# Supporting Information

## A Novel Intramolecular Through-Space Interaction between F and CN: A Strategy for the Conformational Control of an Acyclic System

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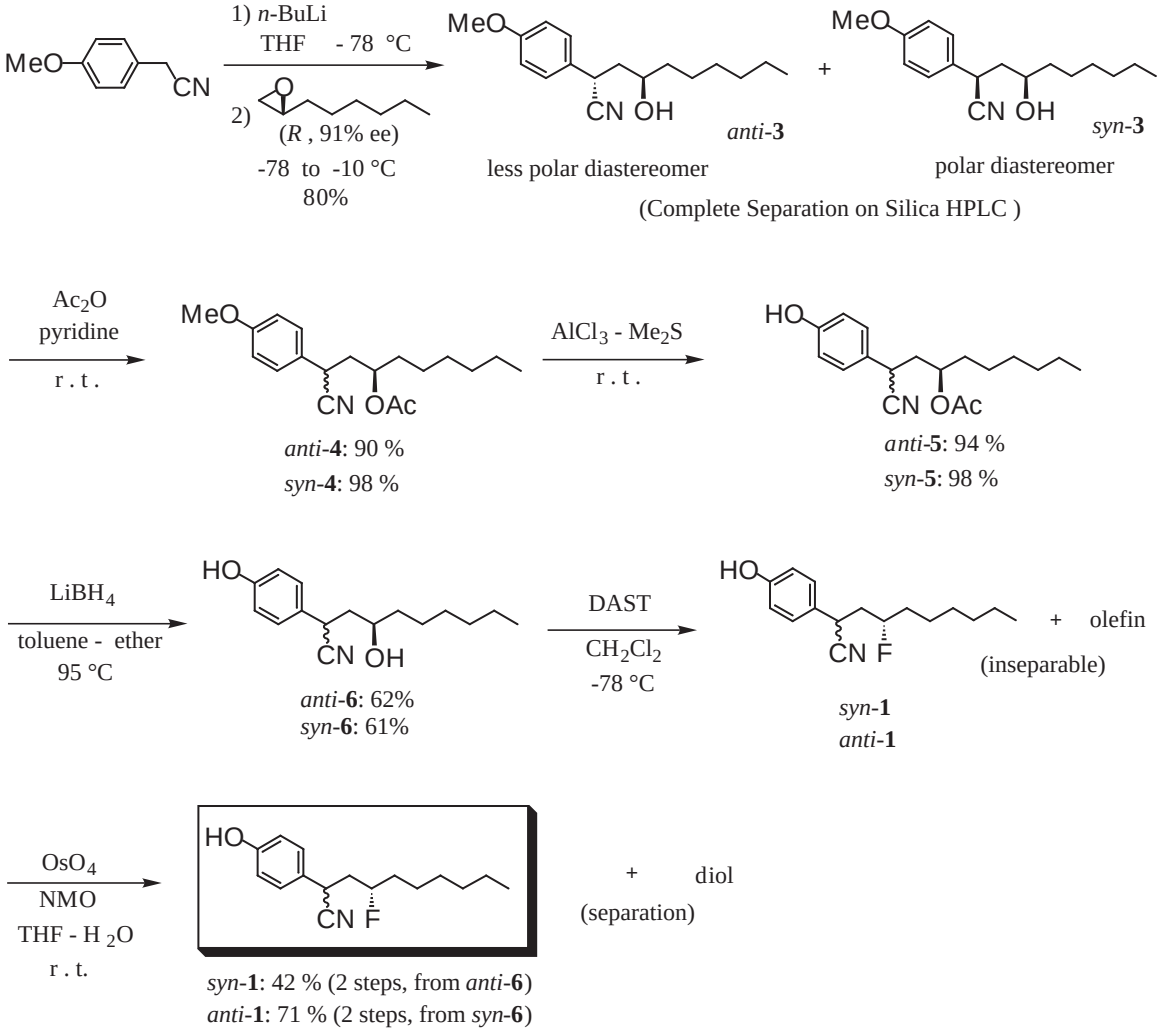
**General.** Melting points were taken on a micro hot-stage apparatus (Yanagimoto) and were uncorrected. Infrared (IR) spectra were recorded on a JASCO IR-810 diffraction grating infrared spectrophotometer and $^1$H-NMR spectra were obtained on a Varian XL-300 or a Varian INOVA 400NB NMR spectrometer with tetramethylsilane as an internal standard. Mass spectra (MS) were determined on a JEOL JMS-SX 102A QQ or a JEOL JMS-GC-mate mass spectrometer. Combustion analysis was done on a Perkin Elmer Series II CHNS/O Analyzer 2400. Specific rotations were recorded on a Horiba SEPA-200 automatic digital polarimeter. Wakogel C-200 (silica gel) (100-200 mesh, Wako) was used for open column chromatography. Flash column chromatography was performed with Silica Gel 60N (Kanto Chemical) or Silica Gel 60H (Nakalai Tesque). Kieselgel 60 F-254 plates (Merck) were used for thin layer chromatography (TLC). When necessary, compounds were further purified by a recycle HPLC (LC-908, Japan Analytical Industry Co., Ltd.) on GPC columns (JAIGEL 1H and 2H) after purification on silica gel.

**Materials.** Toluene, ether, and tetrahydrofuran (THF) were distilled from sodium benzophenone ketyl, and dichloromethane was distilled from $CaH_2$, after ten washings with water to remove methanol contaminants. Most of the reagents were obtained from Wako Pure Chemical Industries, Ltd., Nacalai Tesque, Inc., Kanto Chemical Co., Inc., or Aldrich Chemical Inc. (*R*)-Epoxyoctane was available from the Japan Energy Corporation.

Synthesis of *syn*- and *anti*-4-Fluoro-2-(4-hydroxyphenyl)decanenitrile (**1**)




**(2*S*, 4*R*)- and (2*R*, 4*R*)-4-Hydroxy-2-(4-methoxyphenyl)decanenitrile (*anti*- and *syn*-3)**

To a THF (5 ml) solution of 4-methoxyphenylacetonitrile (750 mg, 5.10 mmol) was added dropwise *n*-BuLi (2.52 M in hexane, 2.43 ml, 6.12 mmol) at –78° C under a nitrogen atmosphere. After stirring for 1 h, a THF (3 ml) solution of (*R*)-epoxyoctane (719 mg, 5.61 mmol) and additional THF (6 ml) were added dropwise to the reaction mixture, which was warmed up to –10 °C and stirred again for 2.5 h. The reaction mixture was poured into a separating funnel replaced with 1*N* hydrochloric acid (10 ml) and crushed ice, adjusted with 1*N* sodium bicarbonate to pH 6, and extracted with ethyl acetate. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 5 / 1) to give (4*R*)-4-hydroxy-2-(4-methoxyphenyl)decanenitriles (*anti* and *syn* = 1.6 : 1) (1.126 g, 80% yield). The diastereomeric mixture (850 mg) was further purified by a recycle HPLC with Kusano pre-packed column Si-10 (hexane / ethyl acetate = 4 / 1, flow rate 9.85 ml / min, pressure 10 kgf / $cm^2$) to give pure (2*S*, 4*R*)-4-hydroxy-2-(4-methoxyphenyl)decanenitrile (*anti*-**3**) (503 mg) and (2*R*, 4*R*)-4-hydroxy-2-(4-methoxyphenyl)decanenitrile (*syn*-**3**) (247 mg).

***anti*-3**: yellowish oil; $[\alpha]_D^{26}$ = -27.7 (2.50, MeOH); $^1$H-NMR (400 MHz, $CDCl_3$) δ: 7.27 (AA'XX', *J* = 8.7 Hz, 2H), 6.90 (AA'XX', *J* = 8.7 Hz, 2H), 4.14 (dd, *J* = 11.5 and 4.4 Hz, 1H), 3.95 (m, 1H), 3.80 (s, 3H), 2.07 (br, 1H), 1.98 (dd, A part of

AB, $J_{AB}$ = 13.9 Hz, $J$ = 11.5 and 2.4 Hz, 1H), 1.80 (dd, B part of AB, $J_{AB}$ = 13.9 Hz, $J$ = 10.6 and 4.4 Hz, 1H), 1.52-1.41 (m, 2H), 1.40-1.24 (m, 8H), 0.88 (t, $J$ = 6.8 Hz, 3H); $^{13}$C-NMR (100 MHz, $CDCl_3$) δ: 159.2, 128.2, 128.1, 121.1, 114.4, 69.2, 55.3, 43.5, 37.8, 33.5, 31.7, 29.1, 25.3, 22.5, 14.0; IR ($CHCl_3$): 3620, 3489, 2959, 2932, 2858, 2241, 1612, 1514, 1466, 1254, 1180, 1036, 831 cm$^{-1}$; MS EI (20 eV) *m/z*: 275 ($M^+$, 12), 257 (22), 231 (5), 159 (100), 147 (46), 134 (10), 121 (9), 108 (15); HRMS calcd for $C_{17}H_{25}NO_2$ ($M^+$): 275.1885, found: 275.1883; $^tR$ 60 min. [Kusano Pre-packed Column Silica Gel (Si-10, ϕ 22 x 300 mm); elute: hexane / ethyl acetate = 4 / 1 ; flow rate: 9.85 ml / min.; pressure: 10 kgf / cm$^2$; detector: UV 254 nm and RI].

***syn*-3**: yellowish oil; $[\alpha]_D^{16}$ = -21.8 (2.03, MeOH); $^1$H-NMR (400 MHz, $CDCl_3$) δ: 7.27 (AA'XX', $J$ = 8.7 Hz, 2H), 6.90 (AA'XX', $J$ = 8.7 Hz, 2H), 4.02 (dd, $J$ = 10.0 and 5.3 Hz, 1H), 3.81 (s, 3H), 3.39 (m, 1H), 2.08 (dd, A part of AB, $J_{AB}$ = 13.7 Hz, $J$ = 9.7 and 5.3 Hz, 1H), 1.96 (dd, B part of AB, $J_{AB}$ = 13.7 Hz, $J$ = 10.0 and 3.3 Hz, 1H), 1.46-1.24 (m, 10H), 0.86 (t, $J$ = 6.9 Hz, 3H), (OH was not observed); $^{13}$C-NMR (100 MHz, $CDCl_3$) δ: 159.3, 128.8, 127.2, 121.9, 114.4, 68.0, 55.3, 42.6, 37.6, 32.5, 31.6, 29.1, 25.3, 22.5, 14.0; IR ($CHCl_3$): 3622, 3495, 2957, 2932, 2858, 2241, 1612, 1514, 1466, 1252, 1180, 1036, 831 cm$^{-1}$; MS EI (20 eV) *m/z*: 275 ($M^+$, 18), 257 (20), 231 (9), 164 (24), 159 (100), 147 (65), 134 (17), 121 (17), 108 (25); HRMS calcd for $C_{17}H_{25}NO_2$ ($M^+$): 275.1885, found: 275.1880; $^tR$ 75 min. [Kusano Pre-packed Column Silica Gel (Si-10, ϕ 22 x 300 mm); elute: hexane / ethyl acetate = 4 / 1 ; flow rate: 9.85 ml / min.; pressure: 10 kgf / cm$^2$; detector: UV 254 nm and RI].

**(2*S*, 4*R*)-4-Acetoxy-2-(4-methoxyphenyl)decanenitrile (*anti*-4)**

A mixture of (2*S*, 4*R*)-4-hydroxy-2-(4-methoxyphenyl)decanenitrile (*anti*-**3**) (291 mg, 1.06 mmol) and acetic anhydride (1.62 g, 15.91 mmol) and pyridine (1.47 g, 18.54 mmol) was stirred for 17.5 h at room temperature. The reaction mixture was concentrated *in vacuo*, and the residue was purified by column chromatography (hexane / ethyl acetate = 8 / 1) to give (2*S*, 4*R*)-4-acetoxy-2-(4-methoxyphenyl)decanenitrile (*anti*-**4**) (301 mg, 90% yield). mp 38.7-39.1 °C (hexane); $[\alpha]_D^{22}$ = -7.58 (1.93, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.24 (AA'XX', $J$ = 8.7 Hz, 2H), 6.90 (AA'XX', $J$ = 8.7 Hz, 2H), 5.03 (m, 1H), 3.83 (dd, $J$ = 9.7 and 5.3 Hz, 1H), 3.81 (s, 3H), 2.19-2.00 (m, 5H), 1.72-1.47 (m, 2H), 1.37-1.16 (m, 8H), 0.87 (t, $J$ = 6.7 Hz, 3H); IR ($CHCl_3$): 2959, 2932, 2860, 2243, 1734, 1612, 1514, 1466, 1375, 1252, 1238, 1180, 1034, 831 cm$^{-1}$; MS FAB(+) *m/z*: 318 [$(M+H)^+$]; HRMS calcd for $C_{19}H_{28}NO_3$ [$(M+H)^+$]: 318.2070, found: 318.2078; Anal. Calcd for $C_{19}H_{27}NO_3$: C, 71.89; H, 8.57; N, 4.41. Found : C, 71.80; H, 8.57; N, 4.61.

**(2*R*, 4*R*)-4-Acetoxy-2-(4-methoxyphenyl)decanenitrile (*syn*-4)**

A mixture of (2*R*, 4*R*)-4-hydroxy-2-(4-methoxyphenyl)decanenitrile (*syn*-**3**) (202 mg, 0.73 mmol), acetic anhydride (1.08 g, 10.60 mmol), and pyridine (978 mg, 12.36 mmol) was stirred for 18 h at room temperature. The reaction mixture was concentrated *in vacuo*, and the residue was purified by column chromatography (hexane / ethyl acetate = 8 / 1) to give (2*R*, 4*R*)-4-acetoxy-2-(4-methoxyphenyl)decanenitrile (*syn*-**4**) (229 mg, 98% yield). yellowish oil: $[\alpha]_D^{21}$ = -0.06 (2.22, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.21 (AA'XX', $J$ = 8.8 Hz, 2H), 6.90 (AA'XX', $J$ = 8.8 Hz, 2H), 4.83 (m, 1H), 3.81 (s, 3H), 3.74 (t, $J$ = 7.4 Hz, 1H),

2.28 (dd, A part of AB, $J_{AB}$ = 14.4 Hz, *J* = 9.5 and 7.4 Hz, 1H), 2.09 (s, 3H), 2.00 (dd, B part of AB, $J_{AB}$ = 14.4 Hz, *J* = 7.4 and 3.0 Hz, 1H), 1.61-1.45 (m, 2H), 1.29-1.18 (m, 8H), 0.86 (t, *J* = 6.7 Hz, 3H); IR ($CHCl_3$): 2959, 2932, 2860, 2243, 1732, 1612, 1514, 1466, 1375, 1250, 1238, 1180, 1034, 831 $cm^{-1}$; MS FAB(+) *m/z*: 318 [$(M+H)^+$]; HRMS calcd for $C_{19}H_{28}NO_3$ [$(M+H)^+$]: 318.2070, found: 318.2078.

**(2*S*, 4*R*)-4-Acetoxy-2-(4-hydroxyphenyl)decanenitrile (*anti*-5)**

Aluminum chloride (648 mg, 4.86 mmol) was added to dimethyl sulfide (10 ml) at 0 °C under a nitrogen atmosphere,[15] followed by the addition of a dichloromethane (1 ml) solution of (2*S*, 4*R*)-4-acetoxy-2-(4-methoxyphenyl)decanenitrile (*anti*-**4**) (257 mg, 0.81 mmol). After stirring for 18 h at room temperature, the reaction mixture was poured into water, and extracted with chloroform. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 4 / 1) to give (2*S*, 4*R*)-4-acetoxy-2-(4-hydroxyphenyl)decanenitrile (*anti*-**5**) (231 mg, 94% yield). yellowish oil; $[\alpha]_D^{26}$ = -7.96 (1.98, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.19 (AA'XX', *J* = 8.5 Hz, 2H), 6.84 (AA'XX', *J* = 8.5 Hz, 2H), 5.27 (br, 1H), 5.02 (m, 1H), 3.83 (dd, *J* = 9.2 and 5.5 Hz, 1H), 2.19-2.00 (m, 5H), 1.70-1.48 (m, 2H), 1.36-1.15 (m, 8H), 0.87 (t, *J* = 6.7 Hz, 3H); IR ($CHCl_3$): 3595, 3312, 2959, 2932, 2860, 2243, 1734, 1616, 1516, 1458, 1439, 1375, 1240, 1175, 1032, 833 $cm^{-1}$; MS FAB(+) *m/z*: 304 [$(M+H)^+$]; HRMS calcd for $C_{18}H_{26}NO_3$ [$(M+H)^+$]: 304.1912, found: 304.1919.

**(2*R*, 4*R*)-4-Acetoxy-2-(4-hydroxyphenyl)decanenitrile (*syn*-5)**

Aluminum chloride (479 mg, 3.59 mmol) was added to dimethyl sulfide (10 ml) at 0 °C under a nitrogen atmosphere,[15] followed by the addition of a dichloromethane (1 ml) solution of (2*R*, 4*R*)-4-acetoxy-2-(4-methoxyphenyl)decanenitrile (*syn*-**4**) (190 mg, 0.60 mmol). After stirring for 28 h at room temperature, the reaction mixture was poured into water, and extracted with chloroform. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 4 / 1) to give (2*R*, 4*R*)-4-acetoxy-2-(4-hydroxyphenyl)decanenitrile (*syn*-**5**) (179 mg, 98% yield). colorless oil; $[\alpha]_D^{21}$ = +1.00 (2.39, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.15 (AA'XX', *J* = 8.7 Hz, 2H), 6.83 (AA'XX', *J* = 8.7 Hz, 2H), 5.37 (br, 1H), 4.83 (m, 1H), 3.72 (t, *J* = 7.4 Hz, 1H), 2.28 (dd, A part of AB, $J_{AB}$ = 14.4 Hz, *J* = 9.6 and 7.4 Hz, 1H), 2.10 (s, 3H), 2.01 (dd, B part of AB, $J_{AB}$ = 14.4 Hz, *J* = 7.4 and 3.0 Hz, 1H), 1.60-1.43 (m, 2H), 1.32-1.14 (m, 8H), 0.86 (t, *J* = 6.7 Hz, 3H); IR ($CHCl_3$): 3595, 3312, 2959, 2932, 2860, 2243, 1732, 1614, 1516, 1456, 1439, 1375, 1238, 1175, 1036, 833 $cm^{-1}$; MS FAB(+) *m/z*: 304 [$(M+H)^+$]; HRMS calcd for $C_{18}H_{26}NO_3$ [$(M+H)^+$]: 304.1913, found: 304.1920.

**(2*S*, 4*R*)-4-Hydroxy-2-(4-hydroxyphenyl)decanenitrile (*anti*-6)**

To an ether (10 ml) suspension of lithium borohydride (73 mg, 3.35 mmol) were added an ether (2 ml) solution of (2*S*, 4*R*)-4-acetoxy-2-(4-hydroxyphenyl)decanenitrile (*anti*-**5**) (185 mg, 0.61 mmol) and additional ether (5 ml) at 0 °C. Toluene (10 ml) was then added to the reaction mixture, which was refluxed at 95 °C for 3 h. After the reaction mixture was cooled to room temperature,

lithium borohydride (27 mg, 1.22 mmol) was added, and the mixture was refluxed at 95 °C for an additional 1.5 h. The reaction mixture was poured into ice-water (salting-out), neutralized with 1*N*-hydrochloric acid to pH 7, then extracted with ethyl acetate. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 3 / 1) to give (2*S*, 4*R*)-4-hydroxy-2-(4-hydroxyphenyl)decanenitrile (*anti*-**6**) (99 mg, 62% yield). colorless oil; $[\alpha]_D^{20}$ = -29.7 (1.63, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.22 (AA'XX', *J* = 8.6 Hz, 2H), 6.83 (AA'XX', *J* = 8.6 Hz, 2H), 4.97 (br, 1H), 4.12 (dd, *J* = 11.5 and 4.5 Hz, 1H), 3.95 (m, 1H), 1.98 (dd, A part of AB, $J_{AB}$ = 14.0 Hz, *J* = 11.5 and 2.5 Hz, 1H), 1.80 (dd, B part of AB, $J_{AB}$ = 14.0 Hz, *J* = 10.5 and 4.5 Hz, 1H), 1.50-1.21 (m, 10H), 0.88 (t, *J* = 6.7 Hz, 3H), (an alcoholic proton was not observed); IR ($CHCl_3$): 3597, 3319, 2959, 2930, 2858, 2241, 1614, 1516, 1456, 1439, 1263, 1175, 1040, 833 $cm^{-1}$; MS EI (20 eV) *m/z*: 261 ($M^+$, 4), 243 (18), 160 (9), 146 (14), 145 (100), 133 (30), 120 (6), 69 (7); HRMS calcd for $C_{16}H_{23}NO_2$ ($M^+$): 261.1729, found: 261.1744

**(2*R*, 4*R*)-4-Hydroxy-2-(4-hydroxyphenyl)decanenitrile (*syn*-6)**

To an ether (10 ml) suspension of lithium borohydride (58 mg, 2.68 mmol) were added an ether (1 ml) solution of (2*R*, 4*R*)-4-acetoxy-2-(4-hydroxyphenyl)decanenitrile (*syn*-**5**) (148 mg, 0.49 mmol) and additional ether (5 ml) at 0 °C. Toluene (10 ml) was then added to the reaction mixture, which was refluxed at 95 °C for 1 h. After the reaction mixture was cooled to the room temperature, lithium borohydride (22 mg, 0.98 mmol) was added, and the mixture was refluxed for at 95 °C additional 2 h. The reaction mixture was poured into ice-water (salting-out), neutralized with 1*N*-hydrochloric acid to pH 7, and extracted with ethyl acetate. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 3 / 1) to give (2*R*, 4*R*)-4-hydroxy-2-(4-hydroxyphenyl)decanenitrile (*syn*-**6**) (78 mg, 61% yield). colorless oil; $[\alpha]_D^{26}$ = -22.0 (2.11, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.23 (AA'XX', *J* = 8.6 Hz, 2H), 6.83 (AA'XX', *J* = 8.6 Hz, 2H), 4.88 (br, 1H), 4.01 (dd, *J* = 10.1 and 5.3 Hz, 1H), 3.38 (m, 1H), 2.08 (dd, A part of AB, $J_{AB}$ = 13.7 Hz, *J* = 9.6 and 5.3 Hz, 1H), 1.95 (dd, B part of AB, $J_{AB}$ = 13.7 Hz, *J* = 10.1 and 3.2 Hz, 1H), 1.48-1.17 (m, 10H), 0.86 (t, *J* = 6.8 Hz, 3H), (an alcoholic proton was not observed); IR ($CHCl_3$): 3595, 3329, 2957, 2930, 2858, 2241, 1614, 1516, 1456, 1441, 1263, 1175, 833 $cm^{-1}$; MS EI (20 eV) *m/z*: 261 ($M^+$, 3), 243 (17), 160 (8), 146 (13), 145 (100), 133 (12), 120 (3), 69 (4); HRMS calcd for $C_{16}H_{23}NO_2$ ($M^+$): 261.1729, found: 261.1723.

**(2*S*, 4*S*)-4-Fluoro-2-(4-hydroxyphenyl)decanenitrile (*syn*-1)**

To a dichloromethane (4 ml) solution of (2*S*, 4*R*)-4-hydroxy-2-(4-hydroxyphenyl)decanenitrile (*anti*-**6**) (53 mg, 0.20 mmol) was added dropwise a dichloromethane (0.5 ml) solution of (diethylamino)sulfur trifluoride (DAST)[16] (82 mg, 0.51 mmol) at –78 °C under a nitrogen atmosphere, and the reaction mixture was stirred for 2 h. Water was added to the reaction mixture, and the solution was neutralized with 1*N*-sodium bicarbonate, then extracted with chloroform. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 4 / 1) to give a mixture of the product and olefin. To a THF (3 ml) solution of the obtained mixture and 4-methylmorpholine *N*-oxide

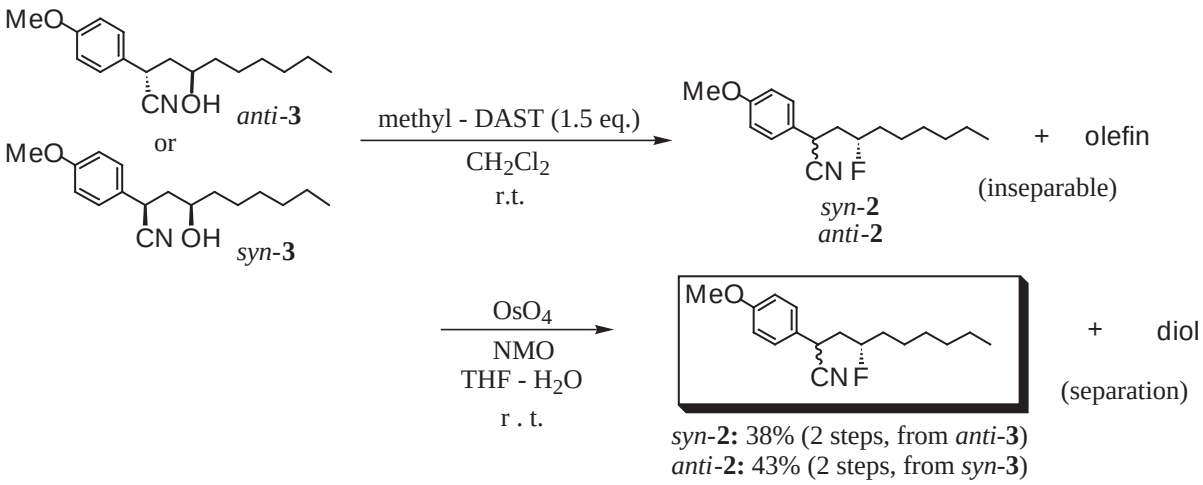
(NMO) (10 mg, 0.085 mmol) was added a water (2 ml) solution of osmium(VIII) oxide (1 mg) at room temperature, and the reaction mixture was stirred for 22 h. The reaction mixture was quenched with 20% sodium bisulfite solution, then extracted with ethyl acetate. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 5 / 1) to give (2*S*, 4*S*)-4-fluoro-2-(4-hydroxyphenyl)decanenitrile (*syn*-**1**) (22 mg, 2 steps 42%). Colorless needles; mp 69.5-70.0 °C (hexane / ethyl acetate = 15 / 1); $[\alpha]_D^{21}$ = +14.5 (1.47, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.22 (AA'XX', *J* = 8.6 Hz, 2H), 6.85 (AA'XX', *J* = 8.6 Hz, 2H), 4.88 (br, 1H), 4.22 (m of d, *J* = 49.5, 1H), 3.92 (dd, *J* = 10.5 and 4.8 Hz, 1H), 2.34 (ddd, A part of AB, $J_{AB}$ = 14.8 Hz, *J* = 11.1, 10.0 and 4.8 Hz, 1H), 1.98 (ddd, B part of AB, $J_{AB}$ = 14.8 Hz, *J* = 35.6, 10.5 and 2.5 Hz, 1H), 1.75-1.16 (m, 10H), 0.86 (t, *J* = 6.7 Hz, 3H); $^{13}$C-NMR (100 MHz, $CDCl_3$) δ: 155.8, 129.1, 126.2, 121.3, 116.1, 90.2 (d, *J* = 169.8 Hz), 40.7 (d, *J* = 20.8 Hz), 34.8 (d, *J* = 20.8 Hz), 32.3 (d, *J* = 4.4 Hz), 31.5, 28.9, 24.8 (d, *J* = 4.4 Hz), 22.4, 14.0; $^{19}$F NMR (282 MHz, $CDCl_3$, external standard: $CF_3CO_2H$) δ: 109.0 (m); IR ($CHCl_3$): 3595, 3300, 2959, 2932, 2860, 2243, 1614, 1516, 1456, 1437, 1265, 1174, 833 cm$^{-1}$; MS EI (20 eV) *m/z*: 263 ($M^+$, 50), 145 (44), 133 (62), 132 (100), 69 (18); HRMS calcd for $C_{16}H_{22}NOF$ ($M^+$): 263.1685, found: 263.1674; Anal. Calcd for $C_{16}H_{22}NOF$: C, 72.97; H, 8.42; N, 5.32. Found : C, 72.93; H, 8.34; N, 5.35.

**(2*R*, 4*S*)-4-Fluoro-2-(4-hydroxyphenyl)decanenitrile (*anti*-1)**

To a dichloromethane (4 ml) solution of (2*R*, 4*R*)-4-hydroxy-2-(4-hydroxyphenyl)decanenitrile (*syn*-**6**) (42 mg, 0.16 mmol) was added dropwise a dichloromethane (0.4 ml) solution of (diethylamino)sulfur trifluoride (DAST)[16] (65 mg, 0.40 mmol) at –78 °C under a nitrogen atmosphere, and the reaction mixture was stirred for 2 h. Water was added to the reaction mixture, and the solution was neutralized with 1*N*-sodium bicarbonate, then extracted with chloroform. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 4 / 1) to give a mixture of the product and olefin. To a THF (3 ml) solution of the obtained mixture and 4-methylmorpholine *N*-oxide (NMO) (10 mg, 0.085 mmol) was added a water (2 ml) solution of osmium(VIII) oxide (1 mg) at room temperature, and then the reaction mixture was stirred for 22 h. The reaction mixture was quenched with 20% sodium bisulfite solution, then extracted with ethyl acetate. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 5 / 1) to give (2*R*, 4*S*)-4-fluoro-2-(4-hydroxyphenyl)decanenitrile (*anti*-**1**) (30 mg, 2 steps 71%). Colorless needles; mp 82.0-82.5 °C (hexane / ethyl acetate = 12 / 1 ); $[\alpha]_D^{14}$ = +29.7 (0.798, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.21 (AA'XX', *J* = 8.6 Hz, 2H), 6.85 (AA'XX', *J* = 8.6 Hz, 2H), 5.46 (br, 1H), 4.79 (m of d, *J* = 49.4, 1H), 4.03 (dd, *J* = 10.9 and 5.5 Hz, 1H), 2.12-1.97 (m, 2H), 1.80-1.21 (m, 10H), 0.89 (t, *J* = 6.8 Hz, 3H); $^{13}$C-NMR (100 MHz, $CDCl_3$) δ: 155.7, 128.4, 127.2, 120.5, 116.1, 91.4 (d, *J* = 169.4 Hz), 41.8 (d, *J* = 20.6 Hz), 35.0 (d, *J* = 20.6 Hz), 33.1 (d, *J* = 4.0 Hz), 31.6, 29.0, 24.7 (d, *J* = 4.0 Hz), 22.5, 14.0; $^{19}$F NMR (282 MHz, $CDCl_3$, external standard: $CF_3CO_2H$) δ: 107.7 (m); IR ($CHCl_3$): 3595, 3312, 2957, 2934, 2860, 2243, 1614, 1516, 1456, 1437, 1265, 1174, 833 cm$^{-1}$; MS EI (20 eV) *m/z*: 263 ($M^+$,

66), 145 (65), 133 (85), 132 (100), 69 (19); HRMS calcd for $C_{16}H_{22}NOF$ ($M^+$): 263.1685, found: 263.1673; Anal. Calcd for $C_{16}H_{22}NOF$: C, 72.97; H, 8.42; N, 5.32. Found: C, 72.74; H, 8.63; N, 5.58.

Synthesis of *syn*- and *anti*-4-Fluoro-2-(4-methoxyphenyl)decanenitrile (**2**)




**(2*S*, 4*S*)-4-Fluoro-2-(4-methoxyphenyl)decanenitrile (*syn*-2)**

To a dichloromethane (7.5 ml) solution of (2*S*, 4*R*)-4-hydroxy-2-(4-methoxyphenyl)decanenitrile (*anti*-**3**) (384 mg, 1.39 mmol) was added dropwise a dichloromethane (2.09 ml) solution of (dimethylamino)sulfur trifluoride (methyl-DAST) (278 mg, 2.09 mmol) at room temperature under a nitrogen atmosphere, and the reaction mixture was stirred for 22.5 h. The reaction mixture was poured into ice-water, and neutralized with 1*N*-sodium bicarbonate (pH 8), then extracted with chloroform. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 20 / 1) to give a mixture of the product and olefin. To a THF (5 ml) solution of the obtained mixture and 4-methylmorpholine *N*-oxide (NMO) (80 mg, 0.68 mmol) was added a water (4 ml) solution of osmium(VIII) oxide (4 mg) at room temperature, and the reaction mixture was stirred for 30 h. The reaction mixture was quenched with 20% sodium bisulfite solution, then extracted with ethyl acetate. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 20 / 1) to give (2*S*, 4*S*)-4-fluoro-2-(4-methoxyphenyl)decanenitrile (*syn*-**2**) (146 mg, 2 steps 38%). Colorless oil; $[\alpha]_D^{19}$ = +12.8 (0.897, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.26 (AA'XX', *J* = 8.7 Hz, 2H), 6.92 (AA'XX', *J* = 8.7 Hz, 2H), 4.21 (m of d, *J* = 49.5, 1H), 3.93 (dd, *J* = 10.6 and 4.8 Hz, 1H), 3.82 (s, 3H), 2.35 (ddd, A part of AB, $J_{AB}$ = 14.4 Hz, *J* = 11.1, 10.0 and 4.8 Hz, 1H), 1.99 (ddd, B part of AB, $J_{AB}$ = 14.4 Hz, *J* = 35.7, 10.6 and 2.6 Hz, 1H), 1.73-1.23 (m, 10H), 0.86 (t, *J* = 6.8 Hz, 3H); $^1$H-NMR (400 MHz, toluene-$d_8$) δ: 6.97 (AA'XX', *J* = 8.7 Hz, 2H), 6.63 (AA'XX', *J* = 8.7 Hz, 2H), 3.98 (m of d, *J* = 49.6, 1H), 3.53 (dd, *J* = 10.6 and 4.9 Hz, 1H), 3.26 (s, 3H), 1.95 (ddd, A part of AB, $J_{AB}$ = 14.2 Hz, *J* = 11.1, 10.0 and 4.9 Hz, 1H), 1.54 (ddd, B part of AB, $J_{AB}$ = 14.2 Hz, *J* = 34.9, 10.6 and 2.7 Hz, 1H), 1.38-0.93 (m, 10H), 0.87 (t, *J* = 7.2 Hz, 3H); $^{13}$C-NMR (100 MHz, $CDCl_3$) δ: 159.5, 128.9, 126.4, 121.2, 114.6, 90.1 (d, *J* = 169.4 Hz), 55.3, 40.8 (d, *J* = 20.7 Hz), 34.8 (d, *J* = 20.7 Hz), 32.3 (d, *J* = 4.4 Hz), 31.6, 28.9, 24.8 (d, *J*

= 4.4 Hz), 22.5, 14.0; $^{13}$C-NMR (100 MHz, toluene-$d_8$) δ: 160.0, 129.2, 127.3, 121.1, 114.7, 90.1 (d, *J* = 170.5 Hz), 54.7, 41.1 (d, *J* = 20.6 Hz), 35.1 (d, *J* = 20.6 Hz), 32.5 (d, *J* = 4.4 Hz), 32.1, 29.5, 25.2 (d, *J* = 4.4 Hz), 23.0, 14.3; $^{19}$F NMR (282 MHz, $CDCl_3$, external standard: $CF_3CO_2H$) δ: 109.0 (m); $^{19}$F NMR (376 MHz, $C_6D_6$, external standard: $CF_3CO_2H$) δ: 102.8 (m); IR ($CHCl_3$): 2959, 2934, 2860, 2243, 1612, 1514, 1466, 1306, 1252, 1180, 1036, 831, 806 cm$^{-1}$; MS EI (20 eV) *m/z*: 277 ($M^+$, 20), 159 (16), 147 (19), 146 (100); HRMS calcd for $C_{17}H_{24}NOF$ ($M^+$): 277.1842, found: 277.1837.

**(2*R*, 4*S*)-4-Fluoro-2-(4-methoxyphenyl)decanenitrile (*anti*-2)**

To a dichloromethane (8.5 ml) solution of (2*R*, 4*R*)-4-hydroxy-2-(4-methoxyphenyl)decanenitrile (*syn*-**3**) (292 mg, 1.06 mmol) was added dropwise a dichloromethane (1.59 ml) solution of (dimethylamino)sulfur trifluoride (methyl-DAST) (212 mg, 1.59 mmol) at room temperature under a nitrogen atmosphere, and the reaction mixture was stirred for 19.5 h. The reaction mixture was poured into ice-water, and neutralized with 1*N*-sodium bicarbonate (pH 8), then extracted with chloroform. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 20 / 1) to give a mixture of the product and olefin. To a THF (5 ml) solution of the obtained mixture and 4-methylmorpholine *N*-oxide (NMO) (80 mg, 0.68 mmol) was added a water (4 ml) solution of osmium(VIII) oxide (4 mg) at room temperature, and the reaction mixture was stirred for 30 h. The reaction mixture was quenched with 20% sodium bisulfite solution, then extracted with ethyl acetate. The extract was washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (hexane / ethyl acetate = 20 / 1) to give (2*R*, 4*S*)-4-fluoro-2-(4-methoxyphenyl)decanenitrile (*anti*-**2**) (127 mg, 2 steps 43%). Colorless needles; mp 50.8-51.4 °C (hexane / ethyl acetate = 100 / 1); $[\alpha]_D^{18}$ = +23.8 (1.03, MeOH); $^1$H-NMR (300 MHz, $CDCl_3$) δ: 7.27 (AA'XX', *J* = 8.7 Hz, 2H), 6.91 (AA'XX', *J* = 8.7 Hz, 2H), 4.80 (m of d, *J* = 49.9 Hz, 1H), 4.04 (dd, *J* = 10.7 and 5.1 Hz, 1H), 3.81 (s, 3H), 2.15-1.97 (m, 1H), 1.75-1.26 (m, 11H), 0.89 (t, *J* = 6.8 Hz, 3H); $^1$H-NMR (400 MHz, toluene-$d_8$) δ: 6.91 (AA'XX', *J* = 8.7 Hz, 2H), 6.62 (AA'XX', *J* = 8.7 Hz, 2H), 4.67 (m of d, *J* = 51.8, 1H), 3.71 (dd, *J* = 11.5 and 4.5 Hz, 1H), 3.28 (s, 3H), 1.68-1.51 (m, 2H), 1.43-1.09 (m, 10H), 0.90 (t, *J* = 7.1 Hz, 3H); $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 159.4, 128.2, 127.5, 120.4, 114.5, 91.3 (d, *J* = 148.1 Hz), 55.3, 42.0 (d, *J* = 20.8 Hz), 35.0 (d, *J* = 20.8 Hz), 33.1 (d, *J* = 3.9 Hz), 31.6, 29.0, 24.8 (d, *J* = 3.9 Hz), 22.5, 14.0; $^{13}$C-NMR (100 MHz, toluene-$d_8$) δ: 159.8, 128.5, 128.2, 120.3, 114.7, 90.5 (d, *J* = 170.1 Hz), 54.7, 42.4 (d, *J* = 20.8 Hz), 35.4 (d, *J* = 20.8 Hz), 33.4 (d, *J* = 4.0 Hz), 32.1, 29.6, 25.3 (d, *J* = 4.0 Hz), 23.0, 14.3; $^{19}$F NMR (282 MHz, $CDCl_3$, external standard: $CF_3CO_2H$) δ: 107.7 (m); $^{19}$F NMR (376 MHz, $C_6D_6$, external standard: $CF_3CO_2H$) δ: 92.6 (m); IR ($CHCl_3$): 2959, 2934, 2860, 2243, 1612, 1514, 1466, 1304, 1254, 1180, 1034, 831, 806 cm$^{-1}$; MS EI (20 eV) *m/z*: 277 ($M^+$, 25), 159 (18), 147 (19), 146 (100); HRMS calcd for $C_{17}H_{24}NOF$ ($M^+$): 277.1842, found: 277.1833; Anal. Calcd for $C_{17}H_{24}NOF$: C, 73.61; H, 8.72; N, 5.05. Found : C, 73.76; H, 8.91; N, 5.35.

**General Procedure for Protonation of *syn*- and *anti*-(4*S*)-4-Fluoro-2-(4-methoxyphenyl)decanenitriles (2) (Table 4)**

To a THF (0.5 ml) solution of (4*S*)-4-fluoro-2-(4-methoxyphenyl)decanenitriles (**2**) (31 mg, 0.112 mmol, *syn* : *anti* = 1.2 : 1) was added dropwise *n*-butyllithium (2.52 M in hexane, 53 μl, 0.134 mmol) at –78 °C under a nitrogen atmosphere, followed by the quick addition of hexamethylphosphramide (HMPA) (97 ml, 0.559 mmol). After stirring for 1 h, a THF (0.3 ml) solution of a proton source (12 equiv.) was added dropwise to the reaction mixture, which was stirred for additional 2 h at the same temperature. The reaction mixture was poured into water, neutralizated with 0.1*N* HCl, and extracted with five portions of ether. The ethereal extract was washed with water, and brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The ratio of *syn* and *anti* was determined by the intergral of the proton at the 2-position on $^1$H-NMR (400 MHz) of the crude residue. The residue was purified by column chromatography (hexane / ethyl acetate = 20 / 1) to give (4*S*)-4-fluoro-2-(4-methoxyphenyl)decanenitriles (**2**) in yield indicated in Table 4.

**References for Supporting Information**


15. (a) Node, M.; Nishide, K.; Sai, M.; Fujita, E. *Tetrahedron Lett.* **1978**, 5211-5214. (b) Node, M.; Nishide, K.; Sai, M.; Fuji, K.; Fujita, E. *J. Org. Chem.* **1981**, *46*, 1991-1993.
16. (a) Middleton, W. *J. Org. Chem.* **1975**, *5*, 574-578. Recent Advances in Selective Formation of the C-F Bond: (b) Wilkinson, J. A. *Chem. Rev.* **1992**, *92*, 505-519. (c) Umemoto, T. *J. Syn. Org. Chem. Jpn* **1992**, *50*, 338-346.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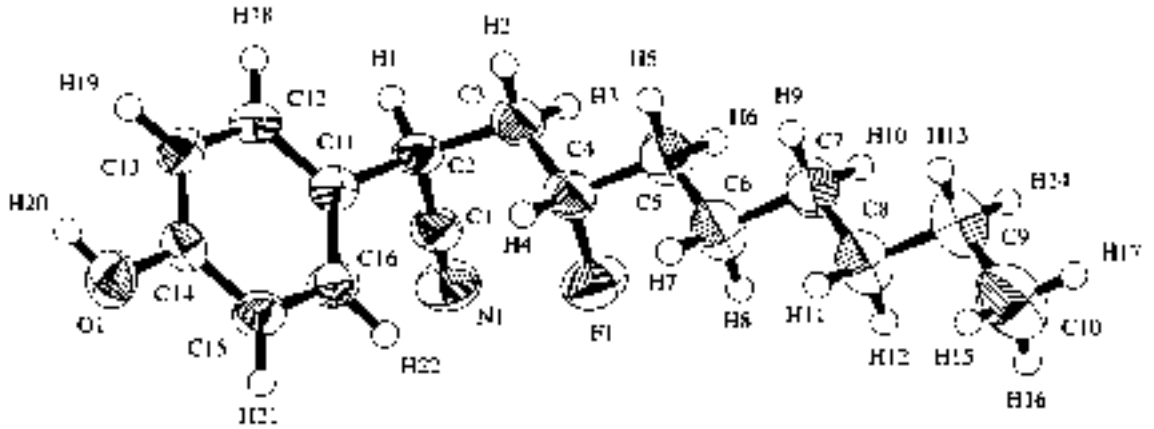
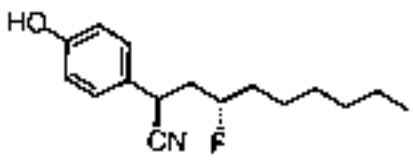
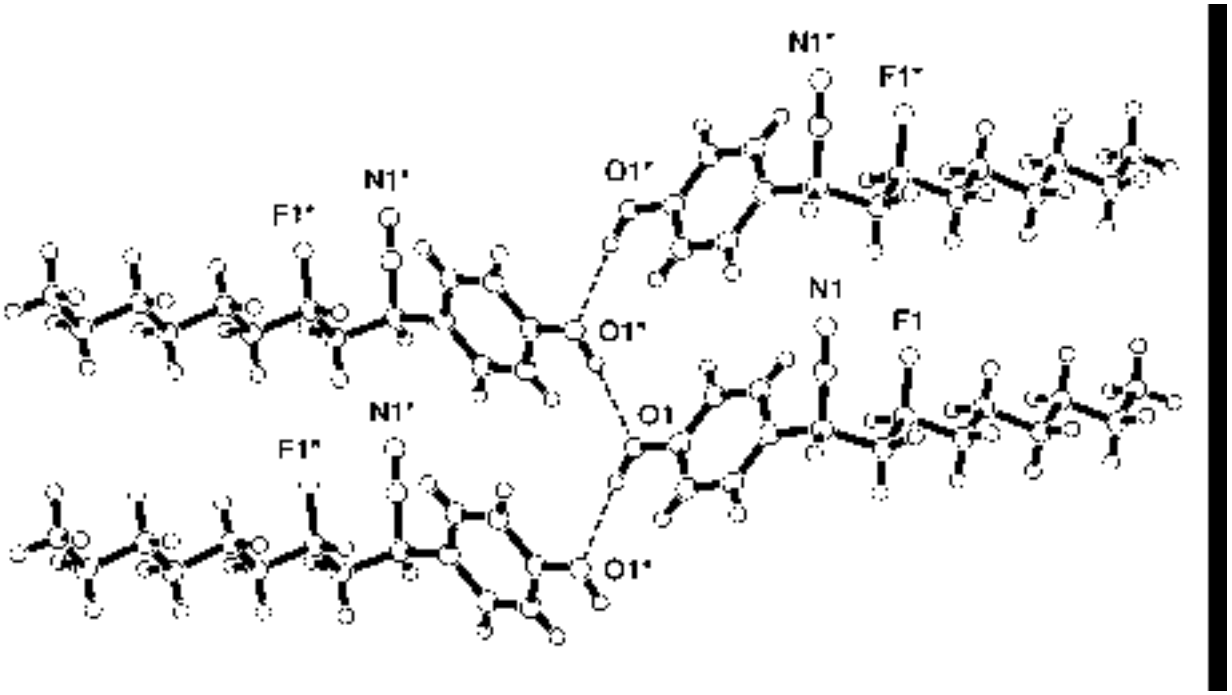



*anti*-**I**

Intermolecular hydrogen bonding of *anti*-**1**

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Molecular Structure Corporation, Rigaku Corporation. (2000). teXsan.
Single Crystal Structure Analysis Software. Version 1.11.
MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Rigaku, 3-9-12 Akishima, Tokyo, Japan.
Zachariasen, W. H. (1967). Acta Cryst. 23, 558-564.
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 H(17)  H  0.4354      0.4358      0.2316      0.1074      Uiso 1.00 calc . . .
 H(18)  H  1.0269      0.0394      0.9255      0.0511      Uiso 1.00 calc . . .
 H(19)  H  0.7787      0.0033      0.9797      0.0526      Uiso 1.00 calc . . .
 H(20)  H  0.5148      0.1705      0.9915      0.1138      Uiso 1.00 calc . . .
 H(21)  H  0.6017      0.6423      0.8806      0.0537      Uiso 1.00 calc . . .
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 O(1)   0.044(1)    0.070(2)    0.059(2)    0.006(2)    0.024(1)    0.011(2)
 N(1)   0.048(2)    0.048(2)    0.077(2)    0.000(2)    0.011(2)    0.004(2)
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 C(2)   0.041(2)    0.038(2)    0.052(2)    0.011(2)    0.013(1)    0.005(2)
 C(3)   0.051(2)    0.045(2)    0.056(2)    0.000(2)    0.019(1)    -0.002(2)
 C(4)   0.049(2)    0.046(2)    0.055(2)    -0.002(2)   0.017(2)    -0.004(2)
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 C(7)   0.072(2)    0.071(3)    0.053(2)    -0.002(2)   0.019(2)    -0.002(2)
 C(8)   0.062(2)    0.078(4)    0.060(2)    0.001(2)    0.016(2)    -0.007(2)
 C(9)   0.070(3)    0.089(4)    0.061(2)    -0.007(3)   0.020(2)    -0.013(2)
 C(10)  0.072(3)    0.121(5)    0.070(3)    0.011(3)    -0.004(2)   -0.026(3)
 C(11)  0.038(2)    0.040(2)    0.041(2)    0.000(1)    0.004(1)    -0.002(2)
 C(12)  0.043(2)    0.037(2)    0.048(2)    0.008(2)    0.008(1)    0.002(2)
 C(13)  0.048(2)    0.041(2)    0.045(2)    -0.001(2)   0.012(2)    0.007(2)
 C(14)  0.040(2)    0.048(2)    0.035(2)    0.000(2)    0.009(1)    -0.006(2)
 C(15)  0.039(2)    0.045(2)    0.051(2)    0.009(2)    0.008(2)    0.003(2)
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 O(1)      C(14)     1.389(4)   . . yes
 N(1)      C(1)      1.140(5)   . . yes
 C(1)      C(2)      1.473(6)   . . yes
 C(2)      C(3)      1.534(6)   . . yes
 C(2)      C(11)     1.530(5)   . . yes
 C(3)      C(4)      1.497(6)   . . yes
 C(4)      C(5)      1.500(6)   . . yes
 C(5)      C(6)      1.502(7)   . . yes
 C(6)      C(7)      1.520(7)   . . yes
 C(7)      C(8)      1.513(7)   . . yes
 C(8)      C(9)      1.511(7)   . . yes
 C(9)      C(10)     1.494(9)   . . yes
 C(11)     C(12)     1.386(5)   . . yes
 C(11)     C(16)     1.378(5)   . . yes
 C(12)     C(13)     1.387(5)   . . yes
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   C(1)      C(2)      C(11)     111.1(3)   . . . yes
   C(1)      F(1)      C(4)      89.1(3)    . . . yes
   C(3)      C(2)      C(11)     114.2(3)   . . . yes
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   F(1)      C(1)      N(1)      103.9(3)   . . . yes
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   F(1)      C(4)      C(3)      108.9(4)   . . . yes
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   C(7)      C(8)      C(9)      114.9(4)   . . . yes
   C(8)      C(9)      C(10)     113.4(5)   . . . yes
   C(2)      C(11)     C(12)     119.6(3)   . . . yes
   C(2)      C(11)     C(16)     122.0(3)   . . . yes
   C(12)     C(11)     C(16)     118.4(3)   . . . yes
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   O(1)      C(14)     C(13)     121.9(4)   . . . yes
   O(1)      C(14)     C(15)     117.5(4)   . . . yes
   C(13)     C(14)     C(15)     120.6(3)   . . . yes
   C(14)     C(15)     C(16)     119.7(4)   . . . yes
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 F(1)      C(4)      C(5)      C(6)      -59.3(5)   . . . . yes
 O(1)      C(14)     C(13)     C(12)     179.7(4)   . . . . yes
 O(1)      C(14)     C(15)     C(16)     179.7(4)   . . . . yes
 N(1)      C(1)      C(2)      C(3)      -124(7)    . . . . yes
 N(1)      C(1)      C(2)      C(11)     106(7)     . . . . yes
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 C(1)      C(2)      C(11)     C(12)     -134.1(4)  . . . . yes
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 C(2)      C(11)     C(12)     C(13)     -177.4(3)  . . . . yes
 C(2)      C(11)     C(16)     C(15)     176.7(4)   . . . . yes
 C(3)      C(2)      C(11)     C(12)     97.9(4)    . . . . yes
 C(3)      C(2)      C(11)     C(16)     -80.4(5)   . . . . yes
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 C(4)      C(3)      C(2)      C(11)     55.8(5)    . . . . yes
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 C(5)      C(6)      C(7)      C(8)      -178.5(5)  . . . . yes
 C(6)      C(7)      C(8)      C(9)      178.6(5)   . . . . yes
 C(7)      C(8)      C(9)      C(10)     -177.8(5)  . . . . yes
 C(11)     C(12)     C(13)     C(14)     0.0(6)     . . . . yes
 C(11)     C(16)     C(15)     C(14)     1.3(6)     . . . . yes
 C(12)     C(11)     C(16)     C(15)     -1.6(5)    . . . . yes
 C(12)     C(13)     C(14)     C(15)     -0.4(6)    . . . . yes
 C(13)     C(12)     C(11)     C(16)     0.9(5)     . . . . yes
 C(13)     C(14)     C(15)     C(16)     -0.3(6)    . . . . yes
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 F(1)      C(3)      3.594(7)   . 1_565 ?
 O(1)      O(1)      3.031(2)   . 2_657 ?
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 N(1)      C(15)     3.579(5)   . 1_655 ?
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 C(12)     C(16)     3.591(6)   . 1_545 ?
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 C(13)     C(15)     3.593(6)    . 1_545 ?
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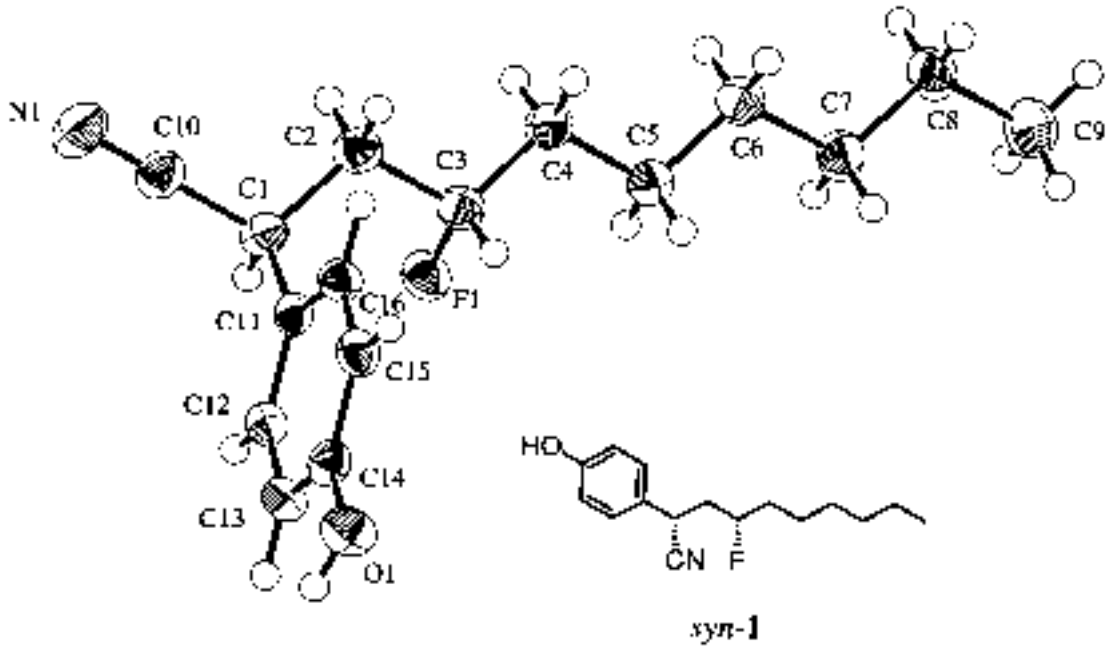
Intermolecular Distances


        atom   atom   distance    ADC(*)

        O(1)   H(20)  2.14(6)     65702

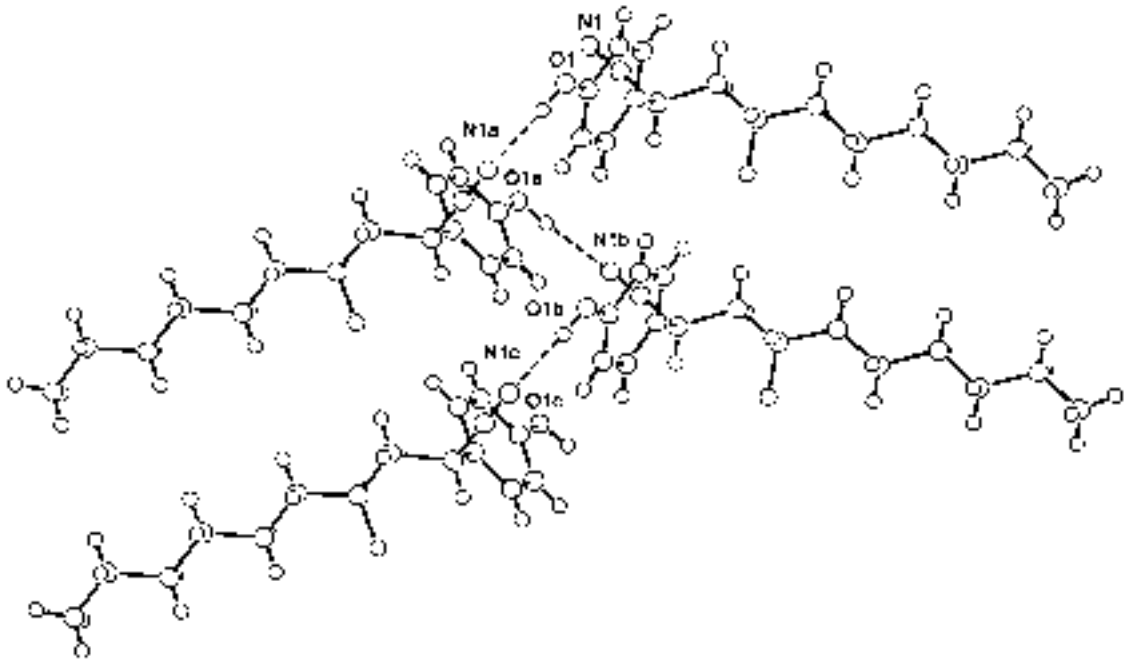

        Contacts out to 3.60 angstroms.  Estimated standard deviations
        in the least significant figure are given in parentheses.
#-----------------------------------------------------------------------------
```

Crystal structure of *syn*-**1**




*syn*-**1**

Intermolecular Hydrogen bonding of syn-**1**



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_publ_contact_author_email              ' node@mb.kyoto-phu.ac.jp '
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    A Novel Intramolecular Through-Space Interaction between F and CN:
A Strategy for the Conformational Control of an Acyclic System
;

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_publ_author_name
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' Kiyoharu Nishide '
;
  Associate Professor
;
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  Kyoto Pharmaceutical University, Misasagi, Yamashina, Kyoto 607-8414, JAPAN
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    X-Ray crystallographic analyses of fluorocyanides anti-1 and 2 revealed a novel
intramolecular through-space interaction between F and CN in an acyclic system, which
was applied to a stereoselective protonation of an acyclic fluorocyanides 2 having
flexible conformation.
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    We are grateful for a Grant-in-Aid (No. 11672126 to KN) from the Ministry of
Education, Science, Sports and Culture of Japan, in partial financial support of this
research.  We are also grateful to Prof. Tamejiro Hiyama, Kyoto University, for helpful
discussions at Sagami Chemical Research Center.   We also thank the Japan Energy
Corporation, Toda, Saitama, Japan, for its kind gift of (R)-epoxyoctane.
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    ENTER OTHER REFERENCES
Molecular Structure Corporation, Rigaku Corporation. (2000). teXsan.
Single Crystal Structure Analysis Software. Version 1.11.
MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Rigaku, 3-9-12 Akishima, Tokyo, Japan.
Zachariasen, W. H. (1967). Acta Cryst. 23, 558-564.
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for calculating R-factor (gt).
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 O(1)   O  0.4202(3)   -0.05599(5) 0.2395(4)   0.0397(6)   Uani 1.00 d . . .
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 C(6)   C  -0.0863(4)  0.18894(8)  0.5790(6)   0.0368(8)   Uani 1.00 d . . .
 C(7)   C  -0.2347(4)  0.19057(8)  0.7621(6)   0.0360(8)   Uani 1.00 d . . .
 C(8)   C  -0.3704(4)  0.22149(8)  0.7173(6)   0.0410(8)   Uani 1.00 d . . .
 C(9)   C  -0.5165(5)  0.22351(9)  0.9017(7)   0.051(1)    Uani 1.00 d . . .
 C(10)  C  0.7813(4)   0.10062(7)  0.2120(6)   0.0358(8)   Uani 1.00 d . . .
 C(11)  C  0.5578(3)   0.05558(7)  0.3351(5)   0.0277(7)   Uani 1.00 d . . .
 C(12)  C  0.5999(4)   0.02948(7)  0.5099(5)   0.0284(7)   Uani 1.00 d . . .
 C(13)  C  0.5548(4)   -0.00786(7) 0.4841(5)   0.0314(8)   Uani 1.00 d . . .
 C(14)  C  0.4676(4)   -0.01963(7) 0.2806(5)   0.0296(7)   Uani 1.00 d . . .
 C(15)  C  0.4232(4)   0.00620(8)  0.1039(6)   0.0316(8)   Uani 1.00 d . . .
 C(16)  C  0.4682(4)   0.04348(7)  0.1336(5)   0.0305(8)   Uani 1.00 d . . .
 H(1)   H  0.6588      0.0989      0.5245      0.0380      Uiso 1.00 calc . . .
 H(1O)  H  0.4732      -0.0691     0.3261      0.0429      Uiso 1.00 calc . . .
 H(2a)  H  0.5400      0.1499      0.3182      0.0406      Uiso 1.00 calc . . .
 H(2b)  H  0.4415      0.1226      0.1487      0.0406      Uiso 1.00 calc . . .
 H(3)   H  0.2654      0.1023      0.4574      0.0373      Uiso 1.00 calc . . .
 H(4a)  H  0.2639      0.1802      0.4592      0.0410      Uiso 1.00 calc . . .
 H(4b)  H  0.1513      0.1560      0.2859      0.0410      Uiso 1.00 calc . . .
 H(5a)  H  -0.0143     0.1344      0.6087      0.0404      Uiso 1.00 calc . . .
 H(5b)  H  0.0948      0.1603      0.7765      0.0404      Uiso 1.00 calc . . .
 H(6a)  H  -0.0239     0.2120      0.5827      0.0442      Uiso 1.00 calc . . .
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 H(6b)  H  -0.1382     0.1856      0.4257      0.0442      Uiso 1.00 calc . . .
 H(7a)  H  -0.2955     0.1673      0.7607      0.0432      Uiso 1.00 calc . . .
 H(7b)  H  -0.1829     0.1945      0.9149      0.0432      Uiso 1.00 calc . . .
 H(8a)  H  -0.3093     0.2447      0.7161      0.0492      Uiso 1.00 calc . . .
 H(8b)  H  -0.4235     0.2173      0.5655      0.0492      Uiso 1.00 calc . . .
 H(9a)  H  -0.4673     0.2306      1.0514      0.0615      Uiso 1.00 calc . . .
 H(9b)  H  -0.6025     0.2415      0.8537      0.0615      Uiso 1.00 calc . . .
 H(9c)  H  -0.5718     0.1997      0.9162      0.0615      Uiso 1.00 calc . . .
 H(12)  H  0.6609      0.0374      0.6498      0.0340      Uiso 1.00 calc . . .
 H(13)  H  0.5838      -0.0253     0.6061      0.0377      Uiso 1.00 calc . . .
 H(15)  H  0.3625      -0.0017     -0.0362     0.0379      Uiso 1.00 calc . . .
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 C(2)   0.039(2)    0.027(1)    0.035(2)    0.002(1)    0.004(1)    0.001(1)
 C(3)   0.035(2)    0.032(1)    0.026(2)    0.001(1)    -0.001(1)   0.000(1)
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 C(7)   0.033(1)    0.034(1)    0.042(2)    0.001(1)    0.001(1)    -0.001(1)
 C(8)   0.039(2)    0.034(1)    0.050(2)    0.006(1)    0.001(2)    -0.001(1)
 C(9)   0.047(2)    0.048(2)    0.058(2)    0.013(2)    0.010(2)    -0.003(2)
 C(10)  0.037(2)    0.027(1)    0.043(2)    -0.003(1)   0.005(2)    -0.001(1)
 C(11)  0.023(1)    0.028(1)    0.032(2)    0.003(1)    0.004(1)    0.000(1)
 C(12)  0.027(1)    0.030(1)    0.028(2)    0.002(1)    -0.001(1)   -0.001(1)
 C(13)  0.031(1)    0.029(1)    0.034(2)    0.005(1)    -0.003(1)   0.001(1)
 C(14)  0.027(1)    0.029(1)    0.032(2)    -0.001(1)   0.005(1)    -0.004(1)
 C(15)  0.028(2)    0.039(1)    0.028(2)    0.002(1)    -0.002(1)   -0.002(1)
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   C(1)      C(2)      C(3)      112.3(2)   . . . yes
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   N(1)      C(10)     C(1)      176.4(3)   . . . yes
   C(1)      C(11)     C(12)     119.2(2)   . . . yes
   C(1)      C(11)     C(16)     122.3(2)   . . . yes
   C(12)     C(11)     C(16)     118.3(2)   . . . yes
   C(11)     C(12)     C(13)     121.3(3)   . . . yes
   C(12)     C(13)     C(14)     119.8(2)   . . . yes
   O(1)      C(14)     C(13)     123.5(2)   . . . yes
   O(1)      C(14)     C(15)     116.7(3)   . . . yes
   C(13)     C(14)     C(15)     119.8(2)   . . . yes
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 F(1)      C(3)      C(4)      C(5)      -58.1(3)   . . . . yes
 O(1)      C(14)     C(13)     C(12)     179.1(3)   . . . . yes
 O(1)      C(14)     C(15)     C(16)     -179.7(3)  . . . . yes
 N(1)      C(10)     C(1)      C(2)      -121(5)    . . . . yes
 N(1)      C(10)     C(1)      C(11)     5(5)       . . . . yes
 C(1)      C(2)      C(3)      C(4)      173.7(2)   . . . . yes
 C(1)      C(11)     C(12)     C(13)     -175.3(2)  . . . . yes
 C(1)      C(11)     C(16)     C(15)     174.7(3)   . . . . yes
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 C(2)      C(1)      C(11)     C(12)     -135.7(3)  . . . . yes
 C(2)      C(1)      C(11)     C(16)     48.8(4)    . . . . yes
 C(2)      C(3)      C(4)      C(5)      -177.3(2)  . . . . yes
 C(3)      C(2)      C(1)      C(10)     -173.2(2)  . . . . yes
 C(3)      C(2)      C(1)      C(11)     63.8(3)    . . . . yes
 C(3)      C(4)      C(5)      C(6)      -177.4(2)  . . . . yes
 C(4)      C(5)      C(6)      C(7)      -177.2(2)  . . . . yes
 C(5)      C(6)      C(7)      C(8)      -178.8(2)  . . . . yes
 C(6)      C(7)      C(8)      C(9)      -179.1(2)  . . . . yes
 C(10)     C(1)      C(11)     C(12)     100.3(3)   . . . . yes
 C(10)     C(1)      C(11)     C(16)     -75.2(3)   . . . . yes
 C(11)     C(12)     C(13)     C(14)     0.5(4)     . . . . yes
 C(11)     C(16)     C(15)     C(14)     0.5(4)     . . . . yes
 C(12)     C(11)     C(16)     C(15)     -0.9(4)    . . . . yes
 C(12)     C(13)     C(14)     C(15)     -0.9(4)    . . . . yes
 C(13)     C(12)     C(11)     C(16)     0.3(4)     . . . . yes
 C(13)     C(14)     C(15)     C(16)     0.4(4)     . . . . yes
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 O(1)      N(1)      2.888(3)   . 2_655 ?
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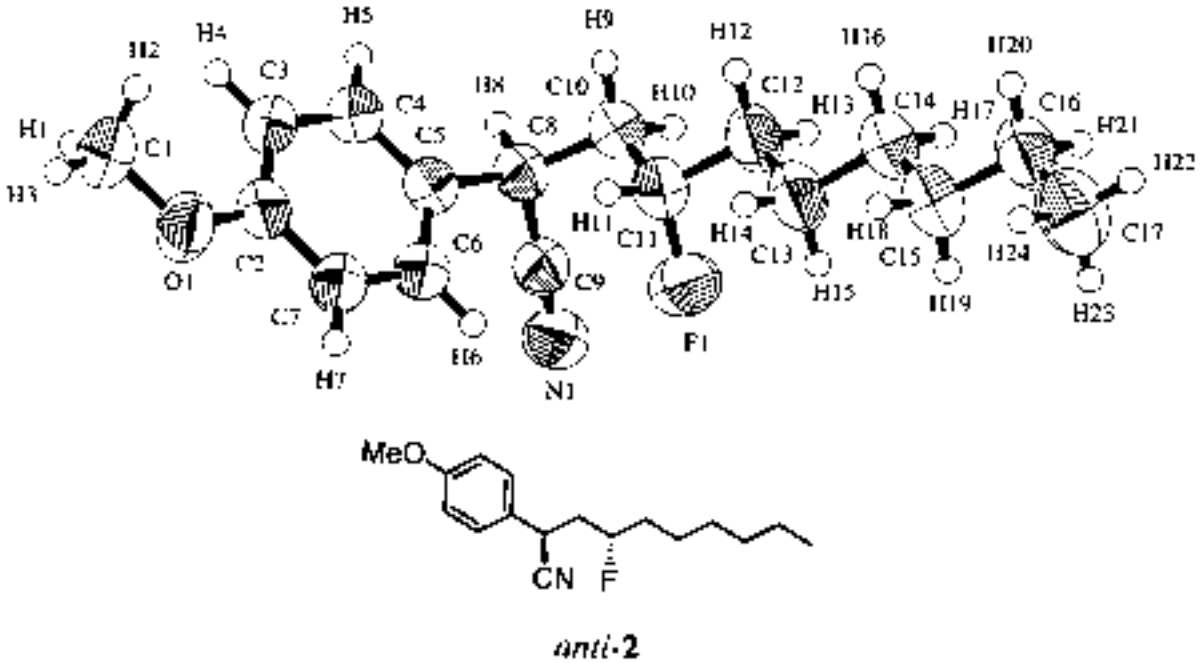
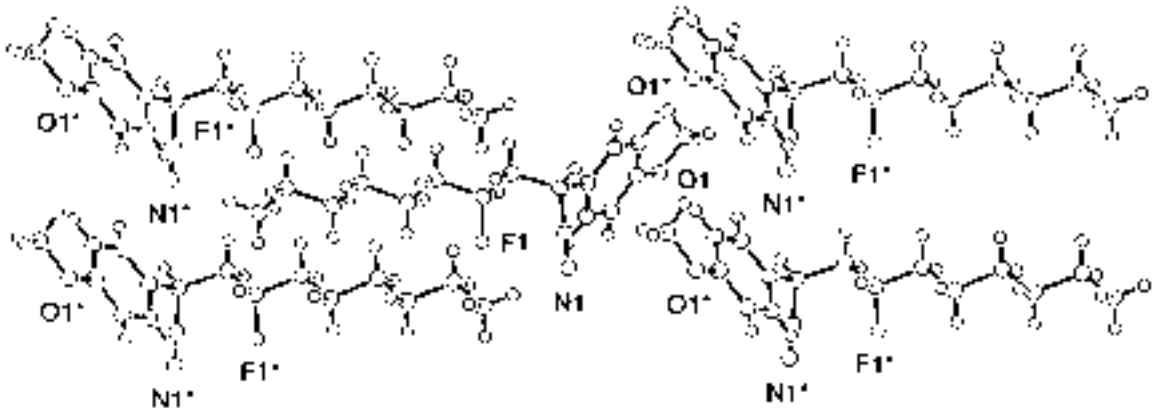
Crystal structure of *anti*-**2**




*anti*-**2**

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A Strategy for the Conformational Control of an Acyclic System
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' Kiyoharu Nishide '
;
  Associate Professor
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;
  Kyoto Pharmaceutical University, Misasagi, Yamashina, Kyoto 607-8414, JAPAN
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    X-Ray crystallographic analyses of fluorocyanides anti-1 and 2 revealed a novel
intramolecular through-space interaction between F and CN in an acyclic system, which
was applied to a stereoselective protonation of an acyclic fluorocyanides 2 having
flexible conformation.
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    We are grateful for a Grant-in-Aid (No. 11672126 to KN) from the Ministry of
Education, Science, Sports and Culture of Japan, in partial financial support of this
research.  We are also grateful to Prof. Tamejiro Hiyama, Kyoto University, for helpful
discussions at Sagami Chemical Research Center.   We also thank the Japan Energy
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Molecular Structure Corporation, Rigaku Corporation. (2000). teXsan.
Single Crystal Structure Analysis Software. Version 1.11.
MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
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Rigaku, 3-9-12 Akishima, Tokyo, Japan.
North, A.C.T., Phillips, D. C. & Mathews, F. S. (1968).
Acta Cryst. A24, 351-359.
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_refine_ls_weighting_scheme            calc
_refine_ls_weighting_details
   'w = 1/[¥s^2^(Fo^2^) + (0.08000(Max(Fo^2^,0) + 2Fc^2^)/3)^2^]'
_refine_ls_shift/su_max                0.0001
_refine_diff_density_max               0.18
_refine_diff_density_min               0.00
_refine_ls_extinction_method           none
_refine_ls_extinction_coef             ?
_refine_ls_abs_structure_details       ?
_refine_ls_abs_structure_Flack         -3.2(9)
loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
  'C' 'C'  0.018 0.009
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'H' 'H'  0.000 0.000
;International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.2)
;
  'F' 'F'  0.073 0.053
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'N' 'N'  0.031 0.018
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
```

```
;
  'O' 'O'  0.049 0.032
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
#---------------------------------------------------------------------------
# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
 F(1)   F  0.3657(4)   -0.5174     -0.1767(2)  0.0956(10)  Uani 1.00 d . . .
 O(1)   O  -0.2743(4)  -0.1691(9)  -0.4381(2)  0.0800(10)  Uani 1.00 d . . .
 N(1)   N  0.5426(5)   -0.660(1)   -0.3251(2)  0.079(1)    Uani 1.00 d . . .
 C(1)   C  -0.3280(6)  0.030(1)    -0.4811(2)  0.087(2)    Uani 1.00 d . . .
 C(2)   C  -0.1026(6)  -0.177(1)   -0.4089(2)  0.063(1)    Uani 1.00 d . . .
 C(3)   C  0.0172(6)   -0.001(1)   -0.4188(2)  0.068(1)    Uani 1.00 d . . .
 C(4)   C  0.1873(6)   -0.025(1)   -0.3859(2)  0.066(1)    Uani 1.00 d . . .
 C(5)   C  0.2337(5)   -0.216(1)   -0.3430(2)  0.060(1)    Uani 1.00 d . . .
 C(6)   C  0.1126(6)   -0.392(1)   -0.3356(2)  0.066(1)    Uani 1.00 d . . .
 C(7)   C  -0.0586(6)  -0.372(1)   -0.3671(2)  0.068(1)    Uani 1.00 d . . .
 C(8)   C  0.4217(6)   -0.238(1)   -0.3079(2)  0.066(1)    Uani 1.00 d . . .
 C(9)   C  0.4906(6)   -0.477(1)   -0.3170(2)  0.068(1)    Uani 1.00 d . . .
 C(10)  C  0.4393(6)   -0.156(1)   -0.2288(2)  0.071(1)    Uani 1.00 d . . .
 C(11)  C  0.3291(7)   -0.278(1)   -0.1780(2)  0.071(1)    Uani 1.00 d . . .
 C(12)  C  0.3572(7)   -0.181(1)   -0.1019(2)  0.080(1)    Uani 1.00 d . . .
 C(13)  C  0.2421(7)   -0.302(1)   -0.0500(2)  0.085(2)    Uani 1.00 d . . .
 C(14)  C  0.2657(7)   -0.198(1)   0.0257(2)   0.083(1)    Uani 1.00 d . . .
 C(15)  C  0.1540(7)   -0.317(1)   0.0784(2)   0.085(2)    Uani 1.00 d . . .
 C(16)  C  0.1780(7)   -0.222(1)   0.1540(2)   0.088(2)    Uani 1.00 d . . .
 C(17)  C  0.0735(8)   -0.349(2)   0.2057(3)   0.105(2)    Uani 1.00 d . . .
 H(1)   H  -0.2601     0.0344      -0.5224     0.1102      Uiso 1.00 calc . . .
 H(2)   H  -0.3109     0.1688      -0.4546     0.1102      Uiso 1.00 calc . . .
 H(3)   H  -0.4476     0.0119      -0.4986     0.1102      Uiso 1.00 calc . . .
 H(4)   H  -0.0167     0.1338      -0.4477     0.0826      Uiso 1.00 calc . . .
 H(5)   H  0.2757      0.0875      -0.3948     0.0820      Uiso 1.00 calc . . .
 H(6)   H  0.1442      -0.5355     -0.3074     0.0784      Uiso 1.00 calc . . .
 H(7)   H  -0.1436     -0.4986     -0.3589     0.0823      Uiso 1.00 calc . . .
 H(8)   H  0.4921      -0.1379     -0.3352     0.0792      Uiso 1.00 calc . . .
 H(9)   H  0.4212      0.0033      -0.2259     0.0877      Uiso 1.00 calc . . .
 H(10)  H  0.5606      -0.1930     -0.2095     0.0877      Uiso 1.00 calc . . .
 H(11)  H  0.2091      -0.2601     -0.1969     0.0838      Uiso 1.00 calc . . .
 H(12)  H  0.3323      -0.0194     -0.1021     0.0998      Uiso 1.00 calc . . .
 H(13)  H  0.4763      -0.2087     -0.0846     0.0998      Uiso 1.00 calc . . .
 H(14)  H  0.1229      -0.2912     -0.0690     0.1028      Uiso 1.00 calc . . .
 H(15)  H  0.2702      -0.4735     -0.0486     0.1028      Uiso 1.00 calc . . .
 H(16)  H  0.2406      -0.0357     0.0239      0.1004      Uiso 1.00 calc . . .
 H(17)  H  0.3866      -0.2197     0.0445      0.1004      Uiso 1.00 calc . . .
 H(18)  H  0.0314      -0.2997     0.0594      0.1084      Uiso 1.00 calc . . .
 H(19)  H  0.1743      -0.4904     0.0773      0.1084      Uiso 1.00 calc . . .
 H(20)  H  0.1531      -0.0593     0.1549      0.1080      Uiso 1.00 calc . . .
 H(21)  H  0.3015      -0.2428     0.1717      0.1080      Uiso 1.00 calc . . .
 H(22)  H  0.0885      -0.2930     0.2528      0.1227      Uiso 1.00 calc . . .
 H(23)  H  0.0983      -0.5201     0.2061      0.1227      Uiso 1.00 calc . . .
 H(24)  H  -0.0506     -0.3377     0.1888      0.1227      Uiso 1.00 calc . . .

loop_
_atom_site_aniso_label
```

```
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
 F(1)   0.125(2)    0.073(2)    0.089(2)    -0.004(2)   0.010(2)    0.004(2)
 O(1)   0.071(2)    0.089(2)    0.077(2)    -0.001(2)   -0.011(1)   0.017(2)
 N(1)   0.077(3)    0.070(2)    0.089(2)    -0.007(2)   -0.001(2)   -0.002(2)
 C(1)   0.094(4)    0.089(4)    0.073(3)    0.010(3)    -0.014(3)   0.013(2)
 C(2)   0.069(2)    0.067(2)    0.051(2)    -0.003(2)   -0.004(2)   -0.003(2)
 C(3)   0.080(2)    0.063(3)    0.058(2)    -0.005(2)   -0.008(2)   0.007(2)
 C(4)   0.077(2)    0.060(2)    0.060(2)    -0.002(2)   -0.002(2)   -0.001(2)
 C(5)   0.064(2)    0.059(2)    0.056(2)    -0.002(2)   -0.003(2)   -0.005(2)
 C(6)   0.069(2)    0.060(3)    0.067(2)    -0.006(2)   -0.004(2)   0.002(2)
 C(7)   0.071(2)    0.067(3)    0.064(2)    -0.004(3)   -0.004(2)   0.007(2)
 C(8)   0.065(2)    0.066(2)    0.065(2)    -0.009(2)   -0.008(2)   0.003(2)
 C(9)   0.071(3)    0.066(2)    0.065(3)    -0.011(2)   -0.007(2)   0.006(2)
 C(10)  0.080(3)    0.066(3)    0.064(2)    -0.004(2)   -0.006(2)   -0.003(2)
 C(11)  0.075(3)    0.074(2)    0.061(2)    0.001(2)    -0.007(2)   0.000(2)
 C(12)  0.087(3)    0.089(4)    0.060(2)    0.009(3)    -0.010(2)   -0.009(2)
 C(13)  0.095(3)    0.095(4)    0.061(2)    -0.007(3)   -0.007(2)   -0.010(2)
 C(14)  0.095(3)    0.090(4)    0.062(2)    -0.005(3)   -0.008(2)   -0.009(2)
 C(15)  0.082(3)    0.102(4)    0.069(2)    -0.005(3)   -0.003(2)   -0.013(2)
 C(16)  0.097(4)    0.098(4)    0.068(2)    0.003(3)    -0.006(2)   -0.009(2)
 C(17)  0.098(4)    0.142(6)    0.078(3)    -0.010(4)   0.020(3)    -0.014(3)
#------------------------------------------------------------------------------
_computing_data_collection            'MSC/AFC Diffractometer Control'
_computing_cell_refinement            'MSC/AFC Diffractometer Control'
_computing_data_reduction             'teXsan Ver. 1.11'
_computing_structure_solution          SHELXS86
_computing_structure_refinement       'teXsan Ver. 1.10'
_computing_publication_material       'teXsan Ver. 1.11'
_computing_molecular_graphics          ?
#------------------------------------------------------------------------------
_geom_special_details
;
 ?
;
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 F(1)      C(9)      2.872(6)   . . yes
 F(1)      C(11)     1.375(10)  . . yes
 O(1)      C(1)      1.417(9)   . . yes
 O(1)      C(2)      1.385(6)   . . yes
 N(1)      C(9)      1.118(8)   . . yes
 C(2)      C(3)      1.376(8)   . . yes
 C(2)      C(7)      1.372(8)   . . yes
 C(3)      C(4)      1.403(7)   . . yes
 C(4)      C(5)      1.367(8)   . . yes
 C(5)      C(6)      1.376(8)   . . yes
 C(5)      C(8)      1.540(8)   . . yes
 C(6)      C(7)      1.399(7)   . . yes
 C(8)      C(9)      1.463(9)   . . yes
 C(8)      C(10)     1.538(7)   . . yes
 C(10)     C(11)     1.493(8)   . . yes
 C(11)     C(12)     1.516(8)   . . yes
 C(12)     C(13)     1.527(9)   . . yes
 C(13)     C(14)     1.522(8)   . . yes
 C(14)     C(15)     1.516(9)   . . yes
 C(15)     C(16)     1.503(8)   . . yes
 C(16)     C(17)     1.49(1)    . . yes
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#------------------------------------------------------------------------------
loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
   C(1)      O(1)      C(2)      117.8(5)   . . . yes
   O(1)      C(2)      C(3)      123.5(5)   . . . yes
   O(1)      C(2)      C(7)      115.3(5)   . . . yes
   C(3)      C(2)      C(7)      121.2(5)   . . . yes
   C(2)      C(3)      C(4)      118.8(5)   . . . yes
   C(3)      C(4)      C(5)      121.1(5)   . . . yes
   C(4)      C(5)      C(6)      118.7(5)   . . . yes
   C(4)      C(5)      C(8)      120.0(5)   . . . yes
   C(6)      C(5)      C(8)      121.2(5)   . . . yes
   C(5)      C(6)      C(7)      121.5(5)   . . . yes
   C(2)      C(7)      C(6)      118.6(5)   . . . yes
   C(5)      C(8)      C(9)      111.3(5)   . . . yes
   C(5)      C(8)      C(10)     112.5(5)   . . . yes
   C(9)      C(8)      C(10)     112.6(5)   . . . yes
   C(9)      F(1)      C(11)     89.4(4)    . . . yes
   N(1)      C(9)      C(8)      178.9(7)   . . . yes
   C(8)      C(10)     C(11)     117.5(5)   . . . yes
   F(1)      C(9)      N(1)      101.6(5)   . . . yes
   F(1)      C(9)      C(8)      79.2(4)    . . . yes
   F(1)      C(11)     C(10)     109.6(5)   . . . yes
   F(1)      C(11)     C(12)     108.9(5)   . . . yes
   C(10)     C(11)     C(12)     112.6(5)   . . . yes
   C(11)     C(12)     C(13)     112.9(6)   . . . yes
   C(12)     C(13)     C(14)     112.9(5)   . . . yes
   C(13)     C(14)     C(15)     113.7(6)   . . . yes
   C(14)     C(15)     C(16)     114.7(6)   . . . yes
   C(15)     C(16)     C(17)     113.9(7)   . . . yes
#------------------------------------------------------------------------------
loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 F(1)      C(11)     C(8)      C(9)      -6.7(5)    . . . . yes
 F(1)      C(11)     C(10)     C(8)      59.0(7)    . . . . yes
 F(1)      C(11)     C(12)     C(13)     -59.4(7)   . . . . yes
 O(1)      C(2)      C(3)      C(4)      179.2(5)   . . . . yes
 O(1)      C(2)      C(7)      C(6)      -179.9(5)  . . . . yes
 N(1)      C(9)      C(8)      C(5)      53(34)     . . . . yes
 N(1)      C(9)      C(8)      C(10)     -179(33)   . . . . yes
 C(1)      O(1)      C(2)      C(3)      0.5(8)     . . . . yes
 C(1)      O(1)      C(2)      C(7)      179.2(5)   . . . . yes
 C(2)      C(3)      C(4)      C(5)      -1.7(8)    . . . . yes
 C(2)      C(7)      C(6)      C(5)      3.0(8)     . . . . yes
 C(3)      C(2)      C(7)      C(6)      -1.3(8)    . . . . yes
 C(3)      C(4)      C(5)      C(6)      3.4(8)     . . . . yes
 C(3)      C(4)      C(5)      C(8)      179.7(5)   . . . . yes
 C(4)      C(3)      C(2)      C(7)      0.6(8)     . . . . yes
 C(4)      C(5)      C(6)      C(7)      -4.1(8)    . . . . yes
 C(4)      C(5)      C(8)      C(9)      -133.2(6)  . . . . yes
 C(4)      C(5)      C(8)      C(10)     99.3(6)    . . . . yes
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 C(5)      C(8)      C(10)     C(11)     58.0(7)    . . . . yes
 C(6)      C(5)      C(8)      C(9)      42.9(7)    . . . . yes
 C(6)      C(5)      C(8)      C(10)     -84.6(7)   . . . . yes
 C(7)      C(6)      C(5)      C(8)      179.7(5)   . . . . yes
 C(8)      C(10)     C(11)     C(12)     -179.6(5)  . . . . yes
 C(9)      C(8)      C(10)     C(11)     -68.8(7)   . . . . yes
 C(10)     C(11)     C(12)     C(13)     178.8(5)   . . . . yes
 C(11)     C(12)     C(13)     C(14)     -178.0(5)  . . . . yes
 C(12)     C(13)     C(14)     C(15)     -179.4(6)  . . . . yes
 C(13)     C(14)     C(15)     C(16)     178.6(6)   . . . . yes
 C(14)     C(15)     C(16)     C(17)     -177.2(6)  . . . . yes
 C(14)     C(15)     C(16)     C(17)     -177.2(6)  . . . . yes
#--------------------------------------------------------------------------------
loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 F(1)      C(9)      2.872(6)   . . ?
 O(1)      C(9)      3.477(7)   . 1_455 ?
 O(1)      C(8)      3.537(7)   . 1_455 ?
 N(1)      C(8)      3.405(9)   . 1_545 ?
 N(1)      C(10)     3.447(8)   . 1_545 ?
 N(1)      C(4)      3.525(8)   . 1_545 ?
#--------------------------------------------------------------------------------
#--------------------------------------------------------------------------------
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