	1.20790300	-0.00102200	-0.71470700
H	3.35995400	-0.00145500	1.94142100
H	-0.95104200	0.00123900	1.93909900
H	1.20392100	-0.00139400	-1.80470300
H	1.20203700	0.00030700	3.16487300
S	4.00820200	-0.00282000	-0.83990700
H	3.53658200	-0.00296000	-2.11021900
S	-1.51035700	0.00057700	-0.98962900
H	-2.37899200	0.00147800	0.05010600

b3lyp/aug-cc-pvdz: SH-C_6H_4-SH, *meta* (conformer no 3)
[total energy (hartree): -1028.69575610]

C	-0.00433700	-0.00003200	-0.00670600
C	-0.00681000	0.00047100	1.39553500
C	1.20991600	-0.00011500	2.08100900

C	2.42658000	-0.00118900	1.39541700
C	2.42397300	-0.00167900	-0.00681900
C	1.20978300	-0.00110000	-0.70662600
H	3.36428000	-0.00164600	1.94969400
H	-0.94445800	0.00131000	1.94989700
H	1.20973300	-0.00147300	-1.79710000
H	1.20997100	0.00026900	3.17170200
S	3.92837600	-0.00307500	-0.97815000
H	4.79485800	-0.00309800	0.06349200
S	-1.50883900	0.00065000	-0.97788600
H	-2.37521700	0.00163600	0.06384400

b3lyp/aug-cc-pvdz: tBu-C_6H_4-tBu, *meta* (conformer no 1)
[total energy (hartree): -546.810551228]

C	-0.00002800	-0.00245000	0.00003900
C	0.00021600	-0.00146200	1.40351300
C	1.20048400	0.00003400	2.11533400
C	2.42288000	0.00057700	1.44228000
C	2.46769600	-0.00036700	0.03951200
C	1.24458300	-0.00186900	-0.65230800
H	3.34400700	0.00174700	2.02423600
H	-0.93879100	-0.00187800	1.95605900
H	1.26191300	-0.00261000	-1.73666700
H	1.18298500	0.00078100	3.20625700
C	-1.33680700	-0.00411400	-0.76583500
C	-2.14492200	-1.26620600	-0.38489400
C	-2.14696200	1.25723400	-0.38678800
C	-1.13893400	-0.00510200	-2.29253800
H	-1.59089600	-2.17835300	-0.64539800
H	-2.36265400	-1.30037800	0.69002500
H	-3.10355200	-1.28189600	-0.92306500
H	-1.59449300	2.16988200	-0.64884800
H	-3.10570800	1.27048400	-0.92482600
H	-2.36456500	1.29276600	0.68811400
H	-2.11829400	-0.00629500	-2.78999400
H	-0.59472900	0.88552900	-2.63468100
H	-0.59322500	-0.89532600	-2.63334400
C	3.82842900	0.00023500	-0.68283800
C	4.62590600	-1.26060200	-0.27606300
C	3.67994500	-0.00085600	-2.21499500
C	4.62397300	1.26281200	-0.27766800
H	4.80783900	-1.29509100	0.80546400
H	4.08274500	-2.17372900	-0.55541700
H	5.60192500	-1.27404800	-0.78206000
H	3.14532700	0.88889400	-2.57412300
H	4.67457500	-0.00038300	-2.68122900
H	3.14671800	-0.89189500	-2.57298900
H	5.59988100	1.27719900	-0.78384700
H	4.07932200	2.17475100	-0.55799700
H	4.80604500	1.29885600	0.80378600

b3lyp/aug-cc-pvdz: tBu-C_6H_4-tBu, *meta* (conformer no 2)
[total energy (hartree): -546.810805083]

C	0.00000000	-0.00015200	-0.00000100
C	0.00000100	0.00000700	1.40334200
C	1.20392500	0.00000700	2.11114300
C	2.42898300	-0.00014800	1.44058400
C	2.47160200	-0.00031400	0.03792100
C	1.24600400	-0.00031600	-0.64757600
H	3.34503900	-0.00013800	2.02649600
H	-0.93345300	0.00013400	1.96111900

H	1.26295600	-0.00045000	-1.73627600
H	1.18717200	0.00012900	3.20185500
C	-1.29426000	-0.00016500	-0.83442800
C	-1.33202500	1.26149300	-1.72769000
C	-1.33222300	-1.26206600	-1.72733900
C	-2.55517900	0.00005900	0.04900300
H	-1.30465500	2.17401400	-1.11683000
H	-0.48170100	1.29484200	-2.42044700
H	-2.25398300	1.27751500	-2.32651400
H	-1.30503900	-2.17442200	-1.11622700
H	-2.25416300	-1.27808700	-2.32619100
H	-0.48187700	-1.29575600	-2.42005300
H	-3.45069800	0.00002700	-0.58697300
H	-2.60391200	-0.88996200	0.69085800
H	-2.60378300	0.89027700	0.69059400
C	3.79054100	-0.00047700	-0.75699900
C	3.85540700	-1.26237400	-1.64826800
C	3.85556000	1.26123800	-1.64851500
C	5.02401800	-0.00046100	0.16443400
H	3.81113300	-2.17472800	-1.03811900
H	3.02538800	-1.29656100	-2.36513600
H	4.79438400	-1.27782000	-2.22002700
H	3.81137900	2.17371700	-1.03854500
H	4.79454600	1.27646900	-2.22026500
H	3.02555500	1.29537900	-2.36540100
H	5.93855900	-0.00057800	-0.44392300
H	5.05313300	0.88971600	0.80725900
H	5.05302400	-0.89051600	0.80743200

[1.4] b3lyp/aug-cc-pvdz: *para*

b3lyp/aug-cc-pvdz: BF_2-C_6H_4-BF_2, *para*
[total energy (hartree): -680.471551483]

C	-0.01676100	0.00005300	-0.01137400
C	-0.00237100	0.00048600	1.39762600
C	1.20399900	0.00003700	2.09650400
C	2.43269200	-0.00085800	1.40679400
C	2.41830200	-0.00129200	-0.00220300
C	1.21192900	-0.00084300	-0.70108300
H	-0.94574800	0.00118400	1.94389300
H	1.21711100	-0.00118300	-1.79125800
H	1.19882000	0.00037800	3.18668000
B	-1.35840700	0.00055800	-0.78411300
F	-2.53850500	0.00140600	-0.14892200
F	-1.40472100	0.00017300	-2.12320900
H	3.36167700	-0.00199000	-0.54847400
B	3.77433600	-0.00136300	2.17953800
F	3.82064500	-0.00097700	3.51863500
F	4.95443700	-0.00221000	1.54435300

b3lyp/aug-cc-pvdz: BH_2-C_6H_4-BH_2, *para*
[total energy (hartree): -283.155347015]

C	-0.02894400	0.00005100	-0.01660500
C	-0.00139500	0.00048500	1.39878500
C	1.20519700	0.00003600	2.09565300
C	2.44488000	-0.00086800	1.41201500
C	2.41733100	-0.00130200	-0.00337500
C	1.21073900	-0.00085400	-0.70024300
H	-0.94509700	0.00118500	1.94669000
H	1.21358200	-0.00119800	-1.79145500
H	1.20235400	0.00038000	3.18686500

B	-1.36740800	0.00055200	-0.78946300
H	-2.40885500	0.00133100	-0.19103400
H	-1.36974200	0.00016700	-1.99057200
B	3.78334400	-0.00137000	2.18487400
H	4.82479200	-0.00216100	1.58644600
H	3.78567800	-0.00097200	3.38598200
H	3.36103400	-0.00200200	-0.55128000

b3lyp/aug-cc-pvdz: Br-C_6H_4-Br, *para*
[total energy (hartree): -5379.38531018]

C	-0.00364500	0.00008300	-0.00175100
C	-0.00371700	0.00053200	1.39684300
C	1.21223100	-0.00001800	2.08230800
C	2.42826200	-0.00101600	1.39696200
C	2.42833400	-0.00147100	-0.00162300
C	1.21237100	-0.00091200	-0.68709300
H	3.37062900	-0.00144600	1.94186000
H	3.37075500	-0.00225300	-0.54642700
Br	1.21216600	0.00060000	3.99841800
H	-0.94614600	0.00131000	1.94163500
Br	1.21249900	-0.00154300	-2.60320300
H	-0.94602000	0.00051000	-0.54663900

b3lyp/aug-cc-pvdz: CHO-C_6H_4-CHO, *para* (conformer no 1)
[total energy (hartree): -458.955687044]

C	-0.00674000	0.00000000	0.01767800
C	0.01743800	0.00000000	1.42326000
C	1.24428300	0.00000000	2.10714100
C	2.43354600	0.00000000	1.38349100
C	2.40936800	0.00000000	-0.02209100
C	1.18252300	0.00000000	-0.70597100
H	3.39273400	0.00000000	1.90416400
H	1.18566500	0.00000000	-1.79523200
H	1.24114100	0.00000000	3.19640100
C	3.69220000	0.00000000	-0.77418500
O	3.77862300	0.00000000	-1.98596400
H	4.60919100	0.00000100	-0.13925400
C	-1.26539400	0.00000000	2.17535400
H	-2.18238500	0.00000100	1.54042300
O	-1.35181800	0.00000100	3.38713400
H	-0.96592800	0.00000000	-0.50299500

b3lyp/aug-cc-pvdz: CHO-C_6H_4-CHO, *para* (conformer no 2)
[total energy (hartree): -458.955561097]

C	-0.01102900	0.00000000	0.02767900
C	-0.01227300	0.00000100	1.43638300
C	1.19046300	0.00000100	2.13036900
C	2.40946700	0.00000100	1.42429300
C	2.41088900	0.00000000	0.02252600
C	1.20188600	0.00000000	-0.67509200
H	-0.96780100	0.00000100	1.95964600
H	1.19470400	-0.00000100	-1.76625000
H	1.21590800	0.00000200	3.21947400
C	-1.29046500	0.00000100	-0.72974400
O	-2.39247200	-0.00000400	-0.21888400
H	-1.17886800	0.00000100	-1.83970700
C	3.70524900	0.00000200	2.15347300
H	4.61075200	0.00000100	1.50191800
O	3.81359300	-0.00000500	3.36330100
H	3.35913000	0.00000000	-0.51742900

b3lyp/aug-cc-pvdz: Cl-C_6H_4-Cl, *para*
[total energy (hartree): -1151.51352635]

C	0.01185100	0.00002600	0.00448600
C	-0.00316900	0.00049400	1.40012400
C	1.20719400	-0.00000600	2.09895400
C	2.40842400	-0.00099300	1.38829600
C	2.42345500	-0.00146400	-0.00733900
C	1.21307600	-0.00093800	-0.70616200
H	3.36919800	-0.00222400	-0.54619700
H	1.20672100	-0.00128800	-1.79455700
Cl	-1.51278000	0.00068500	-0.87619600
H	-0.94892500	0.00125800	1.93896700
Cl	3.93305700	-0.00162900	2.26897500
H	1.21357100	0.00035500	3.18734400

b3lyp/aug-cc-pvdz: CN-C_6H_4-CN, *para*
[total energy (hartree): -416.779161964]

C	-0.00144400	0.00015000	-0.00999800
C	0.00065100	0.00067100	1.39661600
C	1.21770600	0.00004300	2.10185900
C	2.42267700	-0.00109100	1.40617900
C	2.42058300	-0.00161100	-0.00043000
C	1.20352300	-0.00098600	-0.70567700
H	3.36804200	-0.00158500	1.94574800
H	1.20904100	-0.00139100	-1.79416000
H	1.21219500	0.00044800	3.19034300
C	3.66496100	-0.00279100	-0.71884000
N	4.67203600	-0.00375200	-1.30015500
C	-1.24373300	0.00184900	2.11501300
N	-2.25081900	0.00280800	2.69630700
H	-0.94681300	0.00064300	-0.54956200

b3lyp/aug-cc-pvdz: COOH-C_6H_4-COOH, *para* (conformer no 1)
[total energy (hartree): -609.491972633]

C	0.00000500	0.00011900	-0.00001200
C	0.00000400	0.00018000	1.40339500
C	1.20775600	0.00008000	2.10073900
C	2.42300000	-0.00008800	1.39872100
C	2.42159700	-0.00015000	-0.00548600
C	1.21667000	-0.00005100	-0.70117900
H	-0.94312800	0.00030600	1.94502600
H	1.19806200	-0.00010000	-1.78945200
H	1.21017900	0.00012900	3.18834500
C	-1.26552900	0.00022800	-0.78970600
O	-1.32505300	0.00017800	-2.00157500
O	-2.37933100	0.00039400	-0.01047200
H	-3.13816300	0.00045200	-0.61554000
C	3.74003300	-0.00020900	2.09915400
O	4.81895100	-0.00038900	1.54404200
O	3.62295300	-0.00009400	3.45335700
H	4.52656900	-0.00019100	3.80747700
H	3.37339800	-0.00027800	-0.53347000

b3lyp/aug-cc-pvdz: COOH-C_6H_4-COOH, *para* (conformer no 2)
[total energy (hartree): -609.492030850]

C	0.00001600	0.00000200	-0.00001200
C	-0.00001500	-0.00000500	1.40320000
C	1.20468400	-0.00000600	2.10248900
C	2.42151300	-0.00000200	1.40122500
C	2.42154400	0.00000300	-0.00198600
C	1.21684500	0.00000300	-0.70127500

H	-0.95248300	-0.00000700	1.93004100
H	1.21567300	0.00000800	-1.78886500
H	1.20585700	-0.00000900	3.19007800
C	-1.31687300	0.00000400	-0.70081300
O	-2.39604900	0.00000200	-0.14588000
O	-1.19917200	0.00000600	-2.05463300
H	-2.10245900	0.00000600	-2.40958800
C	3.73840200	-0.00000400	2.10202600
O	4.81757800	-0.00000300	1.54709300
O	3.62070100	-0.00000900	3.45584700
H	4.52398800	-0.00001000	3.81080100
H	3.37401200	0.00000600	-0.52882800

b3lyp/aug-cc-pvdz: F-C_6H_4-F, *para*
[total energy (hartree): -430.774470402]

C	-0.00737200	0.00006200	-0.00173000
C	-0.00744100	0.00051400	1.39682300
C	1.21222800	-0.00005400	2.06572100
C	2.43196900	-0.00104400	1.39694300
C	2.43203900	-0.00149000	-0.00160500
C	1.21236400	-0.00093300	-0.67050600
H	3.36240900	-0.00145700	1.96252300
H	3.36253500	-0.00226400	-0.56709200
F	1.21216500	0.00039000	3.42711000
H	-0.93793700	0.00129600	1.96230500
F	1.21243800	-0.00135600	-2.03189500
H	-0.93781200	0.00048000	-0.56730500

b3lyp/aug-cc-pvdz: Li-C_6H_4-Li, *para*
[total energy (hartree): -246.054843999]

C	0.02713900	0.00006100	-0.00501900
C	0.02706800	0.00051400	1.40011200
C	1.21223500	0.00001100	2.17943100
C	2.39748300	-0.00099600	1.40023300
C	2.39755400	-0.00144900	-0.00489600
C	1.21238600	-0.00094300	-0.78421600
H	3.37715500	-0.00146600	1.89967600
H	3.37727800	-0.00224200	-0.50423900
Li	1.21214500	0.00066000	4.13610100
H	-0.95265700	0.00130300	1.89945500
H	-0.95253400	0.00052700	-0.50446200
Li	1.21249000	-0.00156700	-2.74088600

b3lyp/aug-cc-pvdz: N(CH_3)$_2$-C_6H_4-N(CH_3)$_2$, *para* (conformer no 1)
[total energy (hartree): -500.232057641]

C	0.00007300	0.00081200	-0.00026800
C	-0.00015600	0.00025000	1.40997800
C	1.26556700	-0.00051800	2.03193700
C	2.45024200	0.01811500	-0.11581100
C	1.18451900	0.01888200	-0.73777100
H	-0.93539000	-0.00630200	-0.55402800
H	1.34991100	-0.00703800	3.11574100
H	1.10017600	0.02540100	-1.82157400
N	-1.19250700	0.04206500	2.15307300
C	-1.12836200	-0.31292000	3.56092200
H	-0.47055800	0.37603600	4.10678400
C	-2.43081400	-0.29389800	1.47037800
H	-3.26301000	-0.19817300	2.17621000
H	-2.62095500	0.40368000	0.64420600
H	-2.12919500	-0.22170200	3.99678600
H	-2.43664100	-1.32300000	1.05991800

H	-0.76445800	-1.34507200	3.73300800
C	2.45001400	0.01755300	1.29443400
N	3.64259300	-0.02370100	-0.85890800
C	4.88090100	0.31226000	-0.17621300
C	3.57844700	0.33128200	-2.26675600
H	5.71309600	0.21653300	-0.88204500
H	4.88672900	1.34136300	0.23424600
H	5.07104200	-0.38531800	0.64996000
H	4.57928000	0.24006200	-2.70262100
H	2.92064200	-0.35767400	-2.81261700
H	3.21454400	1.36343400	-2.43884300
H	3.38547600	0.02466600	1.84819500

b3lyp/aug-cc-pvdz: $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 2)
[total energy (hartree): -500.232061019]

C	-0.00014900	0.00709900	0.00141100
C	0.00095300	0.00139200	1.41174900
C	1.26744700	-0.00280500	2.03219300
C	2.44861600	-0.07468700	-0.11646700
C	1.18312200	-0.02959400	-0.73735500
H	-0.93542800	0.04464400	-0.55138400
H	1.35351400	0.02533900	3.11550600
H	1.09803700	-0.01966400	-1.82106800
N	-1.19061500	-0.02457900	2.15630300
C	-2.42847300	0.31034300	1.47294300
H	-2.61923000	-0.39047600	0.64960100
C	-1.12332000	0.33736200	3.56206200
H	-2.12401600	0.25254300	3.99958200
H	-0.46762500	-0.35145800	4.11064900
H	-3.26049000	0.21831700	2.17951300
H	-0.75524300	1.36898100	3.72866100
H	-2.43395600	1.33789800	1.05839000
C	2.45072400	-0.03956900	1.29342600
N	3.63713800	-0.17523100	-0.85949100
C	3.58784400	0.16161300	-2.27229300
C	4.89027700	0.11105600	-0.18186200
H	4.58270000	0.01694500	-2.70742200
H	2.89759400	-0.50359100	-2.80743600
H	3.27275100	1.20714400	-2.45938100
H	5.71657500	-0.03593900	-0.88581200
H	4.94671500	1.14488300	0.21281200
H	5.04596200	-0.58227100	0.65510000
H	3.38703400	-0.03679900	1.84572700

b3lyp/aug-cc-pvdz: $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 3)
[total energy (hartree): -500.232056213]

C	-0.00011400	0.00667500	0.00071200
C	0.00011200	0.00010800	1.41094000
C	1.26603400	-0.00640700	2.03246200
C	2.44995700	-0.01805900	-0.11574200
C	1.18403500	-0.01154400	-0.73726400
H	-0.93572000	0.01965500	-0.55269800
H	1.35074400	-0.00557300	3.11625600
H	1.09932500	-0.01237800	-1.82105800
N	-1.19211700	-0.04151600	2.15425000
C	-2.42954400	0.30205900	1.47376000
H	-2.62225000	-0.39052800	0.64399200
C	-1.12624500	0.30621800	3.56383600
H	-2.12727700	0.21650900	3.99955200
H	-0.47079500	-0.38783800	4.10606300
H	-3.26182600	0.20532500	2.17935500

H	-0.75849800	1.33615900	3.74091900
H	-2.43216000	1.33332600	1.06873200
C	2.45018200	-0.02462600	1.29448600
N	3.64218500	0.02356500	-0.85905200
C	3.57631300	-0.32416700	-2.26863900
C	4.87961200	-0.32001300	-0.17856300
H	4.57734500	-0.23445800	-2.70435500
H	3.20856500	-1.35410800	-2.44572300
H	2.92086300	0.36989000	-2.81086400
H	5.71189500	-0.22328100	-0.88415800
H	5.07232000	0.37257300	0.65120500
H	4.88222700	-1.35128000	0.22646400
H	3.38578800	-0.03760600	1.84789600

b3lyp/aug-cc-pvdz: $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 4)
[total energy (hartree): -500.232060775]

C	-0.00116500	-0.00222600	0.00219700
C	0.00146500	0.00133800	1.41253800
C	1.26863000	0.00650000	2.03160800
C	2.44779700	-0.07467400	-0.11783700
C	1.18146000	-0.03887400	-0.73760300
H	-0.93718300	0.02778500	-0.54981100
H	1.35574600	0.04208200	3.11462200
H	1.09513500	-0.03636800	-1.82126200
N	-1.18919700	-0.02478400	2.15850700
C	-2.42922400	0.29996700	1.47418400
H	-2.61784700	-0.40750500	0.65604600
C	-1.12209700	0.34670000	3.56177000
H	-2.12191200	0.26005800	4.00095100
H	-0.46260400	-0.33543400	4.11413900
H	-3.26005500	0.20941100	2.18233500
H	-0.75870200	1.38110600	3.72120800
H	-2.43957400	1.32451000	1.05233400
C	2.45125600	-0.03023300	1.29179300
N	3.63590000	-0.17527500	-0.86155000
C	3.58371400	0.15271400	-2.27634400
C	4.88867000	0.12022800	-0.18720500
H	4.57867600	0.00941200	-2.71168100
H	2.89558400	-0.51852200	-2.80666000
H	3.26418800	1.19580200	-2.46945000
H	5.71478200	-0.02850500	-0.89101600
H	4.94171300	1.15691700	0.20037500
H	5.04779600	-0.56683300	0.65425500
H	3.38812500	-0.01992700	1.84305300

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *para* (conformer no 1)
[total energy (hartree): -343.008771213]

C	0.00003700	0.00008900	0.00001200
C	-0.00003500	0.00003800	1.40352800
C	1.24098800	0.00010000	2.05911200
C	2.43658500	0.00141900	-0.06504600
C	1.19556300	0.00063000	-0.72062900
H	-0.94850500	-0.00618800	-0.54035800
H	1.27565500	-0.00637600	3.15020100
H	1.16090200	-0.00544600	-1.81172100
N	-1.20705600	-0.07252600	2.13114300
H	-1.15030500	0.30942600	3.06768900
H	-2.00944700	0.30572000	1.64195700
C	2.43651400	0.00091100	1.33847100
N	3.64367300	-0.06977200	-0.79268700
H	3.58657800	0.31249400	-1.72908400

H	4.44571800	0.30901500	-0.30335100
H	3.38506100	-0.00473000	1.87883700

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *para* (conformer no 2)
[total energy (hartree): -343.008867224]

C	0.00000900	-0.00030000	0.00005200
C	-0.00001800	-0.00013400	1.40353500
C	1.24097200	0.00006700	2.05910900
C	2.43650600	-0.00217000	-0.06502300
C	1.19551700	-0.00237100	-0.72059600
H	-0.94853600	0.00747800	-0.54028100
H	1.27562900	0.00850900	3.15018000
H	1.16085900	-0.01081300	-1.81166700
N	-1.20715200	0.07396000	2.13122000
H	-2.00877000	-0.30612100	1.64204900
H	-1.14994800	-0.30945400	3.06721400
C	2.43648000	-0.00200400	1.33846100
N	3.64364100	-0.07626500	-0.79270800
H	3.58643700	0.30714900	-1.72870100
H	4.44525900	0.30381700	-0.30353600
H	3.38502400	-0.00978300	1.87879400

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *para* (conformer no 3)
[total energy (hartree): -342.994320017]

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40016200
C	1.20322700	0.00000000	2.11189100
C	2.43441800	0.00000000	0.04015400
C	1.23119100	0.00000000	-0.67157300
H	1.18709600	0.00000000	3.20327900
H	1.24732200	0.00000000	-1.76296300
C	2.43441800	0.00000000	1.44031700
N	3.70533000	0.00000000	2.12719600
H	3.79286600	-0.81591500	2.72971800
H	3.79286600	0.81591400	2.72971700
H	3.39083500	0.00000000	-0.48224500
N	-1.27091200	0.00000000	-0.68687900
H	-1.35844600	0.81591200	-1.28940400
H	-1.35844900	-0.81591700	-1.28939700
H	-0.95641700	0.00000000	1.92256200

b3lyp/aug-cc-pvdz: NH_2-C_6H_4-NH_2, *para* (conformer no 4)
[total energy (hartree): -342.994183117]

C	0.00001800	-0.00000100	0.00002700
C	-0.00001900	0.00000000	1.40365500
C	1.22823700	0.00000100	2.07350700
C	2.43328000	0.00000000	-0.03889900
C	1.20181800	0.00000000	-0.71250500
H	-0.95004000	-0.00000100	-0.53753700
H	1.22800900	0.00000100	3.16320600
H	1.18618000	-0.00000100	-1.80398200
N	-1.21270200	0.00000000	2.18846300
H	-1.78346000	0.81610700	1.97737100
H	-1.78345900	-0.81610800	1.97737300
C	2.43153000	0.00000000	1.36010800
N	3.70367300	-0.00000100	-0.72644700
H	3.79227200	-0.81615900	-1.32840400
H	3.79228500	0.81617300	-1.32838200
H	3.38759600	-0.00000100	1.88299700

b3lyp/aug-cc-pvdz: OCH_3-C_6H_4-OCH_3, *para* (conformer no 1)

[total energy (hartree): -461.347739220]

C	-0.00000600	0.00008200	-0.00002600
C	-0.00001300	0.00077700	1.39683300
C	1.21568600	0.00069600	2.09710900
C	2.41681900	-0.00008200	1.37986100
C	2.41682700	-0.00077600	-0.01699700
C	1.20112800	-0.00069500	-0.71727300
H	-0.95285400	0.00137500	1.92092800
H	-0.93995800	0.00014400	-0.55106300
O	1.32914400	0.00133600	3.46597700
C	0.13257000	0.00208600	4.23207200
H	-0.47250500	-0.89686000	4.03342200
H	0.44798300	0.00246200	5.28027000
H	-0.47191100	0.90125100	4.03260400
H	3.35677200	-0.00014400	1.93089900
O	1.08766900	-0.00133600	-2.08614100
C	2.28424400	-0.00208600	-2.85223600
H	2.88931900	0.89686000	-2.65358700
H	2.88872500	-0.90125100	-2.65276800
H	1.96883000	-0.00246200	-3.90043400
H	3.36966800	-0.00137400	-0.54109200

b3lyp/aug-cc-pvdz: OCH_3-C_6H_4-OCH_3, *para* (conformer no 2)

[total energy (hartree): -461.348044868]

C	0.06506500	-0.02225900	0.10485400
C	0.05345900	0.00092400	1.51082400
C	1.26534900	0.01479400	2.20351600
C	2.48386400	0.00567600	1.50011500
C	2.49006900	-0.01735000	0.10436400
C	1.26657000	-0.03121600	-0.58872700
H	-0.88540700	-0.03303000	-0.42765400
H	1.28075200	-0.04905600	-1.67801300
H	3.41109700	0.01688400	2.06818900
O	3.61864400	-0.02804800	-0.67743600
C	4.87886600	-0.01500700	-0.02231000
H	5.63091900	-0.02721700	-0.81755500
H	5.00539200	0.89463100	0.58632400
H	5.00818200	-0.90322100	0.61661300
O	-1.18796300	0.00797400	2.09710700
C	-1.25100200	0.03175700	3.51605900
H	-0.77663400	0.93868700	3.92397200
H	-2.31591000	0.03390700	3.76929200
H	-0.77309100	-0.85901900	3.95431800
H	1.29354200	0.03262300	3.29042100

b3lyp/aug-cc-pvdz: OH-C_6H_4-OH, *para* (conformer no 1)

[total energy (hartree): -382.746220882]

C	-0.00624800	0.00017800	0.01314600
C	0.00461600	0.00059400	1.41015000
C	1.22034800	0.00002200	2.09902200
C	2.42228700	-0.00096600	1.38205500
C	2.41142300	-0.00138300	-0.01494100
C	1.19568600	-0.00081000	-0.70381600
H	-0.92732900	0.00136900	1.97419900
H	-0.96069800	0.00063400	-0.51759100
O	1.17087300	0.00047200	3.47559800
H	2.06792400	-0.00002000	3.83006800
H	3.37673300	-0.00142300	1.91280100
O	1.24517500	-0.00126100	-2.08039200
H	0.34812800	-0.00076800	-2.43487200
H	3.34336300	-0.00215800	-0.57900100

b3lyp/aug-cc-pvdz: OH-C_6H_4-OH, *para* (conformer no 2)
[total energy (hartree): -382.746076024]

C	0.01827000	0.00010700	0.00069300
C	0.01819500	0.00053400	1.39441100
C	1.22796600	0.00001400	2.09910500
C	2.43616600	-0.00093400	1.39797600
C	2.43624100	-0.00136500	-0.00261000
C	1.22811700	-0.00084500	-0.70387000
H	-0.91872300	0.00127900	1.95031300
H	-0.91858800	0.00051000	-0.55531100
O	1.15962800	0.00047500	3.47482600
H	2.05137100	0.00003000	3.84243500
H	3.38586800	-0.00135000	1.93688000
O	1.15992800	-0.00122800	-2.07959900
H	2.05171200	-0.00189000	-2.44711000
H	3.38600200	-0.00211400	-0.54141100

b3lyp/aug-cc-pvdz: SH-C_6H_4-SH, *para* (conformer no 1)
[total energy (hartree): -1028.69510645]

C	-0.00289000	0.00009600	-0.00546000
C	-0.01576400	0.00058700	1.39550400
C	1.20535800	-0.00000500	2.08575600
C	2.41334600	-0.00105600	1.38834600
C	2.42637600	-0.00156200	-0.01427400
C	1.20674600	-0.00097900	-0.70379100
H	3.35065000	-0.00150000	1.94543300
H	1.18827800	-0.00134700	-1.79371400
H	1.21892900	0.00034400	3.17604500
S	4.01733400	-0.00293100	-0.83803600
H	3.54509200	-0.00302400	-2.10798500
S	-1.52452800	0.00201200	2.36155600
H	-2.38916500	0.00169600	1.31835600
H	-0.93746600	0.00055800	-0.56656500

b3lyp/aug-cc-pvdz: SH-C_6H_4-SH, *para* (conformer no 2)
[total energy (hartree): -1028.69514428]

C	0.00316700	-0.00020100	0.00028300
C	-0.01200900	-0.00003900	1.40234700
C	1.20704800	-0.00063600	2.09394800
C	2.41632000	-0.00137700	1.39692100
C	2.43149600	-0.00154000	-0.00514700
C	1.21244300	-0.00094500	-0.69674600
H	3.35283700	-0.00183400	1.95547100
H	1.19560900	-0.00105500	-1.78661600
H	1.22387600	-0.00052800	3.18381800
S	4.02346400	-0.00251400	-0.82692300
H	3.55264600	-0.00239000	-2.09738300
S	-1.60397200	0.00092700	2.22413100
H	-1.13314600	0.00082700	3.49458800
H	-0.93334700	0.00025700	-0.55827200

b3lyp/aug-cc-pvdz: tBu-C_6H_4-tBu, *para* (conformer no 1)
[total energy (hartree): -546.810989298]

C	0.00000300	-0.00021000	-0.00001200
C	-0.00001700	0.00018700	1.40330100
C	1.18503700	0.00037400	2.14444700
C	2.44198800	0.00017500	1.52057500
C	2.44200800	-0.00022100	0.11726200
C	1.25695400	-0.00040900	-0.62388400
H	1.33438900	-0.00071200	-1.70927800

C	-1.32802400	-0.00039700	-0.77668400
C	-2.14141400	-1.26168000	-0.40481200
C	-2.14134300	1.26114300	-0.40553700
C	-1.10862700	-0.00084400	-2.30023900
H	-1.58567200	-2.17429200	-0.65977300
H	-2.36979700	-1.29555500	0.66807700
H	-3.09469700	-1.27615400	-0.95248900
H	-3.09462400	1.27536100	-0.95322600
H	-2.36973000	1.29564700	0.66733200
H	-1.58554800	2.17357800	-0.66101800
H	-2.08017900	-0.00096400	-2.81269200
H	-0.55782900	0.88925500	-2.63336200
H	-0.55787900	-0.89116600	-2.63284800
H	3.38618200	-0.00038800	-0.42758700
H	-0.94419100	0.00035300	1.94815000
C	3.77001500	0.00036300	2.29724700
C	3.55061800	0.00081100	3.82080200
C	4.58333300	-1.26117800	1.92610200
C	4.58340500	1.26164500	1.92537400
H	2.99987100	0.89113400	4.15341000
H	2.99981800	-0.88928700	4.15392600
H	4.52216900	0.00093000	4.33325500
H	4.81172100	-1.29568300	0.85323200
H	5.53661400	-1.27539600	2.47379100
H	4.02753800	-2.17361300	2.18158300
H	5.53668900	1.27611900	2.47305100
H	4.81178800	1.29551900	0.85248500
H	4.02766400	2.17425800	2.18033500
H	1.10760200	0.00067700	3.22984100

[2.1] b3lyp/6-31G(d,p): *mono*

b3lyp/6-31G(d,p): C_6H_6
[total energy (hartree): -232.258212341]

C	0.00309600	0.00005200	-0.00062100
C	0.00302600	0.00049400	1.39571500
C	1.21221900	-0.00005300	2.09397100
C	2.42149500	-0.00104700	1.39582900
C	2.42156400	-0.00149200	-0.00049400
C	1.21235800	-0.00093900	-0.69875600
H	3.36227400	-0.00147800	1.93905100
H	3.36239700	-0.00226700	-0.54362200
H	-0.93781700	0.00126900	1.93882400
H	-0.93769400	0.00048300	-0.54382400
H	1.21242400	-0.00128400	-1.78510200
H	1.21217800	0.00029200	3.18031700

b3lyp/6-31G(d,p): C_6H_5-BF_2
[total energy (hartree): -456.327985365]

C	-0.03267800	0.00005600	-0.02289500
C	-0.01521200	0.00045600	1.38390300
C	1.18956700	-0.00008000	2.08334500
C	2.39849700	-0.00102600	1.38292900
C	2.40211900	-0.00143600	-0.01430500
C	1.19503600	-0.00089700	-0.70999300
H	3.33907800	-0.00144600	1.92670200
H	3.34378300	-0.00217500	-0.55536300
H	-0.95611400	0.00119600	1.92668800
H	1.19715100	-0.00121300	-1.79630700
H	1.19017500	0.00023700	3.16937700
B	-1.37254800	0.00066300	-0.79305400
F	-2.54114300	0.00157000	-0.15689400

F	-1.41489700	0.00030700	-2.12261900

b3lyp/6-31G(d,p): C_6H_5-BH_2
[total energy (hartree): -257.701103041]

C	-0.03766100	0.00006200	-0.02367800
C	-0.00679400	0.00046000	1.38926800
C	1.19648300	-0.00008000	2.08933900
C	2.40489200	-0.00103500	1.38620100
C	2.40926900	-0.00145200	-0.01189000
C	1.20125300	-0.00090700	-0.70375800
H	3.34607100	-0.00146000	1.92943400
H	3.35159900	-0.00219800	-0.55201500
H	-0.94712100	0.00120700	1.93420500
H	1.20280100	-0.00122900	-1.79056700
H	1.20011200	0.00023800	3.17547900
B	-1.36845800	0.00067200	-0.79156100
H	-1.37824000	0.00032900	-1.98774400
H	-2.40889800	0.00149200	-0.20121200

b3lyp/6-31G(d,p): C_6H_5-Br
[total energy (hartree): -2803.36169124]

C	0.00477500	0.00004400	0.00133500
C	-0.00356800	0.00053800	1.39721800
C	1.21216000	-0.00000100	2.07814900
C	2.42803300	-0.00101400	1.39747000
C	2.41998100	-0.00149700	0.00159000
C	1.21244900	-0.00097200	-0.69841700
H	3.36122600	-0.00141600	1.94921800
H	3.36353100	-0.00229000	-0.53602100
H	-0.93687800	0.00132900	1.94876600
H	-0.93866400	0.00046100	-0.53646800
H	1.21256700	-0.00135000	-1.78398900
Br	1.21196800	0.00068000	3.99243800

b3lyp/6-31G(d,p): C_6H_5-CHO
[total energy (hartree): -345.582698556]

C	0.00000000	0.00000100	-0.00001800
C	0.00000800	0.00000100	1.40063100
C	1.20543700	0.00000100	2.10061000
C	2.41274700	0.00000000	1.39877700
C	2.41792000	-0.00000100	-0.00112900
C	1.21610600	0.00000000	-0.70026200
H	3.35320800	0.00000000	1.94228900
H	3.36106700	-0.00000100	-0.53933200
H	-0.94662700	0.00000200	1.93617100
H	1.18795800	0.00000000	-1.78519700
H	1.20626900	0.00000200	3.18634200
C	-1.28438000	0.00000200	-0.73615400
O	-1.38798500	0.00000100	-1.94802300
H	-2.18865200	0.00000200	-0.08701200

b3lyp/6-31G(d,p): C_6H_5-Cl
[total energy (hartree): -691.852927576]

C	0.00506800	0.00004500	0.00138300
C	-0.00375200	0.00053200	1.39702100
C	1.21216700	0.00000100	2.07914100
C	2.42822300	-0.00101400	1.39725000
C	2.41966900	-0.00150100	0.00161300
C	1.21243000	-0.00096200	-0.69875500
H	3.36081600	-0.00142100	1.95036800
H	3.36307200	-0.00229300	-0.53614500

H	-0.93644900	0.00131700	1.94996000
H	-0.93823600	0.00046400	-0.53654700
H	1.21254100	-0.00133600	-1.78428200
Cl	1.21202100	0.00059500	3.84028100

b3lyp/6-31G(d,p): C_6H_5-CN
[total energy (hartree): -324.500080486]

C	-0.01134000	0.00005400	-0.00864000
C	-0.01233800	0.00050200	1.39636100
C	1.19672800	-0.00004800	2.08663700
C	2.40525400	-0.00103700	1.38638800
C	2.40719100	-0.00148400	-0.01034700
C	1.20480400	-0.00094300	-0.71220500
H	3.34559400	-0.00146400	1.92921000
H	3.34668400	-0.00225700	-0.55401500
H	-0.95620300	0.00127600	1.93085000
H	1.19558700	-0.00128200	-1.79684900
H	1.19577200	0.00029800	3.17209200
C	-1.25395900	0.00062400	-0.72585800
N	-2.26163100	0.00108700	-1.30720000

b3lyp/6-31G(d,p): C_6H_5-COOH (conformer no 1)
[total energy (hartree): -420.835447777]

C	-0.03399700	0.00003700	0.02983700
C	-0.00757700	0.00043300	1.43128600
C	1.21442500	-0.00009800	2.10110800
C	2.40944400	-0.00102100	1.37810500
C	2.38484000	-0.00141700	-0.01911500
C	1.16677600	-0.00089000	-0.69276200
H	3.36015200	-0.00143300	1.90347000
H	3.31440100	-0.00213600	-0.58018200
H	-0.93977400	0.00115300	1.98424100
H	1.11998500	-0.00117800	-1.77635400
H	1.23529300	0.00020800	3.18670600
C	-1.30725100	0.00057800	-0.73767700
O	-1.38959900	0.00026000	-1.95011900
O	-2.40881600	0.00149200	0.05641300
H	-3.16776000	0.00177500	-0.54986600

b3lyp/6-31G(d,p): C_6H_5-COOH (conformer no 2)
[total energy (hartree): -420.824062540]

C	0.00019800	-0.00156600	-0.00001400
C	0.00013200	0.00025200	1.40136900
C	1.20264100	0.00141800	2.10239500
C	2.41672700	0.01918100	1.41059600
C	2.42503400	0.04062400	0.01521500
C	1.22126900	0.02895700	-0.68851600
H	3.35446900	0.02432800	1.95817000
H	3.36620000	0.07452400	-0.52484500
H	-0.95407400	-0.00052700	1.91680100
H	1.24575100	0.08565600	-1.77422700
H	1.19549500	-0.00783800	3.18805600
C	-1.32888500	-0.00155900	-0.69514500
O	-2.35603900	0.34895300	-0.16428500
O	-1.34361800	-0.42387300	-1.98895300
H	-0.49333700	-0.82462600	-2.21742500

b3lyp/6-31G(d,p): C_6H_5-F
[total energy (hartree): -331.490233155]

C	0.00389300	0.00004800	0.00099800
C	-0.00527700	0.00051500	1.39672200

C	1.21221300	-0.00002700	2.06777800
C	2.42978800	-0.00103300	1.39685400
C	2.42078400	-0.00149900	0.00113900
C	1.21237200	-0.00094500	-0.69906600
H	3.35356600	-0.00144100	1.96503400
H	3.36311100	-0.00228300	-0.53847100
H	-0.92912800	0.00128900	1.96478100
H	-0.93837800	0.00047300	-0.53871000
H	1.21244200	-0.00130000	-1.78446400
F	1.21215400	0.00039200	3.41869500

b3lyp/6-31G(d,p): C_6H_5-Li
[total energy (hartree): -239.146362222]

C	0.00444300	0.00004400	-0.00460900
C	0.01690800	0.00053900	1.39398600
C	1.20792000	0.00004900	2.15871700
C	2.39902800	-0.00098300	1.39412100
C	2.41165700	-0.00149500	-0.00446900
C	1.20808900	-0.00098200	-0.71132600
H	-0.94124700	0.00045900	-0.54383300
H	-0.95147000	0.00134600	1.89954500
H	3.36734800	-0.00141900	1.89979400
H	3.35740600	-0.00229500	-0.54358900
H	1.20815500	-0.00137200	-1.79869500
Li	1.20802300	0.00071600	4.13205900

b3lyp/6-31G(d,p): C_6H_5-$N(CH_3)_2$
[total energy (hartree): -366.231208842]

C	-0.00011400	-0.00248100	0.00034500
C	-0.00007900	0.00246700	1.41374100
C	1.25480200	0.00593400	2.06415900
C	2.43940500	0.02761700	1.33262900
C	2.42708300	0.03670900	-0.06218200
C	1.19448900	0.01927400	-0.71490900
H	-0.93417500	-0.02482100	-0.54713900
H	1.31082800	-0.00789100	3.14550300
H	3.38513400	0.03238200	1.86812800
H	1.15427300	0.01684200	-1.80098100
N	-1.19046500	0.01507400	2.13837700
C	-1.14963700	-0.23869000	3.56803900
H	-0.55258500	0.52050200	4.08548200
C	-2.44288100	-0.22762300	1.44397000
H	-3.26585900	-0.15746700	2.15715700
H	-2.61540300	0.52919400	0.67085400
H	-2.16293000	-0.18461800	3.96936100
H	-2.48753300	-1.21818900	0.96320600
H	-0.73189700	-1.22660700	3.82014800
H	3.35429400	0.05074200	-0.62598300

b3lyp/6-31G(d,p): C_6H_5-NH_2
[total energy (hartree): -287.616505050]

C	-0.00003100	0.00020800	0.00002000
C	0.00005000	0.00013900	1.40535900
C	2.42466700	-0.00014300	-0.03550500
C	1.20027100	0.00051600	-0.70652100
H	-0.94725500	0.00444700	-0.53416100
H	1.17552000	-0.00126200	-1.79284300
N	-1.20076200	0.05874900	2.11902400
H	-2.00659100	-0.30001000	1.62501200
H	-1.15282300	-0.30285300	3.06193700
C	2.42865800	-0.00014300	1.36071900

H	3.35765000	-0.00149900	-0.58991600
C	1.23435100	-0.00040500	2.07732100
H	3.37101700	-0.00234600	1.90171500
H	1.25060400	0.00361800	3.16464000

b3lyp/6-31G(d,p): C_6H_5-OCH_3
[total energy (hartree): -346.783317440]

C	0.00000100	-0.00019900	-0.00004800
C	-0.00011200	-0.00036300	1.38971100
C	1.21479200	0.00005800	2.09115800
C	2.42517000	0.00064400	1.38840300
C	2.40758100	0.00080100	-0.01017200
C	1.20483200	0.00038400	-0.71166300
H	-0.92461300	-0.00081500	1.95774800
H	-0.94679200	-0.00053100	-0.53265500
O	1.10873600	-0.00014700	3.45403300
H	3.37394300	0.00098000	1.91158200
H	3.35127300	0.00125800	-0.54849100
C	2.30265600	0.00024500	4.21925400
H	2.90958000	0.89399700	4.02483000
H	1.99093600	-0.00001800	5.26480100
H	2.91031300	-0.89295800	4.02459700
H	1.20171800	0.00051100	-1.79705300

b3lyp/6-31G(d,p): C_6H_5-OH
[total energy (hartree): -307.478469429]

C	0.00248200	0.00005500	-0.00069300
C	-0.01025800	0.00054600	1.39488000
C	1.19751900	0.00001300	2.10039600
C	2.41351800	-0.00100400	1.40797000
C	2.41195300	-0.00148500	0.01546900
C	1.21015400	-0.00096200	-0.69833100
H	3.33865300	-0.00140500	1.97469100
H	3.35903300	-0.00228000	-0.51655300
H	-0.95486800	0.00134400	1.93523900
H	-0.94003600	0.00047500	-0.54066300
H	1.21638600	-0.00134100	-1.78359300
O	1.25297500	0.00044900	3.46719900
H	0.35297600	0.00114200	3.81849600

b3lyp/6-31G(d,p): C_6H_5-SH
[total energy (hartree): -630.445237848]

C	-0.01825300	-0.00002400	-0.00793800
C	-0.01393600	0.00042400	1.39225700
C	1.19640700	-0.00006900	2.08577000
C	2.40906800	-0.00100700	1.39620100
C	2.40265200	-0.00145300	0.00027900
C	1.19898200	-0.00096800	-0.70224300
H	3.34846800	-0.00139000	1.94005800
H	3.33957100	-0.00218600	-0.54917900
H	-0.95018300	0.00115400	1.94283800
H	1.20457600	-0.00131600	-1.78837200
H	1.18613800	0.00028700	3.17195700
S	-1.52578800	0.00055000	-0.97171200
H	-2.38273700	0.00151600	0.06730300

b3lyp/6-31G(d,p): C_6H_5-tBu
[total energy (hartree): -389.524131426]

C	0.03837300	0.00000200	-0.01535100
C	0.04500200	0.00052900	1.39055300
C	1.23501300	0.00005300	2.11490500

C	2.46270200	-0.00098100	1.44995400
C	2.47806200	-0.00153100	0.05741100
C	1.28088300	-0.00104200	-0.66376400
H	3.39245400	-0.00135700	2.01132600
H	3.42379100	-0.00234600	-0.47760800
H	-0.89575700	0.00132900	1.93360100
H	1.33029400	-0.00149100	-1.74653500
H	1.20305700	0.00048900	3.20097400
C	-1.30144200	0.00057900	-0.77610600
C	-2.11153800	-1.26064300	-0.39321800
C	-2.10993400	1.26310800	-0.39413400
C	-1.10729200	-0.00010700	-2.30380500
H	-1.56697500	-2.17178400	-0.66151700
H	-2.31965700	-1.30067600	0.67991100
H	-3.07268100	-1.27124800	-0.91960000
H	-1.56414000	2.17336300	-0.66293700
H	-3.07098600	1.27463200	-0.92065900
H	-2.31815800	1.30410200	0.67893900
H	-2.08334700	0.00031600	-2.79962700
H	-0.56345400	0.88637800	-2.64600800
H	-0.56456800	-0.88752900	-2.64534400

[2.2] b3lyp/6-31G(d,p): *ortho*

b3lyp/6-31G(d,p): BF_2-C_6H_4-BF_2, *ortho*
[total energy (hartree): -680.389865616]

C	-0.00010800	0.00024100	0.00041200
C	-0.00055300	-0.00033100	1.40433500
C	1.24245700	-0.00060700	2.09202300
C	2.43145600	0.02957300	1.34621600
C	2.41196600	0.04026400	-0.04938300
C	1.19264800	0.01948700	-0.72433800
H	3.38419200	0.03446300	1.86747200
H	1.16880300	0.02194600	-1.81016700
B	-1.38185500	0.11961200	2.11130600
F	-1.53085100	0.67836400	3.30486700
F	-2.49215800	-0.26909100	1.49130800
H	-0.94767000	-0.00398100	-0.53027700
B	1.38104600	-0.15182200	3.63493400
F	2.49019100	0.24398200	4.25260800
F	0.46145400	-0.74467100	4.38434900
H	3.34450800	0.06135900	-0.60573600

b3lyp/6-31G(d,p): BH_2-C_6H_4-BH_2, *ortho* (conformer no 1)
[total energy (hartree): -283.130381088]

C	-0.00215600	-0.00003000	-0.00833800
C	0.01822800	0.00054700	1.39081400
C	1.22692900	0.00008400	2.09116600
C	2.44642600	-0.00097700	1.40091200
C	2.43767500	-0.00156700	-0.02383900
C	1.20118900	-0.00107400	-0.70448800
H	1.20056900	-0.00152300	-1.79172800
H	1.20646900	0.00055800	3.17831100
B	3.78631000	-0.00269100	-0.74130600
H	3.90266200	-0.00324000	-1.93003200
H	4.78940300	-0.00303700	-0.06837600
H	-0.94926000	0.00034400	-0.53940100
B	3.83927000	-0.00156600	2.11469800
H	4.36848300	-1.02714000	2.42621400
H	4.36972900	1.02358700	2.42548400
H	-0.91841500	0.00137200	1.94230700

b3lyp/6-31G(d,p): BH_2-C_6H_4-BH_2, *ortho* (conformer no 2)
[total energy (hartree): -283.136409073]

C	-0.00001400	-0.00059100	0.00002000
C	0.00005600	-0.00076700	1.39654500
C	1.19399700	-0.00030700	2.14411200
C	2.44323500	0.00036300	1.43400200
C	2.41178000	0.00052700	0.02568900
C	1.21191500	0.00005900	-0.68888900
H	-0.94847900	-0.00127600	1.92636600
H	1.22317600	0.00019700	-1.77533100
B	3.83780000	0.00093800	2.10730200
H	4.80614700	0.00147900	1.40371800
H	3.99164600	0.00087400	3.28694700
H	3.35225200	0.00103500	-0.51836300
H	-0.93925600	-0.00096400	-0.54616400
B	1.05927900	-0.00059200	3.68684600
H	1.99442800	-0.00029900	4.42213700
H	-0.04050700	-0.00114400	4.15924400

b3lyp/6-31G(d,p): Br-C_6H_4-Br, *ortho*
[total energy (hartree): -5374.46126269]

C	0.00466600	0.00001600	0.00343700
C	0.00438800	0.00052400	1.39640900
C	1.21189400	0.00005300	2.09827800
C	2.42292300	-0.00094700	1.39919200
C	2.41922800	-0.00145100	0.00271300
C	1.21312400	-0.00096600	-0.69405000
H	3.36516100	-0.00222300	-0.52637400
Br	1.15299100	0.00078700	3.99949000
H	-0.92731100	0.00129300	1.95054400
H	-0.93943900	0.00039600	-0.53193100
Br	4.09936900	-0.00164800	2.29835000
H	1.22219100	-0.00136300	-1.77934300

b3lyp/6-31G(d,p): CHO-C_6H_4-CHO, *ortho* (conformer no 1)
[total energy (hartree): -458.898037481]

C	-0.03415400	-0.00000100	-0.00783600
C	-0.03441000	0.00000000	1.40884600
C	1.18981400	0.00000100	2.09474200
C	2.39432600	0.00000000	1.40079100
C	2.39457900	0.00000000	0.00109800
C	1.19031800	-0.00000100	-0.69328800
H	1.16385300	-0.00000200	-1.77763200
H	1.16295700	0.00000200	3.17907600
C	-1.27211700	-0.00000200	-0.83719800
O	-1.25692400	0.00000700	-2.05406600
H	-2.23870400	-0.00000800	-0.30017100
H	3.33417600	-0.00000100	-0.54315200
C	-1.27267300	0.00000200	2.23775700
H	-2.23906300	0.00000800	1.70037600
O	-1.25792600	-0.00000600	3.45463100
H	3.33372700	0.00000100	1.94538100

b3lyp/6-31G(d,p): CHO-C_6H_4-CHO, *ortho* (conformer no 2)
[total energy (hartree): -458.899905239]

C	0.03813000	0.00000000	0.01389400
C	0.05855800	0.00000000	1.40955800
C	1.28052700	0.00000100	2.07836400
C	2.49505500	0.00000100	1.37660700
C	2.47085100	-0.00000100	-0.04213600
C	1.23542300	-0.00000100	-0.69921300

H	1.24486100	-0.00000200	-1.78406900
H	1.30133200	0.00000200	3.16524500
C	3.69957100	-0.00000200	-0.90143600
O	3.63153100	0.00001600	-2.11807800
H	4.66443300	-0.00001900	-0.37470900
H	-0.90906100	-0.00000100	-0.51708100
C	3.72214200	0.00000200	2.21584100
H	3.49888200	-0.00000200	3.30557300
O	4.87617800	0.00000600	1.83236000
H	-0.86985600	0.00000100	1.97220100

b3lyp/6-31G(d,p): CHO-C_6H_4-CHO, *ortho* (conformer no 3)
[total energy (hartree): -458.887512626]

C	0.04298600	-0.00000100	0.06418100
C	0.06013400	-0.00000100	1.45867400
C	1.25327500	0.00000000	2.19406500
C	2.48696700	0.00000100	1.48155900
C	2.44676700	0.00000100	0.08066200
C	1.24776800	0.00000100	-0.63150600
H	-0.88169600	-0.00000200	2.00141700
H	1.25904900	0.00000100	-1.71701800
C	3.87710400	0.00000300	2.04097500
H	4.63741400	-0.00000500	1.22520600
O	4.22817200	-0.00000200	3.19695200
H	3.38777300	0.00000200	-0.46346300
C	1.04283200	-0.00000100	3.67774900
H	-0.04387900	0.00000400	3.92808500
O	1.86825900	0.00000100	4.55996600
H	-0.90270100	-0.00000100	-0.46887300

b3lyp/6-31G(d,p): Cl-C_6H_4-Cl, *ortho*
[total energy (hartree): -1151.44210204]

C	-0.00437400	0.00011700	-0.00425100
C	-0.00442600	0.00059500	1.39688200
C	1.20800700	0.00000300	2.09063200
C	2.41401700	-0.00103900	1.39400400
C	2.41406900	-0.00150800	-0.00119800
C	1.20810900	-0.00094000	-0.69791200
H	3.34968800	-0.00232900	-0.55108600
H	1.19144900	-0.00130600	-1.78197000
Cl	-1.49535400	0.00078700	-0.91734600
H	1.19126700	0.00036900	3.17468800
Cl	-1.49547100	0.00187700	2.30987100
H	3.34959100	-0.00148900	1.94395500

b3lyp/6-31G(d,p): CN-C_6H_4-CN, *ortho*
[total energy (hartree): -416.734557196]

C	-0.01447500	0.00015300	0.02137700
C	-0.02615500	0.00073800	1.42331500
C	1.19972600	0.00017100	2.13157600
C	2.40834500	-0.00096100	1.42105300
C	2.40346700	-0.00152800	0.02836700
C	1.19439600	-0.00097300	-0.67016300
H	3.34252300	-0.00138900	1.97147100
H	1.19147100	-0.00141500	-1.75523500
C	-1.27987000	0.00190200	2.11754600
N	-2.31237800	0.00284800	2.65228100
H	-0.95798000	0.00059300	-0.51288400
C	1.22455400	0.00074000	3.56444400
N	1.27697300	0.00117800	4.72602100
H	3.34491100	-0.00240700	-0.51115300

b3lyp/6-31G(d,p): COOH-C_6H_4-COOH, *ortho* (conformer no 1)
[total energy (hartree): -609.398258205]

C	0.05077000	0.02935300	0.07996500
C	0.05642400	0.13055300	1.46954800
C	1.25869900	0.09967200	2.18521200
C	2.47787100	0.00593900	1.48356500
C	2.45897900	-0.11813500	0.08968200
C	1.25471000	-0.10892900	-0.61092900
H	-0.87072200	0.21889600	2.02525600
H	1.25845500	-0.20015800	-1.69267600
C	3.83245000	0.10395900	2.11100400
O	4.81299100	-0.49014000	1.71542200
O	3.88154200	1.00599000	3.11775200
H	4.79626100	0.99020300	3.44652600
H	3.40596400	-0.20532800	-0.43170000
C	1.13014700	0.09496200	3.67573800
O	0.27597800	0.69882100	4.28944900
O	2.01160800	-0.73638900	4.27700100
H	1.83973500	-0.66356000	5.23103500
H	-0.89130400	0.04938700	-0.45912700

b3lyp/6-31G(d,p): COOH-C_6H_4-COOH, *ortho* (conformer no 2)
[total energy (hartree): -609.398380068]

C	-0.00006900	-0.00063300	0.00004000
C	0.00001700	-0.00052400	1.39444500
C	1.20177700	0.00024700	2.10726300
C	2.42381900	-0.04017900	1.40617700
C	2.41292300	-0.03311100	0.00575000
C	1.20849700	-0.00730800	-0.69538800
H	-0.93241700	0.00939400	1.94856800
H	1.21586200	-0.00581900	-1.78092900
C	3.71360600	-0.23124000	2.13181100
O	3.83239400	-0.76416000	3.21449500
O	4.78047700	0.21598700	1.42318500
H	5.56180400	-0.00666400	1.95653300
H	3.35639600	-0.06896600	-0.52631800
C	1.08918800	0.08297400	3.60062000
O	0.31529100	-0.57760400	4.25851600
O	1.86498700	1.05492700	4.12679200
H	1.74264000	1.00554700	5.08998000
H	-0.94213600	0.00599300	-0.53952100

b3lyp/6-31G(d,p): COOH-C_6H_4-COOH, *ortho* (conformer no 3)
[total energy (hartree): -609.397379073]

C	-0.00008900	0.00003700	0.00000800
C	-0.00010200	-0.00019300	1.40906900
C	1.21716700	-0.00042700	2.09700200
C	2.42627700	-0.02408900	1.40118300
C	2.42588700	-0.05021600	0.00793700
C	1.21662600	-0.03699900	-0.68790400
H	1.20803700	-0.03742200	-1.77203400
H	1.20855700	0.00021000	3.18112900
C	-1.26754900	0.18463700	-0.77397700
O	-2.17578600	0.91785300	-0.45357300
O	-1.26344400	-0.51483600	-1.93525900
H	-2.09675300	-0.28817600	-2.38199300
H	3.36303500	-0.07389600	-0.53959600
C	-1.27270300	-0.14551200	2.18291800
O	-2.20369900	-0.84930500	1.86183000
O	-1.24657800	0.55241800	3.34485800

H	-2.08662700	0.35176000	3.79140500
H	3.36370200	-0.02912100	1.94872700

b3lyp/6-31G(d,p): F-C_6H_4-F, *ortho*
[total energy (hartree): -430.715018015]

C	0.00189200	0.00004500	-0.00121800
C	-0.00407600	0.00051400	1.39610200
C	1.20358900	-0.00001800	2.08006500
C	2.41144200	-0.00100200	1.38265100
C	2.42324000	-0.00147400	-0.00516500
C	1.21031700	-0.00095300	-0.69888400
H	3.37821800	-0.00225100	-0.51943400
F	1.22804000	0.00041100	3.42466700
H	-0.92715600	0.00128500	1.96562300
H	-0.94001100	0.00045700	-0.53987400
H	1.21501000	-0.00132300	-1.78391800
F	3.56377100	-0.00151400	2.07591700

b3lyp/6-31G(d,p): N(CH_3)$_2$-C_6H_4-N(CH_3)$_2$, *ortho* (conformer no 1)
[total energy (hartree): -500.198894192]

C	0.00020300	-0.00053300	-0.00028600
C	0.00003300	-0.00156300	1.38881100
C	1.21482000	-0.00102700	2.07602600
C	2.44757100	-0.06068000	-0.02002300
C	1.21469200	-0.03578000	-0.68711100
H	-0.93268600	0.00725100	-0.55619000
H	1.20087400	0.03780700	3.15905800
H	1.20007800	-0.07407300	-1.77015800
C	2.44813800	-0.01152600	1.40931800
N	3.67259800	-0.10755700	-0.74135500
C	4.49144600	-1.30143800	-0.51145800
C	3.62649700	0.25553100	-2.14862300
H	5.49477400	-1.13356000	-0.91734900
H	4.57485300	-1.48635000	0.55938200
H	4.06763100	-2.19467000	-1.00099800
H	3.14574400	-0.50378700	-2.79153000
H	3.09428000	1.20150100	-2.27691900
H	4.65208200	0.38676100	-2.50826800
N	3.67378900	-0.00029100	2.13087400
C	4.52833200	1.16814000	1.90005700
C	3.61668100	-0.36045400	3.53849800
H	4.61701100	1.34976600	0.82910000
H	4.13191100	2.07405300	2.38925500
H	5.52618700	0.97010000	2.30580300
H	3.15787900	0.41323600	4.18030200
H	3.05723600	-1.29045800	3.66770900
H	4.63789200	-0.52096200	3.89868900
H	-0.93284400	0.01743200	1.94446600

b3lyp/6-31G(d,p): N(CH_3)$_2$-C_6H_4-N(CH_3)$_2$, *ortho* (conformer no 2)
[total energy (hartree): -500.188902662]

C	-0.00305800	-0.01656500	0.00147300
C	0.00018200	-0.02425600	1.40398900
C	1.23359900	-0.00215400	2.09083200
C	2.40503500	0.03392900	-0.05009000
C	1.18496700	0.01220300	-0.72611300
H	-0.95445500	-0.03385300	-0.52397700
H	1.15726500	0.01743400	-1.81210000
N	-1.23851800	-0.05583800	2.14812100
C	-2.00579300	-1.28220900	1.93324700
H	-1.37433900	-2.15198300	2.13142500

C	-2.05984700	1.13775900	1.94851600
H	-2.90238800	1.11463400	2.64840400
H	-1.46758100	2.03243300	2.15667000
H	-2.84914200	-1.30517500	2.63218500
H	-2.47265700	1.22974700	0.92769700
H	-2.41305800	-1.38001600	0.91078200
C	2.41939500	0.02671800	1.34319100
H	3.35482300	0.04313900	1.89346800
N	1.37163900	-0.00625400	3.52194500
C	0.94043500	-1.23214200	4.18581800
C	0.89636200	1.19808500	4.19500200
H	-0.15397900	-1.34261300	4.24372500
H	1.35260600	-2.09762900	3.65885600
H	1.33900900	-1.24159700	5.20769000
H	1.29110200	1.21250500	5.21827700
H	1.27974300	2.08193100	3.67683500
H	-0.20146300	1.26987000	4.25018300
H	3.33937600	0.05627000	-0.60356800

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *ortho* (conformer no 1)
[total energy (hartree): -342.975003002]

C	-0.04146900	0.07576300	0.01023200
C	-0.00084800	-0.02167600	1.39919800
C	1.23115100	-0.03702000	2.05833400
C	2.38706600	0.09730900	-0.07004300
C	1.15040400	0.12811500	-0.71726500
H	1.26846900	-0.09334700	3.14408900
H	1.12467900	0.18449600	-1.80336500
C	2.42786800	0.03117200	1.34247400
N	3.69506500	-0.01530200	1.95891300
H	3.64892200	0.09971400	2.96428100
H	4.33506700	0.66619600	1.56029700
H	-0.91988200	-0.07249300	1.97497200
N	3.61565600	0.18236200	-0.75679300
H	4.29626000	-0.48215600	-0.39880700
H	3.51577400	0.06924300	-1.75849400
H	-0.99259500	0.09787600	-0.51283200

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *ortho* (conformer no 2)
[total energy (hartree): -342.969657852]

C	0.04467300	0.07308100	0.00653200
C	0.02137600	0.03680300	1.39977500
C	1.22873200	0.00712700	2.10155900
C	2.47662300	-0.01984600	0.01946000
C	1.26074300	0.04136100	-0.67522700
H	1.22530600	0.01226600	3.18977400
H	1.27771000	0.03414100	-1.76232900
C	2.45475400	-0.00910600	1.43532500
N	3.70382900	-0.05427100	2.12188700
H	3.57200500	-0.17164400	3.12084500
H	4.23885200	0.80083300	1.98050200
H	-0.92050900	0.04861700	1.93906600
N	3.68795800	-0.14014200	-0.65309500
H	3.77448400	0.30354000	-1.55330500
H	4.52063200	-0.14302000	-0.08632700
H	-0.88308400	0.11221100	-0.55679800

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *ortho* (conformer no 3)
[total energy (hartree): -342.957433212]

C	-0.00142600	0.00000100	-0.01136400
C	0.01204800	0.00000100	1.38723700

C	1.21308000	0.00000000	2.09559800
C	2.42366600	0.00000000	0.00982600
C	1.22255700	0.00000100	-0.70953000
H	1.20299300	-0.00000100	3.18171000
C	2.42528000	-0.00000100	1.40444200
H	3.36486000	0.00000000	-0.53589600
N	-1.27953700	0.00000200	-0.67817100
H	-1.30756300	0.79785300	-1.31245100
H	-1.30757300	-0.79786200	-1.31243600
H	-0.94422600	0.00000100	1.90032300
H	3.36692200	-0.00000100	1.94588000
N	1.18317000	0.00000200	-2.15430200
H	1.68058000	0.81167500	-2.51518100
H	1.68057900	-0.81167000	-2.51518200

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *ortho* (conformer no 4)
[total energy (hartree): -342.949143416]

C	0.01609800	0.00000100	0.01288000
C	-0.01384900	0.00000000	1.41704600
C	1.20696200	-0.00000100	2.12191800
C	2.42288700	-0.00000100	0.00186200
C	1.21430400	0.00000000	-0.69599000
H	-0.93006800	0.00000200	-0.52377900
H	1.20513600	0.00000100	-1.78218200
N	-1.26105600	0.00000100	2.13699500
H	-1.81182200	0.81306900	1.87064500
H	-1.81182100	-0.81306900	1.87065000
C	2.40805800	-0.00000100	1.39395300
H	3.34585200	-0.00000200	1.94514100
N	1.20707600	-0.00000300	3.56202400
H	1.71333700	-0.81308000	3.90548100
H	1.71331800	0.81308500	3.90548400
H	3.36818800	-0.00000100	-0.53322400

b3lyp/6-31G(d,p): OCH_3-C_6H_4-OCH_3, *ortho* (conformer no 1)
[total energy (hartree): -461.300739736]

C	0.00073200	0.00278500	0.00025500
C	-0.00015600	0.00069000	1.39931800
C	1.19889400	-0.00093800	2.10461700
C	2.40813200	-0.01271000	1.40344000
C	2.42748300	-0.01301700	0.01207000
C	1.20817700	0.00389500	-0.70351100
H	-0.94836700	0.00503500	1.92844600
H	-0.94232200	0.01318800	-0.53330100
H	3.36240900	-0.01266400	1.92058600
O	1.31325300	0.02969000	-2.06684400
C	0.11756200	0.08672700	-2.82824600
H	-0.51125700	-0.79804400	-2.66517300
H	-0.46521100	0.98736800	-2.59746500
H	0.42823600	0.11853800	-3.87351000
O	3.64000700	0.04263300	-0.63357600
C	3.99810900	-1.11777600	-1.38737900
H	4.03507300	-2.00698400	-0.74441000
H	3.30151700	-1.29275400	-2.21223600
H	4.99543700	-0.92364900	-1.78752900
H	1.20067700	0.00220700	3.19001900

b3lyp/6-31G(d,p): OCH_3-C_6H_4-OCH_3, *ortho* (conformer no 2)
[total energy (hartree): -461.299229756]

C	0.00019400	-0.00115100	-0.00204400
C	-0.00152200	0.00070800	1.39330600

C	1.22188100	0.00154200	2.09034700
C	2.42126200	0.03440400	1.37811700
C	2.41564100	0.04696100	-0.01757200
C	1.20385500	0.01689400	-0.70850300
H	-0.95686400	-0.01421600	-0.51402900
H	1.19194900	0.01741300	-1.79417700
H	3.34929400	0.04674300	1.94104100
O	-1.20819500	-0.04484500	2.05899100
C	-1.53959800	1.14768200	2.78095000
H	-1.62907000	2.00200300	2.09833100
H	-2.50678100	0.96064000	3.25187200
H	-0.79100100	1.37081300	3.54708000
O	1.26364500	0.01658200	3.46862600
C	0.83675400	-1.20000200	4.09353900
H	-0.20064600	-1.43700900	3.83855700
H	1.48446500	-2.03517900	3.79902800
H	0.92517600	-1.03800000	5.16970500
H	3.35560100	0.07035600	-0.56048800

b3lyp/6-31G(d,p): OCH_3-C_6H_4-OCH_3, *ortho* (conformer no 3)
[total energy (hartree): -461.302485278]

C	-0.00003500	0.00033000	-0.00002800
C	-0.00004000	0.00088400	1.40205000
C	1.20030800	0.00087500	2.10878200
C	2.42877500	0.00030300	1.39886000
C	2.41569800	-0.00024600	0.00591300
C	1.20078500	-0.00023300	-0.69402800
H	-0.94296300	0.00132300	1.93572100
H	-0.94573400	0.00035300	-0.53301500
O	1.31020600	0.00139200	3.46877300
C	0.11497100	0.00193100	4.22931100
H	-0.49260400	-0.89144000	4.03343000
H	0.42477000	0.00224000	5.27545200
H	-0.49221400	0.89542700	4.03279000
H	3.34862100	-0.00069300	-0.54513000
O	3.55194200	0.00034200	2.17339400
C	4.80786500	-0.00027100	1.51812400
H	5.55929100	-0.00014300	2.30915900
H	4.94128500	-0.89397100	0.89431800
H	4.94176900	0.89283700	0.89357300
H	1.21111500	-0.00066500	-1.77952700

b3lyp/6-31G(d,p): OH-C_6H_4-OH, *ortho* (conformer no 1)
[total energy (hartree): -382.699292274]

C	-0.01208400	0.00009700	0.01745900
C	-0.00518900	0.00044600	1.40775700
C	1.21223200	-0.00012300	2.09716900
C	2.41130200	-0.00103600	1.38680100
C	2.40416700	-0.00138800	-0.01089200
C	1.19581100	-0.00082500	-0.70231400
H	-0.94812500	0.00116300	1.95072100
H	3.35879900	-0.00148300	1.91639500
O	1.18531500	-0.00116500	-2.06586800
H	0.25845800	-0.00066300	-2.34874400
H	3.32626200	-0.00210000	-0.58271700
O	-1.14993500	0.00059900	-0.76083500
H	-1.93192700	0.00126200	-0.19535300
H	1.21416900	0.00015200	3.18234200

b3lyp/6-31G(d,p): OH-C_6H_4-OH, *ortho* (conformer no 2)
[total energy (hartree): -382.692652705]

C	-0.00128800	0.00001200	-0.00600000
C	0.00582800	0.00051200	1.39256000
C	1.20507200	0.00006500	2.10245600
C	2.42596600	-0.00090200	1.39755900
C	2.41101900	-0.00139300	0.00404800
C	1.20345100	-0.00094000	-0.70153500
H	-0.93239200	0.00126100	1.94415700
H	-0.94691500	0.00037600	-0.53848400
H	1.21518300	-0.00133500	-1.78670900
O	1.27500600	0.00051500	3.46710500
H	0.37571000	0.00115900	3.81997900
O	3.57261800	-0.00131300	2.14069100
H	4.32822400	-0.00199800	1.53876000
H	3.35787100	-0.00214300	-0.53260600

b3lyp/6-31G(d,p): SH-C_6H_4-SH, *ortho* (conformer no 1)
[total energy (hartree): -1028.62947568]

C	0.00002300	0.00041200	-0.00007700
C	-0.00008200	0.00031700	1.40091200
C	1.22890900	0.00017100	2.08936900
C	2.42362700	0.00814500	1.35777600
C	2.41076800	0.01345900	-0.03413600
C	1.19383200	0.00477700	-0.71590900
H	3.37259800	0.00122100	1.88593400
H	1.16973300	0.00609900	-1.80110100
S	-1.52387800	0.02384600	2.34075300
H	-2.33361300	-0.23700200	1.29682800
H	-0.94584100	0.00652800	-0.53377700
S	1.22403700	-0.03399500	3.87978200
H	2.53061200	0.25718900	4.02623100
H	3.34876400	0.01943200	-0.58034600

b3lyp/6-31G(d,p): SH-C_6H_4-SH, *ortho* (conformer no 2)
[total energy (hartree): -1028.63098221]

C	0.00000300	0.00001100	0.00003400
C	0.00001400	0.00029200	1.40011000
C	1.22697200	0.00051100	2.09310400
C	2.42336000	-0.02344100	1.36313200
C	2.40837700	-0.01925700	-0.02934900
C	1.19453100	0.00060300	-0.71606400
H	3.37363500	-0.02898700	1.88876000
H	1.17509400	0.00112100	-1.80123500
S	-1.58576500	0.07993400	2.23423500
H	-1.33751200	-0.86628500	3.16566800
H	-0.95119800	-0.01302800	-0.52241200
S	1.21771300	0.03706300	3.88098300
H	2.53677800	-0.19660200	4.02742600
H	3.34783600	-0.02947000	-0.57354700

b3lyp/6-31G(d,p): SH-C_6H_4-SH, *ortho* (conformer no 3)
[total energy (hartree): -1028.63145012]

C	0.00038300	0.00103000	0.00088500
C	0.00115200	0.00219100	1.40346200
C	1.23630300	0.00181500	2.08643400
C	2.42851400	-0.03211900	1.35139000
C	2.41369800	-0.04615600	-0.04120500
C	1.19329100	-0.01880000	-0.71601700
H	3.37146200	-0.03189700	1.88815500
H	1.16562900	-0.02497300	-1.80143100
S	-1.58976300	0.05579800	2.21185700
H	-1.17754200	-0.48768200	3.37734100

H	-0.94878300	-0.00332600	-0.52619400
S	1.36981100	-0.04927000	3.87849200
H	0.68572700	1.08658500	4.14032400
H	3.34876800	-0.06783300	-0.59189900

b3lyp/6-31G(d,p): tBu-C_6H_4-tBu, *ortho* (conformer no 1)
[total energy (hartree): -546.750711270]

C	0.00060100	-0.00064400	-0.00060100
C	-0.00017800	0.00047100	1.44349600
C	1.26375100	-0.00230600	2.07234400
C	2.48572700	0.04440900	1.41318000
C	2.48433500	0.10760500	0.03114400
C	1.26223300	0.07945200	-0.62881700
H	1.30496600	0.11762800	-1.70638900
H	1.30813900	-0.03943300	3.14992300
C	-1.20349500	-0.03324700	-1.01279300
C	-2.29900300	-1.07019600	-0.66895400
C	-1.79331200	1.39127800	-1.18378900
C	-0.75304000	-0.46036400	-2.44118200
H	-1.87304700	-2.07900700	-0.64260900
H	-2.80603800	-0.89976700	0.27415100
H	-3.06598800	-1.05743500	-1.45056000
H	-1.02048400	2.06915900	-1.56061700
H	-2.61044900	1.37654700	-1.91487800
H	-2.17789700	1.81896500	-0.25997300
H	-1.64521200	-0.59381500	-3.06049400
H	-0.13849600	0.29118100	-2.94315400
H	-0.20727100	-1.40881900	-2.43437200
H	3.40754000	0.16679900	-0.53812200
C	-1.20276900	-0.04812200	2.45843900
C	-0.78319900	0.43666300	3.87819900
C	-2.38476900	0.88651000	2.10732200
C	-1.67268200	-1.51406600	2.64875300
H	-0.11350800	-0.25728100	4.39226400
H	-0.30881900	1.42251200	3.85216500
H	-1.68087300	0.51521300	4.49883300
H	-2.04553300	1.92646500	2.05263200
H	-2.89085400	0.65098400	1.17743600
H	-3.13689200	0.82884700	2.90127100
H	-2.48919500	-1.55762300	3.37942100
H	-2.01995000	-1.98315000	1.72960500
H	-0.84697200	-2.12149600	3.03338800
H	3.41047300	0.04123500	1.98301700

[2.3] b3lyp/6-31G(d,p): *meta*

b3lyp/6-31G(d,p): BF_2-C_6H_4-BF_2, *meta*
[total energy (hartree): -680.396702686]

C	-0.01621500	0.00003600	-0.03342300
C	0.00499700	0.00047500	1.37398900
C	1.20982600	-0.00012500	2.07512100
C	2.41447100	-0.00117800	1.37367400
C	2.43531800	-0.00164800	-0.03374400
C	1.20946200	-0.00102400	-0.71784100
H	3.35526600	-0.00165100	1.91702100
H	-0.93565600	0.00129900	1.91758200
H	1.20931600	-0.00137100	-1.80442300
H	1.20996900	0.00022600	3.16091900
B	-1.35976400	0.00071900	-0.80184000
B	3.77867100	-0.00283100	-0.80250200
F	4.94263700	-0.00342700	-0.16002300
F	3.82141000	-0.00329800	-2.13022300

F	-2.52356900	0.00171900	-0.15907000
F	-1.40283400	0.00033600	-2.12955000

b3lyp/6-31G(d,p): BH_2-C_6H_4-BH_2, *meta*
[total energy (hartree): -283.143201647]

C	-0.02860100	0.00004000	-0.03024000
C	0.00666700	0.00051800	1.38389100
C	1.20982600	-0.00005800	2.08776900
C	2.41280400	-0.00113500	1.38358100
C	2.44770900	-0.00166500	-0.03055800
C	1.20946700	-0.00105200	-0.70371200
H	3.35330000	-0.00158800	1.92905200
H	-0.93369000	0.00136100	1.92960200
H	1.20932700	-0.00143700	-1.79114300
H	1.20996600	0.00032800	3.17382000
B	-1.36080400	0.00069400	-0.79920400
H	-2.40060300	0.00162600	-0.20836100
H	-1.36776500	0.00028000	-1.99448000
B	3.77971300	-0.00286200	-0.79986500
H	3.78636400	-0.00329400	-1.99514300
H	4.81966600	-0.00337200	-0.20929200

b3lyp/6-31G(d,p): Br-C_6H_4-Br, *meta*
[total energy (hartree): -5374.46363881]

C	0.01616000	0.00004400	0.00793600
C	-0.00686900	0.00054500	1.40139300
C	1.21148600	-0.00000200	2.07825000
C	2.42743400	-0.00101500	1.39762500
C	2.41647500	-0.00149400	0.00250200
C	1.21371300	-0.00097200	-0.70450600
H	3.36071600	-0.00142100	1.94821300
H	3.35667500	-0.00228700	-0.54038200
H	1.20354000	-0.00133900	-1.78788200
Br	1.20561500	0.00068100	3.98846300
Br	-1.64068300	0.00077700	-0.94298600
H	-0.94416400	0.00133900	1.94269900

b3lyp/6-31G(d,p): CHO-C_6H_4-CHO, *meta* (conformer no 1)
[total energy (hartree): -458.904031312]

C	0.00419500	0.00000000	-0.03621900
C	0.00971600	0.00000000	1.36712200
C	1.21364800	0.00000000	2.07016200
C	2.41758000	0.00000000	1.36712200
C	2.42310100	0.00000000	-0.03621900
C	1.21364800	0.00000000	-0.73710400
H	3.36337000	0.00000000	1.90403900
H	-0.93607400	0.00000000	1.90403900
H	1.21364800	0.00000000	-1.82222800
H	1.21364800	0.00000000	3.15546900
C	-1.28740100	0.00000000	-0.76825400
O	-1.39122100	0.00000000	-1.97812500
C	3.71469700	0.00000100	-0.76825400
O	3.81851700	-0.00000100	-1.97812500
H	-2.18886900	0.00000000	-0.11591300
H	4.61616500	-0.00000100	-0.11591300

b3lyp/6-31G(d,p): CHO-C_6H_4-CHO, *meta* (conformer no 2)
[total energy (hartree): -458.905398827]

C	-0.01037100	0.00000000	0.00417600
C	0.01286900	0.00000000	1.41063400
C	1.22579900	0.00000000	2.09087400

C	2.42369100	0.00000000	1.37065000
C	2.41084500	0.00000000	-0.02946700
C	1.18635900	0.00000000	-0.71100900
H	3.37641900	0.00000000	1.89520300
H	-0.93455000	-0.00000100	1.94028400
H	1.19383100	0.00000000	-1.79792900
H	1.24341600	-0.00000100	3.17617500
C	-1.30718900	-0.00000100	-0.71724700
O	-2.39309900	0.00000400	-0.17160300
C	3.68548500	0.00000100	-0.78650400
O	3.76163700	0.00000000	-1.99947200
H	-1.22105700	-0.00000300	-1.82549400
H	4.60112400	0.00000100	-0.15507300

b3lyp/6-31G(d,p): CHO-C_6H_4-CHO, *meta* (conformer no 3)
[total energy (hartree): -458.905267855]

C	0.00130600	-0.00000100	0.00850400
C	0.00686000	0.00000000	1.41194900
C	1.21364800	0.00000000	2.10965400
C	2.42043600	0.00000000	1.41194900
C	2.42599000	-0.00000100	0.00850400
C	1.21364800	-0.00000100	-0.68782200
H	3.37462700	0.00000000	1.92939700
H	-0.94733100	0.00000000	1.92939700
H	1.21364800	-0.00000100	-1.77683900
H	1.21364800	0.00000000	3.19522000
C	-1.28261500	-0.00000100	-0.73300700
O	-2.37850900	0.00000100	-0.20802800
C	3.70991100	0.00000000	-0.73300700
O	4.80580500	0.00000100	-0.20802800
H	-1.17789600	0.00000100	-1.84052100
H	3.60519200	0.00000100	-1.84052100

b3lyp/6-31G(d,p): Cl-C_6H_4-Cl, *meta*
[total energy (hartree): -1151.44590464]

C	0.01594700	0.00004300	0.00735200
C	-0.00699200	0.00053900	1.40140900
C	1.21169700	0.00000000	2.07873600
C	2.42813100	-0.00101600	1.39760100
C	2.41598300	-0.00149600	0.00278400
C	1.21416300	-0.00096400	-0.70529200
H	3.36079400	-0.00142600	1.94948100
H	3.35612400	-0.00228800	-0.53993700
H	1.20278600	-0.00132900	-1.78884900
Cl	1.20490200	0.00059600	3.83555200
Cl	-1.50887400	0.00072300	-0.86531600
H	-0.94466500	0.00132500	1.94279700

b3lyp/6-31G(d,p): CN-C_6H_4-CN, *meta*
[total energy (hartree): -416.737207800]

C	-0.00001800	0.00003700	-0.01756400
C	0.00139400	0.00053200	1.38779700
C	1.20997900	-0.00004600	2.08001200
C	2.41843400	-0.00111200	1.38756900
C	2.41958200	-0.00161000	-0.01779100
C	1.20971500	-0.00103600	-0.72417700
H	3.36200800	-0.00156600	1.92203900
H	-0.94208000	0.00136600	1.92244200
H	1.20961400	-0.00141700	-1.80784800
H	1.21008200	0.00033700	3.16483600
C	-1.24411100	0.00063900	-0.73287200

N	-2.25504600	0.00113200	-1.30730700
C	3.66353800	-0.00271500	-0.73333600
N	4.67436100	-0.00361300	-1.30796700

b3lyp/6-31G(d,p): COOH-C_6H_4-COOH, *meta* (conformer no 1)
[total energy (hartree): -609.410573230]

C	0.00333300	0.05291700	-0.00010500
C	0.00528800	0.02862200	1.40224800
C	1.21364800	0.01664000	2.09708600
C	2.42200800	0.02862200	1.40224800
C	2.42396300	0.05291700	-0.00010500
C	1.21364800	0.06497800	-0.69806800
H	3.36461900	0.01931400	1.93720600
H	-0.93732300	0.01931400	1.93720600
H	1.21364800	0.08360800	-1.78180200
H	1.21364800	-0.00212400	3.18230600
C	-1.25869400	0.06653100	-0.79021900
O	-1.31849700	0.08786200	-2.00215200
O	-2.36950300	0.05253300	-0.01058900
H	-3.12263900	0.06321800	-0.62417400
C	3.68599000	0.06653100	-0.79021900
O	3.74579300	0.08786200	-2.00215200
O	4.79679900	0.05253300	-0.01058900
H	5.54993500	0.06321800	-0.62417400

b3lyp/6-31G(d,p): COOH-C_6H_4-COOH, *meta* (conformer no 2)
[total energy (hartree): -609.411327225]

C	0.00444200	-0.04814400	-0.04023000
C	0.00771600	0.00852700	1.36030200
C	1.21364800	0.03650700	2.05723700
C	2.41958000	0.00852700	1.36030200
C	2.42285400	-0.04814400	-0.04023000
C	1.21364800	-0.07663800	-0.74286600
H	3.37209700	0.02975100	1.87878100
H	-0.94480100	0.02975100	1.87878100
H	1.21364800	-0.12025300	-1.82423700
H	1.21364800	0.08023300	3.14165400
C	-1.31330700	-0.07553700	-0.73199300
O	-2.38981300	-0.05149400	-0.17001800
O	-1.20277000	-0.13117300	-2.08195500
H	-2.11254600	-0.14440300	-2.42238100
C	3.74060300	-0.07553700	-0.73199300
O	4.81710900	-0.05149400	-0.17001800
O	3.63006600	-0.13117300	-2.08195500
H	4.53984200	-0.14440300	-2.42238100

b3lyp/6-31G(d,p): COOH-C_6H_4-COOH, *meta* (conformer no 3)
[total energy (hartree): -609.411145727]

C	0.01657400	0.04435500	-0.02890100
C	0.01085900	0.00082400	1.37275800
C	1.21168100	-0.01349300	2.07727600
C	2.42514800	0.01511300	1.39010100
C	2.43592900	0.05855300	-0.01102400
C	1.23016800	0.07318900	-0.72017800
H	3.36452500	0.00405700	1.93073500
H	-0.94476300	-0.02115100	1.88545500
H	1.25523600	0.10669700	-1.80250300
H	1.20436100	-0.04705700	3.16207200
C	-1.29702100	0.05768300	-0.72983900
O	-2.37640200	0.03249900	-0.17314500
O	-1.17738000	0.10152800	-2.07831200

H	-2.08420800	0.10639300	-2.42671600
C	3.70186900	0.09019600	-0.79348600
O	3.76731400	0.12845600	-2.00527100
O	4.80897000	0.07192100	-0.00951600
H	5.56504100	0.09533300	-0.61912800

b3lyp/6-31G(d,p): F-C_6H_4-F, *meta*
[total energy (hartree): -430.721314704]

C	0.02515900	0.00004000	0.01275600
C	-0.00904700	0.00052100	1.40269400
C	1.21166700	-0.00002800	2.06817500
C	2.43024600	-0.00103500	1.39760000
C	2.41745800	-0.00149500	0.00187100
C	1.21518900	-0.00094900	-0.70725300
H	3.35429100	-0.00144600	1.96379500
H	3.35744900	-0.00227900	-0.54072700
H	1.18711300	-0.00128400	-1.79059500
F	1.20698300	0.00039700	3.41596800
F	-1.14448400	0.00056900	-0.65695500
H	-0.94697800	0.00129400	1.94397200

b3lyp/6-31G(d,p): Li-C_6H_4-Li, *meta*
[total energy (hartree): -246.026946020]

C	-0.03985700	0.00006000	-0.04150400
C	0.03214100	0.00051500	1.37556800
C	1.22267900	0.00002800	2.14748600
C	2.41937000	-0.00100100	1.39460700
C	2.42224700	-0.00150000	-0.00309600
C	1.21099300	-0.00097400	-0.70048600
H	3.38669500	-0.00143800	1.90361100
H	3.36727600	-0.00230100	-0.54816300
H	1.25457600	-0.00138900	-1.79265000
Li	1.16327000	0.00076000	4.11684500
Li	-1.77720600	0.00086100	-0.97037100
H	-0.92001800	0.00132000	1.92487700

b3lyp/6-31G(d,p): N(CH_3)$_2$-C_6H_4-N(CH_3)$_2$, *meta* (conformer no 1)
[total energy (hartree): -500.203527003]

C	-0.02962000	0.06769300	-0.00323800
C	0.00218200	0.09000500	1.40786300
C	1.25368100	0.02376000	2.05245500
C	2.40377400	-0.04587300	-0.08006900
C	1.16575900	0.00694500	-0.71144200
H	-0.96614400	0.10167300	-0.54369200
H	1.28844400	0.03069600	3.13047900
H	1.13111000	0.00034900	-1.79795800
N	-1.17479200	0.19308100	2.15229600
C	-1.13271400	-0.04630200	3.58347800
H	-0.48981200	0.68515000	4.08651200
C	-2.44915400	0.01259100	1.47889200
H	-3.25679300	0.14876000	2.20032200
H	-2.58490100	0.76193500	0.69160600
H	-2.13705100	0.06788900	3.99497600
H	-2.56092300	-0.98298900	1.01980300
H	-0.76632200	-1.05265300	3.84386600
C	2.46154900	-0.05120400	1.33040700
N	3.68358300	-0.14663200	1.99954100
C	3.73272400	0.10877000	3.42791700
C	4.91234700	0.02805500	1.24480400
H	4.76057700	-0.00638000	3.77623500
H	3.38829300	1.11986800	3.69974000

H	3.11954200	-0.61381500	3.97849600
H	5.76424000	-0.10071700	1.91487300
H	4.99896900	-0.72885700	0.45788200
H	4.99391200	1.01920600	0.77006300
H	3.30411800	-0.08716800	-0.67833700

b3lyp/6-31G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *meta* (conformer no 2)
[total energy (hartree): -500.203562089]

C	-0.00264700	-0.05403800	-0.00594200
C	0.00030400	-0.00420600	1.40485600
C	1.24081100	0.01639800	2.07347800
C	2.43404400	-0.09848400	-0.03321600
C	1.20774900	-0.10121500	-0.68916300
H	-0.92859300	-0.04857700	-0.56534800
H	1.25421500	0.08235300	3.14990400
H	1.19499200	-0.13287300	-1.77571400
N	-1.19523800	0.01762700	2.12606400
C	-2.43982900	0.25687900	1.41636600
H	-2.61562100	-0.51802900	0.66254400
C	-1.16408400	0.31976900	3.54524300
H	-2.18050800	0.28311600	3.94111700
H	-0.57410900	-0.42430500	4.09253300
H	-3.26867100	0.21484700	2.12532000
H	-0.74376200	1.31399600	3.76873100
H	-2.46982800	1.23453400	0.90876900
C	2.46441300	-0.04961200	1.37728300
N	3.67586000	-0.07309700	2.07156000
C	3.68779900	0.23062400	3.49085400
C	4.91205700	0.12198000	1.33419500
H	3.31238700	1.24092000	3.72208700
H	3.08072800	-0.48917900	4.05164500
H	4.71040600	0.15339000	3.86433100
H	5.75469300	0.04554800	2.02373900
H	5.04085200	-0.65595800	0.57407600
H	4.96763500	1.09986600	0.82911300
H	3.34685500	-0.12664400	-0.61306600

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *meta* (conformer no 1)
[total energy (hartree): -342.974774345]

C	-0.00162500	0.01961900	-0.00202300
C	-0.00613800	0.05640700	1.40296700
C	1.21364800	0.07801100	2.09317600
C	2.42892100	0.01961900	-0.00202300
C	1.21364800	0.00061600	-0.68151800
H	-0.94128400	0.00034800	-0.54693500
H	1.21364800	0.09629900	3.18137100
H	1.21364800	-0.02459700	-1.76798200
N	-1.21347600	0.01740700	2.10846600
H	-1.17420300	0.40775800	3.04028800
H	-2.01153200	0.36610500	1.59504800
C	2.43343400	0.05640700	1.40296700
N	3.64077200	0.01740700	2.10846600
H	3.60149900	0.40775800	3.04028800
H	4.43882800	0.36610500	1.59504800
H	3.36858000	0.00034800	-0.54693500

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *meta* (conformer no 2)
[total energy (hartree): -342.974991773]

C	0.00388800	0.12609500	-0.08913900
C	-0.04289900	0.08454600	1.31486800
C	1.15504700	0.03065800	2.04040000

C	2.43244200	0.05843400	-0.01778900
C	1.23868300	0.11223600	-0.73271600
H	-0.91834300	0.17505900	-0.66129200
H	1.12217700	-0.00118600	3.12775300
H	1.27154800	0.14417400	-1.81850000
N	-1.26882300	0.15694600	1.98612300
H	-2.06054900	-0.16304900	1.44466600
H	-1.26820400	-0.25145800	2.91124300
C	2.39465700	0.01716700	1.38649500
N	3.57798800	-0.09698600	2.12492000
H	3.52122900	0.25653600	3.07067600
H	4.40057700	0.25208000	1.65173100
H	3.38754700	0.04155800	-0.53526800

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *meta* (conformer no 3)
[total energy (hartree): -342.956564779]

C	0.00582600	0.00000000	-0.00935800
C	-0.01352300	0.00000000	1.39226100
C	1.19804200	0.00000000	2.08707800
C	2.42607100	0.00000000	0.01035200
C	1.22039700	0.00000000	-0.69382000
H	-0.93292000	0.00000000	-0.55813000
H	1.16702700	0.00000000	3.17306700
H	1.22860600	0.00000000	-1.78016300
N	-1.23641400	0.00000000	2.16158400
H	-1.79976000	0.81188300	1.91609400
H	-1.79976000	-0.81188300	1.91609400
C	2.42350400	0.00000000	1.40734200
N	3.69504000	0.00000000	2.09301100
H	3.75627100	-0.81146100	2.70507900
H	3.75627100	0.81146100	2.70507900
H	3.38087900	0.00000000	-0.50490200

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *meta* (conformer no 4)
[total energy (hartree): -342.955935891]

C	0.00416800	0.00000000	-0.01345800
C	-0.00382000	0.00000000	1.38734400
C	1.21364800	0.00000000	2.07445100
C	2.42312800	0.00000000	-0.01345800
C	1.21364800	0.00000000	-0.70874700
H	-0.93831300	0.00000000	-0.55575600
H	1.21364800	0.00000000	3.15854800
H	1.21364800	0.00000000	-1.79522100
N	-1.22164100	0.00000000	2.16403100
H	-1.78632400	0.81230900	1.92358000
H	-1.78632400	-0.81230900	1.92358000
C	2.43111600	0.00000000	1.38734400
N	3.64893700	0.00000000	2.16403100
H	4.21362000	0.81230900	1.92358000
H	4.21362000	-0.81230900	1.92358000
H	3.36560900	0.00000000	-0.55575600

b3lyp/6-31G(d,p): OCH_3-C_6H_4-OCH_3, *meta* (conformer no 1)
[total energy (hartree): -461.308141420]

C	-0.13399200	-0.04539600	-0.07669500
C	-0.15772600	-0.02996700	1.31740300
C	1.06165100	0.00694500	2.01052500
C	2.26955400	0.02760800	1.31041900
C	2.27122200	0.01165100	-0.08579300
C	1.06103400	-0.02524800	-0.79494700
H	-1.10445700	-0.04663200	1.84219100

H	-1.07463800	-0.07410100	-0.61947200
O	1.17483300	0.02520800	3.37245300
C	-0.01457100	0.00655600	4.14449700
H	-0.60201800	-0.90296000	3.96453900
H	0.30372000	0.02611600	5.18794500
H	-0.64346500	0.88339700	3.94367100
H	1.04134100	-0.03815000	-1.87725400
H	3.20783200	0.05629100	1.85190300
O	3.50704000	0.03445200	-0.66886600
C	3.58118200	0.02063700	-2.08498600
H	4.64396500	0.04390600	-2.33079700
H	3.13430700	-0.88867400	-2.50718000
H	3.09063000	0.89749100	-2.52687100

b3lyp/6-31G(d,p): OCH_3-C_6H_4-OCH_3, *meta* (conformer no 2)
[total energy (hartree): -461.307917277]

C	0.05007800	-0.00361800	0.02843500
C	0.03408400	0.01238200	1.42077600
C	1.24804200	0.01385200	2.11603500
C	2.46830600	-0.00047700	1.42544200
C	2.45711000	-0.01647800	0.02338400
C	1.24829600	-0.01807100	-0.68089400
H	-0.89236600	0.02371500	1.98359200
H	-0.89040300	-0.00484500	-0.51492300
O	1.14921900	0.02986100	3.47984400
C	2.34069200	0.03169000	4.24693600
H	2.95356400	0.92007800	4.04557400
H	2.02657500	0.04480100	5.29174900
H	2.94371400	-0.86754900	4.06499200
H	1.27309100	-0.03058300	-1.76460100
H	3.40358000	0.00070700	1.96649500
O	3.58881600	-0.03136900	-0.74391600
C	4.84883800	-0.03075000	-0.09573700
H	5.59660800	-0.04414900	-0.89017700
H	4.99196100	0.86954000	0.51614700
H	4.98205500	-0.91802300	0.53703100

b3lyp/6-31G(d,p): OCH_3-C_6H_4-OCH_3, *meta* (conformer no 3)
[total energy (hartree): -461.308846463]

C	-0.07268000	-0.04088400	0.07649100
C	0.01385100	-0.03506500	1.45985100
C	1.28164000	-0.00958200	2.06688000
C	2.43510700	0.00973800	1.28505400
C	2.32456000	0.00354700	-0.11526000
C	1.07191900	-0.02188700	-0.73171700
H	-0.86830000	-0.04977200	2.08989400
H	-1.05067600	-0.06072900	-0.39586700
O	1.28128400	-0.00563200	3.43249800
C	2.53071100	0.01704400	4.10350200
H	3.10535800	0.91997900	3.86035100
H	2.30027100	0.01476500	5.16992700
H	3.13610500	-0.86628900	3.86304000
H	0.97242900	-0.02706200	-1.80965400
H	3.42876300	0.02987700	1.71356500
O	3.51806100	0.02417000	-0.78207300
C	3.49148000	0.02097500	-2.20017400
H	4.53410300	0.04017700	-2.52122700
H	3.00926500	-0.88242400	-2.59504400
H	2.97526200	0.90392000	-2.59828100

b3lyp/6-31G(d,p): OH-C_6H_4-OH, *meta* (conformer no 1)

[total energy (hartree): -382.699253017]

C	0.00817600	0.00003600	0.01461600
C	0.00285900	0.00057400	1.40549900
C	1.22684500	0.00002800	2.08700700
C	2.43320600	-0.00102800	1.38502100
C	2.41602400	-0.00155100	-0.01295200
C	1.20334600	-0.00102600	-0.70826600
H	-0.91988100	0.00140500	1.97416400
H	-0.93605100	0.00045200	-0.52202900
H	1.19424500	-0.00143900	-1.79533800
O	1.18276700	0.00058800	3.45269300
H	2.08539200	0.00013100	3.79725700
O	3.62912200	-0.00259300	-0.64377900
H	3.48411500	-0.00285500	-1.59892900
H	3.38967800	-0.00145900	1.90039400

b3lyp/6-31G(d,p): OH-C_6H_4-OH, *meta* (conformer no 2)

[total energy (hartree): -382.698191561]

C	0.02735400	0.00004300	0.01587700
C	0.00775800	0.00058700	1.40953400
C	1.22180700	0.00003700	2.10198400
C	2.43592500	-0.00104400	1.40662900
C	2.43112700	-0.00158100	0.00755700
C	1.22452800	-0.00103400	-0.69782200
H	-0.92041300	0.00142500	1.96930300
H	-0.91320700	0.00047000	-0.52723300
H	1.24542900	-0.00146100	-1.78151700
O	1.16799800	0.00059200	3.46809600
H	2.06649300	0.00010600	3.82258000
O	3.58722800	-0.00264500	-0.72221400
H	4.34375200	-0.00294700	-0.12167100
H	3.37940100	-0.00147200	1.95142100

b3lyp/6-31G(d,p): OH-C_6H_4-OH, *meta* (conformer no 3)

[total energy (hartree): -382.698934527]

C	-0.00253100	0.00005500	-0.00128900
C	-0.01619400	0.00056000	1.39225300
C	1.20192900	0.00000800	2.08476200
C	2.41441000	-0.00104000	1.39415000
C	2.40617600	-0.00153500	-0.00120400
C	1.19744100	-0.00098600	-0.70997700
H	-0.95702800	0.00137800	1.93690700
H	-0.94308600	0.00048600	-0.54425300
H	1.19870700	-0.00136800	-1.79709400
O	1.26692800	0.00044200	3.44997100
H	0.36885900	0.00114500	3.80582400
O	3.62103900	-0.00254700	-0.62735700
H	3.48057700	-0.00276700	-1.58311600
H	3.35274600	-0.00146800	1.93591400

b3lyp/6-31G(d,p): SH-C_6H_4-SH, *meta* (conformer no 1)

[total energy (hartree): -1028.63174132]

C	-0.00234800	0.00008300	-0.02172700
C	-0.00295300	0.00053800	1.37850900
C	1.21004900	-0.00006300	2.06366100
C	2.42286400	-0.00109800	1.37817300
C	2.42187400	-0.00155300	-0.02205800
C	1.20966500	-0.00096800	-0.72111800
H	3.36045000	-0.00154900	1.92484100
H	-0.94039000	0.00135800	1.92543100
H	1.20951800	-0.00133200	-1.80699300

H	1.21020200	0.00029100	3.14964300
S	4.00560900	-0.00291000	-0.85222500
H	3.53116200	-0.00291000	-2.11272200
S	-1.58631400	0.00087600	-0.85145400
H	-1.11222300	0.00027000	-2.11208500

b3lyp/6-31G(d,p): SH-C_6H_4-SH, *meta* (conformer no 2)
[total energy (hartree): -1028.63189880]

C	-0.00628300	-0.00004300	-0.01456900
C	-0.00971500	0.00044600	1.38457900
C	1.20393800	-0.00006700	2.07139600
C	2.41702700	-0.00105400	1.38839600
C	2.41833000	-0.00154300	-0.01293700
C	1.20792700	-0.00103800	-0.71210000
H	3.35355700	-0.00144000	1.93684800
H	-0.94528500	0.00121600	1.93467200
H	1.20335800	-0.00141200	-1.79808900
H	1.20174700	0.00031300	3.15747100
S	4.00320500	-0.00282500	-0.83986800
H	3.53058900	-0.00291000	-2.10096400
S	-1.50800200	0.00054500	-0.98612500
H	-2.36798600	0.00154200	0.05006600

b3lyp/6-31G(d,p): SH-C_6H_4-SH, *meta* (conformer no 3)
[total energy (hartree): -1028.63179148]

C	-0.00274800	-0.00004200	-0.00637600
C	-0.00386800	0.00045800	1.39389900
C	1.20991700	-0.00011900	2.07836500
C	2.42363900	-0.00119000	1.39378000
C	2.42238400	-0.00168400	-0.00649100
C	1.20978300	-0.00110600	-0.70403000
H	3.35823400	-0.00164000	1.94550800
H	-0.93841100	0.00128700	1.94571300
H	1.20973300	-0.00147600	-1.79021200
H	1.20997200	0.00026700	3.16453400
S	3.92617900	-0.00308000	-0.97387600
H	4.78320700	-0.00305800	0.06487200
S	-1.50664300	0.00062900	-0.97360900
H	-2.36356600	0.00168600	0.06522500

b3lyp/6-31G(d,p): tBu-C_6H_4-tBu, *meta* (conformer no 1)
[total energy (hartree): -546.789734451]

C	0.02946900	0.01275000	-0.06659000
C	0.03083400	0.00046200	1.34097100
C	1.20429400	-0.01069000	2.10125900
C	2.42714100	-0.00875900	1.40758700
C	2.45425500	0.00356400	0.01872100
C	1.26655100	0.01411000	-0.71720700
H	1.32224800	0.02336600	-1.79938100
C	-1.31230000	0.02418200	-0.82540500
C	-2.12761100	-1.23717900	-0.45420800
C	-2.11681600	1.28665000	-0.43486800
C	-1.11842700	0.03495200	-2.35325200
H	-1.58572000	-2.14783800	-0.72959200
H	-2.33782700	-1.28585700	0.61813500
H	-3.08798300	-1.24012200	-0.98225000
H	-3.07725600	1.30568500	-0.96241600
H	-2.32623200	1.32078100	0.63820000
H	-1.56730100	2.19675900	-0.69661200
H	-2.09436500	0.04254900	-2.84936700
H	-0.57130100	0.92215600	-2.68821600

H	-0.57836500	-0.85147900	-2.70147400
H	3.40796300	0.00491700	-0.50227500
H	3.36542500	-0.01688100	1.95417200
C	1.19969600	-0.02475400	3.64231600
C	1.93538800	1.22982400	4.17003100
C	-0.22394600	-0.02545000	4.23043200
C	1.92681000	-1.29386300	4.14671500
H	2.97224700	1.26949800	3.82407700
H	1.43703500	2.14525800	3.83482600
H	1.94963000	1.23218200	5.26591500
H	-0.79340000	-0.90784900	3.92074600
H	-0.16926800	-0.03560800	5.32377000
H	-0.78775300	0.86610300	3.93703500
H	1.94046800	-1.31691700	5.24236100
H	1.42257700	-2.19950500	3.79415000
H	2.96356600	-1.33394900	3.80050200
H	-0.92350700	-0.00029300	1.85389400

b3lyp/6-31G(d,p): tBu-C_6H_4-tBu, *meta* (conformer no 2)
[total energy (hartree): -546.789671172]

C	0.04666300	0.01320300	-0.06162400
C	0.08389100	0.00080000	1.34053200
C	1.27724500	-0.01077200	2.07769600
C	2.48084800	-0.00887400	1.36001800
C	2.47282500	0.00387600	-0.03362600
C	1.27218900	0.01462600	-0.74140100
H	1.30243800	0.02404000	-1.82458800
C	-1.31204100	0.02412300	-0.79023000
C	-2.11721700	-1.23847800	-0.40166900
C	-2.10880600	1.28524900	-0.38020900
C	-1.15261900	0.03660800	-2.32195100
H	-1.58090700	-2.14841700	-0.69003300
H	-2.30237400	-1.28823200	0.67525000
H	-3.08955500	-1.24211300	-0.90730700
H	-3.08150200	1.30331700	-0.88482100
H	-2.29277200	1.31845000	0.69755200
H	-1.56699100	2.19640500	-0.65406900
H	-2.13933100	0.04434600	-2.79631100
H	-0.61344600	0.92442800	-2.66796000
H	-0.62010500	-0.84920600	-2.68309000
H	3.41483200	0.00524500	-0.57552300
H	3.43210100	-0.01738500	1.87898500
C	1.22501500	-0.02472500	3.61825800
C	0.48595400	1.23739700	4.12229100
C	0.47033700	-1.28673600	4.09893000
C	2.62965400	-0.03925800	4.25086500
H	1.00476000	2.14742800	3.80381700
H	-0.53882500	1.28847900	3.74313100
H	0.43635000	1.23995400	5.21712900
H	0.97752200	-2.19709100	3.76313900
H	0.42100300	-1.30917000	5.19353100
H	-0.55517900	-1.31788100	3.71951000
H	2.54168700	-0.04925400	5.34206700
H	3.19991100	-0.92675400	3.95769600
H	3.21071000	0.84680800	3.97506300
H	-0.85757300	-0.00001100	1.88165400

b3lyp/6-31G(d,p): tBu-C_6H_4-tBu, *meta* (conformer no 3)
[total energy (hartree): -546.789515747]

C	-0.03542300	0.00463900	-0.01456300
C	0.00453300	-0.00460600	1.38791700

C	1.20515200	0.01560000	2.11359900
C	2.40443000	0.04607700	1.38788800
C	2.39272400	0.05568500	-0.00475400
C	1.18675200	0.03539300	-0.70110500
H	1.20406900	0.04355900	-1.78689600
C	-1.35753900	-0.01738100	-0.80664700
C	-1.44848500	1.24946200	-1.69029000
C	-1.39463900	-1.27321900	-1.70976500
C	-2.59580700	-0.05105800	0.10889800
H	-1.43242800	2.15634700	-1.07703600
H	-0.61688300	1.31148700	-2.39809800
H	-2.37927800	1.24644800	-2.26888000
H	-2.32551400	-1.30178600	-2.28755700
H	-0.56223100	-1.28825500	-2.41912000
H	-1.33838600	-2.18773400	-1.11035500
H	-3.50465600	-0.06563300	-0.50130500
H	-2.61033800	-0.94349600	0.74306000
H	-2.64813700	0.82987700	0.75699000
H	3.33132500	0.07931500	-0.55194600
H	3.35792000	0.06254700	1.90731900
C	1.24266700	0.00542400	3.65471200
C	2.01360600	-1.24443500	4.14185000
C	1.96188600	1.27868200	4.16000200
C	-0.16383500	-0.02749000	4.28217300
H	1.52152600	-2.16299300	3.80584800
H	3.04092900	-1.26089900	3.76658300
H	2.05848400	-1.26380000	5.23672800
H	1.43270000	2.18095900	3.83651000
H	2.00545600	1.28444600	5.25510700
H	2.98773800	1.34246500	3.78603000
H	-0.07849700	-0.03318400	5.37362800
H	-0.75685500	0.84953200	4.00291400
H	-0.72074000	-0.92397300	3.99067700
H	-0.92890600	-0.02842900	1.93258700

[2.4] b3lyp/6-31G(d,p): *para*

b3lyp/6-31G(d,p): BF_2-C_6H_4-BF_2, *para*
[total energy (hartree): -680.395684889]

C	0.00167700	-0.00117500	-0.00083100
C	-0.01336300	0.00048100	1.40592200
C	1.21325300	0.00115500	2.09469100
C	2.41739400	0.00021400	1.39760800
C	2.43243400	-0.00143700	-0.00914100
C	1.20581600	-0.00211600	-0.69791200
H	3.35841400	0.00074900	1.93983900
H	1.20364000	-0.00338200	-1.78404800
H	1.21543300	0.00242600	3.18082700
B	3.77653400	-0.00247200	-0.78251100
F	3.81380400	-0.00398800	-2.11018700
F	4.94162900	-0.00186900	-0.14424900
B	-1.35746800	0.00154500	2.17928600
F	-1.39475100	0.00309200	3.50696000
F	-2.52255800	0.00095600	1.54101500
H	-0.93934500	-0.00172200	-0.54305800

b3lyp/6-31G(d,p): BH_2-C_6H_4-BH_2, *para*
[total energy (hartree): -283.140994504]

C	-0.02619200	0.00004800	-0.01509200
C	0.00091300	0.00048300	1.39793900
C	1.20468300	0.00003600	2.09324700
C	2.44212900	-0.00086600	1.41050200

C	2.41502300	-0.00130000	-0.00252800
C	1.21125400	-0.00085400	-0.69783700
H	-0.94005300	0.00118000	1.94166500
H	1.21199200	-0.00120000	-1.78459300
H	1.20394500	0.00038100	3.18000300
B	-1.36335000	0.00055000	-0.78711700
H	-2.40180400	0.00132000	-0.19538300
H	-1.37027300	0.00017400	-1.98227800
B	3.77928600	-0.00136900	2.18252700
H	4.81774100	-0.00215000	1.59079500
H	3.78621000	-0.00098000	3.37768800
H	3.35598900	-0.00199700	-0.54625500

b3lyp/6-31G(d,p): Br-C_6H_4-Br, *para*
[total energy (hartree): -5374.46370835]

C	-0.00137300	0.00008200	0.00005100
C	-0.00144400	0.00053100	1.39504100
C	1.21223100	-0.00001800	2.07993100
C	2.42598800	-0.00101500	1.39516000
C	2.42605900	-0.00146900	0.00017800
C	1.21237100	-0.00091100	-0.68471600
H	3.36226900	-0.00144100	1.94143600
H	3.36239400	-0.00224700	-0.54600300
Br	1.21217000	0.00059600	3.98956200
H	-0.93778700	0.00130400	1.94121400
Br	1.21250300	-0.00154100	-2.59434700
H	-0.93766100	0.00050400	-0.54621700

b3lyp/6-31G(d,p): CHO-C_6H_4-CHO, *para* (conformer no 1)
[total energy (hartree): -458.904717936]

C	-0.00413300	0.00000000	0.01378000
C	0.01785100	0.00000000	1.41702500
C	1.24082500	0.00000000	2.10389100
C	2.43093900	0.00000000	1.38738900
C	2.40895500	0.00000000	-0.01585500
C	1.18598000	0.00000000	-0.70272100
H	3.38564700	0.00000000	1.90779000
H	1.19998300	0.00000000	-1.78762800
H	1.22682300	0.00000000	3.18879700
C	3.68557800	0.00000000	-0.77353600
O	3.76206800	0.00000000	-1.98627100
H	4.60065200	0.00000000	-0.14179200
C	-1.25877200	0.00000000	2.17470600
H	-2.17384600	0.00000000	1.54296100
O	-1.33526200	0.00000000	3.38744000
H	-0.95884100	0.00000000	-0.50662000

b3lyp/6-31G(d,p): CHO-C_6H_4-CHO, *para* (conformer no 2)
[total energy (hartree): -458.904595192]

C	-0.00530800	0.00000000	0.02494400
C	-0.00762400	0.00000100	1.43091300
C	1.19275200	0.00000100	2.12365700
C	2.40890800	0.00000000	1.41812800
C	2.41165200	-0.00000100	0.01794700
C	1.20559900	-0.00000100	-0.67807600
H	-0.96273100	0.00000200	1.94597000
H	1.19654900	-0.00000100	-1.76518600
H	1.22481100	0.00000100	3.20830400
C	-1.28833200	0.00000000	-0.72145600
O	-2.38504400	-0.00000500	-0.19860500
H	-1.18143100	0.00000500	-1.82847100

C	3.69703900	0.00000000	2.15571700
H	4.60217400	0.00000400	1.50946900
O	3.79271000	-0.00000300	3.36691600
H	3.35740800	-0.00000200	-0.51821500

b3lyp/6-31G(d,p): Cl-C_6H_4-Cl, *para*
[total energy (hartree): -1151.44604267]

C	0.01230200	0.00002700	0.00466800
C	-0.00057400	0.00049600	1.39882700
C	1.20697300	-0.00001100	2.09622700
C	2.40797600	-0.00098900	1.38811300
C	2.42086000	-0.00145800	-0.00604200
C	1.21329700	-0.00094000	-0.70343600
H	3.36294700	-0.00221600	-0.54231900
H	1.20688800	-0.00129100	-1.78743400
Cl	-1.50914400	0.00068200	-0.87367400
H	-0.94267400	0.00125700	1.93508900
Cl	3.92942000	-0.00162900	2.26645500
H	1.21340400	0.00034800	3.18022000

b3lyp/6-31G(d,p): CN-C_6H_4-CN, *para*
[total energy (hartree): -416.737796340]

C	0.00034500	0.00014900	-0.00950800
C	0.00221000	0.00066900	1.39576300
C	1.21823700	0.00004200	2.10007000
C	2.42088800	-0.00109100	1.40568900
C	2.41902400	-0.00161000	0.00042300
C	1.20299300	-0.00098400	-0.70388800
H	3.36335700	-0.00158200	1.94163600
H	1.21012700	-0.00139000	-1.78805300
H	1.21111000	0.00044700	3.18423600
C	3.66114700	-0.00278800	-0.71665500
N	4.66844300	-0.00374800	-1.29793600
C	-1.23991900	0.00184600	2.11282800
N	-2.24722700	0.00280500	2.69408800
H	-0.94212800	0.00064000	-0.54545000

b3lyp/6-31G(d,p): COOH-C_6H_4-COOH, *para* (conformer no 1)
[total energy (hartree): -609.410696320]

C	-0.00657300	0.04726300	0.02370400
C	-0.00800900	0.07745000	1.42485100
C	1.19713800	0.07756200	2.12089500
C	2.40990700	0.04747500	1.41914900
C	2.40984000	0.01732100	0.01763000
C	1.20729800	0.01731000	-0.67689800
H	-0.95001700	0.10062800	1.95981200
H	1.18248600	-0.00553600	-1.76066700
H	1.20449600	0.10075100	3.20418900
C	-1.26795800	0.04581300	-0.76929900
O	-1.32213700	0.01998600	-1.98200300
O	-2.38083400	0.07677000	0.00463200
H	-3.13234400	0.07275100	-0.61111900
C	3.72748300	0.04582200	2.11481000
O	4.80465800	0.01950200	1.55508200
O	3.61398200	0.07711300	3.46552200
H	4.52302700	0.07286200	3.80834900
H	3.36098700	-0.00574600	-0.50246200

b3lyp/6-31G(d,p): COOH-C_6H_4-COOH, *para* (conformer no 2)
[total energy (hartree): -609.410753480]

C	0.01083100	0.05028000	-0.00631300

C	0.00086500	0.05028600	1.39474900
C	1.19794200	0.05027700	2.10157900
C	2.41646500	0.05028000	1.40771300
C	2.42643100	0.05028600	0.00665100
C	1.22935400	0.05027700	-0.70017900
H	-0.95447800	0.05029400	1.90765400
H	1.23056400	0.05028200	-1.78373200
H	1.19673200	0.05028200	3.18513200
C	-1.30240000	0.05028600	-0.71023300
O	-2.38343000	0.05030600	-0.15708000
O	-1.17973500	0.05026500	-2.06021200
H	-2.08633300	0.05027300	-2.40947100
C	3.72969600	0.05028600	2.11163300
O	4.81072600	0.05030600	1.55848000
O	3.60703100	0.05026500	3.46161200
H	4.51362900	0.05027300	3.81087100
H	3.38177400	0.05029400	-0.50625400

b3lyp/6-31G(d,p): F-C_6H_4-F, *para*
[total energy (hartree): -430.720171045]

C	-0.00434700	0.00007100	-0.00000800
C	-0.00441800	0.00051100	1.39510100
C	1.21222400	-0.00004400	2.06871800
C	2.42894600	-0.00103500	1.39521600
C	2.42901700	-0.00148600	0.00012200
C	1.21236100	-0.00091500	-0.67350300
H	3.35434600	-0.00145300	1.96015500
H	3.35447200	-0.00226700	-0.56472600
F	1.21217900	0.00037900	3.41913800
H	-0.92988500	0.00127700	1.95993800
F	1.21245200	-0.00137300	-2.02392300
H	-0.92976000	0.00048000	-0.56493700

b3lyp/6-31G(d,p): Li-C_6H_4-Li, *para*
[total energy (hartree): -246.027951744]

C	0.02570600	0.00005900	-0.00250700
C	0.02563500	0.00051300	1.39760000
C	1.21223700	0.00000800	2.16868300
C	2.39891900	-0.00100000	1.39772100
C	2.39899000	-0.00145500	-0.00238400
C	1.21238700	-0.00094400	-0.77346800
H	3.37152900	-0.00146300	1.90055900
H	3.37165200	-0.00224500	-0.50512300
Li	1.21213700	0.00067400	4.13566500
H	-0.94702800	0.00129800	1.90033800
H	-0.94690500	0.00051500	-0.50534400
Li	1.21248200	-0.00154600	-2.74045000

b3lyp/6-31G(d,p): N(CH_3)$_2$-C_6H_4-N(CH_3)$_2$, *para* (conformer no 1)
[total energy (hartree): -500.200578497]

C	-0.00010000	0.00059800	-0.00007200
C	-0.00000300	0.00013400	1.40807900
C	1.26388300	-0.00036300	2.02881600
C	2.44422300	0.06852400	-0.11466200
C	1.18102000	0.03368200	-0.73585100
H	-0.93339200	-0.03198900	-0.54901100
H	1.34526500	-0.03238900	3.10854800
H	1.10045300	0.02635200	-1.81609200
N	-1.19225200	0.01333800	2.15163200
C	-1.12428000	-0.34655300	3.55707100
H	-0.48574200	0.35224800	4.10729200

C	-2.42946000	-0.31110800	1.46373900
H	-3.25934200	-0.23771300	2.16966200
H	-2.62479300	0.40474700	0.65865700
H	-2.12409800	-0.27952700	3.99100700
H	-2.43763700	-1.32380300	1.02521100
H	-0.73955200	-1.36589100	3.73199600
C	2.44501500	0.03245700	1.29299500
N	3.63460000	0.14901100	-0.85706400
C	4.88432300	-0.14137600	-0.17658900
C	3.58090600	-0.18011100	-2.27072600
H	5.71042200	-0.01485600	-0.87941000
H	5.04932600	0.56079800	0.64709200
H	4.93480000	-1.16391800	0.23553300
H	4.57672200	-0.06077600	-2.70263100
H	3.23914400	-1.21030700	-2.46952600
H	2.91319600	0.50402900	-2.80445700
H	3.37915400	0.02281700	1.84134600

b3lyp/6-31G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 2)
[total energy (hartree): -500.200336590]

C	0.00029200	0.00103400	-0.00072100
C	-0.00000200	-0.00324400	1.40113800
C	1.18675000	-0.00278000	2.13543200
C	2.44203000	-0.01389200	0.09308500
C	1.25753100	0.00623000	-0.63057600
H	1.11351100	0.00817800	3.21599600
H	1.31343900	0.05578300	-1.71371000
C	2.44444100	-0.03005900	1.50568900
N	3.63845500	-0.08414700	2.23807600
C	3.58487500	0.20237800	3.66081900
C	4.88211300	0.23121300	1.55634800
H	4.58737300	0.10637900	4.08236100
H	3.20886800	1.21382700	3.88980400
H	2.94420100	-0.51903400	4.17881500
H	5.71019100	0.12654700	2.26011500
H	5.06490600	-0.46962000	0.73516000
H	4.90858800	1.25294600	1.14172400
H	3.37509500	0.00119900	-0.45684800
N	-1.18621800	0.05781300	-0.77930600
C	-2.42801000	0.30122000	-0.06821800
C	-1.33464700	-0.96544800	-1.81041900
H	-2.32872500	1.18236000	0.57125400
H	-3.21962000	0.49995500	-0.79732300
H	-2.75777900	-0.54701700	0.56025500
H	-2.12548600	-0.66744800	-2.50671700
H	-0.41224700	-1.07652900	-2.38115400
H	-1.59770400	-1.95498300	-1.39516600
H	-0.93547500	-0.00452300	1.94893200

b3lyp/6-31G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 3)
[total energy (hartree): -500.200284614]

C	0.00011500	0.00483700	0.00108500
C	0.00094100	0.00477200	1.40327100
C	1.25815300	0.00719800	2.03248700
C	2.44442500	-0.00195100	-0.10458100
C	1.18599100	-0.00249500	-0.73382900
H	-0.93575100	0.02114300	-0.54584400
H	1.31537000	-0.01725000	3.11637700
H	1.11233000	0.00026200	-1.81449900
N	-1.18661700	-0.04008100	2.18104400
C	-2.42846100	-0.28576000	1.47086600

H	-2.32941400	-1.16984000	0.83549900
C	-1.33323200	0.99076500	3.20459600
H	-2.12739100	0.70108400	3.90060800
H	-0.41224800	1.10175900	3.77760300
H	-3.22038900	-0.48051400	2.20074600
H	-1.59088500	1.97862000	2.78185800
H	-2.75772900	0.55977700	0.83842800
C	2.44255200	0.01837800	1.30777700
N	3.63794200	-0.04374500	-0.83809500
C	3.58360900	0.25928800	-2.25744500
C	4.88199500	0.25871900	-0.15204900
H	4.58720500	0.17612900	-2.67903500
H	2.94922600	-0.46053500	-2.78553100
H	3.20019100	1.27046100	-2.47451700
H	5.70945700	0.16710500	-0.85830100
H	4.90904200	1.27274300	0.28134700
H	5.06530800	-0.45700500	0.65614500
H	3.37582700	0.02654000	1.85744600

b3lyp/6-31G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 4)
[total energy (hartree): -500.200532064]

C	-0.00973900	-0.01294900	-0.01341900
C	-0.00772100	-0.00079100	1.39459400
C	1.25682000	0.01318400	2.01380600
C	2.43509000	0.02217500	-0.13180600
C	1.17055100	0.00819800	-0.75101700
H	-0.94429800	-0.03311900	-0.56085600
H	1.33910700	0.01576900	3.09395700
H	1.08826400	0.00560800	-1.83116800
N	-1.19918800	0.02517700	2.13933400
C	-1.12781600	-0.31016000	3.55080700
H	-0.49477000	0.40296000	4.08902100
C	-2.43595300	-0.31659800	1.45861000
H	-3.26465000	-0.24029100	2.16556900
H	-2.63905300	0.38743500	0.64498800
H	-2.12794200	-0.24390100	3.98405800
H	-2.43734900	-1.33467900	1.03295200
H	-0.73450600	-1.32310300	3.74250300
C	2.43710900	0.03433000	1.27620900
N	3.62655700	-0.00379200	-0.87654500
C	4.86332200	0.33798900	-0.19582500
C	3.55517800	0.33151900	-2.28802300
H	5.69201600	0.26169300	-0.90278700
H	4.86471200	1.35606700	0.22984000
H	5.06643100	-0.36604700	0.61779400
H	4.55530700	0.26528400	-2.72127100
H	2.92215500	-0.38163000	-2.82622800
H	3.16183700	1.34444500	-2.47973700
H	3.37166900	0.05449700	1.82364400

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *para* (conformer no 1)
[total energy (hartree): -342.970778450]

C	0.01043800	0.04307700	0.00939800
C	-0.01700900	0.04328300	1.41142800
C	1.21102300	0.04297400	2.08844800
C	2.44430500	0.04328300	-0.01002800
C	1.21627300	0.04297400	-0.68704800
H	-0.92519300	0.04062400	-0.54503600
H	1.22352600	0.04027200	3.17591900
H	1.20377000	0.04027200	-1.77451900
N	-1.23550400	-0.02038500	2.11511200

H	-1.18747500	0.37798200	3.04452200
H	-2.01700000	0.37498100	1.60744500
C	2.41685800	0.04307700	1.39200200
N	3.66280000	-0.02038500	-0.71371200
H	3.61477100	0.37798200	-1.64312200
H	4.44429600	0.37498100	-0.20604500
H	3.35248900	0.04062400	1.94643600

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *para* (conformer no 2)
[total energy (hartree): -342.970933159]

C	0.00004800	0.00018500	-0.00018100
C	0.00003100	-0.00024300	1.40207600
C	1.19198000	-0.00036700	2.12201900
C	2.43300600	0.00181100	0.06690400
C	1.24105700	0.00193500	-0.65304000
H	1.15817400	-0.00840300	3.20900700
H	1.27486400	0.00997100	-1.74002800
C	2.43298900	0.00138300	1.46916000
N	3.63758900	-0.06620000	2.19657200
H	3.57104800	0.33262300	3.12474900
H	4.42816900	0.33161100	1.70493700
H	3.37932100	-0.00421500	-0.46905600
N	-1.20455100	0.06776900	-0.72759200
H	-1.13801200	-0.33105000	-1.65577200
H	-1.99513400	-0.33003700	-0.23595900
H	-0.94628400	0.00578400	1.93803600

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *para* (conformer no 3)
[total energy (hartree): -342.956307964]

C	-0.00324800	0.00000100	-0.01445700
C	0.00112200	0.00000000	1.38381700
C	1.20329000	0.00000000	2.09096700
C	2.42617400	0.00000100	0.01758300
C	1.22400600	0.00000100	-0.68956700
H	1.19145800	-0.00000100	3.17857800
H	1.23583800	0.00000100	-1.77717800
C	2.43054400	0.00000000	1.41585700
N	3.70449100	0.00000000	2.09584300
H	3.77292400	-0.81224200	2.70578800
H	3.77292400	0.81224100	2.70578900
H	3.38023700	0.00000100	-0.49978100
N	-1.27719500	0.00000100	-0.69444300
H	-1.34562600	0.81224000	-1.30439200
H	-1.34563000	-0.81224400	-1.30438500
H	-0.95294100	0.00000000	1.90118100

b3lyp/6-31G(d,p): NH_2-C_6H_4-NH_2, *para* (conformer no 4)
[total energy (hartree): -342.956141338]

C	-0.00015900	-0.00000100	-0.00802200
C	-0.01609700	0.00000000	1.39379200
C	1.20250300	0.00000100	2.07716200
C	2.42884700	-0.00000100	-0.01768900
C	1.20691500	-0.00000200	-0.70491100
H	-0.94106000	-0.00000200	-0.55384700
H	1.18306700	0.00000200	3.16222200
H	1.20475400	-0.00000300	-1.79266600
N	-1.23594400	0.00000100	2.16629000
H	-1.80062800	0.81245600	1.92657200
H	-1.80062800	-0.81245400	1.92657300
C	2.41127700	0.00000000	1.37931700
N	3.70773900	-0.00000200	-0.68804700

H	3.78219100	-0.81248600	-1.29689200
H	3.78220200	0.81249400	-1.29687300
H	3.36058000	0.00000000	1.90522400

b3lyp/6-31G(d,p): OCH_3-C_6H_4-OCH_3, *para* (conformer no 1)
[total energy (hartree): -461.306105482]

C	-0.00048100	-0.00110100	-0.00001300
C	-0.00047300	-0.00106100	1.38450400
C	1.21022000	-0.00309200	2.09662600
C	2.41441800	-0.00518300	1.39371900
C	2.41441000	-0.00522400	-0.00925600
C	1.21020400	-0.00317300	-0.71214900
H	-0.93063900	0.00055200	1.94314800
H	-0.93065300	0.00047900	-0.55864700
O	1.09619800	-0.00285400	3.46257100
C	2.28885600	-0.00475700	4.22615900
H	2.89880400	0.88750000	4.03104500
H	1.97965500	-0.00414000	5.27263900
H	2.89585100	-0.89907200	4.03123800
H	3.36473100	-0.00682500	1.91418600
O	1.09616700	-0.00301500	-2.07809300
C	2.28881700	-0.00496000	-2.84169400
H	2.89876600	0.88730900	-2.64663600
H	2.89581400	-0.89926400	-2.64672900
H	1.97960300	-0.00440200	-3.88817000
H	3.36471700	-0.00689500	-0.52973300

b3lyp/6-31G(d,p): OCH_3-C_6H_4-OCH_3, *para* (conformer no 2)
[total energy (hartree): -461.305834141]

C	-0.00015100	-0.00024100	0.00019300
C	0.00007800	0.00048400	1.39370800
C	1.21421500	0.00075500	2.09279200
C	2.41403500	0.00029100	1.37570700
C	2.41380600	-0.00043500	-0.01780800
C	1.19967000	-0.00070600	-0.71689100
H	-0.94728800	0.00083000	1.91952000
H	-0.93412600	-0.00045700	-0.55214100
O	1.33062600	0.00145200	3.45897500
C	0.14013400	0.00193500	4.22637000
H	-0.46923700	-0.89141900	4.03484700
H	0.45326800	0.00243200	5.27170700
H	-0.46909200	0.89519600	4.03395500
H	3.34801000	0.00050700	1.92804100
O	1.08325700	-0.00140300	-2.08307500
C	2.27374900	-0.00188500	-2.85047000
H	2.88312000	0.89146900	-2.65894700
H	2.88297600	-0.89514500	-2.65805500
H	1.96061500	-0.00238200	-3.89580700
H	3.36117200	-0.00078000	-0.54361900

b3lyp/6-31G(d,p): OH-C_6H_4-OH, *para* (conformer no 1)
[total energy (hartree): -382.695762140]

C	-0.00359200	0.00017800	0.01344900
C	0.00585200	0.00059300	1.40699000
C	1.21899600	0.00002400	2.09904700
C	2.41963200	-0.00096500	1.38175300
C	2.41018800	-0.00138200	-0.01178200
C	1.19703900	-0.00080800	-0.70384200
H	-0.92148000	0.00136200	1.96981200
H	-0.95364500	0.00063000	-0.51690500
O	1.16887200	0.00047000	3.47028700

H	2.07061200	-0.00002600	3.81590800
H	3.36968100	-0.00141900	1.91211400
O	1.24717600	-0.00126100	-2.07508100
H	0.34543900	-0.00076400	-2.42071100
H	3.33751400	-0.00215300	-0.57461400

b3lyp/6-31G(d,p): OH-C_6H_4-OH, *para* (conformer no 2)
[total energy (hartree): -382.695626704]

C	0.01878600	0.00010400	0.00265700
C	0.01871100	0.00053200	1.39244700
C	1.22723400	0.00001200	2.09903500
C	2.43285200	-0.00093700	1.39646100
C	2.43292700	-0.00136800	-0.00109500
C	1.22738500	-0.00085100	-0.70380000
H	-0.91270600	0.00127600	1.94868600
H	-0.91257100	0.00050400	-0.55368300
O	1.15930500	0.00047800	3.46945200
H	2.05615700	0.00003300	3.82759400
H	3.37892000	-0.00134900	1.93356200
O	1.15960500	-0.00122800	-2.07422500
H	2.05649700	-0.00186800	-2.43226800
H	3.37905300	-0.00211400	-0.53809400

b3lyp/6-31G(d,p): SH-C_6H_4-SH, *para* (conformer no 1)
[total energy (hartree):] -1028.63140028

C	-0.00069300	0.00017500	-0.00428500
C	-0.01441600	0.00066400	1.39430600
C	1.20580600	0.00001900	2.08272600
C	2.41044100	-0.00106600	1.38713800
C	2.42453200	-0.00158100	-0.01379600
C	1.20650700	-0.00096300	-0.70131200
H	3.34447400	-0.00154300	1.94115200
H	1.18778000	-0.00134300	-1.78721900
H	1.21853100	0.00034800	3.16866700
S	4.01171800	-0.00302800	-0.83774100
H	3.53814700	-0.00299500	-2.09845200
S	-1.52162400	0.00221800	2.35676700
H	-2.37717000	0.00129300	1.31669500
H	-0.93173600	0.00069000	-0.56347400

b3lyp/6-31G(d,p): SH-C_6H_4-SH, *para* (conformer no 2)
[total energy (hartree): -1028.63145304]

C	0.00569700	-0.00020600	0.00138800
C	-0.01058100	-0.00006900	1.40123200
C	1.20731800	-0.00066400	2.09110800
C	2.41379300	-0.00137700	1.39581500
C	2.43007100	-0.00151500	-0.00402900
C	1.21217200	-0.00092100	-0.69390500
H	3.34669300	-0.00183800	1.95187900
H	1.19579000	-0.00100200	-1.77977500
H	1.22370100	-0.00058400	3.17697800
S	4.01818100	-0.00242500	-0.82623300
H	3.54592000	-0.00249600	-2.08739100
S	-1.59869100	0.00083800	2.22343600
H	-1.12643000	0.00095700	3.48459400
H	-0.92720300	0.00025700	-0.55467600

b3lyp/6-31G(d,p): tBu-C_6H_4-tBu, *para* (conformer no 1)
[total energy (hartree): -546.790135443]

C	-0.02057000	0.00997700	-0.05428600
C	-0.01051000	-0.01269200	1.34748400

C	1.17768900	-0.02238700	2.07748000
C	2.42762900	-0.00987600	1.44396900
C	2.41756900	0.01279300	0.04220100
C	1.22936900	0.02248700	-0.68779600
H	1.29341900	0.04012000	-1.76996300
C	-1.35520700	0.01948100	-0.82185100
C	-2.16358900	-1.25043900	-0.46525700
C	-2.17053900	1.27222100	-0.42281300
C	-1.15076800	0.04591900	-2.34798500
H	-1.61442100	-2.15520000	-0.74556300
H	-2.37682300	-1.30870700	0.60610200
H	-3.12199700	-1.25562200	-0.99688100
H	-3.12956400	1.28924600	-0.95305500
H	-2.38294400	1.29390400	0.65004300
H	-1.62702600	2.18896000	-0.67367000
H	-2.12320300	0.05222300	-2.85096800
H	-0.60677000	0.93967700	-2.67056700
H	-0.60267800	-0.83378900	-2.70081800
H	3.35639600	0.02317100	-0.50470300
H	-0.94933800	-0.02307300	1.89438600
C	3.76226500	-0.01938800	2.21153700
C	3.55782400	-0.04581500	3.73767000
C	4.57758600	-1.27213700	1.81250300
C	4.57066200	1.25052300	1.85494000
H	3.00974000	0.83390000	4.09049600
H	3.01382000	-0.93956600	4.06026000
H	4.53025900	-0.05212300	4.24065400
H	4.78998800	-1.29382500	0.73964600
H	5.53661100	-1.28916900	2.34274400
H	4.03406500	-2.18887200	2.06336400
H	5.52906900	1.25569400	2.38656600
H	4.78389800	1.30878500	0.78358100
H	4.02150400	2.15529000	2.13524300
H	1.11364100	-0.04002000	3.15964700

b3lyp/6-31G(d,p): tBu-C_6H_4-tBu, *para* (conformer no 2)
[total energy (hartree): -546.790167174]

C	-0.01136100	0.00983400	-0.07050500
C	0.02811300	-0.01346100	1.33450900
C	1.23014500	-0.02262000	2.03282500
C	2.47038400	-0.00846600	1.37104500
C	2.43134700	0.01511600	-0.02594700
C	1.22165400	0.02380800	-0.72866700
H	1.26260600	0.04194900	-1.81195400
C	-1.36273700	0.01945300	-0.80761600
C	-2.16574600	-1.24752200	-0.42892400
C	-2.16601000	1.27538700	-0.39420100
C	-1.19232700	0.04043200	-2.33782600
H	-1.62530600	-2.15441200	-0.71915300
H	-2.35514000	-1.30252600	0.64707700
H	-3.13595700	-1.25173700	-0.93863600
H	-3.13723600	1.29236800	-0.90172400
H	-2.35309700	1.30168800	0.68328800
H	-1.62675400	2.19002900	-0.66140700
H	-2.17542200	0.04632800	-2.81968600
H	-0.65426000	0.93230500	-2.67510700
H	-0.65291800	-0.84116500	-2.69917400
H	3.35249200	0.02721500	-0.59777900
H	-0.89908300	-0.02464200	1.90086700
C	3.78031100	-0.01926300	2.17870900
C	3.83029500	1.22523500	3.09653500

C	3.83903400	-1.29742900	3.04843900
C	5.02533500	0.00243000	1.27226700
H	3.79627600	2.14734800	2.50725000
H	2.99096400	1.24665400	3.79771700
H	4.75540400	1.23064400	3.68416900
H	3.81478700	-2.19675900	2.42447300
H	4.76261600	-1.31708900	3.63816400
H	2.99791800	-1.35284300	3.74567100
H	5.93084400	-0.00659700	1.88751800
H	5.06472900	-0.87170600	0.61412000
H	5.05889200	0.90152300	0.64829700
H	1.19687000	-0.04108500	3.11866000

[3.1] b3lyp/6-311++G(d,p): *mono*

b3lyp/6-311++G(d,p): C_6H_6
[total energy (hartree): -232.311304370]

C	0.00453700	0.00005100	0.00021600
C	0.00446700	0.00049200	1.39487900
C	1.21221900	-0.00005300	2.09230700
C	2.42005500	-0.00104600	1.39499300
C	2.42012500	-0.00149000	0.00034300
C	1.21235700	-0.00093900	-0.69709200
H	3.35917300	-0.00147700	1.93724300
H	3.35929700	-0.00226500	-0.54181400
H	-0.93471700	0.00126700	1.93701500
H	-0.93459400	0.00048100	-0.54201400
H	1.21242300	-0.00128200	-1.78151000
H	1.21217700	0.00029000	3.17672500

b3lyp/6-311++G(d,p): C_6H_5-BF_2
[total energy (hartree): -456.454232394]

C	-0.03078400	0.00005800	-0.02206100
C	-0.01407600	0.00045700	1.38353100
C	1.18952900	-0.00008000	2.08131200
C	2.39689800	-0.00102800	1.38206100
C	2.40054400	-0.00143600	-0.01323200
C	1.19562600	-0.00089500	-0.70901100
H	3.33578300	-0.00145200	1.92496100
H	3.34057600	-0.00217600	-0.55323000
H	-0.95249000	0.00119900	1.92685600
H	1.19974000	-0.00120900	-1.79342900
H	1.18998200	0.00023500	3.16539500
B	-1.36677400	0.00066000	-0.78971600
F	-2.54258700	0.00156100	-0.15954200
F	-1.41915400	0.00032100	-2.12238200

b3lyp/6-311++G(d,p): C_6H_5-BH_2
[total energy (hartree): -257.756689208]

C	-0.03680400	0.00005500	-0.02311400
C	-0.00631600	0.00045500	1.38831800
C	1.19610100	-0.00008100	2.08687200
C	2.40308000	-0.00103100	1.38513700
C	2.40689900	-0.00144600	-0.01099600
C	1.20059200	-0.00090700	-0.70282700
H	3.34264300	-0.00145500	1.92739700
H	3.34770800	-0.00218800	-0.55016300
H	-0.94463600	0.00119900	1.93318400
H	1.20301700	-0.00122500	-1.78785800
H	1.19983800	0.00023600	3.17120700
B	-1.36734800	0.00065300	-0.79093400
H	-1.37497800	0.00032000	-1.98438600

H	-2.40448800	0.00151400	-0.20033600

b3lyp/6-311++G(d,p): C_6H_5-Br
[total energy (hartree): -2805.85393978]

C	0.00684700	0.00004100	0.00196100
C	-0.00184100	0.00053400	1.39646600
C	1.21215200	0.00000300	2.07691400
C	2.42630300	-0.00101100	1.39672200
C	2.41791600	-0.00149900	0.00222500
C	1.21244900	-0.00096800	-0.69726800
H	3.36020700	-0.00141600	1.94387400
H	3.36005200	-0.00229200	-0.53415900
H	-0.93586900	0.00132300	1.94340500
H	-0.93518700	0.00046000	-0.53461100
H	1.21257900	-0.00134400	-1.78097000
Br	1.21197200	0.00068300	3.99672900

b3lyp/6-311++G(d,p): C_6H_5-CHO
[total energy (hartree): -345.669195380]

C	-0.00851700	0.00005600	-0.01074600
C	-0.00516300	0.00046800	1.38821300
C	1.19968700	-0.00008200	2.08637400
C	2.40399600	-0.00104500	1.38414100
C	2.40634400	-0.00145900	-0.01415000
C	1.20551600	-0.00091100	-0.71130600
H	3.34386900	-0.00147900	1.92495200
H	3.34707600	-0.00221200	-0.55286100
H	-0.94863200	0.00122600	1.92556100
H	1.18187900	-0.00121100	-1.79472800
H	1.20165500	0.00023600	3.17023100
C	-1.29978800	0.00065600	-0.73558800
O	-1.42008600	0.00037900	-1.94054100
H	-2.19655000	0.00141600	-0.07995500

b3lyp/6-311++G(d,p): C_6H_5-Cl
[total energy (hartree): -691.934292455]

C	0.00681300	0.00004400	0.00226400
C	-0.00139800	0.00053100	1.39621700
C	1.21216600	0.00000600	2.07709200
C	2.42586900	-0.00101100	1.39644500
C	2.41792500	-0.00149900	0.00249400
C	1.21242900	-0.00096100	-0.69721700
H	3.35737700	-0.00142000	1.94799600
H	3.35989400	-0.00229300	-0.53403000
H	-0.93301000	0.00131300	1.94758900
H	-0.93506100	0.00046200	-0.53443300
H	1.21254100	-0.00133600	-1.78088100
Cl	1.21202400	0.00059000	3.83775400

b3lyp/6-311++G(d,p): C_6H_5-CN
[total energy (hartree): -324.577839150]

C	-0.01073600	0.00005500	-0.00829000
C	-0.01148300	0.00050200	1.39430900
C	1.19587800	-0.00004700	2.08395400
C	2.40284900	-0.00103600	1.38499600
C	2.40444200	-0.00148100	-0.00973400
C	1.20345500	-0.00094100	-0.71044700
H	3.34160900	-0.00146400	1.92689300
H	3.34222900	-0.00225400	-0.55276500
H	-0.95337100	0.00127500	1.92881400
H	1.19526900	-0.00127900	-1.79338800

H	1.19459800	0.00029600	3.16761000
C	-1.25081000	0.00062100	-0.72402400
N	-2.25178800	0.00108000	-1.30150600

b3lyp/6-311++G(d,p): C_6H_5-COOH (conformer no 1)
[total energy (hartree): -420.948281748]

C	-0.03165500	0.00003700	0.02614900
C	-0.00684800	0.00043600	1.42594400
C	1.21231700	-0.00009500	2.09738200
C	2.40699100	-0.00102100	1.37784400
C	2.38450900	-0.00141900	-0.01750400
C	1.16936800	-0.00089100	-0.69289100
H	3.35519200	-0.00143600	1.90388600
H	3.31340200	-0.00214300	-0.57605600
H	-0.93752100	0.00116100	1.97784700
H	1.12960300	-0.00118200	-1.77513500
H	1.23092800	0.00021400	3.18114800
C	-1.30524000	0.00057900	-0.74045200
O	-1.39049000	0.00028400	-1.94655100
O	-2.40571100	0.00146900	0.05624100
H	-3.17430200	0.00176900	-0.53276300

b3lyp/6-311++G(d,p): C_6H_5-COOH (conformer no 2)
[total energy (hartree): -420.937391975]

C	0.00020200	-0.00183200	0.00001900
C	0.00015000	0.00038000	1.39965400
C	1.20095500	0.00173500	2.10023400
C	2.41391500	0.02162800	1.41075000
C	2.42253900	0.04093600	0.01750800
C	1.22055700	0.02604000	-0.68611500
H	3.34971800	0.02881300	1.95794200
H	3.36216300	0.07525000	-0.52143800
H	-0.95046800	-0.00057500	1.91824900
H	1.25100100	0.07577400	-1.77014700
H	1.19267800	-0.00771600	3.18402800
C	-1.32893800	-0.00059800	-0.69574300
O	-2.34918000	0.36274700	-0.17518200
O	-1.34799100	-0.44070800	-1.98384800
H	-0.49636400	-0.82375700	-2.22514700

b3lyp/6-311++G(d,p): C_6H_5-F
[total energy (hartree): -331.580194865]

C	0.00553100	0.00004900	0.00182400
C	-0.00364100	0.00051000	1.39614400
C	1.21221700	-0.00005800	2.06204400
C	2.42815300	-0.00104100	1.39628100
C	2.41914000	-0.00148700	0.00196400
C	1.21237400	-0.00095300	-0.69700200
H	3.35116500	-0.00144400	1.96253800
H	3.35982100	-0.00226400	-0.53656800
H	-0.92671700	0.00129400	1.96229100
H	-0.93508700	0.00047800	-0.53681100
H	1.21243900	-0.00130500	-1.78049300
F	1.21214200	0.00041200	3.41907900

b3lyp/6-311++G(d,p): C_6H_5-Li
[total energy (hartree): -239.203491278]

C	0.00637600	0.00004200	-0.00327900
C	0.01961100	0.00053500	1.39452400
C	1.20792100	0.00004500	2.16117900
C	2.39632800	-0.00098400	1.39465600

C	2.40972500	-0.00149300	-0.00314100
C	1.20808800	-0.00098000	-0.71022700
H	-0.93800900	0.00046000	-0.54098900
H	-0.94864300	0.00133900	1.89643500
H	3.36452500	-0.00142200	1.89668100
H	3.35416700	-0.00229200	-0.54075000
H	1.20815400	-0.00136500	-1.79553100
Li	1.20801600	0.00072300	4.12214200

b3lyp/6-311++G(d,p): C_6H_5-N$(CH_3)_2$
[total energy (hartree): -366.314146016]

C	0.00003100	-0.00557200	0.00064700
C	0.00028100	0.00099700	1.41287700
C	1.25558600	0.00674800	2.05998900
C	2.43805300	0.03257700	1.32796000
C	2.42423300	0.04266400	-0.06516900
C	1.19232900	0.02024900	-0.71546200
H	-0.93202000	-0.03056300	-0.54649100
H	1.31491600	-0.00665700	3.13932000
H	3.38298100	0.03999100	1.86097000
H	1.15136400	0.01712300	-1.79959300
N	-1.18826400	0.01611100	2.13821000
C	-1.14897800	-0.25449800	3.56629800
H	-0.52963500	0.48018200	4.08758200
C	-2.44139100	-0.24497800	1.44871100
H	-3.26282700	-0.14963700	2.15826600
H	-2.60984200	0.48664700	0.65425200
H	-2.15778400	-0.17438000	3.97019900
H	-2.48441100	-1.25062700	1.00300800
H	-0.76125000	-1.25753800	3.80100300
H	3.34908000	0.06001600	-0.62905400

b3lyp/6-311++G(d,p): C_6H_5-NH_2
[total energy (hartree): -287.687735522]

C	-0.00000500	-0.00027800	0.00016500
C	0.00008200	0.00008500	1.40306900
C	2.42168700	-0.00006600	-0.03523500
C	1.19889400	-0.00093700	-0.70575800
H	-0.94470900	0.00441300	-0.53473100
H	1.17492500	-0.00280700	-1.79013200
N	-1.20097600	0.05776800	2.11651600
H	-2.01677300	-0.27836500	1.62639400
H	-1.16139100	-0.28070700	3.06657000
C	2.42536700	0.00174400	1.35933200
H	3.35314500	-0.00133400	-0.58843100
C	1.23194800	0.00251700	2.07444800
H	3.36613700	0.00213600	1.89916100
H	1.24949200	0.00979700	3.15988700

b3lyp/6-311++G(d,p): C_6H_5-OCH_3
[total energy (hartree): -346.867621020]

C	0.01962700	0.00017400	-0.11805700
C	-0.06858400	0.00065600	1.27674100
C	1.10220700	0.00003400	2.03965400
C	2.34939300	-0.00105100	1.40189600
C	2.42002200	-0.00151500	0.01592100
C	1.25467400	-0.00091000	-0.75608800
H	-1.04222500	0.00151400	1.74801200
H	-0.89379100	0.00066400	-0.70271500
O	1.13524200	0.00042700	3.40528600
H	3.24373300	-0.00151900	2.01341600

H	3.39099000	-0.00236500	-0.46697300
C	-0.09492200	0.00136400	4.11549900
H	-0.68751100	-0.89253900	3.89175100
H	0.17113000	0.00139700	5.17135000
H	-0.68636100	0.89594500	3.89141400
H	1.31350300	-0.00127700	-1.83797700

b3lyp/6-311++G(d,p): C_6H_5-OH
[total energy (hartree): -307.558732401]

C	0.00383300	0.00005200	-0.00119700
C	-0.00903000	0.00054500	1.39296500
C	1.19662100	0.00001600	2.09651800
C	2.41054200	-0.00100100	1.40742200
C	2.41012500	-0.00148400	0.01638100
C	1.21036700	-0.00096200	-0.69715300
H	3.33503500	-0.00140400	1.97206000
H	3.35581200	-0.00227900	-0.51416000
H	-0.95256700	0.00134300	1.93126400
H	-0.93659700	0.00047200	-0.54088100
H	1.21717500	-0.00134000	-1.78049200
O	1.25091500	0.00045500	3.46555300
H	0.35825500	0.00113400	3.82622600

b3lyp/6-311++G(d,p): C_6H_5-SH
[total energy (hartree): -630.525369663]

C	-0.01744800	-0.00003900	-0.00743400
C	-0.01279100	0.00040600	1.39092700
C	1.19583300	-0.00007100	2.08373700
C	2.40738300	-0.00100000	1.39543100
C	2.40052400	-0.00144700	0.00129200
C	1.19820300	-0.00097100	-0.70033000
H	3.34513400	-0.00137400	1.93831800
H	3.33571000	-0.00217400	-0.54750300
H	-0.94675100	0.00112300	1.94155900
H	1.20466500	-0.00131400	-1.78465100
H	1.18560700	0.00028400	3.16809200
S	-1.52256500	0.00049800	-0.97127000
H	-2.37853800	0.00159700	0.06905100

b3lyp/6-311++G(d,p): C_6H_5-tBu
[total energy (hartree): -389.607188651]

C	0.03829200	0.00000600	-0.01488400
C	0.04560000	0.00054500	1.38919000
C	1.23442700	0.00006600	2.11233500
C	2.46074500	-0.00098400	1.44822000
C	2.47547600	-0.00154400	0.05769100
C	1.27899100	-0.00105300	-0.66243700
H	3.38896600	-0.00136400	2.00845700
H	3.41958600	-0.00237200	-0.47647100
H	-0.89222400	0.00135900	1.93340400
H	1.32949800	-0.00150900	-1.74336000
H	1.20313000	0.00051000	3.19658100
C	-1.30081400	0.00058000	-0.77541700
C	-2.11045800	-1.26048200	-0.39287500
C	-2.10886800	1.26293700	-0.39378000
C	-1.10694500	-0.00009700	-2.30254400
H	-1.56421100	-2.16990800	-0.65813200
H	-2.32160300	-1.29826000	0.67822300
H	-3.06818600	-1.27175500	-0.92261100
H	-1.56139200	2.17148500	-0.65951100
H	-3.06649300	1.27512600	-0.92367500

H	-2.32014100	1.30165600	0.67726100
H	-2.08291000	0.00032700	-2.79560300
H	-0.56482900	0.88572200	-2.64467800
H	-0.56593800	-0.88684500	-2.64402300

[3.2] b3lyp/6-311++G(d,p): *ortho*

b3lyp/6-311++G(d,p): BF_2-C_6H_4-BF_2, *ortho*
[total energy (hartree): -680.586898593]

C	-0.00005100	0.00054900	0.00042400
C	-0.00039300	-0.00030300	1.40300500
C	1.24333600	-0.00082300	2.08863500
C	2.42894300	0.03823200	1.34036300
C	2.40760000	0.05260800	-0.05343300
C	1.19002800	0.02523300	-0.72525800
H	3.38159500	0.04496800	1.85776300
H	1.16368900	0.02913800	-1.80909600
B	-1.38388600	0.12443500	2.09819900
F	-1.55111900	0.67444300	3.29490400
F	-2.49688700	-0.24751500	1.46563600
H	-0.94575500	-0.00547500	-0.52967100
B	1.39824700	-0.16629000	3.62549000
F	2.52069600	0.21180200	4.23754300
F	0.48926700	-0.75809700	4.39090800
H	3.33808900	0.07932400	-0.60922900

b3lyp/6-311++G(d,p): BH_2-C_6H_4-BH_2, *ortho* (conformer no 1)
[total energy (hartree): -283.188670784]

C	0.00271400	-0.00006100	-0.00694200
C	0.02353800	0.00058000	1.39013200
C	1.23124800	0.00015200	2.08846400
C	2.44924900	-0.00097500	1.39852100
C	2.44054100	-0.00162100	-0.02430200
C	1.20406300	-0.00113300	-0.70291700
H	1.20174400	-0.00160400	-1.78843800
H	1.21009500	0.00069700	3.17405700
B	3.78525200	-0.00271400	-0.74870000
H	3.88988200	-0.00321600	-1.93596400
H	4.78956700	-0.00305400	-0.08311600
H	-0.94303300	0.00030100	-0.53674300
B	3.83454000	-0.00156900	2.12313300
H	4.35719100	-1.02675900	2.43705500
H	4.35815200	1.02318000	2.43690900
H	-0.91123400	0.00144200	1.94125000

b3lyp/6-311++G(d,p): BH_2-C_6H_4-BH_2, *ortho* (conformer no 2)
[total energy (hartree): -283.194684748]

C	-0.00001300	-0.00025800	0.00002100
C	0.00005600	-0.00056100	1.39464100
C	1.19309000	-0.00038700	2.14135500
C	2.44086000	0.00010500	1.43140600
C	2.40858600	0.00040100	0.02436400
C	1.20979800	0.00022700	-0.68831900
H	-0.94696000	-0.00094500	1.92362900
H	1.22043300	0.00046900	-1.77297800
B	3.83506300	0.00036200	2.10458200
H	4.79936400	0.00074800	1.40018200
H	3.98696300	0.00019900	3.28143100
H	3.34716600	0.00077600	-0.51949900
H	-0.93784800	-0.00040700	-0.54503200
B	1.05970100	-0.00076900	3.68379700
H	1.99399500	-0.00070200	4.41527800

H	-0.03833100	-0.00115000	4.15319200

b3lyp/6-311++G(d,p): Br-C_6H_4-Br, *ortho*
[total energy (hartree): -5379.39058763]

C	0.00662500	0.00001300	0.00464300
C	0.00695700	0.00051900	1.39530800
C	1.21266400	0.00004900	2.09898300
C	2.42312400	-0.00094700	1.40021700
C	2.41706600	-0.00145200	0.00433400
C	1.21320800	-0.00096400	-0.69177000
H	3.35955900	-0.00222200	-0.52757300
Br	1.13359600	0.00080500	4.00658600
H	-0.92528300	0.00128900	1.94517700
H	-0.93625400	0.00039700	-0.52924200
Br	4.11508500	-0.00166000	2.28530900
H	1.22283800	-0.00135600	-1.77525800

b3lyp/6-311++G(d,p): CHO-C_6H_4-CHO, *ortho* (conformer no 1)
[total energy (hartree): -459.017255033]

C	-0.03111700	-0.00000100	-0.00715100
C	-0.03137100	-0.00000100	1.40816200
C	1.19169200	-0.00000100	2.09306000
C	2.39386200	0.00000000	1.39991600
C	2.39411300	0.00000000	0.00197300
C	1.19219400	0.00000000	-0.69160600
H	1.17119600	0.00000100	-1.77449900
H	1.17030100	-0.00000100	3.17594500
C	-1.27342500	-0.00000100	-0.83168000
O	-1.26787700	0.00000000	-2.04310500
H	-2.23625600	-0.00000200	-0.29309300
H	3.33218700	0.00000100	-0.54129000
C	-1.27397800	-0.00000200	2.23224000
H	-2.23661100	0.00000300	1.69330100
O	-1.26887200	0.00000200	3.44366700
H	3.33174000	0.00000000	1.94351700

b3lyp/6-311++G(d,p): CHO-C_6H_4-CHO, *ortho* (conformer no 2)
[total energy (hartree): -459.018464102]

C	0.03928000	0.00001000	0.01609800
C	0.06148400	-0.00000300	1.40921400
C	1.28314200	-0.00001200	2.07470500
C	2.49528700	0.00000000	1.37217100
C	2.46931700	0.00000500	-0.04490200
C	1.23398700	0.00000800	-0.69812200
H	1.23521000	0.00000700	-1.78149800
H	1.30514200	-0.00002100	3.15966500
C	3.70047200	-0.00003300	-0.90284800
O	3.63836900	0.00006200	-2.11421300
H	4.66443000	-0.00015800	-0.37875400
H	-0.90681100	0.00001500	-0.51312700
C	3.72028400	0.00003200	2.21688800
H	3.49256000	-0.00004500	3.30354400
O	4.87083200	0.00014000	1.84162600
H	-0.86442800	-0.00000700	1.97247300

b3lyp/6-311++G(d,p): CHO-C_6H_4-CHO, *ortho* (conformer no 3)
[total energy (hartree): -459.006141622]

C	0.04577100	0.00000000	0.06624800
C	0.06330700	0.00000000	1.45931300
C	1.25437200	-0.00000100	2.19431700
C	2.48662700	-0.00000100	1.48270600

C	2.44573300	0.00000000	0.08381700
C	1.24817400	0.00000000	-0.62802400
H	-0.87715800	0.00000000	2.00069500
H	1.25990500	0.00000000	-1.71171400
C	3.87991500	-0.00000200	2.03756100
H	4.63551400	0.00000200	1.22021400
O	4.23594800	0.00000100	3.18564900
H	3.38488100	-0.00000100	-0.45978800
C	1.03841800	-0.00000200	3.67838300
H	-0.04727600	0.00000100	3.92395800
O	1.85465400	0.00000100	4.56081700
H	-0.89855900	0.00000100	-0.46551900

b3lyp/6-311++G(d,p): Cl-C_6H_4-Cl, *ortho*
[total energy (hartree): -1151.55186209]

C	-0.00212800	0.00009900	-0.00276500
C	-0.00217800	0.00056800	1.39539500
C	1.20792200	0.00000000	2.08831700
C	2.41233900	-0.00103800	1.39313600
C	2.41238700	-0.00151500	-0.00032800
C	1.20802200	-0.00094100	-0.69560000
H	3.34642200	-0.00232800	-0.54933400
H	1.19215800	-0.00129300	-1.77799600
Cl	-1.49328300	0.00080100	-0.91497300
H	1.19197700	0.00037900	3.17071300
Cl	-1.49339800	0.00188200	2.30749600
H	3.34633300	-0.00147700	1.94220900

b3lyp/6-311++G(d,p): CN-C_6H_4-CN, *ortho*
[total energy (hartree): -416.836662367]

C	-0.01345800	0.00015400	0.02480100
C	-0.02527900	0.00073500	1.42471900
C	1.19808100	0.00017300	2.13152900
C	2.40488200	-0.00095900	1.42187700
C	2.40041600	-0.00152600	0.03148200
C	1.19321700	-0.00096900	-0.66596900
H	3.33790600	-0.00138800	1.97097800
H	1.19006400	-0.00140700	-1.74930200
C	-1.27803000	0.00189700	2.11451500
N	-2.30475300	0.00283500	2.64319100
H	-0.95527400	0.00059600	-0.50906400
C	1.22625100	0.00074000	3.56134200
N	1.28100800	0.00117500	4.71488200
H	3.34047500	-0.00240500	-0.50696500

b3lyp/6-311++G(d,p): COOH-C_6H_4-COOH, *ortho* (conformer no 1)
[total energy (hartree): -609.570857599]

C	0.00003500	-0.00091800	0.00025600
C	0.00042500	0.00022400	1.39173700
C	1.20166200	0.00076700	2.10541100
C	2.42124800	0.03458800	1.40412800
C	2.40939500	0.01472600	0.00705300
C	1.20743100	-0.00463900	-0.69370700
H	-0.93056000	-0.01558000	1.94476900
H	1.21567900	-0.01425100	-1.77737800
C	3.76445100	0.17086200	2.04795300
O	4.77239100	-0.35303700	1.64192300
O	3.75387900	1.02432100	3.09756600
H	4.65601100	1.05271000	3.45045000
H	3.35587300	0.03114600	-0.51898400
C	1.08296200	-0.11425200	3.59213100

O	0.22673400	0.42103500	4.25202100
O	1.99350500	-0.96297000	4.12189200
H	1.84586100	-0.97738500	5.07959600
H	-0.94050900	-0.00703500	-0.53814000

b3lyp/6-311++G(d,p): COOH-C_6H_4-COOH, *ortho* (conformer no 2)
[total energy (hartree): -609.571138546]

C	-0.00030400	-0.00218700	-0.00037900
C	-0.00056200	-0.00142600	1.39233900
C	1.19966800	0.00037200	2.10304300
C	2.41974200	-0.03154200	1.40308000
C	2.40883900	-0.02531200	0.00441300
C	1.20592800	-0.00689700	-0.69530400
H	-0.93387800	0.00685200	1.94195800
H	1.21279000	-0.00720300	-1.77898400
C	3.70916000	-0.20699200	2.13112800
O	3.82715400	-0.71570000	3.21878700
O	4.77535800	0.22949600	1.41495800
H	5.56446900	0.03208700	1.94104900
H	3.35014900	-0.05566500	-0.52813500
C	1.09187300	0.07510500	3.59778900
O	0.38381300	-0.63947500	4.26128800
O	1.79860400	1.10410800	4.11243100
H	1.70633200	1.06138800	5.07640400
H	-0.94113600	0.00194600	-0.53847500

b3lyp/6-311++G(d,p): COOH-C_6H_4-COOH, *ortho* (conformer no 3)
[total energy (hartree): -609.570331398]

C	0.00002600	0.00055800	-0.00000200
C	-0.00005200	0.00010700	1.40637100
C	1.21487900	-0.00044800	2.09392800
C	2.42221400	-0.02560300	1.39881200
C	2.42185300	-0.05111400	0.00781600
C	1.21438200	-0.03778300	-0.68742900
H	1.20761300	-0.03883200	-1.76988200
H	1.20797400	0.00061600	3.17636500
C	-1.26624000	0.18914100	-0.77420500
O	-2.15450800	0.94299600	-0.46859000
O	-1.27918200	-0.53795300	-1.91750900
H	-2.10662700	-0.32607300	-2.37559600
H	3.35737300	-0.07523500	-0.53882800
C	-1.27205500	-0.14748100	2.17977200
O	-2.18701200	-0.86695700	1.86989500
O	-1.25919200	0.57308300	3.32726800
H	-2.09366400	0.38809600	3.78422800
H	3.35798600	-0.03159400	1.94551800

b3lyp/6-311++G(d,p): F-C_6H_4-F, *ortho*
[total energy (hartree): -430.841702147]

C	0.00390600	0.00004400	0.00052100
C	-0.00184600	0.00050800	1.39506800
C	1.20407400	-0.00002700	2.07685500
C	2.40845400	-0.00100100	1.38147700
C	2.42123700	-0.00147400	-0.00373800
C	1.21081200	-0.00095400	-0.69626400
H	3.37439200	-0.00224800	-0.51801600
F	1.22237000	0.00042200	3.42362000
H	-0.92402500	0.00128100	1.96301700
H	-0.93634300	0.00046000	-0.53714600
H	1.21552500	-0.00131800	-1.77936900
F	3.56571800	-0.00151600	2.07050500

b3lyp/6-311++G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *ortho* (conformer no 1)
[total energy (hartree): -500.310312750]

C	0.00063100	0.00188100	-0.00040500
C	-0.00020400	-0.00119000	1.39375900
C	1.18507300	-0.00194700	2.13993400
C	2.40258900	0.01891600	0.03724700
C	1.20871300	-0.00734100	-0.68227900
H	1.23386400	-0.01495100	-1.76607000
C	2.42869600	0.04426300	1.43733000
N	3.65755400	0.09019100	2.14683300
C	3.86481000	1.27980100	2.97780300
C	4.86146600	-0.28258400	1.42109000
H	4.09488300	2.16791600	2.36697800
H	2.97386300	1.47695500	3.57067400
H	4.70431700	1.10376100	3.65607400
H	5.67368700	-0.41347700	2.14070400
H	4.71155200	-1.22953000	0.89953100
H	5.18802500	0.47347900	0.68642200
H	3.33657900	0.05067100	-0.50827900
H	-0.94948600	-0.03425500	1.91211900
N	1.15799500	-0.02471900	3.55920300
C	-0.08874800	0.34768500	4.20878500
C	1.77454200	-1.19735600	4.18598300
H	-0.46625600	1.28465800	3.79541900
H	-0.87956800	-0.41713200	4.12115200
H	0.10634000	0.49792100	5.27373700
H	1.13945900	-2.09274600	4.08726300
H	2.74218900	-1.39515900	3.72904800
H	1.92466400	-0.99956700	5.25095500
H	-0.94019000	-0.00865200	-0.53897000

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *ortho* (conformer no 1)
[total energy (hartree): -343.063795877]

C	0.00005800	-0.00025300	0.00004400
C	-0.00011000	-0.00001600	1.39186200
C	1.21099500	-0.00002000	2.08376000
C	2.42756400	-0.04657600	-0.00925900
C	1.21102200	-0.02803800	-0.69154400
H	1.21556700	0.01988800	3.16954300
H	1.21542000	-0.04804600	-1.77732700
C	2.42781900	-0.00935500	1.40178100
N	3.66956200	-0.04401500	2.06745800
H	3.59947100	0.11607400	3.06325200
H	4.35943200	0.57549000	1.65629600
H	-0.93400000	0.01175700	1.94153800
N	3.66995000	-0.04038500	-0.67463200
H	3.59640900	-0.19847900	-1.67049800
H	4.34524400	-0.67581100	-0.26356900
H	-0.93371700	0.00959100	-0.54986500

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *ortho* (conformer no 2)
[total energy (hartree): -343.046378195]

C	0.00582600	0.00000200	-0.01605400
C	0.01623600	0.00000100	1.38116100
C	1.21238800	-0.00000100	2.09348700
C	2.42776400	0.00000000	0.01522500
C	1.23117000	0.00000200	-0.70942000
H	1.19735100	-0.00000200	3.17762400
C	2.42533100	-0.00000100	1.40778700
H	3.36918000	0.00000000	-0.52583000

N	-1.27212600	0.00000300	-0.67996000
H	-1.33294600	0.80364700	-1.29957200
H	-1.33296300	-0.80366100	-1.29954400
H	-0.93921000	0.00000200	1.89221000
H	3.36357200	-0.00000200	1.95126900
N	1.20640200	0.00000400	-2.15260800
H	1.67872000	0.81658300	-2.52763500
H	1.67871600	-0.81657700	-2.52763800

b3lyp/6-311++G(d,p): OCH_3-C_6H_4-OCH_3, *ortho* (conformer no 1)
[total energy (hartree): -461.414575487]

C	0.00012100	0.00066000	0.00016300
C	-0.00006100	-0.00000200	1.39391100
C	1.20076300	-0.00064900	2.10071200
C	2.41908200	0.02485900	1.40006800
C	2.41261500	0.00969300	0.00679300
C	1.20806300	-0.00502500	-0.69431800
H	-0.92640000	-0.00218900	1.95683600
H	-0.94043800	-0.00091000	-0.53849100
O	1.17259200	0.02654200	3.47714400
C	1.56018000	-1.19874400	4.11552200
H	2.57910900	-1.48150600	3.83975100
H	1.50445100	-1.01351500	5.18789600
H	0.86740000	-2.00398900	3.84856900
H	3.36508400	0.01193700	-0.51070000
O	3.62253400	0.01276100	2.06940900
C	3.97331600	1.24988000	2.70605400
H	4.09129300	2.04324000	1.96017800
H	3.21869100	1.54243000	3.44039100
H	4.92692400	1.07593900	3.20383900
H	1.21577600	-0.01436400	-1.77812000

b3lyp/6-311++G(d,p): OCH_3-C_6H_4-OCH_3, *ortho* (conformer no 2)
[total energy (hartree): -461.416658605]

C	0.00073500	0.00249500	0.00031500
C	-0.00016200	0.00035300	1.39739300
C	1.19810100	-0.00084900	2.10001500
C	2.40462200	-0.01069700	1.39800600
C	2.42396100	-0.01326800	0.00857300
C	1.20547200	0.00431100	-0.70476100
H	-0.94621900	0.00429200	1.92644300
H	-0.94170400	0.01444800	-0.53075200
H	3.35669900	-0.00590000	1.91594300
O	1.30371700	0.03373200	-2.06634000
C	0.10903900	0.11857700	-2.83163700
H	-0.52905400	-0.75852600	-2.67821300
H	-0.45433800	1.02641600	-2.59121200
H	0.42598500	0.15619700	-3.87266600
O	3.63483100	0.05011400	-0.63526500
C	4.00886800	-1.10189500	-1.39941100
H	4.06179700	-1.98759000	-0.75620800
H	3.30969700	-1.27863700	-2.21899300
H	4.99879200	-0.88735500	-1.80116700
H	1.20152000	0.00400100	3.18351300

b3lyp/6-311++G(d,p): OCH_3-C_6H_4-OCH_3, *ortho* (conformer no 3)
[total energy (hartree): -461.418389955]

C	-0.00003600	0.00015600	-0.00005700
C	-0.00006000	0.00072200	1.40041700
C	1.19716000	0.00117700	2.10889400
C	2.42498300	0.00106500	1.40103700

C	2.41168200	0.00049700	0.00989600
C	1.19956400	0.00004200	-0.69172400
H	-0.94278500	0.00079800	1.93091100
H	-0.94368200	-0.00018900	-0.53276100
O	1.29895400	0.00175000	3.46661600
C	0.10323300	0.00186800	4.23115300
H	-0.49883800	-0.89246800	4.03499200
H	0.41876000	0.00234200	5.27332700
H	-0.49912900	0.89585100	4.03427200
H	3.34290800	0.00039100	-0.54063100
O	3.54869600	0.00154300	2.16970000
C	4.80950600	0.00141800	1.51827500
H	5.55323700	0.00186300	2.31359000
H	4.94146700	-0.89296100	0.89901900
H	4.94124300	0.89528800	0.89823600
H	1.21131400	-0.00038800	-1.77527800

b3lyp/6-311++G(d,p): OH-C_6H_4-OH, *ortho* (conformer no 1)
[total energy (hartree): -382.807092773]

C	0.00000400	-0.00001600	-0.00002900
C	0.00010200	0.00091200	1.39638600
C	1.20481200	0.00131700	2.08718500
C	2.42279300	0.00080400	1.39306400
C	2.41751500	-0.00012200	0.00296700
C	1.20816800	-0.00053100	-0.69228700
H	-0.93607100	0.00132100	1.94712200
H	-0.94128100	-0.00033100	-0.53611500
O	1.31552600	0.00222500	3.46191000
H	0.44453600	0.00257000	3.87042300
H	3.36778700	-0.00051200	-0.51742100
O	3.60754600	0.00120100	2.06886000
H	3.41819700	0.00183200	3.01606800
H	1.21485300	-0.00124900	-1.77575600

b3lyp/6-311++G(d,p): OH-C_6H_4-OH, *ortho* (conformer no 2)
[total energy (hartree): -382.800298433]

C	-0.00000800	0.00000400	0.00000400
C	0.00001600	0.00000100	1.39594500
C	1.19393900	-0.00000400	2.11146900
C	2.41521100	-0.00000500	1.41561800
C	2.40848900	0.00000100	0.02374200
C	1.20760500	0.00000400	-0.68806200
H	-0.94005000	0.00000400	1.94060100
H	-0.94074600	0.00000700	-0.53715700
H	1.22511000	0.00000600	-1.77120900
O	1.25076100	-0.00000500	3.47683400
H	0.35588100	-0.00005300	3.83178600
O	3.56062600	-0.00000900	2.16093400
H	4.32258000	0.00000600	1.57250000
H	3.35629000	-0.00000100	-0.50733300

b3lyp/6-311++G(d,p): SH-C_6H_4-SH, *ortho* (conformer no 1)
[total energy (hartree): -1028.73672531]

C	0.00004700	0.00234800	-0.00044000
C	-0.00020400	0.00255300	1.39879900
C	1.22610000	0.00140200	2.08661000
C	2.42003700	-0.00170000	1.35701100
C	2.40797200	0.00152100	-0.03283400
C	1.19241500	-0.00308600	-0.71463400
H	3.36719000	-0.01529900	1.88440300
H	1.16940600	-0.00333800	-1.79803400

S	-1.52291700	0.04654100	2.33857700
H	-2.32437000	-0.30367000	1.31372400
H	-0.94363600	0.01545400	-0.53400500
S	1.21857200	-0.03795100	3.87632000
H	2.50612000	0.32983900	4.02454800
H	3.34446500	-0.00006700	-0.57805400

b3lyp/6-311++G(d,p): $SH-C_6H_4-SH$, *ortho* (conformer no 2)
[total energy (hartree): -1028.73813554]

C	0.00008700	-0.00097000	-0.00070700
C	-0.00039400	-0.00087500	1.39759400
C	1.22475000	0.00000200	2.08929700
C	2.41966700	-0.01827300	1.36027100
C	2.40560100	-0.01481800	-0.03003700
C	1.19277600	0.00168400	-0.71571400
H	3.36851400	-0.01991200	1.88463700
H	1.17300800	0.00211600	-1.79905600
S	-1.58617800	0.07916300	2.22815500
H	-1.30877600	-0.81987900	3.19762300
H	-0.94890300	-0.01684200	-0.52372400
S	1.21649700	0.04158500	3.87574300
H	2.53202700	-0.21331200	4.02191000
H	3.34335800	-0.02247000	-0.57351400

b3lyp/6-311++G(d,p): $SH-C_6H_4-SH$, *ortho* (conformer no 3)
[total energy (hartree): -1028.73858002]

C	0.00001100	0.00004900	0.00015800
C	0.00012800	0.00001300	1.39888000
C	1.22794200	0.00004400	2.09100200
C	2.42006100	-0.03405700	1.35562900
C	2.40372400	-0.04901000	-0.03378700
C	1.19061200	-0.02300200	-0.71844200
H	3.36652400	-0.03003700	1.88419700
H	1.16823900	-0.02754400	-1.80173000
S	-1.59483400	0.09974900	2.22520200
H	-1.51598100	-1.07433500	2.89104500
H	-0.95038100	0.00261900	-0.51961500
S	1.37973700	-0.00411400	3.86699500
H	0.14635400	0.48899100	4.11243300
H	3.34044700	-0.07045700	-0.57890800

[3.3] b3lyp/6-311++G(d,p): *meta*

b3lyp/6-311++G(d,p): $BF_2-C_6H_4-BF_2$, *meta*
[total energy (hartree): -680.595785004]

C	-0.01402400	0.00003700	-0.03290300
C	0.00629000	0.00047900	1.37305100
C	1.20982700	-0.00012400	2.07222900
C	2.41318100	-0.00118100	1.37273300
C	2.43312600	-0.00165000	-0.03322600
C	1.20946000	-0.00102600	-0.71836400
H	3.35146400	-0.00165600	1.91669400
H	-0.93185100	0.00130800	1.91725900
H	1.20931400	-0.00137200	-1.80310000
H	1.20997200	0.00022700	3.15607800
B	-1.35454700	0.00071600	-0.79845700
B	3.77345300	-0.00282800	-0.79912200
F	4.94306000	-0.00343700	-0.16026700
F	3.82731500	-0.00329200	-2.12915300
F	-2.52399400	0.00172100	-0.15931100
F	-1.40874000	0.00033600	-2.12847600

b3lyp/6-311++G(d,p): BH_2-C_6H_4-BH_2, *meta*
[total energy (hartree): -283.201509687]

C	-0.02672100	0.00003900	-0.02967500
C	0.00757200	0.00051900	1.38276000
C	1.20982600	-0.00006000	2.08466900
C	2.41189900	-0.00113800	1.38245000
C	2.44582900	-0.00166500	-0.02999300
C	1.20946700	-0.00105200	-0.70368800
H	3.35046900	-0.00159300	1.92774100
H	-0.93085800	0.00136600	1.92829200
H	1.20932700	-0.00143500	-1.78941000
H	1.20996600	0.00032600	3.16901300
B	-1.35846400	0.00068900	-0.79849300
H	-2.39508700	0.00162000	-0.20753300
H	-1.36377600	0.00026900	-1.99106800
B	3.77737300	-0.00285600	-0.79915500
H	3.78237700	-0.00327700	-1.99173100
H	4.81414900	-0.00336600	-0.20846200

b3lyp/6-311++G(d,p): Br-C_6H_4-Br, *meta*
[total energy (hartree): -5379.39511438]

C	0.01825400	0.00004100	0.00824600
C	-0.00522200	0.00054200	1.40036100
C	1.21202000	0.00000200	2.07631800
C	2.42641200	-0.00101300	1.39704000
C	2.41449400	-0.00149400	0.00365900
C	1.21383500	-0.00096900	-0.70361400
H	3.36033200	-0.00142200	1.94319400
H	3.35329600	-0.00228800	-0.53815900
H	1.20815700	-0.00133800	-1.78542500
Br	1.20470400	0.00068400	3.99235600
Br	-1.64494600	0.00078000	-0.94340900
H	-0.94123900	0.00133300	1.94075700

b3lyp/6-311++G(d,p): CHO-C_6H_4-CHO, *meta* (conformer no 1)
[total energy (hartree): -459.023745934]

C	0.00594800	0.00000000	-0.04030200
C	0.01175600	0.00000000	1.36133500
C	1.21364800	0.00000000	2.06374100
C	2.41554000	0.00000000	1.36133500
C	2.42134800	0.00000000	-0.04030200
C	1.21364800	0.00000000	-0.74060700
H	3.35927200	0.00000000	1.89818500
H	-0.93197600	0.00000000	1.89818500
H	1.21364800	0.00000000	-1.82439100
H	1.21364800	0.00000000	3.14721600
C	-1.29144900	0.00000000	-0.76374400
O	-1.40976400	0.00000000	-1.96654500
C	3.71874500	0.00000000	-0.76374400
O	3.83706000	-0.00000100	-1.96654500
H	-2.18647000	-0.00000100	-0.10610900
H	4.61376600	0.00000000	-0.10610900

b3lyp/6-311++G(d,p): CHO-C_6H_4-CHO, *meta* (conformer no 2)
[total energy (hartree): -459.025267840]

C	-0.01238000	0.00000000	0.00892700
C	0.01485600	0.00000000	1.41382900
C	1.22814700	0.00000000	2.08835600
C	2.42271800	0.00000100	1.36528300
C	2.40659900	0.00000100	-0.03241400
C	1.18072300	0.00000100	-0.70856700

H	3.37455100	0.00000100	1.88769500
H	-0.92681800	-0.00000100	1.95043900
H	1.18042800	0.00000100	-1.79395800
H	1.24928800	-0.00000100	3.17178400
C	-1.30642600	0.00000000	-0.71890600
O	-2.39253900	-0.00000100	-0.18621900
C	3.68444200	0.00000100	-0.78487500
O	3.77144000	-0.00000300	-1.99155700
H	-1.21562100	0.00000100	-1.82463300
H	4.59579900	-0.00000100	-0.15098400

b3lyp/6-311++G(d,p): CHO-C_6H_4-CHO, *meta* (conformer no 3)
[total energy (hartree): -459.025111931]

C	0.00169800	0.00000000	0.01450300
C	0.00761400	0.00000000	1.41570900
C	1.21364800	0.00000000	2.11120200
C	2.41968200	0.00000000	1.41570900
C	2.42559800	0.00000000	0.01450300
C	1.21364800	0.00000000	-0.67942400
H	3.36931000	0.00000000	1.93823600
H	-0.94201400	0.00000000	1.93823600
H	1.21364800	0.00000000	-1.76664600
H	1.21364800	0.00000000	3.19498400
C	-1.27650500	0.00000000	-0.73776200
O	-2.37435900	0.00000000	-0.23002000
C	3.70380100	0.00000000	-0.73776200
O	4.80165500	0.00000000	-0.23002000
H	-1.16329500	-0.00000100	-1.84232400
H	3.59059100	0.00000000	-1.84232400

b3lyp/6-311++G(d,p): Cl-C_6H_4-Cl, *meta*
[total energy (hartree): -1151.55575315]

C	0.01809300	0.00004200	0.00845800
C	-0.00440900	0.00053800	1.39993000
C	1.21182500	0.00000500	2.07633700
C	2.42598900	-0.00101300	1.39684100
C	2.41409000	-0.00149300	0.00387400
C	1.21374400	-0.00096200	-0.70307100
H	3.35755100	-0.00142500	1.94720700
H	3.35268000	-0.00228700	-0.53792600
H	1.20311600	-0.00132800	-1.78493200
Cl	1.20471200	0.00059200	3.83298000
Cl	-1.50672600	0.00072100	-0.86386500
H	-0.94067000	0.00132200	1.94048600

b3lyp/6-311++G(d,p): CN-C_6H_4-CN, *meta*
[total energy (hartree): -416.839662624]

C	0.00185900	0.00003600	-0.01738700
C	0.00315300	0.00053100	1.38539300
C	1.20997800	-0.00004700	2.07650900
C	2.41667400	-0.00111200	1.38516600
C	2.41770500	-0.00160900	-0.01761300
C	1.20971500	-0.00103500	-0.72240800
H	3.35835000	-0.00156700	1.91961400
H	-0.93842300	0.00136500	1.92001600
H	1.20961500	-0.00141500	-1.80451300
H	1.21008100	0.00033400	3.15962000
C	-1.23950500	0.00063500	-0.73149900
N	-2.24354800	0.00112500	-1.30222400
C	3.65893200	-0.00271100	-0.73196100
N	4.66286400	-0.00360200	-1.30288100

b3lyp/6-311++G(d,p): COOH-C_6H_4-COOH, *meta* (conformer no 1)
[total energy (hartree): -609.583078910]

C	0.00491500	0.05282900	-0.00440300
C	0.00707300	0.02931600	1.39607000
C	1.21364800	0.01768400	2.08979900
C	2.42022300	0.02931600	1.39607000
C	2.42238100	0.05282900	-0.00440300
C	1.21364800	0.06444700	-0.70161900
H	3.36049500	0.02028200	1.93147100
H	-0.93319900	0.02028200	1.93147100
H	1.21364800	0.08234600	-1.78396600
H	1.21364800	-0.00045200	3.17320200
C	-1.25876500	0.06601800	-0.79199500
O	-1.32351600	0.08618300	-1.99726300
O	-2.36706700	0.05293800	-0.00771100
H	-3.13103600	0.06296800	-0.60289900
C	3.68606100	0.06601800	-0.79199500
O	3.75081200	0.08618300	-1.99726300
O	4.79436300	0.05293800	-0.00771100
H	5.55833200	0.06296800	-0.60289900

b3lyp/6-311++G(d,p): COOH-C_6H_4-COOH, *meta* (conformer no 2)
[total energy (hartree): -609.583813610]

C	0.00549000	-0.04791600	-0.03522000
C	0.00891600	0.00904200	1.36327800
C	1.21364800	0.03710500	2.05845100
C	2.41838000	0.00904200	1.36327800
C	2.42180600	-0.04791600	-0.03522000
C	1.21364800	-0.07655400	-0.73609200
H	3.36706500	0.03060600	1.88541300
H	-0.93976900	0.03060600	1.88541300
H	1.21364800	-0.12018300	-1.81565600
H	1.21364800	0.08088700	3.14103400
C	-1.31015700	-0.07554300	-0.73098200
O	-2.38382000	-0.05113500	-0.17702300
O	-1.19352500	-0.13212400	-2.08057000
H	-2.09259100	-0.14610600	-2.44036500
C	3.73745300	-0.07554200	-0.73098200
O	4.81111600	-0.05113500	-0.17702300
O	3.62082100	-0.13212500	-2.08057000
H	4.51988700	-0.14610600	-2.44036500

b3lyp/6-311++G(d,p): COOH-C_6H_4-COOH, *meta* (conformer no 3)
[total energy (hartree): -609.583630905]

C	0.01520600	0.04402500	-0.02518100
C	0.01309400	0.00054000	1.37466400
C	1.21429000	-0.01348200	2.07439700
C	2.42442500	0.01534900	1.38526300
C	2.43195700	0.05867800	-0.01380800
C	1.22556300	0.07301700	-0.71846800
H	3.36270800	0.00443900	1.92417000
H	-0.93752800	-0.02174200	1.89321800
H	1.24478000	0.10626900	-1.79930100
H	1.20985100	-0.04688800	3.15738100
C	-1.29831400	0.05726400	-0.72647600
O	-2.37326000	0.03169000	-0.17470900
O	-1.17640600	0.10178800	-2.07477700
H	-2.07341300	0.10714600	-2.43991100
C	3.69731900	0.09040600	-0.79716000
O	3.76450100	0.12790500	-2.00248900

O	4.80398800	0.07286900	-0.01155600
H	5.56913800	0.09582600	-0.60487900

b3lyp/6-311++G(d,p): F-C_6H_4-F, *meta*
[total energy (hartree): -430.847772456]

C	0.03020700	0.00004100	0.01535500
C	-0.00744500	0.00051700	1.40176800
C	1.21194900	-0.00005500	2.06250400
C	2.42847000	-0.00104100	1.39680300
C	2.41577900	-0.00148600	0.00284000
C	1.21498800	-0.00095500	-0.70533000
H	3.35169500	-0.00144700	1.96122900
H	3.35406900	-0.00226200	-0.53875200
H	1.18804000	-0.00129000	-1.78707600
F	1.20599300	0.00041100	3.41537600
F	-1.14447800	0.00057300	-0.65578700
H	-0.94422200	0.00130000	1.94237200

b3lyp/6-311++G(d,p): Li-C_6H_4-Li, *meta*
[total energy (hartree): -246.086683606]

C	-0.04496800	0.00006400	-0.04093800
C	0.03320200	0.00051200	1.37528200
C	1.22015400	0.00002900	2.15178900
C	2.41454700	-0.00100000	1.39702500
C	2.41666300	-0.00149500	0.00004000
C	1.20618100	-0.00096700	-0.69732100
H	3.38245800	-0.00144300	1.90143000
H	3.36015400	-0.00229500	-0.54433900
H	1.25375300	-0.00137800	-1.78771500
Li	1.17873100	0.00075500	4.10768700
Li	-1.76079400	0.00084200	-0.98036200
H	-0.91791500	0.00131800	1.92414600

b3lyp/6-311++G(d,p): N$(CH_3)_2$-C_6H_4-N$(CH_3)_2$, *meta* (conformer no 1)
[total energy (hartree): -500.316187297]

C	0.00029100	0.00356700	0.00185100
C	0.00046800	0.00229500	1.41231400
C	1.23986500	-0.00025600	2.08074200
C	2.43435400	-0.04368000	-0.02399800
C	1.21010200	-0.02641100	-0.68028500
H	-0.92242400	0.02021600	-0.55899800
H	1.25167900	0.00966600	3.15740400
H	1.19837000	-0.03660900	-1.76537800
N	-1.19498400	-0.01601700	2.13252900
C	-2.44127600	0.25087400	1.43239300
H	-2.59929600	-0.47262200	0.62899600
C	-1.17055000	0.27135100	3.55682700
H	-2.18437500	0.20129600	3.95032000
H	-0.56196400	-0.46036500	4.09528600
H	-3.27017700	0.14592500	2.13222200
H	-0.78022600	1.27539200	3.78481600
H	-2.48185300	1.26091300	0.99623700
C	2.46450200	-0.01558300	1.38588300
N	3.67526200	0.01656700	2.07955400
C	3.68185700	-0.24301800	3.50948300
C	4.90607600	-0.26467900	1.35798100
H	4.70384700	-0.16400300	3.87942700
H	3.08381700	0.49835600	4.04652600
H	3.29811800	-1.24287100	3.76532100
H	5.74998900	-0.14586500	2.03734000
H	4.93736200	-1.28329600	0.94146400

H	5.04646800	0.44249000	0.53700600
H	3.34482400	-0.07102200	-0.60408300

b3lyp/6-311++G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *meta* (conformer no 2)
[total energy (hartree): -500.316192770]

C	0.00022500	0.00890400	0.00032500
C	-0.00000900	0.00382600	1.41082900
C	1.23934500	0.00162900	2.07963800
C	2.43441900	-0.03273800	-0.02505800
C	1.21037800	-0.01007400	-0.68153600
H	-0.92218300	0.03484300	-0.56067400
H	1.25105000	0.02282300	3.15612600
H	1.19924000	0.00094500	-1.76662800
N	-1.19563600	-0.00975400	2.13025200
C	-2.44082500	0.26581700	1.43172800
H	-2.60210000	-0.45277200	0.62453800
C	-1.17106200	0.26157000	3.55736700
H	-2.18473800	0.18609800	3.95027800
H	-0.56143700	-0.47597800	4.08674400
H	-3.27008000	0.16076300	2.13113000
H	-0.78155100	1.26312600	3.79737400
H	-2.47722900	1.27825700	1.00089000
C	2.46378000	-0.03852700	1.38514000
N	3.67318400	-0.09432500	2.07920700
C	3.68829300	0.17739600	3.50652400
C	4.91164600	0.14179000	1.35466600
H	3.34357700	1.19348400	3.75391400
H	3.06102300	-0.53577900	4.04835800
H	4.70601500	0.06159600	3.87865100
H	5.75160200	0.00913900	2.03636600
H	5.03261600	-0.58061100	0.54386200
H	4.97157900	1.15306700	0.92372700
H	3.34535500	-0.03870600	-0.60500700

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *meta* (conformer no 1)
[total energy (hartree): -343.064236784]

C	-0.00016400	0.02221500	-0.00157300
C	-0.00427900	0.06443500	1.40095500
C	1.21364800	0.08497000	2.08998600
C	2.42746000	0.02221500	-0.00157300
C	1.21364800	0.00216300	-0.68056000
H	-0.93737800	-0.00010200	-0.54687500
H	1.21364800	0.10100300	3.17642200
H	1.21364800	-0.02841100	-1.76490400
N	-1.21102600	0.02761500	2.10724300
H	-1.18138800	0.40214900	3.04403300
H	-2.02070300	0.34663500	1.59607900
C	2.43157500	0.06443500	1.40095500
N	3.63832200	0.02761500	2.10724300
H	3.60868400	0.40214900	3.04403300
H	4.44799900	0.34663500	1.59607900
H	3.36467400	-0.00010200	-0.54687500

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *meta* (conformer no 2)
[total energy (hartree): -343.046576786]

C	0.00780400	0.00000000	-0.01538200
C	-0.01714900	0.00000000	1.38387100
C	1.19011200	0.00000000	2.08302900
C	2.42564300	0.00000000	0.01488600
C	1.22441900	0.00000000	-0.69314100
H	-0.92645400	0.00000000	-0.56762300

H	1.15698500	0.00000000	3.16710300
H	1.23781100	0.00000000	-1.77749700
N	-1.24203300	0.00000000	2.14792500
H	-1.80577700	0.81719800	1.93554000
H	-1.80577700	-0.81719800	1.93554000
C	2.41701400	0.00000000	1.40961000
N	3.68422300	0.00000000	2.10076400
H	3.77440700	-0.81687300	2.69690100
H	3.77440700	0.81687300	2.69690100
H	3.37992400	0.00000000	-0.49776100

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *meta* (conformer no 3)
[total energy (hartree): -343.046063508]

C	0.00519100	0.00000000	-0.02127800
C	-0.00228900	0.00000000	1.37732800
C	1.21364800	0.00000000	2.06321300
C	2.42210500	0.00000000	-0.02127800
C	1.21364800	0.00000000	-0.71520900
H	-0.93525100	0.00000000	-0.56288600
H	1.21364800	0.00000000	3.14580400
H	1.21364800	0.00000000	-1.79972800
N	-1.21863700	0.00000000	2.15420900
H	-1.78440800	0.81767000	1.94971200
H	-1.78440800	-0.81767000	1.94971200
C	2.42958500	0.00000000	1.37732800
N	3.64593300	0.00000000	2.15420900
H	4.21170400	0.81767000	1.94971200
H	4.21170400	-0.81767000	1.94971200
H	3.36254700	0.00000000	-0.56288600

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *meta* (conformer no 4)
[total energy (hartree): -343.064373508]

C	-0.00412300	0.11055600	-0.11463100
C	-0.05632400	0.05057800	1.28621300
C	1.13640700	-0.02235800	2.01444300
C	2.42049100	0.02003100	-0.03496000
C	1.23154700	0.09374000	-0.75315800
H	-0.92117800	0.17558300	-0.68994600
H	1.09904100	-0.06735900	3.09941800
H	1.26889300	0.13900700	-1.83634200
N	-1.28383300	0.12240000	1.95397200
H	-2.08644200	-0.15726100	1.40946300
H	-1.29888900	-0.27668800	2.88109900
C	2.37651600	-0.03770700	1.36626800
N	3.55557500	-0.16862200	2.10816800
H	3.50618000	0.15201400	3.06411900
H	4.39285300	0.15281300	1.64497800
H	3.37502300	0.00096500	-0.54949700

b3lyp/6-311++G(d,p): OCH_3-C_6H_4-OCH_3, *meta* (conformer no 1)
[total energy (hartree): -461.424518006]

C	0.00015600	0.00053600	0.00089000
C	0.00051300	0.00095200	1.40136300
C	1.22454600	-0.00097200	2.06750200
C	2.43048000	-0.00328700	1.35044200
C	2.40347000	-0.00367100	-0.04034400
C	1.17786100	-0.00173500	-0.72522700
H	-0.93645500	0.00274800	1.93999700
H	-0.94842600	0.00204700	-0.52454300
O	1.36596300	-0.00081100	3.42675900
C	0.19347800	0.00147900	4.22943100

H	-0.41495500	-0.89158600	4.05051600
H	0.53970300	0.00119500	5.26181900
H	-0.41184900	0.89654400	4.04996700
H	1.18160100	-0.00205900	-1.80769300
H	3.35306600	-0.00472300	1.91348100
O	3.51958300	-0.00585500	-0.82553500
C	4.79405200	-0.00786700	-0.19732600
H	5.52384300	-0.00933400	-1.00540300
H	4.93718500	0.88607700	0.41929900
H	4.93412900	-0.90196400	0.41978100

b3lyp/6-311++G(d,p): OCH_3-C_6H_4-OCH_3, *meta* (conformer no 2)
[total energy (hartree): -461.423783409]

C	-0.13432700	-0.04544100	-0.07679400
C	-0.15741600	-0.03016900	1.31561600
C	1.06057200	0.00682000	2.00729100
C	2.26626500	0.02768900	1.30846500
C	2.26779600	0.01186500	-0.08519100
C	1.05949900	-0.02505100	-0.79378400
H	-1.10316800	-0.04708800	1.83848100
H	-1.07333700	-0.07425400	-0.61856100
O	1.17094700	0.02492100	3.36856000
C	-0.01666300	0.00654800	4.14796600
H	-0.59946300	-0.90356100	3.96916200
H	0.30978300	0.02632400	5.18659900
H	-0.64081900	0.88427300	3.94809300
H	1.03850000	-0.03773200	-1.87429000
H	3.20337900	0.05651400	1.84917600
O	3.50161800	0.03482200	-0.67036200
C	3.58310400	0.02050400	-2.08859800
H	4.64581800	0.04366300	-2.32487200
H	3.13942900	-0.88957400	-2.50685200
H	3.09592600	0.89805800	-2.52742000

b3lyp/6-311++G(d,p): OCH_3-C_6H_4-OCH_3, *meta* (conformer no 3)
[total energy (hartree): -461.423333497]

C	0.05229300	-0.00362900	0.02965500
C	0.03546400	0.01237600	1.42024600
C	1.24697700	0.01380700	2.11421200
C	2.46540600	-0.00059600	1.42369900
C	2.45504300	-0.01659600	0.02326700
C	1.24858400	-0.01815300	-0.67955200
H	-0.89096300	0.02378200	1.97992300
H	-0.88659600	-0.00477600	-0.51275900
O	1.15268300	0.02989000	3.47770300
C	2.34329700	0.03166900	4.25046300
H	2.95144900	0.92081800	4.04980900
H	2.02233300	0.04499000	5.29092500
H	2.94124400	-0.86854700	4.06950500
H	1.27067500	-0.03055900	-1.76167000
H	3.39932100	0.00058800	1.96389700
O	3.58874700	-0.03145200	-0.73991700
C	4.85314800	-0.03065200	-0.09513700
H	5.59386500	-0.04395800	-0.89320100
H	4.99422600	0.87051100	0.51207800
H	4.98466200	-0.91879600	0.53303900

b3lyp/6-311++G(d,p): OH-C_6H_4-OH, *meta* (conformer no 1)
[total energy (hartree): -382.806619669]

C	0.00866000	0.00003500	0.01609700
C	0.00521000	0.00057300	1.40529300

C	1.22730200	0.00003000	2.08295600
C	2.43125400	-0.00102900	1.38178400
C	2.41199200	-0.00155500	-0.01311500
C	1.20192300	-0.00102800	-0.70699500
H	-0.91650900	0.00140500	1.97251200
H	-0.93457800	0.00045400	-0.51832200
H	1.19098900	-0.00143600	-1.79208300
O	1.18550700	0.00058700	3.45049600
H	2.08102400	0.00013800	3.80422600
O	3.62661700	-0.00259700	-0.64514000
H	3.49418600	-0.00285200	-1.59876800
H	3.38626900	-0.00146000	1.89641900

b3lyp/6-311++G(d,p): OH-C_6H_4-OH, *meta* (conformer no 2)
[total energy (hartree): -382.805437538]

C	0.02954900	0.00004000	0.01714900
C	0.01015000	0.00058500	1.40915100
C	1.22149900	0.00003500	2.09908200
C	2.43389400	-0.00104200	1.40544200
C	2.42846100	-0.00157600	0.00873900
C	1.22539700	-0.00103500	-0.69557000
H	-0.91766500	0.00142400	1.96637900
H	-0.90934400	0.00046700	-0.52497300
H	1.24428700	-0.00146000	-1.77768400
O	1.16873400	0.00059600	3.46722000
H	2.05974500	0.00011100	3.83138800
O	3.58684600	-0.00264300	-0.72114900
H	4.34798800	-0.00295800	-0.13190200
H	3.37563700	-0.00146900	1.94925200

b3lyp/6-311++G(d,p): OH-C_6H_4-OH, *meta* (conformer no 3)
[total energy (hartree): -382.806447475]

C	-0.00276300	0.00005400	-0.00141500
C	-0.01590200	0.00055800	1.39056300
C	1.20048000	0.00000400	2.08025900
C	2.41062200	-0.00103900	1.39195900
C	2.40154600	-0.00153000	-0.00019700
C	1.19613000	-0.00098600	-0.70887800
H	-0.95530900	0.00138000	1.93374500
H	-0.94161600	0.00048500	-0.54338900
H	1.19682400	-0.00136700	-1.79401400
O	1.26644000	0.00044700	3.44714600
H	0.37625100	0.00114000	3.81368300
O	3.61835800	-0.00255000	-0.62635900
H	3.49110600	-0.00276700	-1.58063100
H	3.34780800	-0.00146700	1.93301900

b3lyp/6-311++G(d,p): SH-C_6H_4-SH, *meta* (conformer no 1)
[total energy (hartree): -1028.73905646]

C	-0.00094800	0.00007800	-0.02147600
C	-0.00166500	0.00054200	1.37678900
C	1.21004500	-0.00005600	2.06074300
C	2.42157500	-0.00110800	1.37645300
C	2.42047900	-0.00157300	-0.02180400
C	1.20966500	-0.00098700	-0.71934300
H	3.35714600	-0.00155800	1.92305500
H	-0.93709000	0.00137100	1.92363700
H	1.20952200	-0.00135300	-1.80326400
H	1.21020200	0.00030500	3.14495800
S	4.00310700	-0.00294100	-0.85012700
H	3.52710500	-0.00282600	-2.11052300

S	-1.58381500	0.00088300	-0.84934700
H	-1.10816400	0.00025700	-2.10987600

b3lyp/6-311++G(d,p): SH-C_6H_4-SH, *meta* (conformer no 2)
[total energy (hartree): -1028.73920252]

C	-0.00483200	-0.00006800	-0.01438200
C	-0.00848000	0.00042700	1.38304400
C	1.20357500	-0.00006700	2.06876400
C	2.41558500	-0.00105200	1.38700400
C	2.41690300	-0.00155500	-0.01218300
C	1.20780600	-0.00106500	-0.71018900
H	3.35009800	-0.00142300	1.93538700
H	-0.94180000	0.00119200	1.93313200
H	1.20319100	-0.00144400	-1.79435400
H	1.20167100	0.00032100	3.15307300
S	4.00046700	-0.00284000	-0.83752600
H	3.52614100	-0.00282800	-2.09851400
S	-1.50434000	0.00047500	-0.98594100
H	-2.36357600	0.00165900	0.05146300

b3lyp/6-311++G(d,p): SH-C_6H_4-SH, *meta* (conformer no 3)
[total energy (hartree): -1028.73913028]

C	-0.00130300	-0.00661000	-0.00542400
C	-0.00243900	-0.00374900	1.39295100
C	1.21002100	-0.00120500	2.07618000
C	2.42231800	-0.00573500	1.39267300
C	2.42085600	-0.00852700	-0.00570200
C	1.20969700	-0.00812700	-0.70175800
H	3.35470000	-0.00698800	1.94432200
H	-0.93469400	-0.00339700	1.94481500
H	1.20957600	-0.00613200	-1.78623500
H	1.21014800	0.00186200	3.16058100
S	3.92211100	-0.01847700	-0.97351200
H	4.77827700	0.03399800	0.06521500
S	-1.50278600	-0.01390200	-0.97289900
H	-2.35867000	0.03791800	0.06609400

b3lyp/6-311++G(d,p): tBu-C_6H_4-tBu, *meta* (conformer no 2)
[total energy (hartree): -546.902622657]

C	0.03035700	0.01295500	-0.06536900
C	0.03248200	0.00054000	1.34080600
C	1.20421400	-0.01052900	2.09996600
C	2.42552400	-0.00822300	1.40710900
C	2.45188100	0.00421800	0.02028200
C	1.26515100	0.01457800	-0.71517500
H	1.32221000	0.02381200	-1.79547800
C	-1.31083700	0.02430000	-0.82395100
C	-2.12610700	-1.23659900	-0.45307200
C	-2.11517900	1.28648700	-0.43402200
C	-1.11751600	0.03484800	-2.35126700
H	-1.58278500	-2.14578700	-0.72519100
H	-2.33955200	-1.28267900	0.61723700
H	-3.08304800	-1.24007300	-0.98451700
H	-3.07205100	1.30621300	-0.96520000
H	-2.32809100	1.31816800	0.63692400
H	-1.56400400	2.19494500	-0.69241900
H	-2.09351100	0.04234700	-2.84435700
H	-0.57215700	0.92129600	-2.68645300
H	-0.57922300	-0.85093000	-2.69941300
H	3.40391900	0.00580700	-0.50011500
H	3.36335300	-0.01617800	1.95057000

C	1.19929500	-0.02497600	3.64039200
C	1.93384200	1.22937300	4.16887400
C	-0.22383100	-0.02621000	4.22833200
C	1.92587700	-1.29382000	4.14479800
H	2.97064000	1.26713400	3.82731600
H	1.43745300	2.14319000	3.83067800
H	1.94274500	1.23204800	5.26347300
H	-0.79214500	-0.90812300	3.92017300
H	-0.16681000	-0.03662600	5.32022800
H	-0.78702600	0.86464300	3.93692100
H	1.93393700	-1.31796900	5.23913500
H	1.42424400	-2.19781100	3.78841500
H	2.96269300	-1.33120200	3.80325400
H	-0.91973000	-0.00041600	1.85381900

[3.4] b3lyp/6-311++G(d,p): para

b3lyp/6-311++G(d,p): BF_2-C_6H_4-BF_2, *para*
[total energy (hartree): -680.594691370]

C	0.00274300	0.00039000	0.00010400
C	-0.01111500	0.00264800	1.40522000
C	1.21397300	0.00173900	2.09334700
C	2.41632400	-0.00132800	1.39667100
C	2.43018200	-0.00358700	-0.00844400
C	1.20509300	-0.00267700	-0.69657100
H	3.35493200	-0.00200600	1.93929100
H	1.20047200	-0.00438100	-1.78079800
H	1.21859400	0.00344600	3.17757400
B	3.77085600	-0.00701200	-0.78005000
F	3.81670700	-0.00917000	-2.11027600
F	4.94228700	-0.00796500	-0.14743500
B	-1.35178700	0.00606500	2.17682700
F	-1.39763500	0.00821400	3.50705200
F	-2.52321800	0.00701500	1.54421500
H	-0.93586600	0.00106700	-0.54251500

b3lyp/6-311++G(d,p): BH_2-C_6H_4-BH_2, *para*
[total energy (hartree): -283.199435150]

C	-0.02471400	0.00005000	-0.01417400
C	0.00225700	0.00048400	1.39713700
C	1.20478700	0.00003600	2.09167200
C	2.44065100	-0.00086800	1.40958400
C	2.41368000	-0.00130200	-0.00172700
C	1.21115000	-0.00085400	-0.69626200
H	-0.93690100	0.00118400	1.94059200
H	1.21246600	-0.00119800	-1.78131100
H	1.20347100	0.00038000	3.17672100
B	-1.36134200	0.00055100	-0.78595300
H	-2.39657300	0.00131500	-0.19406600
H	-1.36628000	0.00017600	-1.97840100
B	3.77727800	-0.00136800	2.18136300
H	4.81251000	-0.00213600	1.58947800
H	3.78221600	-0.00099100	3.37381100
H	3.35283700	-0.00200100	-0.54518100

b3lyp/6-311++G(d,p): Br-C_6H_4-Br, *para*
[total energy (hartree): -5379.39515046]

C	0.00080100	0.00008000	0.00057500
C	0.00073000	0.00052900	1.39451700
C	1.21223200	-0.00002200	2.07900900
C	2.42381700	-0.00101500	1.39463500
C	2.42388800	-0.00146700	0.00070300

C	1.21237100	-0.00091300	-0.68379400
H	3.36098100	-0.00144200	1.93607100
H	3.36110500	-0.00224300	-0.54063900
Br	1.21216600	0.00060000	3.99447200
H	-0.93649800	0.00130300	1.93584600
Br	1.21250100	-0.00154000	-2.59925700
H	-0.93637400	0.00050600	-0.54084800

b3lyp/6-311++G(d,p): CHO-C_6H_4-CHO, *para* (conformer no 1)
[total energy (hartree): -459.024533639]

C	-0.00337300	0.00000000	0.01942000
C	0.02095900	0.00000000	1.42089200
C	1.24429000	0.00000000	2.10226600
C	2.43017900	0.00000000	1.38174900
C	2.40584700	0.00000000	-0.01972200
C	1.18251500	0.00000000	-0.70109700
H	3.38412100	0.00000000	1.89976300
H	1.18670100	0.00000000	-1.78450100
H	1.24010500	0.00000000	3.18567000
C	3.68639800	0.00000000	-0.77217500
O	3.77370500	0.00000100	-1.97851800
H	4.59713800	-0.00000100	-0.13788800
C	-1.25959300	0.00000000	2.17334400
H	-2.17033200	-0.00000100	1.53905700
O	-1.34689900	0.00000000	3.37968700
H	-0.95731500	0.00000000	-0.49859300

b3lyp/6-311++G(d,p): CHO-C_6H_4-CHO, *para* (conformer no 2)
[total energy (hartree): -459.024419367]

C	-0.00731200	0.00000000	0.02975000
C	-0.00829500	0.00000000	1.43406300
C	1.19047200	0.00000000	2.12577300
C	2.40580400	0.00000000	1.42212300
C	2.40724500	0.00000000	0.02435400
C	1.20213500	0.00000000	-0.67103000
H	-0.95910800	0.00000000	1.95372400
H	1.19498400	0.00000000	-1.75631800
H	1.21663200	0.00000000	3.20899600
C	-1.28576600	0.00000000	-0.72579200
O	-2.38354500	0.00000000	-0.21855100
H	-1.17148000	0.00000000	-1.82994800
C	3.69947700	0.00000000	2.15137500
H	4.59858000	0.00000000	1.50035000
O	3.80889200	0.00000000	3.35573100
H	3.35041800	0.00000000	-0.51264400

b3lyp/6-311++G(d,p): Cl-C_6H_4-Cl, *para*
[total energy (hartree): -1151.55581733]

C	0.01411800	0.00002700	0.00573300
C	0.00141600	0.00049400	1.39703600
C	1.20754800	-0.00001200	2.09361700
C	2.40615900	-0.00099000	1.38704900
C	2.41887200	-0.00145600	-0.00425200
C	1.21272100	-0.00093900	-0.70082500
H	3.35896100	-0.00221300	-0.54057400
H	1.20736700	-0.00128900	-1.78313200
Cl	-1.50739800	0.00068000	-0.87268400
H	-0.93868900	0.00125400	1.93334400
Cl	3.92767500	-0.00162800	2.26546500
H	1.21292500	0.00034600	3.17591900

b3lyp/6-311++G(d,p): CN-C_6H_4-CN, *para*
[total energy (hartree): -416.840263379]

C	0.00241700	0.00014800	-0.00781500
C	0.00382800	0.00066800	1.39482200
C	1.21779800	0.00004200	2.09743900
C	2.41881700	-0.00108900	1.40399600
C	2.41740700	-0.00160800	0.00136600
C	1.20343100	-0.00098400	-0.70125600
H	3.35922800	-0.00158000	1.94023600
H	1.20926500	-0.00138700	-1.78378600
H	1.21197300	0.00044400	3.17997000
C	3.65698800	-0.00278300	-0.71423800
N	4.65749000	-0.00373800	-1.29162800
C	-1.23576000	0.00184100	2.11041000
N	-2.23627700	0.00279400	2.68777400
H	-0.93799900	0.00063800	-0.54404700

b3lyp/6-311++G(d,p): COOH-C_6H_4-COOH, *para* (conformer no 1)
[total energy (hartree): -609.583154543]

C	0.00000600	0.00000800	-0.00001200
C	0.00000100	0.00006200	1.39923700
C	1.20411000	-0.00002300	2.09383900
C	2.41520900	-0.00016600	1.39296400
C	2.41383500	-0.00022400	-0.00693200
C	1.21238700	-0.00014300	-0.69998400
H	-0.93919800	0.00016600	1.93598300
H	1.19228700	-0.00019300	-1.78249300
H	1.20966700	0.00002600	3.17559100
C	-1.26362900	0.00010800	-0.78965300
O	-1.32292700	0.00008200	-1.99604300
O	-2.37362100	0.00023900	-0.01036200
H	-3.13628000	0.00029900	-0.60743400
C	3.73172600	-0.00026000	2.09090100
O	4.80544400	-0.00040700	1.53768700
O	3.61343500	-0.00016300	3.44189300
H	4.51217700	-0.00024800	3.80297500
H	3.36097900	-0.00033400	-0.53148000

b3lyp/6-311++G(d,p): COOH-C_6H_4-COOH, *para* (conformer no 2)
[total energy (hartree): -609.583196011]

C	0.00001500	0.00000100	-0.00001000
C	-0.00001300	0.00000000	1.39892300
C	1.20068900	-0.00000200	2.09631200
C	2.41330500	-0.00000300	1.39615900
C	2.41333300	-0.00000200	-0.00277300
C	1.21263100	0.00000000	-0.70016200
H	-0.94795300	0.00000000	1.92208800
H	1.20860200	0.00000100	-1.78189900
H	1.20471800	-0.00000200	3.17804900
C	-1.31621100	0.00000200	-0.69861200
O	-2.39037100	-0.00000200	-0.14595700
O	-1.19684300	0.00000500	-2.04918200
H	-2.09512100	0.00000500	-2.41141000
C	3.72953100	-0.00000500	2.09476200
O	4.80369100	-0.00001100	1.54210700
O	3.61016300	-0.00000400	3.44533200
H	4.50844100	-0.00000800	3.80756000
H	3.36127300	-0.00000200	-0.52593800

b3lyp/6-311++G(d,p): F-C_6H_4-F, *para*
[total energy (hartree): -430.846851626]

C	-0.00260500	0.00005900	0.00063400
C	-0.00267500	0.00050900	1.39445800
C	1.21222800	-0.00005700	2.06267600
C	2.42720300	-0.00104100	1.39457700
C	2.42727300	-0.00148700	0.00076000
C	1.21236400	-0.00093300	-0.66746100
H	3.35191100	-0.00145100	1.95743800
H	3.35203600	-0.00225600	-0.56200900
F	1.21216600	0.00038900	3.41859600
H	-0.92744000	0.00128800	1.95722100
F	1.21243900	-0.00135200	-2.02338100
H	-0.92731500	0.00047700	-0.56222000

b3lyp/6-311++G(d,p): Li-C_6H_4-Li, *para*
[total energy (hartree): -246.088112858]

C	0.02965800	0.00005900	-0.00269100
C	0.02958700	0.00051000	1.39778500
C	1.21223600	0.00000500	2.17240500
C	2.39496700	-0.00099800	1.39790500
C	2.39503800	-0.00144800	-0.00256900
C	1.21238700	-0.00094100	-0.77719000
H	3.36849600	-0.00146400	1.89578900
H	3.36861800	-0.00223500	-0.50035300
Li	1.21213900	0.00066700	4.12522100
H	-0.94399500	0.00129400	1.89556800
H	-0.94387200	0.00052200	-0.50057400
Li	1.21248300	-0.00155600	-2.73000600

b3lyp/6-311++G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 1)
[total energy (hartree): -500.312901154]

C	0.00006800	0.00090700	-0.00024400
C	-0.00014600	0.00025200	1.40606500
C	1.26299400	-0.00064500	2.02429900
C	2.44326400	0.02142000	-0.11809400
C	1.18012400	0.02231700	-0.73632800
H	-0.93170200	-0.00589800	-0.54916400
H	1.34634500	-0.00686700	3.10253300
H	1.09677300	0.02854000	-1.81456200
N	-1.19176700	0.03447500	2.14995300
C	-1.12817000	-0.32827100	3.55624800
H	-0.46669800	0.34739900	4.10335300
C	-2.43050800	-0.30537300	1.46918700
H	-3.25923700	-0.20273600	2.17021500
H	-2.62016700	0.38141900	0.64107900
H	-2.12241700	-0.22975400	3.99282800
H	-2.43834900	-1.33325500	1.07046800
H	-0.77708600	-1.36013800	3.72169700
C	2.44305100	0.02076600	1.28821500
N	3.63488500	-0.01280200	-0.86198200
C	4.87362600	0.32704500	-0.18121500
C	3.57128900	0.34994300	-2.26827700
H	5.70235500	0.22440800	-0.88224300
H	4.88146700	1.35492700	0.21750300
H	5.06328500	-0.35974700	0.64689200
H	4.56553600	0.25142700	-2.70485600
H	2.90981700	-0.32572600	-2.81538300
H	3.22020500	1.38181100	-2.43372600
H	3.37482000	0.02757000	1.83713500

b3lyp/6-311++G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 2)
[total energy (hartree): -500.312667427]

C	0.00023800	0.00766100	-0.00166300
C	0.00013200	0.00464500	1.39867700
C	1.25784900	0.00391500	2.02451700
C	2.44271500	0.04131600	-0.11156200
C	1.18553600	0.00994300	-0.73703100
H	-0.93252300	0.00306800	-0.55010300
H	1.32077600	-0.04249200	3.10523200
H	1.10821300	0.00000500	-1.81552600
N	-1.18651000	-0.05829500	2.17245700
C	-2.43484500	-0.24734900	1.45488100
H	-2.36387600	-1.11273400	0.79346100
C	-1.31276800	0.91239100	3.25641100
H	-2.12714600	0.60913500	3.91904100
H	-0.40125500	0.95589200	3.84958200
H	-3.22967700	-0.44170200	2.17835000
H	-1.52774200	1.92929700	2.88537700
H	-2.73374100	0.62872100	0.85211000
C	2.43977800	0.02427200	1.29936600
N	3.63608000	0.10655700	-0.84458600
C	3.58531800	-0.19274800	-2.26595300
C	4.88006800	-0.22744700	-0.16959800
H	4.58090000	-0.06423900	-2.69116000
H	3.24645500	-1.21963100	-2.47933900
H	2.91863700	0.49973900	-2.78527100
H	5.70759000	-0.09227200	-0.86631800
H	5.05650200	0.44155500	0.67578700
H	4.90583000	-1.26450300	0.20238300
H	3.37077500	0.01330700	1.84938000

b3lyp/6-311++G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 3)
[total energy (hartree): -500.312914231]

C	0.00134300	-0.00310700	0.00206700
C	0.00063800	0.00034400	1.40848400
C	1.26374800	-0.00216700	2.02684100
C	2.44362000	0.06866500	-0.11483800
C	1.18134500	0.02997800	-0.73370700
H	-0.92966500	-0.03526800	-0.54719700
H	1.34730300	-0.03186400	3.10466500
H	1.09856100	0.02308900	-1.81197900
N	-1.19098200	0.02428400	2.15229000
C	-1.12858600	-0.35025100	3.55538900
H	-0.46489900	0.31873700	4.10796400
C	-2.43053700	-0.30421300	1.46818500
H	-3.25950300	-0.20073800	2.16885100
H	-2.61427900	0.38894300	0.64402400
H	-2.12254900	-0.25213700	3.99277600
H	-2.44478000	-1.32964900	1.06313100
H	-0.78106500	-1.38466000	3.71251800
C	2.44376000	0.03067300	1.29106200
N	3.63294700	0.15967300	-0.85707500
C	4.88515900	-0.13381300	-0.18010700
C	3.58574100	-0.18353600	-2.26882800
H	5.70901400	0.02011100	-0.87750900
H	5.04044500	0.54667100	0.66030700
H	4.94143100	-1.16704000	0.20075100
H	4.57450400	-0.03318100	-2.70312900
H	3.28180700	-1.22756200	-2.45061400
H	2.89427800	0.46996400	-2.80563000
H	3.37560800	0.02325700	1.83977600

b3lyp/6-311++G(d,p): $N(CH_3)_2$-C_6H_4-$N(CH_3)_2$, *para* (conformer no 4)

[total energy (hartree): -500.312595994]

C	0.00121500	-0.01104000	-0.00124000
C	-0.00217000	0.00218100	1.39922100
C	1.25334600	0.01840800	2.02821200
C	2.44391100	-0.01411200	-0.10493400
C	1.18777000	-0.02170100	-0.73376100
H	-0.93068800	-0.00590100	-0.55128100
H	1.31355400	0.00854600	3.11006700
H	1.11340600	-0.03158100	-1.81252500
N	-1.19169300	-0.04436100	2.17024800
C	-2.43613100	-0.26074100	1.45369900
H	-2.35382800	-1.13839200	0.81003800
C	-1.32767400	0.95548900	3.22601800
H	-2.14175600	0.66556200	3.89498700
H	-0.41797300	1.02209500	3.81985700
H	-3.23085100	-0.44872200	2.17911800
H	-1.54883800	1.96000600	2.82576100
H	-2.74321800	0.59971200	0.83270300
C	2.43738900	0.02348100	1.30545900
N	3.63919600	-0.07030100	-0.83503000
C	3.59051400	0.22969100	-2.25646100
C	4.88036900	0.26360000	-0.15557300
H	4.58920900	0.11368800	-2.67785600
H	2.93443100	-0.47008100	-2.77974900
H	3.24014700	1.25252600	-2.46999700
H	5.70978100	0.13598400	-0.85141900
H	4.90193200	1.29836000	0.22327800
H	5.05738200	-0.41025700	0.68588200
H	3.36696200	0.03848900	1.85772200

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *para* (conformer no 1)

[total energy (hartree): -343.059980704]

C	0.01198100	0.04887700	0.01107900
C	-0.01501400	0.05076600	1.41035100
C	1.21049200	0.04867100	2.08625600
C	2.44231000	0.05076600	-0.00895100
C	1.21680400	0.04867100	-0.68485600
H	-0.92126200	0.04240900	-0.54372000
H	1.22457000	0.04175400	3.17183400
H	1.20272600	0.04175400	-1.77043400
N	-1.23375500	-0.01324100	2.11445800
H	-1.19523100	0.36484100	3.05071600
H	-2.02674300	0.35873200	1.61068000
C	2.41531500	0.04887700	1.39032100
N	3.66105100	-0.01324100	-0.71305800
H	3.62252700	0.36484100	-1.64931600
H	4.45403900	0.35873200	-0.20928000
H	3.34855800	0.04240900	1.94512000

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *para* (conformer no 2)

[total energy (hartree): -343.060072198]

C	0.00012200	0.00021500	-0.00031800
C	-0.00001900	-0.00045600	1.39918300
C	1.19104000	-0.00064200	2.11840500
C	2.42954700	0.00488600	0.06692800
C	1.23848800	0.00507200	-0.65229500
H	1.15585300	-0.01028100	3.20348000
H	1.27367600	0.01471300	-1.73737000
C	2.42940500	0.00421700	1.46642800
N	3.63445600	-0.06131600	2.19394900
H	3.57697700	0.31619800	3.12953600

H	4.43592200	0.31425600	1.70638200
H	3.37339500	0.00021700	-0.46964300
N	-1.20492800	0.06574800	-0.72783800
H	-1.14745100	-0.31176300	-1.66342600
H	-2.00639600	-0.30982000	-0.24027100
H	-0.94386700	0.00421400	1.93575400

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *para* (conformer no 3)
[total energy (hartree): -343.046391712]

C	0.00109000	0.00000000	-0.01927700
C	-0.00024100	0.00000000	1.37665500
C	1.19758800	0.00000000	2.08871200
C	2.42753700	0.00000000	0.02474500
C	1.22970800	0.00000100	-0.68731200
H	1.17993600	-0.00000100	3.17413500
H	1.24736000	0.00000100	-1.77273500
C	2.42620600	0.00000000	1.42067700
N	3.69602000	0.00000000	2.10606700
H	3.79346600	-0.81759600	2.69974100
H	3.79346600	0.81759500	2.69974100
H	3.38089200	0.00000100	-0.49036800
N	-1.26872400	0.00000100	-0.70466700
H	-1.36616800	0.81759400	-1.29834400
H	-1.36617200	-0.81759700	-1.29833800
H	-0.95359600	0.00000000	1.89176800

b3lyp/6-311++G(d,p): NH_2-C_6H_4-NH_2, *para* (conformer no 4)
[total energy (hartree): -343.046217250]

C	-0.00261700	-0.00000100	-0.01314100
C	-0.01890900	0.00000000	1.38641200
C	1.19808800	0.00000100	2.06798300
C	2.42378900	-0.00000100	-0.02384900
C	1.20360200	-0.00000100	-0.70958100
H	-0.94136600	-0.00000100	-0.55844100
H	1.18217400	0.00000100	3.15141800
H	1.20078400	-0.00000200	-1.79519900
N	-1.23788500	0.00000100	2.15829400
H	-1.80349200	0.81784900	1.95447500
H	-1.80349200	-0.81784800	1.95447600
C	2.40552600	0.00000000	1.37085900
N	3.70168300	-0.00000200	-0.69375200
H	3.80798700	-0.81791500	-1.28535900
H	3.80799500	0.81792000	-1.28534600
H	3.35169100	0.00000000	1.89895700

b3lyp/6-311++G(d,p): OCH_3-C_6H_4-OCH_3, *para* (conformer no 1)
[total energy (hartree): -461.421212150]

C	-0.00012400	-0.00024500	0.00018200
C	0.00006300	0.00122900	1.39250400
C	1.21129700	0.00151300	2.09199500
C	2.40893500	0.00030700	1.37707200
C	2.40874800	-0.00116700	-0.01525000
C	1.19751400	-0.00145100	-0.71474100
H	-0.94701900	0.00214400	1.91527900
H	-0.93386800	-0.00047200	-0.54932900
O	1.32305700	0.00291800	3.45835900
C	0.13307200	0.00410900	4.23087500
H	-0.47151000	-0.88995000	4.03976800
H	0.45238900	0.00502700	5.27205600
H	-0.47088100	0.89821500	4.03800200
H	3.34267900	0.00053400	1.92658300

O	1.08575400	-0.00285600	-2.08110500
C	2.27573900	-0.00404900	-2.85362100
H	2.88032200	0.89000900	-2.66251500
H	2.87969100	-0.89815500	-2.66074700
H	1.95642200	-0.00496900	-3.89480200
H	3.35583000	-0.00208200	-0.53802500

b3lyp/6-311++G(d,p): OCH_3-C_6H_4-OCH_3, *para* (conformer no 2)
[total energy (hartree): -461.421503914]

C	0.00001300	0.00016000	0.00001400
C	-0.00003900	0.00031200	1.40254000
C	1.21397500	0.00031400	2.08198900
C	2.42289600	0.00016700	1.36998900
C	2.41760600	0.00001800	-0.02121100
C	1.19105300	0.00001600	-0.70145300
H	-0.95077400	0.00016000	-0.51941400
H	1.19794800	-0.00009900	-1.78484200
H	3.35091600	0.00017200	1.92594500
O	3.53722500	-0.00013200	-0.81118900
C	4.80600100	-0.00015300	-0.17729900
H	5.54212100	-0.00028900	-0.97986300
H	4.94599700	0.89396800	0.44117500
H	4.94587100	-0.89416500	0.44136300
O	-1.23387900	0.00044700	1.99849300
C	-1.29518600	0.00061600	3.41563500
H	-0.82219900	0.89463600	3.83830500
H	-2.35414800	0.00070800	3.66979600
H	-0.82230300	-0.89335800	3.83851600
H	1.25002700	0.00042800	3.16314100

b3lyp/6-311++G(d,p): OH-C_6H_4-OH, *para* (conformer no 1)
[total energy (hartree): -382.803211153]

C	-0.00189500	0.00017400	0.01547200
C	0.00885200	0.00059100	1.40781900
C	1.22016200	0.00002300	2.09564500
C	2.41793500	-0.00096300	1.37973000
C	2.40718800	-0.00138000	-0.01261100
C	1.19587300	-0.00081000	-0.70043900
H	-0.91760900	0.00136100	1.96890400
H	-0.95124500	0.00062600	-0.51210100
O	1.17154300	0.00047400	3.46928600
H	2.06576200	-0.00002600	3.82490200
H	3.36728000	-0.00141600	1.90731000
O	1.24450500	-0.00126400	-2.07408000
H	0.35028900	-0.00075800	-2.42970600
H	3.33364300	-0.00215100	-0.57370500

b3lyp/6-311++G(d,p): OH-C_6H_4-OH, *para* (conformer no 2)
[total energy (hartree): -382.803034616]

C	0.02263600	0.00010100	0.00331200
C	0.02256100	0.00053000	1.39179200
C	1.22837100	0.00001500	2.09568200
C	2.43200800	-0.00093300	1.39594300
C	2.43208300	-0.00137000	-0.00057800
C	1.22852200	-0.00085200	-0.70044700
H	-0.90861800	0.00127400	1.94522500
H	-0.90848400	0.00050200	-0.55022100
O	1.16033500	0.00048200	3.46844900
H	2.04906700	0.00003200	3.83755500
H	3.37674900	-0.00134700	1.93137300
O	1.16063500	-0.00124200	-2.07322100

H	2.04940700	-0.00184600	-2.44223000
H	3.37688200	-0.00212200	-0.53590600

b3lyp/6-311++G(d,p): SH-C_6H_4-SH, *para* (conformer no 1)
[total energy (hartree): -1028.73851349]

C	0.00006100	0.00275700	-0.00033700
C	-0.00019600	0.00201800	1.39691000
C	1.22409800	0.00068500	2.07210300
C	2.42132100	0.00694800	1.36513700
C	2.42178600	-0.00487600	-0.03288600
C	1.19839500	-0.01705900	-0.70768800
H	3.35903400	0.02133200	1.90909000
H	1.16950100	-0.03731600	-1.79125500
H	1.24751400	-0.00316200	3.15604200
S	3.99857100	-0.04861900	-0.87488700
H	3.53770400	0.29350600	-2.09374500
S	-1.49853000	0.04397800	2.37103700
H	-2.34808500	-0.25834500	1.37010200
H	-0.93472600	0.01313500	-0.54940100

b3lyp/6-311++G(d,p): SH-C_6H_4-SH, *para* (conformer no 2)
[total energy (hartree): -1028.73850759]

C	0.00744000	0.00036400	0.00279100
C	-0.00947300	0.00122300	1.40048800
C	1.20691400	0.00106300	2.08879100
C	2.41206300	-0.00064800	1.39441800
C	2.42897400	-0.00139000	-0.00327500
C	1.21258500	-0.00076200	-0.69158100
H	3.34305400	-0.00108100	1.95036700
H	1.19471700	-0.00141000	-1.77556400
H	1.22478800	0.00219000	3.17277400
S	4.01643800	-0.00324100	-0.82375900
H	3.54291000	-0.00385500	-2.08489600
S	-1.59694300	0.00431600	2.22095900
H	-1.12348000	-0.00813500	3.48206100
H	-0.92355700	0.00031800	-0.55315300