Electronic Supplemental Information for "Computational simulation of the anion binding association mechanism contributed to rotation of pyrrole ring for dipyrrolyldiketone BF_2 complexes"

Osamu Kobayashi,[a] Tomoki Kato,[a] Takako Mashiko,[a] Yohei Haketa,[b] Hiromitsu Maeda[b] and Masanori Tachikawa*[a]

a. Graduate School of Nanobioscience, Yokohama City University, 22-2 Seto, Kanazawa-ku, Yokohama, Kanagawa 236-0027, Japan, E-mail: tachi@yokohama-cu.ac.jp

b. Department of Applied Chemistry, College of Life Sciences, Ritsumeikan University, 1-1-1 Nojihigashi, Kusatsu, Shiga 525-8577, Japan

Figures for molecule 1

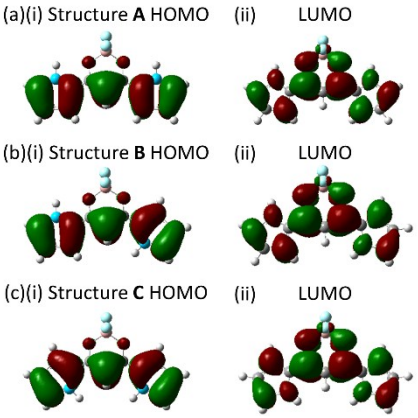

Fig. S1 The MOs of the Structures (a) **A** (b) **B** and (c) **C**. (i) HOMO and (ii) LUMO of corresponding to each structures are shown.

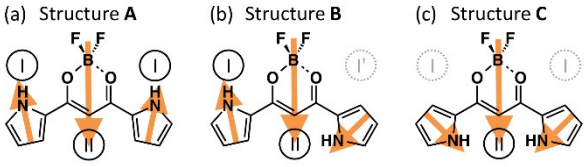

Fig. S2 The schematic representation of the divided dipole moments of 1 (Structures (a) **A**, (b) **B** and (c) **C**). The orange arrows show the divided dipole moments and the black circles are the actual anion-binding sites and the grey circles are disappeared sites.

The structures of the **1**-X^- shown in Table 2 and Fig. 6.

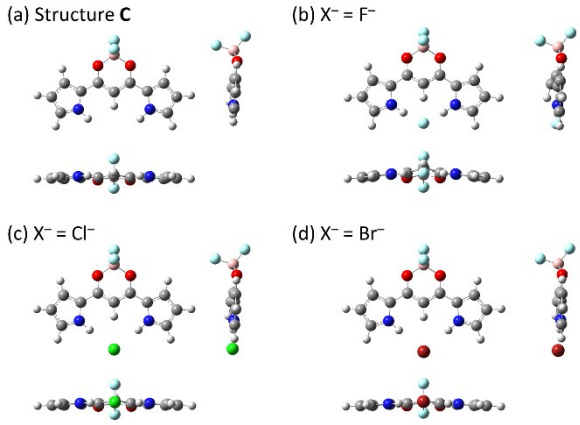

Fig. S3 The structure of C-II capturing (a) no anion, (b) fluoride anion, (c) chloride anion and (d) bromide anion. In (b), the hydrogen atom of backbone is shifted out of the molecular plane because of the strong hydrogen bonding between the hydrogen of pyrrolyl group and F–.

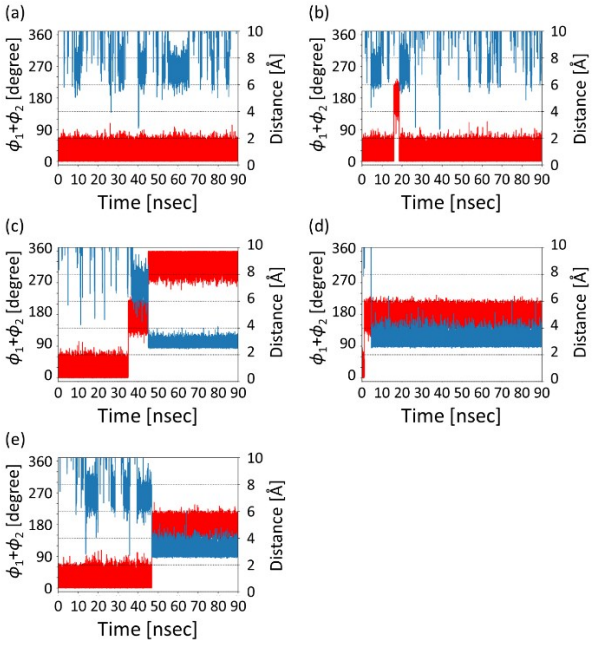

Fig. S4 The distance between CH of 1 and TBA (blue curve) and the sum of the absolute value of two dihedral angles of N–C–C=O (red curve) along the typical trajectories: (a) no isomerisation, (b) isomerisation to the Structure **B** followed by the reverse rotation, (c) isomerisation to the Structure **C** via the Structure **B**-I, (d) isomerisation to the Structure **B** followed by Cl^- capturing and (e) isomerisation to the Structure **B**-II. The horizontal, left vertical and the right vertical axes show time, sum of the dihedral angles and the CH···Cl^- distances. The red curves between 0° and 120°, 120° and 240°, 240° and 360° are corresponding to the Structures A, B and C. The blue curve around 4, 7, and over 10 Å are corresponding to the site II, site I, and free Cl^-, respectively.

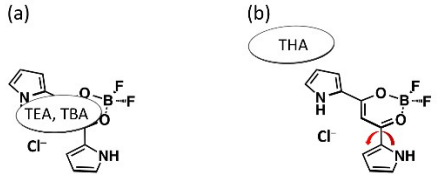

Fig. S5 The schematic structure of the ion pairs of 1 and (a) TEA or TBA and (b) THA. While the TEA and TBA are strongly bound with 1 (as shown in (a)), THA often moves away from **1** (as shown in (b)). This behaviour should lead to the rotation of pyrrole ring from Structure **B**-II to **C**-II.

The coordinates of the DFT-optimized structures corresponding to Fig. S3

```
27
Optimized structure of 1
C   0.54778800 -0.03546500  2.49654000
C   2.17190100  0.01380900  4.02763500
C   0.97161000 -0.08853600  4.71164200
H  -1.11834200 -0.19118800  3.91679600
H   2.61943300  0.09856200  1.98379500
H   3.18785900  0.06310500  4.39438300
H   0.85693200 -0.13378000  5.78590400
C  -0.08404700 -0.01986900  1.20282600
C   0.60134400  0.16077900  0.00000000
C  -0.08404700 -0.01986900 -1.20282600
O  -1.37354800 -0.22237800 -1.21893200
H   1.66377800  0.36071700  0.00000000
C   0.54778800 -0.03546500 -2.49654000
C   2.17190100  0.01380900 -4.02763500
H   2.61943300  0.09856200 -1.98379500
C   0.97161000 -0.08853600 -4.71164200
H  -1.11834200 -0.19118800 -3.91679600
H   3.18785900  0.06310500 -4.39438300
H   0.85693200 -0.13378000 -5.78590400
B  -2.19035100  0.02929400  0.00000000
O  -1.37354800 -0.22237800  1.21893200
F  -3.27010800 -0.83845800  0.00000000
F  -2.60034200  1.36708300  0.00000000
C  -0.05262300 -0.12044200 -3.74634700
C  -0.05262300 -0.12044200  3.74634700
```

N 1.91024600 0.04722900 -2.69917800
N 1.91024600 0.04722900 2.69917800

28
Optimized structure of 1-F^-
C -0.30437500 0.00999200 -2.39685000
C -2.16372000 -0.09377500 -3.60265800
C -1.09879100 -0.20206000 -4.49059900
H 1.10245900 -0.19065400 -4.07869000
H -2.26266700 0.06280200 -1.47525500
H -3.22955100 -0.11469900 -3.78784300
H -1.17624500 -0.31150100 -5.56425300
C 0.47405600 0.11865800 -1.19077500
C -0.13134900 0.49643400 0.00000000
C 0.47405600 0.11865800 1.19077500
O 1.73343700 -0.23937800 1.22545800
H -1.16619700 0.80404800 0.00000000
C -0.30437500 0.00999200 2.39685000
C -2.16372000 -0.09377500 3.60265800
H -2.26266700 0.06280200 1.47525500
C -1.09879100 -0.20206000 4.49059900
H 1.10245900 -0.19065400 4.07869000
H -3.22955100 -0.11469900 3.78784300
H -1.17624500 -0.31150100 5.56425300
B 2.55752900 -0.01331700 0.00000000
O 1.73343700 -0.23937800 -1.22545800
F 3.60474800 -0.92536700 0.00000000
F 3.02972200 1.30742000 0.00000000
C 0.08080500 -0.14381800 3.72425600
C 0.08080500 -0.14381800 -3.72425600
N -1.68429800 0.03986800 2.34815300
N -1.68429800 0.03986800 -2.34815300
F -3.04689900 0.10638900 0.00000000

28
Optimized structure of 1-Cl^-

C 0.06275600 -0.04674200 2.46575600
C 1.77647000 -0.05399000 3.88555500
C 0.61874500 -0.13576100 4.64725800
H -1.51981400 -0.18060300 3.98463700
H 2.11121400 0.03152300 1.80766200
H 2.81505300 -0.03656400 4.18722500
H 0.57194500 -0.19013400 5.72656800
C -0.61852900 -0.00019200 1.19901200
C 0.05368800 0.21451200 0.00000000
C -0.61852900 -0.00019200 -1.19901200
O -1.90927500 -0.21621900 -1.22416700
H 1.11730200 0.40932900 0.00000000
C 0.06275600 -0.04674200 -2.46575600
C 1.77647000 -0.05399000 -3.88555500
H 2.11121400 0.03152300 -1.80766200
C 0.61874500 -0.13576100 -4.64725800
H -1.51981400 -0.18060300 -3.98463700
H 2.81505300 -0.03656400 -4.18722500
H 0.57194500 -0.19013400 -5.72656800
B -2.71701400 0.04258000 0.00000000
O -1.90927500 -0.21621900 1.22416700
F -3.80970900 -0.81438700 0.00000000
F -3.12183800 1.38535300 0.00000000
C -0.46491000 -0.13340200 -3.74880300
C -0.46491000 -0.13340200 3.74880300
N 1.43726000 0.00242900 -2.57856200
N 1.43726000 0.00242900 2.57856200
Cl 3.55912600 0.09235900 0.00000000

28
Optimized structure of 1-Br^-
C -0.35961800 -0.08691000 2.46934100
C 1.34227200 -0.12995300 3.90304800
C 0.17711100 -0.18967700 4.65518200
H -1.95646400 -0.19051400 3.97566400
H 1.69643000 -0.03127900 1.83194700

H 2.37866900 -0.13143500 4.21285100
H 0.12038100 -0.24554400 5.73393000
C -1.03403700 -0.02161400 1.19958200
C -0.35293100 0.16061600 0.00000000
C -1.03403700 -0.02161400 -1.19958200
O -2.33200600 -0.18906500 -1.22425400
H 0.71698400 0.31491500 0.00000000
C -0.35961800 -0.08691000 -2.46934100
C 1.34227200 -0.12995300 -3.90304800
H 1.69643000 -0.03127900 -1.83194700
C 0.17711100 -0.18967700 -4.65518200
H -1.95646400 -0.19051400 -3.97566400
H 2.37866900 -0.13143500 -4.21285100
H 0.12038100 -0.24554400 -5.73393000
B -3.13104200 0.09375200 0.00000000
O -2.33200600 -0.18906500 1.22425400
F -4.24918000 -0.72990800 0.00000000
F -3.49538600 1.44799300 0.00000000
C -0.89902600 -0.16376800 -3.74813200
C -0.89902600 -0.16376800 3.74813200
N 1.01432700 -0.06599100 -2.59378700
N 1.01432700 -0.06599100 2.59378700
Br 3.27628500 0.11541100 0.00000000

The coordinates of the DFT-optimized structures corresponding to Fig. 4

27
Optimized structure of 1 (A)
C 2.48503900 -0.67280200 -0.01406500
C 2.85115500 -2.01165400 0.07267600
C 4.25635200 -2.06572600 0.00471900
C 4.71061400 -0.76110800 -0.12248300
N 3.63998400 0.06461500 -0.13309300
H 3.66292800 1.07120800 -0.21300400
H 2.17442100 -2.85072300 0.16919700
H 4.87587900 -2.95129000 0.04180900

H   5.71573000 -0.37151600 -0.20542300
C   1.19789300 -0.03111600 0.00000100
C   0.00000000 -0.72400300 0.15518400
C -1.19789200 -0.03111700 -0.00000100
O -1.22112900 1.26566800 -0.17671700
H   0.00000100 -1.79456500 0.30888100
C -2.48503800 -0.67280300 -0.01406600
C -2.85115500 -2.01165400 0.07268400
N -3.63998200 0.06461400 -0.13310100
C -4.25635200 -2.06572500 0.00472500
H -2.17442200 -2.85072200 0.16921300
C -4.71061300 -0.76110800 -0.12248500
H -3.66292700 1.07120600 -0.21301900
H -4.87587900 -2.95128900 0.04182000
H -5.71572900 -0.37151700 -0.20542900
B -0.00000100 2.09127800 0.04021300
O   1.22113000 1.26566900 -0.17671100
F -0.00000400 2.55813500 1.35793400
F   0.00000100 3.13524500 -0.87189900

27
Transition state of 1 (A->B)
C   2.54073600 -0.53345400 -0.11473200
C   4.50504100 -1.47981000 -0.67261700
C   4.46559300 -1.33284100 0.69478700
H   2.97499800 -0.52469200 1.96081400
H   2.97120500 -0.92866700 -2.22604800
H   5.32038100 -1.90569700 -1.24213200
H   5.18642300 -1.58833400 1.45853100
C   1.19665700 0.08659400 -0.06831900
C   0.05962100 -0.66392300 0.10644600
C -1.19759600 -0.02741400 -0.00211200
O -1.27917400 1.25923500 -0.15567000
H   0.13009400 -1.73580100 0.23105700
C -2.43492100 -0.73954400 0.00541400
C -4.64882800 -0.97282300 -0.06399500

H -3.73409200 0.92318700 -0.17830500
C -4.10791000 -2.24791000 0.05918700
H -1.98121600 -2.89512700 0.19046500
H -5.67975000 -0.65353000 -0.13023000
H -4.66846200 -3.17100300 0.10975400
B -0.08215600 2.15451500 -0.00111000
O   1.16638000 1.38377000 -0.23300200
F -0.07766400 2.64749800 1.30409300
F -0.17589400 3.16832400 -0.93793600
C -2.71291200 -2.10269500 0.10246800
N -3.64015700 -0.07930700 -0.09531700
C   3.28019500 -0.97113500 -1.18973600
N   3.26894600 -0.75920900 1.02458500

27
Optimized structure of 1 (B)
C   2.53599800 -0.51923900 -0.03691300
C   3.76786800 0.11526900 -0.13267000
C   4.76143100 -0.88210300 -0.10332000
C   4.11158500 -2.10045700 0.00862600
N   2.77680700 -1.87480000 0.04962200
H   2.08052900 -2.60176400 0.11202400
H   3.90856200 1.18486500 -0.20964900
H   5.83183900 -0.73834900 -0.15677700
H   4.50634300 -3.10574700 0.06032400
C   1.22254600 0.07068500 -0.01488300
C   0.04594900 -0.65535600 0.16371800
C -1.17692700 -0.00603200 -0.00256700
O -1.24367300 1.28512000 -0.19336500
H   0.06350200 -1.72152400 0.34358800
C -2.43918100 -0.69475800 -0.01276100
C -2.75502600 -2.04618700 0.07783800
N -3.62105700 -0.00149100 -0.13337600
C -4.15698000 -2.15303400 0.01126600
H -2.04766400 -2.85956200 0.17484900
C -4.65974300 -0.86649200 -0.11940600

H -3.68150700 1.00334000 -0.21629000
H -4.74269100 -3.06116700 0.05127600
H -5.67898500 -0.51552900 -0.20240100
B -0.04359400 2.14438800 0.03591600
O   1.19569400 1.36299500 -0.21129200
F -0.05370600 2.57591900 1.36615300
F -0.08779500 3.20950800 -0.84910400

27
Transition state of 1 (B->C)
C   2.50142400 -0.55420400 -0.11161100
C   4.43715900 -1.55975200 -0.66487200
C   4.40221700 -1.40495800 0.70175700
H   2.93784300 -0.54451500 1.96374500
H   2.92023200 -0.97122100 -2.22115500
H   5.23988000 -2.01150100 -1.23234500
H   5.11596100 -1.67641700 1.46664400
C   1.17692300 0.10737100 -0.06966000
C   0.01658800 -0.60771900 0.11592600
C -1.22413100 0.05904500 -0.01119700
O -1.26250800 1.34464100 -0.17913500
H   0.07355100 -1.67743600 0.26327100
C -2.49060100 -0.60509600 -0.01173600
C -3.97001700 -2.27248800 0.04690700
H -1.91726900 -2.66584400 0.09099400
C -4.69337800 -1.08962000 -0.03013600
H -3.96514200 1.02086000 -0.12529400
H -4.30789900 -3.29870800 0.09105000
H -5.77115400 -1.00789500 -0.05428900
B -0.04717200 2.20306000 -0.00925600
O   1.18395800 1.40003400 -0.24940400
F -0.02503500 2.67741500 1.30303700
F -0.10553600 3.23106400 -0.93270700
C -3.76272100 -0.04018500 -0.06845700
N -2.65294900 -1.97579700 0.06027700
C   3.22754900 -1.01837900 -1.18455100

N 3.22256500 -0.79569000 1.02897700

27
Optimized structure of 1 (C)
C 0.54778800 -0.03546500 2.49654000
C 2.17190100 0.01380900 4.02763500
C 0.97161000 -0.08853600 4.71164200
H -1.11834200 -0.19118800 3.91679600
H 2.61943300 0.09856200 1.98379500
H 3.18785900 0.06310500 4.39438300
H 0.85693200 -0.13378000 5.78590400
C -0.08404700 -0.01986900 1.20282600
C 0.60134400 0.16077900 0.00000000
C -0.08404700 -0.01986900 -1.20282600
O -1.37354800 -0.22237800 -1.21893200
H 1.66377800 0.36071700 0.00000000
C 0.54778800 -0.03546500 -2.49654000
C 2.17190100 0.01380900 -4.02763500
H 2.61943300 0.09856200 -1.98379500
C 0.97161000 -0.08853600 -4.71164200
H -1.11834200 -0.19118800 -3.91679600
H 3.18785900 0.06310500 -4.39438300
H 0.85693200 -0.13378000 -5.78590400
B -2.19035100 0.02929400 0.00000000
O -1.37354800 -0.22237800 1.21893200
F -3.27010800 -0.83845800 0.00000000
F -2.60034200 1.36708300 0.00000000
C -0.05262300 -0.12044200 -3.74634700
C -0.05262300 -0.12044200 3.74634700
N 1.91024600 0.04722900 -2.69917800
N 1.91024600 0.04722900 2.69917800

The coordinates of the DFT-optimized structures corresponding to Fig. 6

28
Optimized structure of 1-Cl^- (A-I)

C -1.65201200 1.40899400 0.02373700
C -1.66827100 2.80415900 0.07561400
C -3.01296800 3.20557900 0.03687300
C -3.77807000 2.04514100 -0.03815900
N -2.95612400 0.97899000 -0.04658100
H -3.29294000 0.00715000 -0.09228300
H -0.80090500 3.44985200 0.12940800
H -3.39364900 4.21782800 0.05896800
H -4.85077600 1.91196600 -0.08514700
C -0.55037500 0.49124200 0.03561700
C   0.78119600 0.90828700 0.15717700
C   1.79140600 -0.02654500 -0.00823000
O   1.53198000 -1.30227800 -0.16310100
H   1.01804700 1.95474400 0.29180900
C   3.19184500 0.31958500 -0.05559700
C   3.84317200 1.54505900 -0.00443600
N   4.15342900 -0.65596300 -0.16768900
C   5.22685600 1.28684200 -0.08702600
H   3.36852800 2.51408100 0.07950000
C   5.38180300 -0.08679600 -0.18703000
H   3.95070700 -1.64378200 -0.22233500
H   6.02564100 2.01591500 -0.07661000
H   6.27553200 -0.68961000 -0.26876700
B   0.16772500 -1.83091400 0.12700700
O -0.85162300 -0.77154000 -0.10698800
F   0.11799000 -2.21821400 1.47085900
F -0.08289600 -2.89570600 -0.72309100
Cl -4.74153700 -1.62577700 -0.18883200

28
Transition state of 1-Cl^- (A-I -> B->II)
C   2.62856000 -0.59966300 -0.45718300
C   2.86882200 -1.76520500 -1.18128000
C   4.23216400 -2.07209900 -1.03697700
C   4.78978400 -1.08976800 -0.22803200
N   3.82165000 -0.21358100 0.11175500

H 3.93338500 0.60060400 0.69915700
H 2.13387800 -2.32618100 -1.74365300
H 4.75868300 -2.91319000 -1.46642100
H 5.80461500 -0.96330100 0.12302500
C 1.43363600 0.16172400 -0.25789400
C 0.19246800 -0.18967200 -0.82605000
C -0.93244400 0.49737700 -0.43005700
O -0.87351200 1.54091500 0.35529800
H 0.10200600 -1.05443500 -1.46875900
C -2.28892300 0.08468900 -0.85517500
C -2.99842500 0.42582900 -1.98785900
N -3.05749200 -0.74927300 -0.09289900
C -4.25334600 -0.23819700 -1.89852900
H -2.65265600 1.08066500 -2.77767100
C -4.25126700 -0.95388600 -0.71955400
H -2.75262500 -1.18680300 0.78722600
H -5.06137900 -0.19455700 -2.61731100
H -5.00198300 -1.59562200 -0.27900500
B 0.42708400 2.19392900 0.64338000
O 1.54260200 1.19755400 0.51919800
F 0.42319700 2.68835500 1.93497700
F 0.64716500 3.20471900 -0.29822800
Cl -1.89768200 -2.12876700 2.52584400

28
Optimized structure of 1-Cl^- (A-II)
C 2.48152200 -0.14794500 -0.04439600
C 2.83257700 -1.49247500 0.00623900
C 4.23953800 -1.55288800 -0.05293500
C 4.70658800 -0.24964100 -0.13843100
N 3.64242500 0.58643900 -0.13267900
H 3.67339400 1.59423900 -0.18339000
H 2.13634200 -2.32352400 0.07225400
H 4.85166700 -2.44452600 -0.03713800
H 5.71564500 0.13376800 -0.20281000
C 1.19545900 0.49470000 -0.01860200

C   0.00000100 -0.20798100 0.09662800
C -1.19545500 0.49470400 -0.01859400
O -1.22216900 1.80099100 -0.14014400
H -0.00000100 -1.29024500 0.18821500
C -2.48152000 -0.14793900 -0.04439800
C -2.83257900 -1.49246700 0.00621900
N -3.64241600 0.58644500 -0.13276900
C -4.23954300 -1.55287300 -0.05290600
H -2.13635000 -2.32352200 0.07223900
C -4.70658900 -0.24962300 -0.13837700
H -3.67337700 1.59424200 -0.18354500
H -4.85167600 -2.44450600 -0.03707000
H -5.71564600 0.13379300 -0.20271300
B   0.00000400 2.61971900 0.07225500
O   1.22217600 1.80098800 -0.14014300
F   0.00000400 3.10071100 1.38813400
F   0.00000700 3.66771700 -0.84228600
Cl -0.00001400 -3.94374200 0.10222400

28
Optimized structure of 1-X^-
C   2.44972200 0.34569700 -0.00964300
C   4.64660800 0.69093900 -0.11893700
C   4.04063500 1.93697800 -0.00529300
H   1.87119400 2.47268900 0.14397600
H   3.83104400 -1.25285700 -0.18999500
H   5.69202900 0.42526000 -0.19686700
H   4.55355300 2.88856500 0.02228000
C   1.24760500 -0.42230500 0.01381200
C -0.03179400 0.16307400 0.15304400
C -1.13381400 -0.64337200 0.02971800
O -1.05155000 -1.94321400 -0.13520100
H -0.14604800 1.23782000 0.26748300
C -2.50931800 -0.09455400 0.04685900
C -4.40227900 0.74369400 -0.79824000
H -2.75091000 0.25678300 -2.02833500

C -4.56646100 0.65858800 0.56505400
H -3.13731200 -0.07078100 2.14506300
H -5.06591800 1.09953800 -1.57360800
H -5.44917800 0.95129500 1.11803100
B   0.23606000 -2.65617900 0.02435000
O   1.38617600 -1.70746400 -0.13278700
F   0.34423900 -3.63325700 -0.95700400
F   0.30246700 -3.21081600 1.30538900
C -3.36130400 0.12604600 1.10474800
C   2.65395200 1.72342300 0.06350100
N -3.15275500 0.27989400 -1.10343200
N   3.68588900 -0.25582900 -0.12197500
Cl -0.41231600 3.79629300 0.08757400

28
Optimized structure of 1-Cl^- (B-II)
C   2.44969000 0.22695800 -0.08613200
C   3.62499000 0.96655100 -0.18707300
C   4.69381300 0.05284200 -0.19165000
C   4.13873100 -1.21740300 -0.09272400
N   2.79531800 -1.10602600 -0.02982500
H   2.15588900 -1.90954100 0.03990200
H   3.67744800 2.04556200 -0.24724900
H   5.74917200 0.28067900 -0.25844900
H   4.61269800 -2.18945800 -0.06369900
C   1.09135700 0.69511900 -0.03834000
C -0.00640200 -0.15241100 0.10858600
C -1.28316900 0.38003800 -0.02749600
O -1.48524900 1.66814300 -0.16405400
H   0.12478400 -1.22277500 0.22383400
C -2.46520800 -0.44054400 -0.06437500
C -2.61956800 -1.82166300 -0.02533000
N -3.71873300 0.11842400 -0.15595500
C -4.00273000 -2.08472600 -0.09354500
H -1.81404400 -2.54598400 0.03930700
C -4.65190100 -0.86196000 -0.17384300

H -3.89461900 1.11173500 -0.19891300
H -4.48030600 -3.05515300 -0.08730800
H -5.70547200 -0.62851400 -0.24181900
B -0.37383200 2.62546000 0.09872900
O   0.93621600 1.98930200 -0.17926000
F -0.42194600 3.00624900 1.44766300
F -0.52822800 3.72435000 -0.73782000
Cl 0.88433700 -3.67014200 0.18768600

28
Optimized structure of 1-Cl^- (C-II)
C   0.06275600 -0.04674200 2.46575600
C   1.77647000 -0.05399000 3.88555500
C   0.61874500 -0.13576100 4.64725800
H -1.51981400 -0.18060300 3.98463700
H   2.11121400 0.03152300 1.80766200
H   2.81505300 -0.03656400 4.18722500
H   0.57194500 -0.19013400 5.72656800
C -0.61852900 -0.00019200 1.19901200
C   0.05368800 0.21451200 0.00000000
C -0.61852900 -0.00019200 -1.19901200
O -1.90927500 -0.21621900 -1.22416700
H   1.11730200 0.40932900 0.00000000
C   0.06275600 -0.04674200 -2.46575600
C   1.77647000 -0.05399000 -3.88555500
H   2.11121400 0.03152300 -1.80766200
C   0.61874500 -0.13576100 -4.64725800
H -1.51981400 -0.18060300 -3.98463700
H   2.81505300 -0.03656400 -4.18722500
H   0.57194500 -0.19013400 -5.72656800
B -2.71701400 0.04258000 0.00000000
O -1.90927500 -0.21621900 1.22416700
F -3.80970900 -0.81438700 0.00000000
F -3.12183800 1.38535300 0.00000000
C -0.46491000 -0.13340200 -3.74880300
C -0.46491000 -0.13340200 3.74880300

```
N   1.43726000  0.00242900 -2.57856200
N   1.43726000  0.00242900  2.57856200
Cl  3.55912600  0.09235900  0.00000000
```

The coordinates of the partially optimized structures using DFT corresponding to Fig. 7

```
28
Rotation of py ring w/ anion = 0.0, Rotation of py ring w/o anion = 0.0
C  -1.65774200  1.40298000  0.08246200
C  -1.68636900  2.79765000  0.14267400
C  -3.03395100  3.18809800  0.09148000
C  -3.78767000  2.02231000 -0.01093600
N  -2.95674000  0.96330100 -0.01446800
H  -3.28442600 -0.00904800 -0.10192400
H  -0.82587600  3.45000400  0.22152500
H  -3.42348100  4.19677900  0.12100500
H  -4.85762800  1.87978600 -0.08481000
C  -0.55118100  0.49115600  0.09841600
C   0.78116900  0.91659100  0.16795700
C   1.79036400 -0.02188000  0.01762000
O   1.53243800 -1.30320000 -0.08109700
H   1.01715700  1.96910000  0.24408000
C   3.18767700  0.32582700 -0.08371400
C   3.83819600  1.55274700 -0.07278700
N   4.14506800 -0.64902600 -0.23181700
C   5.21731200  1.29597900 -0.21501700
H   3.36616600  2.52170500  0.02536300
C   5.37017400 -0.07814100 -0.31157700
H   3.94179000 -1.63751000 -0.26983300
H   6.01440000  2.02633300 -0.24566800
H   6.26039600 -0.68009400 -0.42979600
B   0.17495100 -1.82959800  0.24151200
O  -0.85225000 -0.77689200  0.01556100
F   0.15175700 -2.20131900  1.59058500
F  -0.08984900 -2.90641400 -0.58969500
Cl -4.71812300 -1.61874000 -0.40510100
```

28
Rotation of py ring w/ anion = 0.0, Rotation of py ring w/o anion = 30.0
C -1.64377400 1.39605500 0.09145300
C -1.65241900 2.78942300 0.19765100
C -2.99373400 3.19911900 0.18393800
C -3.76579300 2.04624400 0.06185000
N -2.95134300 0.97734800 0.00589000
H -3.29709700 0.01093300 -0.08212300
H -0.78108100 3.42727600 0.27545400
H -3.36876000 4.21130500 0.25259500
H -4.83921900 1.92060000 0.00985000
C -0.54857000 0.47627400 0.04081400
C   0.79362300 0.88668600 0.11235000
C   1.78632600 -0.04641900 -0.12276200
O   1.52252900 -1.32552400 -0.24741500
H   1.04557600 1.92770600 0.26094100
C   3.19214800 0.29700800 -0.18734200
C   3.82923100 1.49606600 -0.46670000
N   4.15540600 -0.60971400 0.18428300
C   5.21353500 1.28785800 -0.27703000
H   3.34475500 2.40829200 -0.79068500
C   5.37782300 -0.02433900 0.13125800
H   3.96484000 -1.56784200 0.43982000
H   6.00528100 2.01045200 -0.42180000
H   6.27162900 -0.57562100 0.38816500
B   0.17255100 -1.84599600 0.10833900
O -0.85560300 -0.78451600 -0.09118400
F   0.17825100 -2.21621500 1.45836900
F -0.12215600 -2.91877400 -0.71630800
Cl -4.76516200 -1.57912800 -0.28045600

28
Rotation of py ring w/ anion = 0.0, Rotation of py ring w/o anion = 60.0
C -1.60949400 1.39354400 0.11363500
C -1.57566600 2.78727900 0.23502000
C -2.90235700 3.23371400 0.26581800

C -3.71072300 2.10330200 0.14876100
N -2.93168300 1.01303600 0.05839700
H -3.30847700 0.05880000 -0.04860900
H -0.68454800 3.39863300 0.29889700
H -3.24671100 4.25483300 0.35751600
H -4.78847800 2.01083100 0.12090900
C -0.54382000 0.44933700 0.03441000
C   0.81850600 0.83012500 0.07763700
C   1.77707200 -0.11675000 -0.19571500
O   1.48834700 -1.39223300 -0.31425100
H   1.10044800 1.86382400 0.22242500
C   3.20429900 0.20795800 -0.25676500
C   3.86904900 1.21787600 -0.92352600
N   4.10108800 -0.39816100 0.58829400
C   5.22096500 1.18493200 -0.49399800
H   3.42645500 1.88834800 -1.64910600
C   5.32610300 0.17991900 0.44537800
H   3.88637900 -1.17337400 1.19801700
H   6.02572200 1.82388500 -0.83230500
H   6.17317100 -0.16561900 1.02132700
B   0.14270000 -1.88599200 0.07970800
O -0.87438200 -0.80171200 -0.09375200
F   0.17386500 -2.24609000 1.43199100
F -0.20087300 -2.95381600 -0.73010400
Cl -4.78797400 -1.48888400 -0.31596000

28
Rotation of py ring w/ anion = 0.0, Rotation of py ring w/o anion = 90.0
C -1.60214300 1.40170700 0.07934000
C -1.55321300 2.79933100 0.15655000
C -2.87328900 3.26192800 0.14448400
C -3.69384000 2.13699900 0.04938600
N -2.92830000 1.03559100 0.01057900
H -3.31601600 0.08255100 -0.07078200
H -0.65618100 3.40200400 0.21906300
H -3.20667200 4.28944700 0.19522100

H -4.77205200 2.05696300 0.00413500
C -0.54792900 0.44587200 0.05477100
C   0.82182900 0.81960300 0.09641300
C   1.77634800 -0.14474500 -0.08838700
O   1.48354200 -1.41811000 -0.19768100
H   1.10831900 1.85905300 0.17747600
C   3.21659100 0.18952700 -0.18529600
C   3.98753200 0.51211000 -1.27876400
N   4.01696000 0.23300100 0.92692800
C   5.30808000 0.75107300 -0.80266700
H   3.63654000 0.56821300 -2.30102200
C   5.29074500 0.57063700 0.56125900
H   3.71605100 0.03243600 1.86880900
H   6.17013000 1.02589100 -1.39600800
H   6.07490800 0.65384300 1.30048800
B   0.12016900 -1.90427300 0.13953200
O -0.88373000 -0.80387200 -0.03616100
F   0.10206300 -2.29680100 1.48128400
F -0.21236000 -2.94577900 -0.70823000
Cl -4.79803400 -1.46084400 -0.29805100

28
Rotation of py ring w/ anion = 0.0, Rotation of py ring w/o anion = 120.0
C -1.60402900 1.40930300 0.01522900
C -1.56417200 2.80762000 0.01466200
C -2.88822800 3.26084700 -0.04163400
C -3.70035900 2.12829400 -0.08080300
N -2.92604800 1.03085300 -0.04700100
H -3.30552700 0.07231500 -0.08033300
H -0.67181300 3.41920200 0.05444800
H -3.22773700 4.28761800 -0.05496000
H -4.77734500 2.03854200 -0.13310300
C -0.54220500 0.45630400 0.06009900
C   0.81818400 0.83665500 0.07957700
C   1.78605200 -0.13856200 -0.00563100
O   1.49345800 -1.41170400 -0.07177400

H   1.09618500 1.88186400 0.06568400
C   3.20922800 0.18742600 -0.16711300
C   4.11662600 -0.25179800 -1.10892000
N   3.89174300 0.93731100 0.75888500
C   5.38079200 0.28766600 -0.75408200
H   3.88248200 -0.87659500 -1.96078000
C   5.20838200 1.00721000 0.40922000
H   3.48629500 1.35157500 1.58489900
H   6.31318500 0.15995500 -1.28773400
H   5.91481300 1.55552300 1.01645200
B   0.11964000 -1.89452000 0.23494200
O -0.88004800 -0.79813200 0.03948700
F   0.07609200 -2.29175700 1.57425600
F -0.19124500 -2.93788100 -0.62122100
Cl -4.78006600 -1.49381800 -0.24736000

28
Rotation of py ring w/ anion = 0.0, Rotation of py ring w/o anion = 150.0
C -1.59564300 1.41181500 0.03181400
C -1.56471600 2.80844200 0.04152400
C -2.89249900 3.25485200 -0.02959400
C -3.69651900 2.11915900 -0.08536100
N -2.91363800 1.02580300 -0.04776000
H -3.28498900 0.06557700 -0.09276600
H -0.67681800 3.42550500 0.09589300
H -3.23738200 4.27995500 -0.04068500
H -4.77197800 2.02168600 -0.15192200
C -0.52947700 0.45668500 0.07895300
C   0.82364900 0.83289200 0.11676200
C   1.79592900 -0.14832300 0.01484300
O   1.48885300 -1.41703300 -0.06470300
H   1.09166400 1.88093400 0.10904900
C   3.20895700 0.14792400 -0.13196500
C   4.20666000 -0.61388200 -0.71594200
N   3.79791000 1.27864500 0.38734100
C   5.42016600 0.09465100 -0.56456700

H   4.05509800 -1.56558900 -1.20738100
C   5.13248500 1.25320800 0.13255800
H   3.32996900 1.98871900 0.93029800
H   6.39692600 -0.20475700 -0.91987400
H   5.77786600 2.05133500 0.47210000
B   0.11556900 -1.89222000 0.25118000
O -0.87762500 -0.79775300 0.04226500
F   0.07437800 -2.27598000 1.59596300
F -0.19635200 -2.94751500 -0.59129300
Cl -4.77024100 -1.50518900 -0.29555000

28
Rotation of py ring w/ anion = 0.0, Rotation of py ring w/o anion = 180.0
C -1.60445100 1.40127000 0.08055100
C -1.58395900 2.79632400 0.14103900
C -2.91539300 3.23551400 0.08018600
C -3.71010700 2.09734000 -0.02556700
N -2.91832700 1.00917700 -0.02555300
H -3.28234100 0.04855200 -0.10401800
H -0.70105400 3.41755300 0.22281500
H -3.26791100 4.25776800 0.10675400
H -4.78428300 1.99336200 -0.10260300
C -0.53106600 0.45092900 0.08650700
C   0.81692400 0.83016200 0.16721200
C   1.79798400 -0.13619700 -0.00501600
O   1.49128300 -1.40260300 -0.13274100
H   1.06932000 1.87659400 0.26961700
C   3.21032700 0.15232200 -0.10363700
C   4.26353100 -0.73691900 -0.25886600
N   3.74703800 1.42017700 -0.03815400
C   5.45445900 0.01782200 -0.29060800
H   4.15945300 -1.81053600 -0.33785000
C   5.09689700 1.34746800 -0.15072800
H   3.23188400 2.28073100 0.06750800
H   6.46205900 -0.35911800 -0.40150600
H   5.70408300 2.24168500 -0.12435500

B   0.12845100 -1.88578800 0.21027500
O -0.87307300 -0.80328800 -0.01431000
F   0.10341300 -2.24163900 1.56434500
F -0.18137400 -2.96076100 -0.60697000
Cl -4.76760900 -1.51709500 -0.35107000

28
Rotation of py ring w/ anion = 30.0, Rotation of py ring w/o anion = 0.0
C   1.67259700 1.38396100 0.23193700
C   1.66766600 2.77261900 0.34539200
C   3.00458800 3.20130200 0.25460600
C   3.77933400 2.06425000 0.05819500
N   2.97343300 0.98282200 0.04304100
H   3.31689000 0.02312800 -0.10768300
H   0.79327300 3.39043200 0.50718200
H   3.37143500 4.21646800 0.32631300
H   4.84693800 1.95410000 -0.07788200
C   0.56952400 0.46017400 0.16308800
C -0.72559000 0.86697500 -0.16309700
C -1.77300200 -0.03148300 0.01326200
O -1.55657300 -1.27589700 0.35520600
H -0.91664900 1.88498700 -0.47391800
C -3.16047900 0.33255800 -0.12442800
C -3.77277200 1.54353700 -0.42363700
N -4.15458000 -0.59890400 0.06176500
C -5.16411200 1.32099400 -0.41761200
H -3.26718500 2.47982700 -0.62135600
C -5.36347800 -0.01674700 -0.11242200
H -3.98470100 -1.56794200 0.29003200
H -5.93976700 2.04904900 -0.61222000
H -6.27736400 -0.58500000 -0.00861000
B -0.17655300 -1.84587100 0.27540000
O   0.82496200 -0.77256600 0.51491500
F   0.00936700 -2.37651500 -1.00420500
F -0.04486400 -2.81214000 1.25949100
Cl 4.64556800 -1.62390300 -0.56133800

28

Rotation of py ring w/ anion = 30.0, Rotation of py ring w/o anion = 30.0

C 1.66813000 1.38933000 0.20325100
C 1.65675400 2.78133100 0.28072800
C 2.98557500 3.21597700 0.13485700
C 3.76211000 2.07858600 -0.05835800
N 2.96549400 0.99216900 -0.01946100
H 3.31197000 0.03042800 -0.15075400
H 0.78302100 3.39681600 0.45430300
H 3.34725900 4.23494600 0.16741800
H 4.82558100 1.97290300 -0.22658500
C 0.56914100 0.46243800 0.19360700
C -0.74134100 0.85605000 -0.10665700
C -1.77658400 -0.03166300 0.15020000
O -1.54863800 -1.27687100 0.48447800
H -0.94845900 1.85705200 -0.45946600
C -3.17177700 0.31959100 0.00246800
C -3.81091200 1.55054200 0.01889000
N -4.10585700 -0.62973500 -0.33786900
C -5.16767200 1.32103700 -0.29610900
H -3.34642400 2.49997900 0.25260400
C -5.31206600 -0.03842900 -0.51710000
H -3.90846700 -1.61637700 -0.42320700
H -5.95516200 2.05997600 -0.35608800
H -6.18219900 -0.61872400 -0.79088700
B -0.17119600 -1.84077700 0.35517400
O 0.83417000 -0.76091000 0.56421700
F -0.02418300 -2.36415900 -0.93256300
F 0.00166900 -2.80838200 1.33025400
Cl 4.63891900 -1.63081100 -0.57325600

28

Rotation of py ring w/ anion = 30.0, Rotation of py ring w/o anion = 60.0

C 1.63037700 1.39640400 0.18809700
C 1.58199700 2.79103500 0.23590900

C 2.89027800 3.25859900 0.03915000
C 3.69334200 2.13784800 -0.15533600
N 2.93233400 1.03151900 -0.06891200
H 3.30577200 0.07638100 -0.18180100
H 0.69611900 3.38554600 0.42049000
H 3.22352700 4.28760600 0.03784600
H 4.75415900 2.05947500 -0.35345700
C 0.55894800 0.44556500 0.21118800
C -0.77799100 0.80990200 -0.05224100
C -1.77833400 -0.09604600 0.23270400
O -1.51932100 -1.33946600 0.55363200
H -1.02130100 1.80502100 -0.39810500
C -3.19660100 0.22847700 0.07349400
C -3.91878800 1.32540100 0.50132300
N -3.99455000 -0.49196900 -0.78109700
C -5.20774000 1.23212700 -0.08251000
H -3.55569000 2.09185300 1.17407300
C -5.21563700 0.10295500 -0.87563800
H -3.71980600 -1.34407800 -1.24736200
H -6.03558000 1.91405700 0.05882400
H -5.99116800 -0.31827100 -1.49995600
B -0.13661700 -1.87354200 0.39277700
O 0.85407700 -0.76793400 0.57564500
F -0.00452500 -2.38948100 -0.89902500
F 0.08735400 -2.83395000 1.36261700
Cl 4.67529100 -1.54648500 -0.53692700

28
Rotation of py ring w/ anion = 30.0, Rotation of py ring w/o anion = 90.0
C -1.61826100 1.39347600 -0.20342900
C -1.54816700 2.78802200 -0.26462600
C -2.85317900 3.27656200 -0.11317000
C -3.67844400 2.16943100 0.07261200
N -2.93332500 1.05165400 0.02110400
H -3.32496200 0.10403600 0.14062900
H -0.64895500 3.36792900 -0.43023100

H -3.17078100 4.31019100 -0.13466800
H -4.74519000 2.10979900 0.24375600
C -0.56342900 0.42811800 -0.17480400
C   0.77923500 0.78621800 0.10067800
C   1.76907900 -0.13860500 -0.12268000
O   1.51043100 -1.37686500 -0.45684300
H   1.02916700 1.79457700 0.40098600
C   3.20457300 0.20676100 -0.00113600
C   4.08510200 0.70171700 -0.93585900
N   3.87483000 0.07533300 1.18751200
C   5.33905800 0.86574600 -0.28177400
H   3.85020400 0.91696800 -1.97015000
C   5.17375500 0.47088400 1.02576200
H   3.47575600 -0.27427700 2.04571400
H   6.25534500 1.23470700 -0.72321500
H   5.86949800 0.43976300 1.85240700
B   0.12208100 -1.90361200 -0.33678300
O -0.86081500 -0.78613100 -0.52222500
F -0.04581200 -2.43654400 0.94252900
F -0.09063300 -2.84365900 -1.32773500
Cl -4.72328600 -1.48463200 0.49931300

28
Rotation of py ring w/ anion = 30.0, Rotation of py ring w/o anion = 120.0
C -1.62210100 1.38015300 -0.26107500
C -1.56008400 2.76506700 -0.42196200
C -2.87365500 3.25245700 -0.33149900
C -3.69396300 2.15574100 -0.08444000
N -2.93758600 1.04264100 -0.04111200
H -3.32363500 0.10217700 0.13412000
H -0.66255000 3.33960200 -0.61348600
H -3.19777200 4.27926900 -0.43439700
H -4.76360300 2.09794200 0.06780000
C -0.56022800 0.42015200 -0.16087700
C   0.76946400 0.79958700 0.10686700
C   1.77243800 -0.13925100 -0.03105800

```
O   1.52194800 -1.38302300 -0.33708000
H   1.00899600  1.83091400  0.32950000
C   3.19423800  0.22323400  0.01985600
C   4.20567300 -0.04957000 -0.87812500
N   3.75712400  0.81568100  1.12340300
C   5.41164700  0.43322000 -0.30695000
H   4.07759400 -0.52835200 -1.83999300
C   5.10086000  0.95030200  0.93291700
H   3.25848400  1.08318000  1.95899400
H   6.39683700  0.40233400 -0.75282000
H   5.72722600  1.39498600  1.69338800
B   0.13198600 -1.91686300 -0.24360100
O  -0.85544200 -0.81242300 -0.44878100
F  -0.05200100 -2.45431900  1.03131600
F  -0.05039200 -2.86132600 -1.23852700
Cl -4.71732500 -1.48048000  0.57345400

28
Rotation of py ring w/ anion = 30.0, Rotation of py ring w/o anion = 150.0
C  -1.61115400  1.37767300 -0.27921900
C  -1.55178600  2.75851800 -0.45919200
C  -2.86669500  3.24684300 -0.36124900
C  -3.68377300  2.15327000 -0.09824900
N  -2.92383200  1.04060300 -0.04900200
H  -3.30650000  0.10182700  0.13671800
H  -0.65640200  3.33167100 -0.66470200
H  -3.19217100  4.27236800 -0.47328800
H  -4.75250100  2.09460500  0.05959400
C  -0.54621400  0.41484900 -0.17559500
C   0.77432100  0.79156300  0.09852100
C   1.78363300 -0.15502800 -0.02697400
O   1.52048000 -1.39819100 -0.32494200
H   1.00286400  1.82764000  0.30954700
C   3.19269000  0.17771100  0.04469200
C   4.27735600 -0.47997300 -0.51184200
N   3.67995000  1.22643500  0.79223700
```

C   5.44078700 0.21244800 -0.10875800
H   4.21583300 -1.35080900 -1.15071800
C   5.03509200 1.25263600 0.70716600
H   3.12957200 1.84230800 1.37185800
H   6.46262700 -0.01985500 -0.37634600
H   5.60973500 1.99851100 1.23844800
B   0.12786900 -1.92308800 -0.22631600
O -0.85204500 -0.82098300 -0.45302900
F -0.06113000 -2.44207200 1.05686400
F -0.05203300 -2.88611800 -1.20555500
Cl -4.71998600 -1.47929700 0.59200000

28
Rotation of py ring w/ anion = 30.0, Rotation of py ring w/o anion = 180.0
C   1.61452000 1.38362300 0.22602700
C   1.56587700 2.77037800 0.35376900
C   2.88644800 3.24395400 0.25503600
C   3.69634600 2.13486800 0.04097400
N   2.92662300 1.02780800 0.02247400
H   3.30311700 0.07998100 -0.12540900
H   0.67324200 3.35754200 0.52975000
H   3.21966900 4.27015900 0.33302600
H   4.76609300 2.06115100 -0.10291600
C   0.54442100 0.42235100 0.15745100
C -0.76886200 0.78747300 -0.15342500
C -1.78797600 -0.14284300 0.03668700
O -1.52002400 -1.37776300 0.36975100
H -0.97673800 1.80238800 -0.46352100
C -3.19377600 0.16498400 -0.06462300
C -4.27734800 -0.69039700 0.08020300
N -3.69294500 1.41560500 -0.36137400
C -5.44683000 0.06770800 -0.12872900
H -4.20563300 -1.74552600 0.30698600
C -5.04679700 1.36532800 -0.40004200
H -3.15218000 2.25307700 -0.51444500
H -6.46836100 -0.28516400 -0.09021600

H -5.62782300 2.25109500 -0.61666900
B -0.13035300 -1.90193800 0.24405400
O   0.84435700 -0.80221600 0.49490400
F   0.05118100 -2.38738500 -1.05455000
F   0.05574000 -2.89013000 1.19634100
Cl 4.71832600 -1.51447100 -0.51281600

28
Rotation of py ring w/ anion = 60.0, Rotation of py ring w/o anion = 0.0
C -1.77802600 1.22092500 -0.51417000
C -1.83359900 2.53928800 -0.93780700
C -3.15631600 2.99097400 -0.71625300
C -3.84351000 1.94654300 -0.12353400
N -3.00523400 0.88713400 -0.00098600
H -3.27988600 -0.00342200 0.43570300
H -1.01396200 3.09076400 -1.38148000
H -3.56202000 3.96431700 -0.95881300
H -4.86517300 1.87874100 0.22545100
C -0.61525700 0.34216100 -0.40841800
C   0.58403000 0.78731400 0.12200800
C   1.72759000 -0.00867400 -0.03724700
O   1.65213900 -1.19912400 -0.56133500
H   0.64639800 1.76352000 0.58250400
C   3.04796300 0.42986300 0.31525400
C   3.51248400 1.62778200 0.85003900
N   4.13651900 -0.39323100 0.13782200
C   4.90675200 1.50776300 0.99329100
H   2.90595800 2.48696400 1.10551500
C   5.25753400 0.24283500 0.54136000
H   4.08295200 -1.33020900 -0.23573200
H   5.58821700 2.25284800 1.38027500
H   6.22392700 -0.23827800 0.48229200
B   0.32179700 -1.86800800 -0.74761100
O -0.72696300 -0.83866600 -0.96057200
F   0.03566000 -2.59980300 0.40486000
F   0.39704300 -2.67561900 -1.87057700

```
Cl -4.37694100 -1.52717900  1.52965000

28
Rotation of py ring w/ anion = 60.0, Rotation of py ring w/o anion = 30.0
C   1.80659800  1.23797800  0.47785300
C   1.88523000  2.56851200  0.85968700
C   3.19622800  3.00752400  0.56153700
C   3.85134200  1.94298400 -0.03344300
N   3.00654000  0.88386700 -0.08435000
H   3.25195700 -0.02133300 -0.51121100
H   1.08911100  3.13606900  1.32530400
H   3.61660500  3.98532200  0.75621700
H   4.85423900  1.86302500 -0.43091700
C   0.63424000  0.36872200  0.44984900
C  -0.58745500  0.80921500 -0.04328400
C  -1.72551500  0.03179100  0.19296900
O  -1.63790500 -1.15979300  0.71323000
H  -0.66422800  1.76326200 -0.54601700
C  -3.05317600  0.44667500 -0.18581600
C  -3.58205800  1.70618400 -0.43670100
N  -4.01420800 -0.48068200 -0.51582000
C  -4.90003400  1.52039800 -0.90039600
H  -3.07204500  2.64813900 -0.28062200
C  -5.12958500  0.15399300 -0.94458800
H  -3.89164800 -1.48014800 -0.43775200
H  -5.60782900  2.29006100 -1.17635400
H  -6.00257700 -0.40254800 -1.25599200
B  -0.30466800 -1.82962600  0.86447000
O   0.75647900 -0.79863300  1.02223300
F  -0.06127500 -2.58196300 -0.28400000
F  -0.33927400 -2.61526000  2.00435500
Cl  4.19322900 -1.63396700 -1.58333600

28
Rotation of py ring w/ anion = 60.0, Rotation of py ring w/o anion = 60.0
C   1.77874200  1.25348700  0.44410100
```

```
C   1.81939600  2.59064200  0.81193500
C   3.11206800  3.06586900  0.49521300
C   3.79077600  2.01747800 -0.10373700
N   2.97970200  0.93285100 -0.13574600
H   3.24807100  0.02922700 -0.55381200
H   1.01200300  3.13738300  1.28286400
H   3.50476600  4.05755800  0.67663300
H   4.78929600  1.96659800 -0.51670200
C   0.63123400  0.35538200  0.44701700
C  -0.62105000  0.76904600 -0.01755100
C  -1.72981200 -0.01867700  0.26531500
O  -1.61337800 -1.20542500  0.78914500
H  -0.73392700  1.71701800 -0.52458500
C  -3.08331800  0.36649700 -0.12761100
C  -3.74796500  1.57051300  0.01008800
N  -3.82701300 -0.43025600 -0.96409300
C  -4.95382300  1.46894500 -0.72640400
H  -3.40296500  2.41515600  0.59267600
C  -4.96357200  0.22421300 -1.32403600
H  -3.57610900 -1.36708600 -1.24445100
H  -5.72638600  2.22085900 -0.81433400
H  -5.68728000 -0.24043000 -1.97897600
B  -0.27216400 -1.85128200  0.94692000
O   0.78672100 -0.79902100  1.02312000
F  -0.04139200 -2.66078900 -0.16164300
F  -0.26492500 -2.56875200  2.13013500
Cl  4.17874000 -1.59276300 -1.60091600

28
Rotation of py ring w/ anion = 60.0, Rotation of py ring w/o anion = 90.0
C  -1.76038600  1.26830700 -0.44520900
C  -1.74670700  2.61117700 -0.79641100
C  -3.03453600  3.12150800 -0.52171400
C  -3.76581800  2.08779500  0.04078100
N  -2.99103700  0.97850800  0.08775900
H  -3.29474100  0.08070300  0.49574700
```

H -0.90692900 3.13858200 -1.23142100
H -3.38997800 4.12651200 -0.70641500
H -4.77887900 2.06491000 0.41943200
C -0.64203300 0.33742900 -0.40561700
C   0.61308900 0.72518000 0.09203400
C   1.70259000 -0.09107400 -0.14530000
O   1.58689600 -1.25639400 -0.70954100
H   0.73694500 1.68182700 0.58021900
C   3.07910100 0.31695900 0.21815200
C   4.01890100 1.01810700 -0.50209900
N   3.61016500 0.02833600 1.44813400
C   5.16702300 1.14722500 0.32925100
H   3.89043400 1.39250000 -1.50934500
C   4.88100100 0.52692300 1.52352500
H   3.14199400 -0.48463200 2.18013100
H   6.09569300 1.64167500 0.07705700
H   5.47221300 0.39927300 2.41929600
B   0.24279100 -1.88043400 -0.91814100
O -0.80353000 -0.80829500 -0.98701000
F -0.02895600 -2.71341000 0.16092500
F   0.25035200 -2.55942100 -2.12201000
Cl -4.22632000 -1.53713600 1.53015100

28
Rotation of py ring w/ anion = 60.0, Rotation of py ring w/o anion = 120.0
C   1.75000700 -1.21658000 -0.56040400
C   1.75721300 -2.52792800 -1.01184800
C   3.05648600 -3.03653000 -0.78460100
C   3.77768300 -2.03334300 -0.16008400
N   2.98341400 -0.94356000 -0.02533600
H   3.28204100 -0.07591300 0.44354800
H   0.92180300 -3.03737700 -1.47583300
H   3.42589500 -4.01940900 -1.04568300
H   4.79572500 -2.01725800 0.20531900
C   0.62149400 -0.30121600 -0.43099000
C -0.61042500 -0.73484000 0.06157000

C -1.71467800 0.10359100 -0.05511800
O -1.61672700 1.29628700 -0.55717200
H -0.71756100 -1.73815100 0.45142400
C -3.07537100 -0.35944600 0.22662300
C -4.21738000 -0.25814900 -0.54339900
N -3.43882500 -0.84463600 1.45959000
C -5.29256900 -0.74614700 0.24079600
H -4.25771800 0.11206400 -1.55938200
C -4.77899500 -1.08705500 1.47527100
H -2.81409100 -0.98235800 2.24039700
H -6.32740500 -0.83521800 -0.06142900
H -5.26122500 -1.47573000 2.36114600
B -0.27851300 1.94008100 -0.76180800
O   0.76885900 0.88829900 -0.93193600
F   0.01715600 2.70192700 0.36432300
F -0.32929400 2.70254800 -1.91483800
Cl 4.32261000 1.40912900 1.60766800

28
Rotation of py ring w/ anion = 60.0, Rotation of py ring w/o anion = 150.0
C   1.73487300 -1.19658500 -0.57974600
C   1.74364300 -2.49087900 -1.07528200
C   3.04803800 -3.00175300 -0.87600200
C   3.77079100 -2.01655000 -0.22686500
N   2.97175600 -0.93505800 -0.04876400
H   3.27167500 -0.08169100 0.44351200
H   0.90688100 -2.98717900 -1.55098000
H   3.41889500 -3.97409100 -1.17240400
H   4.79249000 -2.00676300 0.12839100
C   0.60630900 -0.28064100 -0.42838700
C -0.61457100 -0.71638100 0.06868400
C -1.73082500 0.12196100 -0.04743000
O -1.62198900 1.32051100 -0.53710500
H -0.70787200 -1.72785400 0.44043500
C -3.07728400 -0.31810000 0.23374600
C -4.27984000 0.17830300 -0.24775000

N -3.37172700 -1.29853500 1.15643300
C -5.31432100 -0.54585100 0.37953100
H -4.37696700 0.96392700 -0.98505900
C -4.71653400 -1.43993700 1.25169400
H -2.70130700 -1.79631700 1.72336800
H -6.37789500 -0.43015000 0.22184500
H -5.15133800 -2.15548800 1.93559700
B -0.28079700 1.96460100 -0.70723500
O   0.75973300 0.91912300 -0.91507000
F   0.01091300 2.68293300 0.45103100
F -0.32547500 2.77771300 -1.82744700
Cl 4.34333200 1.36372600 1.64057500

28
Rotation of py ring w/ anion = 60.0, Rotation of py ring w/o anion = 180.0
C -1.72733900 1.20855500 -0.53801800
C -1.72763400 2.51951200 -0.98797800
C -3.02868300 3.03165500 -0.77080600
C -3.75810800 2.02828200 -0.15770200
N -2.96600600 0.93620500 -0.01703200
H -3.27506800 0.06691200 0.44030500
H -0.88693800 3.02649800 -1.44507500
H -3.39362000 4.01624300 -1.03213700
H -4.78082300 2.01141700 0.19447600
C -0.59874500 0.28784100 -0.42018000
C   0.61826300 0.70400900 0.09817900
C   1.74201800 -0.12090700 -0.06411500
O   1.62409400 -1.31303900 -0.57212900
H   0.69169500 1.68509200 0.54622500
C   3.08362000 0.28277900 0.25669200
C   4.25962900 -0.45199400 0.15948900
N   3.41486800 1.52473000 0.75921000
C   5.30985500 0.36943000 0.60838600
H   4.32486100 -1.47103800 -0.19734200
C   4.74944600 1.58423800 0.97193400
H   2.77652100 2.28481000 0.93871300

H   6.35903800 0.11460600 0.66765900
H   5.20866300 2.48032200 1.36596100
B   0.27850400 -1.94931200 -0.72357200
O -0.75081500 -0.89679300 -0.94747000
F -0.01687400 -2.64593900 0.44833800
F   0.31266500 -2.78269700 -1.82946900
Cl -4.39654000 -1.40111000 1.56444100

28
Rotation of py ring w/ anion = 90.0, Rotation of py ring w/o anion = 0.0
C   2.33185500 0.11722000 -0.78548400
C   3.13334800 0.55729900 -1.81827000
C   4.35841400 -0.15849500 -1.71811800
C   4.25338000 -0.99247700 -0.62452500
N   3.02434300 -0.81313800 -0.06197000
H   2.64393400 -1.32964000 0.74258500
H   2.86332700 1.30344200 -2.55477300
H   5.21634900 -0.06885600 -2.37189900
H   4.95460200 -1.69987400 -0.20343000
C   0.96826300 0.54036400 -0.39440500
C -0.15190600 -0.13167200 -0.82692200
C -1.40152300 0.21045200 -0.27149900
O -1.52169000 1.23252100 0.52178100
H -0.05332000 -0.98179900 -1.48779800
C -2.59307800 -0.54724100 -0.50176000
C -2.82183700 -1.70011900 -1.24940600
N -3.79322400 -0.17553300 0.06190900
C -4.18571400 -2.01354200 -1.12563600
H -2.07874000 -2.24898700 -1.81298500
C -4.75488300 -1.04819600 -0.30437600
H -3.91339300 0.62658100 0.66405400
H -4.70486700 -2.84849800 -1.57551800
H -5.77371200 -0.93148100 0.03839000
B -0.40219200 2.21718800 0.69421600
O   0.89952500 1.56026800 0.42111500
F -0.42311300 2.67896600 1.99800500

F -0.59458200 3.25270100 -0.22622100
Cl 1.62103600 -2.39500000 2.31317000

28
Rotation of py ring w/ anion = 90.0, Rotation of py ring w/o anion = 30.0
C   2.34793400 0.05635700 -0.75831600
C   3.22928600 0.46810100 -1.73612300
C   4.40736200 -0.31323100 -1.57895000
C   4.19388100 -1.16038800 -0.51167200
N   2.94510000 -0.92516500 -0.01766300
H   2.49354800 -1.42959500 0.75723300
H   3.04413200 1.24126900 -2.47092200
H   5.30589000 -0.25856000 -2.17984200
H   4.83028300 -1.91258600 -0.06597200
C   0.99530800 0.55514500 -0.42247300
C -0.14484300 -0.05417800 -0.90038800
C -1.39068500 0.34662300 -0.38376200
O -1.48066800 1.33470200 0.45402500
H -0.06926800 -0.91393100 -1.55175700
C -2.60264300 -0.39141500 -0.61372400
C -2.94302500 -1.29584600 -1.61316100
N -3.62217600 -0.38938100 0.31004500
C -4.21000300 -1.81680200 -1.28934500
H -2.34454600 -1.53112000 -2.48386600
C -4.59339500 -1.24202800 -0.08628300
H -3.62674500 0.16633200 1.15346100
H -4.78363500 -2.53476900 -1.85921300
H -5.48224800 -1.39046900 0.51099400
B -0.32513100 2.26048300 0.69531500
O   0.95391300 1.56300100 0.40581600
F -0.34650900 2.65152600 2.02172000
F -0.45594600 3.34941100 -0.17035400
Cl 1.33522700 -2.44948600 2.26416500

28
Rotation of py ring w/ anion = 90.0, Rotation of py ring w/o anion = 60.0

C   2.37903500 -0.10633900 -0.69116200
C   3.33568800 0.19321800 -1.63795100
C   4.41701200 -0.70519300 -1.42023400
C   4.07042200 -1.50997400 -0.35511100
N   2.83423200 -1.13658400 0.08263800
H   2.28490700 -1.57069300 0.83558800
H   3.26443400 0.97013300 -2.38830000
H   5.34066600 -0.75449100 -1.98215200
H   4.60400900 -2.31898800 0.12448000
C   1.06926600 0.52661100 -0.42069200
C -0.10941900 0.01504700 -0.94010800
C -1.31980600 0.48131700 -0.41811900
O -1.35527200 1.46126000 0.43122000
H -0.08974500 -0.85211700 -1.58541600
C -2.57447600 -0.23413000 -0.61943400
C -3.12854700 -0.75476600 -1.77447500
N -3.30414100 -0.69985400 0.44616400
C -4.25814000 -1.51558800 -1.38704900
H -2.76472700 -0.58293800 -2.77945000
C -4.32682200 -1.47168700 -0.00806200
H -3.10063800 -0.50588000 1.41598400
H -4.94170300 -2.04149400 -2.03978700
H -5.01821300 -1.93599800 0.68099700
B -0.15365200 2.33239000 0.63870100
O   1.08375200 1.53486600 0.39766500
F -0.15627800 2.79089600 1.94043700
F -0.20309600 3.37338400 -0.28924200
Cl 0.73881500 -2.24547300 2.19796900

28
Rotation of py ring w/ anion = 90.0, Rotation of py ring w/o anion = 90.0
C   2.44516200 -0.20981400 -0.62900900
C   3.56551000 0.00501900 -1.40103400
C   4.47403200 -1.04762000 -1.09876200
C   3.87426800 -1.84787300 -0.14959500
N   2.64516200 -1.32894400 0.13361600

H   1.94353700 -1.71101200 0.77408700
H   3.70973600 0.82042700 -2.09790200
H   5.45508000 -1.19742100 -1.53014200
H   4.22401400 -2.74321000 0.34526200
C   1.19850000 0.56496900 -0.45183000
C   0.00875300 0.16730500 -1.05544100
C -1.16861300 0.54861000 -0.41998300
O -1.19336100 1.50100600 0.45565200
H   0.00471400 -0.65150700 -1.76163000
C -2.42962100 -0.19850500 -0.61523500
C -3.47081200 -0.02224100 -1.49936000
N -2.73278300 -1.23953100 0.21967600
C -4.44108800 -1.01526300 -1.18527200
H -3.52916300 0.73668500 -2.26870400
C -3.94992600 -1.74919400 -0.12679800
H -2.07343900 -1.61974500 0.90358600
H -5.39102800 -1.16918900 -1.68021600
H -4.36665300 -2.59513000 0.40189700
B   0.01674700 2.36592200 0.63179400
O   1.23093000 1.51206100 0.42942500
F   0.02932500 2.87055900 1.91310600
F   0.00016100 3.36667600 -0.33832900
Cl -0.03824100 -2.06659900 1.87188500

28
Rotation of py ring w/ anion = 90.0, Rotation of py ring w/o anion = 120.0
C   2.44320400 -0.11904700 -0.54053200
C   3.56563100 0.18911600 -1.27807800
C   4.54918000 -0.78554900 -0.95235200
C   3.99181600 -1.63194700 -0.01783100
N   2.72183400 -1.20789000 0.24373700
H   2.01281600 -1.72006400 0.77537300
H   3.66562400 1.02347400 -1.96035700
H   5.54941500 -0.85647300 -1.35930700
H   4.39498600 -2.50545100 0.47561500
C   1.17122200 0.60901100 -0.34808600

```
C  -0.01622200  0.15300900 -0.89733200
C  -1.20659800  0.57604200 -0.29737200
O  -1.24475100  1.61926900  0.46829300
H  -0.01528600 -0.69180100 -1.57245600
C  -2.46364400 -0.13788300 -0.50529800
C  -3.71387200  0.32340800 -0.87574100
N  -2.57906200 -1.45607100 -0.13865300
C  -4.60064600 -0.77576900 -0.77287300
H  -3.94302500  1.32956300 -1.20218900
C  -3.86889400 -1.84936900 -0.29747600
H  -1.81486100 -2.00972100  0.26540400
H  -5.65543700 -0.78300300 -1.01392900
H  -4.17336500 -2.85848300 -0.05608300
B  -0.01574900  2.46803300  0.61762500
O   1.18751300  1.58849000  0.50772500
F  -0.03137200  3.05514600  1.86590700
F   0.00749300  3.40802000 -0.41264400
Cl  0.03672000 -2.80924500  1.27262000

0
Rotation of py ring w/ anion = 90.0, Rotation of py ring w/o anion = 150.0

28
Rotation of py ring w/ anion = 90.0, Rotation of py ring w/o anion = 180.0
C   2.31990700  0.10359300 -0.73709900
C   3.16479400  0.53697000 -1.73756800
C   4.36991100 -0.20669500 -1.60512700
C   4.20984000 -1.05087100 -0.52616200
N   2.96804700 -0.84885100 -0.00062900
H   2.54178600 -1.38812800  0.76491600
H   2.93885100  1.30214800 -2.46935700
H   5.25104400 -0.12915800 -2.22884900
H   4.87883700 -1.78241400 -0.09400100
C   0.97018700  0.58132100 -0.36099700
C  -0.17352800 -0.05774700 -0.78635100
C  -1.41075600  0.31479700 -0.21831900
```

```
O  -1.49101300  1.34788600  0.56362500
H  -0.08506800 -0.90880400 -1.44748300
C  -2.62535100 -0.42269700 -0.39967300
C  -3.89869500 -0.13177000  0.08127300
N  -2.72310700 -1.57850500 -1.14873000
C  -4.76491700 -1.13558700 -0.38264300
H  -4.14732200  0.72352700  0.69498200
C  -4.00117200 -2.01487300 -1.13770700
H  -1.96124700 -2.06355500 -1.59824400
H  -5.82645900 -1.22102200 -0.19588500
H  -4.28282000 -2.91839500 -1.66065700
B  -0.35338600  2.31210800  0.68283900
O   0.93399600  1.60639300  0.44697800
F  -0.35668500  2.84424300  1.95906700
F  -0.51313300  3.30107900 -0.29415400
Cl  1.41576100 -2.60141300  2.15641700

28
Rotation of py ring w/ anion = 120.0, Rotation of py ring w/o anion = 0.0
C   1.58601100  1.43014700  0.01266500
C   1.54144500  2.82805700  0.00391600
C   2.86314900  3.28568400 -0.07233000
C   3.67906700  2.15613800 -0.11045100
N   2.90925600  1.05600800 -0.05760300
H   3.29121300  0.09844600 -0.08511500
H   0.64735100  3.43648500  0.05227800
H   3.19827400  4.31364100 -0.09825200
H   4.75580800  2.07008800 -0.17291900
C   0.52898700  0.47365200  0.09394200
C  -0.83186100  0.84947200  0.13522500
C  -1.79360800 -0.13178900  0.18598000
O  -1.50001500 -1.40860300  0.16049800
H  -1.12000800  1.89052000  0.09358100
C  -3.22494100  0.17641400  0.11148000
C  -3.97916300  1.10455600  0.80087200
N  -4.00501500 -0.33497200 -0.89557600
```

C -5.27063700 1.11497900 0.21215600
H -3.63642900 1.69074900 1.64393700
C -5.24824700 0.22003700 -0.83690100
H -3.70882200 -1.04059000 -1.55368500
H -6.12095400 1.70746000 0.52242600
H -6.01516600 -0.06281400 -1.54426900
B -0.09966000 -1.90641200 0.22252900
O   0.87576100 -0.77790000 0.09863200
F   0.10720000 -2.78869100 -0.83183900
F   0.10096600 -2.52700100 1.45447600
Cl 4.75862800 -1.49000000 -0.24673400

28
Rotation of py ring w/ anion = 120.0, Rotation of py ring w/o anion = 30.0
C   1.63699700 1.39989100 0.19640100
C   1.58564100 2.79437200 0.24053100
C   2.89522400 3.26334300 0.05457300
C   3.70115200 2.14353500 -0.13299900
N   2.94134600 1.03599500 -0.04847000
H   3.31148900 0.08097200 -0.17440200
H   0.69772400 3.38766100 0.41907200
H   3.22716200 4.29278200 0.05447200
H   4.76303600 2.06688200 -0.32581800
C   0.56595900 0.44836200 0.22196000
C -0.76929000 0.81039100 -0.05341800
C -1.77176600 -0.09153300 0.23633600
O -1.51522100 -1.33102800 0.57431400
H -1.00987900 1.80134700 -0.41284000
C -3.18883500 0.23156900 0.06455500
C -3.91183000 1.33645100 0.47025200
N -3.98154000 -0.49918500 -0.78623600
C -5.19607700 1.23779400 -0.12282400
H -3.55257800 2.11141500 1.13529200
C -5.20017800 0.09722400 -0.89971100
H -3.70449700 -1.35780400 -1.23900900
H -6.02324800 1.92385400 0.00140200

H -5.97148700 -0.33098000 -1.52450200
B -0.13246900 -1.86843000 0.42797100
O   0.85891600 -0.76118700 0.59994600
F   0.00576500 -2.40313300 -0.85530400
F   0.08612300 -2.81474400 1.41296600
Cl 4.62043800 -1.57184900 -0.60573800

28
Rotation of py ring w/ anion = 120.0, Rotation of py ring w/o anion = 60.0
C   2.41432400 -0.02650600 -0.46982700
C   3.63992000 0.50146600 -0.84347900
C   4.60016200 -0.52055500 -0.66448600
C   3.93305500 -1.61576500 -0.14246900
N   2.61809400 -1.30728500 -0.02115900
H   1.89365300 -1.93891600 0.35311500
H   3.80416400 1.50362100 -1.21836800
H   5.65838700 -0.46418100 -0.88308800
H   4.30052700 -2.58717300 0.15962600
C   1.12657500 0.64256300 -0.31349000
C -0.06441800 0.05434900 -0.73843700
C -1.26917600 0.60463800 -0.31594700
O -1.30886800 1.70361900 0.38209700
H -0.04959600 -0.88864800 -1.26822500
C -2.53751900 -0.10511500 -0.46009300
C -3.07261300 -0.75532600 -1.55579900
N -3.30700800 -0.41787700 0.63305800
C -4.22994800 -1.44025900 -1.10988900
H -2.67549400 -0.72067700 -2.56222000
C -4.33569300 -1.22141100 0.24890400
H -3.12860600 -0.10539400 1.57609200
H -4.90499800 -2.03371300 -1.71155900
H -5.05638900 -1.58085100 0.96982100
B -0.10035000 2.57447000 0.49704600
O   1.13258200 1.74154000 0.38198700
F -0.10848100 3.18649700 1.73757600
F -0.12060500 3.50293000 -0.54549500

```
Cl  0.45450300 -3.32087500  1.12735000

28
Rotation of py ring w/ anion = 120.0, Rotation of py ring w/o anion = 90.0
C   2.48018800 -0.13369100 -0.53736500
C   3.77043100  0.27342300 -0.82929200
C   4.59834000 -0.86608200 -0.69693100
C   3.79068100 -1.91240500 -0.28541400
N   2.51261500 -1.46537600 -0.19930800
H   1.71508000 -1.98467700  0.18690000
H   4.06349800  1.27199600 -1.12675300
H   5.66390600 -0.91993800 -0.87675300
H   4.03524600 -2.93640700 -0.03860400
C   1.24532700  0.62337100 -0.37663000
C   0.03277400  0.14895600 -0.89439400
C  -1.13088500  0.56144500 -0.27168500
O  -1.14698200  1.57299200  0.54650100
H   0.01991000 -0.69960600 -1.56463200
C  -2.42009600 -0.13061800 -0.48666000
C  -3.47394900  0.18361600 -1.31622600
N  -2.79443300 -1.17177600  0.32057100
C  -4.51593000 -0.73952700 -1.01931200
H  -3.49416600  0.99093200 -2.03697100
C  -4.05815600 -1.56401300 -0.01452100
H  -2.13290100 -1.69684500  0.89590600
H  -5.48936800 -0.78876000 -1.48953500
H  -4.52636800 -2.40275900  0.48166500
B   0.04330600  2.47332300  0.60524600
O   1.28086500  1.64477900  0.41963400
F   0.09667000  3.07336700  1.84663900
F  -0.03857500  3.40327400 -0.43170300
Cl -0.09440600 -2.79054400  1.27063300

28
Rotation of py ring w/ anion = 120.0, Rotation of py ring w/o anion = 120.0
C  -2.47032800  0.08582900 -0.44265500
```

C -3.74235100 -0.37210700 -0.74284400
C -4.62694800 0.71441600 -0.55225500
C -3.86978200 1.78066000 -0.09715200
N -2.57242000 1.39193000 -0.02686500
H -1.78624900 1.97509300 0.28407800
H -3.98743900 -1.37272300 -1.07507300
H -5.69569600 0.72082500 -0.72108400
H -4.16199600 2.78258200 0.18634300
C -1.21226000 -0.63674000 -0.29867500
C -0.01034200 -0.10432600 -0.76139100
C   1.17255800 -0.57720100 -0.20070400
O   1.20625800 -1.69070000 0.47108500
H -0.00667800 0.79349300 -1.36502200
C   2.44730600 0.10752000 -0.39451400
C   3.68378700 -0.40211300 -0.75173800
N   2.62206000 1.40584900 0.01932000
C   4.61898800 0.64966200 -0.60655700
H   3.87270000 -1.41225300 -1.09145800
C   3.92864300 1.74517600 -0.11780000
H   1.86625600 2.01989700 0.34395400
H   5.67761000 0.61246500 -0.82731800
H   4.27368000 2.73604800 0.14418500
B -0.00517300 -2.56833200 0.48903200
O -1.22985900 -1.71239200 0.43470600
F -0.01841900 -3.28589600 1.67029800
F   0.02361200 -3.40049800 -0.63262400
Cl 0.01486100 3.16820100 0.87890400

28
Rotation of py ring w/ anion = 120.0, Rotation of py ring w/o anion = 150.0
C -2.44858400 0.11000500 -0.34600100
C -3.71857300 -0.33906300 -0.66624700
C -4.61608300 0.71639000 -0.38087600
C -3.86732000 1.75502700 0.14437200
N -2.56515100 1.37469100 0.18071400
H -1.77725900 1.97674600 0.44244200

H -3.95576300 -1.31726900 -1.06450900
H -5.68716700 0.71998000 -0.53463500
H -4.16686000 2.73308800 0.49558500
C -1.19066900 -0.62535800 -0.24852800
C   0.01206000 -0.05696000 -0.63365300
C   1.20053400 -0.62374600 -0.15337700
O   1.20935200 -1.81091400 0.38103900
H   0.02331500 0.89831600 -1.14124800
C   2.46428500 0.06201200 -0.22523600
C   3.75555000 -0.45001800 -0.27005100
N   2.55214100 1.43612800 -0.17923300
C   4.63532200 0.64944300 -0.27723900
H   4.00838000 -1.50100400 -0.32019400
C   3.85455700 1.79550900 -0.20182200
H   1.76468500 2.07685100 -0.01784800
H   5.71539800 0.61997800 -0.33019500
H   4.14128900 2.83713800 -0.14950500
B -0.02805000 -2.64971700 0.32736500
O -1.22634500 -1.76673600 0.38988100
F -0.03677700 -3.49325500 1.42524400
F -0.03816200 -3.36195600 -0.87716600
Cl 0.02877800 3.34633400 0.55440000

28
Rotation of py ring w/ anion = 120.0, Rotation of py ring w/o anion = 180.0
C   2.44700100 -0.15289000 -0.24696000
C   3.72826100 0.27074900 -0.55255600
C   4.61202700 -0.76874600 -0.17513900
C   3.84312600 -1.76858100 0.39160200
N   2.54203000 -1.37788100 0.37258800
H   1.74456800 -1.98161600 0.58577500
H   3.98347800 1.22429000 -0.99677800
H   5.68728600 -0.78560600 -0.29513900
H   4.12519700 -2.72780500 0.80370000
C   1.19911400 0.60946800 -0.22294700
C -0.00291600 0.01648400 -0.55184900

C -1.19602600 0.64459000 -0.15245500
O -1.18518700 1.87755700 0.26897700
H -0.00918200 -0.98842400 -0.95198200
C -2.44538000 -0.04926900 -0.05124000
C -3.71815600 0.46929900 0.17618200
N -2.58360400 -1.39327000 -0.33726700
C -4.62925200 -0.59309700 0.05523800
H -3.93792300 1.50946600 0.37738400
C -3.88717500 -1.72960300 -0.24643400
H -1.81552100 -2.07490600 -0.34863400
H -5.70397500 -0.54852700 0.16854700
H -4.20323700 -2.75504400 -0.38368600
B   0.06727500 2.68747000 0.16666000
O   1.24751000 1.79728400 0.33036200
F   0.06828600 3.62763200 1.18410700
F   0.11104000 3.29239800 -1.09637400
Cl -0.10190100 -3.42826700 0.22560600

28
Rotation of py ring w/ anion = 150.0, Rotation of py ring w/o anion = 0.0
C -2.45489100 -0.17700800 -0.09684900
C -3.65212000 -0.88227300 -0.14963200
C -4.69215500 0.04863600 0.03799100
C -4.09543200 1.28786500 0.22769200
N -2.75364400 1.14260400 0.15957000
H -2.08352100 1.92180300 0.21027400
H -3.74115200 -1.94850600 -0.31140400
H -5.75554100 -0.15045300 0.03921100
H -4.53630300 2.25897100 0.40880400
C -1.10542000 -0.68938500 -0.10161000
C   0.00603400 0.11200900 -0.34238900
C   1.27283300 -0.41026300 -0.08645500
O   1.44715100 -1.67461300 0.20571700
H -0.11209200 1.16017800 -0.59266400
C   2.45958200 0.40055800 -0.06790500
C   2.63018800 1.77230500 -0.22093700

```
N   3.69496600 -0.14887400  0.18850700
C   4.00469600  2.03774500 -0.06200900
H   1.83599800  2.49033800 -0.39681700
C   4.63240200  0.82653400  0.18996600
H   3.85672000 -1.13342200  0.34324200
H   4.49038800  3.00250100 -0.11713800
H   5.67430300  0.59912800  0.36858900
B   0.31988100 -2.63732900  0.03387000
O  -0.97474500 -1.94671600  0.24836200
F   0.45311100 -3.64501400  0.97964600
F   0.36465200 -3.15113600 -1.26953900
Cl -0.76417000  3.65915500  0.02654400

28
Rotation of py ring w/ anion = 150.0, Rotation of py ring w/o anion = 30.0
C  -2.43923400 -0.13668600 -0.07956600
C  -3.65048700 -0.82121600 -0.09307500
C  -4.66686100  0.12724700  0.12691200
C  -4.04160600  1.35534400  0.30056400
N  -2.70614900  1.18707100  0.18941800
H  -2.02272500  1.95703300  0.22148400
H  -3.76272300 -1.88557600 -0.25249200
H  -5.73291800 -0.05312800  0.16345000
H  -4.45904300  2.33357100  0.49844500
C  -1.10381700 -0.67901200 -0.13124800
C   0.02233700  0.10154800 -0.39415500
C   1.28114900 -0.45955600 -0.20863400
O   1.43260200 -1.72292900  0.10067600
H  -0.07622700  1.16057400 -0.60683800
C   2.49143200  0.32827100 -0.18228400
C   2.75668200  1.60434200 -0.65876000
N   3.57473900 -0.07086200  0.56522000
C   4.04877000  1.95527100 -0.21348900
H   2.08409900  2.20777500 -1.25529900
C   4.52140700  0.89858200  0.54719200
H   3.64494100 -0.96310900  1.03253000
```

H   4.57596000 2.87817900 -0.41344200
H   5.45616400 0.77390300 1.07597000
B   0.28227100 -2.66406000 -0.00945000
O -0.99358500 -1.93794200 0.21094800
F   0.41491900 -3.64201300 0.96696300
F   0.28051000 -3.22187300 -1.29447100
Cl -0.72286100 3.67733800 0.03969500

28
Rotation of py ring w/ anion = 150.0, Rotation of py ring w/o anion = 60.0
C -2.42629800 -0.03105400 -0.11923600
C -3.67904900 -0.63911400 -0.16618700
C -4.63847700 0.37073000 0.01729700
C -3.94171000 1.55980000 0.20346100
N -2.61869100 1.31047400 0.12872100
H -1.88956200 2.03625000 0.20406400
H -3.85218500 -1.69500600 -0.32764100
H -5.71426400 0.25765400 0.02000500
H -4.30320400 2.56248100 0.38907900
C -1.12987500 -0.65113000 -0.14303400
C   0.05235900 0.06270000 -0.40530500
C   1.26572700 -0.56832400 -0.21240200
O   1.34688600 -1.82623100 0.14344000
H   0.02047400 1.12083100 -0.63982400
C   2.53204500 0.16578100 -0.21336100
C   3.02215300 1.09903100 -1.10515900
N   3.35178600 0.16496100 0.88822800
C   4.20345300 1.64039100 -0.53678400
H   2.57634800 1.34925000 -2.05921500
C   4.37093600 1.04864300 0.69789000
H   3.22463700 -0.41606400 1.70345000
H   4.85380100 2.38431900 -0.97690300
H   5.12959800 1.19095100 1.45464500
B   0.15280900 -2.70852000 0.05584100
O -1.09231900 -1.90396700 0.21379100
F   0.20738200 -3.64225500 1.08032900

F   0.13708400 -3.32358600 -1.20064300
Cl -0.52151000 3.68313600 0.17390500

28
Rotation of py ring w/ anion = 150.0, Rotation of py ring w/o anion = 90.0
C -2.43893500 -0.07204500 -0.19043800
C -3.68216200 -0.70194100 -0.25616000
C -4.66065000 0.29718800 -0.14720200
C -3.98745100 1.50532300 0.01347300
N -2.66099700 1.27693100 -0.00961400
H -1.94630200 2.01594700 0.08854100
H -3.83406200 -1.76615600 -0.38029900
H -5.73404500 0.16757600 -0.17800300
H -4.37138700 2.50765100 0.14986200
C -1.13677800 -0.66603500 -0.12837200
C   0.05161400 0.05707400 -0.38362600
C   1.25572500 -0.52098800 -0.06233400
O   1.35530400 -1.76514800 0.33348000
H   0.01390500 1.09250400 -0.70181300
C   2.53032000 0.22915000 -0.13939400
C   3.43807900 0.32277100 -1.16962700
N   3.02162900 0.93447000 0.92744900
C   4.51399800 1.13040400 -0.70368300
H   3.33495300 -0.13932400 -2.14276300
C   4.22359900 1.49240400 0.59152100
H   2.54383800 1.06765700 1.80597500
H   5.39798500 1.41382700 -1.25948400
H   4.76716300 2.10386500 1.29784100
B   0.19101300 -2.67847300 0.19393600
O -1.08389700 -1.89804700 0.28196600
F   0.21049700 -3.60039600 1.22794500
F   0.24726000 -3.30058400 -1.05718200
Cl -0.62275000 3.67197500 0.17177800

28
Rotation of py ring w/ anion = 150.0, Rotation of py ring w/o anion = 120.0

C -2.48539500 0.05486400 -0.24319100
C -3.78187200 -0.44460900 -0.29082200
C -4.65129000 0.66236400 -0.29731600
C -3.85962100 1.80155800 -0.22416100
N -2.56084600 1.43092700 -0.20450100
H -1.76964500 2.06380600 -0.03298600
H -4.04473300 -1.49311500 -0.34224800
H -5.73167000 0.64309200 -0.34823500
H -4.13716100 2.84557100 -0.16991900
C -1.22466800 -0.63342500 -0.17647100
C -0.02552500 -0.03477500 -0.58964200
C   1.16245900 -0.56005500 -0.11455600
O   1.21554000 -1.74627700 0.43302200
H -0.03036700 0.93149100 -1.07573800
C   2.43720800 0.13148600 -0.29376700
C   3.66334500 -0.36951600 -0.69490600
N   2.64000000 1.38998200 0.22236200
C   4.61797300 0.65348000 -0.48180000
H   3.83469800 -1.35839900 -1.10019100
C   3.94968800 1.72211600 0.08869600
H   1.88825000 2.02227900 0.51337000
H   5.67460400 0.61460400 -0.71177100
H   4.31085700 2.69042600 0.40719300
B   0.02554700 -2.63782400 0.32868900
O -1.22462700 -1.81686000 0.36758100
F   0.01633500 -3.50299600 1.41000400
F   0.07653800 -3.32669800 -0.88840000
Cl -0.01491900 3.32673000 0.58237700

28
Rotation of py ring w/ anion = 150.0, Rotation of py ring w/o anion = 150.0
C -2.46425900 0.06531400 -0.16043000
C -3.75763800 -0.43903400 -0.21462100
C -4.63544800 0.66001100 -0.13648200
C -3.85062300 1.79769300 -0.00685400
N -2.54877100 1.43358500 -0.02145700

H -1.75785500 2.07761900 0.09403100
H -4.01450200 -1.48506800 -0.31880800
H -5.71654600 0.63518000 -0.16694000
H -4.13212700 2.83610700 0.10453000
C -1.20259500 -0.63162800 -0.12799600
C -0.00156200 -0.01041500 -0.46449300
C   1.19042200 -0.61507600 -0.07366600
O   1.21765300 -1.85343100 0.34404400
H   0.00195400 0.99567500 -0.86230100
C   2.45799600 0.07102400 -0.13728300
C   3.74442400 -0.44524500 -0.22422900
N   2.55854900 1.43708900 0.01106700
C   4.63405500 0.64595900 -0.16315800
H   3.98888900 -1.49312900 -0.33865600
C   3.86380700 1.79000400 -0.00797100
H   1.77394100 2.08751600 0.13362900
H   5.71363800 0.61127900 -0.22341000
H   4.15764200 2.82559700 0.09757200
B -0.00052000 -2.69742800 0.17886100
O -1.22218300 -1.85658400 0.32969000
F -0.00577400 -3.66910700 1.16806500
F   0.00967400 -3.26612200 -1.10163000
Cl 0.00287000 3.47454100 0.29259300

0
Rotation of py ring w/ anion = 150.0, Rotation of py ring w/o anion = 180.0

28
Rotation of py ring w/ anion = 180.0, Rotation of py ring w/o anion = 0.0
C -2.44835800 -0.22428600 -0.11432200
C -3.61864600 -0.96648800 -0.24741800
C -4.69177900 -0.05769300 -0.23603200
C -4.14412900 1.21150400 -0.09175800
N -2.80081100 1.10447200 -0.01822000
H -2.16541200 1.90845900 0.07737200
H -3.66501200 -2.04345600 -0.33965700

H -5.74532200 -0.28797800 -0.32085500
H -4.62320700 2.17988000 -0.03643600
C -1.09003300 -0.69161900 -0.05284600
C   0.00737000 0.15784100 0.08443500
C   1.28453200 -0.37860900 -0.02772400
O   1.48642400 -1.66894400 -0.14234800
H -0.12398500 1.23048700 0.17563500
C   2.46756200 0.44021000 -0.07085300
C   2.62393500 1.82099300 -0.03110300
N   3.71884400 -0.11997800 -0.18233700
C   4.00634500 2.08267800 -0.11786200
H   1.82003900 2.54575800 0.04747000
C   4.65284500 0.85938000 -0.21094700
H   3.89263900 -1.11340800 -0.23090600
H   4.48520700 3.05247900 -0.11547900
H   5.70496600 0.62501700 -0.29605300
B   0.37351300 -2.62241400 0.12628500
O -0.93613600 -1.98882400 -0.16134600
F   0.41630000 -2.98927800 1.47912800
F   0.53023500 -3.73012200 -0.69819000
Cl -0.88780600 3.66686300 0.23006200

28
Rotation of py ring w/ anion = 180.0, Rotation of py ring w/o anion = 30.0
C -2.43900700 -0.23711500 -0.02114800
C -3.61155800 -0.98988700 -0.02720900
C -4.68524800 -0.08609800 0.04138200
C -4.13603300 1.19087000 0.09749200
N -2.79168300 1.09254300 0.06231800
H -2.15869600 1.90566300 0.07045400
H -3.65649300 -2.06973700 -0.07688400
H -5.74057200 -0.32329500 0.05512600
H -4.61604200 2.15834400 0.16018000
C -1.07845800 -0.69422100 -0.05370200
C   0.02553800 0.16400800 -0.00455100
C   1.29258500 -0.37255700 -0.16658400

O   1.50236800 -1.66497100 -0.23339500
H -0.10008700 1.23667100 0.09582500
C   2.48581800 0.44391600 -0.17635000
C   2.64937400 1.80366400 -0.39720400
N   3.68795400 -0.05629400 0.26616200
C   3.99848900 2.11100000 -0.11419900
H   1.87169500 2.48752900 -0.71726400
C   4.60861700 0.93873800 0.30005700
H   3.84716800 -1.02279000 0.51059300
H   4.47438400 3.07889800 -0.19526300
H   5.62288300 0.74783500 0.62234800
B   0.40278900 -2.64289300 -0.01698200
O -0.92467600 -1.98997000 -0.13444700
F   0.53121400 -3.18414800 1.26819400
F   0.49517900 -3.63873200 -0.98658800
Cl -0.96187300 3.69253700 0.04710700

28
Rotation of py ring w/ anion = 180.0, Rotation of py ring w/o anion = 60.0
C -2.42817100 -0.16792200 -0.05205200
C -3.63761800 -0.86587700 -0.06284300
C -4.66637300 0.08060200 0.03739500
C -4.05711400 1.33090300 0.11786900
N -2.72198500 1.17507200 0.06723400
H -2.05466100 1.96180600 0.09325500
H -3.73321200 -1.94107500 -0.13598900
H -5.73109500 -0.10868300 0.05705400
H -4.49347000 2.31685200 0.20850800
C -1.09656900 -0.68513300 -0.09836900
C   0.05731700 0.12503900 -0.03079700
C   1.28527800 -0.45784800 -0.25247900
O   1.43935300 -1.75842100 -0.35198400
H -0.01592900 1.19980800 0.09710000
C   2.52582400 0.31853000 -0.25560900
C   2.83353400 1.51556800 -0.87243700
N   3.53213300 0.03580900 0.63658700

C   4.09092600 1.93528500 -0.36903100
H   2.21663500 2.02261800 -1.60330100
C   4.48824300 1.00263200 0.56736100
H   3.56372500 -0.77836200 1.23214900
H   4.63988300 2.82320300 -0.65265200
H   5.37117800 0.95552600 1.18939500
B   0.31572200 -2.66778500 -0.01485600
O -0.99137100 -1.97962900 -0.21329200
F   0.42309700 -3.03918500 1.33248800
F   0.36379700 -3.77633100 -0.84912100
Cl -0.82648600 3.69790700 0.14469800

28
Rotation of py ring w/ anion = 180.0, Rotation of py ring w/o anion = 90.0
C -2.43111500 -0.12616000 -0.09011200
C -3.64928000 -0.80645000 -0.17403300
C -4.66528600 0.15655800 -0.16069900
C -4.04141400 1.39977700 -0.06200000
N -2.70979900 1.22405700 -0.02046700
H -2.03464500 2.00150600 0.05689300
H -3.75682700 -1.88091200 -0.24030000
H -5.73176000 -0.01517100 -0.21388300
H -4.46740800 2.39341600 -0.01701800
C -1.11240800 -0.66808200 -0.05805300
C   0.05985700 0.12671800 0.01274300
C   1.27945500 -0.48722100 -0.11199000
O   1.41545600 -1.78905300 -0.19475700
H   0.00210900 1.20840300 0.07416000
C   2.54102200 0.28610600 -0.18034300
C   3.22153400 0.78756200 -1.26618500
N   3.24505600 0.61007100 0.95011700
C   4.38423700 1.43874500 -0.76502200
H   2.91287300 0.69569300 -2.29937900
C   4.36647800 1.31231500 0.60486500
H   2.97048400 0.37883800 1.89294400
H   5.14201700 1.94749500 -1.34609700

H   5.05283400 1.66646200 1.36101600
B   0.26582800 -2.68128200 0.09164800
O -1.02481000 -1.96335000 -0.13380200
F   0.31993000 -3.07495600 1.43415200
F   0.31437000 -3.77599600 -0.75981900
Cl -0.80693900 3.72531500 0.22531400

28
Rotation of py ring w/ anion = 180.0, Rotation of py ring w/o anion = 120.0
C -2.43739200 -0.13801100 0.05684200
C -3.65114700 -0.81777700 0.16974800
C -4.67416000 0.13385800 0.05149800
C -4.05709200 1.36911000 -0.13008600
N -2.72203400 1.19853700 -0.13595000
H -2.04655400 1.97588200 -0.18810700
H -3.75414200 -1.88564700 0.30924900
H -5.74048800 -0.04259900 0.09226800
H -4.48750800 2.35396800 -0.25420700
C -1.11157400 -0.67381200 0.04891700
C   0.04403900 0.10810300 -0.15713100
C   1.27843900 -0.47032800 0.04814100
O   1.42759100 -1.75677800 0.24363900
H -0.02736800 1.17228100 -0.35547900
C   2.52264400 0.29879200 -0.04562200
C   3.67916200 0.01281300 -0.74453100
N   2.77756000 1.37943100 0.76325100
C   4.63871400 0.99211000 -0.38366900
H   3.80142600 -0.80332000 -1.44459500
C   4.05018200 1.81634100 0.55398000
H   2.10486800 1.81690400 1.37641600
H   5.64648800 1.08527300 -0.76608000
H   4.43647600 2.67495100 1.08497500
B   0.27804200 -2.67506300 0.03493800
O -1.01280100 -1.95812300 0.24646200
F   0.36100000 -3.71403400 0.95168200
F   0.30873200 -3.15068500 -1.28166400

```
Cl -0.74993500  3.68801900 -0.12822000

28
Rotation of py ring w/ anion = 180.0, Rotation of py ring w/o anion = 150.0
C  -2.46539100  0.05372300  0.02971900
C  -3.74183900 -0.48164600  0.16661400
C  -4.65591800  0.58089500  0.04778800
C  -3.91115900  1.73302600 -0.16874200
N  -2.60006000  1.40921700 -0.19720600
H  -1.83887300  2.09526800 -0.21666300
H  -3.96234400 -1.52942200  0.32220300
H  -5.73452500  0.52393300  0.10546200
H  -4.22896600  2.75878200 -0.29876100
C  -1.19534700 -0.61741700  0.00000100
C   0.00116200  0.05212800 -0.26277800
C   1.20029700 -0.59302600 -0.00167800
O   1.24529700 -1.87274400  0.27165300
H   0.00175400  1.10698300 -0.50181300
C   2.46742800  0.09771800 -0.07486300
C   3.74776400 -0.41694300 -0.22482700
N   2.58391300  1.44490600  0.19671200
C   4.64855400  0.65962700 -0.09076700
H   3.98232400 -1.45538900 -0.41833800
C   3.89187700  1.79200900  0.17110400
H   1.80754000  2.10277500  0.30655600
H   5.72658600  0.62199600 -0.17279800
H   4.19492200  2.81645300  0.33964100
B   0.03447600 -2.70905100  0.04761800
O  -1.20879500 -1.90288200  0.23186800
F   0.03135800 -3.74480500  0.97211100
F   0.05665700 -3.19752800 -1.26611600
Cl -0.05979400  3.53238000  0.08049100

28
Rotation of py ring w/ anion = 180.0, Rotation of py ring w/o anion = 180.0
C  -2.46924300  0.06366200 -0.08982800
```

```
C  -3.74457300 -0.47404300 -0.21680300
C  -4.65619500  0.59810400 -0.18574100
C  -3.91083800  1.75821500 -0.02880400
N  -2.60031600  1.43266500  0.03177800
H  -1.83849200  2.11371000  0.09744800
H  -3.96649200 -1.52804500 -0.31881600
H  -5.73361200  0.54182400 -0.26316200
H  -4.22648100  2.79065500  0.03784100
C  -1.19830900 -0.60971100 -0.03647900
C   0.00104000  0.07689000  0.11672100
C   1.20161000 -0.60945500 -0.03014800
O   1.22799000 -1.90980100 -0.17507000
H   0.00039800  1.15189600  0.23573000
C   2.47097300  0.06629600 -0.08974600
C   3.74970200 -0.46999000 -0.18665800
N   2.59573700  1.43823800 -0.00646500
C   4.65737300  0.60583700 -0.16690500
H   3.97571800 -1.52574100 -0.25679900
C   3.90580000  1.76750900 -0.05674400
H   1.83179600  2.11799700  0.04300400
H   5.73604700  0.55175000 -0.22672400
H   4.21605100  2.80290100 -0.01571500
B   0.00280100 -2.71326700  0.08858700
O  -1.22584900 -1.91147700 -0.16638700
F   0.00671300 -3.11405400  1.43209200
F   0.00034200 -3.81123800 -0.76350800
Cl -0.00597400  3.57123700  0.15225100
```

The comparison between wB97x and MP2. The potential energies are calculated in gas phase and the energies includes ZPE. Units in kcal/mol.

	A	TS1(A→B)	B	TS2(B→C)	C
wB97x	0	12.2	4.1	16.4	9.0
MP2	0	12.2	4.5	16.6	9.7

The detail of the initial settings for MD simulation at NVT condition

input	description

ntx=1,	The coordinates continue the NPT calc., but the velocity were not continued.
irest=...,	Flag for restart MD simulation or not.
nstlim=...,	The steps of MD simulation (the actual numbers are summarized in next table).
dt=0.002,	The time step was 2 ns.
tempi=300.0,	The initial temperature was set to be 300 K. (This simulation follows MD simulation under NPT ensenble)
temp0=300.0,	The reference temperature was set to be 300 K
ntpr=100,	Energy etc. were output by each 100 steps
ntwx=100,	The coordinates were output by each 100 steps
ntb=1,	NVT ensemble
cut=12.0,	The cutoff of the direct space sum of PME were 12.0 Angstroms.
ntp=0,	No pressure control
ntt=3,	Langevin dynamics was employed for the temperature control.
iwrap=1,	The coordinates were output so that all atoms are in "primary box"
ntwr=100,	Restart file are output by 100 steps
ntwe=100,	energies and temperature are output by 100 steps
gamma_ln=2.0,	collision frequency are 2.0 ps^{-1}
ntc=2,	SHAKE algorithm was employed and the bonds including hydrogen are constrained.
ntf=2,	The force calculation for the bond including H atoms are omitted.
ntxo=1,	ASCII formatted output were written
ioutfm=0	The coordinates were output in ASCII format.

The details of the steps were following:

section	component	detail	total
4.1	TBA	7,500,000 * 2 +10,000,000 *3	45,000,000
4.2	TEA	7,500,000 * 6	45,000,000
4.3	THA	7,500,000 * 6	45,000,000
4.4	Na^+	7,500,000 * 1+10,000,000 * 3+7,500,000 * 1	45,000,000
4.5	Absent of salts	7,500,000 * 6	45,000,000

Frcmod file for the system including boron atom

```
remark goes here
MASS
```

```
B 10.810        0.000              modified by authors

BOND
cp-cd  411.70   1.434      same as ca-cd
cp-cc  411.70   1.434      same as ca-cc
cp-os  372.40   1.373      same as ca-os
os-B   301.50   1.500      os-c3 modified by authors
B -f   290.00   1.390      c3-f  modified by authors

ANGLE
cp-cd-cd   67.660    111.040   same as ca-cd-cd
cp-cd-ha   46.400    124.040   same as ca-cd-ha
cp-na-cd   68.460    113.150   same as ca-na-cd
cp-na-hn   47.630    125.590   same as ca-na-hn
cp-cp-cc   64.630    124.300   same as cc-ca-cp
cp-cp-os   71.040    121.890   same as c2-c2-os
cd-cp-na   70.330    124.550   same as c2-c2-n3
cd-cp-cp   64.880    120.660   same as ca-ca-ce
na-cp-cp   72.910    108.790   same as cp-ca-na
cp-cc-cp   63.940    117.580   same as ca-ce-ca
cp-cc-ha   46.400    124.040   same as ca-cc-ha
cp-os-B    63.310    119.950   c3-os-ca by kato
cc-cp-os   71.040    121.890   same as c2-c2-os
os-B -os   71.720    113.730   os-c3-os
os-B -f    70.660    110.610   f -c3-os
f -B -f    71.260    107.160   f -c3-f

DIHE
cp-cp-cc-cp   1    6.650       180.000          2.000      same as X -c2-
c2-X
cp-cp-cc-ha   1    6.650       180.000          2.000      same as X -c2-
c2-X
cp-cp-os-B    1    0.900      180.000         2.000     same as X -ca-os-X

cd-cp-na-cd   1    0.300       180.000          2.000      same as X -ca-
na-X
```

```
cd-cp-na-hn   1    0.300      180.000          2.000     same as X -ca-na-X

cd-cd-cp-na   1    6.650       180.000           2.000      same as X -c2-
c2-X
cd-cd-cp-cp   1    6.650       180.000           2.000      same as X -c2-
c2-X
cd-na-cp-cp   1    0.300       180.000           2.000      same as X -ca-
na-X
na-cp-cd-ha   1    6.650       180.000           2.000      same as X -c2-
c2-X
hn-na-cp-cp   1    0.300       180.000           2.000      same as X -ca-
na-X
ha-cd-cp-cp   1    6.650       180.000           2.000      same as X -c2-
c2-X
cp-cc-cp-os   1    6.650       180.000           2.000      same as X -c2-
c2-X
cp-os-B -os   3    1.150        0.000          3.000     X-c3-os-X
cp-os-B -f    3    1.150        0.000          3.000     X-c3-os-X
cc-cp-os-B    1    0.900       180.000           2.000      same as X -ca-
os-X
os-cp-cc-ha   1    6.650       180.000           2.000      same as X -c2-
c2-X

IMPROPER
cd-cp-cp-na        1.1         180.0        2.0         Using default value
cd-cp-cd-ha        1.1         180.0        2.0         Using default value
cd-cd-cd-ha        1.1         180.0        2.0         Using default value
cd-ha-cd-na        1.1         180.0        2.0         Using default value
cd-cp-na-hn         1.1          180.0         2.0          General improper
torsional angle (2 general atom types)
cc-cp-cp-os        1.1         180.0        2.0         Using default value
cp-cp-cc-ha        1.1         180.0        2.0         Using default value

NONBON
  B          2.010  0.095            ATTN, need revision
```

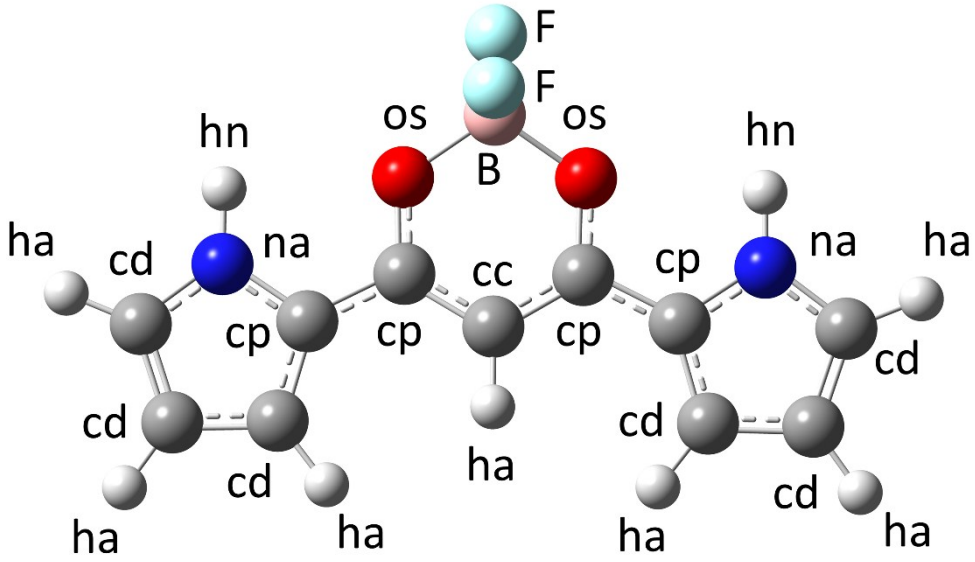

Fig. S6 The atomtype corresponding to the frcmod file above.

The comparison of optimized structure between DFT and MM

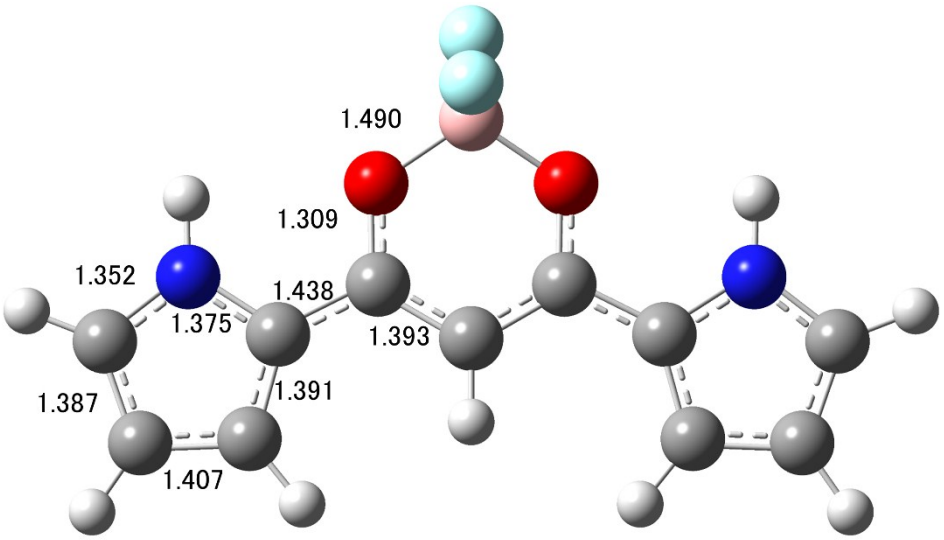

Fig. S7 The structure **A** of **1** optimized with DFT method.

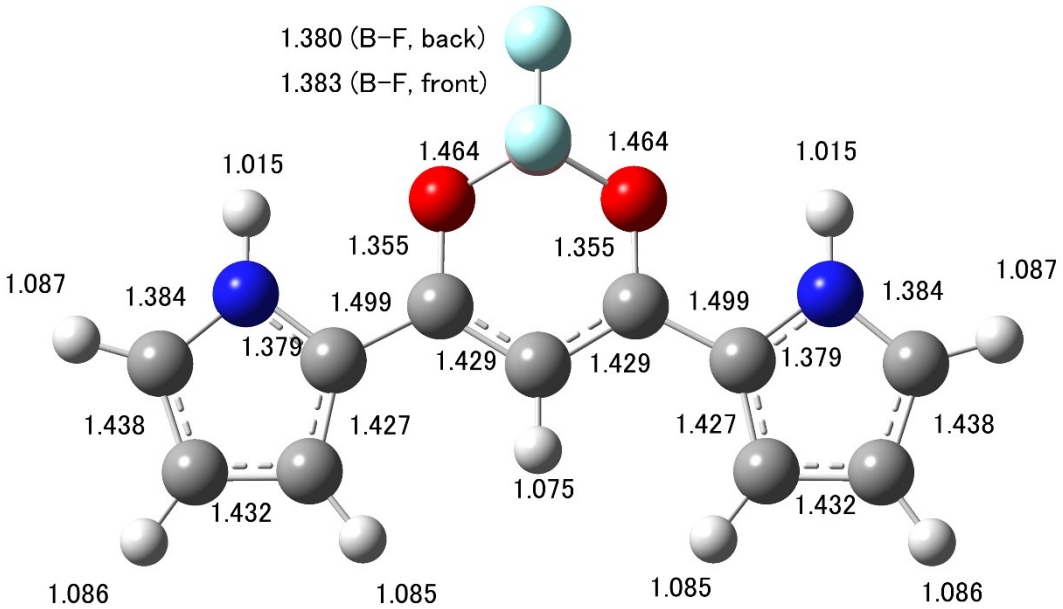

Fig. S8 The structure **A** of **1** optimized with MM method.

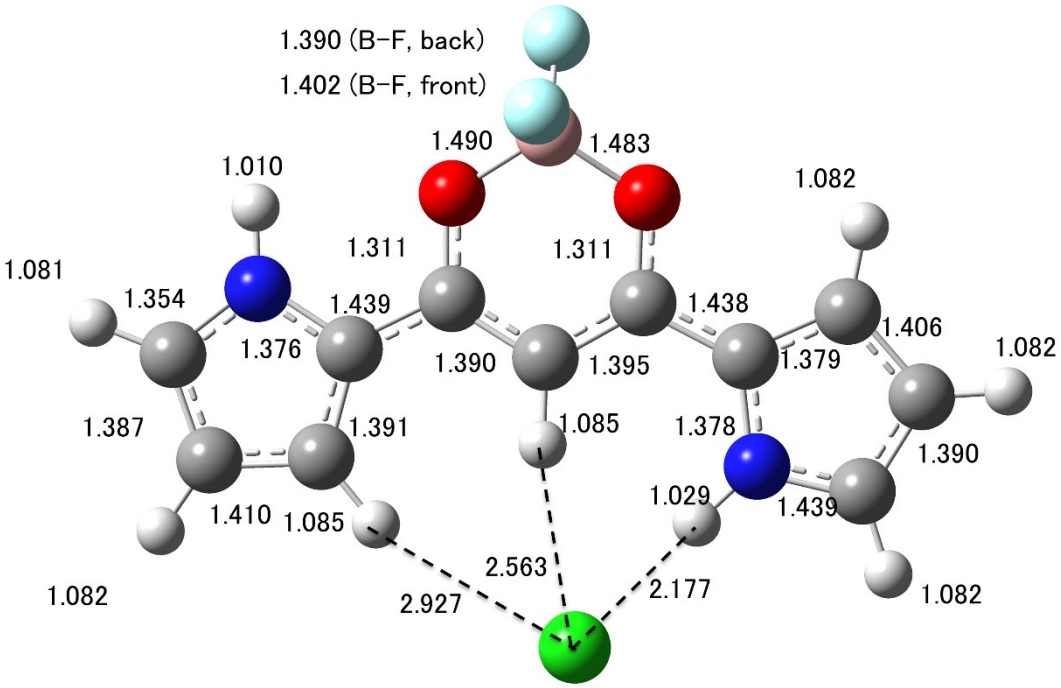

Fig. S9 The structure **B**-I of **1**-Cl^- optimized with DFT method.

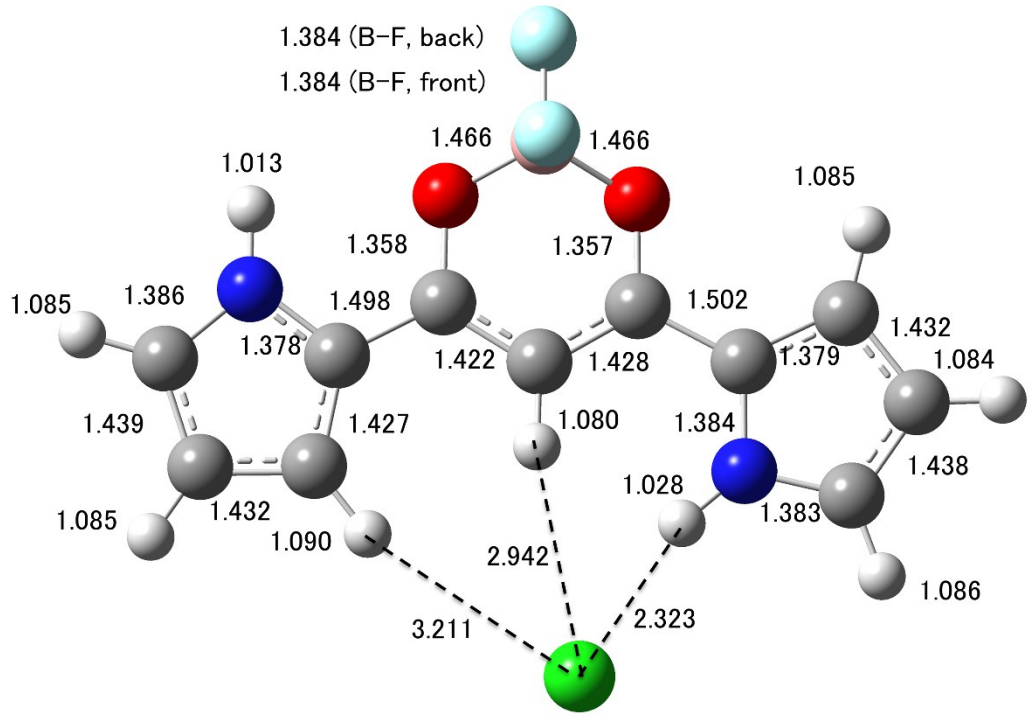

Fig. S10 The structure **B**-I of **1**-Cl^- optimized with MM method.

The Single-crystal X-ray structures[1]

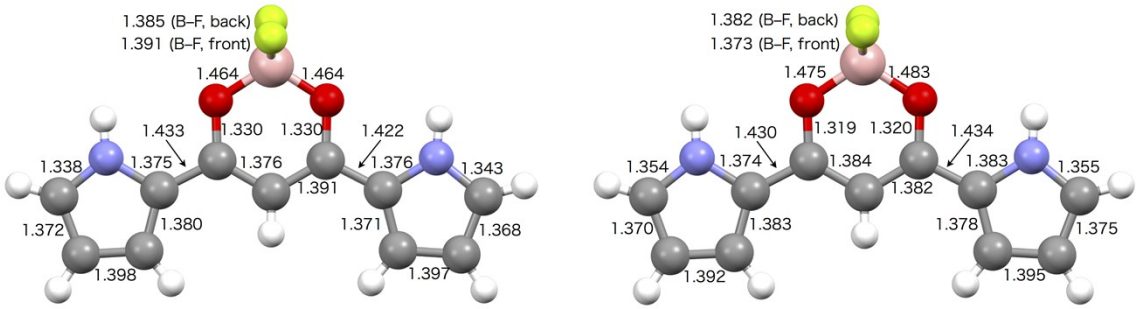

Fig. S11 The structure **A** of **1** (two independent structures).

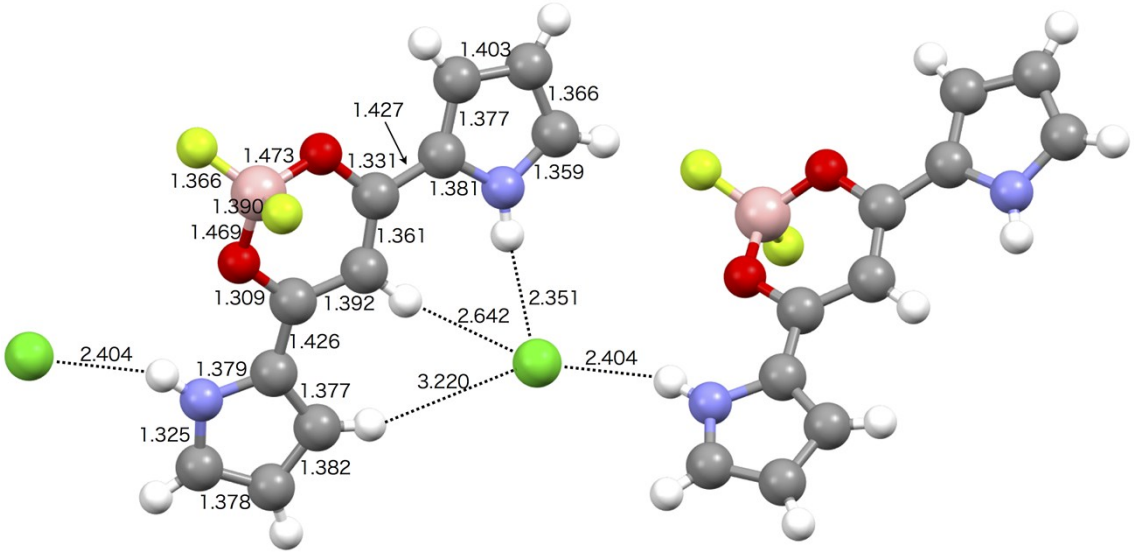

Fig. S12 The structure **B-I** of **1**-Cl^{-}.

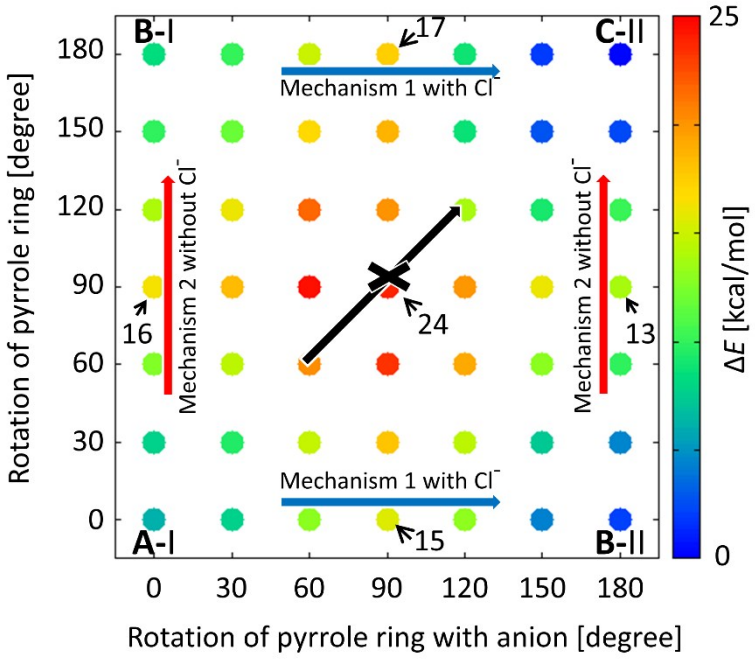

Fig. S13 Scatter plot version of PES of **1** corresponding to the actually computed structures without interpolations. The potential energies were calculated for each 30 degrees for each direction. The blue and red arrows show the mechanism 1 with Cl^- and mechanism 2 without Cl^-, respectively. The numbers in the graph are corresponding to the potential energies at (0°, 90°), (90°, 0°), (180°, 90°), (90°, 180°), and (90°, 90°). The diagonal black arrow shows the concerted pyrrole ring rotation from the Structure **A**-I to **C**-II.

References

1. H. Maeda and Y. Kusunose, *Chem. Eur. J.,* 2005, **11**, 5661-5666.