Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

of

Planar Tetracoordinate Fluorine Atom: Global Minimum with Viable Possibility

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Cartesian coordinates and electronic energies (a. u.) calculated at CCSD(T)/aug-cc-pVTZ/J//TPSSh-def2-TZVP level.

^{2}A

E = -131.256783

3	1.478871000	-1.278089000	-0.000506000
3	-1.477338000	-1.279065000	0.000351000
3	-1.252740000	1.192417000	0.000256000
3	1.251299000	1.193314000	-0.000097000
1	-0.001205000	2.468234000	0.000411000
1	-2.645748000	0.062919000	-0.000566000
1	2.645542000	0.065410000	0.000821000
9	0.000126000	-0.231366000	-0.000075000

^{2}B

E = -131.238836

3	1.528147000	1.156043000	-0.000029000
3	-0.963219000	0.795072000	0.000191000
3	-4.116909000	-0.463801000	-0.000005000
3	1.968827000	-1.158136000	0.000144000
1	0.197864000	2.261478000	-0.000172000
1	-2.642472000	0.371993000	0.000142000
1	3.100948000	0.110434000	0.000219000
9	0.454791000	-0.414604000	-0.000121000

^{2}C

E = -131.237502

3	-0.260824000	1.228361000	0.093398000
3	1.581516000	0.000153000	0.936279000
3	-0.260941000	-1.228321000	0.093726000
3	-3.418179000	0.000085000	0.139797000
1	-1.690882000	0.000124000	0.182884000
9	0.764281000	-0.000174000	-0.740374000

1	0.943643000	-1.669380000	1.345818000
1	0.943991000	1.669982000	1.345064000

^{2}D

E = -131.236143

1	-0.047553000	-0.410433000	-3.618745000
3	-0.068658000	-0.602774000	-5.319498000
3	-0.025638000	-0.222903000	-1.967331000
3	0.018344000	0.160570000	1.407208000
3	0.062318000	0.537645000	4.765121000
1	0.038201000	0.346391000	3.060544000
9	-0.003531000	-0.031005000	-0.280336000
1	0.082037000	0.725476000	6.424722000

^{2}E

E = -131.235812

3	-0.325571000	1.250817000	-0.000003000
3	-0.325300000	-1.250773000	0.000040000
3	2.172556000	-1.458113000	-0.000022000
3	2.172304000	1.458339000	-0.000056000
9	-1.543075000	-0.000108000	0.000017000
1	0.830657000	-2.620160000	-0.000124000
1	0.830292000	2.620262000	-0.000056000
1	1.144758000	0.000059000	0.000148000

^{2}F

E = -131.233584

3	-0.135606000	-0.000086000	0.000165000
3	-2.895190000	-1.288547000	0.000006000
3	-2.894699000	1.288875000	-0.000052000
3	3.288301000	0.000631000	-0.000020000
1	-1.252834000	-1.534534000	0.000156000
1	-4.054689000	0.000574000	-0.000291000

1	-1.252403000	1.534012000	0.000301000
9	1.607945000	-0.000297000	-0.000051000

^{2}G

E = -131.203455

3	0.621088000	1.376904000	0.060962000
3	0.487547000	-1.301818000	0.434594000
3	-2.078271000	1.354740000	0.262950000
3	-2.176203000	-1.330590000	-0.111461000
9	1.566974000	-0.047349000	-0.108250000
1	-0.753770000	2.386803000	-0.296979000
1	-3.124661000	0.090628000	-0.401309000
1	-0.786822000	-2.349001000	-0.268592000

^{2}H

E = -131.185492

3	4.148685000	1.908534000	-0.000017000
3	4.088367000	-0.913285000	-0.000804000
3	-1.746519000	-0.106578000	0.000822000
3	1.603578000	-0.754638000	0.000690000
1	2.884606000	-2.088549000	-0.000436000
9	-3.360014000	0.170820000	-0.000393000
1	3.128280000	0.539756000	0.000168000
1	-0.055088000	-0.390691000	0.001737000

Cartesian coordinate of the lowest energy isomer (**^{2}A**) calculated at CCSD(T)/aug-cc-pVQZ level.

^{2}A

3	1.510127000	-1.270539000	0.000080000
3	-1.508966000	-1.271948000	-0.000281000
3	-1.264216000	1.174249000	0.000093000
3	1.263013000	1.175344000	0.000284000
1	-0.001196000	2.515200000	0.000303000
1	-2.743596000	0.075973000	-0.000185000

1	2.743507000	0.078544000	0.000318000
9	0.000135000	-0.283049000	-0.000016000