

Supplementary Information for

Impacts of External Fields on Aromaticity and Acidity for Benzoic Acid: A Density Functional Theory, Conceptual Density Functional Theory and Information-Theoretic Approach Study

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7. The optimized molecular coordinates.

1. Benchmark Results

Table S1 Benchmark tests for benzoic acid under electric field with 9 basis sets and 9 functionals/methods to examine the impact of the methodology dependence on the NICS(0) values.

Functional	Basis set
B3LYP	6-311G(d)
pw91pw91	6-311G(d,p)
CAM-B3LYP	6-311+G(d)
b3pw91	6-311+G(d,p)
pbepbe	Def2SVPP
tpsstpss	Def2TZVP
ω b97xd	cc-pVDZ
M062X	cc-pVTZ
MP2	aug-cc-pVTZ

When basis sets were tested, the M062X functional was employed. When functionals were tested, 6-311+G(d) basis set was employed. Units in ppm.

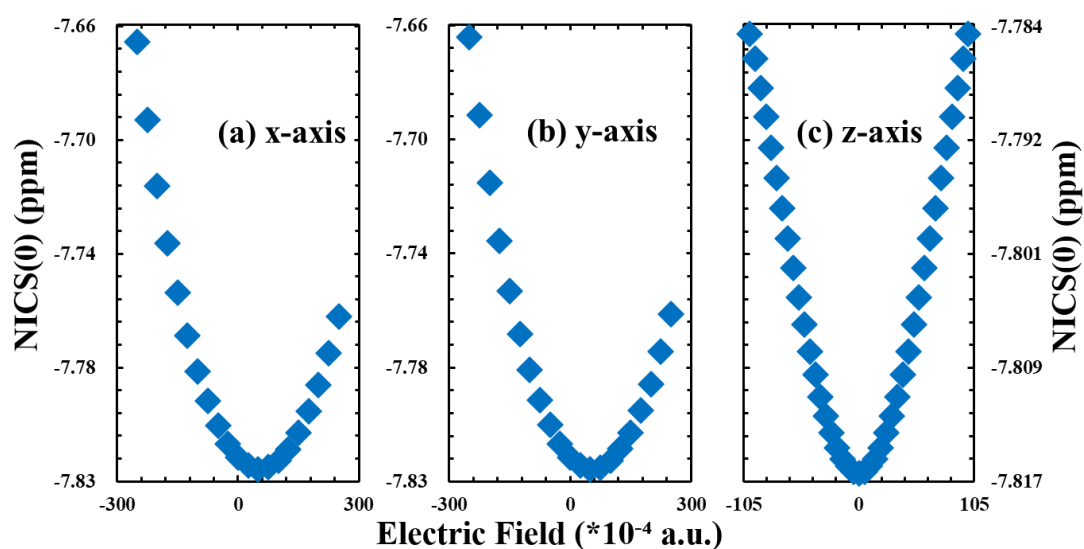


Figure S1 Profiles of aromaticity index NICS(0) values at B3LYP/6-311+G(d) level as a function of the applied external electric field along (a) x-axis; (b) y-axis; and (c) z-axis directions.

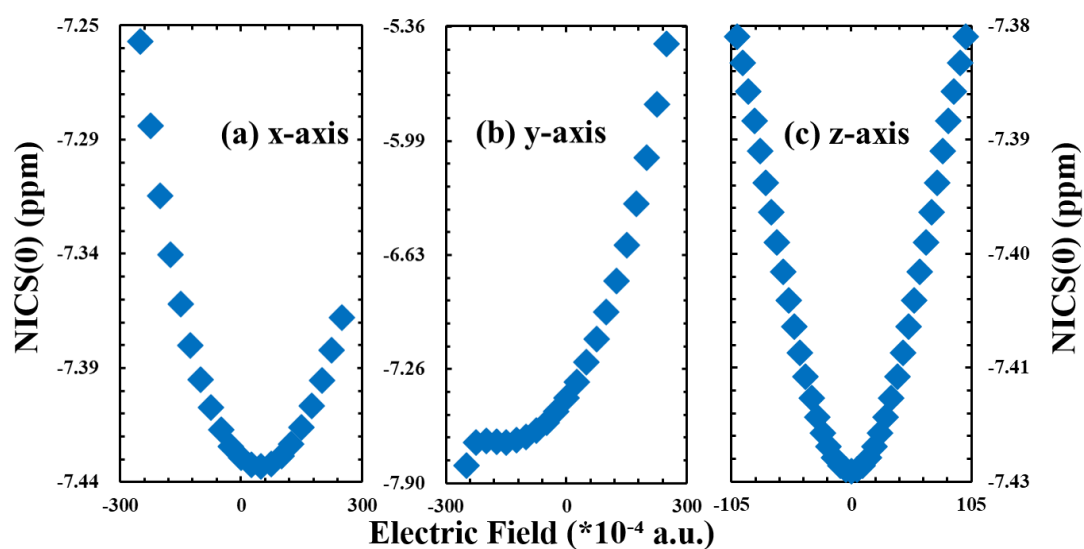


Figure S2 Profiles of aromaticity index NICS(0) values at pw91pw91/6-311+G(d) level as a function of the applied external electric field along (a) x-axis; (b) y-axis; and (c) z-axis directions.

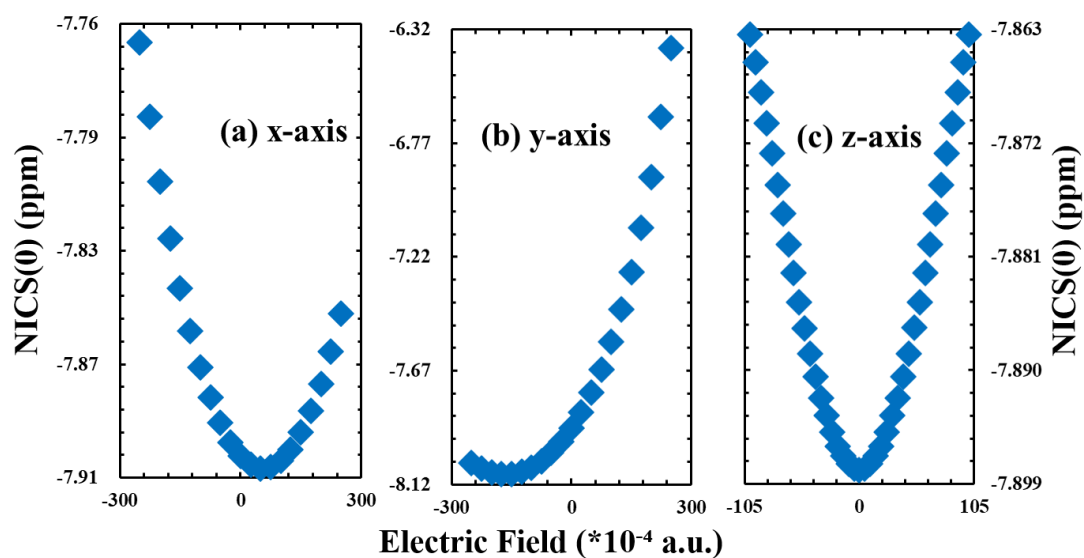


Figure S3 Profiles of aromaticity index NICS(0) values at CAM-B3LYP/6-311+G(d) level as a function of the applied external electric field along (a) x-axis; (b) y-axis; and (c) z-axis directions.

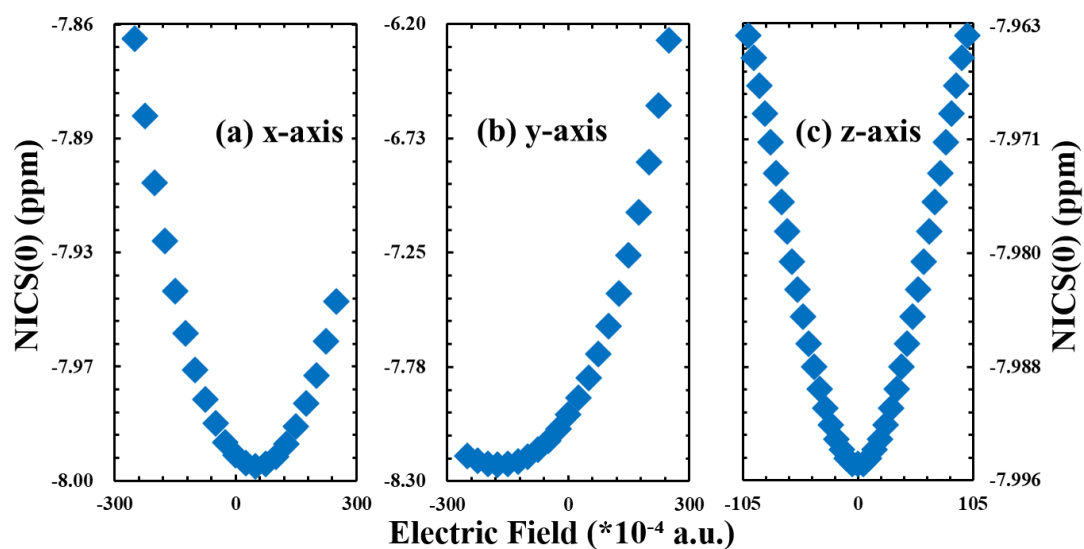


Figure S4 Profiles of aromaticity index NICS(0) values at b3pw91/6-311+G(d) level as a function of the applied external electric field along (a) x-axis; (b) y-axis; and (c) z-axis directions.

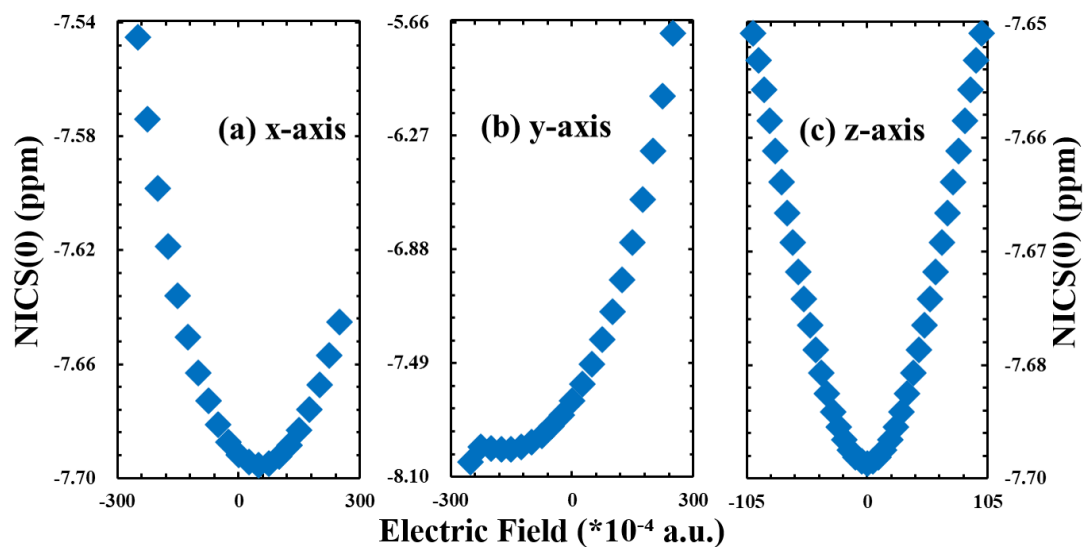


Figure S5 Profiles of aromaticity index NICS(0) values at tpsstpss/6-311+G(d) level as a function of the applied external electric field along (a) x-axis; (b) y-axis; and (c) z-axis directions.

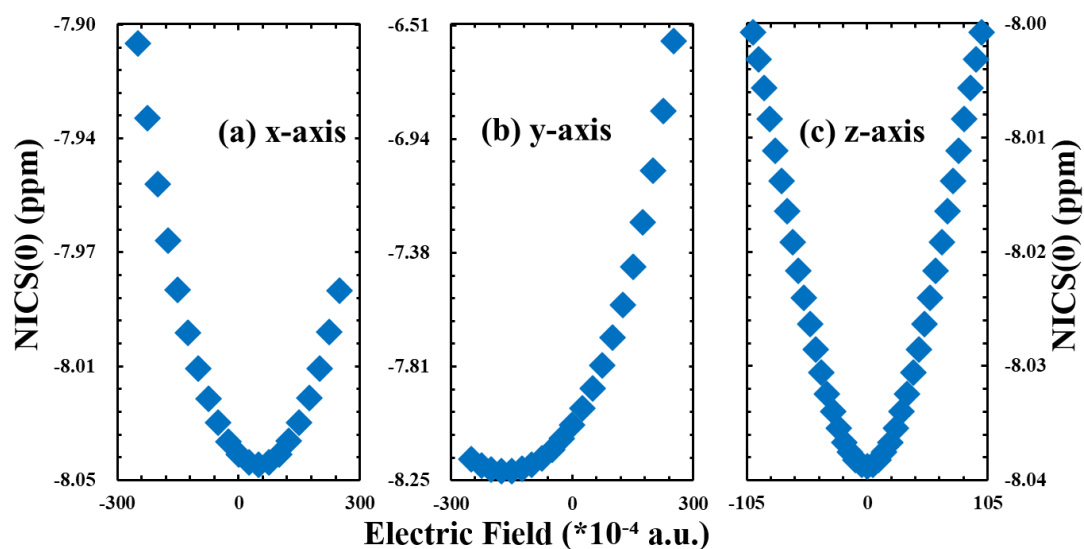


Figure S6 Profiles of aromaticity index NICS(0) values at ω b97xd/6-311+G(d) level as a function of the applied external electric field along (a) x-axis; (b) y-axis; and (c) z-axis directions.

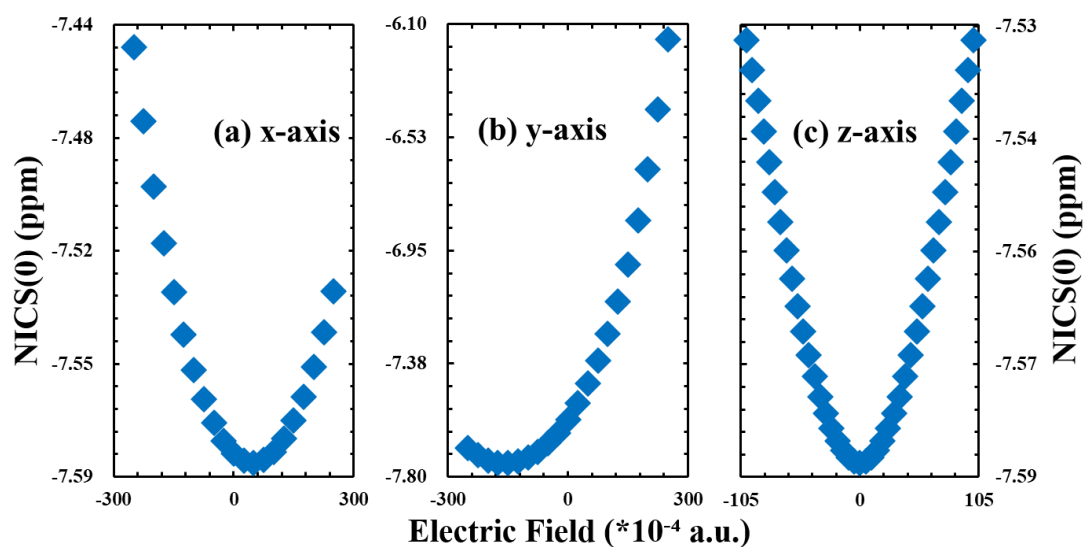


Figure S7 Profiles of aromaticity index NICS(0) values at M062X/6-311+G(d) level as a function of the applied external electric field along (a) x-axis; (b) y-axis; and (c) z-axis directions.

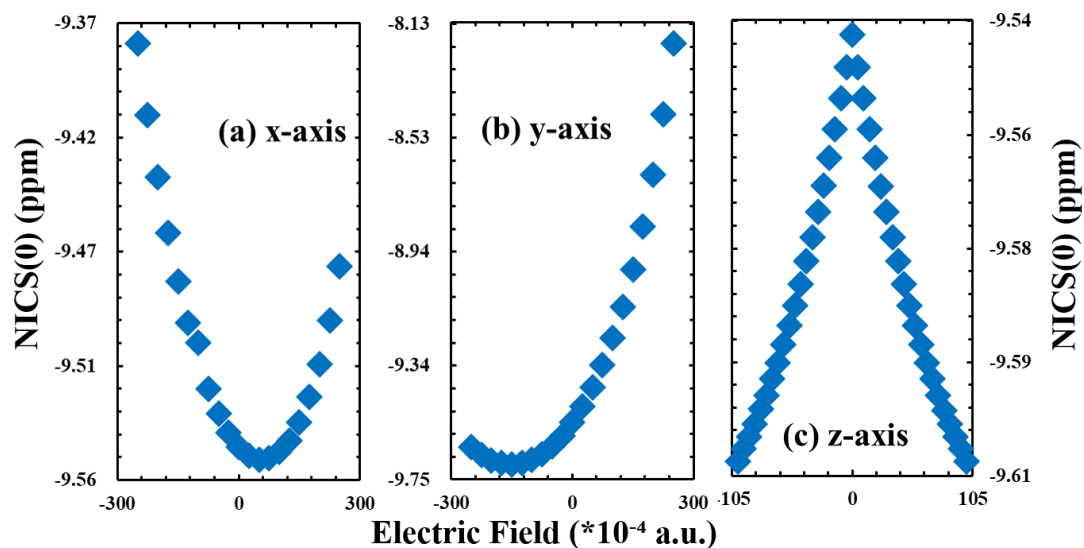


Figure S8 Profiles of aromaticity index NICS(0) values at MP2/6-311+G(d) level as a function of the applied external electric field along (a) x-axis; (b) y-axis; and (c) z-axis directions.

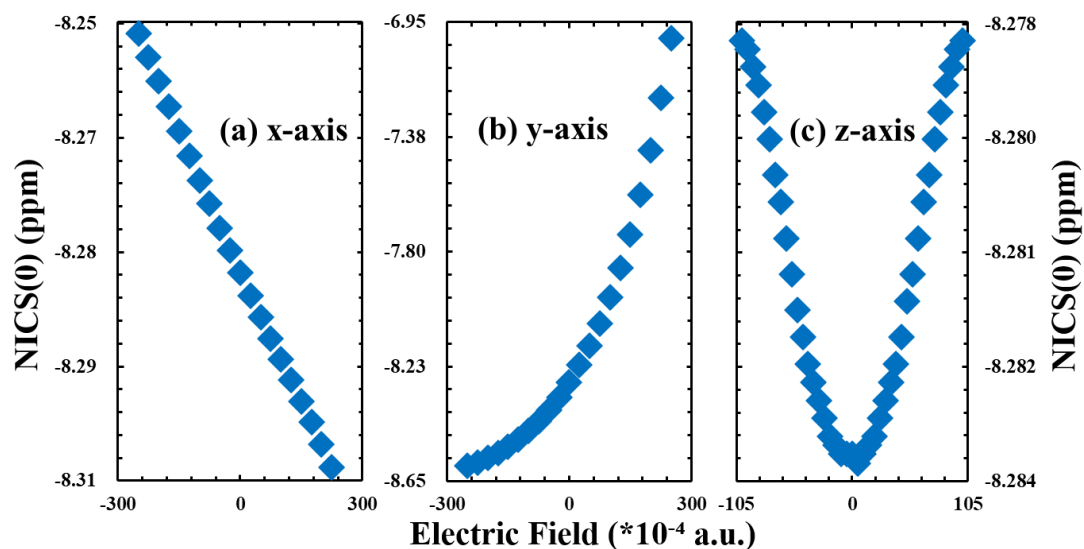


Figure S9 NICS(0) values of calculated benzoic acid under the electric field at m062x/6-311G(d) level.

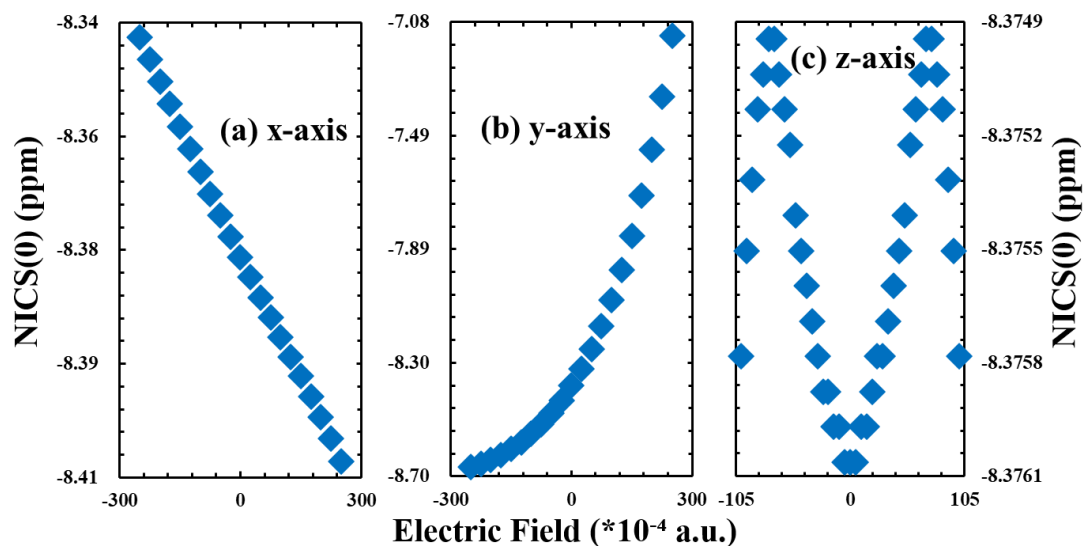


Figure S10 NICS(0) values of calculated benzoic acid under the electric field at M062X/6-311G(d,p) level.

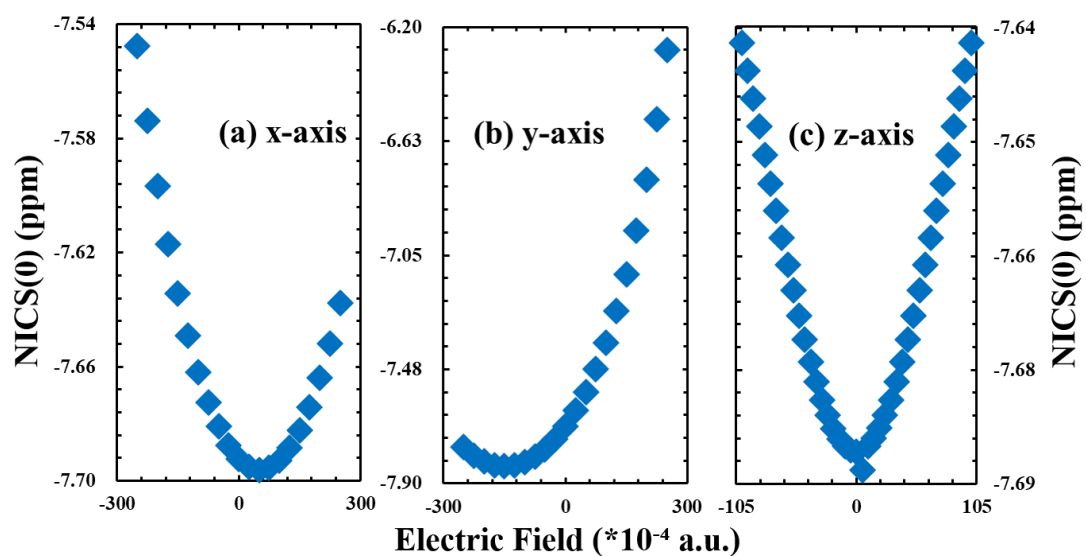


Figure S11 NICS(0) values of calculated benzoic acid under the electric field at M062X/6-311+G(d,p) level.

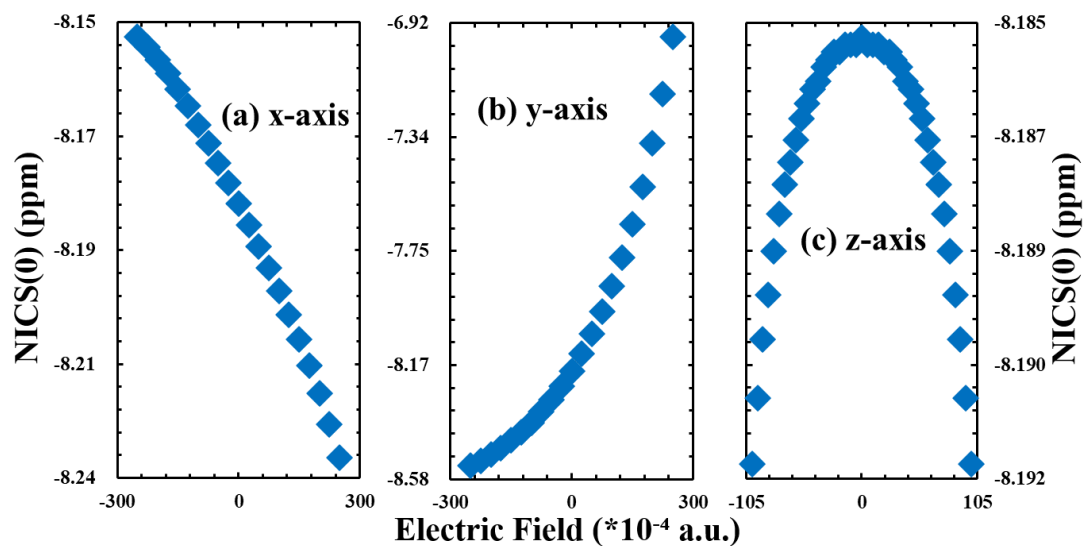


Figure S12 NICS(0) values of calculated benzoic acid under the electric field at M062X/Def2SVPP level.

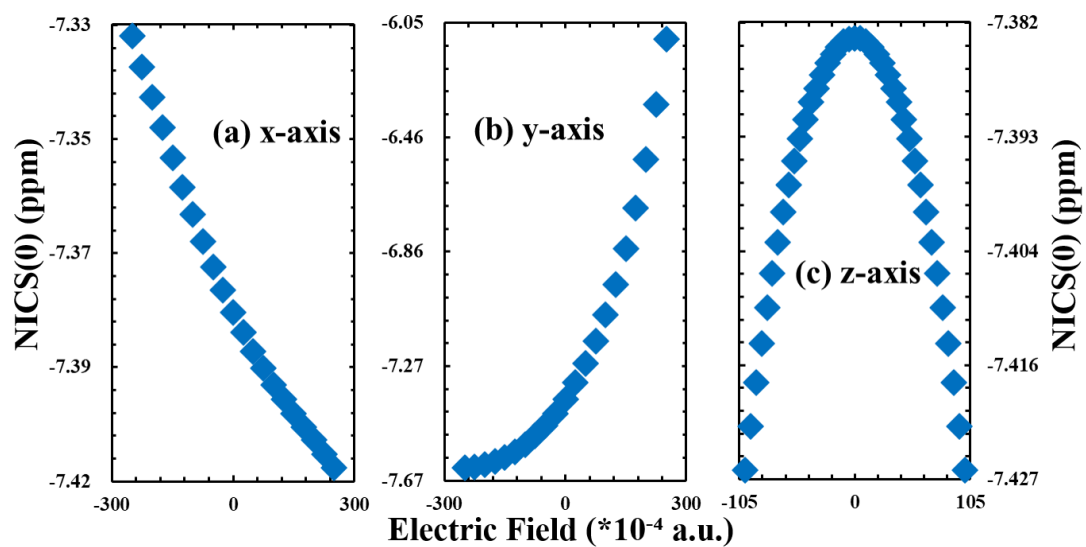


Figure S13 NICS(0) values of calculated benzoic acid under the electric field at M062X/Def2TZVP level.

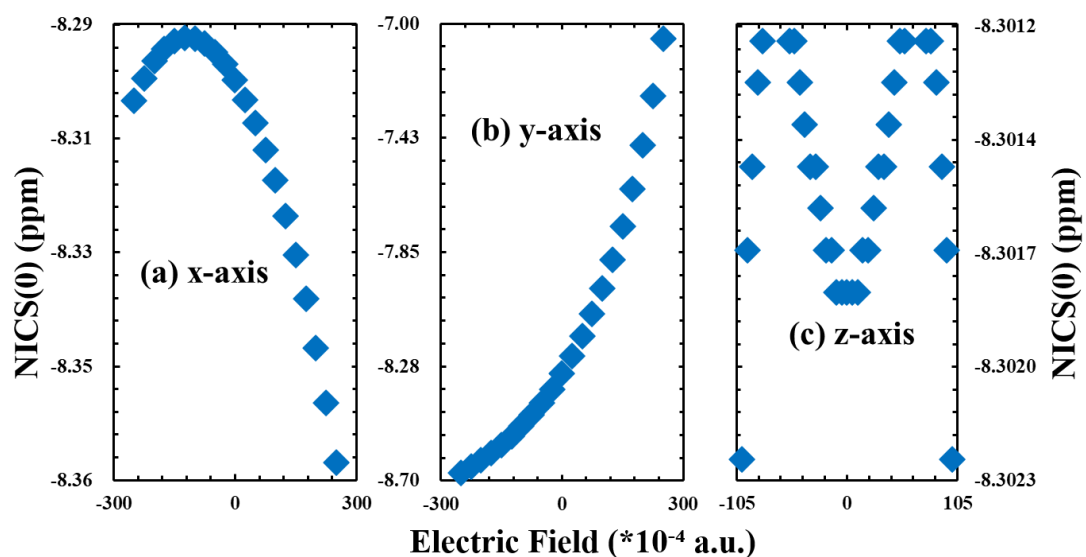


Figure S14 NICS(0) values of calculated benzoic acid under the electric field at M062X/cc-pVDZ level.

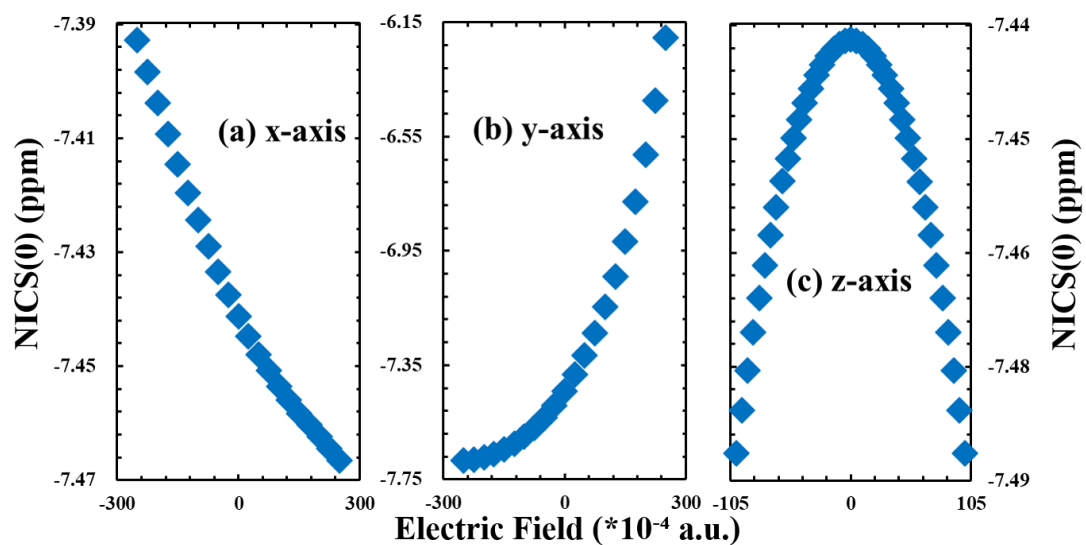


Figure S15 NICS(0) values of calculated benzoic acid under the electric field at M062X/cc-pVTZ level.

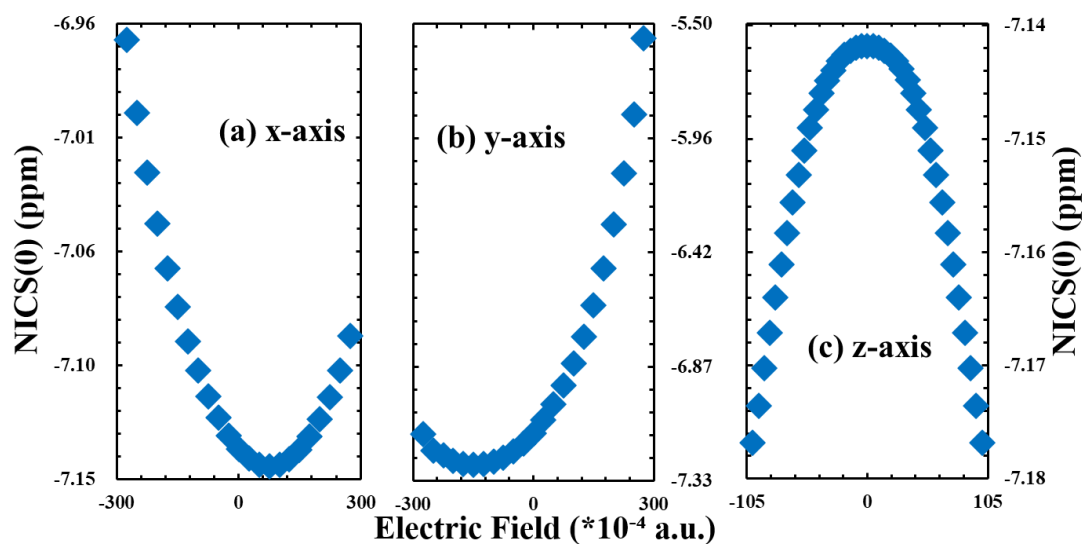


Figure S16 NICS(0) values of calculated benzoic acid under the electric field at M062X/aug-cc-pVTZ level.

2. Profiles of average C-C bond distance of the ring change as a function of the strength of the applied external electric field.

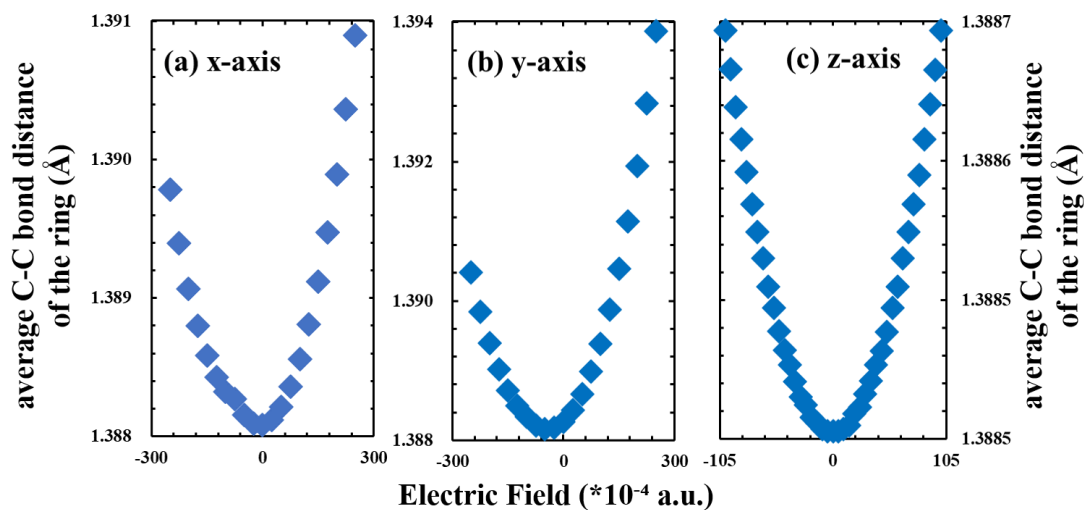


Figure S17 Profiles of average C-C bond distance of the ring change as a function of the strength of the applied external electric field along (a) x-axis; (b) y-axis; and (c) z-axis.

3. Aromaticity results characterized by other indicators (such as NICS(1)_{zz}, PDI, HOMA, FLU) of benzoic acid under the external electric field.

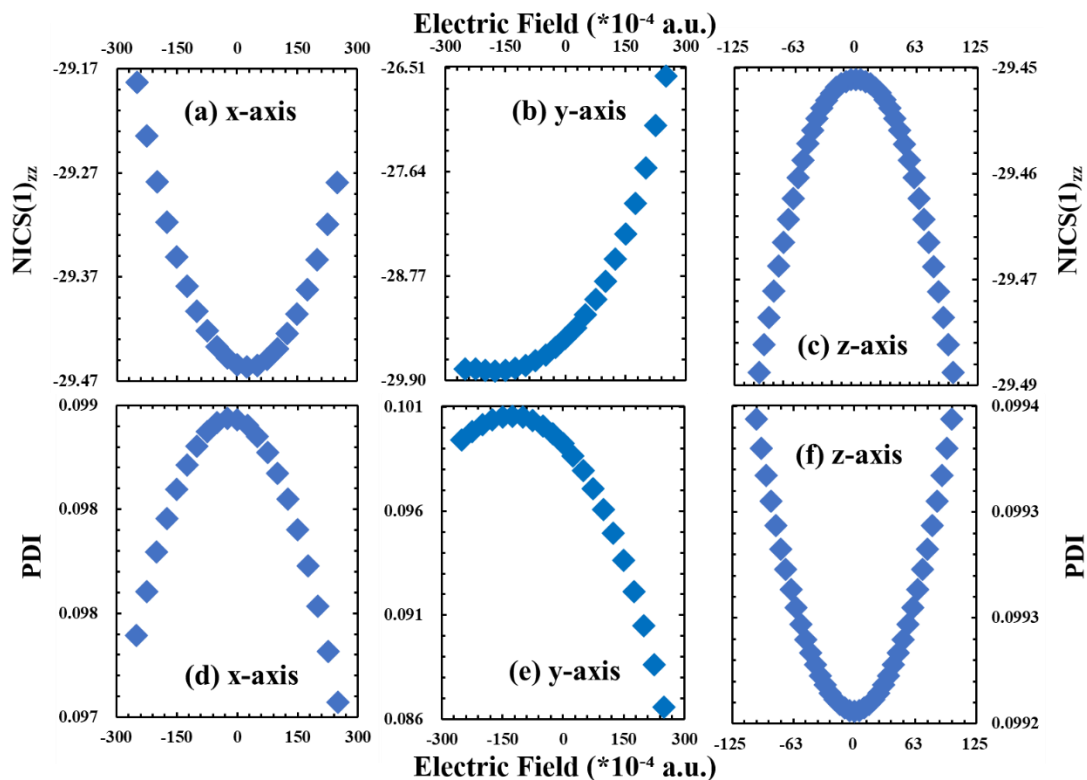


Figure S18 Changes in NICS(1)_{zz} and PDI values of benzoic acid with electric field changes, shown here are changes in all three directions: (a) (d) x-axis; (b) (e) y-axis; (c) (f) z-axis.

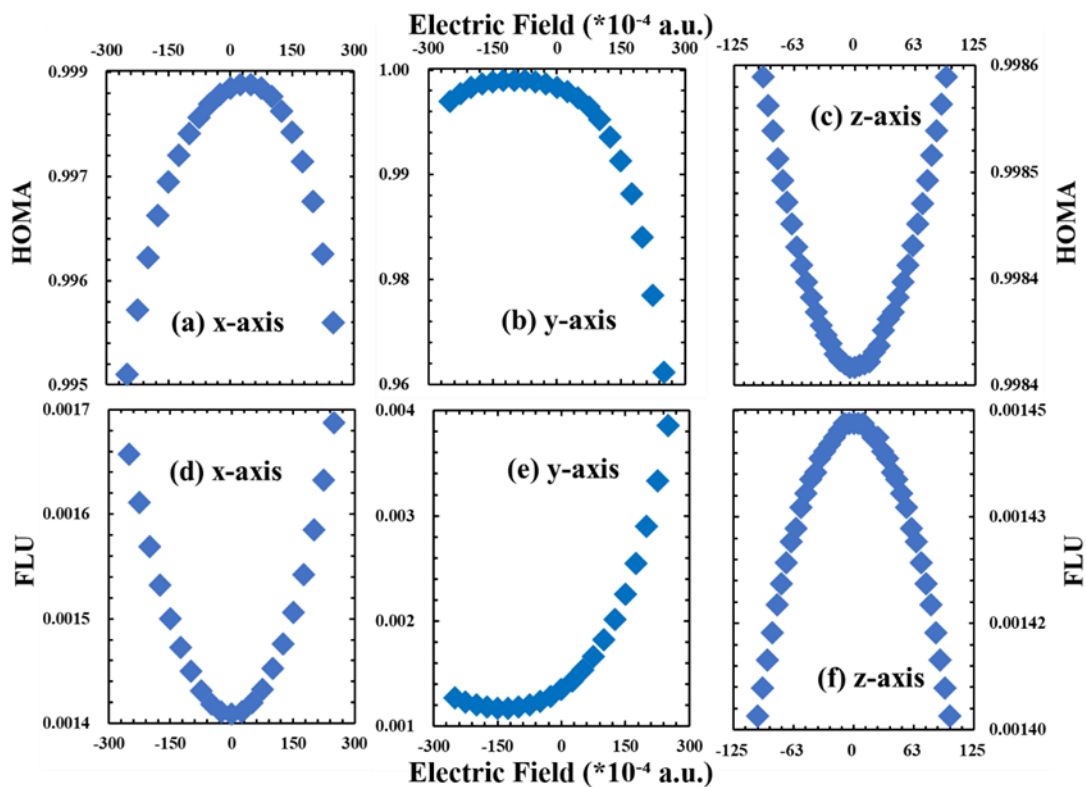


Figure S19 Changes in HOMA and FLU values of benzoic acid with electric field changes, shown here are changes in all three directions: (a) (d) x-axis; (b) (e) y-axis; (c) (f) z-axis.

4. Profiles of the molecular electrostatic potential (MEP) values and natural valence atomic orbital energy (NAO) values of the dissociating proton on benzoic acid as a function of the applied external electric field strength for p-fluorobenzoic acid and 3,5-difluorobenzoic acid in three directions.

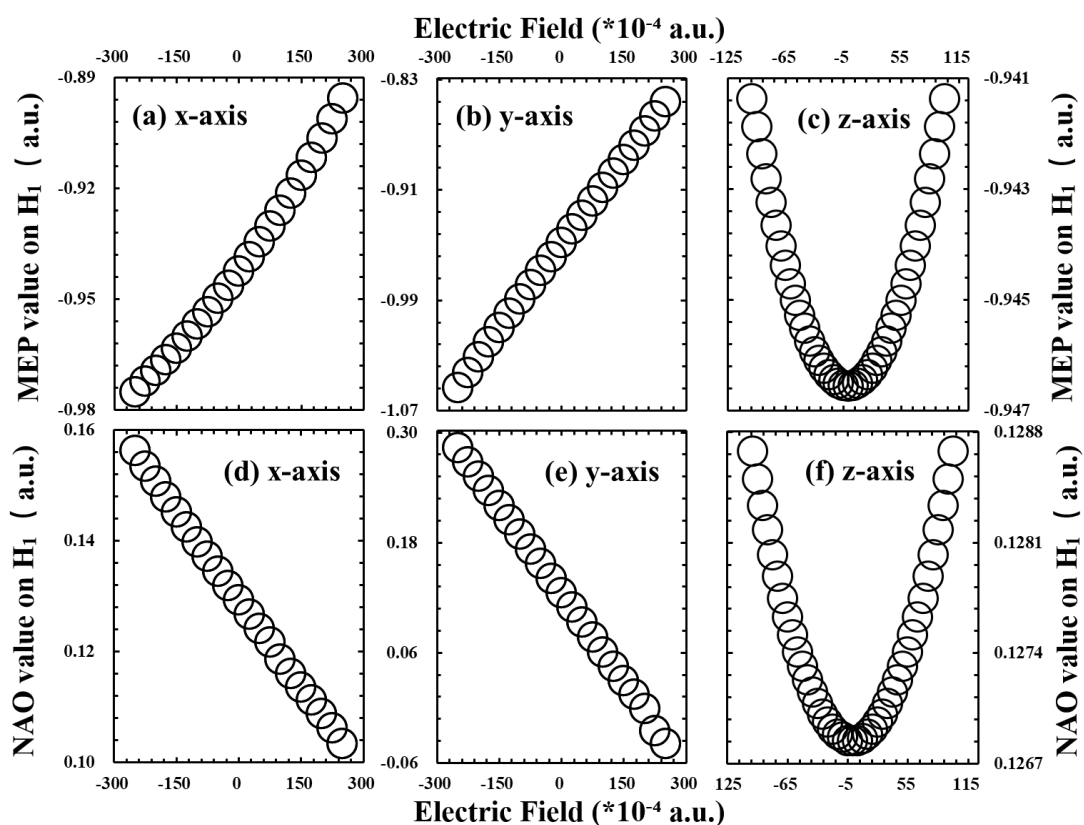


Figure S20 Profiles of the molecular electrostatic potential (MEP) values and natural valence atomic orbital energy (NAO) values of the dissociating proton on benzoic acid (H_1 in Scheme 1) as a function of p-fluorobenzoic acid applied external electric field strength in three directions.

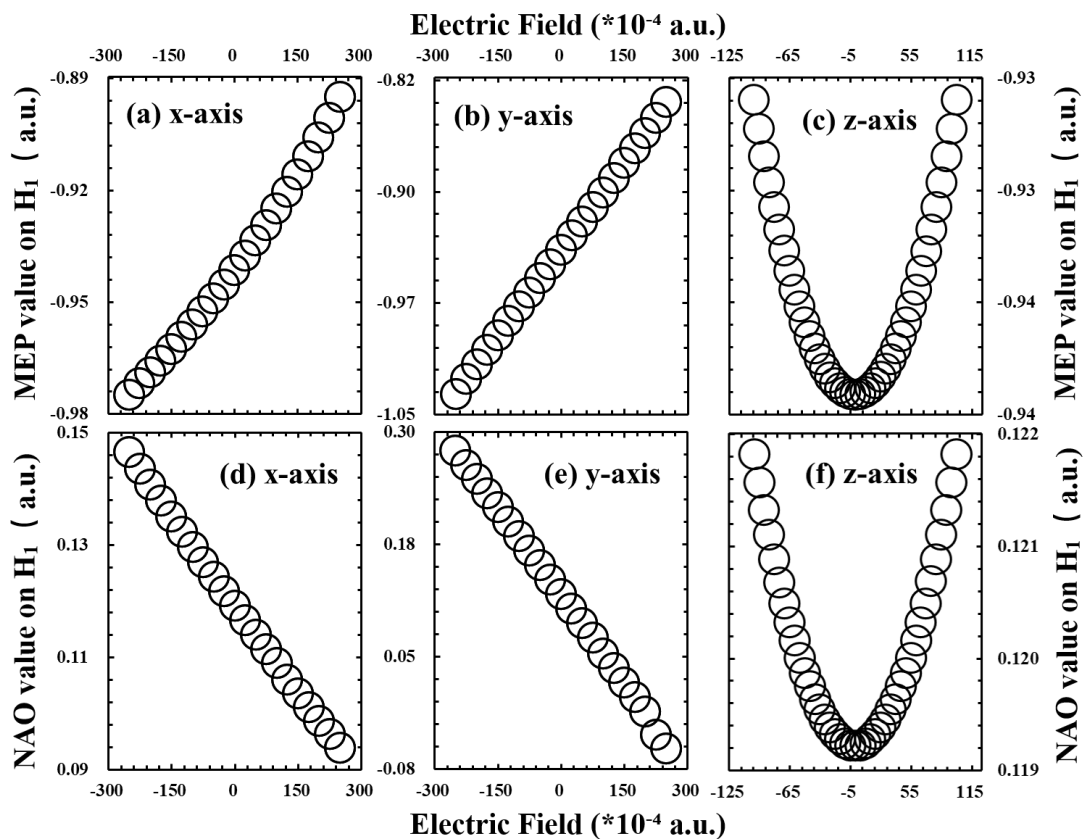


Figure S21 Profiles of the molecular electrostatic potential (MEP) values and natural valence atomic orbital energy (NAO) values of the dissociating proton on benzoic acid (H₁ in Scheme 1) as a function of 3,5-difluorobenzoic acid applied external electric field strength in three directions.

5. Predicted pKa values as a function of p-fluorobenzoic acid and 3,5-difluorobenzoic applied external electric field strength in three directions.

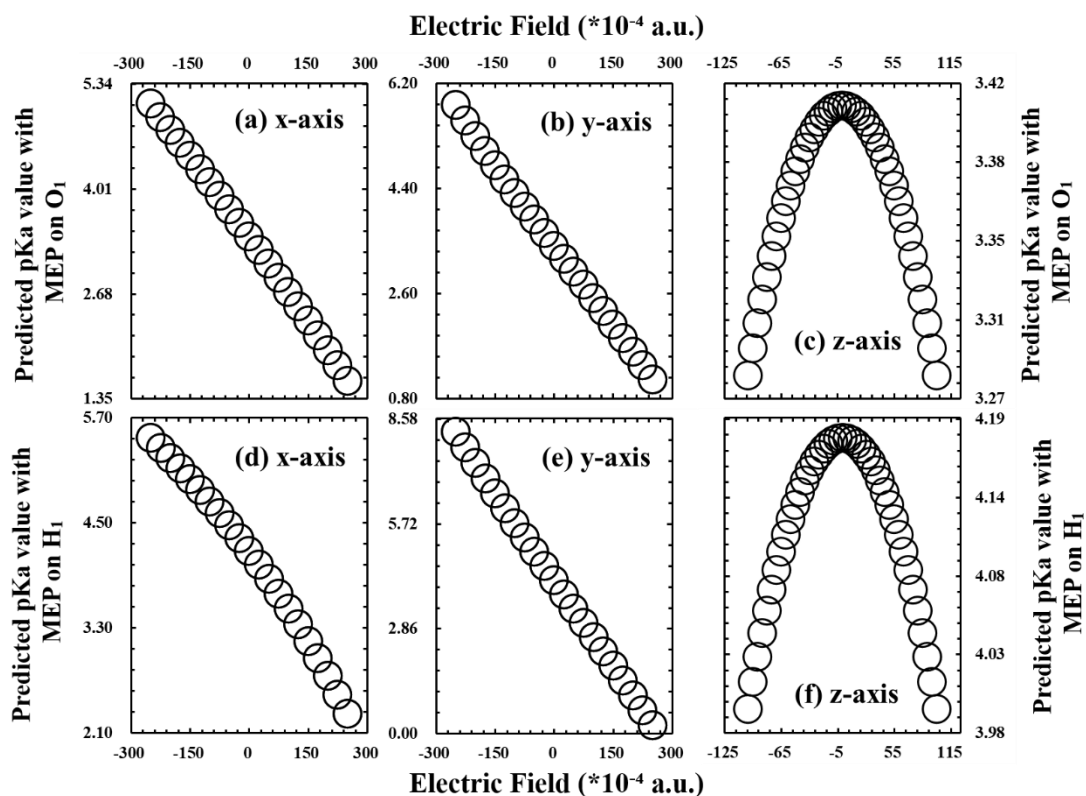


Figure S22 Predicted pKa values as a function of p-fluorobenzoic acid applied external electric field strength in three different directions. (a) - (c) are predicted pKa values using MEP results from O₁ in Scheme 1 and (d) - (f) are values using MEP data from H₁.

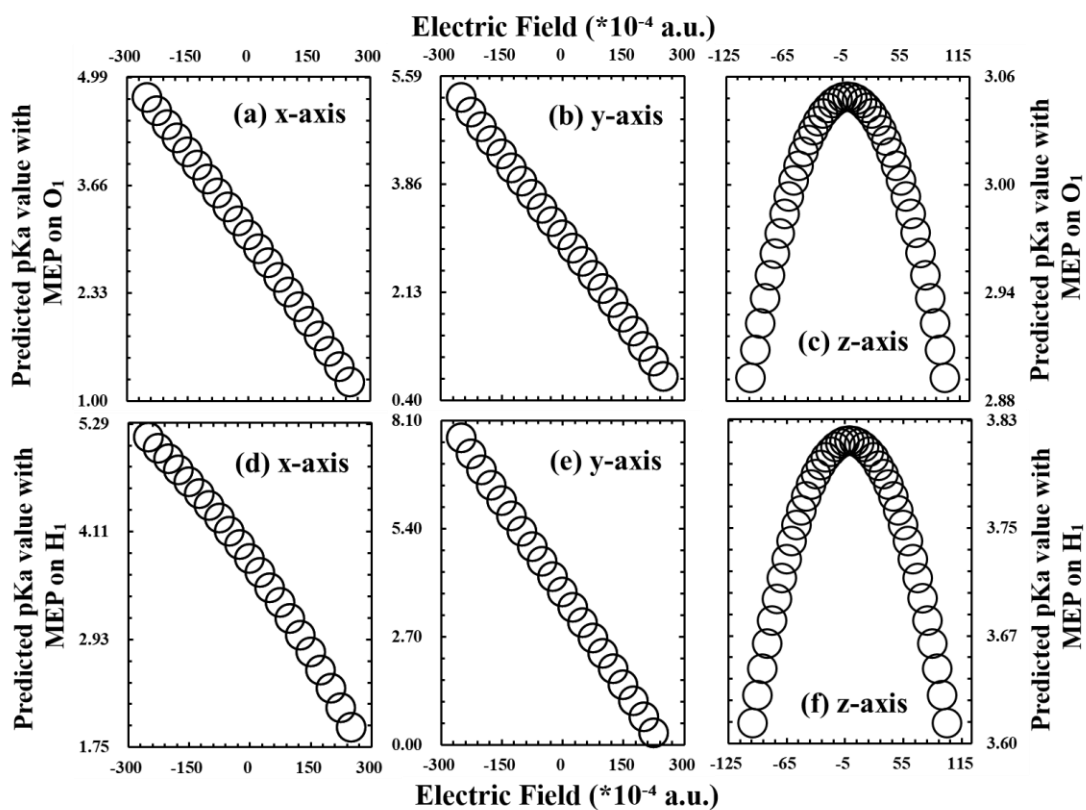


Figure S23 Predicted pKa values as a function of 3,5-difluorobenzoic applied external electric field strength in three different directions. (a) - (c) are predicted pKa values using MEP results from O_1 in Scheme 1 and (d) - (f) are values using MEP data from H_1 .

6. Strong linear correlations of MEP values of p-fluorobenzoic acid and 3,5-difluorobenzoic with NPA partial charges on both O₁ and H₁ for when the external electric field is applied to any of the three directions.

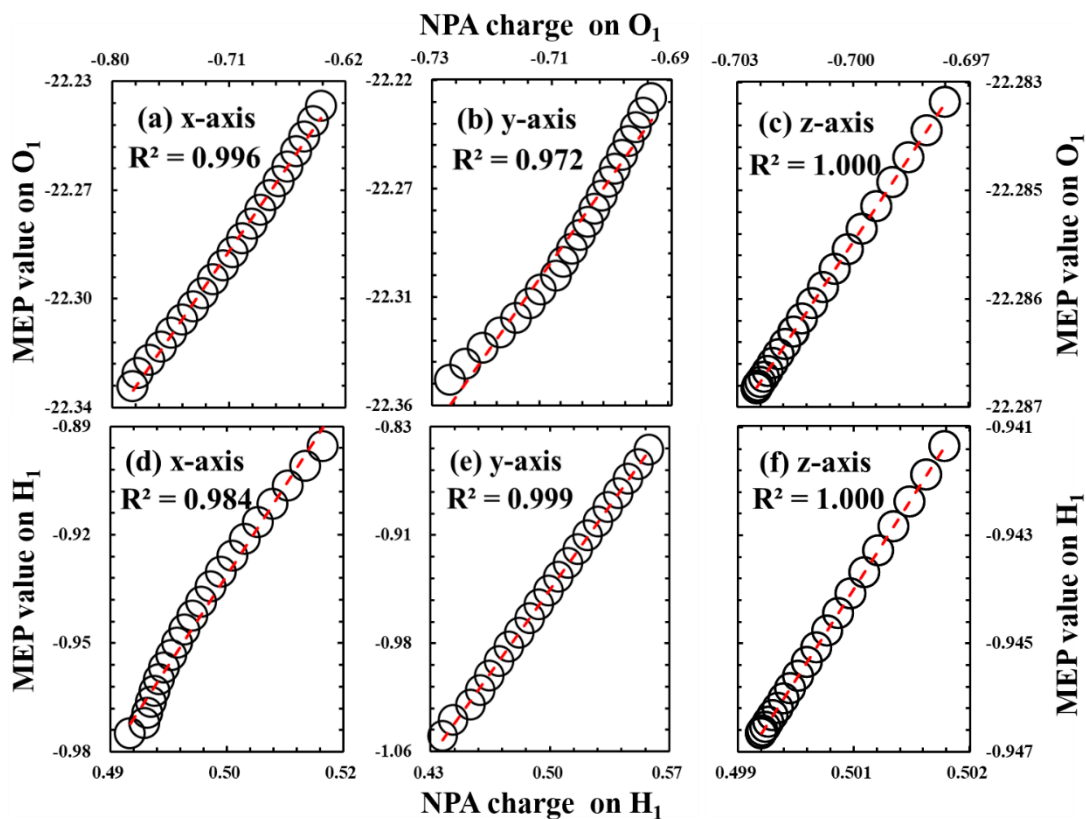


Figure S24 Strong linear correlations of MEP values of p-fluorobenzoic acid with NPA partial charges on both O₁ and H₁ for when the external electric field is applied to any of the three directions. (a) - (c) are for O₁ in Scheme 1 and (d) - (f) are for H₁ in Scheme 1.

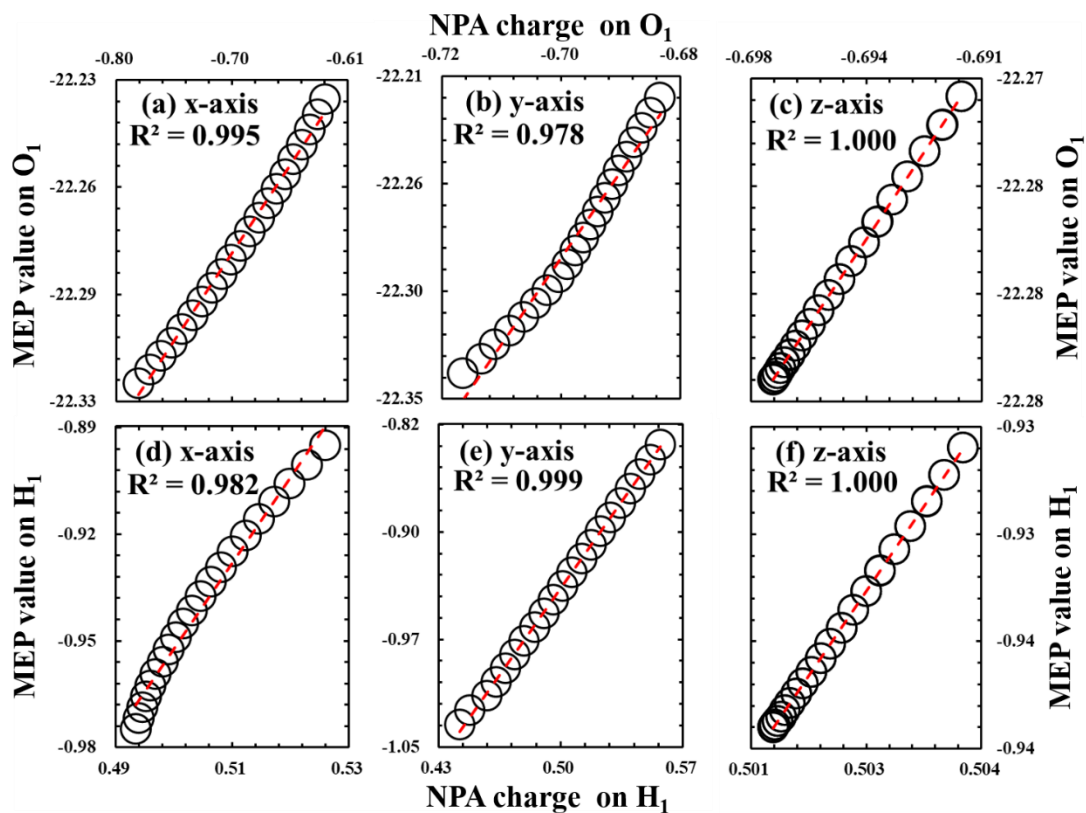


Figure S25 Strong linear correlations of MEP values of 3,5-difluorobenzoic with NPA partial charges on both O₁ and H₁ for when the external electric field is applied to any of the three directions. (a) - (c) are for O₁ in Scheme 1 and (d) - (f) are for H₁ in Scheme 1.

7. The optimized molecular coordinates

==> 1_H_x+00.gjf <==

C	1.23575700	0.69015800	-0.00000100
C	0.04075400	1.40227300	-0.00000600
C	-1.17756700	0.73058100	-0.00000700
C	-1.20059800	-0.65365900	-0.00000300
C	-0.00776300	-1.36629700	0.00000100
C	1.20790200	-0.69590500	0.00000300
H	2.17567300	1.22236900	0.00000100
H	-2.09022400	1.31000800	-0.00001000
H	-2.14569300	-1.17847800	-0.00000400
H	-0.02623100	-2.44775500	0.00000400
H	2.13408000	-1.25348400	0.00000600
C	0.01470400	2.88752700	-0.00000800
O	-0.98381200	3.55582800	-0.00000600
O	1.24428300	3.43827400	-0.00001300
H	1.11980700	4.39627300	-0.00001500

==> 1_H_x-100.gjf <==

C	1.23236500	0.69425800	-0.00000100
C	0.03596300	1.40448300	-0.00000400
C	-1.18111500	0.72988900	-0.00000600
C	-1.20118500	-0.65370100	-0.00000400
C	-0.00590800	-1.36530500	0.00000000
C	1.20779100	-0.69344100	0.00000200
H	2.17447200	1.22308900	0.00000100
H	-2.09244500	1.31229700	-0.00000900
H	-2.14565300	-1.18269800	-0.00000500
H	-0.01816400	-2.44693700	0.00000200
H	2.13638400	-1.24645200	0.00000500
C	0.01015000	2.89222300	-0.00000600
O	-1.00044000	3.55510400	0.00000100
O	1.23102900	3.42575000	-0.00001700
H	1.15782700	4.38915500	-0.00001700

==> 1_H_x+100.gjf <==

C	1.23907700	0.68710500	-0.00000600
C	0.04415300	1.40038300	-0.00000500
C	-1.17597400	0.73104600	-0.00000200
C	-1.20101000	-0.65478300	0.00000100
C	-0.00931400	-1.36761900	0.00000000
C	1.20876300	-0.69812900	-0.00000300
H	2.17760000	1.22313700	-0.00000800

H	-2.09163900	1.30660300	-0.00000200
H	-2.14772000	-1.17615700	0.00000400
H	-0.03329400	-2.44902300	0.00000200
H	2.13422900	-1.25963300	-0.00000500
C	0.01815400	2.88361100	-0.00000900
O	-0.96811600	3.55827900	-0.00001400
O	1.25869100	3.45093100	-0.00000500
H	1.08747100	4.40196200	-0.00000700

==> 1_H_x-125.gjf <==

C	1.23149900	0.69545200	-0.00000400
C	0.03453300	1.40509800	-0.00000600
C	-1.18230700	0.72968200	-0.00000500
C	-1.20147700	-0.65389900	-0.00000200
C	-0.00539300	-1.36510800	0.00000100
C	1.20788900	-0.69277500	0.00000000
H	2.17427500	1.22351500	-0.00000500
H	-2.09358400	1.31267600	-0.00000700
H	-2.14595600	-1.18405100	0.00000000
H	-0.01597100	-2.44680100	0.00000400
H	2.13734300	-1.24454800	0.00000200
C	0.00883200	2.89354300	-0.00000800
O	-1.00478900	3.55519200	-0.00001100
O	1.22783000	3.42263900	-0.00000700
H	1.16834900	4.38709800	-0.00000900

==> 1_H_x+125.gjf <==

C	1.23988600	0.68649500	-0.00000300
C	0.04478700	1.39995600	-0.00000100
C	-1.17590100	0.73110800	0.00000000
C	-1.20127700	-0.65525600	-0.00000100
C	-0.00965100	-1.36800700	-0.00000200
C	1.20909500	-0.69865700	-0.00000400
H	2.17816900	1.22358700	-0.00000600
H	-2.09255900	1.30559100	0.00000000
H	-2.14853200	-1.17589400	-0.00000100
H	-0.03491200	-2.44941700	-0.00000200
H	2.13465900	-1.26103700	-0.00000500
C	0.01883500	2.88274100	-0.00000300
O	-0.96431100	3.55917500	0.00001200
O	1.26253300	3.45411400	-0.00002200
H	1.08025200	4.40321300	-0.00002100

==> 1_H_x-150.gjf <==

C	1.23062400	0.69671800	-0.00000700
C	0.03300200	1.40574000	-0.00000800
C	-1.18362200	0.72946400	-0.00000400
C	-1.20182400	-0.65417700	0.00000100
C	-0.00485700	-1.36493100	0.00000200
C	1.20804000	-0.69208400	-0.00000200
H	2.17411600	1.22404400	-0.00001000
H	-2.09496900	1.31296800	-0.00000400
H	-2.14638800	-1.18552500	0.00000500
H	-0.01370000	-2.44669100	0.00000500
H	2.13845600	-1.24258400	-0.00000200
C	0.00744400	2.89492800	-0.00001200
O	-1.00922500	3.55538900	-0.00002900
O	1.22466300	3.41953900	0.00000600
H	1.17931200	4.38491400	0.00000100

==> 1_H_x+150.gjf <==

C	1.24067100	0.68600500	-0.00000900
C	0.04528100	1.39954000	-0.00000300
C	-1.17598400	0.73115800	0.00000300
C	-1.20162900	-0.65581100	0.00000400
C	-0.00996400	-1.36840900	-0.00000200
C	1.20944900	-0.69913400	-0.00000900
H	2.17879200	1.22412600	-0.00001600
H	-2.09378200	1.30445000	0.00000800
H	-2.14947400	-1.17579000	0.00001000
H	-0.03642900	-2.44983500	-0.00000200
H	2.13526500	-1.26230700	-0.00001500
C	0.01940500	2.88190400	-0.00000500
O	-0.96051900	3.56023200	-0.00000400
O	1.26653300	3.45723800	-0.00000800
H	1.07345700	4.40434500	-0.00000900

==> 1_H_x-175.gjf <==

C	1.22973900	0.69805200	-0.00000600
C	0.03137600	1.40641300	-0.00000700
C	-1.18505800	0.72923200	-0.00000400
C	-1.20222400	-0.65453200	0.00000100
C	-0.00430000	-1.36477700	0.00000200
C	1.20824500	-0.69137200	-0.00000200
H	2.17399800	1.22467200	-0.00000900
H	-2.09659600	1.31317400	-0.00000400
H	-2.14695100	-1.18711800	0.00000400
H	-0.01135400	-2.44660900	0.00000500

H	2.13972700	-1.24055800	-0.00000100
C	0.00598000	2.89638400	-0.00001100
O	-1.01375700	3.55569600	-0.00002400
O	1.22151800	3.41645900	0.00000100
H	1.19073000	4.38259700	-0.00000100

==> 1_H_x+175.gjf <==

C	1.24143500	0.68557400	-0.00001500
C	0.04568100	1.39914300	-0.00000300
C	-1.17621300	0.73117400	0.00000900
C	-1.20204800	-0.65645400	0.00001200
C	-0.01025300	-1.36883800	-0.00000200
C	1.20985100	-0.69960000	-0.00001700
H	2.17942800	1.22479000	-0.00002700
H	-2.09524200	1.30324200	0.00001700
H	-2.15053900	-1.17582900	0.00002200
H	-0.03788500	-2.45028800	-0.00000200
H	2.13603800	-1.26351800	-0.00003000
C	0.01989000	2.88110800	-0.00000900
O	-0.95676700	3.56141600	-0.00002900
O	1.27066200	3.46036800	0.00001000
H	1.06703500	4.40542600	0.00000600

==> 1_H_x-200.gjf <==

C	1.22884900	0.69945500	-0.00000500
C	0.02965400	1.40711700	-0.00000600
C	-1.18661300	0.72899000	-0.00000400
C	-1.20267600	-0.65496500	0.00000000
C	-0.00372200	-1.36464700	0.00000100
C	1.20850500	-0.69063900	-0.00000100
H	2.17392400	1.22540000	-0.00000700
H	-2.09846900	1.31329300	-0.00000500
H	-2.14765100	-1.18882600	0.00000200
H	-0.00893100	-2.44655700	0.00000400
H	2.14115500	-1.23847700	0.00000000
C	0.00444800	2.89791200	-0.00001000
O	-1.01838500	3.55610800	-0.00002000
O	1.21839100	3.41340900	-0.00000200
H	1.20259300	4.38014100	-0.00000400

==> 1_H_x+200.gjf <==

C	1.24217500	0.68522400	-0.00001300
C	0.04597400	1.39876000	0.00000100
C	-1.17660800	0.73115900	0.00001100

C	-1.20254600	-0.65718000	0.00001000
C	-0.01051300	-1.36929100	-0.00000500
C	1.21029400	-0.70004800	-0.00001700
H	2.18007600	1.22559700	-0.00002400
H	-2.09696600	1.30196400	0.00002000
H	-2.15172300	-1.17603600	0.00001800
H	-0.03928100	-2.45077400	-0.00000800
H	2.13698900	-1.26465000	-0.00003100
C	0.02028000	2.88033400	-0.00000100
O	-0.95303600	3.56272400	0.00001000
O	1.27495600	3.46349100	-0.00001500
H	1.06100100	4.40644000	-0.00001300

==> 1_H_x-225.gjf <==

C	1.22795400	0.70092300	0.00000100
C	0.02783900	1.40785400	-0.00000500
C	-1.18828300	0.72874000	-0.00000600
C	-1.20317700	-0.65547600	-0.00000300
C	-0.00312400	-1.36454300	0.00000200
C	1.20882300	-0.68988800	0.00000400
H	2.17390000	1.22622200	0.00000100
H	-2.10058900	1.31332200	-0.00001100
H	-2.14849300	-1.19064400	-0.00000500
H	-0.00643000	-2.44653600	0.00000500
H	2.14274100	-1.23634700	0.00000800
C	0.00285100	2.89951700	-0.00001000
O	-1.02311100	3.55662700	-0.00001600
O	1.21527900	3.41040200	-0.00001000
H	1.21489300	4.37754100	-0.00001300

==> 1_H_x+225.gjf <==

C	1.24288800	0.68496700	-0.00002100
C	0.04612700	1.39839000	-0.00000200
C	-1.17715400	0.73111300	0.00001600
C	-1.20312600	-0.65801200	0.00001400
C	-0.01075800	-1.36977100	-0.00000600
C	1.21076000	-0.70045300	-0.00002300
H	2.18076600	1.22647900	-0.00003700
H	-2.09898600	1.30054500	0.00003100
H	-2.15304900	-1.17639800	0.00002500
H	-0.04056700	-2.45129600	-0.00000800
H	2.13812200	-1.26565800	-0.00003900
C	0.02055300	2.87961700	0.00000000
O	-0.94931400	3.56423400	0.00000400

O	1.27943100	3.46658200	-0.00000300
H	1.05537700	4.40737400	-0.00001000

==> 1_H_x-250.gjf <==

C	1.22705800	0.70245800	0.00000200
C	0.02592900	1.40862300	-0.00000300
C	-1.19006900	0.72848500	-0.00000600
C	-1.20372600	-0.65606700	-0.00000300
C	-0.00250700	-1.36446500	0.00000200
C	1.20920000	-0.68911600	0.00000500
H	2.17392800	1.22714000	0.00000400
H	-2.10296400	1.31325600	-0.00001200
H	-2.14948500	-1.19257100	-0.00000700
H	-0.00384800	-2.44654600	0.00000400
H	2.14448700	-1.23417000	0.00000900
C	0.00119400	2.90120000	-0.00001000
O	-1.02793600	3.55725300	-0.00001600
O	1.21217600	3.40744600	-0.00001100
H	1.22763500	4.37478600	-0.00001500

==> 1_H_x+250.gjf <==

C	1.24356300	0.68479800	-0.00001800
C	0.04615700	1.39803300	0.00000400
C	-1.17788500	0.73102800	0.00001800
C	-1.20378900	-0.65893900	0.00001100
C	-0.01097100	-1.37027900	-0.00000800
C	1.21126400	-0.70083400	-0.00002300
H	2.18145400	1.22751700	-0.00003200
H	-2.10129700	1.29903800	0.00003400
H	-2.15449800	-1.17694900	0.00002000
H	-0.04178700	-2.45185600	-0.00001400
H	2.13944800	-1.26656700	-0.00004100
C	0.02071700	2.87891700	0.00001100
O	-0.94559500	3.56589400	0.00005100
O	1.28412200	3.46966700	-0.00003500
H	1.05016600	4.40824600	-0.00003500

==> 1_H_x-25.gjf <==

C	1.23491500	0.69108500	-0.00000100
C	0.03968700	1.40279200	-0.00000600
C	-1.17827400	0.73042700	-0.00000600
C	-1.20065500	-0.65356000	-0.00000300
C	-0.00732800	-1.36601800	0.00000100
C	1.20780100	-0.69531300	0.00000300

H	2.17530500	1.22240900	0.00000100
H	-2.09043900	1.31068700	-0.00001000
H	-2.14549600	-1.17935800	-0.00000400
H	-0.02431100	-2.44751000	0.00000400
H	2.13442800	-1.25180700	0.00000600
C	0.01366800	2.88862100	-0.00000800
O	-0.98786800	3.55548800	-0.00000700
O	1.24088300	3.43512600	-0.00001200
H	1.12875500	4.39464300	-0.00001500

==> 1_H_x+25.gjf <==

C	1.23659500	0.68929500	0.00000100
C	0.04173500	1.40177400	-0.00000400
C	-1.17698000	0.73072100	-0.00000700
C	-1.20060300	-0.65382900	-0.00000600
C	-0.00817900	-1.36659600	0.00000000
C	1.20805000	-0.69648300	0.00000500
H	2.17608800	1.22241900	0.00000400
H	-2.09023600	1.30925900	-0.00001100
H	-2.14601400	-1.17771400	-0.00000900
H	-0.02809000	-2.44803000	0.00000200
H	2.13388600	-1.25510500	0.00001000
C	0.01567300	2.88648200	-0.00000500
O	-0.97981400	3.55627400	0.00001000
O	1.24775400	3.44143000	-0.00002500
H	1.11120800	4.39781600	-0.00002300

==> 1_H_x-50.gjf <==

C	1.23407000	0.69207600	0.00000300
C	0.03853600	1.40333300	-0.00000300
C	-1.17910100	0.73026000	-0.00000700
C	-1.20077300	-0.65353300	-0.00000700
C	-0.00687400	-1.36576100	0.00000000
C	1.20774800	-0.69470800	0.00000600
H	2.17498300	1.22253900	0.00000700
H	-2.09087700	1.31129600	-0.00001200
H	-2.14542400	-1.18035400	-0.00001200
H	-0.02233000	-2.44729200	0.00000100
H	2.13492900	-1.25007600	0.00001100
C	0.01256400	2.88976700	-0.00000300
O	-0.99198700	3.55525400	0.00001900
O	1.23754700	3.43199200	-0.00003200
H	1.13806100	4.39291800	-0.00002800

==> 1_H_x+50.gjf <==

C	1.23743000	0.68849800	-0.00000200
C	0.04263000	1.40129300	-0.00000500
C	-1.17651700	0.73084700	-0.00000500
C	-1.20067200	-0.65407300	-0.00000200
C	-0.00857700	-1.36691600	0.00000100
C	1.20824400	-0.69704700	0.00000100
H	2.17654900	1.22256300	-0.00000200
H	-2.09047200	1.30844400	-0.00000800
H	-2.14645900	-1.17707100	-0.00000100
H	-0.02988700	-2.44833100	0.00000400
H	2.13384300	-1.25667500	0.00000300
C	0.01657300	2.88548200	-0.00000900
O	-0.97586900	3.55682900	-0.00001100
O	1.25130600	3.44459500	-0.00000900
H	1.10295000	4.39927500	-0.00001200

==> 1_H_x-75.gjf <==

C	1.23322200	0.69313300	0.00000000
C	0.03729600	1.40389600	-0.00000500
C	-1.18004700	0.73008100	-0.00000600
C	-1.20095000	-0.65357900	-0.00000400
C	-0.00640100	-1.36552300	0.00000100
C	1.20774400	-0.69408400	0.00000200
H	2.17470700	1.22276500	0.00000100
H	-2.09154400	1.31183500	-0.00000900
H	-2.14547600	-1.18146700	-0.00000500
H	-0.02028200	-2.44710100	0.00000300
H	2.13558000	-1.24829400	0.00000600
C	0.01139300	2.89096600	-0.00000700
O	-0.99617500	3.55512500	-0.00000100
O	1.23426500	3.42886700	-0.00001600
H	1.14774000	4.39109200	-0.00001700

==> 1_H_x+75.gjf <==

C	1.23825800	0.68776600	-0.00000500
C	0.04343700	1.40083000	-0.00000600
C	-1.17618000	0.73095600	-0.00000400
C	-1.20080700	-0.65439000	0.00000000
C	-0.00895600	-1.36725700	0.00000100
C	1.20848200	-0.69759600	-0.00000200
H	2.17705400	1.22280100	-0.00000600
H	-2.09093800	1.30756000	-0.00000500
H	-2.14702800	-1.17654900	0.00000300

H	-0.03162200	-2.44866300	0.00000400
H	2.13395600	-1.25818600	-0.00000100
C	0.01740100	2.88452500	-0.00001000
O	-0.97197100	3.55749500	-0.00001900
O	1.25494800	3.44776300	-0.00000300
H	1.09503600	4.40065700	-0.00000600

==> 1_H_y-100.gjf <==

C	1.24025300	0.68633500	0.00000000
C	0.04891000	1.40114400	-0.00000600
C	-1.17013900	0.73277700	-0.00000800
C	-1.19951000	-0.65200500	-0.00000500
C	-0.00934800	-1.36967200	0.00000100
C	1.20785000	-0.70167400	0.00000300
H	2.17927900	1.22103000	0.00000200
H	-2.07650500	1.32294100	-0.00001100
H	-2.15011500	-1.16878600	-0.00000600
H	-0.03179700	-2.45293300	0.00000400
H	2.13502200	-1.25951200	0.00000800
C	0.01082000	2.89923200	-0.00000800
O	-1.00960900	3.52342500	-0.00000500
O	1.23099900	3.44519900	-0.00001300
H	1.13496200	4.41021200	-0.00001400

==> 1_H_y+100.gjf <==

C	1.23271900	0.69250200	-0.00000400
C	0.03395400	1.40575600	-0.00000600
C	-1.18467600	0.72809400	-0.00000400
C	-1.20238800	-0.65556900	-0.00000100
C	-0.00657400	-1.36551800	0.00000100
C	1.20865900	-0.69186300	0.00000000
H	2.17416300	1.22188200	-0.00000500
H	-2.10325000	1.29804100	-0.00000600
H	-2.14248200	-1.18859000	0.00000100
H	-0.02182400	-2.44692800	0.00000400
H	2.13358000	-1.25089000	0.00000100
C	0.01868800	2.87765800	-0.00000800
O	-0.95822000	3.58974100	-0.00001000
O	1.25784100	3.43642700	-0.00001000
H	1.10088100	4.38697100	-0.00001200

==> 1_H_y-125.gjf <==

C	1.24162100	0.68512200	-0.00000500
C	0.05121000	1.40116900	-0.00001000

C	-1.16818100	0.73330300	-0.00000800
C	-1.19932300	-0.65163800	-0.00000300
C	-0.00981900	-1.37094500	0.00000300
C	1.20792900	-0.70344100	0.00000200
H	2.18055400	1.22033900	-0.00000600
H	-2.07290600	1.32637200	-0.00001000
H	-2.15139900	-1.16640100	-0.00000200
H	-0.03340900	-2.45494500	0.00000800
H	2.13530100	-1.26162900	0.00000700
C	0.00985800	2.90255100	-0.00001200
O	-1.01610000	3.51548100	-0.00002200
O	1.22762700	3.44780400	0.00000000
H	1.13810900	4.41457100	-0.00000100

==> 1_H_y+125.gjf <==

C	1.23217400	0.69286100	-0.00000200
C	0.03242300	1.40709000	-0.00000400
C	-1.18646000	0.72738700	-0.00000200
C	-1.20297800	-0.65608100	-0.00000100
C	-0.00632600	-1.36573300	0.00000100
C	1.20898400	-0.69107400	0.00000000
H	2.17407900	1.22150400	-0.00000300
H	-2.10649700	1.29507600	-0.00000400
H	-2.14188800	-1.19120700	-0.00000100
H	-0.02087400	-2.44740400	0.00000200
H	2.13355700	-1.25071800	0.00000200
C	0.01971300	2.87541500	-0.00000800
O	-0.95185600	3.59857900	-0.00000300
O	1.26138700	3.43673900	-0.00001600
H	1.09563300	4.38527900	-0.00001800

==> 1_H_y-150.gjf <==

C	1.24310400	0.68378700	0.00000400
C	0.05363800	1.40130300	-0.00000500
C	-1.16616000	0.73382800	-0.00001100
C	-1.19916600	-0.65128800	-0.00000900
C	-0.01033000	-1.37240100	0.00000000
C	1.20804600	-0.70536000	0.00000800
H	2.18200400	1.21947000	0.00000900
H	-2.06920300	1.32991600	-0.00001600
H	-2.15275900	-1.16401500	-0.00001400
H	-0.03512100	-2.45726400	0.00000200
H	2.13559100	-1.26402800	0.00001600
C	0.00889400	2.90605600	-0.00000400

O	-1.02262700	3.50756700	0.00002000
O	1.22419800	3.45080200	-0.00003100
H	1.14096400	4.41934100	-0.00002800

==> 1_H_y+150.gjf <==

C	1.23173000	0.69311600	-0.00000400
C	0.03096000	1.40863300	-0.00000600
C	-1.18825500	0.72663900	-0.00000300
C	-1.20363800	-0.65659800	0.00000100
C	-0.00609700	-1.36611800	0.00000300
C	1.20937800	-0.69037000	0.00000000
H	2.17412400	1.22101600	-0.00000700
H	-2.10974700	1.29211500	-0.00000500
H	-2.14139200	-1.19385700	0.00000400
H	-0.01998800	-2.44816100	0.00000600
H	2.13358600	-1.25074300	0.00000100
C	0.02075400	2.87324200	-0.00001200
O	-0.94552300	3.60757800	-0.00002400
O	1.26501500	3.43738300	-0.00000200
H	1.09016600	4.38383800	-0.00001000

==> 1_H_y-175.gjf <==

C	1.24471000	0.68231100	0.00000100
C	0.05618800	1.40154300	-0.00000400
C	-1.16406400	0.73435900	-0.00000700
C	-1.19903100	-0.65097400	-0.00000300
C	-0.01089600	-1.37404800	0.00000100
C	1.20820600	-0.70742600	0.00000300
H	2.18363000	1.21842200	0.00000300
H	-2.06540100	1.33355200	-0.00001100
H	-2.15420400	-1.16160900	-0.00000400
H	-0.03690600	-2.45990700	0.00000300
H	2.13587300	-1.26674500	0.00000600
C	0.00793200	2.90977800	-0.00000900
O	-1.02918700	3.49970100	-0.00001800
O	1.22069100	3.45421000	-0.00000700
H	1.14353100	4.42454700	-0.00001200

==> 1_H_y+175.gjf <==

C	1.23139600	0.69325600	0.00000000
C	0.02956900	1.41040000	-0.00000400
C	-1.19006300	0.72583900	-0.00000500
C	-1.20437700	-0.65712100	-0.00000100
C	-0.00588900	-1.36668200	0.00000300

C	1.20984900	-0.68975300	0.00000300
H	2.17429900	1.22041100	0.00000000
H	-2.11299600	1.28915100	-0.00000900
H	-2.14099900	-1.19654500	-0.00000100
H	-0.01917200	-2.44921400	0.00000600
H	2.13367000	-1.25097100	0.00000600
C	0.02180700	2.87114500	-0.00000800
O	-0.93924400	3.61676200	-0.00001200
O	1.26874100	3.43838200	-0.00001400
H	1.08448200	4.38265300	-0.00002100

==> 1_H_y-200.gjf <==

C	1.24642600	0.68071100	0.00000000
C	0.05888800	1.40188700	-0.00000500
C	-1.16190900	0.73487900	-0.00000700
C	-1.19893100	-0.65065900	-0.00000300
C	-0.01148600	-1.37589100	0.00000200
C	1.20839600	-0.70967600	0.00000200
H	2.18546200	1.21713600	0.00000200
H	-2.06150000	1.33729700	-0.00001100
H	-2.15570900	-1.15922200	-0.00000300
H	-0.03884700	-2.46288100	0.00000500
H	2.13618300	-1.26974200	0.00000600
C	0.00697400	2.91372300	-0.00001100
O	-1.03577200	3.49185500	-0.00002200
O	1.21712300	3.45806000	-0.00000400
H	1.14577300	4.43023600	-0.00000800

==> 1_H_y+200.gjf <==

C	1.23116800	0.69326800	-0.00000200
C	0.02825800	1.41241900	-0.00000500
C	-1.19188700	0.72497800	-0.00000400
C	-1.20520400	-0.65764400	0.00000000
C	-0.00570700	-1.36744700	0.00000300
C	1.21040100	-0.68922500	0.00000300
H	2.17462800	1.21964200	-0.00000300
H	-2.11624500	1.28618100	-0.00000700
H	-2.14072900	-1.19925700	0.00000000
H	-0.01841700	-2.45059000	0.00000600
H	2.13382100	-1.25139800	0.00000500
C	0.02288600	2.86911100	-0.00000900
O	-0.93302500	3.62614400	-0.00000600
O	1.27257100	3.43977500	-0.00001900
H	1.07855300	4.38175700	-0.00002200

==> 1_H_y-225.gjf <==

C	1.24828000	0.67894800	-0.00000100
C	0.06177700	1.40232700	-0.00000600
C	-1.15966300	0.73538800	-0.00000700
C	-1.19886400	-0.65034500	-0.00000300
C	-0.01211600	-1.37794500	0.00000200
C	1.20862000	-0.71213800	0.00000300
H	2.18753200	1.21556600	0.00000000
H	-2.05744900	1.34119000	-0.00001100
H	-2.15728200	-1.15683600	-0.00000400
H	-0.04097000	-2.46621300	0.00000500
H	2.13651500	-1.27306200	0.00000700
C	0.00600500	2.91793100	-0.00001200
O	-1.04242100	3.48400000	-0.00002300
O	1.21345500	3.46241800	-0.00000300
H	1.14765100	4.43648400	-0.00000600

==> 1_H_y+225.gjf <==

C	1.23107700	0.69313100	-0.00000100
C	0.02703500	1.41469100	-0.00000300
C	-1.19372800	0.72404800	-0.00000200
C	-1.20613100	-0.65816800	0.00000200
C	-0.00554800	-1.36842300	0.00000400
C	1.21105000	-0.68879400	0.00000200
H	2.17511600	1.21871300	-0.00000300
H	-2.11948100	1.28321000	-0.00000500
H	-2.14058500	-1.20200100	0.00000200
H	-0.01774500	-2.45230100	0.00000600
H	2.13404400	-1.25205200	0.00000400
C	0.02398500	2.86715200	-0.00000900
O	-0.92689800	3.63575700	-0.00000600
O	1.27651800	3.44159700	-0.00002200
H	1.07236600	4.38115300	-0.00002600

==> 1_H_y-250.gjf <==

C	1.25041000	0.67693700	-0.00000200
C	0.06492000	1.40281000	-0.00000800
C	-1.15725400	0.73595900	-0.00000800
C	-1.19883400	-0.65002200	-0.00000300
C	-0.01286300	-1.38019500	0.00000300
C	1.20891300	-0.71481200	0.00000300
H	2.18995200	1.21365900	-0.00000100
H	-2.05315700	1.34533200	-0.00001200

H	-2.15897900	-1.15433400	-0.00000300
H	-0.04323700	-2.46990100	0.00000700
H	2.13678500	-1.27692500	0.00000800
C	0.00509900	2.92236700	-0.00001200
O	-1.04917000	3.47596400	-0.00002400
O	1.20955600	3.46743100	-0.00000200
H	1.14893100	4.44344200	-0.00000300

==> 1_H_y+250.gjf <==

C	1.23112900	0.69282500	-0.00000400
C	0.02590600	1.41723600	-0.00000600
C	-1.19558900	0.72303700	-0.00000100
C	-1.20716900	-0.65869000	0.00000400
C	-0.00541900	-1.36964100	0.00000600
C	1.21180500	-0.68847000	0.00000200
H	2.17578400	1.21758500	-0.00000800
H	-2.12270900	1.28022500	-0.00000300
H	-2.14059000	-1.20476800	0.00000700
H	-0.01715700	-2.45438700	0.00001000
H	2.13435100	-1.25294200	0.00000300
C	0.02512500	2.86527900	-0.00001300
O	-0.92087400	3.64564300	-0.00001600
O	1.28059000	3.44390400	-0.00001600
H	1.06588900	4.38087600	-0.00002300

==> 1_H_y-25.gjf <==

C	1.23673200	0.68935100	-0.00000200
C	0.04264100	1.40179700	-0.00000600
C	-1.17576300	0.73114500	-0.00000700
C	-1.20026900	-0.65322200	-0.00000300
C	-0.00811600	-1.36689300	0.00000100
C	1.20782900	-0.69716400	0.00000200
H	2.17635600	1.22223100	0.00000000
H	-2.08690000	1.31310700	-0.00001000
H	-2.14668800	-1.17603000	-0.00000200
H	-0.02749700	-2.44863400	0.00000400
H	2.13428500	-1.25463700	0.00000500
C	0.01372800	2.89025500	-0.00000900
O	-0.99023000	3.54763500	-0.00001100
O	1.24097600	3.43950000	-0.00000900
H	1.12398600	4.39927200	-0.00001300

==> 1_H_y+25.gjf <==

C	1.23487500	0.69087200	-0.00000200
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C	0.03895400	1.40289200	-0.00000600
C	-1.17934800	0.73000100	-0.00000600
C	-1.20097100	-0.65411000	-0.00000300
C	-0.00743600	-1.36586100	0.00000100
C	1.20801900	-0.69475600	0.00000200
H	2.17512300	1.22239300	-0.00000100
H	-2.09349600	1.30698400	-0.00000900
H	-2.14477400	-1.18095100	-0.00000300
H	-0.02503900	-2.44714500	0.00000400
H	2.13390200	-1.25254600	0.00000500
C	0.01568500	2.88490900	-0.00000900
O	-0.97741000	3.56410700	-0.00000900
O	1.24760200	3.43736300	-0.00001100
H	1.11538400	4.39356100	-0.00001300

==> 1_H_y-50.gjf <==

C	1.23780900	0.68844500	-0.00000200
C	0.04463000	1.40145200	-0.00000700
C	-1.17392600	0.73169900	-0.00000700
C	-1.19998000	-0.65279900	-0.00000200
C	-0.00849700	-1.36765100	0.00000100
C	1.20779800	-0.69854200	0.00000200
H	2.17718500	1.22196500	0.00000000
H	-2.08349900	1.31630700	-0.00001000
H	-2.14775800	-1.17359900	-0.00000100
H	-0.02884600	-2.44978600	0.00000500
H	2.13451200	-1.25602400	0.00000500
C	0.01275400	2.89310200	-0.00001000
O	-0.99667400	3.53950000	-0.00001500
O	1.23766400	3.44105800	-0.00000600
H	1.12790000	4.40258400	-0.00001000

==> 1_H_y+50.gjf <==

C	1.23407500	0.69150100	-0.00000400
C	0.03722300	1.40367100	-0.00000600
C	-1.18112200	0.72939600	-0.00000400
C	-1.20139000	-0.65457900	0.00000000
C	-0.00712900	-1.36558600	0.00000200
C	1.20818200	-0.69370300	0.00000000
H	2.17469000	1.22231800	-0.00000500
H	-2.09674900	1.30399200	-0.00000600
H	-2.14393000	-1.18345900	0.00000100
H	-0.02390800	-2.44680300	0.00000500
H	2.13375600	-1.25180600	0.00000100

C	0.01667400	2.88239700	-0.00001000
O	-0.97101000	3.57250900	-0.00001900
O	1.25095800	3.43675100	-0.00000300
H	1.11075100	4.39111300	-0.00000700

==> 1_H_y-75.gjf <==

C	1.23898400	0.68744000	-0.00000300
C	0.04672000	1.40123500	-0.00000600
C	-1.17205200	0.73224300	-0.00000500
C	-1.19972800	-0.65239200	0.00000000
C	-0.00890800	-1.36857600	0.00000200
C	1.20780600	-0.70004400	0.00000000
H	2.17816000	1.22156600	-0.00000400
H	-2.08003000	1.31959200	-0.00000800
H	-2.14890100	-1.17118400	0.00000100
H	-0.03028000	-2.45121600	0.00000500
H	2.13475800	-1.25764800	0.00000200
C	0.01178400	2.89608800	-0.00001200
O	-1.00313600	3.53142700	-0.00003000
O	1.23433900	3.44295600	0.00000300
H	1.13155500	4.40622500	-0.00000200

==> 1_H_y+75.gjf <==

C	1.23335500	0.69204600	-0.00000100
C	0.03555600	1.40462200	-0.00000400
C	-1.18289700	0.72876200	-0.00000500
C	-1.20186100	-0.65506800	-0.00000300
C	-0.00684200	-1.36547100	0.00000000
C	1.20839300	-0.69273800	0.00000100
H	2.17436800	1.22215000	-0.00000100
H	-2.10000000	1.30101100	-0.00000700
H	-2.14316400	-1.18600600	-0.00000400
H	-0.02283600	-2.44673000	0.00000200
H	2.13364800	-1.25125300	0.00000400
C	0.01767500	2.87998400	-0.00000600
O	-0.96461000	3.58105300	0.00000300
O	1.25436800	3.43643600	-0.00001900
H	1.10591900	4.38891600	-0.00001900

==> 1_H_z-05.gjf <==

C	1.23575800	0.69015700	-0.00447100
C	0.04075300	1.40227400	-0.00355100
C	-1.17756600	0.73058800	-0.00026300
C	-1.20059500	-0.65365200	0.00227800

C	-0.00776400	-1.36629200	0.00035300
C	1.20790200	-0.69590400	-0.00333900
H	2.17567100	1.22237500	-0.00503000
H	-2.09021800	1.31001800	0.00229000
H	-2.14567900	-1.17846500	0.00755400
H	-0.02622400	-2.44774600	0.00351100
H	2.13407600	-1.25349000	-0.00331400
C	0.01472600	2.88752900	-0.00455100
O	-0.98369900	3.55583600	-0.01821900
O	1.24420400	3.43824700	0.01125000
H	1.11972700	4.39623800	0.01544400

==> 1_H_z+05.gjf <==

C	1.23575700	0.69015600	0.00447300
C	0.04075500	1.40227400	0.00354000
C	-1.17756400	0.73058900	0.00024400
C	-1.20059300	-0.65365000	-0.00228100
C	-0.00776300	-1.36629300	-0.00034400
C	1.20790100	-0.69590600	0.00334600
H	2.17567400	1.22236700	0.00503600
H	-2.09021900	1.31001600	-0.00232000
H	-2.14567800	-1.17846200	-0.00755600
H	-0.02622900	-2.44774700	-0.00349700
H	2.13407800	-1.25348600	0.00332500
C	0.01472700	2.88753000	0.00452500
O	-0.98369900	3.55583500	0.01816700
O	1.24420500	3.43825000	-0.01125300
H	1.11972200	4.39624000	-0.01546400

==> 1_H_z-100.gjf <==

C	1.23646400	0.68874500	-0.08941600
C	0.04261600	1.40265800	-0.07188700
C	-1.17561500	0.73425600	-0.00614500
C	-1.19902900	-0.64965200	0.04604200
C	-0.00827500	-1.36485100	0.00931400
C	1.20711100	-0.69712300	-0.06450300
H	2.17718000	1.22017200	-0.10039000
H	-2.08671700	1.31421800	0.04401300
H	-2.14073300	-1.17047900	0.14971500
H	-0.02627500	-2.44440600	0.07391400
H	2.13281200	-1.25571500	-0.06234900
C	0.02351100	2.88841300	-0.09094400
O	-0.94005500	3.55638400	-0.36105100
O	1.21303300	3.43035000	0.22076000

H	1.08504300	4.38474200	0.30286900
==> 1_H_z+100.gjf <==			
C	1.23646400	0.68874500	0.08941600
C	0.04261600	1.40265900	0.07187700
C	-1.17561500	0.73425600	0.00613100
C	-1.19902900	-0.64965200	-0.04605000
C	-0.00827400	-1.36485100	-0.00931200
C	1.20711100	-0.69712200	0.06450900
H	2.17718000	1.22017200	0.10039100
H	-2.08671700	1.31421700	-0.04403400
H	-2.14073200	-1.17048000	-0.14972500
H	-0.02627500	-2.44440600	-0.07390600
H	2.13281200	-1.25571400	0.06236300
C	0.02351100	2.88841400	0.09092700
O	-0.94005500	3.55638500	0.36103300
O	1.21303200	3.43034900	-0.22078300
H	1.08504300	4.38474100	-0.30289500

==> 1_H_z-10.gjf <==			
C	1.23575600	0.69015000	-0.00892000
C	0.04076200	1.40227900	-0.00712900
C	-1.17755600	0.73061500	-0.00055400
C	-1.20058100	-0.65362200	0.00456700
C	-0.00776400	-1.36628100	0.00077100
C	1.20789500	-0.69591100	-0.00660400
H	2.17567800	1.22235700	-0.01004300
H	-2.09020400	1.31003700	0.00451500
H	-2.14563700	-1.17841000	0.01510600
H	-0.02622500	-2.44772100	0.00712800
H	2.13407200	-1.25349200	-0.00650400
C	0.01479500	2.88753700	-0.00916900
O	-0.98335500	3.55585600	-0.03660300
O	1.24397100	3.43817800	0.02251300
H	1.11946400	4.39614100	0.03087000

==> 1_H_z+10.gjf <==			
C	1.23575600	0.69015000	0.00891400
C	0.04076200	1.40227900	0.00712000
C	-1.17755600	0.73061500	0.00054600
C	-1.20058200	-0.65362200	-0.00457200
C	-0.00776400	-1.36628100	-0.00077400
C	1.20789400	-0.69591100	0.00660000
H	2.17567800	1.22235700	0.01003700

H	-2.09020400	1.31003700	-0.00452500
H	-2.14563700	-1.17841000	-0.01511100
H	-0.02622500	-2.44772100	-0.00712900
H	2.13407200	-1.25349200	0.00650300
C	0.01479500	2.88753700	0.00915600
O	-0.98335400	3.55585600	0.03658800
O	1.24397100	3.43817800	-0.02252500
H	1.11946400	4.39614100	-0.03088500

==> 1_H_z-15.gjf <==

C	1.23575900	0.69013500	-0.01335500
C	0.04077200	1.40228600	-0.01070200
C	-1.17754000	0.73065800	-0.00085100
C	-1.20056300	-0.65358000	0.00685600
C	-0.00777100	-1.36626200	0.00119800
C	1.20788600	-0.69591800	-0.00985300
H	2.17568300	1.22234700	-0.01502900
H	-2.09017400	1.31008100	0.00672100
H	-2.14557200	-1.17832100	0.02265500
H	-0.02621200	-2.44767900	0.01075500
H	2.13405500	-1.25351700	-0.00967900
C	0.01490900	2.88754900	-0.01379100
O	-0.98278000	3.55588900	-0.05499000
O	1.24358000	3.43806400	0.03375900
H	1.11903800	4.39598200	0.04624700

==> 1_H_z+15.gjf <==

C	1.23575900	0.69012200	0.01334800
C	0.04076800	1.40229300	0.01069300
C	-1.17753100	0.73065300	0.00084200
C	-1.20055400	-0.65358900	-0.00686500
C	-0.00777900	-1.36626200	-0.00119200
C	1.20789100	-0.69591100	0.00986600
H	2.17566300	1.22236400	0.01501500
H	-2.09016500	1.31007600	-0.00673100
H	-2.14557600	-1.17830400	-0.02267500
H	-0.02619400	-2.44767800	-0.01074300
H	2.13404900	-1.25352300	0.00970700
C	0.01490000	2.88755500	0.01377300
O	-0.98278700	3.55590300	0.05494500
O	1.24357800	3.43804900	-0.03376300
H	1.11905100	4.39596500	-0.04627800

==> 1_H_z-20.gjf <==

C	1.23576400	0.69011700	-0.01780600
C	0.04079400	1.40229500	-0.01427100
C	-1.17751400	0.73072100	-0.00113400
C	-1.20053400	-0.65351200	0.00915000
C	-0.00777900	-1.36623200	0.00161000
C	1.20787300	-0.69592900	-0.01313000
H	2.17569500	1.22232700	-0.02003800
H	-2.09012600	1.31014600	0.00895700
H	-2.14547800	-1.17819000	0.03020900
H	-0.02620300	-2.44761700	0.01435800
H	2.13403400	-1.25354400	-0.01289700
C	0.01506700	2.88756100	-0.01838400
O	-0.98198600	3.55591900	-0.07327800
O	1.24303200	3.43789900	0.04498100
H	1.11843200	4.39575300	0.06161600

==> 1_H_z+20.gjf <==

C	1.23575600	0.69012300	0.01781700
C	0.04079100	1.40229700	0.01426200
C	-1.17751800	0.73072000	0.00111200
C	-1.20053400	-0.65351100	-0.00916300
C	-0.00777400	-1.36623500	-0.00160400
C	1.20787000	-0.69593200	0.01314700
H	2.17569900	1.22231300	0.02006200
H	-2.09013800	1.31013100	-0.00899800
H	-2.14547400	-1.17819500	-0.03022700
H	-0.02621000	-2.44761900	-0.01434700
H	2.13404200	-1.25352900	0.01292500
C	0.01506900	2.88756700	0.01836900
O	-0.98197800	3.55592800	0.07329200
O	1.24303700	3.43790000	-0.04503100
H	1.11843500	4.39575500	-0.06167100

==> 1_H_z-25.gjf <==

C	1.23576300	0.69009800	-0.02225700
C	0.04081900	1.40230900	-0.01783000
C	-1.17748500	0.73080100	-0.00140700
C	-1.20049900	-0.65342500	0.01144100
C	-0.00778300	-1.36620000	0.00202000
C	1.20785200	-0.69595100	-0.01640300
H	2.17572000	1.22227700	-0.02505200
H	-2.09007900	1.31021000	0.01121400
H	-2.14535500	-1.17802900	0.03773900
H	-0.02620200	-2.44754200	0.01795700

H	2.13401600	-1.25356600	-0.01610200
C	0.01527100	2.88758600	-0.02295500
O	-0.98096500	3.55596600	-0.09148600
O	1.24233800	3.43770300	0.05613900
H	1.11765900	4.39547600	0.07692600

==> 1_H_z+25.gjf <==

C	1.23576900	0.69009500	0.02225500
C	0.04081900	1.40230800	0.01781800
C	-1.17748100	0.73080100	0.00139300
C	-1.20049700	-0.65342800	-0.01144600
C	-0.00778800	-1.36619500	-0.00201400
C	1.20785600	-0.69594200	0.01641200
H	2.17571100	1.22229700	0.02504700
H	-2.09007100	1.31021900	-0.01123200
H	-2.14535800	-1.17802200	-0.03775100
H	-0.02619000	-2.44753800	-0.01794100
H	2.13400900	-1.25357400	0.01612700
C	0.01526700	2.88758100	0.02292700
O	-0.98097400	3.55596300	0.09142300
O	1.24233700	3.43768900	-0.05614200
H	1.11766400	4.39545900	-0.07693600

==> 1_H_z-30.gjf <==

C	1.23578000	0.69006300	-0.02668000
C	0.04085800	1.40232200	-0.02137800
C	-1.17743700	0.73089900	-0.00169300
C	-1.20045400	-0.65332200	0.01371100
C	-0.00780000	-1.36615400	0.00243200
C	1.20783400	-0.69596800	-0.01964900
H	2.17574100	1.22224900	-0.03001000
H	-2.08999300	1.31032000	0.01343600
H	-2.14521500	-1.17781600	0.04522500
H	-0.02618400	-2.44744600	0.02155100
H	2.13397700	-1.25362300	-0.01927300
C	0.01551000	2.88760700	-0.02748500
O	-0.97975700	3.55599900	-0.10946300
O	1.24149100	3.43745800	0.06712700
H	1.11672200	4.39512600	0.09209000

==> 1_H_z+30.gjf <==

C	1.23577600	0.69005500	0.02671100
C	0.04084800	1.40233600	0.02134100
C	-1.17742900	0.73090500	0.00164300

C	-1.20044400	-0.65333600	-0.01372800
C	-0.00780700	-1.36615900	-0.00237300
C	1.20783700	-0.69595800	0.01974000
H	2.17572900	1.22225400	0.03005600
H	-2.08999800	1.31029200	-0.01353300
H	-2.14522000	-1.17779500	-0.04527100
H	-0.02616200	-2.44744900	-0.02146100
H	2.13397500	-1.25361500	0.01942300
C	0.01550300	2.88760900	0.02741600
O	-0.97975200	3.55599900	0.10939200
O	1.24149100	3.43745300	-0.06719300
H	1.11672500	4.39512200	-0.09222200

==> 1_H_z-35.gjf <==

C	1.23579500	0.69002400	-0.03112600
C	0.04090900	1.40233800	-0.02490100
C	-1.17738200	0.73101500	-0.00195400
C	-1.20040300	-0.65319800	0.01596200
C	-0.00781000	-1.36610900	0.00278900
C	1.20780800	-0.69600500	-0.02294400
H	2.17578700	1.22217500	-0.03499200
H	-2.08989600	1.31043400	0.01572600
H	-2.14504300	-1.17757500	0.05266800
H	-0.02618100	-2.44734000	0.02506900
H	2.13394200	-1.25368300	-0.02250100
C	0.01579600	2.88764300	-0.03193700
O	-0.97834800	3.55603100	-0.12723100
O	1.24049900	3.43720900	0.07806400
H	1.11559900	4.39475400	0.10724900

==> 1_H_z+35.gjf <==

C	1.23579500	0.69001500	0.03111400
C	0.04090100	1.40235100	0.02488100
C	-1.17737200	0.73102200	0.00194500
C	-1.20039400	-0.65321100	-0.01597500
C	-0.00782200	-1.36611300	-0.00278400
C	1.20781100	-0.69599300	0.02296400
H	2.17577400	1.22218800	0.03498100
H	-2.08990000	1.31041300	-0.01573600
H	-2.14505400	-1.17754800	-0.05269600
H	-0.02616000	-2.44734200	-0.02505700
H	2.13393600	-1.25368000	0.02254200
C	0.01578800	2.88764000	0.03191900
O	-0.97834200	3.55602900	0.12721300

O	1.24050200	3.43719800	-0.07806300
H	1.11560900	4.39474400	-0.10730600

==> 1_H_z-40.gjf <==

C	1.23582100	0.68997400	-0.03553000
C	0.04097700	1.40235500	-0.02844400
C	-1.17731100	0.73115300	-0.00226200
C	-1.20034500	-0.65305000	0.01820300
C	-0.00782900	-1.36605500	0.00320700
C	1.20777900	-0.69604800	-0.02615400
H	2.17584400	1.22209400	-0.03991300
H	-2.08977200	1.31058500	0.01791700
H	-2.14485400	-1.17728400	0.06006900
H	-0.02618300	-2.44721600	0.02867900
H	2.13389600	-1.25376300	-0.02559300
C	0.01612200	2.88767600	-0.03642300
O	-0.97674700	3.55604900	-0.14495200
O	1.23936000	3.43692000	0.08886400
H	1.11431200	4.39432100	0.12227400

==> 1_H_z+40.gjf <==

C	1.23582100	0.68997500	0.03553100
C	0.04097700	1.40235600	0.02843200
C	-1.17731000	0.73115300	0.00224700
C	-1.20034400	-0.65305100	-0.01820900
C	-0.00782900	-1.36605500	-0.00320100
C	1.20777900	-0.69604700	0.02616400
H	2.17584400	1.22209500	0.03991600
H	-2.08977200	1.31058400	-0.01794200
H	-2.14485400	-1.17728400	-0.06007800
H	-0.02618200	-2.44721700	-0.02866400
H	2.13389600	-1.25376200	0.02561400
C	0.01612200	2.88767700	0.03640000
O	-0.97674800	3.55605000	0.14491900
O	1.23936100	3.43691900	-0.08888400
H	1.11431300	4.39432000	-0.12230200

==> 1_H_z-45.gjf <==

C	1.23585500	0.68991500	-0.03994800
C	0.04106100	1.40237300	-0.03200000
C	-1.17722500	0.73131100	-0.00257500
C	-1.20027900	-0.65287900	0.02045300
C	-0.00785100	-1.36599300	0.00363800
C	1.20774700	-0.69610000	-0.02936200

H	2.17591500	1.22199800	-0.04485300
H	-2.08962100	1.31076400	0.02010200
H	-2.14464200	-1.17694700	0.06747600
H	-0.02618900	-2.44707500	0.03231300
H	2.13384200	-1.25386000	-0.02868100
C	0.01649200	2.88771300	-0.04091100
O	-0.97494700	3.55605700	-0.16266400
O	1.23806800	3.43660000	0.09966100
H	1.11284600	4.39383700	0.13729300

==> 1_H_z+45.gjf <==

C	1.23585500	0.68991500	0.03994900
C	0.04106100	1.40237300	0.03198800
C	-1.17722500	0.73131100	0.00255900
C	-1.20027800	-0.65288000	-0.02045900
C	-0.00785100	-1.36599400	-0.00363200
C	1.20774700	-0.69609900	0.02937200
H	2.17591500	1.22199800	0.04485600
H	-2.08962200	1.31076300	-0.02012800
H	-2.14464200	-1.17694700	-0.06748500
H	-0.02618800	-2.44707600	-0.03229900
H	2.13384300	-1.25385900	0.02870200
C	0.01649200	2.88771400	0.04088800
O	-0.97494800	3.55605800	0.16263100
O	1.23806900	3.43659900	-0.09968000
H	1.11284700	4.39383600	-0.13732100

==> 1_H_z-50.gjf <==

C	1.23589800	0.68984500	-0.04439300
C	0.04116200	1.40239200	-0.03557400
C	-1.17712600	0.73149000	-0.00288700
C	-1.20020500	-0.65268500	0.02272600
C	-0.00787800	-1.36592400	0.00408500
C	1.20771100	-0.69616200	-0.03258000
H	2.17600000	1.22188400	-0.04983400
H	-2.08944500	1.31097300	0.02229100
H	-2.14440600	-1.17656300	0.07491600
H	-0.02620100	-2.44691700	0.03598000
H	2.13378100	-1.25397600	-0.03178500
C	0.01690800	2.88775300	-0.04541700
O	-0.97293400	3.55605600	-0.18045900
O	1.23661300	3.43624800	0.11051900
H	1.11119400	4.39330100	0.15235400

==> 1_H_z+50.gjf <==

C	1.23589700	0.68984500	0.04439400
C	0.04116100	1.40239200	0.03556200
C	-1.17712500	0.73149000	0.00287100
C	-1.20020400	-0.65268500	-0.02273200
C	-0.00787700	-1.36592500	-0.00407900
C	1.20771100	-0.69616100	0.03259000
H	2.17599900	1.22188500	0.04983700
H	-2.08944500	1.31097200	-0.02231700
H	-2.14440600	-1.17656400	-0.07492500
H	-0.02620000	-2.44691700	-0.03596600
H	2.13378100	-1.25397500	0.03180500
C	0.01690700	2.88775400	0.04539500
O	-0.97293500	3.55605700	0.18042600
O	1.23661400	3.43624700	-0.11053800
H	1.11119400	4.39330000	-0.15238100

==> 1_H_z-55.gjf <==

C	1.23594800	0.68976300	-0.04886400
C	0.04127800	1.40241100	-0.03916900
C	-1.17701100	0.73169000	-0.00319800
C	-1.20012200	-0.65246700	0.02502500
C	-0.00790800	-1.36584800	0.00455400
C	1.20767100	-0.69623400	-0.03580400
H	2.17609800	1.22175300	-0.05485600
H	-2.08924100	1.31121100	0.02448100
H	-2.14414700	-1.17613200	0.08239500
H	-0.02621800	-2.44674100	0.03968500
H	2.13371000	-1.25411000	-0.03490200
C	0.01737100	2.88779700	-0.04995400
O	-0.97069400	3.55604500	-0.19839300
O	1.23498800	3.43586200	0.12147000
H	1.10934900	4.39271400	0.16747100

==> 1_H_z+55.gjf <==

C	1.23594800	0.68976400	0.04886300
C	0.04127800	1.40241100	0.03915700
C	-1.17701100	0.73168900	0.00318400
C	-1.20012200	-0.65246700	-0.02503100
C	-0.00790800	-1.36584800	-0.00454900
C	1.20767100	-0.69623400	0.03581200
H	2.17609700	1.22175400	0.05485700
H	-2.08924100	1.31121000	-0.02450400
H	-2.14414600	-1.17613300	-0.08240300

H	-0.02621700	-2.44674200	-0.03967300
H	2.13371000	-1.25410900	0.03491900
C	0.01737000	2.88779700	0.04993300
O	-0.97069600	3.55604600	0.19836300
O	1.23498800	3.43586100	-0.12148900
H	1.10935000	4.39271300	-0.16749700

==> 1_H_z-60.gjf <==

C	1.23600700	0.68967100	-0.05333300
C	0.04141000	1.40243000	-0.04278500
C	-1.17688200	0.73191000	-0.00353100
C	-1.20003200	-0.65222500	0.02733800
C	-0.00794300	-1.36576500	0.00506000
C	1.20762700	-0.69631600	-0.03899900
H	2.17620800	1.22160500	-0.05987500
H	-2.08901300	1.31147800	0.02662800
H	-2.14386500	-1.17565300	0.08988400
H	-0.02624000	-2.44654700	0.04345100
H	2.13363100	-1.25426200	-0.03797300
C	0.01788200	2.88784400	-0.05453700
O	-0.96821600	3.55602600	-0.21649400
O	1.23318800	3.43544100	0.13249600
H	1.10731200	4.39207600	0.18261200

==> 1_H_z+60.gjf <==

C	1.23600600	0.68967200	0.05333200
C	0.04140900	1.40243100	0.04277400
C	-1.17688200	0.73191000	0.00351700
C	-1.20003200	-0.65222600	-0.02734400
C	-0.00794300	-1.36576500	-0.00505500
C	1.20762700	-0.69631600	0.03900600
H	2.17620800	1.22160600	0.05987600
H	-2.08901300	1.31147700	-0.02665000
H	-2.14386400	-1.17565400	-0.08989100
H	-0.02623900	-2.44654800	-0.04344000
H	2.13363100	-1.25426200	0.03798800
C	0.01788100	2.88784400	0.05451700
O	-0.96821800	3.55602800	0.21646600
O	1.23318900	3.43544000	-0.13251500
H	1.10731300	4.39207500	-0.18263800

==> 1_H_z-65.gjf <==

C	1.23606700	0.68957400	-0.05780800
C	0.04155300	1.40245200	-0.04641600

C	-1.17674500	0.73215200	-0.00386700
C	-1.19993500	-0.65196100	0.02966300
C	-0.00798000	-1.36567600	0.00558200
C	1.20757700	-0.69640700	-0.04218500
H	2.17633100	1.22144100	-0.06491100
H	-2.08877200	1.31176500	0.02877800
H	-2.14356300	-1.17513000	0.09737000
H	-0.02626700	-2.44634000	0.04724100
H	2.13355100	-1.25441900	-0.04102200
C	0.01844000	2.88789300	-0.05913600
O	-0.96550200	3.55601200	-0.23465400
O	1.23122800	3.43497900	0.14354100
H	1.10508900	4.39138000	0.19776700

==> 1_H_z+65.gjf <==

C	1.23606600	0.68957400	0.05780600
C	0.04155200	1.40245200	0.04640400
C	-1.17674500	0.73215200	0.00385400
C	-1.19993500	-0.65196100	-0.02966800
C	-0.00798000	-1.36567600	-0.00557800
C	1.20757700	-0.69640700	0.04219100
H	2.17633100	1.22144200	0.06491000
H	-2.08877200	1.31176400	-0.02879800
H	-2.14356200	-1.17513100	-0.09737700
H	-0.02626700	-2.44634000	-0.04723000
H	2.13355100	-1.25441900	0.04103600
C	0.01844000	2.88789300	0.05911600
O	-0.96550400	3.55601300	0.23462500
O	1.23122900	3.43497800	-0.14355800
H	1.10509000	4.39137900	-0.19779100

==> 1_H_z-70.gjf <==

C	1.23613100	0.68946700	-0.06228900
C	0.04169900	1.40247400	-0.05004300
C	-1.17659800	0.73240800	-0.00420200
C	-1.19983000	-0.65168100	0.03199100
C	-0.00802200	-1.36557800	0.00610700
C	1.20752500	-0.69650000	-0.04537000
H	2.17645200	1.22127700	-0.06994200
H	-2.08850900	1.31207500	0.03092000
H	-2.14323500	-1.17456900	0.10485900
H	-0.02628500	-2.44611300	0.05103500
H	2.13345700	-1.25459600	-0.04407800
C	0.01903800	2.88795000	-0.06371900

O	-0.96256500	3.55600600	-0.25279100
O	1.22910500	3.43447000	0.15458700
H	1.10270900	4.39062300	0.21287700

==> 1_H_z+70.gjf <==

C	1.23613100	0.68946700	0.06228700
C	0.04169900	1.40247500	0.05003100
C	-1.17659800	0.73240700	0.00418800
C	-1.19983000	-0.65168100	-0.03199600
C	-0.00802100	-1.36557800	-0.00610200
C	1.20752500	-0.69650000	0.04537600
H	2.17645200	1.22127800	0.06994100
H	-2.08850800	1.31207500	-0.03094000
H	-2.14323400	-1.17457000	-0.10486600
H	-0.02628500	-2.44611300	-0.05102500
H	2.13345700	-1.25459600	0.04409100
C	0.01903800	2.88795000	0.06369900
O	-0.96256700	3.55600700	0.25276300
O	1.22910500	3.43447000	-0.15460500
H	1.10271000	4.39062200	-0.21290100

==> 1_H_z-75.gjf <==

C	1.23619400	0.68935900	-0.06677000
C	0.04184700	1.40249900	-0.05366200
C	-1.17644500	0.73267500	-0.00453100
C	-1.19971300	-0.65138700	0.03431000
C	-0.00805800	-1.36547400	0.00662200
C	1.20747100	-0.69659400	-0.04855400
H	2.17657400	1.22111200	-0.07496600
H	-2.08823600	1.31239300	0.03307900
H	-2.14287800	-1.17398000	0.11231800
H	-0.02629200	-2.44587000	0.05481200
H	2.13336500	-1.25476900	-0.04712600
C	0.01967000	2.88801200	-0.06826800
O	-0.95942400	3.55601300	-0.27080200
O	1.22683100	3.43391900	0.16555900
H	1.10016500	4.38980600	0.22791900

==> 1_H_z+75.gjf <==

C	1.23619400	0.68936000	0.06676800
C	0.04184700	1.40250000	0.05365000
C	-1.17644500	0.73267500	0.00451800
C	-1.19971300	-0.65138800	-0.03431500
C	-0.00805800	-1.36547400	-0.00661700

C	1.20747100	-0.69659300	0.04856000
H	2.17657300	1.22111300	0.07496500
H	-2.08823600	1.31239300	-0.03310000
H	-2.14287700	-1.17398100	-0.11232500
H	-0.02629100	-2.44587000	-0.05480200
H	2.13336500	-1.25476800	0.04713900
C	0.01966900	2.88801200	0.06824800
O	-0.95942500	3.55601400	0.27077500
O	1.22683100	3.43391800	-0.16557700
H	1.10016500	4.38980500	-0.22794400

==> 1_H_z-80.gjf <==

C	1.23625500	0.68924300	-0.07126500
C	0.04199500	1.40253000	-0.05727500
C	-1.17628800	0.73295600	-0.00485900
C	-1.19959400	-0.65108000	0.03663200
C	-0.00810300	-1.36536100	0.00714500
C	1.20741100	-0.69669000	-0.05173400
H	2.17668500	1.22094900	-0.07997700
H	-2.08794900	1.31273000	0.03522000
H	-2.14249900	-1.17335200	0.11979100
H	-0.02629100	-2.44560600	0.05860400
H	2.13325700	-1.25495500	-0.05017700
C	0.02034000	2.88808100	-0.07281500
O	-0.95604700	3.55603300	-0.28882200
O	1.22440700	3.43331200	0.17653100
H	1.09749500	4.38892300	0.24294300

==> 1_H_z+80.gjf <==

C	1.23625400	0.68924600	0.07124800
C	0.04199600	1.40252700	0.05727400
C	-1.17628900	0.73296000	0.00485000
C	-1.19959200	-0.65107600	-0.03663600
C	-0.00810000	-1.36536300	-0.00713800
C	1.20741000	-0.69669100	0.05173600
H	2.17669300	1.22094200	0.07997900
H	-2.08795300	1.31273000	-0.03525400
H	-2.14250000	-1.17335400	-0.11977500
H	-0.02629700	-2.44561100	-0.05858800
H	2.13326400	-1.25495000	0.05017200
C	0.02034600	2.88808100	0.07278700
O	-0.95604900	3.55604600	0.28875800
O	1.22440900	3.43331000	-0.17653400
H	1.09748000	4.38891900	-0.24293700

==> 1_H_z-85.gjf <==

C	1.23630900	0.68912800	-0.07577700
C	0.04215000	1.40255700	-0.06092200
C	-1.17612800	0.73326200	-0.00518100
C	-1.19946400	-0.65074400	0.03897800
C	-0.00814200	-1.36524500	0.00767900
C	1.20734300	-0.69679500	-0.05492500
H	2.17681600	1.22075700	-0.08507300
H	-2.08766000	1.31308200	0.03742200
H	-2.14209600	-1.17268700	0.12725600
H	-0.02630200	-2.44533400	0.06241200
H	2.13316000	-1.25513300	-0.05321700
C	0.02107700	2.88815300	-0.07736100
O	-0.95239900	3.55609400	-0.30691300
O	1.22180400	3.43264700	0.18759600
H	1.09460500	4.38797000	0.25797000

==> 1_H_z+85.gjf <==

C	1.23631000	0.68912900	0.07577500
C	0.04214700	1.40255700	0.06091400
C	-1.17612900	0.73326100	0.00516400
C	-1.19946400	-0.65074600	-0.03898400
C	-0.00814100	-1.36524400	-0.00767400
C	1.20734400	-0.69679300	0.05492700
H	2.17681300	1.22076400	0.08506800
H	-2.08766100	1.31308200	-0.03744100
H	-2.14209500	-1.17269100	-0.12726400
H	-0.02629700	-2.44533400	-0.06239800
H	2.13315900	-1.25513400	0.05323200
C	0.02107200	2.88815700	0.07734400
O	-0.95240200	3.55610300	0.30688700
O	1.22180400	3.43264100	-0.18761800
H	1.09461300	4.38796300	-0.25798900

==> 1_H_z-90.gjf <==

C	1.23636300	0.68900500	-0.08031300
C	0.04230200	1.40258900	-0.06457000
C	-1.17596300	0.73357900	-0.00549800
C	-1.19932700	-0.65039600	0.04133600
C	-0.00818500	-1.36511900	0.00821900
C	1.20727100	-0.69690000	-0.05812400
H	2.17693500	1.22057100	-0.09017100
H	-2.08735800	1.31344600	0.03961800

H	-2.14166600	-1.17198700	0.13475600
H	-0.02629800	-2.44504000	0.06623500
H	2.13304900	-1.25532100	-0.05628000
C	0.02184800	2.88823300	-0.08191000
O	-0.94850800	3.55617100	-0.32504000
O	1.21903400	3.43192800	0.19869100
H	1.09157500	4.38695300	0.27299300

==> 1_H_z+90.gjf <==

C	1.23636200	0.68900600	0.08031400
C	0.04230200	1.40258900	0.06456000
C	-1.17596300	0.73357900	0.00548300
C	-1.19932600	-0.65039600	-0.04134500
C	-0.00818500	-1.36511900	-0.00821600
C	1.20727100	-0.69689900	0.05813100
H	2.17693500	1.22057200	0.09017600
H	-2.08735700	1.31344600	-0.03964100
H	-2.14166400	-1.17198700	-0.13476900
H	-0.02629700	-2.44504000	-0.06622700
H	2.13304900	-1.25532100	0.05629800
C	0.02184800	2.88823400	0.08189400
O	-0.94850600	3.55617200	0.32503300
O	1.21903100	3.43192700	-0.19872200
H	1.09157200	4.38695200	-0.27302500

==> 1_H_z-95.gjf <==

C	1.23641400	0.68887800	-0.08486300
C	0.04245700	1.40262300	-0.06822600
C	-1.17579200	0.73391100	-0.00581500
C	-1.19918200	-0.65003200	0.04369900
C	-0.00823000	-1.36498800	0.00876700
C	1.20719300	-0.69700900	-0.06132000
H	2.17705600	1.22037600	-0.09528600
H	-2.08704400	1.31382500	0.04182100
H	-2.14121000	-1.17125000	0.14225600
H	-0.02628900	-2.44473000	0.07007200
H	2.13293200	-1.25551500	-0.05933400
C	0.02266200	2.88832000	-0.08644700
O	-0.94438000	3.55626800	-0.34313800
O	1.21610200	3.43116000	0.20977900
H	1.08838200	4.38587600	0.28797700

==> 1_H_z+95.gjf <==

C	1.23641300	0.68887800	0.08486200
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C	0.04245700	1.40262300	0.06821500
C	-1.17579200	0.73391100	0.00580100
C	-1.19918100	-0.65003200	-0.04370500
C	-0.00822900	-1.36498800	-0.00876400
C	1.20719300	-0.69700800	0.06132600
H	2.17705600	1.22037700	0.09528600
H	-2.08704300	1.31382500	-0.04184200
H	-2.14120900	-1.17125100	-0.14226500
H	-0.02628800	-2.44473100	-0.07006400
H	2.13293200	-1.25551400	0.05934700
C	0.02266100	2.88832000	0.08642900
O	-0.94438100	3.55626900	0.34311600
O	1.21610200	3.43115900	-0.20979900
H	1.08838100	4.38587500	-0.28800200