Supporting Information

Anion Binding Modes in *meso*-Substituted Hexapyrrolic Calix[4]pyrrole Isomers

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Page No. Contents

Materials and methods: All other chemicals and solvents were purchased from commercial sources and were used as such, unless otherwise mentioned. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker DRX 500 NMR spectrometer. Chemical shifts were calibrated to the corresponding deuterated solvents. The UV spectra were measured using a Hitachi U-3010 double beam spectrophotometer. Electronspray ionization mass spectrometry was measured by a Shimadzu 2010A LCMS.

Titration curves obtained by plotting the change in optical density were analyzed by nonlinear least-squares method using an equation for 1:1 binding model.[1] The equations 1 and 2 were used to fit the experimental data,

$$[G] = \frac{K_a[G]_t - K_a[H]_t - 1 + \{(K_a[H]_t - K_a[G]_t + 1)^2 + 4K_a[G]_t\}^{1/2}}{2K_a} \quad (1)$$

$$[HG] = \frac{K_a[G][H]_t}{1 + K_a[G]} = \frac{A - A_0}{A_i - A_0} \quad (2)$$

where $[G]_t$, $[H]_t$ are total concentrations of guest and host, respectively. K_a is a binding constant and $[G]$, and $[HG]$ are unknown concentration of guest and complex, respectively. Eqn (1) defines value of unknown $[G]$ based on K_a and experimentally obtained values $[H]_t$ and $[G]_t$. A, A_0, and A_i are the guest (G) concentration-dependent absorbance, absorbance at no guest concentration and infinite guest concentration, respectively.

Calculated geometries of *cis*-**1** and *trans*-**1** without and with fluoride were fully optimized with the Gaussian 09 package[2] at the density functional theory (DFT) level of theory by using the B3LYP (Becke's three parameters hybrid functional with the Lee-Yang-Parr correlation functional) and the 6-31G* basis set. The global minimum conformations of *cis*-**1**, *trans*-**1,** *cis*-**1** with fluoride and *trans*-**1** with fluoride were reached starting from the single crystal structures obtained from X-ray diffraction analyses of *cis*-**1** and *trans*-**1** by means of the appropriate manual search in the conformational space by low-level calculations (PM3 method). Solvent (acetonitrile) effects were applied on the gas-phase optimized geometries, using the Tomasi's polarizable continuum model (PCM). The gauge-including atomic orbital (GIAO) method was used to calculate ^{1}H nuclear magnetic shielding tensors at the DFT (B3LYP/6-31G*) level of theory was applied to *cis*-**1** with fluoride and *trans*-**1** with fluoride in acetonitrile (PCM).

Synthesis of compound 1: To the solution of compound **4** (500 mg, 1.47 mmol) in anhydrous acetonitrile (50 mL) was added acetone (18.4 mL, 250 mmol), then trifluoroacetic acid (0.57 mL, 7.4 mmol) was added under nitrogen atmosphere. The mixture was stirred for 24 h at room temperature. The reaction mixture was quenched upon addition of triethylamine and extracted with ethyl acetate (50 mL × 2). The organic layer was dried over anhydrous $MgSO_4$ and the solvent was removed under reduced pressure to afford the crude reaction mixture, which was

purified by a silica-gel column chromatography [ethyl acetate/ hexanes = 1/4, R_f = 0.50 (*cis*-**1**), 0.59 (*trans*-**1**)] to afford pure product **1** with *cis*-**1** (78 mg, 7%) and *trans*-**1** (112 mg, 10%) isomers as white solid.

*Data for cis-**1***: Mp: 204-206 ^oC; ^1H NMR (500 MHz, CD_3CN) δ = 8.01 (br s, 4H, pyrrole-NH), 7.92 (br s, 2H, pyrrole-NH), 5.90 (m, 4H, pyrrole-β-H), 5.82 (m, 4H, pyrrole-*β*-H), 4.16 (q, *J* = 7.0 Hz, 4H, O*CH*$_2$CH$_3$), 2.69 (q, *J* = 7.5 Hz, 4H, *CH*$_2$CH$_3$), 1.86 (s, 6H, CH_3), 1.66 (s, 6H, CH_3), 1.62 (s, 6H, CH_3), 1.50(s, 6H, CH_3), 1.23 (t, *J* = 7.0 Hz, 6H, OCH$_2$*CH*$_3$). 1.05 ppm (t, *J* = 7.5 Hz, 6H, CH$_2$*CH*$_3$); ^{13}C APT NMR (125 MHz, CD_3CN) δ = 161.5 (Cq), 140.3 (Cq), 138.7 (Cq), 135.6 (Cq), 135.2 (Cq), 116.8 (Cq), 115.8 (Cq), 106.1 (CH), 104.0 (CH), 60.3 (CH_2), 41.6 (Cq), 35.7 (Cq), 30.4 (CH_3), 27.4 (CH_3), 25.5 (CH_3), 18.7 (CH_2), 15.4 (CH_3), 14.7 (CH_3), 9.4 ppm (CH_3); ESI-MS *m/z* 781 (M + Na^+).

*Data for trans-**1***: Mp: 210-212 ^oC; ^1H NMR (500 MHz, CD_3CN) δ = 8.14 (br s, 4H, pyrrole-NH), 8.08 (br s, 2H, pyrrole-NH), 5.95-5.89 (m, 8H, pyrrole-*β*-H), 4.16 (q, *J* = 7.0 Hz, 4H, O*CH*$_2$CH$_3$), 2.66 (q, *J* = 7.5 Hz, 4H, *CH*$_2$CH$_3$), 1.86 (s, 6H, CH_3), 1.53 (s, 12H, CH_3), 1.51 (s, 6H, CH_3), 1.23 (t, *J* = 7.0 Hz, 6H, OCH$_2$*CH*$_3$). 1.02 ppm (t, *J* = 7.5 Hz, 6H, CH$_2$*CH*$_3$); ^{13}C APT NMR (125 MHz, CD_3CN) δ = 161.5 (Cq), 140.0 (Cq), 138.3 (Cq), 135.7 (Cq), 135.3 (Cq), 116.8 (Cq), 115.8 (Cq), 105.8 (CH), 104.3 (CH), 60.2 (CH_2), 41.4 (Cq), 36.2 (Cq), 30.4 (CH_3), 26.5 (CH_3), 18.6 (CH_2), 15.4 (CH_3), 14.7 (CH_3), 8.9 ppm (CH_3); ESI-MS *m/z* 781 (M + Na^+).

Synthesis of compound 4: A solution of **3**[3] (500 mg, 2.24 mmol) in anhydrous dichloromethane (15 mL) was treated with pyrrole (6.2 mL, 89.6 mmol) under nitrogen atmosphere, then trifluoroacetic acid (0.86 mL, 11.2 mmol) was added dropwise over a period of 5 minutes at 0 °C. The mixture was stirred for 3 days at room temperature. The reaction mixture was quenched upon addition of triethylamine and extracted with dichloromethane (50 mL × 2). The organic layer was dried over anhydrous $MgSO_4$ and the solvent was removed under reduced pressure to afford the crude reaction mixture. The crude mixture was added sodium borohydride in ethanol (50 mL) and stirred for 5 h at room temperature. The ethanol was removed under reduced pressure and the mixture was extracted with dichloromethane (50 mL × 2). The organic layer was dried over anhydrous $MgSO_4$ and the solvent was removed under reduced pressure to afford the crude reaction mixture, which was purified by a silica-gel column chromatography (ethyl acetate/ hexanes = 1/9, R_f = 0.11) to afford pure product **4** as white solid. Yield: 440 mg (58%). Mp: 102-105 °C; ^1H NMR (500 MHz, $CDCl_3$) δ = 8.34 (br s, 1H, NH), 7.87 (br s, 2H, NH), 6.72-6.65 (m, 2H, pyrrole-H), 6.25-6.19 (m, 2H, pyrrole-H), 6.15-6.09 (m, 2H, pyrrole-H), 4.23 (q, *J* = 7.0 Hz, 2H, O*CH*$_2$CH$_3$), 2.70 (q, *J* = 7.5 Hz, 2H, *CH*$_2$CH$_3$), 2.00 (s, 3H, CH_3), 1.65 (s, 3H, CH_3), 1.30 (t, J = 7.0 Hz, 3H, OCH$_2$*CH*$_3$). 1.10 ppm (t, J = 7.5 Hz, 3H, CH$_2$*CH*$_3$); ^{13}C APT NMR (125 MHz, $CDCl_3$) δ = 161.5 (Cq), 136.7 (Cq), 135.4 (Cq), 135.0 (Cq), 117.3 (CH), 116.1 (Cq), 115.5 (Cq), 109.0 (CH), 106.0 (CH), 59.8 (CH_2), 41.1 (Cq), 26.9 (CH_3), 18.4 (CH_2), 15.2 (CH_3), 14.5 (CH_3), 9.2 ppm (CH_3); ESI-MS *m/z* 340 (M + H^+).

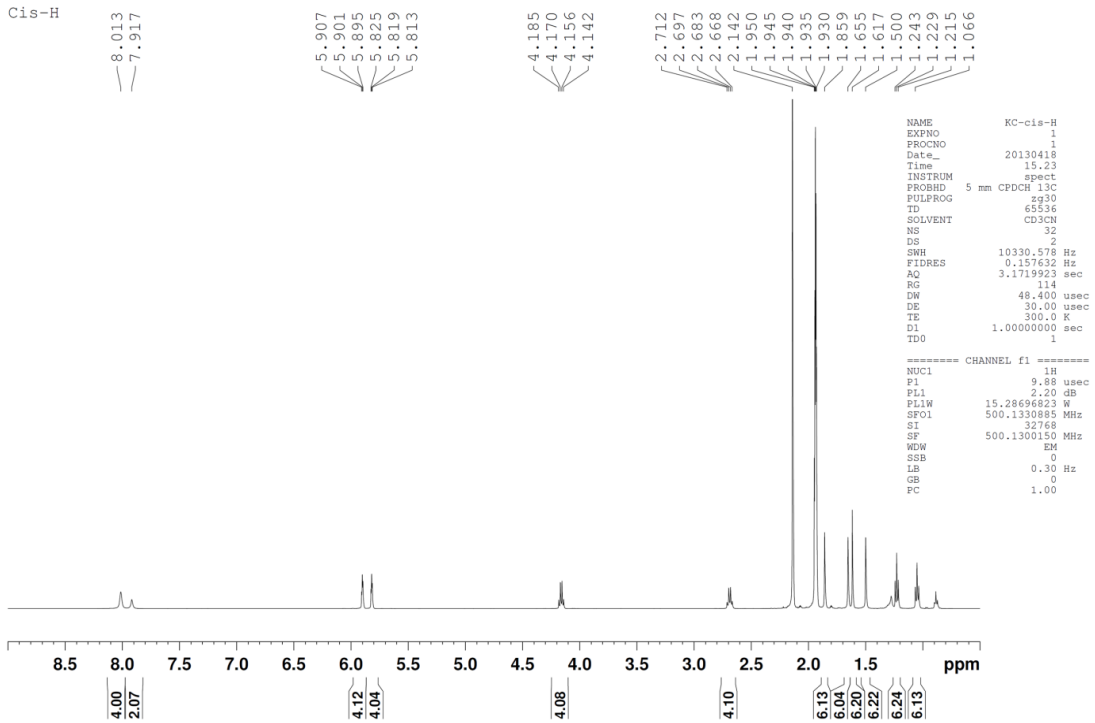

Figure S1. ^{1}H NMR (500 MHz) spectrum of *cis*-**1** in CD_3CN.

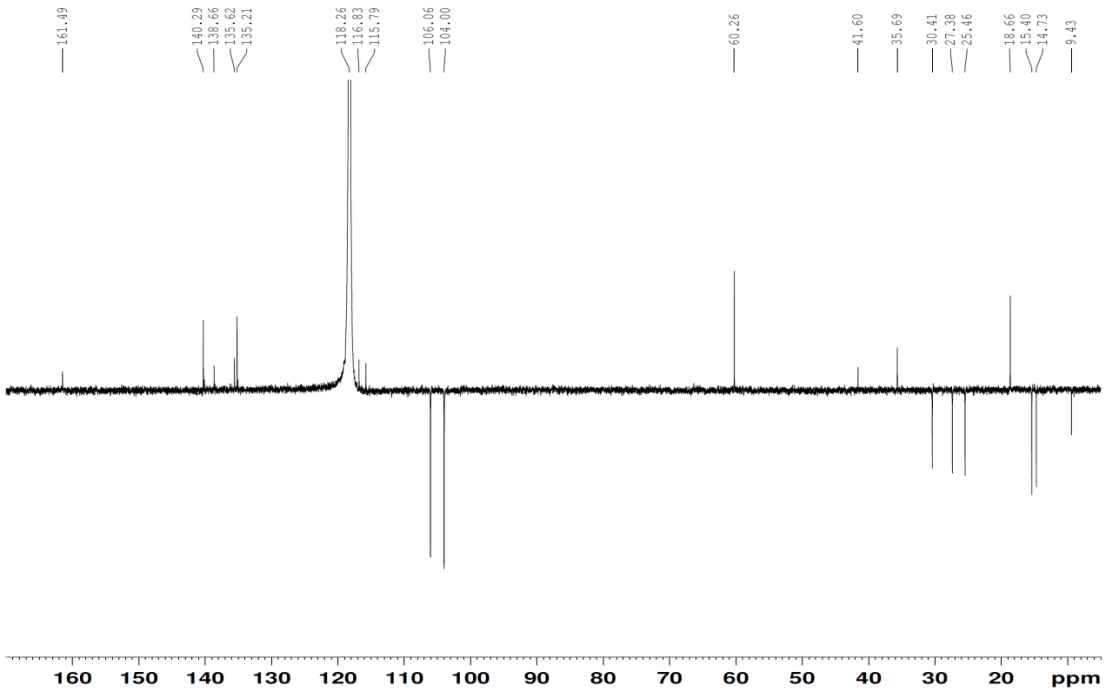

Figure S2. ^{13}C APT NMR (125 MHz) spectrum of *cis*-**1** in CD_3CN.

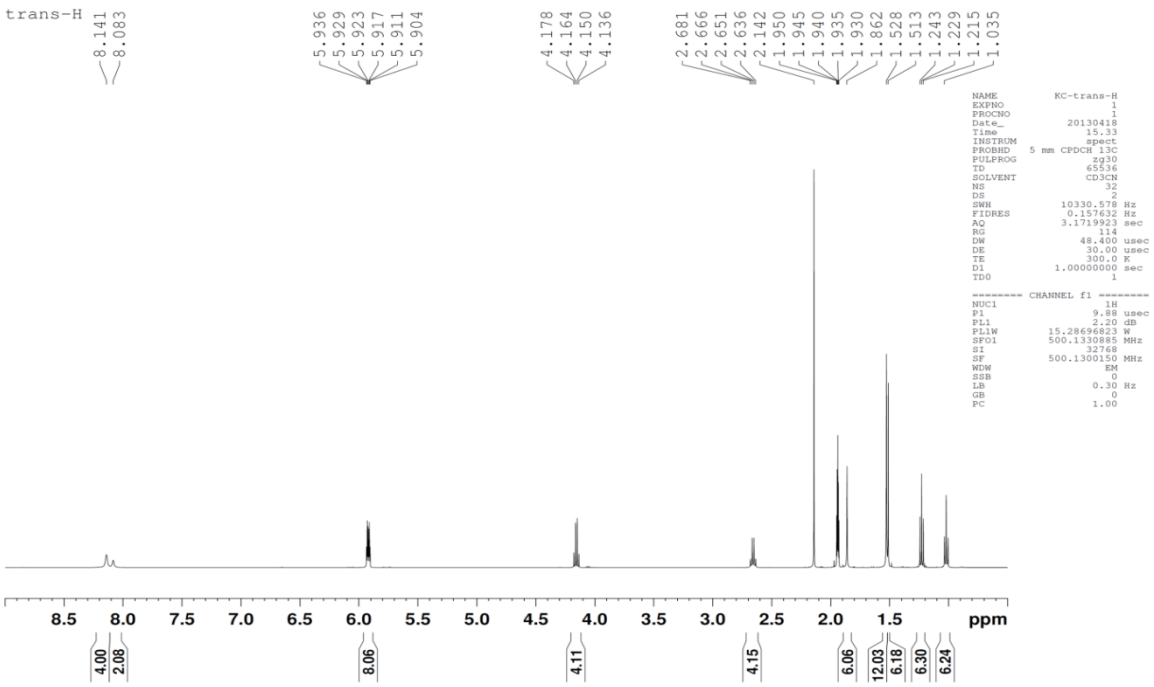

Figure S3. ^{1}H NMR (500 MHz) spectrum of *trans*-**1** in CD_3CN.

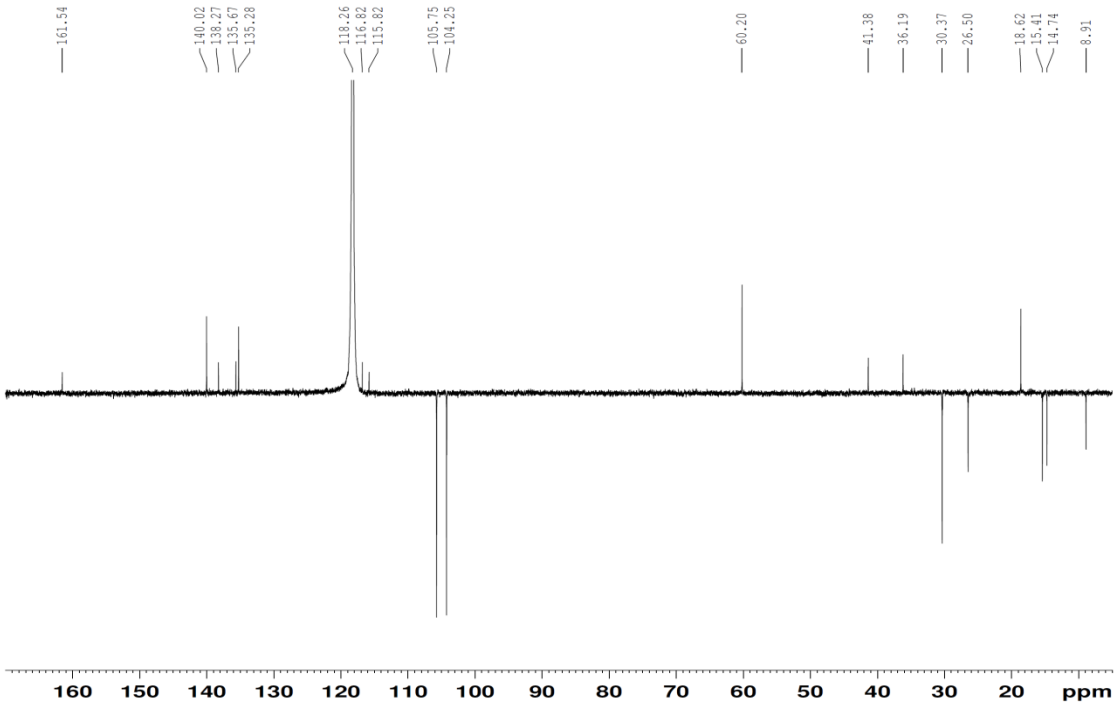

Figure S4. ^{13}C APT NMR (125 MHz) spectrum of *trans*-**1** in CD_3CN.

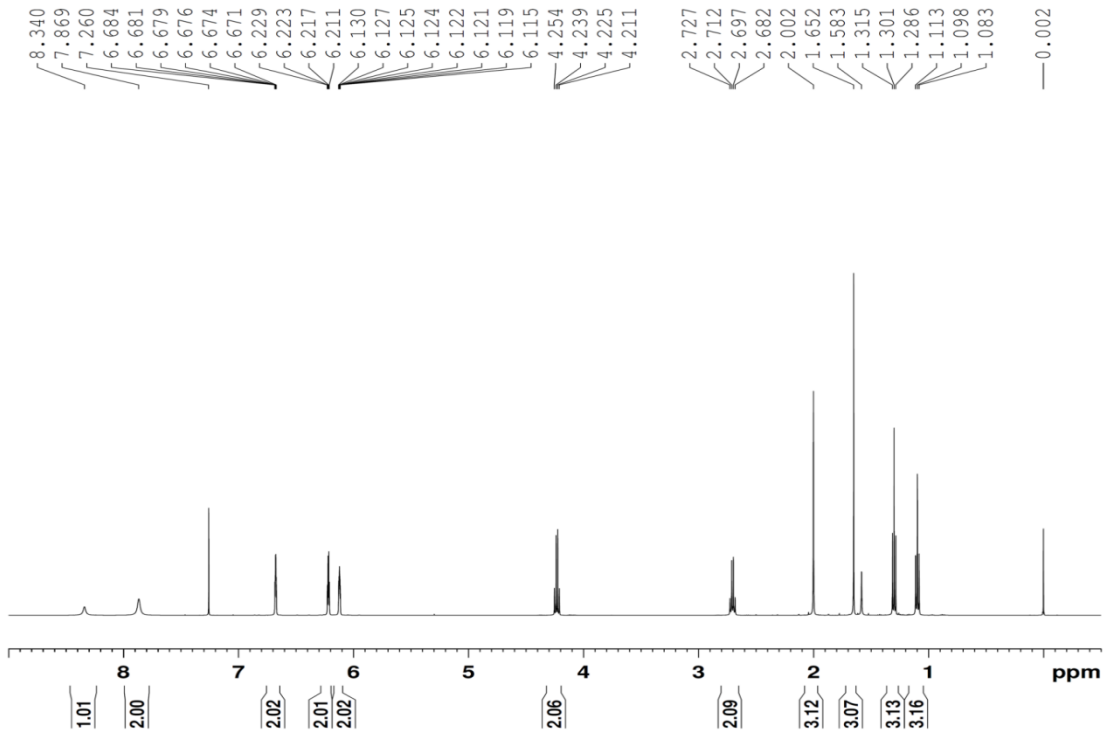

Figure S5. ^{1}H NMR (500 MHz) spectrum of **4** in $CDCl_3$.

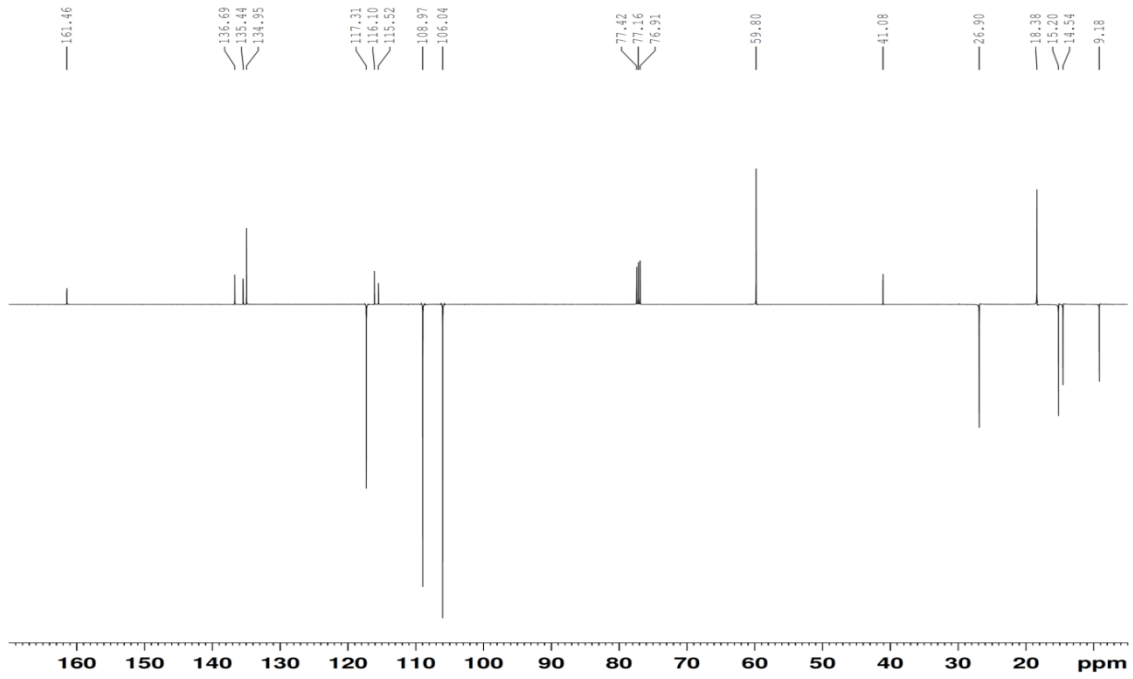

Figure S6. ^{13}C APT NMR (125 MHz) spectrum of **4** in $CDCl_3$.

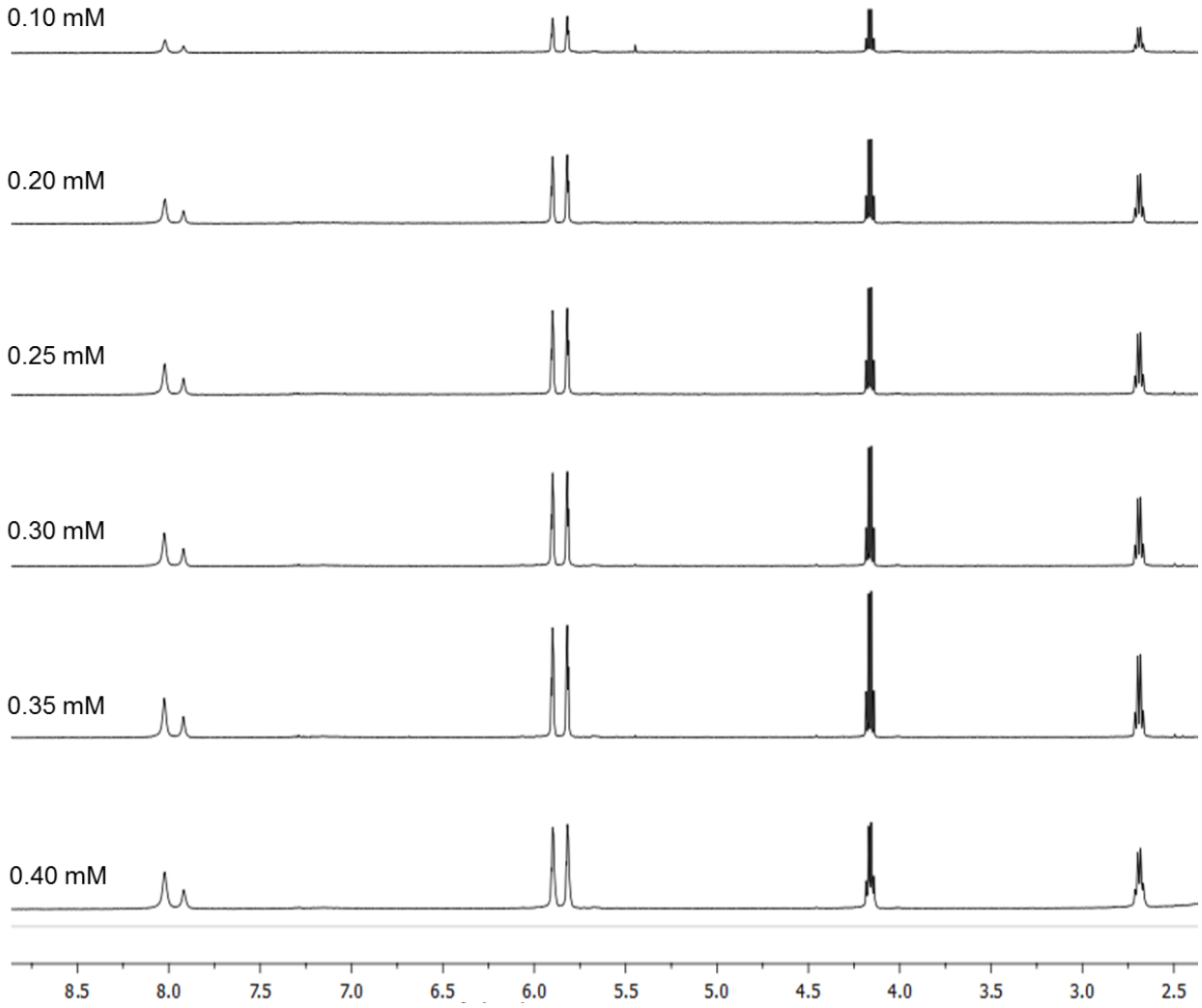

Figure S7. Variable-concentration ^{1}H NMR spectra of *cis*-**1** in CD_3CN (maximum solubility of *cis*-**1** in CD_3CN is 0.40 mM).

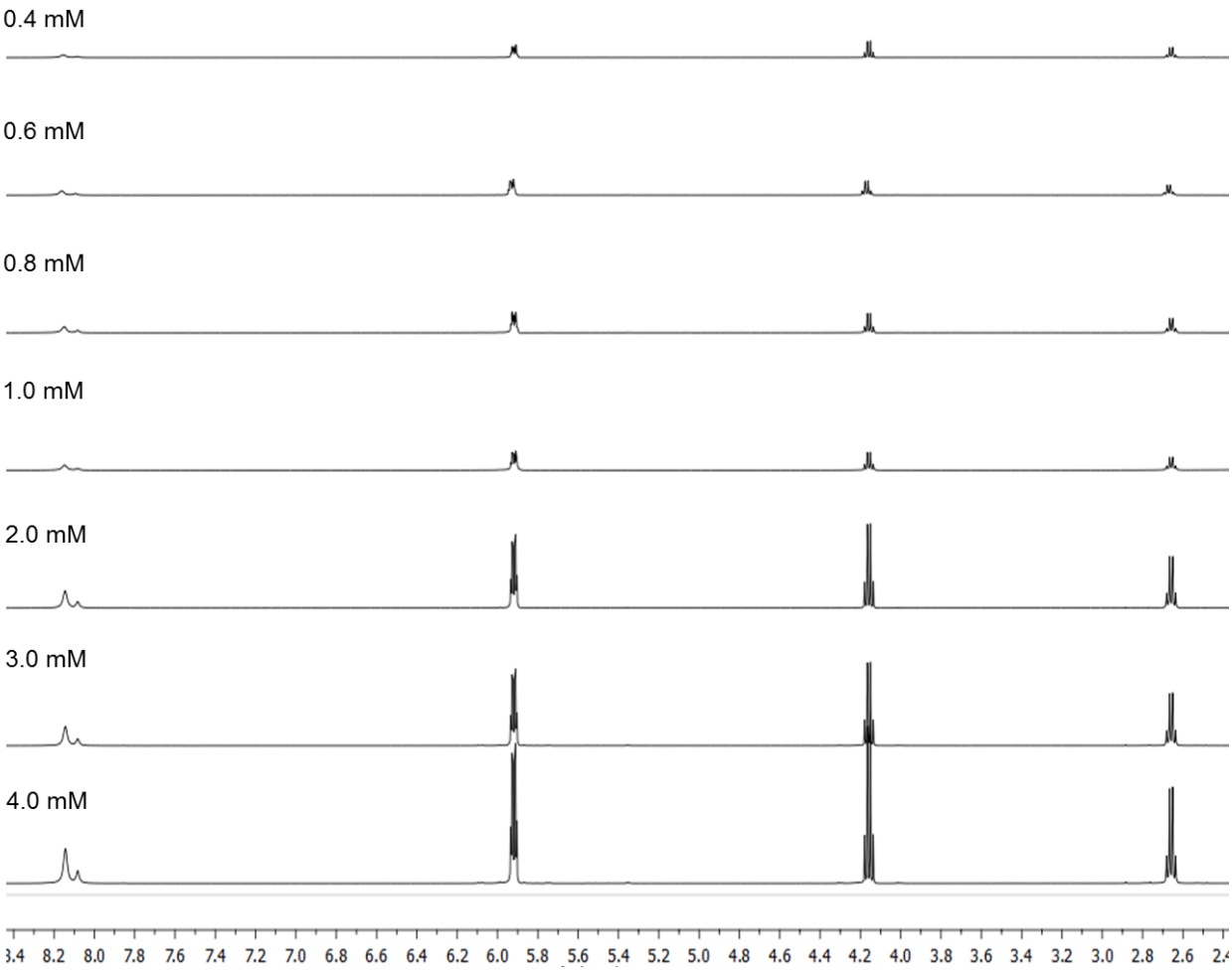

Figure S8. Variable-concentration ^{1}H NMR spectra of *trans*-**1** in CD_3CN.

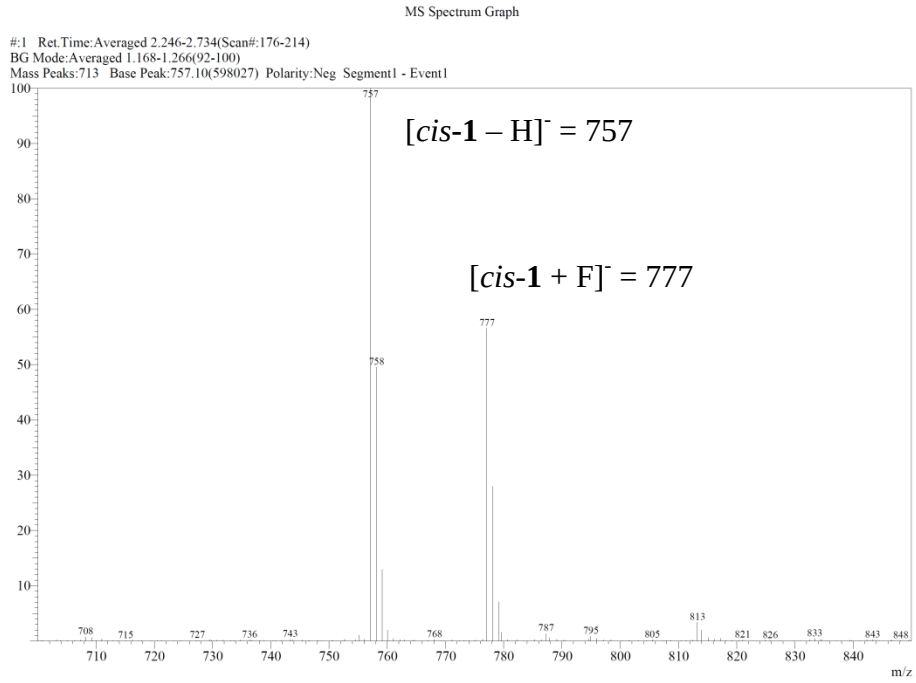

Figure S9. ESI MS spectrum of a mixture of *cis*-**1** and fluoride in MeCN. The spectrum showed 1:1 complex.

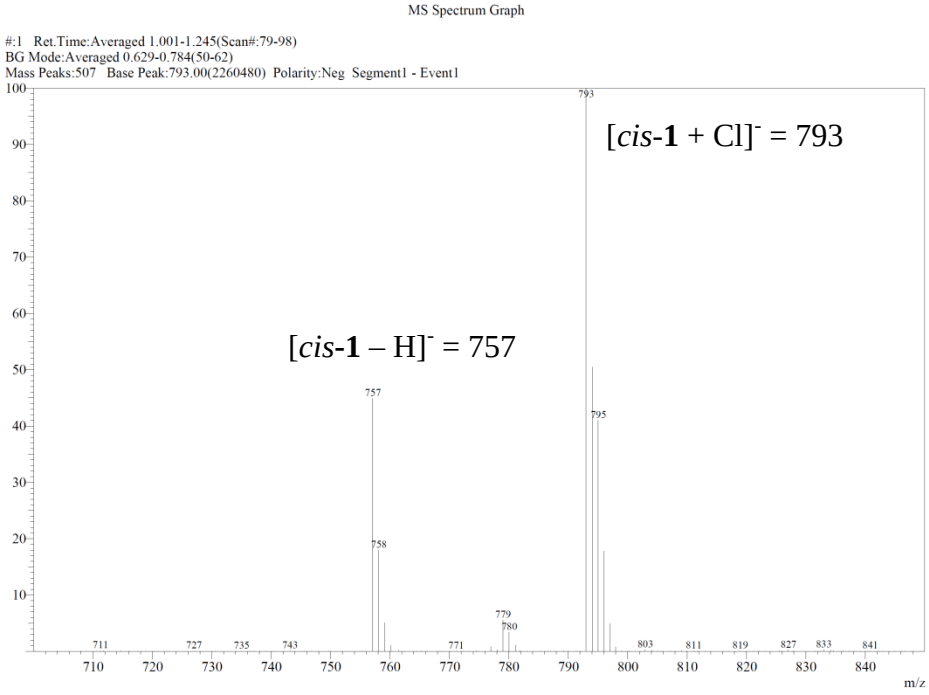

Figure S10. ESI MS spectrum of a mixture of *cis*-**1** and chloride in MeCN. The spectrum showed 1:1 complex.

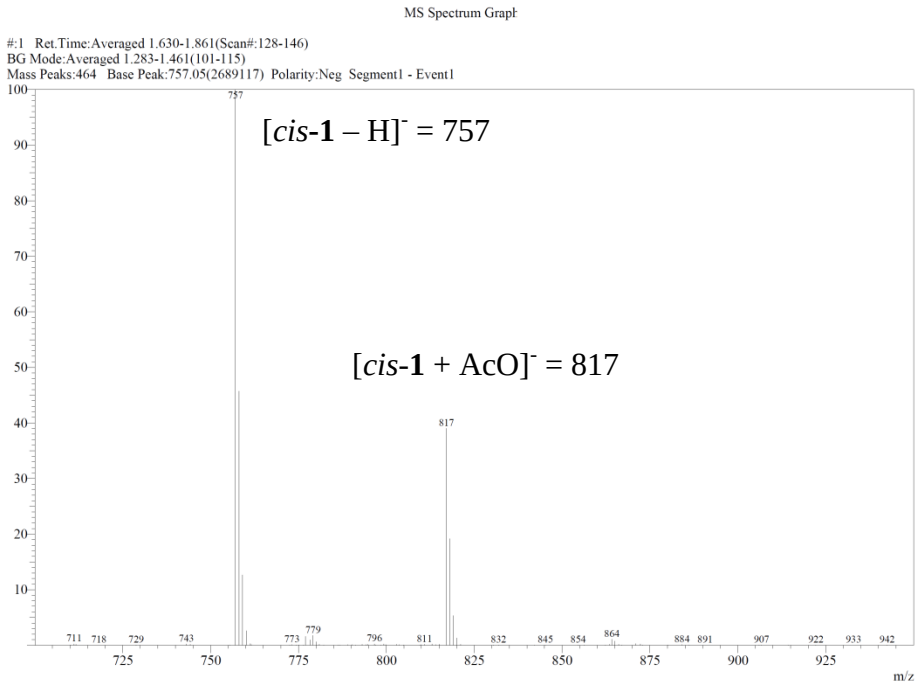

Figure S11. ESI MS spectrum of a mixture of *cis*-**1** and acetate in MeCN. The spectrum showed 1:1 complex.

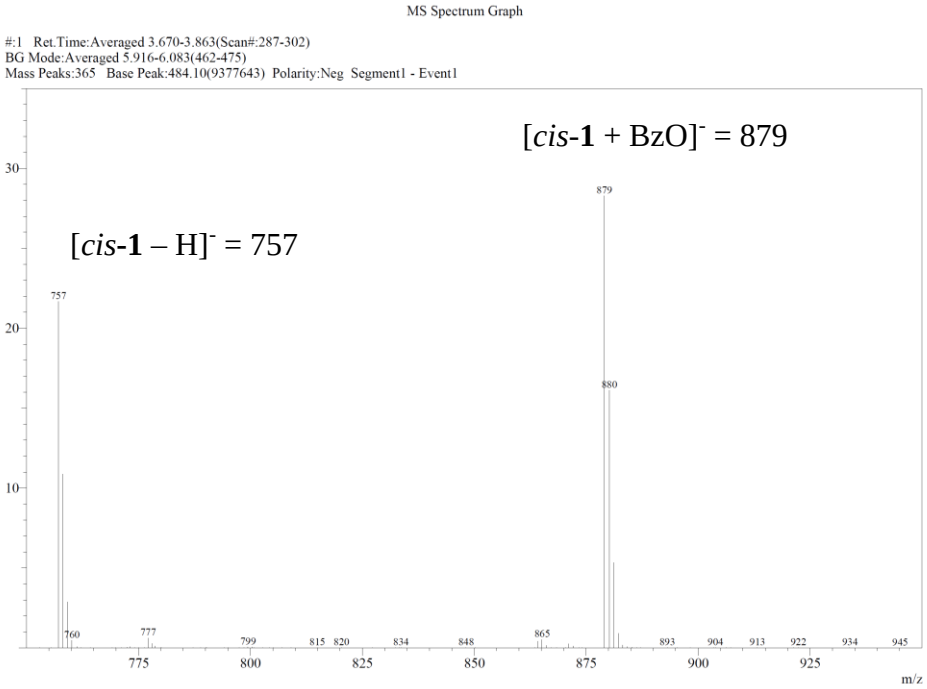

Figure S12. ESI MS spectrum of a mixture of *cis*-**1** and benzoate in MeCN. The spectrum showed 1:1 complex.

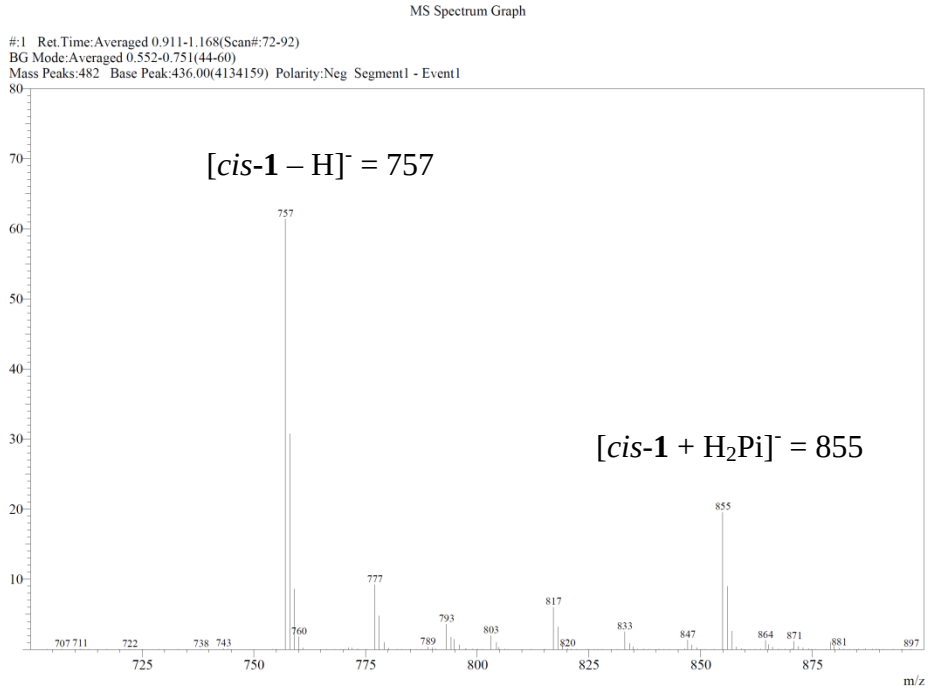

Figure S13. ESI MS spectrum of a mixture of *cis*-**1** and dihydrogenphosphate in MeCN. The spectrum showed 1:1 complex.

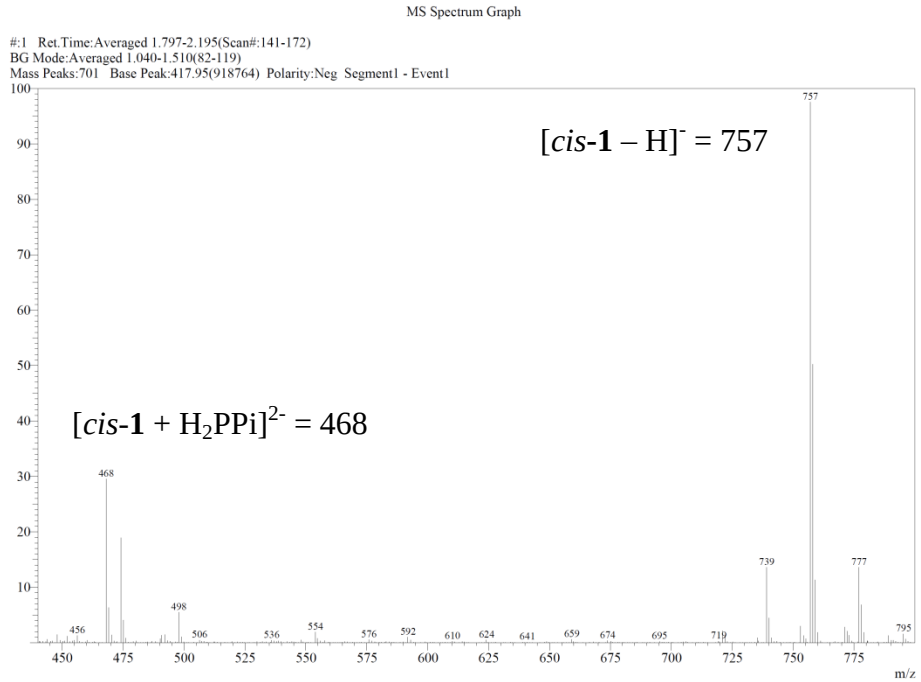

Figure S14. ESI MS spectrum of a mixture of *cis*-**1** and pyrophosphate in MeCN. The spectrum showed 1:1 complex.

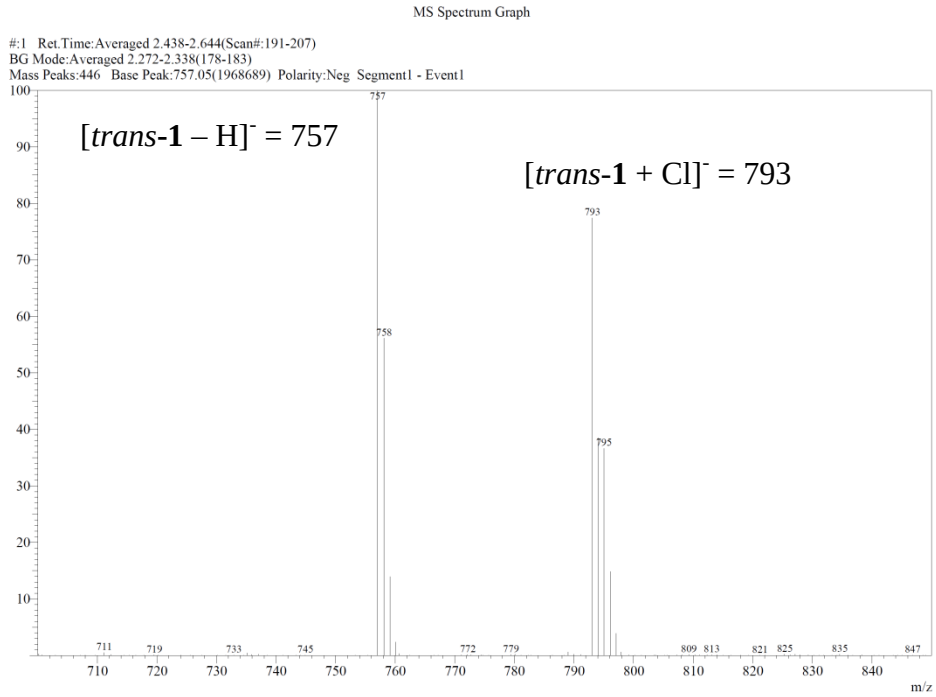

Figure S15. ESI MS spectrum of a mixture of *trans*-**1** and chloride in MeCN. The spectrum showed 1:1 complex.

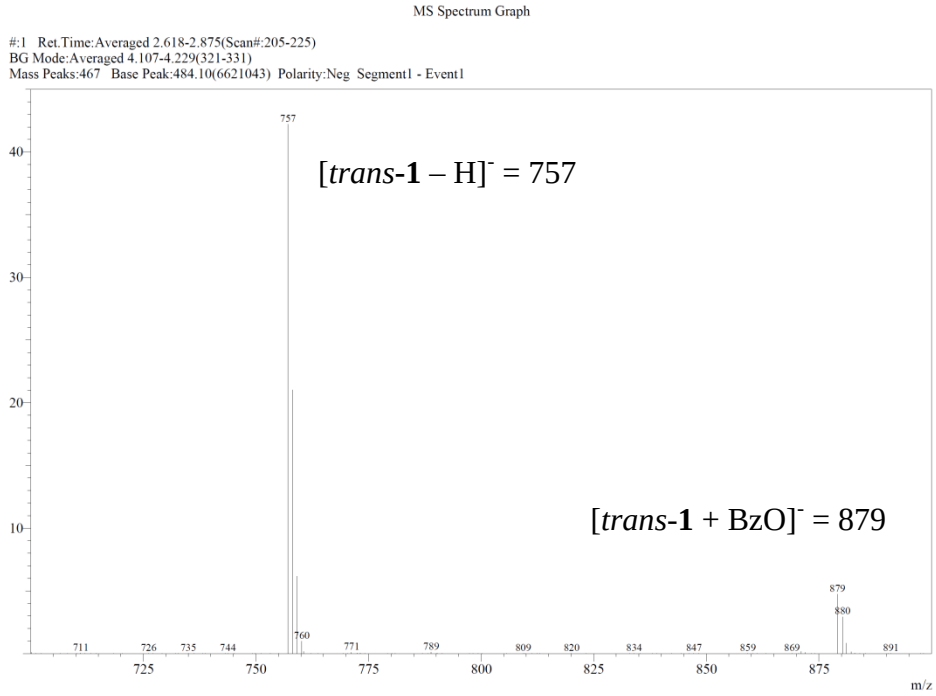

Figure S16. ESI MS spectrum of a mixture of *trans*-**1** and benzoate in MeCN. The spectrum showed 1:1 complex.

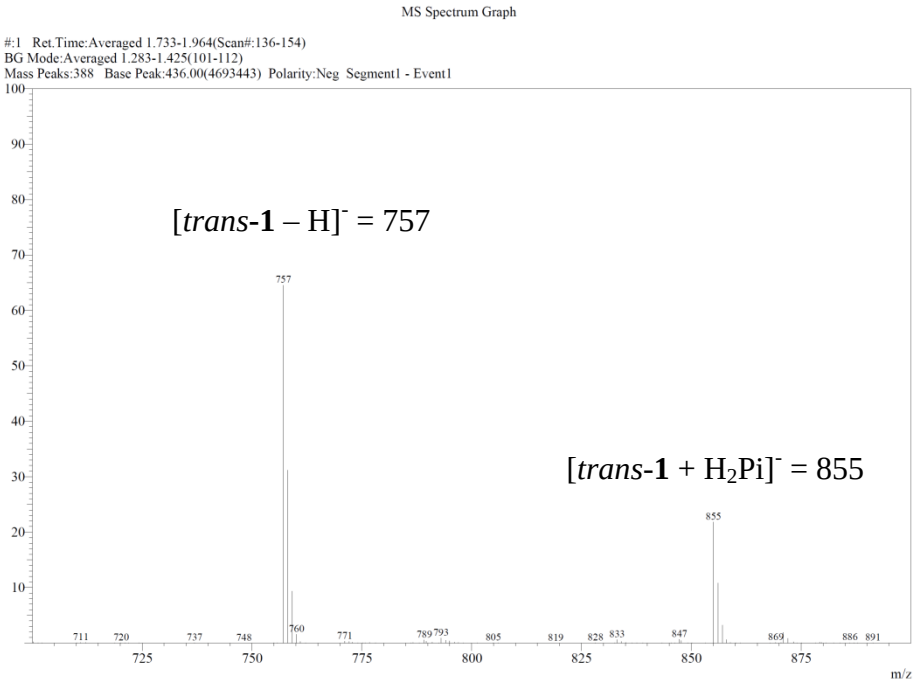

Figure S17. ESI MS spectrum of a mixture of *trans*-**1** and dihydrogenphosphate in MeCN. The spectrum showed 1:1 complex.

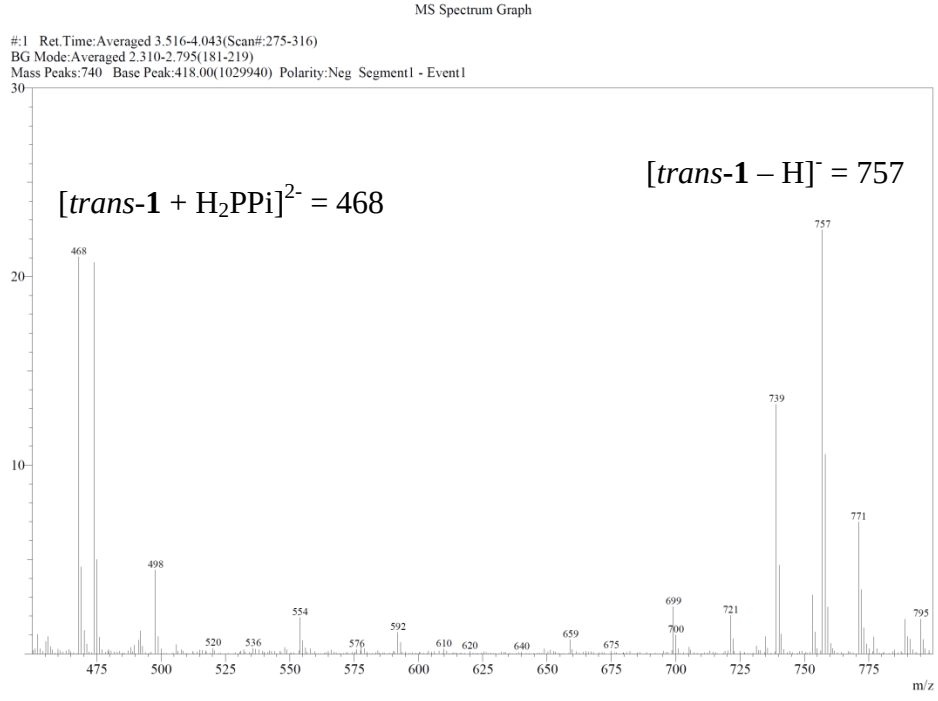

Figure S18. ESI MS spectrum of a mixture of *trans*-**1** and pyrophosphate in MeCN. The spectrum showed 1:1 complex.

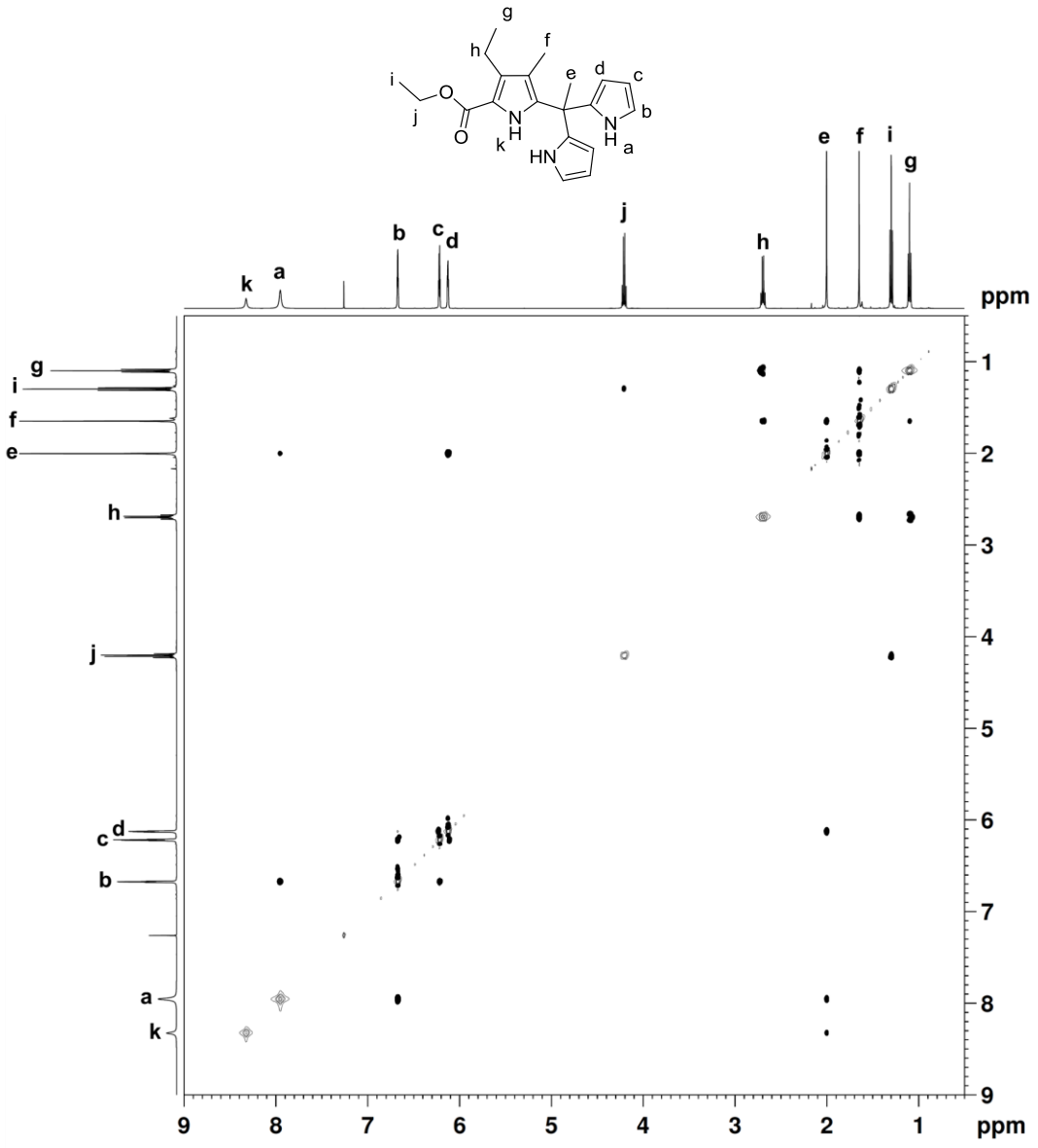

Figure S19. 2D NOESY NMR spectrum of **4** recorded in $CDCl_3$.

Note: The NOESY spectrum supports the following contentions:

1. The pyrrole *α*-protons (b) have corresponding signals with the pyrrole *β*-protons (c) and pyrrole NH (a).
2. The pyrrole *β*-protons (c) have corresponding signals with both the pyrrole *β*-protons (d) and pyrrole *α*-protons (b) protons.

3. The pyrrole *β*-protons (d) have corresponding signals with CH_3 (e) and pyrrole *β*-protons (c) protons.

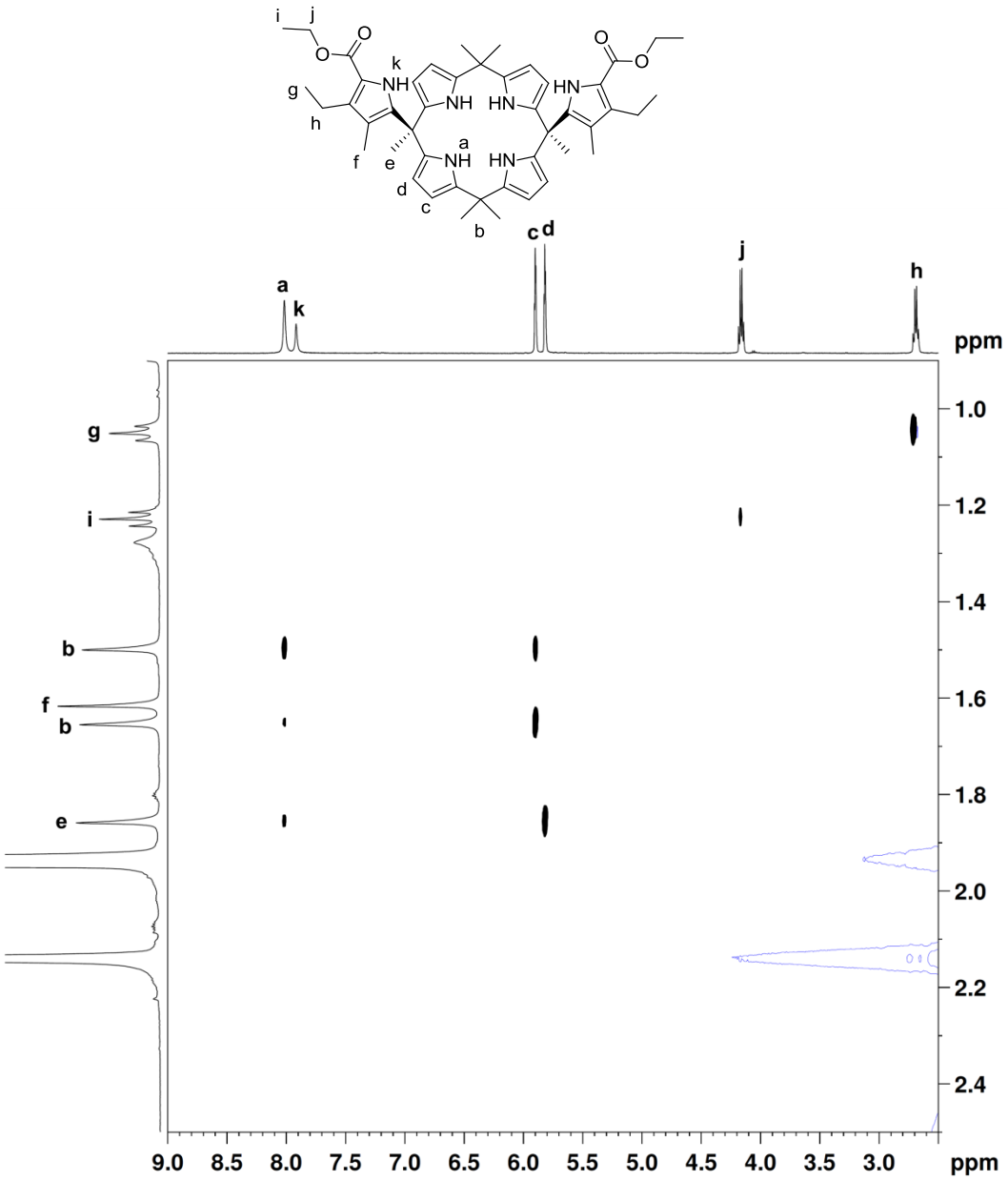

Figure S20. 2D NOESY NMR spectrum of *cis*-**1** (0.4 mM) recorded in CD_3CN.

Note: The NOESY spectrum supports the following contentions:

1. The pyrrole *β*-protons (c) have corresponding signals with two CH_3 (b) protons.
2. The pyrrole *β*-protons (d) have corresponding signals with one CH_3 (e) protons.
3. The side-pyrrole NH protons (k) have no corresponding signals.

4. The side-pyrrole β-methyl protons (f) have no corresponding signals.
5. The pyrrole NH protons (a) have corresponding signals with two CH_3 (b) and one CH_3 (e).

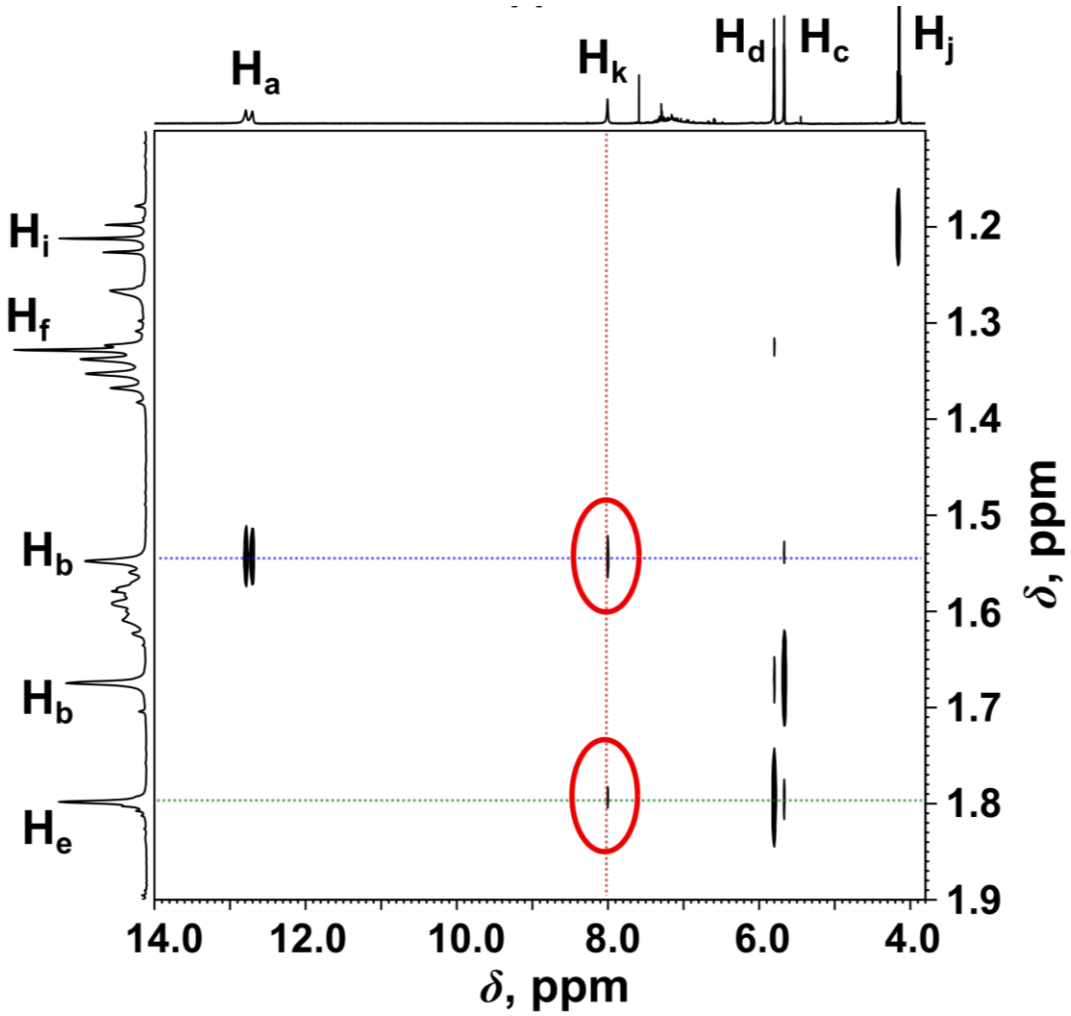

Figure S21. 2D NOESY NMR spectrum of *cis*-**1** (0.4 mM) with fluoride (1.0 mM) recorded in CD_3CN.

Note: The NOESY spectrum supports the following contentions:

1. The side-pyrrole NH protons (k) have corresponding signals with one CH_3 (b) protons.
2. The side-pyrrole NH protons (k) have corresponding signals with the CH_3 (e) protons.

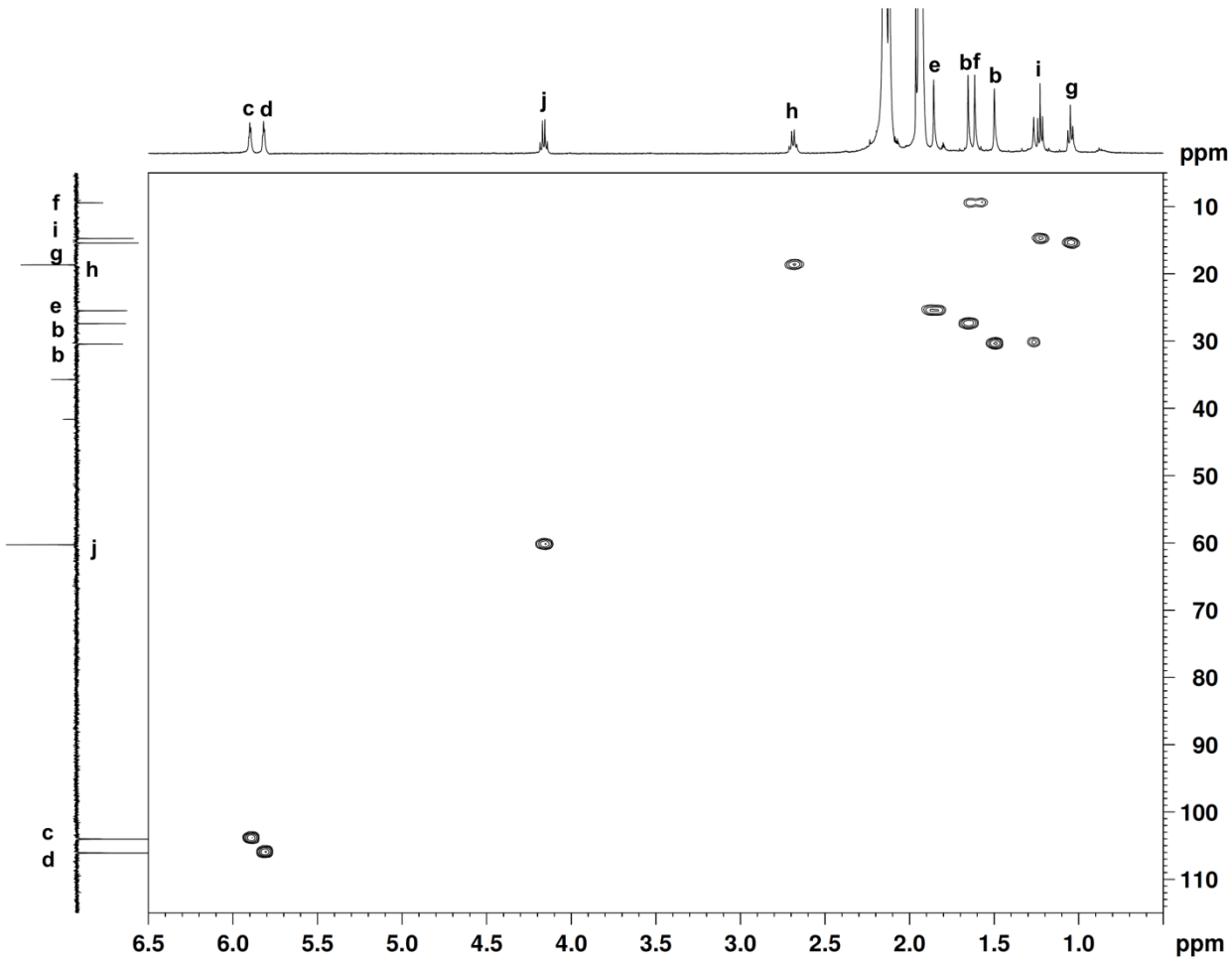

Figure S22. 2D HSQC NMR spectrum of *cis*-**1** (0.4 mM) recorded in CD_3CN.

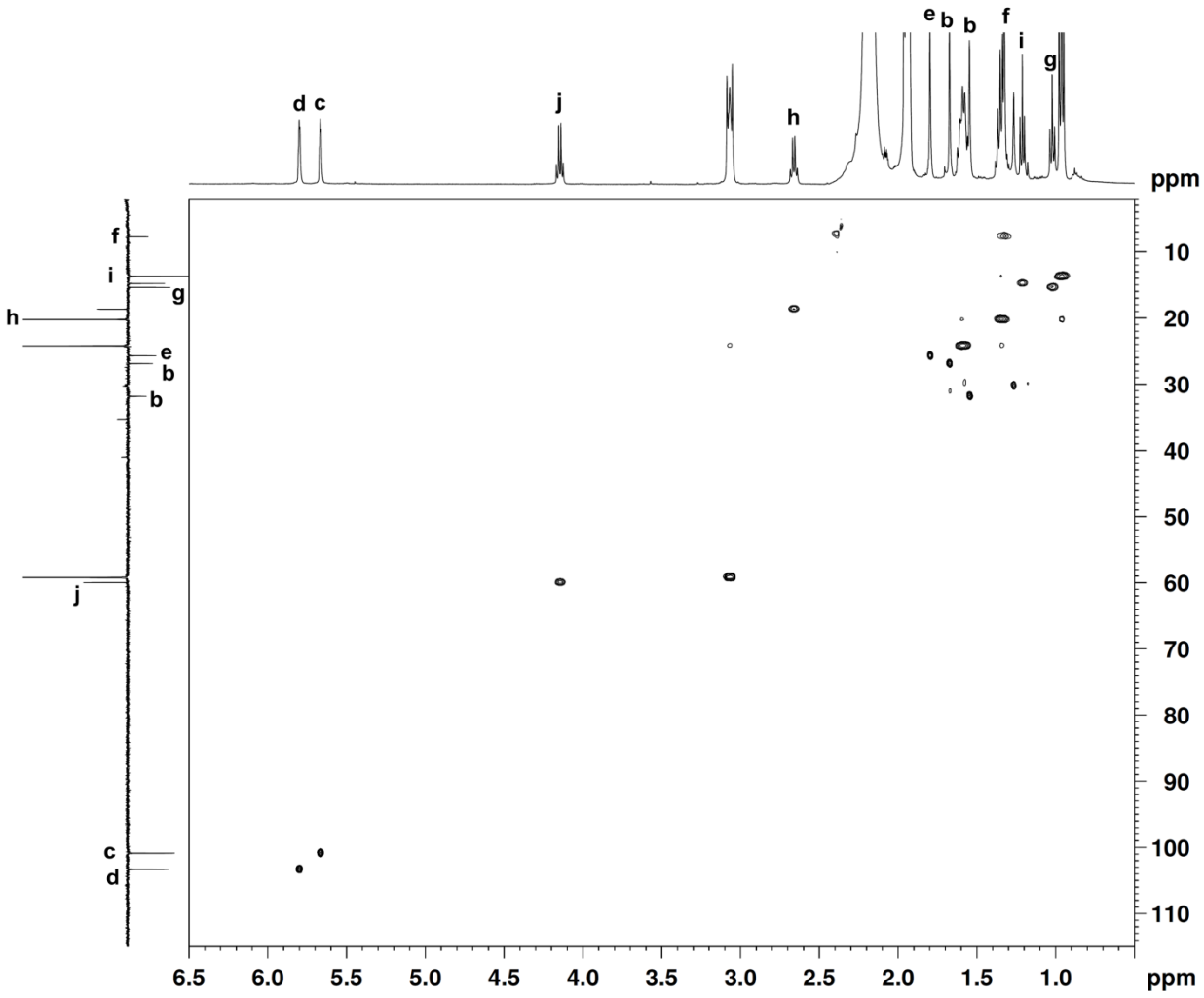

Figure S23. 2D HSQC NMR spectrum of *cis*-**1** (0.4 mM) with fluoride (1.0 mM) recorded in CD_3CN.

Note: The 2D HSQC spectrum supports the following contentions (Figures S20 and S21):

1. The side-pyrrole methyl-carbons (f) move upfield from 9.4 ppm to 7.6 ppm.
2. The pyrrole *β*-carbons (c) move upfield from 104.0 ppm to 100.9 ppm.
3. The pyrrole *β*-protons (d) move upfield from 106.1 ppm to 103.3 ppm.

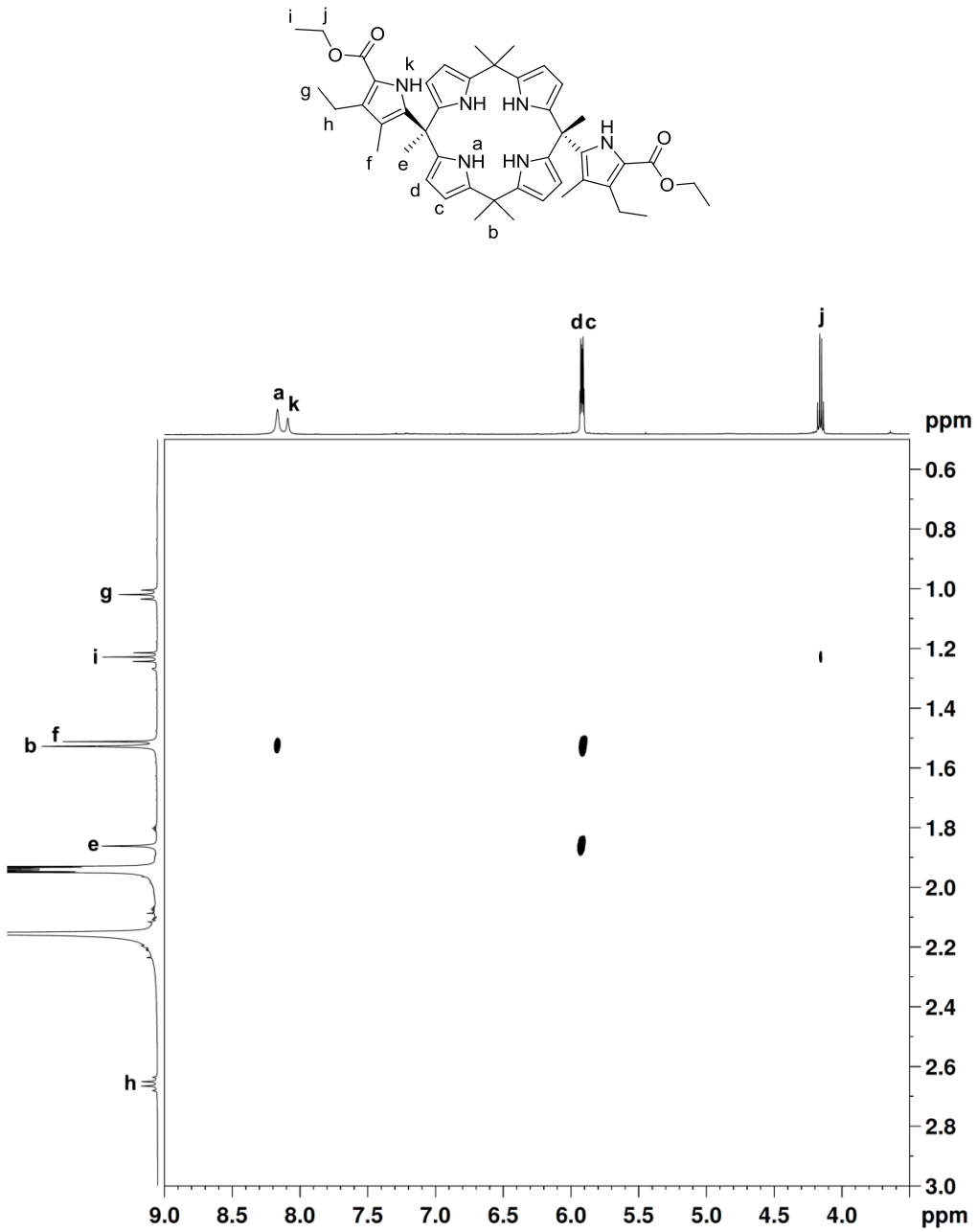

Figure S24. 2D NOESY NMR spectrum of *trans*-**1** (0.4 mM) recorded in CD_3CN.

Note: The NOESY spectrum supports the following contentions:

1. The pyrrole NH protons (a) have corresponding signals with two CH_3 (b).
2. The pyrrole *β*-protons (c) have corresponding signals with two CH_3 (b) protons.
3. The pyrrole *β*-protons (d) have corresponding signals with one CH_3 (e) protons.
4. The side-pyrrole NH protons (k) have no corresponding signals.

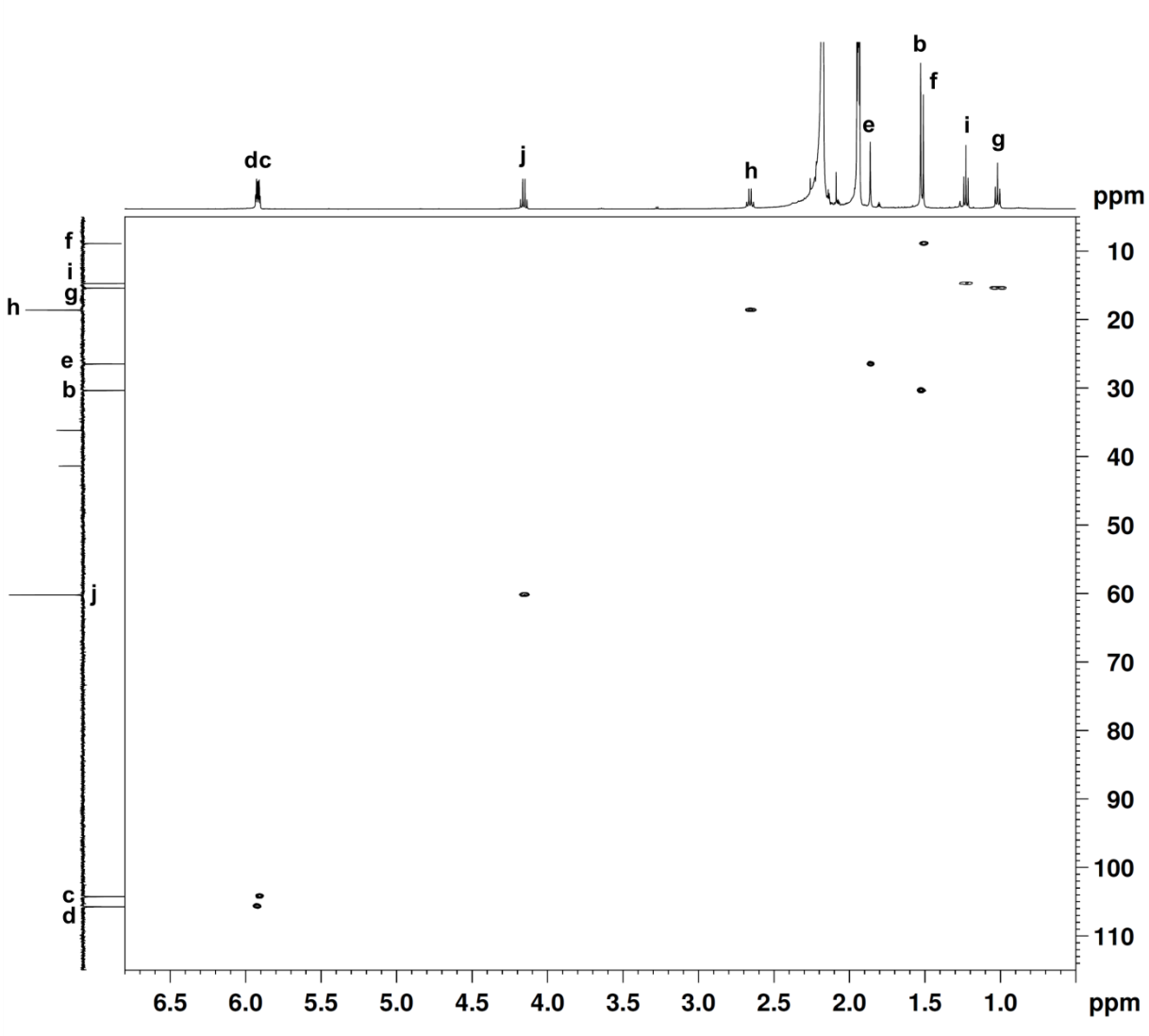

Figure S25. 2D HSQC NMR spectrum of *trans*-**1** (0.4 mM) recorded in CD_3CN.

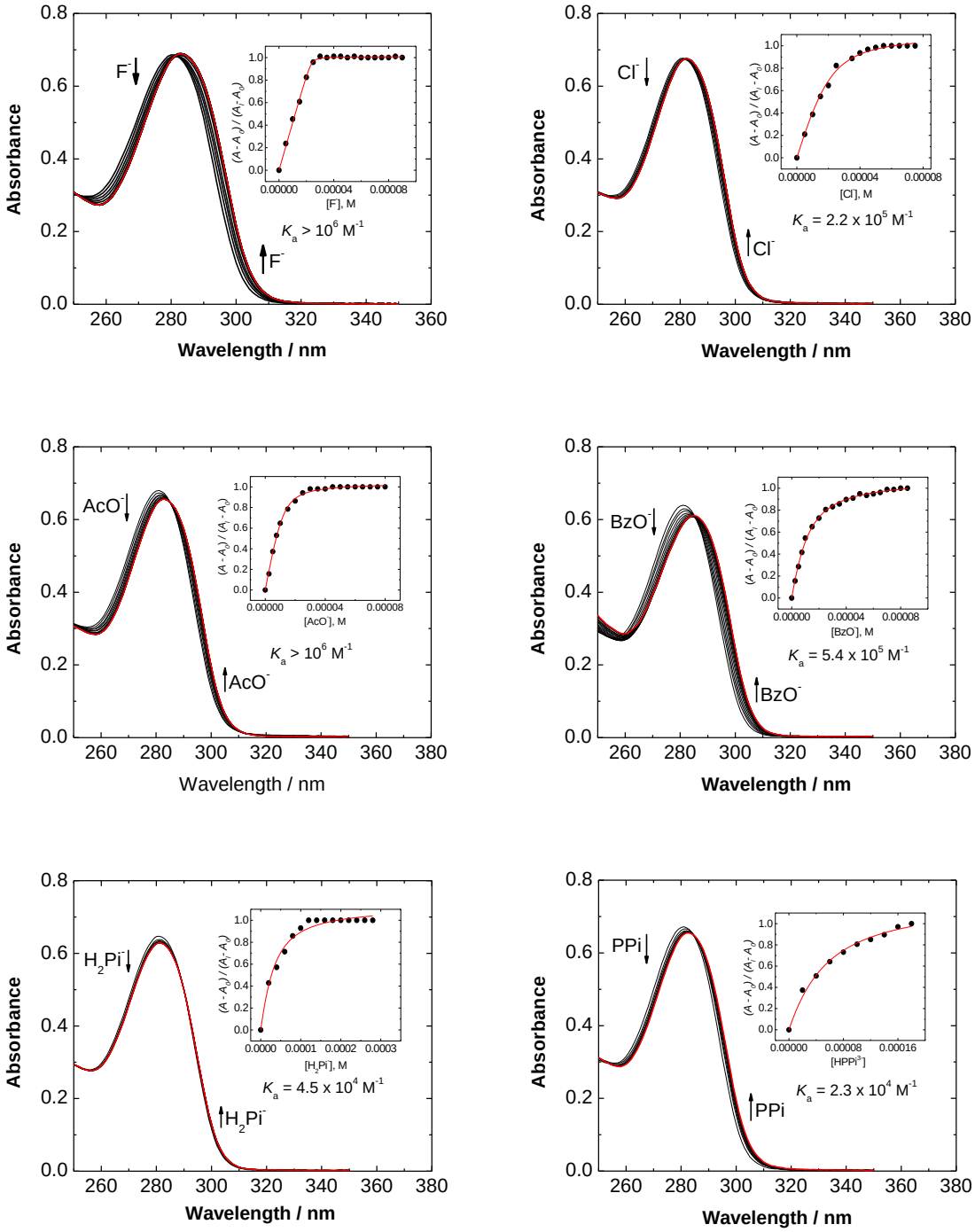

Figure S26. Absorption spectra of *cis*-**1** (20 μM) upon the addition of tetrabutylammonium anions in anhydrous MeCN.

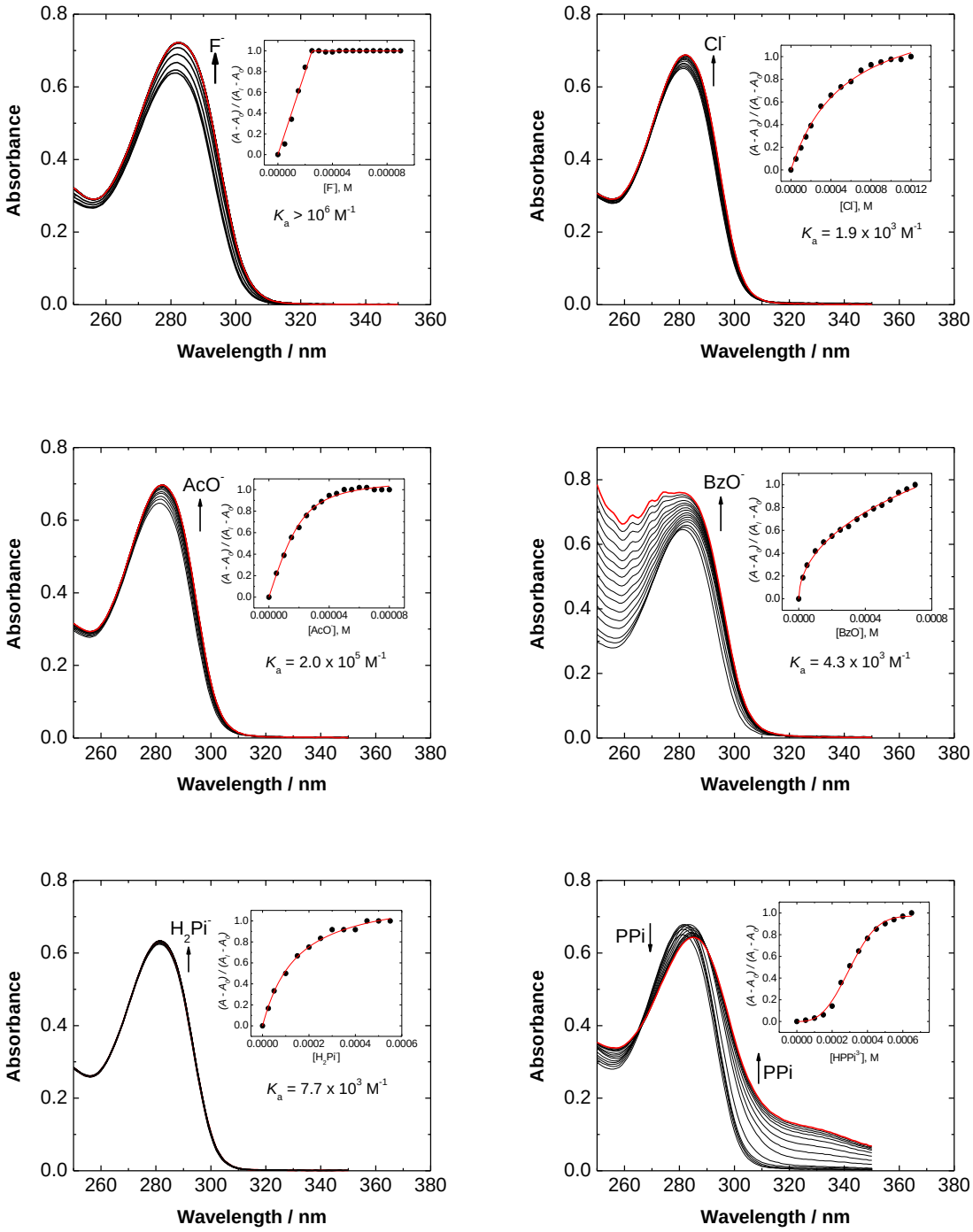

Figure S27. Absorption spectra of *trans*-**1** (20 μM) upon the addition of tetrabutylammonium anions in anhydrous MeCN.

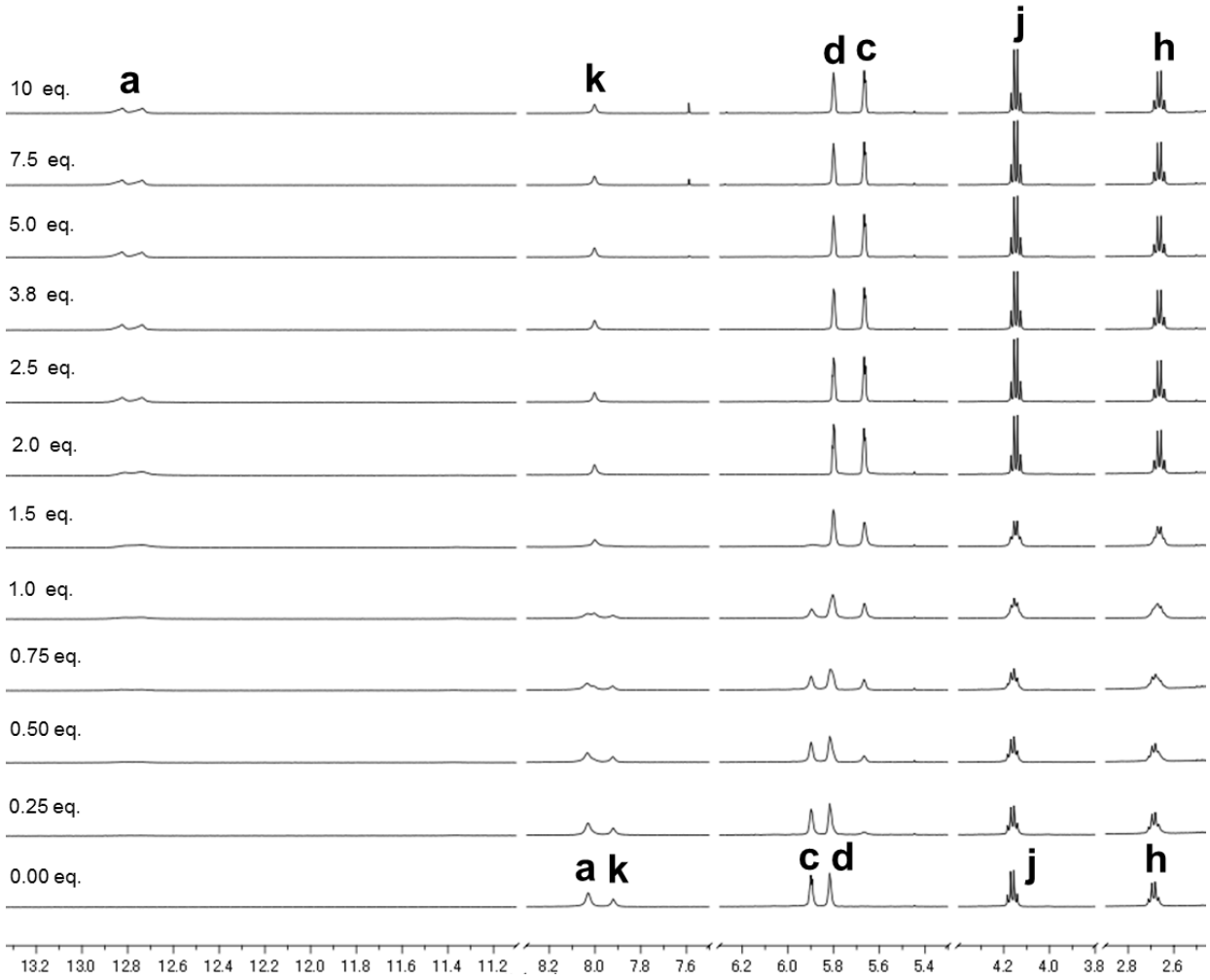

Figure S28. ^{1}H NMR (500 MHz) spectra of *cis*-**1** (0.4 mM) upon the addition of fluoride in CD_3CN.

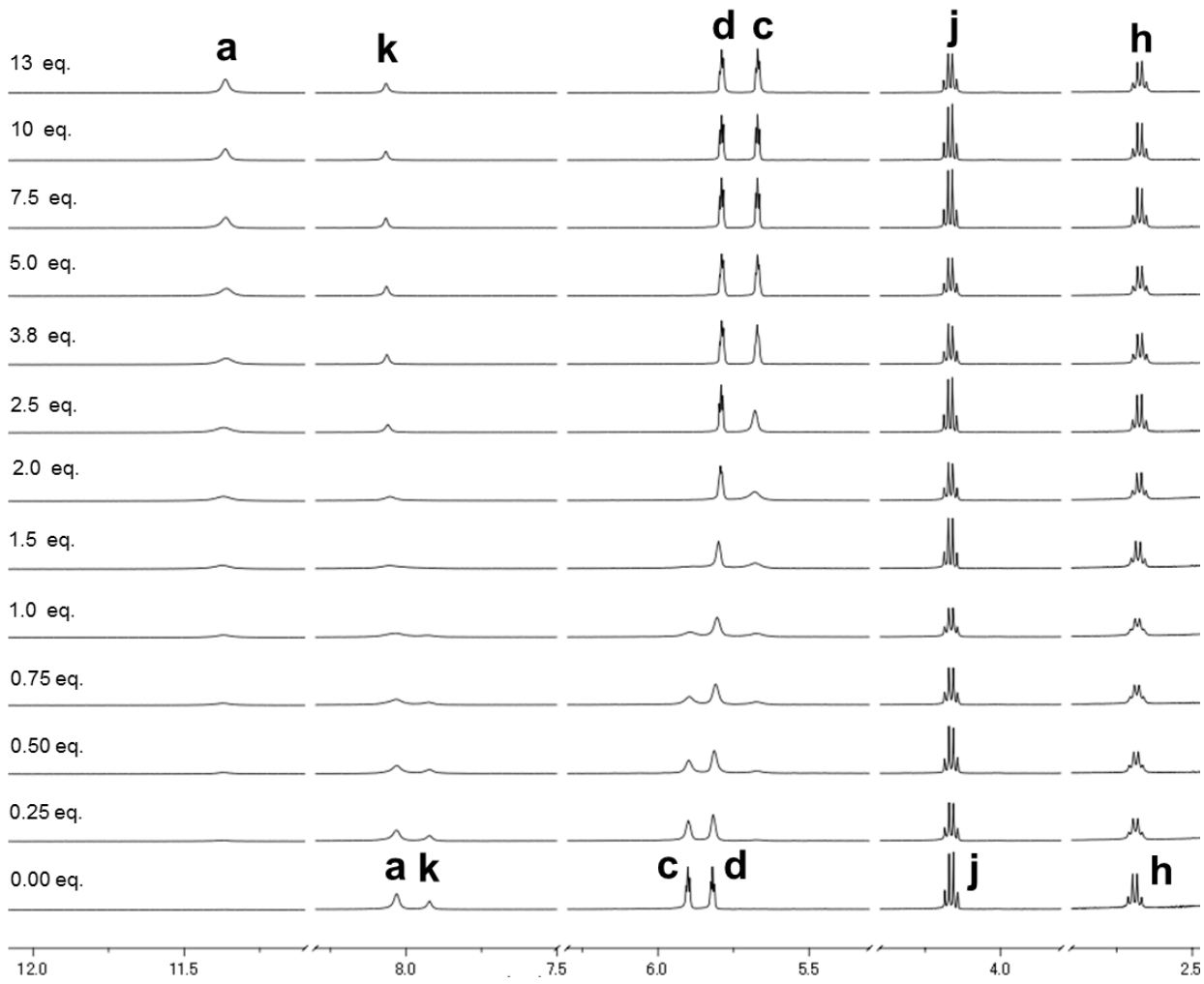

Figure S29. ^{1}H NMR (500 MHz) spectra of *cis*-**1** (0.4 mM) upon the addition of chloride in CD_3CN.

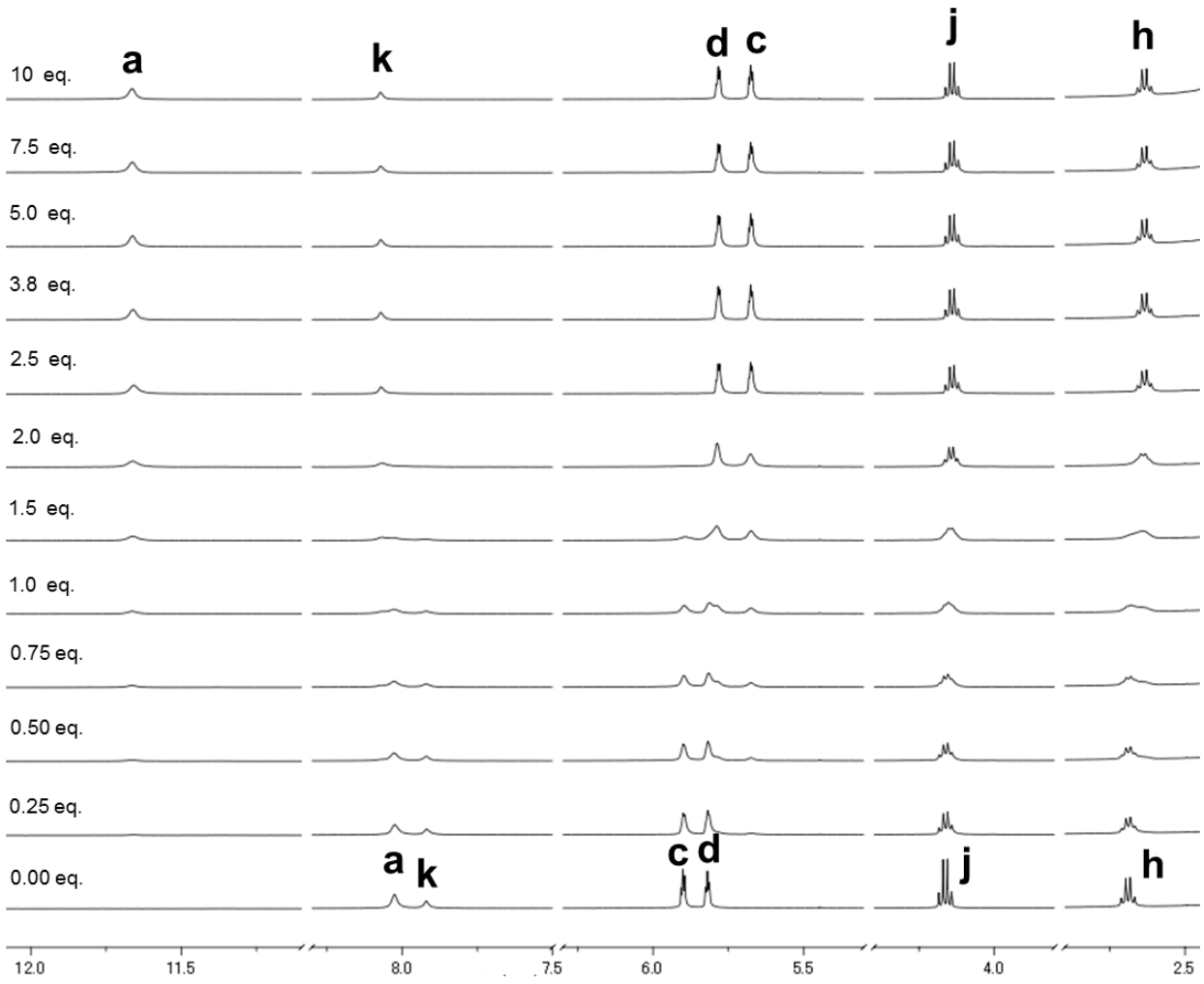

Figure S30. ^{1}H NMR (500 MHz) spectra of *cis*-1 (0.4 mM) upon the addition of acetate in CD_3CN.

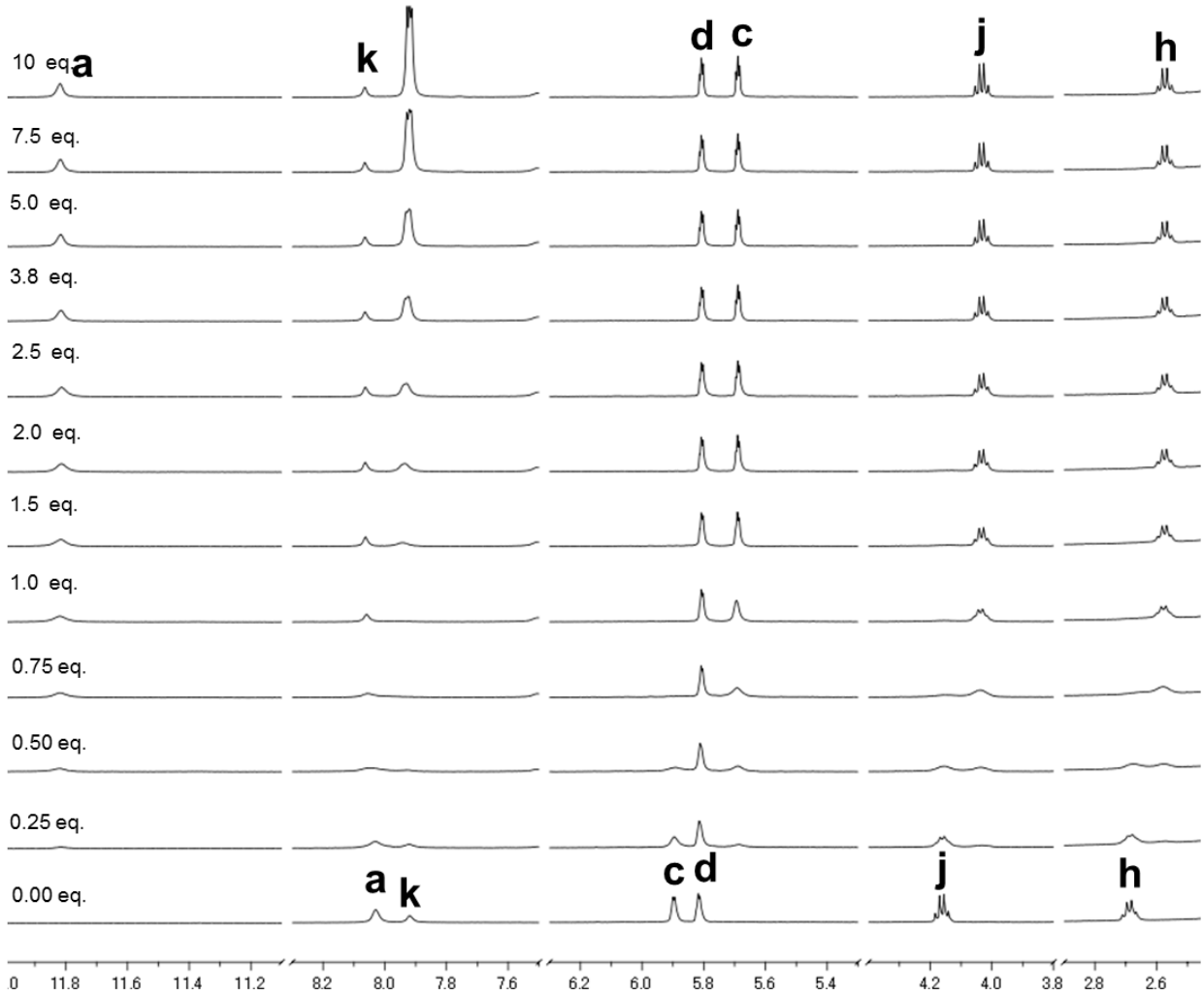

Figure S31. ^{1}H NMR (500 MHz) spectra of *cis*-**1** (0.4 mM) upon the addition of benzoate in CD_3CN.

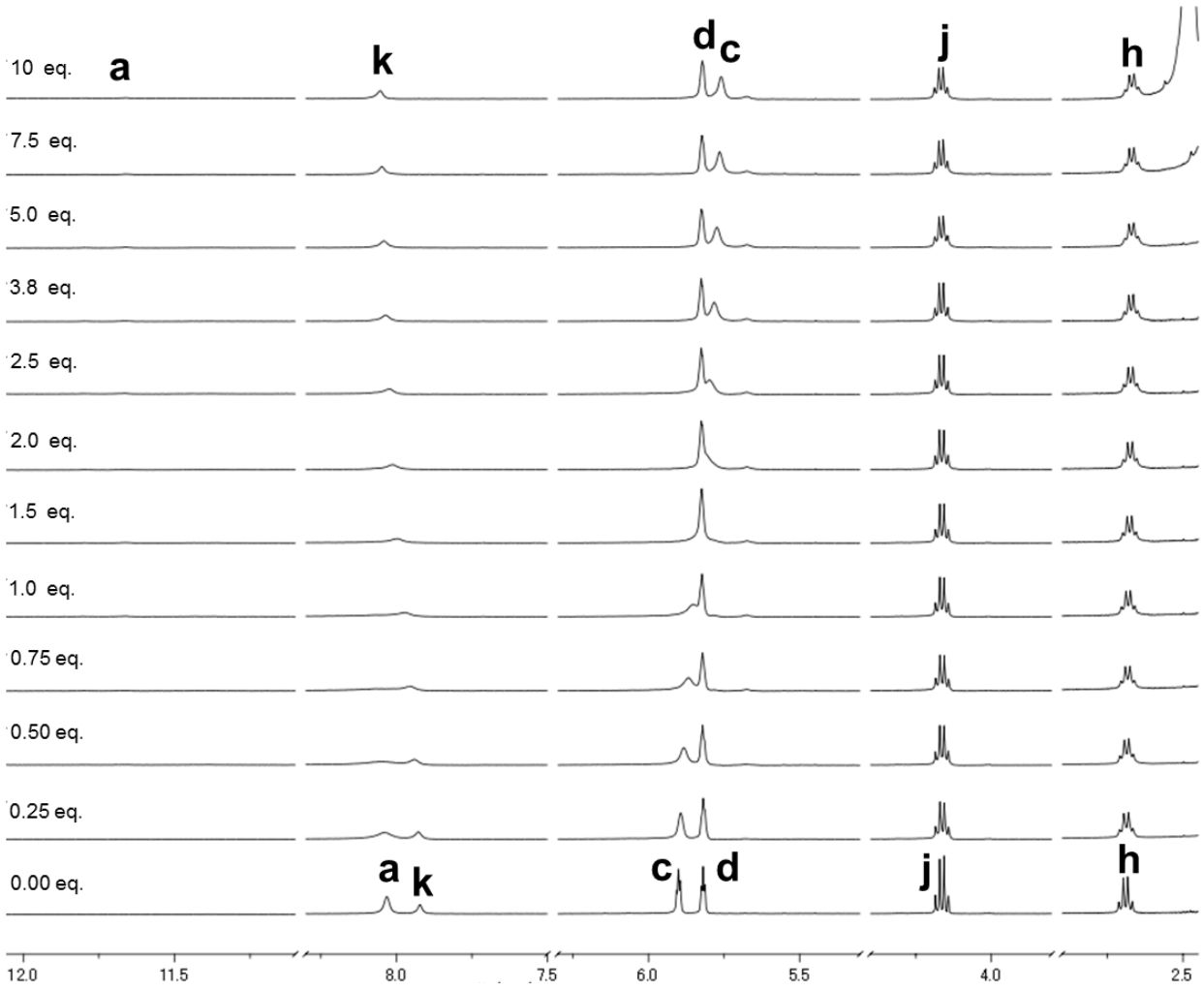

Figure S32. ^{1}H NMR (500 MHz) spectra of *cis*-**1** (0.4 mM) upon the addition of dihydrogen phosphate in CD_3CN.

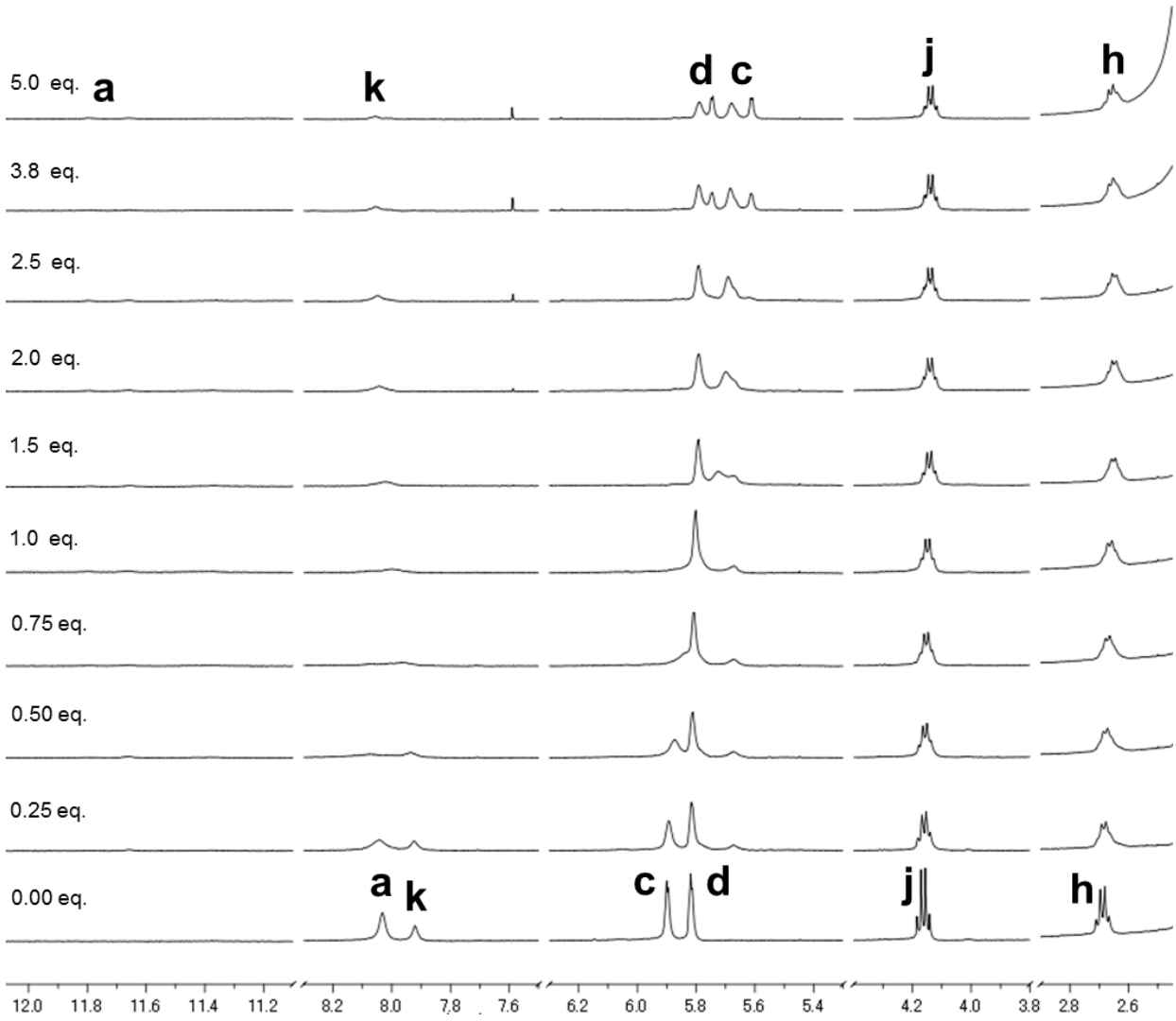

Figure S33. ^{1}H NMR (500 MHz) spectra of *cis*-**1** (0.4 mM) upon the addition of pyrophosphate in CD_3CN.

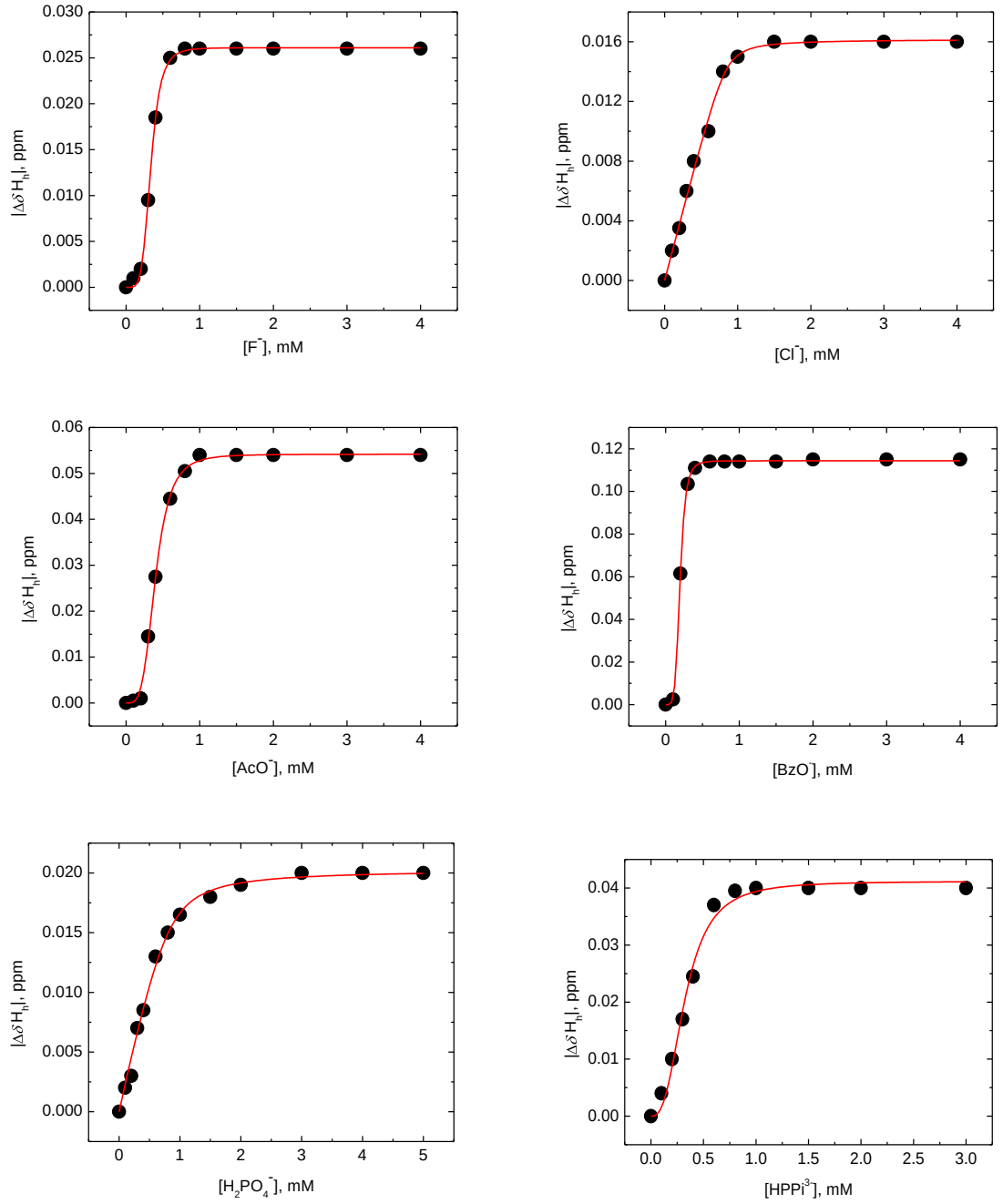

Figure S34. ^{1}H NMR titration plots of ethylene protons (H_h) of *cis*-**1** upon addition of anions in CD_3CN.

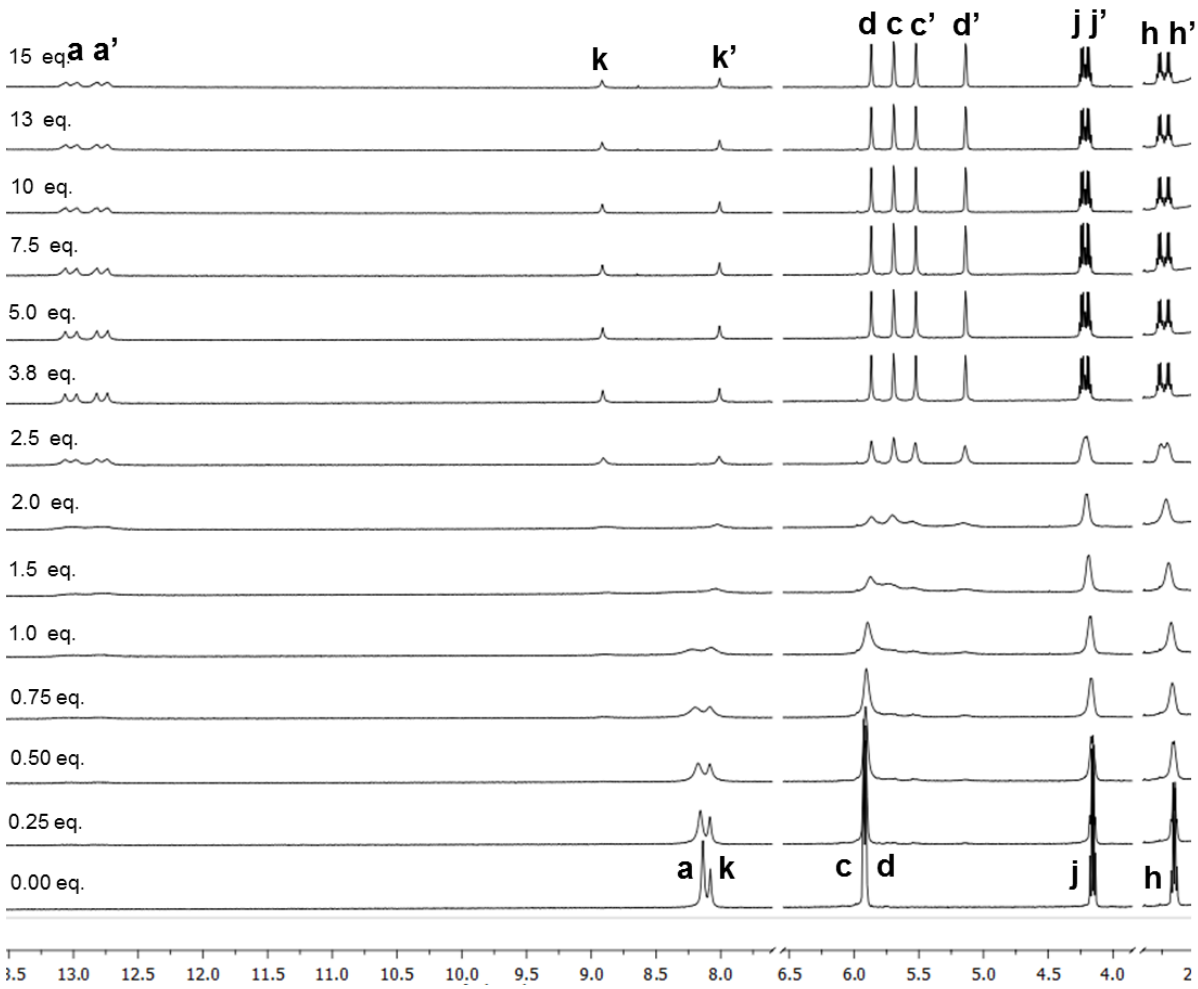

Figure S35. ^{1}H NMR (500 MHz) spectra of *trans*-**1** (0.4 mM) upon the addition of fluoride in CD_3CN.

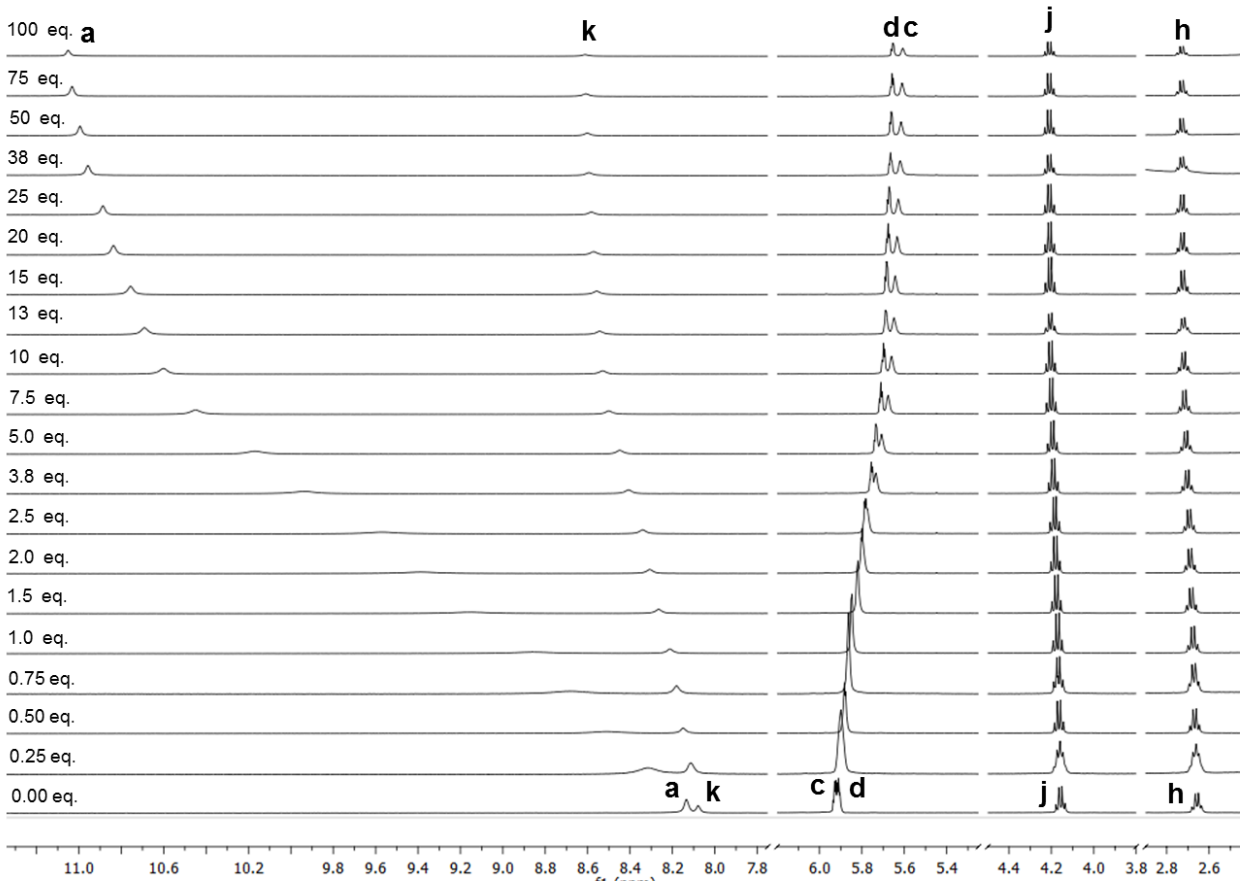

Figure S36. ^{1}H NMR (500 MHz) spectra of *trans*-**1** (0.4 mM) upon the addition of chloride in CD_3CN.

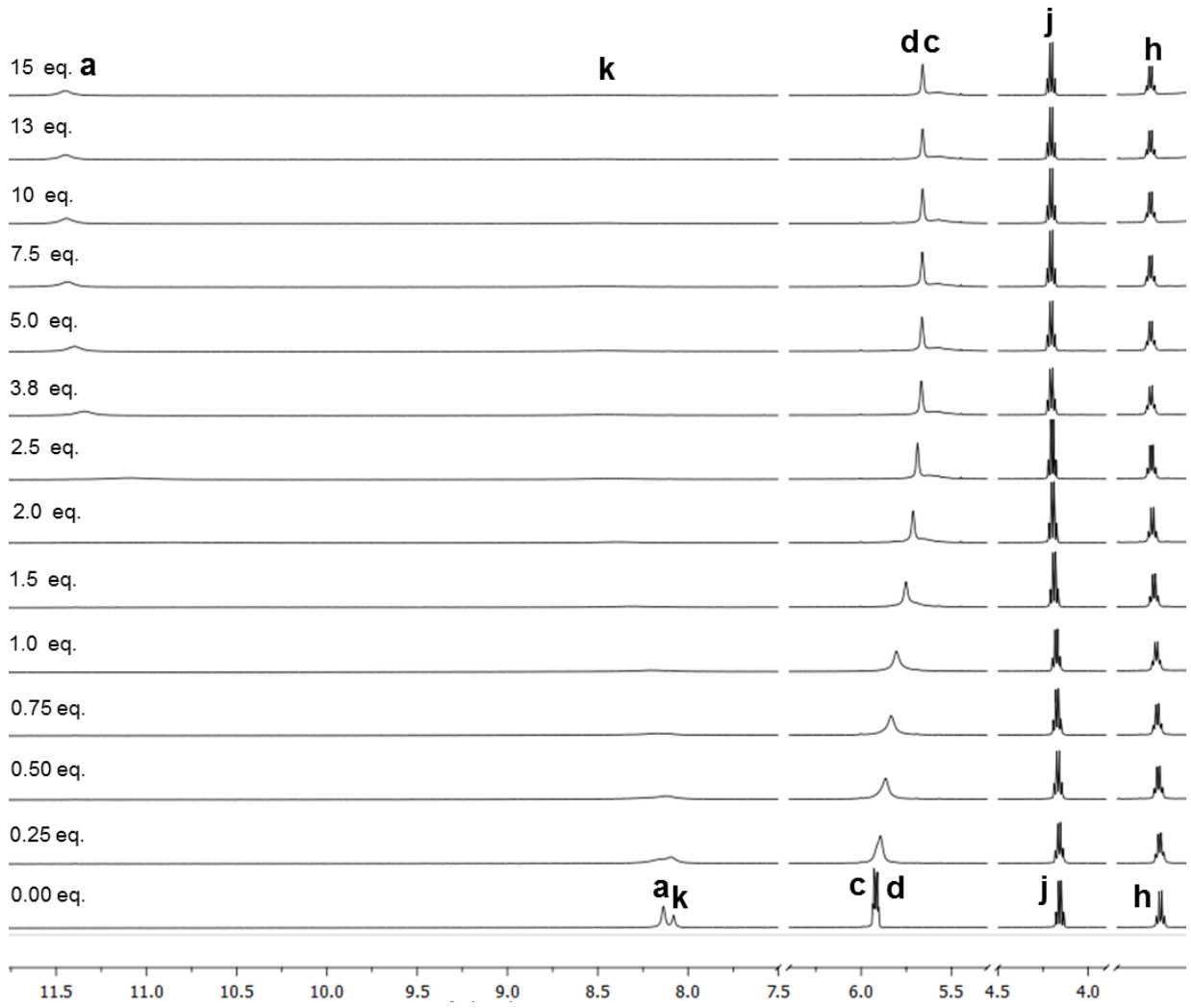

Figure S37. ^{1}H NMR (500 MHz) spectra of *trans*-**1** (0.4 mM) upon the addition of acetate in CD_3CN.

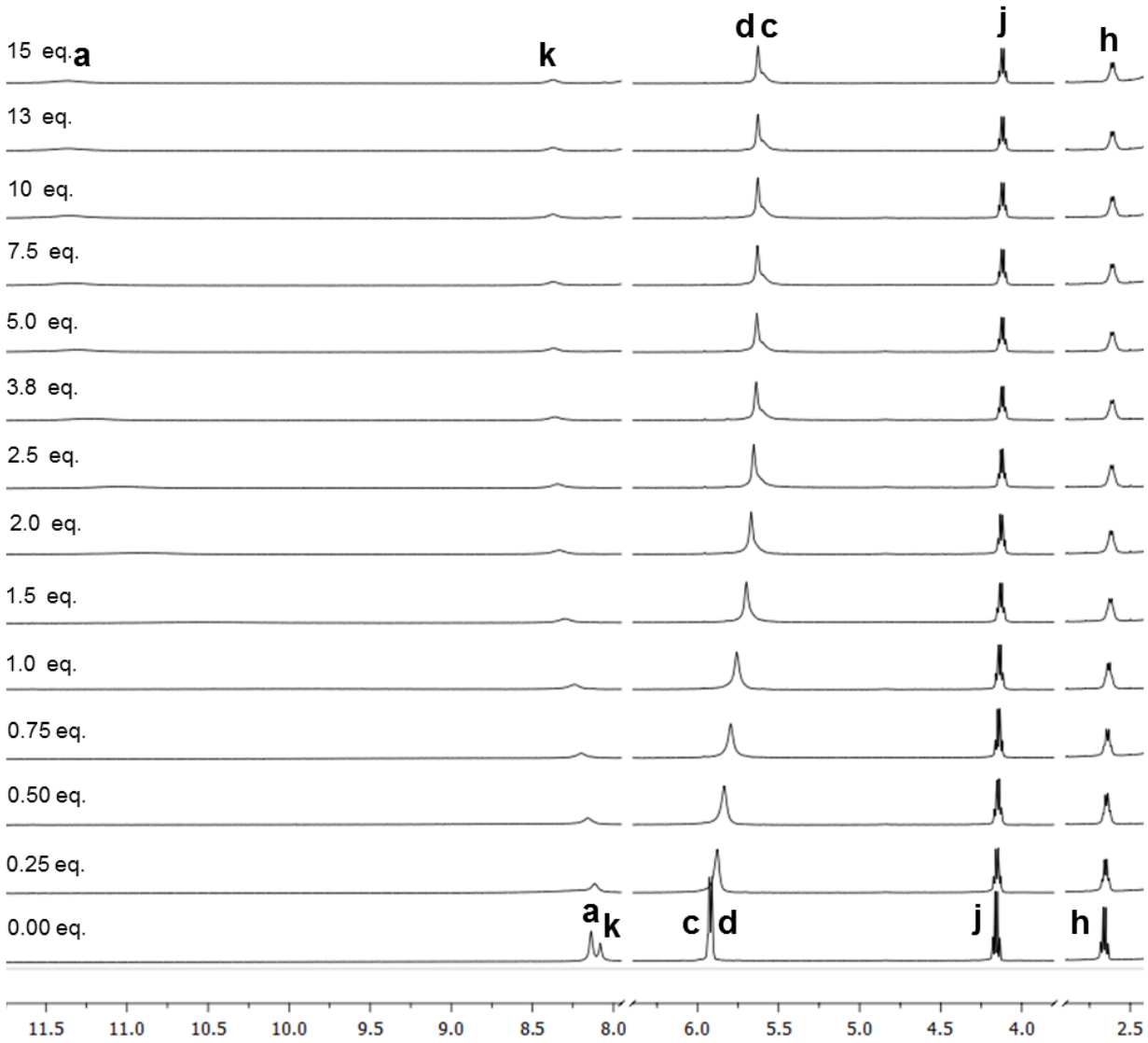

Figure S38. ^{1}H NMR (500 MHz) spectra of *trans*-**1** (0.4 mM) upon the addition of benzoate in CD_3CN.

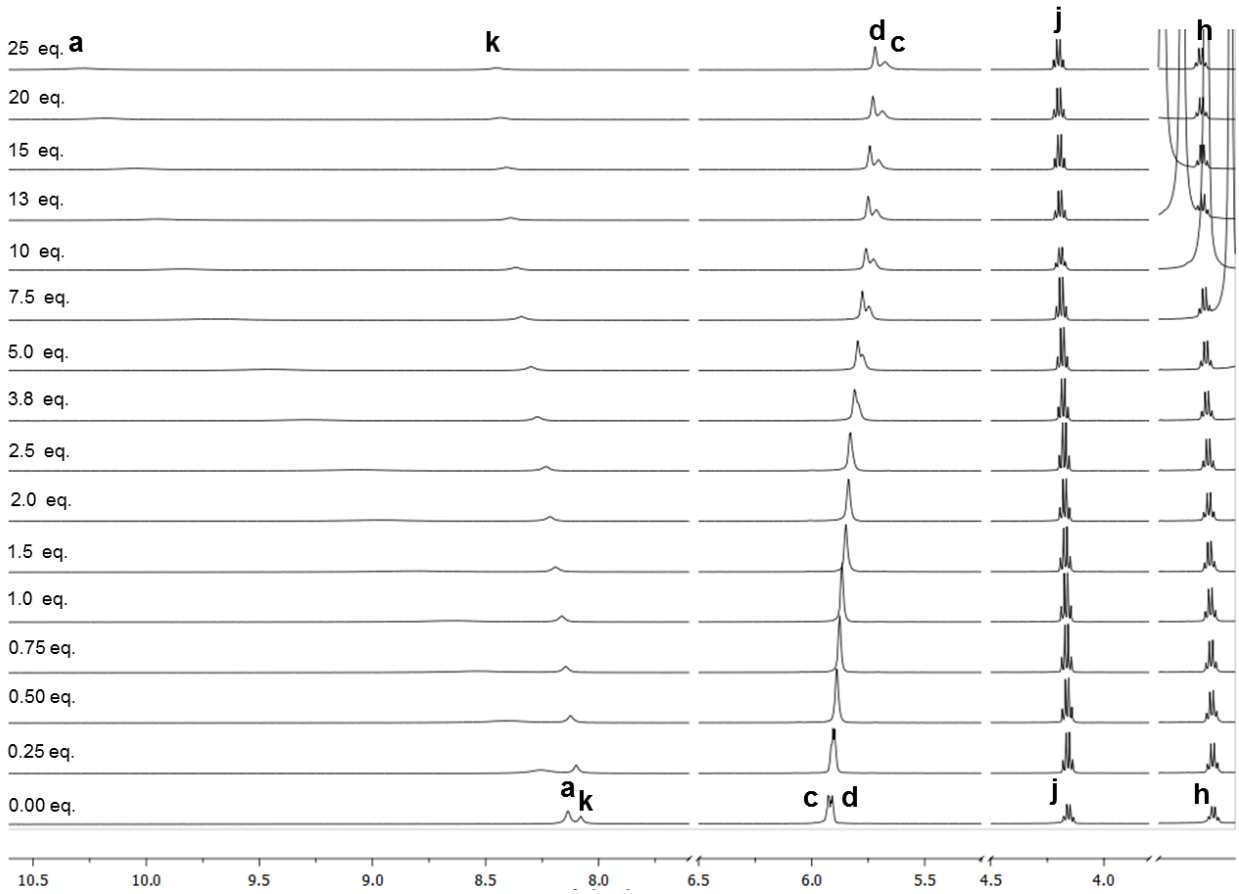

Figure S39. ^{1}H NMR (500 MHz) spectra of *trans*-**1** (0.4 mM) upon the addition of dihydrogen phosphate in CD_3CN.

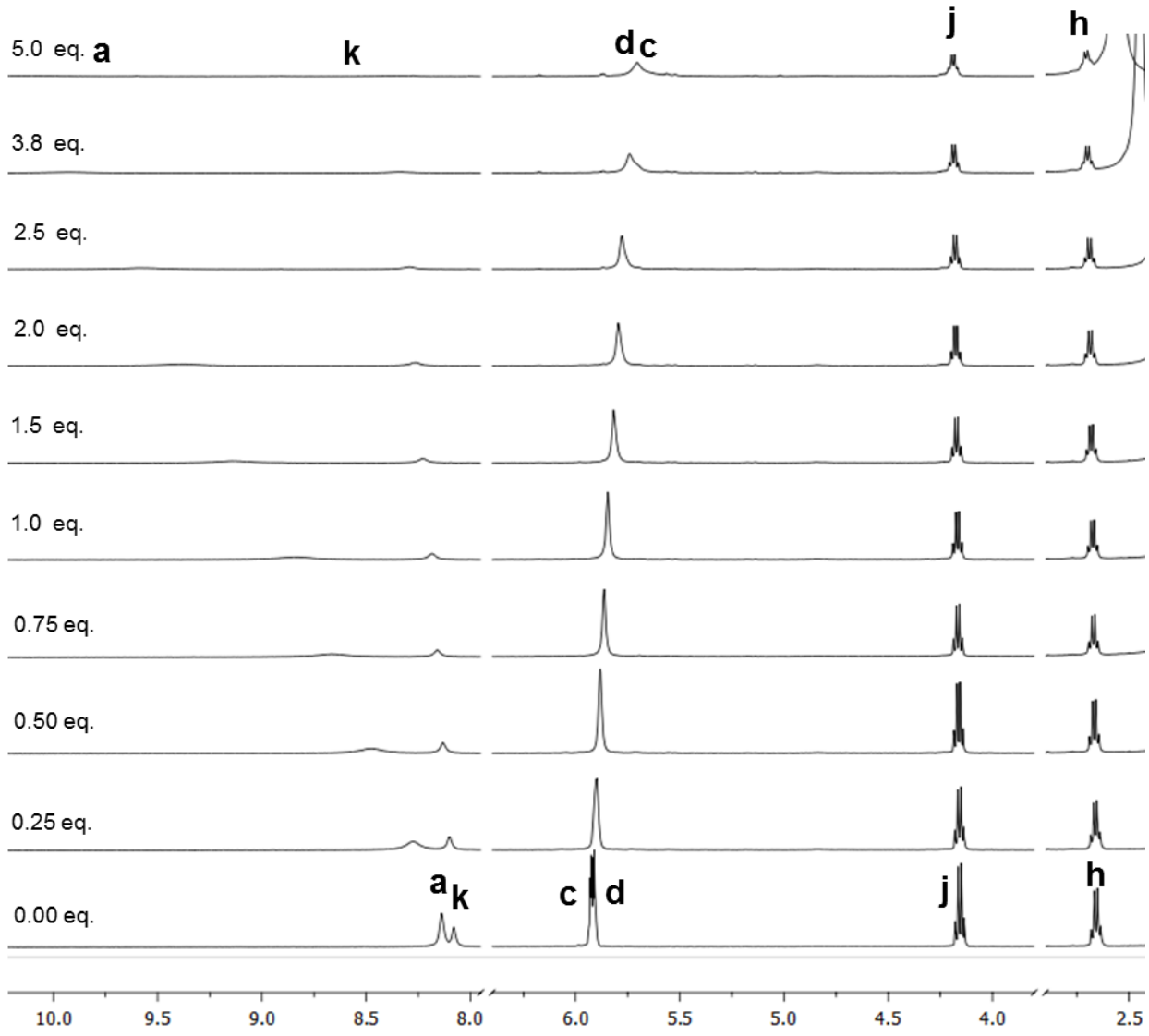

Figure S40. ^{1}H NMR (500 MHz) spectra of *trans*-**1** (0.4 mM) upon the addition of pyrophosphate in CD_3CN.

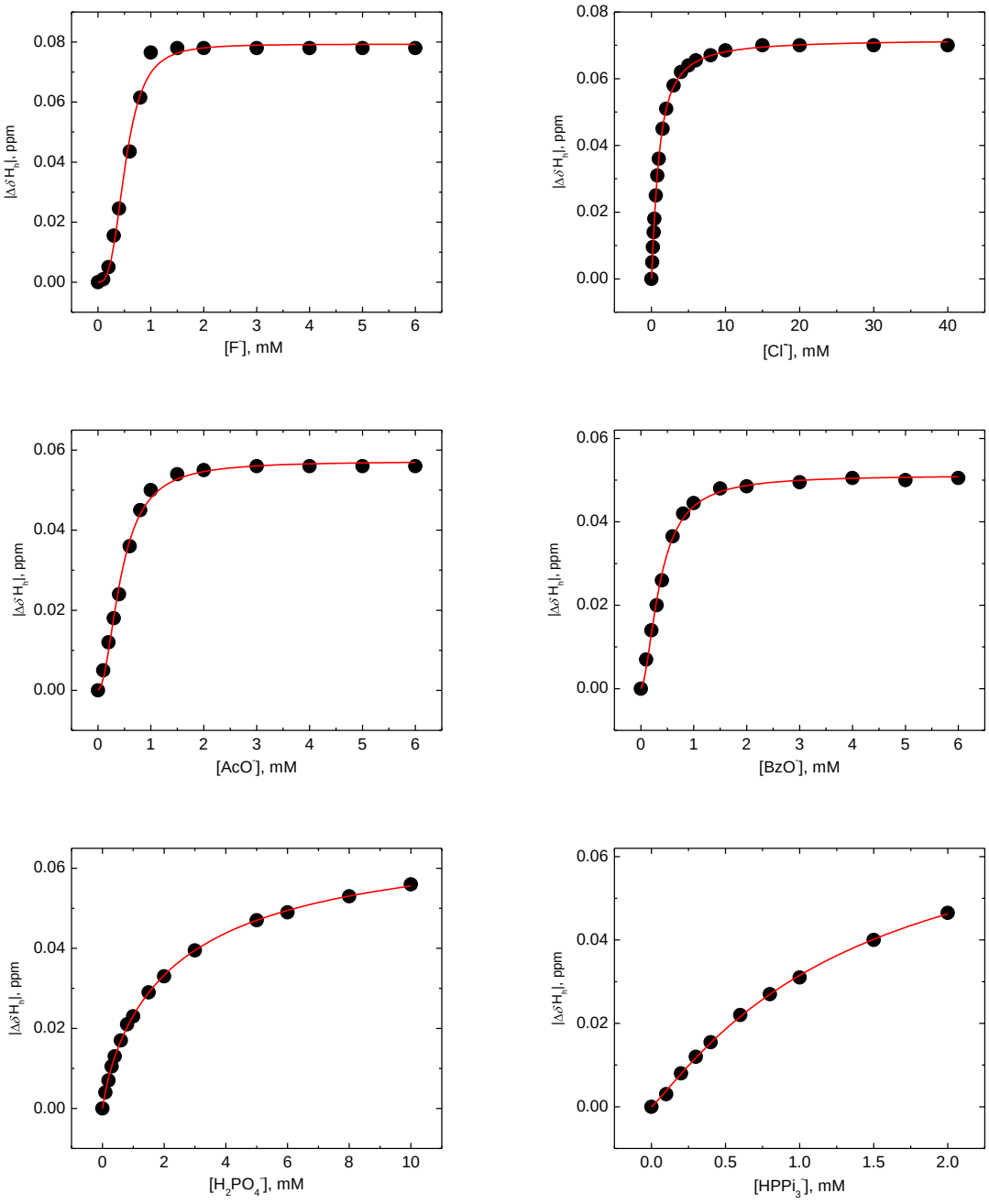

Figure S41. ^{1}H NMR titration plots of ethylene protons (H_h) of *trans*-**1** upon addition of anions in CD_3CN.

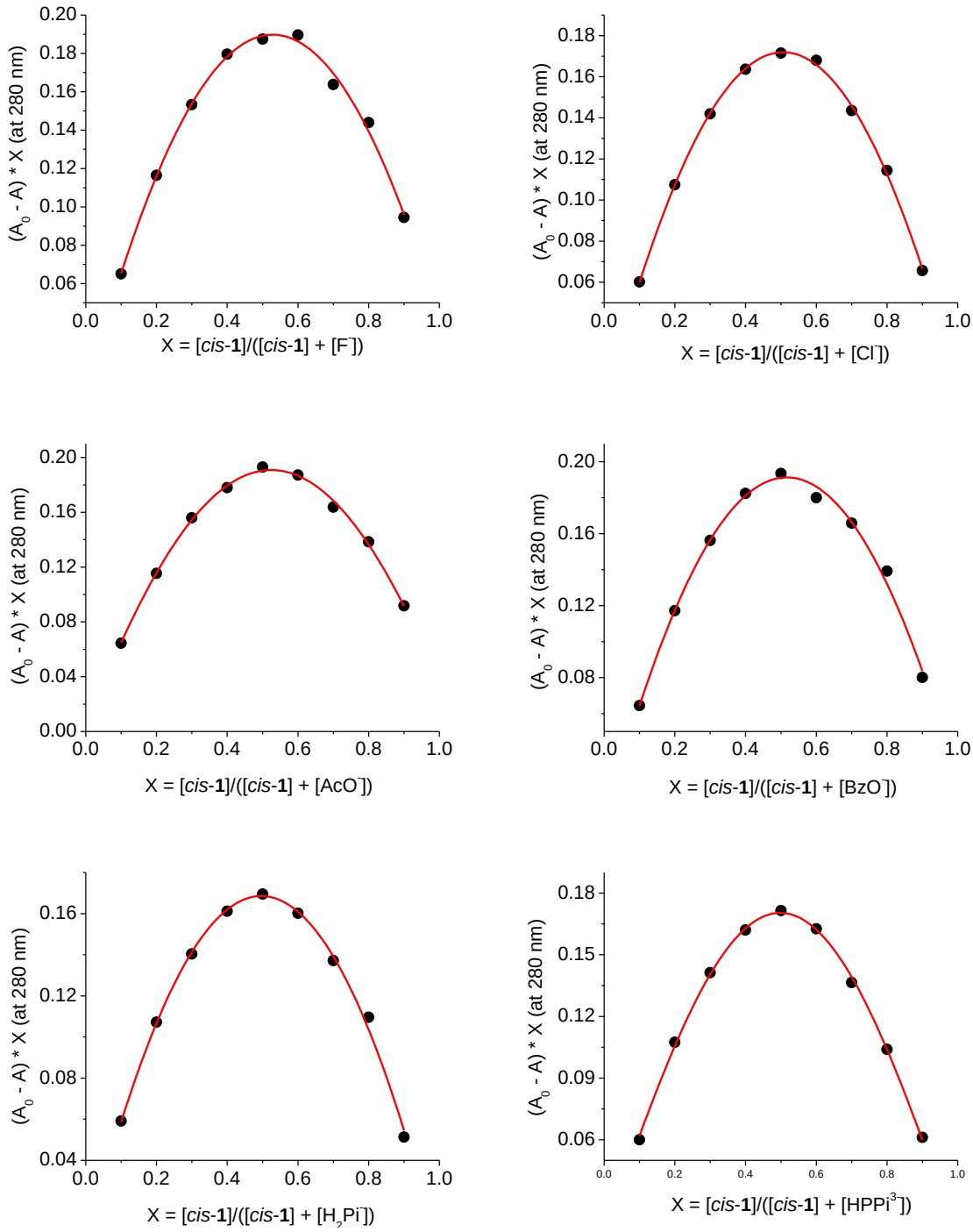

Figure S42. Job's plots of a 1:1 complex of *cis*-**1** and tetrabutylammonium anions, where the absorption at 280 nm was plotted against the mole fraction of *cis*-**1** at invariant total concentration of 20 μM in anhydrous MeCN.

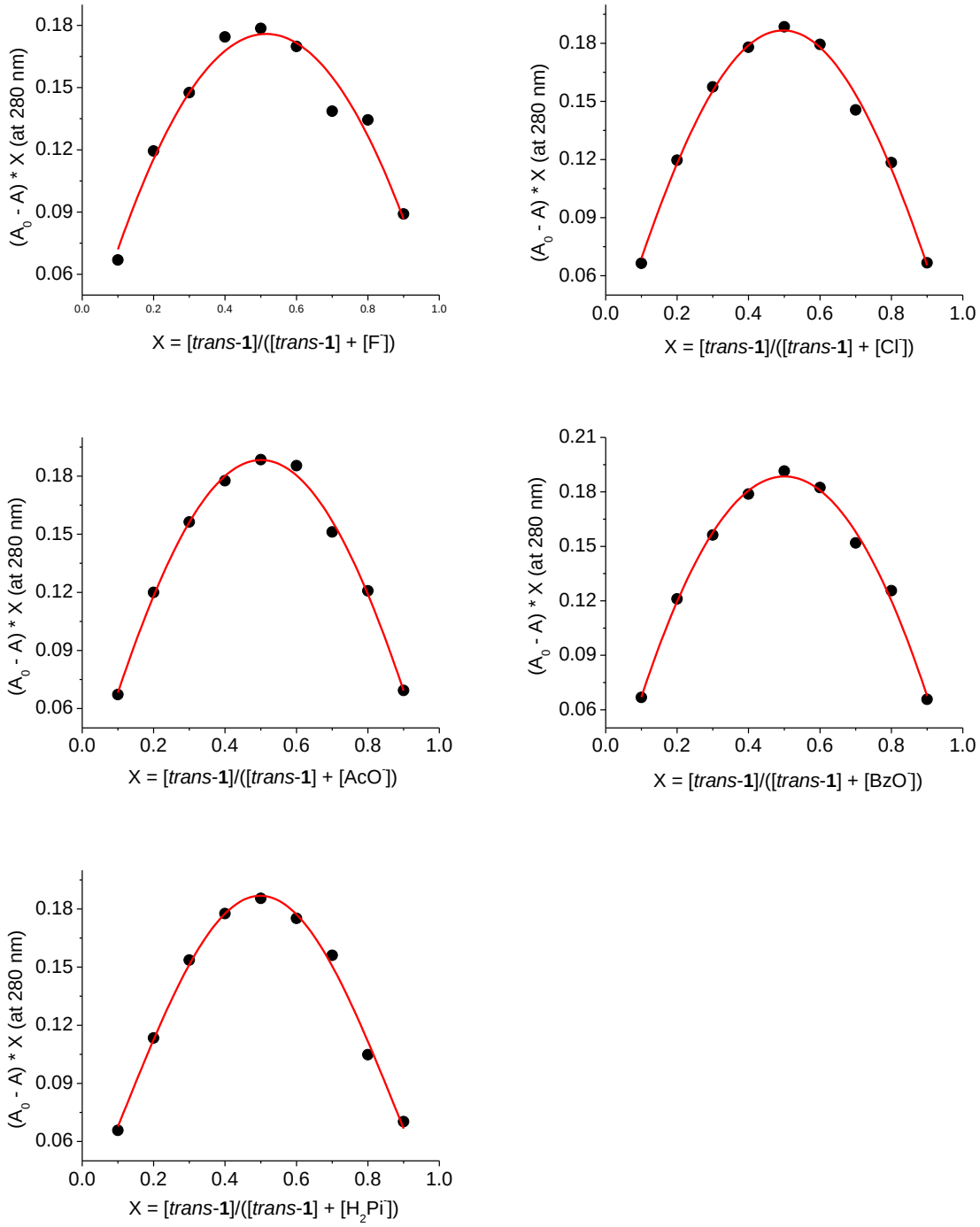

Figure S43. Job's plots of a 1:1 complex of *trans*-**1** and tetrabutylammonium anions, where the absorption at 280 nm was plotted against the mole fraction of *trans*-**1** at invariant total concentration of 20 μM in anhydrous MeCN.

X-ray structural analysis

The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromatized Mo-K_α radiation (λ = 0.71070 Å) at 153 K using an Oxford Cryostream low temperature device. Data reduction was performed using DENZO-SMN.[4] The structure was solved by direct methods using SIR97[5] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[6] The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2 x Ueq of the attached atom (1.5 x Ueq for methyl hydrogen atoms). The function, $\sum w(|Fo|^2 - |Fc|^2)^2$, was minimized, where $w = 1/[(\sigma(Fo))^2 + (0.0499*P)^2 + (1.0626*P)]$ and $P = (|Fo|^2 + 2|Fc|^2)/3$. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the *International Tables for X-ray Crystallography*.[7] All figures were generated using Mercury from CCDC.

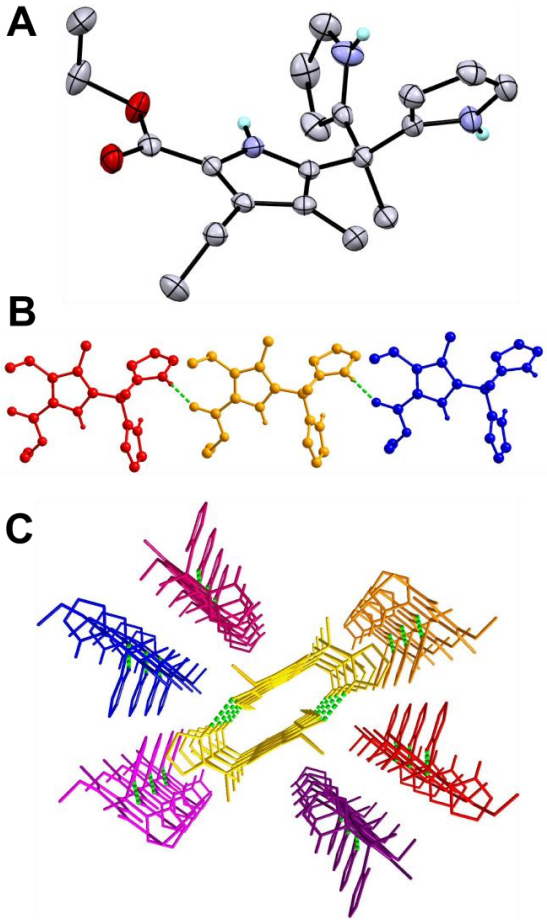

Figure S44. X-ray diffraction analysis of **4** (A). The X-ray analysis reveals an intermolecular hydrogen bond between pyrrole NH and acyl oxygen in the solid state (B). Packing diagram (C) highlights the intermolecular hydrogen bonding. Thermal ellipsoids are scaled to the 50% probability level. All hydrogen atoms bound to carbon atoms are omitted.

Table S1. Crystallographic data and structure refinement for **4**.

Identification code	pa1222
Empirical formula	C20 H25 N3 O2
Formula weight	339.43
Temperature	153(2) K
Wavelength	0.71070 Å
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 32.6975(7) Å alpha = 90 deg. b = 10.0081(3) Å beta = 114.622(2)deg. c = 24.9344(8) Å gamma = 90 deg.
Volume	7417.6(4) A^3
Z, Calculated density	16, 1.216 Mg/m^3
Absorption coefficient	0.080 mm^{-1}
F(000)	2912
Crystal size	0.2 x 0.1 x 0.1 mm
Theta range for data collection	1.80 to 27.48 deg.
Limiting indices	-41<=h<=42, -12<=k<=12, -32<=l<=32
Reflections collected / unique	15372 / 8481 [R(int) = 0.0510]
Completeness to theta =	27.48 99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8481 / 0 / 459
Goodness-of-fit on F^2	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0557, wR2 = 0.1056

R indices (all data)	R1 = 0.1219, wR2 = 0.1260
Largest diff. peak and hole	0.306 and -0.309 e. $Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	4491(1)	9021(1)	7002(1)	35(1)
O(2)	4145(1)	7169(1)	7122(1)	40(1)
N(1)	4987(1)	7581(2)	6555(1)	27(1)
N(2)	6035(1)	9058(2)	6500(1)	34(1)
N(3)	6175(1)	6152(2)	7043(1)	37(1)
C(1)	4696(1)	6970(2)	6750(1)	27(1)
C(2)	4734(1)	5602(2)	6694(1)	32(1)
C(3)	5056(1)	5398(2)	6460(1)	32(1)
C(4)	5205(1)	6643(2)	6375(1)	28(1)
C(5)	5540(1)	7010(2)	6120(1)	30(1)
C(6)	5624(1)	8504(2)	6158(1)	30(1)
C(7)	5341(1)	9547(2)	5888(1)	39(1)
C(8)	5586(1)	10747(2)	6073(1)	45(1)
C(9)	6012(1)	10423(2)	6446(1)	43(1)
C(10)	5978(1)	6257(2)	6441(1)	32(1)
C(11)	6255(1)	5620(2)	6236(1)	39(1)
C(12)	6625(1)	5116(2)	6724(1)	47(1)
C(13)	6568(1)	5451(2)	7216(1)	44(1)
C(14)	4420(1)	7692(2)	6973(1)	30(1)

C(15)	4211(1)	9788(2)	7217(1)	44(1)
C(16)	4406(1)	11134(2)	7384(1)	48(1)
C(17)	4477(1)	4538(2)	6846(1)	42(1)
C(18)	4007(1)	4322(2)	6363(1)	55(1)
C(19)	5206(1)	4058(2)	6337(1)	46(1)
C(20)	5339(1)	6605(2)	5462(1)	40(1)
O(1A)	6485(1)	3958(1)	4990(1)	37(1)
O(2A)	7028(1)	2506(1)	5525(1)	37(1)
N(1A)	6988(1)	6095(1)	5503(1)	25(1)
N(2A)	6343(1)	8824(2)	5390(1)	39(1)
N(3A)	7214(1)	10461(2)	6396(1)	33(1)
C(1A)	7160(1)	4831(2)	5653(1)	25(1)
C(2A)	7589(1)	4953(2)	6101(1)	25(1)
C(3A)	7671(1)	6335(2)	6219(1)	27(1)
C(4A)	7289(1)	7019(2)	5837(1)	25(1)
C(5A)	7179(1)	8506(2)	5744(1)	27(1)
C(6A)	6709(1)	8710(2)	5265(1)	28(1)
C(7A)	6550(1)	8777(2)	4664(1)	44(1)
C(8A)	6080(1)	8945(2)	4430(1)	47(1)
C(9A)	5961(1)	8972(2)	4886(1)	44(1)
C(10A)	7205(1)	9104(2)	6317(1)	27(1)
C(11A)	7196(1)	8526(2)	6811(1)	32(1)
C(12A)	7204(1)	9576(2)	7197(1)	38(1)
C(13A)	7214(1)	10744(2)	6931(1)	38(1)
C(14A)	6900(1)	3651(2)	5396(1)	28(1)
C(15A)	6173(1)	2849(2)	4751(1)	45(1)
C(16A)	5935(1)	2585(3)	5126(2)	87(1)
C(17A)	7906(1)	3818(2)	6394(1)	30(1)
C(18A)	8105(1)	3174(2)	5998(1)	42(1)
C(19A)	8091(1)	6934(2)	6683(1)	34(1)

C(20A)	7519(1)	9193(2)	5547(1)	36(1)

Table S3. Bond lengths [Å] and angles [deg] for **4.**

O(1)-C(14)	1.346(2)
O(1)-C(15)	1.456(2)
O(2)-C(14)	1.224(2)
N(1)-C(4)	1.363(2)
N(1)-C(1)	1.378(2)
N(1)-H(1A)	0.8800
N(2)-C(9)	1.371(3)
N(2)-C(6)	1.373(2)
N(2)-H(2A)	0.8800
N(3)-C(13)	1.367(3)
N(3)-C(10)	1.369(2)
N(3)-H(3A)	0.8800
C(1)-C(2)	1.386(3)
C(1)-C(14)	1.437(3)
C(2)-C(3)	1.416(3)
C(2)-C(17)	1.499(3)
C(3)-C(4)	1.386(3)
C(3)-C(19)	1.503(3)
C(4)-C(5)	1.525(3)
C(5)-C(6)	1.516(3)
C(5)-C(10)	1.518(3)
C(5)-C(20)	1.544(3)
C(6)-C(7)	1.371(3)
C(7)-C(8)	1.410(3)

C(7)-H(7A)	0.9500
C(8)-C(9)	1.352(3)
C(8)-H(8A)	0.9500
C(9)-H(9A)	0.9500
C(10)-C(11)	1.370(3)
C(11)-C(12)	1.404(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.358(3)
C(12)-H(12A)	0.9500
C(13)-H(13A)	0.9500
C(15)-C(16)	1.474(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.522(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
O(1A)-C(14A)	1.347(2)
O(1A)-C(15A)	1.456(2)

O(2A)-C(14A)	1.217(2)
N(1A)-C(4A)	1.355(2)
N(1A)-C(1A)	1.372(2)
N(1A)-H(1AA)	0.8800
N(2A)-C(6A)	1.361(2)
N(2A)-C(9A)	1.362(3)
N(2A)-H(2AA)	0.8800
N(3A)-C(13A)	1.361(2)
N(3A)-C(10A)	1.371(2)
N(3A)-H(3AA)	0.8800
C(1A)-C(2A)	1.388(2)
C(1A)-C(14A)	1.440(3)
C(2A)-C(3A)	1.417(3)
C(2A)-C(17A)	1.506(3)
C(3A)-C(4A)	1.394(3)
C(3A)-C(19A)	1.503(3)
C(4A)-C(5A)	1.525(3)
C(5A)-C(6A)	1.518(3)
C(5A)-C(10A)	1.520(2)
C(5A)-C(20A)	1.548(3)
C(6A)-C(7A)	1.367(3)
C(7A)-C(8A)	1.409(3)
C(7A)-H(7AA)	0.9500
C(8A)-C(9A)	1.347(3)
C(8A)-H(8AA)	0.9500
C(9A)-H(9AA)	0.9500
C(10A)-C(11A)	1.372(3)
C(11A)-C(12A)	1.418(3)
C(11A)-H(11B)	0.9500
C(12A)-C(13A)	1.351(3)

C(12A)-H(12B)	0.9500
C(13A)-H(13B)	0.9500
C(15A)-C(16A)	1.471(3)
C(15A)-H(15C)	0.9900
C(15A)-H(15D)	0.9900
C(16A)-H(16D)	0.9800
C(16A)-H(16E)	0.9800
C(16A)-H(16F)	0.9800
C(17A)-C(18A)	1.532(3)
C(17A)-H(17C)	0.9900
C(17A)-H(17D)	0.9900
C(18A)-H(18D)	0.9800
C(18A)-H(18E)	0.9800
C(18A)-H(18F)	0.9800
C(19A)-H(19D)	0.9800
C(19A)-H(19E)	0.9800
C(19A)-H(19F)	0.9800
C(20A)-H(20D)	0.9800
C(20A)-H(20E)	0.9800
C(20A)-H(20F)	0.9800
C(14)-O(1)-C(15)	114.91(15)
C(4)-N(1)-C(1)	110.06(15)
C(4)-N(1)-H(1A)	125.0
C(1)-N(1)-H(1A)	125.0
C(9)-N(2)-C(6)	109.98(17)
C(9)-N(2)-H(2A)	125.0
C(6)-N(2)-H(2A)	125.0
C(13)-N(3)-C(10)	109.57(17)
C(13)-N(3)-H(3A)	125.2
C(10)-N(3)-H(3A)	125.2

N(1)-C(1)-C(2)	107.46(16)
N(1)-C(1)-C(14)	123.39(17)
C(2)-C(1)-C(14)	129.14(18)
C(1)-C(2)-C(3)	107.20(17)
C(1)-C(2)-C(17)	126.45(19)
C(3)-C(2)-C(17)	126.34(18)
C(4)-C(3)-C(2)	107.66(17)
C(4)-C(3)-C(19)	127.22(18)
C(2)-C(3)-C(19)	125.12(18)
N(1)-C(4)-C(3)	107.61(16)
N(1)-C(4)-C(5)	122.51(16)
C(3)-C(4)-C(5)	129.86(17)
C(6)-C(5)-C(10)	110.55(16)
C(6)-C(5)-C(4)	110.69(15)
C(10)-C(5)-C(4)	110.07(15)
C(6)-C(5)-C(20)	108.14(16)
C(10)-C(5)-C(20)	108.76(15)
C(4)-C(5)-C(20)	108.57(15)
C(7)-C(6)-N(2)	106.40(17)
C(7)-C(6)-C(5)	130.80(18)
N(2)-C(6)-C(5)	122.80(17)
C(6)-C(7)-C(8)	108.26(19)
C(6)-C(7)-H(7A)	125.9
C(8)-C(7)-H(7A)	125.9
C(9)-C(8)-C(7)	107.56(19)
C(9)-C(8)-H(8A)	126.2
C(7)-C(8)-H(8A)	126.2
C(8)-C(9)-N(2)	107.79(19)
C(8)-C(9)-H(9A)	126.1
N(2)-C(9)-H(9A)	126.1

N(3)-C(10)-C(11)	107.06(17)
N(3)-C(10)-C(5)	121.76(16)
C(11)-C(10)-C(5)	131.16(18)
C(10)-C(11)-C(12)	107.90(19)
C(10)-C(11)-H(11A)	126.0
C(12)-C(11)-H(11A)	126.0
C(13)-C(12)-C(11)	107.57(19)
C(13)-C(12)-H(12A)	126.2
C(11)-C(12)-H(12A)	126.2
C(12)-C(13)-N(3)	107.90(19)
C(12)-C(13)-H(13A)	126.1
N(3)-C(13)-H(13A)	126.1
O(2)-C(14)-O(1)	122.49(18)
O(2)-C(14)-C(1)	124.14(18)
O(1)-C(14)-C(1)	113.37(16)
O(1)-C(15)-C(16)	108.83(16)
O(1)-C(15)-H(15A)	109.9
C(16)-C(15)-H(15A)	109.9
O(1)-C(15)-H(15B)	109.9
C(16)-C(15)-H(15B)	109.9
H(15A)-C(15)-H(15B)	108.3
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(2)-C(17)-C(18)	112.83(17)
C(2)-C(17)-H(17A)	109.0
C(18)-C(17)-H(17A)	109.0

C(2)-C(17)-H(17B)	109.0
C(18)-C(17)-H(17B)	109.0
H(17A)-C(17)-H(17B)	107.8
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(3)-C(19)-H(19A)	109.5
C(3)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(3)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(5)-C(20)-H(20A)	109.5
C(5)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(5)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(14A)-O(1A)-C(15A)	116.56(15)
C(4A)-N(1A)-C(1A)	110.54(15)
C(4A)-N(1A)-H(1AA)	124.7
C(1A)-N(1A)-H(1AA)	124.7
C(6A)-N(2A)-C(9A)	110.67(17)
C(6A)-N(2A)-H(2AA)	124.7
C(9A)-N(2A)-H(2AA)	124.7
C(13A)-N(3A)-C(10A)	109.77(16)
C(13A)-N(3A)-H(3AA)	125.1

C(10A)-N(3A)-H(3AA)	125.1
N(1A)-C(1A)-C(2A)	107.52(15)
N(1A)-C(1A)-C(14A)	122.38(16)
C(2A)-C(1A)-C(14A)	129.94(17)
C(1A)-C(2A)-C(3A)	107.04(16)
C(1A)-C(2A)-C(17A)	125.84(16)
C(3A)-C(2A)-C(17A)	127.11(17)
C(4A)-C(3A)-C(2A)	107.43(16)
C(4A)-C(3A)-C(19A)	126.95(17)
C(2A)-C(3A)-C(19A)	125.60(17)
N(1A)-C(4A)-C(3A)	107.47(16)
N(1A)-C(4A)-C(5A)	120.51(16)
C(3A)-C(4A)-C(5A)	132.00(16)
C(6A)-C(5A)-C(10A)	109.08(14)
C(6A)-C(5A)-C(4A)	110.37(15)
C(10A)-C(5A)-C(4A)	108.89(14)
C(6A)-C(5A)-C(20A)	108.39(15)
C(10A)-C(5A)-C(20A)	110.95(15)
C(4A)-C(5A)-C(20A)	109.16(15)
N(2A)-C(6A)-C(7A)	106.18(17)
N(2A)-C(6A)-C(5A)	121.96(15)
C(7A)-C(6A)-C(5A)	131.83(17)
C(6A)-C(7A)-C(8A)	108.12(19)
C(6A)-C(7A)-H(7AA)	125.9
C(8A)-C(7A)-H(7AA)	125.9
C(9A)-C(8A)-C(7A)	107.51(19)
C(9A)-C(8A)-H(8AA)	126.2
C(7A)-C(8A)-H(8AA)	126.2
C(8A)-C(9A)-N(2A)	107.51(19)
C(8A)-C(9A)-H(9AA)	126.2

N(2A)-C(9A)-H(9AA)	126.2
N(3A)-C(10A)-C(11A)	107.16(16)
N(3A)-C(10A)-C(5A)	121.03(16)
C(11A)-C(10A)-C(5A)	131.70(17)
C(10A)-C(11A)-C(12A)	107.21(18)
C(10A)-C(11A)-H(11B)	126.4
C(12A)-C(11A)-H(11B)	126.4
C(13A)-C(12A)-C(11A)	107.74(18)
C(13A)-C(12A)-H(12B)	126.1
C(11A)-C(12A)-H(12B)	126.1
C(12A)-C(13A)-N(3A)	108.12(18)
C(12A)-C(13A)-H(13B)	125.9
N(3A)-C(13A)-H(13B)	125.9
O(2A)-C(14A)-O(1A)	122.86(17)
O(2A)-C(14A)-C(1A)	125.40(17)
O(1A)-C(14A)-C(1A)	111.74(16)
O(1A)-C(15A)-C(16A)	110.04(18)
O(1A)-C(15A)-H(15C)	109.7
C(16A)-C(15A)-H(15C)	109.7
O(1A)-C(15A)-H(15D)	109.7
C(16A)-C(15A)-H(15D)	109.7
H(15C)-C(15A)-H(15D)	108.2
C(15A)-C(16A)-H(16D)	109.5
C(15A)-C(16A)-H(16E)	109.5
H(16D)-C(16A)-H(16E)	109.5
C(15A)-C(16A)-H(16F)	109.5
H(16D)-C(16A)-H(16F)	109.5
H(16E)-C(16A)-H(16F)	109.5
C(2A)-C(17A)-C(18A)	113.32(15)
C(2A)-C(17A)-H(17C)	108.9

C(18A)-C(17A)-H(17C)	108.9
C(2A)-C(17A)-H(17D)	108.9
C(18A)-C(17A)-H(17D)	108.9
H(17C)-C(17A)-H(17D)	107.7
C(17A)-C(18A)-H(18D)	109.5
C(17A)-C(18A)-H(18E)	109.5
H(18D)-C(18A)-H(18E)	109.5
C(17A)-C(18A)-H(18F)	109.5
H(18D)-C(18A)-H(18F)	109.5
H(18E)-C(18A)-H(18F)	109.5
C(3A)-C(19A)-H(19D)	109.5
C(3A)-C(19A)-H(19E)	109.5
H(19D)-C(19A)-H(19E)	109.5
C(3A)-C(19A)-H(19F)	109.5
H(19D)-C(19A)-H(19F)	109.5
H(19E)-C(19A)-H(19F)	109.5
C(5A)-C(20A)-H(20D)	109.5
C(5A)-C(20A)-H(20E)	109.5
H(20D)-C(20A)-H(20E)	109.5
C(5A)-C(20A)-H(20F)	109.5
H(20D)-C(20A)-H(20F)	109.5
H(20E)-C(20A)-H(20F)	109.5

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **4**.
The anisotropic displacement factor exponent takes the form:

$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
O(1)	33(1)	32(1)	44(1)	-2(1)	22(1)	1(1)
O(2)	34(1)	46(1)	44(1)	6(1)	21(1)	-4(1)
N(1)	28(1)	23(1)	29(1)	-1(1)	11(1)	-1(1)
N(2)	32(1)	36(1)	37(1)	-4(1)	17(1)	0(1)
N(3)	36(1)	42(1)	36(1)	2(1)	18(1)	12(1)
C(1)	22(1)	30(1)	25(1)	2(1)	7(1)	-2(1)
C(2)	30(1)	31(1)	28(1)	5(1)	5(1)	-3(1)
C(3)	33(1)	27(1)	33(1)	0(1)	10(1)	0(1)
C(4)	28(1)	25(1)	27(1)	-2(1)	9(1)	3(1)
C(5)	33(1)	28(1)	29(1)	-3(1)	15(1)	3(1)
C(6)	33(1)	31(1)	33(1)	-1(1)	20(1)	3(1)
C(7)	38(1)	33(1)	51(1)	6(1)	24(1)	6(1)
C(8)	55(2)	29(1)	65(2)	5(1)	40(1)	6(1)
C(9)	53(1)	33(1)	56(1)	-10(1)	35(1)	-10(1)
C(10)	36(1)	27(1)	36(1)	-2(1)	18(1)	3(1)
C(11)	43(1)	39(1)	43(1)	-4(1)	25(1)	3(1)
C(12)	39(1)	46(1)	61(2)	1(1)	27(1)	12(1)
C(13)	35(1)	46(1)	49(1)	12(1)	15(1)	12(1)
C(14)	25(1)	35(1)	25(1)	4(1)	5(1)	-2(1)
C(15)	41(1)	44(1)	59(2)	-7(1)	30(1)	0(1)
C(16)	50(1)	42(1)	60(2)	-9(1)	29(1)	-1(1)
C(17)	40(1)	34(1)	49(1)	10(1)	15(1)	-5(1)
C(18)	47(1)	43(1)	68(2)	6(1)	18(1)	-16(1)

C(19)	53(1)	28(1)	55(1)	1(1)	22(1)	3(1)
C(20)	45(1)	40(1)	35(1)	-4(1)	16(1)	-1(1)
O(1A)	36(1)	29(1)	37(1)	1(1)	5(1)	-8(1)
O(2A)	45(1)	22(1)	45(1)	0(1)	19(1)	-1(1)
N(1A)	24(1)	24(1)	28(1)	0(1)	12(1)	0(1)
N(2A)	39(1)	53(1)	30(1)	5(1)	18(1)	7(1)
N(3A)	44(1)	25(1)	34(1)	-3(1)	20(1)	-3(1)
C(1A)	30(1)	21(1)	28(1)	0(1)	17(1)	0(1)
C(2A)	28(1)	25(1)	30(1)	1(1)	19(1)	2(1)
C(3A)	27(1)	30(1)	30(1)	-1(1)	17(1)	-3(1)
C(4A)	29(1)	24(1)	29(1)	-3(1)	19(1)	-4(1)
C(5A)	34(1)	22(1)	32(1)	0(1)	20(1)	-2(1)
C(6A)	39(1)	19(1)	32(1)	1(1)	21(1)	1(1)
C(7A)	57(1)	50(1)	31(1)	1(1)	24(1)	6(1)
C(8A)	55(2)	44(1)	29(1)	3(1)	5(1)	8(1)
C(9A)	37(1)	46(1)	44(1)	6(1)	12(1)	9(1)
C(10A)	27(1)	24(1)	31(1)	-2(1)	13(1)	0(1)
C(11A)	35(1)	31(1)	34(1)	3(1)	18(1)	4(1)
C(12A)	39(1)	51(1)	28(1)	-2(1)	17(1)	3(1)
C(13A)	41(1)	38(1)	38(1)	-12(1)	17(1)	0(1)
C(14A)	35(1)	26(1)	27(1)	1(1)	18(1)	-3(1)
C(15A)	42(1)	38(1)	40(1)	-3(1)	3(1)	-14(1)
C(16A)	69(2)	79(2)	142(3)	-56(2)	72(2)	-42(2)
C(17A)	31(1)	28(1)	34(1)	1(1)	16(1)	1(1)
C(18A)	43(1)	40(1)	47(1)	0(1)	22(1)	12(1)
C(19A)	31(1)	33(1)	38(1)	-2(1)	15(1)	-2(1)
C(20A)	47(1)	27(1)	46(1)	0(1)	32(1)	-3(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **4**.

	x	y	z	U(eq)
H(1A)	5026	8449	6547	32
H(2A)	6277	8605	6721	41
H(3A)	6065	6485	7283	45
H(7A)	5033	9474	5622	47
H(8A)	5472	11624	5957	54
H(9A)	6252	11032	6637	52
H(11A)	6206	5535	5834	47
H(12A)	6870	4628	6712	56
H(13A)	6767	5236	7610	53
H(15A)	4198	9336	7563	53
H(15B)	3901	9855	6905	53
H(16A)	4203	11689	7489	72
H(16B)	4445	11541	7051	72
H(16C)	4698	11068	7723	72
H(17A)	4452	4789	7215	51
H(17B)	4646	3688	6918	51
H(18A)	3859	3595	6477	82
H(18B)	4029	4088	5994	82
H(18C)	3831	5144	6306	82
H(19A)	5242	3441	6659	68
H(19B)	5493	4155	6305	68
H(19C)	4979	3704	5965	68
H(20A)	5266	5651	5426	60
H(20B)	5559	6784	5298	60
H(20C)	5066	7125	5246	60
H(1AA)	6719	6280	5228	30

H(2AA)	6353	8805	5748	47
H(3AA)	7218	11059	6140	39
H(7AA)	6726	8719	4443	52
H(8AA)	5882	9024	4024	56
H(9AA)	5665	9076	4861	53
H(11B)	7187	7596	6881	39
H(12B)	7203	9476	7575	46
H(13B)	7220	11611	7089	46
H(15C)	6341	2040	4731	54
H(15D)	5953	3067	4346	54
H(16D)	5719	1856	4955	131
H(16E)	5774	3392	5151	131
H(16F)	6152	2331	5522	131
H(17C)	7744	3128	6513	36
H(17D)	8155	4155	6756	36
H(18D)	8305	2441	6211	63
H(18E)	8275	3844	5888	63
H(18F)	7861	2824	5640	63
H(19D)	8034	7867	6750	51
H(19E)	8334	6896	6550	51
H(19F)	8179	6429	7051	51
H(20D)	7448	10147	5483	54
H(20E)	7498	8786	5179	54
H(20F)	7824	9081	5854	54

Table S6. Torsion angles [deg] for **4**.

C(4)-N(1)-C(1)-C(2)	0.26(19)
C(4)-N(1)-C(1)-C(14)	179.33(16)
N(1)-C(1)-C(2)-C(3)	0.0(2)
C(14)-C(1)-C(2)-C(3)	-179.00(17)
N(1)-C(1)-C(2)-C(17)	-179.20(17)
C(14)-C(1)-C(2)-C(17)	1.8(3)
C(1)-C(2)-C(3)-C(4)	-0.2(2)
C(17)-C(2)-C(3)-C(4)	178.95(17)
C(1)-C(2)-C(3)-C(19)	179.03(18)
C(17)-C(2)-C(3)-C(19)	-1.8(3)
C(1)-N(1)-C(4)-C(3)	-0.41(19)
C(1)-N(1)-C(4)-C(5)	178.24(15)
C(2)-C(3)-C(4)-N(1)	0.4(2)
C(19)-C(3)-C(4)-N(1)	-178.86(18)
C(2)-C(3)-C(4)-C(5)	-178.12(17)
C(19)-C(3)-C(4)-C(5)	2.6(3)
N(1)-C(4)-C(5)-C(6)	5.9(2)
C(3)-C(4)-C(5)-C(6)	-175.77(18)
N(1)-C(4)-C(5)-C(10)	128.40(17)
C(3)-C(4)-C(5)-C(10)	-53.3(2)
N(1)-C(4)-C(5)-C(20)	-112.66(19)
C(3)-C(4)-C(5)-C(20)	65.7(2)
C(9)-N(2)-C(6)-C(7)	-0.1(2)
C(9)-N(2)-C(6)-C(5)	179.69(17)
C(10)-C(5)-C(6)-C(7)	172.58(19)
C(4)-C(5)-C(6)-C(7)	-65.2(3)
C(20)-C(5)-C(6)-C(7)	53.6(3)
C(10)-C(5)-C(6)-N(2)	-7.1(2)

C(4)-C(5)-C(6)-N(2)	115.11(18)
C(20)-C(5)-C(6)-N(2)	-126.07(18)
N(2)-C(6)-C(7)-C(8)	-0.3(2)
C(5)-C(6)-C(7)-C(8)	179.99(19)
C(6)-C(7)-C(8)-C(9)	0.5(2)
C(7)-C(8)-C(9)-N(2)	-0.6(2)
C(6)-N(2)-C(9)-C(8)	0.4(2)
C(13)-N(3)-C(10)-C(11)	-0.5(2)
C(13)-N(3)-C(10)-C(5)	-178.72(18)
C(6)-C(5)-C(10)-N(3)	77.8(2)
C(4)-C(5)-C(10)-N(3)	-44.8(2)
C(20)-C(5)-C(10)-N(3)	-163.63(18)
C(6)-C(5)-C(10)-C(11)	-99.9(2)
C(4)-C(5)-C(10)-C(11)	137.5(2)
C(20)-C(5)-C(10)-C(11)	18.7(3)
N(3)-C(10)-C(11)-C(12)	0.3(2)
C(5)-C(10)-C(11)-C(12)	178.3(2)
C(10)-C(11)-C(12)-C(13)	0.0(3)
C(11)-C(12)-C(13)-N(3)	-0.3(3)
C(10)-N(3)-C(13)-C(12)	0.5(2)
C(15)-O(1)-C(14)-O(2)	-0.6(2)
C(15)-O(1)-C(14)-C(1)	178.95(15)
N(1)-C(1)-C(14)-O(2)	176.32(16)
C(2)-C(1)-C(14)-O(2)	-4.8(3)
N(1)-C(1)-C(14)-O(1)	-3.2(2)
C(2)-C(1)-C(14)-O(1)	175.67(17)
C(14)-O(1)-C(15)-C(16)	164.13(17)
C(1)-C(2)-C(17)-C(18)	81.2(3)
C(3)-C(2)-C(17)-C(18)	-97.8(2)
C(4A)-N(1A)-C(1A)-C(2A)	-0.08(19)

C(4A)-N(1A)-C(1A)-C(14A)	175.63(16)
N(1A)-C(1A)-C(2A)-C(3A)	0.20(19)
C(14A)-C(1A)-C(2A)-C(3A)	-175.07(17)
N(1A)-C(1A)-C(2A)-C(17A)	-178.87(15)
C(14A)-C(1A)-C(2A)-C(17A)	5.9(3)
C(1A)-C(2A)-C(3A)-C(4A)	-0.25(19)
C(17A)-C(2A)-C(3A)-C(4A)	178.81(16)
C(1A)-C(2A)-C(3A)-C(19A)	178.43(16)
C(17A)-C(2A)-C(3A)-C(19A)	-2.5(3)
C(1A)-N(1A)-C(4A)-C(3A)	-0.07(19)
C(1A)-N(1A)-C(4A)-C(5A)	178.68(15)
C(2A)-C(3A)-C(4A)-N(1A)	0.20(19)
C(19A)-C(3A)-C(4A)-N(1A)	-178.46(16)
C(2A)-C(3A)-C(4A)-C(5A)	-178.35(17)
C(19A)-C(3A)-C(4A)-C(5A)	3.0(3)
N(1A)-C(4A)-C(5A)-C(6A)	1.5(2)
C(3A)-C(4A)-C(5A)-C(6A)	179.94(17)
N(1A)-C(4A)-C(5A)-C(10A)	121.26(17)
C(3A)-C(4A)-C(5A)-C(10A)	-60.3(2)
N(1A)-C(4A)-C(5A)-C(20A)	-117.48(17)
C(3A)-C(4A)-C(5A)-C(20A)	60.9(2)
C(9A)-N(2A)-C(6A)-C(7A)	-0.6(2)
C(9A)-N(2A)-C(6A)-C(5A)	-178.72(17)
C(10A)-C(5A)-C(6A)-N(2A)	-27.1(2)
C(4A)-C(5A)-C(6A)-N(2A)	92.5(2)
C(20A)-C(5A)-C(6A)-N(2A)	-147.96(17)
C(10A)-C(5A)-C(6A)-C(7A)	155.3(2)
C(4A)-C(5A)-C(6A)-C(7A)	-85.1(2)
C(20A)-C(5A)-C(6A)-C(7A)	34.4(3)
N(2A)-C(6A)-C(7A)-C(8A)	0.5(2)

C(5A)-C(6A)-C(7A)-C(8A)	178.38(19)
C(6A)-C(7A)-C(8A)-C(9A)	-0.2(3)
C(7A)-C(8A)-C(9A)-N(2A)	-0.1(3)
C(6A)-N(2A)-C(9A)-C(8A)	0.4(2)
C(13A)-N(3A)-C(10A)-C(11A)	0.4(2)
C(13A)-N(3A)-C(10A)-C(5A)	177.06(16)
C(6A)-C(5A)-C(10A)-N(3A)	-73.2(2)
C(4A)-C(5A)-C(10A)-N(3A)	166.34(16)
C(20A)-C(5A)-C(10A)-N(3A)	46.2(2)
C(6A)-C(5A)-C(10A)-C(11A)	102.6(2)
C(4A)-C(5A)-C(10A)-C(11A)	-17.9(3)
C(20A)-C(5A)-C(10A)-C(11A)	-138.1(2)
N(3A)-C(10A)-C(11A)-C(12A)	-0.5(2)
C(5A)-C(10A)-C(11A)-C(12A)	-176.65(18)
C(10A)-C(11A)-C(12A)-C(13A)	0.4(2)
C(11A)-C(12A)-C(13A)-N(3A)	-0.2(2)
C(10A)-N(3A)-C(13A)-C(12A)	-0.2(2)
C(15A)-O(1A)-C(14A)-O(2A)	6.6(3)
C(15A)-O(1A)-C(14A)-C(1A)	-172.95(15)
N(1A)-C(1A)-C(14A)-O(2A)	-177.53(17)
C(2A)-C(1A)-C(14A)-O(2A)	-2.9(3)
N(1A)-C(1A)-C(14A)-O(1A)	2.0(2)
C(2A)-C(1A)-C(14A)-O(1A)	176.68(17)
C(14A)-O(1A)-C(15A)-C(16A)	87.3(2)
C(1A)-C(2A)-C(17A)-C(18A)	72.0(2)
C(3A)-C(2A)-C(17A)-C(18A)	-106.9(2)

Table S7. Hydrogen bonds for **4** [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...N(3)	0.88	2.65	3.160(2)	118.3
N(3)-H(3A)...O(2)#1	0.88	2.00	2.878(2)	175.5
N(2A)-H(2AA)...N(2)	0.88	2.51	3.325(2)	154.9
N(3A)-H(3AA)...O(2A)#2	0.88	2.01	2.861(2)	161.9

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2 #2 x,y+1,z

Table S8. Crystallographic data and structure refinement for *cis*-**1**.

Identification code	spa242
Empirical formula	C26 H18 N3 O6
Formula weight	468.43
Temperature	153(2) K
Wavelength	0.71070 Å
Unit cell dimensions	a = 10.4590(2) Å alpha = 103.891(2) deg. b = 14.6430(4) Å beta = 106.045(2) deg. c = 18.3230(5) Å gamma = 107.1360(10) deg.
Volume	2414.06(10) A^3
Z, Calculated density	4, 1.289 Mg/m^3
Absorption coefficient	0.093 mm^{-1}
F(000)	972

Theta range for data collection	1.55 to 25.00 deg.
Limiting indices	-12<=h<=11, -17<=k<=17, -21<=l<=21
Reflections collected / unique	13201 / 8448 [R(int) = 0.0343]
Completeness to theta =	25.00 99.2 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8448 / 372 / 573
Goodness-of-fit on F^2	1.624
Final R indices [I>2sigma(I)]	R1 = 0.0710, wR2 = 0.1239
R indices (all data)	R1 = 0.1270, wR2 = 0.1340
Largest diff. peak and hole	0.763 and -0.585 e. $Å^{-3}$

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for *cis*-**1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	1689(3)	992(2)	8480(1)	65(1)
O(2)	937(2)	2299(2)	8588(1)	61(1)
O(3)	2471(3)	8352(2)	3287(1)	77(1)
O(4)	4126(3)	8212(3)	4304(1)	98(1)
N(1)	5748(2)	6183(2)	7698(1)	27(1)
N(2)	2606(2)	5331(2)	8030(1)	29(1)
N(3)	1085(2)	6748(2)	7119(1)	28(1)
N(4)	3929(2)	7297(2)	6534(1)	28(1)

N(5)	3299(3)	3557(2)	8548(1)	32(1)
N(6)	2491(3)	8020(2)	5163(1)	37(1)
C(1)	5617(3)	6044(2)	6904(2)	27(1)
C(2)	4934(3)	5028(3)	6490(2)	41(1)
C(3)	4635(3)	4527(2)	7032(2)	36(1)
C(4)	5143(3)	5256(2)	7776(2)	25(1)
C(5)	5005(3)	5180(2)	8565(1)	26(1)
C(6)	3819(3)	5542(2)	8682(2)	29(1)
C(7)	3607(3)	5975(2)	9362(2)	34(1)
C(8)	2224(3)	6027(2)	9107(2)	34(1)
C(9)	1617(3)	5629(2)	8279(2)	28(1)
C(10)	134(3)	5397(2)	7682(2)	30(1)
C(11)	257(3)	5760(2)	6989(2)	29(1)
C(12)	-371(3)	5279(2)	6168(2)	44(1)
C(13)	95(3)	5993(2)	5802(2)	42(1)
C(14)	993(3)	6904(2)	6392(2)	28(1)
C(15)	1893(3)	7913(2)	6378(2)	28(1)
C(16)	3481(3)	8093(2)	6707(2)	28(1)
C(17)	4700(3)	8964(2)	7081(2)	34(1)
C(18)	5911(3)	8689(2)	7145(2)	35(1)
C(19)	5419(3)	7658(2)	6804(2)	29(1)
C(20)	6175(3)	6936(2)	6646(2)	31(1)
C(21)	6431(3)	5849(2)	9299(1)	34(1)
C(22)	-734(3)	4241(2)	7344(2)	37(1)
C(23)	-663(3)	5925(2)	8117(2)	37(1)
C(24)	1652(3)	8806(2)	6893(2)	34(1)
C(25)	5848(3)	6535(2)	5725(2)	42(1)
C(26)	7808(3)	7519(2)	7098(2)	42(1)
C(27)	4576(3)	4077(2)	8506(1)	28(1)
C(28)	5276(3)	3410(2)	8411(1)	29(1)

C(29)	4375(3)	2461(2)	8391(1)	30(1)
C(30)	3150(3)	2577(2)	8483(2)	32(1)
C(31)	1895(4)	1867(3)	8514(2)	46(1)
C(32)	-426(5)	1680(4)	8601(3)	98(2)
C(33)	-728(6)	2249(5)	9197(4)	170(3)
C(34)	6731(3)	3646(2)	8351(2)	43(1)
C(35)	4680(4)	1510(2)	8294(2)	41(1)
C(36)	5248(4)	1346(3)	9092(2)	49(1)
C(37)	1486(3)	7904(2)	5509(2)	29(1)
C(38)	234(3)	7861(2)	4956(2)	33(1)
C(39)	524(3)	7974(2)	4266(2)	36(1)
C(40)	1932(3)	8069(2)	4409(2)	39(1)
C(41)	2831(4)	8235(3)	3934(2)	58(1)
C(42)	5223(6)	8329(5)	3921(3)	123(2)
C(43)	6166(6)	9291(4)	4273(3)	140(2)
C(44)	-1182(3)	7708(3)	5055(2)	49(1)
C(45)	-490(4)	8044(2)	3538(2)	49(1)
C(46)	-307(4)	9148(3)	3645(2)	71(1)
O(1A)	7058(2)	8193(2)	9010(1)	44(1)
O(2A)	6795(2)	9575(2)	9692(1)	38(1)
C(1A)	4679(3)	8192(2)	8768(2)	46(1)
C(2A)	6287(3)	8631(3)	9155(2)	35(1)
C(3A)	8351(3)	10055(2)	10101(2)	43(1)
C(4A)	8691(4)	11021(3)	10769(2)	72(1)

Table S10. Bond lengths [Å] and angles [deg] for *cis*-**1**.

O(1)-C(31)	1.218(4)
O(2)-C(31)	1.352(4)
O(2)-C(32)	1.457(4)
O(3)-C(41)	1.210(4)
O(4)-C(41)	1.351(4)
O(4)-C(42)	1.492(4)
N(1)-C(4)	1.379(3)
N(1)-C(1)	1.382(3)
N(1)-H(1)	0.8800
N(2)-C(6)	1.373(3)
N(2)-C(9)	1.379(3)
N(2)-H(2)	0.8800
N(3)-C(11)	1.371(3)
N(3)-C(14)	1.388(3)
N(3)-H(3)	0.8800
N(4)-C(16)	1.380(3)
N(4)-C(19)	1.384(3)
N(4)-H(4)	0.8800
N(5)-C(27)	1.362(3)
N(5)-C(30)	1.369(3)
N(5)-H(5)	0.8800
N(6)-C(37)	1.360(3)
N(6)-C(40)	1.372(3)
N(6)-H(6)	0.8800
C(1)-C(2)	1.353(4)
C(1)-C(20)	1.507(4)
C(2)-C(3)	1.417(4)
C(2)-H(2A)	0.9500

C(3)-C(4)	1.360(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.517(3)
C(5)-C(27)	1.511(4)
C(5)-C(6)	1.532(3)
C(5)-C(21)	1.546(4)
C(6)-C(7)	1.363(3)
C(7)-C(8)	1.422(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.366(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.513(4)
C(10)-C(11)	1.512(3)
C(10)-C(22)	1.534(4)
C(10)-C(23)	1.543(3)
C(11)-C(12)	1.366(4)
C(12)-C(13)	1.413(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.356(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.509(4)
C(15)-C(16)	1.517(4)
C(15)-C(37)	1.526(3)
C(15)-C(24)	1.549(3)
C(16)-C(17)	1.365(4)
C(17)-C(18)	1.422(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.359(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.516(4)

C(20)-C(26)	1.533(4)
C(20)-C(25)	1.549(3)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.390(3)
C(28)-C(29)	1.417(4)
C(28)-C(34)	1.500(4)
C(29)-C(30)	1.390(4)
C(29)-C(35)	1.498(4)
C(30)-C(31)	1.440(4)
C(32)-C(33)	1.377(5)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-H(33A)	0.9800

C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.525(4)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.390(4)
C(38)-C(39)	1.415(4)
C(38)-C(44)	1.500(4)
C(39)-C(40)	1.381(4)
C(39)-C(45)	1.504(4)
C(40)-C(41)	1.455(4)
C(42)-C(43)	1.328(6)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-C(46)	1.527(4)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-H(46A)	0.9800

C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
O(1A)-C(2A)	1.214(3)
O(2A)-C(2A)	1.337(3)
O(2A)-C(3A)	1.450(3)
C(1A)-C(2A)	1.493(4)
C(1A)-H(1A1)	0.9800
C(1A)-H(1A2)	0.9800
C(1A)-H(1A3)	0.9800
C(3A)-C(4A)	1.501(4)
C(3A)-H(3A1)	0.9900
C(3A)-H(3A2)	0.9900
C(4A)-H(4A1)	0.9800
C(4A)-H(4A2)	0.9800
C(4A)-H(4A3)	0.9800
C(31)-O(2)-C(32)	118.6(3)
C(41)-O(4)-C(42)	120.8(3)
C(4)-N(1)-C(1)	110.1(2)
C(4)-N(1)-H(1)	125.0
C(1)-N(1)-H(1)	125.0
C(6)-N(2)-C(9)	110.98(19)
C(6)-N(2)-H(2)	124.5
C(9)-N(2)-H(2)	124.5
C(11)-N(3)-C(14)	111.2(2)
C(11)-N(3)-H(3)	124.4
C(14)-N(3)-H(3)	124.4
C(16)-N(4)-C(19)	110.6(2)
C(16)-N(4)-H(4)	124.7
C(19)-N(4)-H(4)	124.7
C(27)-N(5)-C(30)	110.7(2)

C(27)-N(5)-H(5)	124.7
C(30)-N(5)-H(5)	124.7
C(37)-N(6)-C(40)	110.3(2)
C(37)-N(6)-H(6)	124.8
C(40)-N(6)-H(6)	124.8
C(2)-C(1)-N(1)	106.5(2)
C(2)-C(1)-C(20)	132.3(2)
N(1)-C(1)-C(20)	121.2(2)
C(1)-C(2)-C(3)	108.9(2)
C(1)-C(2)-H(2A)	125.5
C(3)-C(2)-H(2A)	125.5
C(4)-C(3)-C(2)	107.4(3)
C(4)-C(3)-H(3A)	126.3
C(2)-C(3)-H(3A)	126.3
C(3)-C(4)-N(1)	107.2(2)
C(3)-C(4)-C(5)	130.7(3)
N(1)-C(4)-C(5)	121.8(2)
C(27)-C(5)-C(4)	108.7(2)
C(27)-C(5)-C(6)	109.0(2)
C(4)-C(5)-C(6)	108.5(2)
C(27)-C(5)-C(21)	110.0(2)
C(4)-C(5)-C(21)	111.7(2)
C(6)-C(5)-C(21)	108.9(2)
C(7)-C(6)-N(2)	107.0(2)
C(7)-C(6)-C(5)	131.8(2)
N(2)-C(6)-C(5)	120.7(2)
C(6)-C(7)-C(8)	107.4(2)
C(6)-C(7)-H(7)	126.3
C(8)-C(7)-H(7)	126.3
C(9)-C(8)-C(7)	108.7(2)

C(9)-C(8)-H(8)	125.6
C(7)-C(8)-H(8)	125.6
C(8)-C(9)-N(2)	105.9(2)
C(8)-C(9)-C(10)	132.4(2)
N(2)-C(9)-C(10)	121.4(2)
C(11)-C(10)-C(9)	110.3(2)
C(11)-C(10)-C(22)	109.1(2)
C(9)-C(10)-C(22)	109.1(2)
C(11)-C(10)-C(23)	109.9(2)
C(9)-C(10)-C(23)	109.7(2)
C(22)-C(10)-C(23)	108.7(2)
C(12)-C(11)-N(3)	106.2(2)
C(12)-C(11)-C(10)	132.0(3)
N(3)-C(11)-C(10)	121.8(2)
C(11)-C(12)-C(13)	108.1(3)
C(11)-C(12)-H(12)	125.9
C(13)-C(12)-H(12)	125.9
C(14)-C(13)-C(12)	108.9(2)
C(14)-C(13)-H(13)	125.6
C(12)-C(13)-H(13)	125.6
C(13)-C(14)-N(3)	105.6(3)
C(13)-C(14)-C(15)	133.1(2)
N(3)-C(14)-C(15)	121.0(2)
C(14)-C(15)-C(16)	110.1(2)
C(14)-C(15)-C(37)	109.9(2)
C(16)-C(15)-C(37)	108.3(2)
C(14)-C(15)-C(24)	111.1(2)
C(16)-C(15)-C(24)	109.0(2)
C(37)-C(15)-C(24)	108.4(2)
C(17)-C(16)-N(4)	106.4(2)

C(17)-C(16)-C(15)	132.1(3)
N(4)-C(16)-C(15)	120.7(3)
C(16)-C(17)-C(18)	108.2(3)
C(16)-C(17)-H(17)	125.9
C(18)-C(17)-H(17)	125.9
C(19)-C(18)-C(17)	108.2(3)
C(19)-C(18)-H(18)	125.9
C(17)-C(18)-H(18)	125.9
C(18)-C(19)-N(4)	106.6(2)
C(18)-C(19)-C(20)	132.6(3)
N(4)-C(19)-C(20)	120.7(3)
C(1)-C(20)-C(19)	110.1(2)
C(1)-C(20)-C(26)	111.4(2)
C(19)-C(20)-C(26)	109.3(2)
C(1)-C(20)-C(25)	108.8(2)
C(19)-C(20)-C(25)	108.5(2)
C(26)-C(20)-C(25)	108.8(2)
C(5)-C(21)-H(21A)	109.5
C(5)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(5)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(10)-C(22)-H(22A)	109.5
C(10)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(10)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(10)-C(23)-H(23A)	109.5

C(10)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(10)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(15)-C(24)-H(24A)	109.5
C(15)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(15)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(20)-C(25)-H(25A)	109.5
C(20)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(20)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(20)-C(26)-H(26A)	109.5
C(20)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(20)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(5)-C(27)-C(28)	107.2(3)
N(5)-C(27)-C(5)	121.2(2)
C(28)-C(27)-C(5)	131.6(3)
C(27)-C(28)-C(29)	107.7(3)
C(27)-C(28)-C(34)	126.6(3)
C(29)-C(28)-C(34)	125.7(2)
C(30)-C(29)-C(28)	107.0(2)

C(30)-C(29)-C(35)	126.3(3)
C(28)-C(29)-C(35)	126.7(3)
N(5)-C(30)-C(29)	107.4(3)
N(5)-C(30)-C(31)	121.7(3)
C(29)-C(30)-C(31)	130.8(3)
O(1)-C(31)-O(2)	123.1(3)
O(1)-C(31)-C(30)	126.1(3)
O(2)-C(31)-C(30)	110.8(3)
C(33)-C(32)-O(2)	109.0(4)
C(33)-C(32)-H(32A)	109.9
O(2)-C(32)-H(32A)	109.9
C(33)-C(32)-H(32B)	109.9
O(2)-C(32)-H(32B)	109.9
H(32A)-C(32)-H(32B)	108.3
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(28)-C(34)-H(34A)	109.5
C(28)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(28)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(29)-C(35)-C(36)	113.4(2)
C(29)-C(35)-H(35A)	108.9
C(36)-C(35)-H(35A)	108.9
C(29)-C(35)-H(35B)	108.9

C(36)-C(35)-H(35B)	108.9
H(35A)-C(35)-H(35B)	107.7
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
N(6)-C(37)-C(38)	107.3(2)
N(6)-C(37)-C(15)	119.9(2)
C(38)-C(37)-C(15)	132.6(2)
C(37)-C(38)-C(39)	107.5(2)
C(37)-C(38)-C(44)	127.0(2)
C(39)-C(38)-C(44)	125.5(3)
C(40)-C(39)-C(38)	107.3(2)
C(40)-C(39)-C(45)	126.7(3)
C(38)-C(39)-C(45)	126.0(3)
N(6)-C(40)-C(39)	107.6(2)
N(6)-C(40)-C(41)	120.3(3)
C(39)-C(40)-C(41)	132.1(3)
O(3)-C(41)-O(4)	123.9(3)
O(3)-C(41)-C(40)	125.5(4)
O(4)-C(41)-C(40)	110.6(3)
C(43)-C(42)-O(4)	107.4(4)
C(43)-C(42)-H(42A)	110.2
O(4)-C(42)-H(42A)	110.2
C(43)-C(42)-H(42B)	110.2
O(4)-C(42)-H(42B)	110.2
H(42A)-C(42)-H(42B)	108.5
C(42)-C(43)-H(43A)	109.5

C(42)-C(43)-H(43B) 109.5
H(43A)-C(43)-H(43B) 109.5
C(42)-C(43)-H(43C) 109.5
H(43A)-C(43)-H(43C) 109.5
H(43B)-C(43)-H(43C) 109.5
C(38)-C(44)-H(44A) 109.5
C(38)-C(44)-H(44B) 109.5
H(44A)-C(44)-H(44B) 109.5
C(38)-C(44)-H(44C) 109.5
H(44A)-C(44)-H(44C) 109.5
H(44B)-C(44)-H(44C) 109.5
C(39)-C(45)-C(46) 111.5(3)
C(39)-C(45)-H(45A) 109.3
C(46)-C(45)-H(45A) 109.3
C(39)-C(45)-H(45B) 109.3
C(46)-C(45)-H(45B) 109.3
H(45A)-C(45)-H(45B) 108.0
C(45)-C(46)-H(46A) 109.5
C(45)-C(46)-H(46B) 109.5
H(46A)-C(46)-H(46B) 109.5
C(45)-C(46)-H(46C) 109.5
H(46A)-C(46)-H(46C) 109.5
H(46B)-C(46)-H(46C) 109.5
C(2A)-O(2A)-C(3A) 115.5(2)
C(2A)-C(1A)-H(1A1) 109.5
C(2A)-C(1A)-H(1A2) 109.5
H(1A1)-C(1A)-H(1A2) 109.5
C(2A)-C(1A)-H(1A3) 109.5
H(1A1)-C(1A)-H(1A3) 109.5
H(1A2)-C(1A)-H(1A3) 109.5

O(1A)-C(2A)-O(2A)	123.2(3)
O(1A)-C(2A)-C(1A)	124.9(3)
O(2A)-C(2A)-C(1A)	111.9(3)
O(2A)-C(3A)-C(4A)	107.5(2)
O(2A)-C(3A)-H(3A1)	110.2
C(4A)-C(3A)-H(3A1)	110.2
O(2A)-C(3A)-H(3A2)	110.2
C(4A)-C(3A)-H(3A2)	110.2
H(3A1)-C(3A)-H(3A2)	108.5
C(3A)-C(4A)-H(4A1)	109.5
C(3A)-C(4A)-H(4A2)	109.5
H(4A1)-C(4A)-H(4A2)	109.5
C(3A)-C(4A)-H(4A3)	109.5
H(4A1)-C(4A)-H(4A3)	109.5
H(4A2)-C(4A)-H(4A3)	109.5

Table S11. Anisotropic displacement parameters ($Å^2$ x 10^3) for *cis*-**1**.

The anisotropic displacement factor exponent takes the form:

$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
O(1)	57(2)	51(2)	77(2)	39(2)	16(1)	2(1)
O(2)	44(2)	71(2)	73(2)	35(1)	34(1)	10(1)
O(3)	87(2)	87(2)	32(1)	25(1)	19(1)	-2(2)
O(4)	43(2)	180(3)	47(2)	32(2)	25(2)	9(2)

N(1)	31(2)	26(2)	21(1)	7(1)	9(1)	9(1)
N(2)	36(2)	36(2)	19(1)	11(1)	12(1)	16(1)
N(3)	31(2)	27(2)	20(1)	7(1)	7(1)	7(1)
N(4)	29(2)	24(2)	26(1)	10(1)	8(1)	7(1)
N(5)	35(2)	35(2)	28(1)	15(1)	13(1)	13(1)
N(6)	31(2)	50(2)	29(1)	19(1)	8(1)	13(1)
C(1)	30(2)	35(2)	22(2)	11(2)	10(1)	16(2)
C(2)	56(2)	44(2)	23(2)	11(2)	16(2)	19(2)
C(3)	52(2)	25(2)	30(2)	10(2)	16(2)	12(2)
C(4)	27(2)	25(2)	25(2)	10(1)	9(1)	11(2)
C(5)	28(2)	28(2)	22(1)	11(1)	8(1)	11(2)
C(6)	36(2)	30(2)	23(2)	14(1)	9(2)	12(2)
C(7)	43(2)	40(2)	19(1)	12(1)	10(2)	19(2)
C(8)	40(2)	40(2)	31(2)	16(2)	19(2)	20(2)
C(9)	31(2)	30(2)	30(2)	15(1)	16(2)	15(2)
C(10)	33(2)	27(2)	33(2)	14(2)	16(2)	12(2)
C(11)	30(2)	25(2)	29(2)	8(1)	11(2)	10(2)
C(12)	55(2)	29(2)	33(2)	9(2)	11(2)	2(2)
C(13)	57(2)	35(2)	25(2)	12(2)	12(2)	9(2)
C(14)	30(2)	30(2)	26(2)	11(2)	11(2)	12(2)
C(15)	28(2)	30(2)	26(2)	10(1)	10(1)	11(2)
C(16)	35(2)	28(2)	21(1)	11(1)	9(1)	13(2)
C(17)	39(2)	26(2)	37(2)	9(2)	13(2)	13(2)
C(18)	29(2)	36(2)	37(2)	14(2)	10(2)	8(2)
C(19)	28(2)	34(2)	27(2)	17(2)	10(1)	10(2)
C(20)	31(2)	38(2)	29(2)	18(2)	13(2)	14(2)
C(21)	40(2)	34(2)	27(2)	11(1)	12(2)	15(2)
C(22)	38(2)	35(2)	43(2)	18(2)	18(2)	13(2)
C(23)	38(2)	39(2)	43(2)	19(2)	22(2)	19(2)
C(24)	34(2)	36(2)	34(2)	15(2)	11(2)	15(2)

C(25)	51(2)	54(2)	38(2)	27(2)	25(2)	27(2)
C(26)	36(2)	51(2)	49(2)	28(2)	19(2)	20(2)
C(27)	31(2)	32(2)	19(1)	11(1)	8(1)	9(2)
C(28)	39(2)	29(2)	23(2)	13(1)	12(2)	14(2)
C(29)	39(2)	29(2)	18(1)	10(1)	6(1)	9(2)
C(30)	37(2)	29(2)	26(2)	15(1)	9(2)	5(2)
C(31)	46(2)	50(3)	32(2)	19(2)	9(2)	6(2)
C(32)	74(3)	124(4)	91(3)	58(3)	41(3)	5(3)
C(33)	148(5)	152(5)	283(6)	97(5)	164(5)	62(4)
C(34)	43(2)	40(2)	49(2)	17(2)	19(2)	18(2)
C(35)	54(2)	29(2)	36(2)	13(2)	14(2)	13(2)
C(36)	61(2)	44(2)	48(2)	23(2)	16(2)	26(2)
C(37)	31(2)	29(2)	29(2)	12(1)	13(2)	10(2)
C(38)	35(2)	36(2)	32(2)	15(2)	11(2)	16(2)
C(39)	43(2)	34(2)	26(2)	13(2)	5(2)	13(2)
C(40)	42(2)	44(2)	26(2)	17(2)	9(2)	8(2)
C(41)	52(3)	71(3)	37(2)	18(2)	15(2)	5(2)
C(42)	101(4)	156(5)	75(3)	28(3)	51(3)	-5(4)
C(43)	159(5)	97(4)	139(4)	31(3)	95(4)	-11(4)
C(44)	44(2)	63(2)	43(2)	19(2)	11(2)	27(2)
C(45)	59(2)	47(2)	31(2)	16(2)	4(2)	18(2)
C(46)	107(3)	64(3)	44(2)	24(2)	10(2)	47(3)
O(1A)	48(2)	38(1)	43(1)	11(1)	15(1)	20(1)
O(2A)	35(1)	34(1)	38(1)	10(1)	11(1)	11(1)
C(1A)	40(2)	51(2)	39(2)	21(2)	6(2)	8(2)
C(2A)	41(2)	35(2)	27(2)	19(2)	8(2)	11(2)
C(3A)	37(2)	38(2)	42(2)	11(2)	9(2)	9(2)
C(4A)	70(3)	56(3)	57(2)	-3(2)	0(2)	19(2)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for *cis*-**1**.

	x	y	z	U(eq)
H(1)	6159	6777	8096	32
H(2)	2478	5044	7520	35
H(3)	1607	7220	7601	34
H(4)	3348	6650	6287	33
H(5)	2659	3815	8609	38
H(6)	3373	8059	5391	44
H(2A)	4693	4704	5927	49
H(3A)	4168	3813	6899	44
H(7)	4262	6200	9905	40
H(8)	1795	6294	9454	41
H(12)	-1010	4584	5890	53
H(13)	-177	5856	5235	50
H(17)	4734	9638	7267	41
H(18)	6894	9147	7385	42
H(21A)	6306	5777	9796	50
H(21B)	6690	6564	9341	50
H(21C)	7200	5628	9227	50
H(22A)	-267	3899	7041	56
H(22B)	-1715	4090	6983	56
H(22C)	-775	3995	7793	56
H(23A)	-733	5691	8568	55
H(23B)	-1635	5755	7733	55
H(23C)	-129	6666	8326	55
H(24A)	1962	8847	7460	52

H(24B)	626	8690	6690	52
H(24C)	2217	9447	6856	52
H(25A)	6357	6085	5615	63
H(25B)	6172	7111	5546	63
H(25C)	4807	6153	5430	63
H(26A)	8025	7793	7681	63
H(26B)	8143	8081	6907	63
H(26C)	8300	7055	6996	63
H(32A)	-1209	1461	8068	118
H(32B)	-358	1063	8711	118
H(33A)	-13	2392	9730	255
H(33B)	-1693	1866	9170	255
H(33C)	-693	2892	9117	255
H(34A)	6905	4166	8098	64
H(34B)	6764	3025	8021	64
H(34C)	7476	3903	8895	64
H(35A)	5398	1545	8034	49
H(35B)	3782	916	7927	49
H(36A)	6108	1948	9470	74
H(36B)	5499	746	8994	74
H(36C)	4503	1239	9326	74
H(42A)	5717	7858	4000	147
H(42B)	4754	8170	3331	147
H(43A)	5682	9746	4149	209
H(43B)	6951	9379	4068	209
H(43C)	6562	9456	4861	209
H(44A)	-1238	7390	5465	74
H(44B)	-1973	7265	4537	74
H(44C)	-1261	8370	5228	74
H(45A)	-1497	7640	3452	58

H(45B)	-305	7750	3051	58
H(46A)	-459	9448	4137	107
H(46B)	-1015	9164	3174	107
H(46C)	669	9539	3693	107
H(1A1)	4384	7898	8179	70
H(1A2)	4317	8732	8897	70
H(1A3)	4280	7660	8973	70
H(3A1)	8808	10211	9716	51
H(3A2)	8721	9593	10329	51
H(4A1)	8228	11437	10544	108
H(4A2)	9738	11402	11018	108
H(4A3)	8329	10852	11179	108

Table S13. Torsion angles [deg] for *cis*-**1**.

C(4)-N(1)-C(1)-C(2)	-0.3(3)
C(4)-N(1)-C(1)-C(20)	179.3(2)
N(1)-C(1)-C(2)-C(3)	0.0(3)
C(20)-C(1)-C(2)-C(3)	-179.5(3)
C(1)-C(2)-C(3)-C(4)	0.3(3)
C(2)-C(3)-C(4)-N(1)	-0.5(3)
C(2)-C(3)-C(4)-C(5)	173.7(3)
C(1)-N(1)-C(4)-C(3)	0.5(3)
C(1)-N(1)-C(4)-C(5)	-174.3(2)
C(3)-C(4)-C(5)-C(27)	17.5(4)
N(1)-C(4)-C(5)-C(27)	-169.1(2)
C(3)-C(4)-C(5)-C(6)	-101.0(3)
N(1)-C(4)-C(5)-C(6)	72.4(3)

C(3)-C(4)-C(5)-C(21)	139.0(3)
N(1)-C(4)-C(5)-C(21)	-47.6(3)
C(9)-N(2)-C(6)-C(7)	0.4(3)
C(9)-N(2)-C(6)-C(5)	173.6(2)
C(27)-C(5)-C(6)-C(7)	89.4(4)
C(4)-C(5)-C(6)-C(7)	-152.3(3)
C(21)-C(5)-C(6)-C(7)	-30.6(4)
C(27)-C(5)-C(6)-N(2)	-81.8(3)
C(4)-C(5)-C(6)-N(2)	36.5(3)
C(21)-C(5)-C(6)-N(2)	158.2(2)
N(2)-C(6)-C(7)-C(8)	-0.2(3)
C(5)-C(6)-C(7)-C(8)	-172.3(3)
C(6)-C(7)-C(8)-C(9)	-0.1(3)
C(7)-C(8)-C(9)-N(2)	0.4(3)
C(7)-C(8)-C(9)-C(10)	173.5(3)
C(6)-N(2)-C(9)-C(8)	-0.5(3)
C(6)-N(2)-C(9)-C(10)	-174.5(2)
C(8)-C(9)-C(10)-C(11)	135.4(3)
N(2)-C(9)-C(10)-C(11)	-52.4(3)
C(8)-C(9)-C(10)-C(22)	-104.8(3)
N(2)-C(9)-C(10)-C(22)	67.5(3)
C(8)-C(9)-C(10)-C(23)	14.2(4)
N(2)-C(9)-C(10)-C(23)	-173.6(2)
C(14)-N(3)-C(11)-C(12)	0.1(3)
C(14)-N(3)-C(11)-C(10)	-178.2(2)
C(9)-C(10)-C(11)-C(12)	127.9(3)
C(22)-C(10)-C(11)-C(12)	8.0(4)
C(23)-C(10)-C(11)-C(12)	-111.1(3)
C(9)-C(10)-C(11)-N(3)	-54.3(3)
C(22)-C(10)-C(11)-N(3)	-174.2(2)

C(23)-C(10)-C(11)-N(3)	66.8(3)
N(3)-C(11)-C(12)-C(13)	0.1(3)
C(10)-C(11)-C(12)-C(13)	178.2(3)
C(11)-C(12)-C(13)-C(14)	-0.3(3)
C(12)-C(13)-C(14)-N(3)	0.4(3)
C(12)-C(13)-C(14)-C(15)	174.9(3)
C(11)-N(3)-C(14)-C(13)	-0.3(3)
C(11)-N(3)-C(14)-C(15)	-175.6(2)
C(13)-C(14)-C(15)-C(16)	-108.2(3)
N(3)-C(14)-C(15)-C(16)	65.6(3)
C(13)-C(14)-C(15)-C(37)	11.0(4)
N(3)-C(14)-C(15)-C(37)	-175.2(2)
C(13)-C(14)-C(15)-C(24)	131.0(3)
N(3)-C(14)-C(15)-C(24)	-55.2(3)
C(19)-N(4)-C(16)-C(17)	0.7(3)
C(19)-N(4)-C(16)-C(15)	172.1(2)
C(14)-C(15)-C(16)-C(17)	-153.2(3)
C(37)-C(15)-C(16)-C(17)	86.6(3)
C(24)-C(15)-C(16)-C(17)	-31.1(4)
C(14)-C(15)-C(16)-N(4)	38.1(3)
C(37)-C(15)-C(16)-N(4)	-82.1(3)
C(24)-C(15)-C(16)-N(4)	160.2(2)
N(4)-C(16)-C(17)-C(18)	-0.8(3)
C(15)-C(16)-C(17)-C(18)	-170.7(2)
C(16)-C(17)-C(18)-C(19)	0.6(3)
C(17)-C(18)-C(19)-N(4)	-0.1(3)
C(17)-C(18)-C(19)-C(20)	175.7(2)
C(16)-N(4)-C(19)-C(18)	-0.4(3)
C(16)-N(4)-C(19)-C(20)	-176.7(2)
C(2)-C(1)-C(20)-C(19)	119.0(3)

N(1)-C(1)-C(20)-C(19)	-60.5(3)
C(2)-C(1)-C(20)-C(26)	-119.7(3)
N(1)-C(1)-C(20)-C(26)	60.9(3)
C(2)-C(1)-C(20)-C(25)	0.2(4)
N(1)-C(1)-C(20)-C(25)	-179.2(2)
C(18)-C(19)-C(20)-C(1)	134.2(3)
N(4)-C(19)-C(20)-C(1)	-50.5(3)
C(18)-C(19)-C(20)-C(26)	11.5(4)
N(4)-C(19)-C(20)-C(26)	-173.2(2)
C(18)-C(19)-C(20)-C(25)	-106.9(3)
N(4)-C(19)-C(20)-C(25)	68.4(3)
C(30)-N(5)-C(27)-C(28)	-0.1(3)
C(30)-N(5)-C(27)-C(5)	-179.8(2)
C(4)-C(5)-C(27)-N(5)	-117.4(2)
C(6)-C(5)-C(27)-N(5)	0.7(3)
C(21)-C(5)-C(27)-N(5)	120.0(2)
C(4)-C(5)-C(27)-C(28)	62.9(4)
C(6)-C(5)-C(27)-C(28)	-178.9(2)
C(21)-C(5)-C(27)-C(28)	-59.6(3)
N(5)-C(27)-C(28)-C(29)	0.4(3)
C(5)-C(27)-C(28)-C(29)	-179.9(2)
N(5)-C(27)-C(28)-C(34)	-178.8(2)
C(5)-C(27)-C(28)-C(34)	0.8(4)
C(27)-C(28)-C(29)-C(30)	-0.6(3)
C(34)-C(28)-C(29)-C(30)	178.6(2)
C(27)-C(28)-C(29)-C(35)	179.6(2)
C(34)-C(28)-C(29)-C(35)	-1.1(4)
C(27)-N(5)-C(30)-C(29)	-0.3(3)
C(27)-N(5)-C(30)-C(31)	179.7(2)
C(28)-C(29)-C(30)-N(5)	0.6(3)

C(35)-C(29)-C(30)-N(5)	-179.7(2)
C(28)-C(29)-C(30)-C(31)	-179.5(3)
C(35)-C(29)-C(30)-C(31)	0.3(4)
C(32)-O(2)-C(31)-O(1)	-2.1(5)
C(32)-O(2)-C(31)-C(30)	178.0(3)
N(5)-C(30)-C(31)-O(1)	-178.2(3)
C(29)-C(30)-C(31)-O(1)	1.8(5)
N(5)-C(30)-C(31)-O(2)	1.7(4)
C(29)-C(30)-C(31)-O(2)	-178.3(3)
C(31)-O(2)-C(32)-C(33)	136.8(4)
C(30)-C(29)-C(35)-C(36)	-80.4(4)
C(28)-C(29)-C(35)-C(36)	99.4(3)
C(40)-N(6)-C(37)-C(38)	0.9(3)
C(40)-N(6)-C(37)-C(15)	-175.3(2)
C(14)-C(15)-C(37)-N(6)	-118.6(3)
C(16)-C(15)-C(37)-N(6)	1.6(3)
C(24)-C(15)-C(37)-N(6)	119.7(3)
C(14)-C(15)-C(37)-C(38)	66.2(4)
C(16)-C(15)-C(37)-C(38)	-173.5(3)
C(24)-C(15)-C(37)-C(38)	-55.4(4)
N(6)-C(37)-C(38)-C(39)	-1.1(3)
C(15)-C(37)-C(38)-C(39)	174.5(3)
N(6)-C(37)-C(38)-C(44)	178.2(3)
C(15)-C(37)-C(38)-C(44)	-6.2(5)
C(37)-C(38)-C(39)-C(40)	0.8(3)
C(44)-C(38)-C(39)-C(40)	-178.4(3)
C(37)-C(38)-C(39)-C(45)	-175.6(3)
C(44)-C(38)-C(39)-C(45)	5.1(5)
C(37)-N(6)-C(40)-C(39)	-0.4(3)
C(37)-N(6)-C(40)-C(41)	177.4(3)

C(38)-C(39)-C(40)-N(6)	-0.3(3)
C(45)-C(39)-C(40)-N(6)	176.1(3)
C(38)-C(39)-C(40)-C(41)	-177.8(3)
C(45)-C(39)-C(40)-C(41)	-1.3(6)
C(42)-O(4)-C(41)-O(3)	-0.2(6)
C(42)-O(4)-C(41)-C(40)	177.9(3)
N(6)-C(40)-C(41)-O(3)	-175.2(3)
C(39)-C(40)-C(41)-O(3)	1.9(6)
N(6)-C(40)-C(41)-O(4)	6.6(5)
C(39)-C(40)-C(41)-O(4)	-176.2(3)
C(41)-O(4)-C(42)-C(43)	99.8(6)
C(40)-C(39)-C(45)-C(46)	-86.1(4)
C(38)-C(39)-C(45)-C(46)	89.7(4)
C(3A)-O(2A)-C(2A)-O(1A)	-0.2(4)
C(3A)-O(2A)-C(2A)-C(1A)	179.5(2)
C(2A)-O(2A)-C(3A)-C(4A)	-170.7(2)

Table S14. Crystallographic data and structure refinement for *trans*-**1**.

Identification code	spa-24-1
Empirical formula	C26 H18 N2 O2
Formula weight	390.42
Temperature	153(2) K
Wavelength	0.71070 Å
Unit cell dimensions	a = 10.2870(13) Å alpha = 111.592(5) deg. b = 11.1500(10) Å beta = 92.851(4) deg.

	c = 13.0400(17) Å gamma = 113.076(4) deg.
Volume	1246.1(3) A^3
Z, Calculated density	2, 1.041 Mg/m^3
Absorption coefficient	0.067 mm^{-1}
F(000)	408
Theta range for data collection	1.72 to 25.00 deg.
Limiting indices	0<=h<=12, -12<=k<=9, -15<=l<=15
Reflections collected / unique	3762 / 3762 [R(int) = 0.0000]
Completeness to theta = 25.00	85.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3762 / 192 / 297
Goodness-of-fit on F^2	1.484
Final R indices [I>2sigma(I)]	R1 = 0.1123, wR2 = 0.1998
R indices (all data)	R1 = 0.1829, wR2 = 0.2212
Largest diff. peak and hole	0.497 and -0.425 e. $Å^{-3}$

Table S15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for *trans*-**1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)	
N(1)	4922(4)	2809(3)	4862(3)	36(1)	
N(2)	3584(4)	4826(3)	6319(3)	36(1)	

C(3)	2741(5)	5475(4)	6205(4)	34(1)
O(4)	3318(4)	3454(3)	3396(3)	48(1)
N(5)	4265(4)	858(4)	2392(3)	36(1)
C(7)	5312(5)	2124(4)	1438(4)	33(1)
C(8)	6147(5)	2684(4)	4549(4)	34(1)
O(9)	1766(4)	-1438(3)	1915(3)	59(1)
C(10)	2782(5)	3393(5)	6067(4)	37(1)
C(11)	6668(5)	2958(4)	3537(4)	34(1)
C(12)	4734(5)	2555(5)	5807(4)	38(1)
C(13)	1958(6)	-1063(5)	1043(5)	44(1)
C(14)	3345(5)	661(5)	-443(4)	45(1)
C(15)	5458(5)	2061(4)	2475(4)	34(1)
C(16)	3974(5)	954(5)	725(4)	35(1)
C(17)	2080(5)	2989(5)	2881(4)	39(1)
C(18)	6715(5)	2332(5)	5290(4)	43(1)
C(19)	1360(5)	3132(5)	5775(4)	43(1)
C(20)	7892(5)	2474(5)	3312(4)	44(1)
C(21)	3420(5)	2489(5)	6297(4)	42(1)
C(22)	2405(6)	1438(5)	-440(4)	55(2)
C(23)	1321(5)	4424(5)	5862(4)	42(1)
C(24)	3369(5)	191(5)	1332(4)	37(1)
C(25)	928(5)	1560(5)	2730(5)	52(1)
C(26)	5807(6)	2226(5)	6075(4)	45(1)
C(27)	1619(6)	3820(5)	2409(5)	57(2)
C(28)	6394(5)	3184(5)	1076(4)	49(1)
C(29)	3879(7)	3030(6)	7580(5)	63(2)
C(30)	2255(6)	915(5)	5789(5)	71(2)
C(31)	375(6)	-2711(6)	1711(5)	72(2)
O(32)	1116(4)	-1687(4)	137(3)	58(1)
C(33)	706(8)	-3894(7)	1584(7)	107(3)

Table S16. Bond lengths [Å] and angles [deg] for *trans*-**1**.

N(1)-C(8)	1.386(6)
N(1)-C(12)	1.368(5)
N(1)-H(1)	0.8800
N(2)-C(3)	1.362(5)
N(2)-C(10)	1.376(5)
N(2)-H(2)	0.8800
C(3)-C(23)	1.383(6)
C(3)-C(11)#1	1.500(6)
O(4)-C(17)	1.218(5)
N(5)-C(24)	1.376(5)
N(5)-C(15)	1.381(5)
N(5)-H(5)	0.8800
C(7)-C(15)	1.383(6)
C(7)-C(16)	1.426(6)
C(7)-C(28)	1.514(6)
C(8)-C(18)	1.354(6)
C(8)-C(11)	1.537(6)
O(9)-C(13)	1.347(6)
O(9)-C(31)	1.492(6)
C(10)-C(19)	1.377(6)
C(10)-C(21)	1.503(6)
C(11)-C(15)	1.517(6)
C(11)-C(3)#1	1.500(6)
C(11)-C(20)	1.554(6)
C(12)-C(26)	1.359(6)
C(12)-C(21)	1.511(7)
C(13)-O(32)	1.204(5)

C(13)-C(24)	1.474(6)
C(14)-C(16)	1.488(6)
C(14)-C(22)	1.530(7)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(16)-C(24)	1.367(6)
C(17)-C(27)	1.482(6)
C(17)-C(25)	1.500(6)
C(18)-C(26)	1.425(7)
C(18)-H(18)	0.9500
C(19)-C(23)	1.420(6)
C(19)-H(19)	0.9500
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(29)	1.531(7)
C(21)-C(30)	1.540(6)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23)	0.9500
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26)	0.9500
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800

C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(33)	1.443(8)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(8)-N(1)-C(12)	109.7(4)
C(8)-N(1)-H(1)	125.2
C(12)-N(1)-H(1)	125.2
C(3)-N(2)-C(10)	112.6(4)
C(3)-N(2)-H(2)	123.7
C(10)-N(2)-H(2)	123.7
N(2)-C(3)-C(23)	106.2(4)
N(2)-C(3)-C(11)#1	123.7(4)
C(23)-C(3)-C(11)#1	130.1(4)
C(24)-N(5)-C(15)	109.5(3)
C(24)-N(5)-H(5)	125.3
C(15)-N(5)-H(5)	125.3
C(15)-C(7)-C(16)	108.0(4)
C(15)-C(7)-C(28)	127.2(4)
C(16)-C(7)-C(28)	124.7(4)
C(18)-C(8)-N(1)	107.5(4)
C(18)-C(8)-C(11)	130.7(5)

N(1)-C(8)-C(11)	121.8(4)
C(13)-O(9)-C(31)	115.3(4)
C(19)-C(10)-N(2)	104.9(4)
C(19)-C(10)-C(21)	131.0(4)
N(2)-C(10)-C(21)	123.2(4)
C(15)-C(11)-C(3)#1	110.7(4)
C(15)-C(11)-C(8)	111.1(4)
C(3)#1-C(11)-C(8)	110.8(4)
C(15)-C(11)-C(20)	107.4(3)
C(3)#1-C(11)-C(20)	109.2(4)
C(8)-C(11)-C(20)	107.6(4)
C(26)-C(12)-N(1)	107.3(4)
C(26)-C(12)-C(21)	130.0(4)
N(1)-C(12)-C(21)	122.2(4)
O(32)-C(13)-O(9)	125.0(5)
O(32)-C(13)-C(24)	124.2(5)
O(9)-C(13)-C(24)	110.7(4)
C(16)-C(14)-C(22)	111.8(4)
C(16)-C(14)-H(14A)	109.3
C(22)-C(14)-H(14A)	109.3
C(16)-C(14)-H(14B)	109.3
C(22)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	107.9
C(7)-C(15)-N(5)	106.9(4)
C(7)-C(15)-C(11)	132.2(4)
N(5)-C(15)-C(11)	120.7(4)
C(24)-C(16)-C(7)	106.9(4)
C(24)-C(16)-C(14)	127.0(4)
C(7)-C(16)-C(14)	126.1(4)
O(4)-C(17)-C(27)	122.2(4)

O(4)-C(17)-C(25)	121.3(4)
C(27)-C(17)-C(25)	116.6(4)
C(8)-C(18)-C(26)	107.4(5)
C(8)-C(18)-H(18)	126.3
C(26)-C(18)-H(18)	126.3
C(10)-C(19)-C(23)	109.1(4)
C(10)-C(19)-H(19)	125.5
C(23)-C(19)-H(19)	125.5
C(11)-C(20)-H(20A)	109.5
C(11)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(11)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(10)-C(21)-C(12)	113.2(4)
C(10)-C(21)-C(29)	108.4(4)
C(12)-C(21)-C(29)	108.2(4)
C(10)-C(21)-C(30)	108.9(4)
C(12)-C(21)-C(30)	108.8(4)
C(29)-C(21)-C(30)	109.4(4)
C(14)-C(22)-H(22A)	109.5
C(14)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(14)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(3)-C(23)-C(19)	107.2(4)
C(3)-C(23)-H(23)	126.4
C(19)-C(23)-H(23)	126.4
C(16)-C(24)-N(5)	108.6(4)

C(16)-C(24)-C(13)	130.4(5)
N(5)-C(24)-C(13)	120.8(4)
C(17)-C(25)-H(25A)	109.5
C(17)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(17)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(12)-C(26)-C(18)	108.1(4)
C(12)-C(26)-H(26)	126.0
C(18)-C(26)-H(26)	126.0
C(17)-C(27)-H(27A)	109.5
C(17)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(17)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(7)-C(28)-H(28A)	109.5
C(7)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(7)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(21)-C(29)-H(29A)	109.5
C(21)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(21)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(21)-C(30)-H(30A)	109.5

C(21)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(21)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
O(9)-C(31)-C(33)	107.7(5)
O(9)-C(31)-H(31A)	110.2
C(33)-C(31)-H(31A)	110.2
O(9)-C(31)-H(31B)	110.2
C(33)-C(31)-H(31B)	110.2
H(31A)-C(31)-H(31B)	108.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

Table S17. Anisotropic displacement parameters ($Å^2$ x 10^3) for *trans*-**1**.

The anisotropic displacement factor exponent takes the form:

$-2\,pi^2\,[\,h^2\,a^{*2}\,U11 + ... + 2\,h\,k\,a^*\,b^*\,U12\,]$

	U11	U22	U33	U23	U13	U12
N(1)	27(2)	36(2)	43(3)	16(2)	6(2)	15(2)

N(2)	20(2)	29(2)	46(3)	14(2)	7(2)	2(2)
C(3)	22(3)	32(3)	40(3)	13(2)	6(2)	8(2)
O(4)	26(2)	53(2)	63(2)	25(2)	8(2)	15(2)
N(5)	23(2)	38(2)	40(2)	16(2)	8(2)	9(2)
C(7)	17(3)	35(3)	40(3)	11(2)	7(2)	9(2)
C(8)	22(3)	31(2)	39(3)	9(2)	2(2)	9(2)
O(9)	39(2)	45(2)	68(3)	23(2)	5(2)	-3(2)
C(10)	22(3)	31(3)	50(3)	15(2)	17(2)	4(2)
C(11)	23(3)	38(3)	36(3)	11(2)	6(2)	14(2)
C(12)	34(3)	37(3)	41(3)	15(2)	6(2)	15(2)
C(13)	31(3)	44(3)	42(3)	8(3)	3(3)	14(2)
C(14)	31(3)	48(3)	42(3)	15(2)	7(2)	8(2)
C(15)	22(3)	33(3)	38(3)	9(2)	4(2)	11(2)
C(16)	24(3)	39(3)	36(3)	10(2)	6(2)	14(2)
C(17)	21(3)	40(3)	44(3)	10(2)	10(2)	10(2)
C(18)	30(3)	45(3)	49(3)	18(2)	2(2)	15(2)
C(19)	24(3)	39(3)	55(3)	16(2)	15(2)	6(2)
C(20)	29(3)	45(3)	47(3)	10(2)	5(2)	16(2)
C(21)	30(3)	35(3)	60(4)	26(2)	19(2)	6(2)
C(22)	41(3)	62(3)	56(3)	28(3)	3(3)	16(3)
C(23)	20(3)	41(3)	51(3)	13(2)	5(2)	8(2)
C(24)	21(3)	37(3)	42(3)	12(2)	1(2)	8(2)
C(25)	22(3)	44(3)	75(4)	18(3)	10(3)	6(2)
C(26)	47(3)	46(3)	46(3)	23(2)	10(3)	20(2)
C(27)	34(3)	52(3)	78(4)	28(3)	3(3)	13(2)
C(28)	32(3)	50(3)	53(3)	18(3)	15(2)	9(2)
C(29)	71(4)	79(4)	71(4)	51(3)	37(3)	43(3)
C(30)	49(4)	47(3)	120(5)	43(3)	27(3)	14(3)
C(31)	49(4)	60(4)	86(4)	31(3)	16(3)	3(3)
O(32)	29(2)	59(2)	55(2)	11(2)	-4(2)	3(2)

C(33)	70(5)	78(4)	158(6)	65(4)	-3(4)	7(4)

Table S18. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for *trans*-**1**.

	x	y	z	U(eq)
H(1)	4351	3019	4507	43
H(2)	4536	5274	6531	43
H(5)	4102	564	2934	43
H(14A)	2749	-387	-882	54
H(14B)	4141	977	-822	54
H(18)	7563	2183	5288	51
H(19)	538	2232	5551	52
H(20A)	7511	1450	3142	66
H(20B)	8694	3034	3984	66
H(20C)	8244	2632	2666	66
H(22A)	1596	1102	-89	82
H(22B)	2023	1233	-1220	82
H(22C)	2992	2476	-8	82
H(23)	478	4544	5712	50
H(25A)	1369	1070	3008	78
H(25B)	457	971	1925	78
H(25C)	204	1704	3158	78
H(26)	5929	1970	6679	54
H(27A)	1066	4231	2893	85
H(27B)	1009	3182	1644	85
H(27C)	2477	4596	2377	85
H(28A)	7152	3966	1739	74
H(28B)	5896	3579	730	74

H(28C)	6835	2693	524	74
H(29A)	4609	4037	7906	95
H(29B)	4290	2446	7745	95
H(29C)	3031	2955	7911	95
H(30A)	1451	841	6173	107
H(30B)	2679	307	5891	107
H(30C)	1893	595	4979	107
H(31A)	-298	-2957	1017	86
H(31B)	-92	-2497	2357	86
H(33A)	1295	-4004	1019	161
H(33B)	-198	-4780	1335	161
H(33C)	1247	-3702	2312	161

Table S19. Output file z-matrix (Å and degrees) of the *cis*-**1** with fluoride (B3LYP/6-31G*).

C	3.15614	-0.43033	-2.01129
C	3.87518	-1.32374	-2.78911
H	4.80107	-1.11732	-3.3059
C	3.18296	-2.57006	-2.77129
H	3.49205	-3.47683	-3.27057
C	2.04279	-2.40982	-1.99883
C	3.46918	1.01686	-1.62631
C	4.80574	1.42988	-2.30449
H	5.6158	0.78743	-1.95367
H	5.05458	2.4629	-2.05747
H	4.74125	1.34148	-3.3917
C	2.37324	1.96668	-2.10595
C	2.37887	2.88167	-3.14597
H	3.2017	3.07929	-3.81773
C	0.98014	-3.42284	-1.5792
C	0.97581	-3.53911	-0.02935
H	0.73143	-2.59095	0.455
H	1.96492	-3.84942	0.32052
H	0.24344	-4.28606	0.29255
C	1.35086	-4.80693	-2.15079
H	0.60932	-5.54744	-1.84057
H	2.32845	-5.1222	-1.7758
H	1.39217	-4.80028	-3.24311
C	-0.41392	-3.0457	-2.07518
C	-1.18128	-3.58002	-3.09913
H	-0.88974	-4.38398	-3.76006
N	2.03986	-1.10494	-1.54724

H	1.30142	-0.69624	-0.95382
N	1.14632	2.06783	-1.48499
H	0.81004	1.42737	-0.75986
N	-1.18824	-2.08452	-1.45697
H	-0.83059	-1.42259	-0.7592
C	-2.08471	2.39771	-1.99096
C	-3.23425	2.55372	-2.75116
H	-3.5456	3.45549	-3.258
C	-3.93524	1.31333	-2.74051
H	-4.87232	1.10583	-3.23682
C	-3.19961	0.42175	-1.97652
C	-1.01871	3.41311	-1.5893
C	-0.99859	3.54337	-0.0404
H	-0.76607	2.59521	0.45023
H	-0.25121	4.28092	0.26839
H	-1.97953	3.87206	0.31566
C	-1.39501	4.7911	-2.17179
H	-2.36787	5.11084	-1.78902
H	-0.64992	5.53512	-1.8786
H	-1.44917	4.77228	-3.26343
C	0.36884	3.03061	-2.0972
C	1.1176	3.54755	-3.14313
H	0.81143	4.33519	-3.8168
C	-3.51041	-1.02319	-1.58623
C	-4.85288	-1.42479	-2.25524
H	-5.10569	-2.4554	-2.00356
H	-5.65642	-0.77551	-1.90132
H	-4.7942	-1.33876	-3.34307
C	-2.41987	-1.97865	-2.06921
C	-2.43134	-2.89201	-3.11102
H	-3.25928	-3.08905	-3.77663
N	-2.07339	1.0958	-1.53447
H	-1.33015	0.6887	-0.94716
F	-0.02242	-0.03018	-0.04502
C	3.67964	1.12609	-0.10724
C	3.78396	2.23951	0.74767
N	3.92634	0.01153	0.63081
C	4.1074	1.75037	2.05042
C	4.20221	0.35096	1.93958
H	3.86165	-0.93679	0.28718
C	-3.71956	-1.13866	-0.06868
C	-3.80169	-2.25944	0.77193
N	-4.02495	-0.04395	0.68189
C	-4.14006	-1.79599	2.07984
C	-4.26296	-0.39952	1.99628
H	-3.99414	0.90905	0.34825
C	4.53795	-0.65556	2.92547
C	-4.5866	0.61047	2.99187
O	4.82438	-0.44325	4.10265
O	-4.84672	0.4126	4.17765
O	4.54352	-1.90742	2.39023
O	-4.56901	1.86124	2.45768
C	-4.93342	2.95737	3.33544
H	-5.89497	2.72496	3.80236
H	-4.17975	3.03673	4.12567
C	4.9317	-2.99572	3.26704
H	4.18056	-3.09184	4.058

H	5.88931	-2.74539	3.73341
C	-5.00626	4.2194	2.49759
H	-4.04308	4.43716	2.02682
H	-5.76628	4.13081	1.71527
H	-5.27212	5.06523	3.13994
C	5.02807	-4.25508	2.4278
H	5.31128	-5.09673	3.06851
H	4.06853	-4.49068	1.95763
H	5.78506	-4.14973	1.64459
C	-4.35311	-2.62831	3.32114
H	-4.69487	-1.96096	4.11858
H	-5.16763	-3.34218	3.14586
C	4.36375	2.47649	3.35543
H	3.84133	1.9206	4.14161
H	5.4301	2.37247	3.6048
C	3.98442	3.95678	3.47369
H	2.91223	4.11583	3.3083
H	4.21882	4.30328	4.48626
H	4.53775	4.59274	2.77824
C	-3.09932	-3.35049	3.86077
H	-2.28895	-2.63696	4.03433
H	-3.32669	-3.83327	4.81839
H	-2.71954	-4.12717	3.19182
C	-3.74951	-3.69632	0.3254
H	-3.29014	-3.79448	-0.6603
H	-3.18807	-4.32613	1.01249
H	-4.75727	-4.12019	0.25702
C	3.65451	3.67412	0.29997
H	3.28174	3.72039	-0.72209
H	2.96249	4.24604	0.9216
H	4.61816	4.19356	0.32217

Table S20. Output file z-matrix (Å and degrees) of the *trans*-**1** with fluoride (B3LYP/6-31G*).

C	-2.9835	-2.24785	-1.22477
C	-2.94852	-3.21105	-2.19269
H	-3.4359	-4.02684	-2.18725
C	-2.05795	-2.78105	-3.20408
H	-1.8511	-3.25042	-4.00434
C	-1.54356	-1.5614	-2.82085
C	-3.83212	-2.12476	0.02879
C	-4.88243	-3.25029	0.04834
H	-5.40689	-3.2214	-0.77822
H	-5.47777	-3.12855	0.81683
H	-4.43106	-4.11805	0.11836
C	-3.00012	-2.22369	1.2958
C	-2.92561	-3.19805	2.26427
H	-3.39192	-4.0268	2.26305
C	-0.62412	-0.57852	-3.54602
C	-1.32684	0.80009	-3.64246
H	-1.5008	1.14108	-2.74042
H	-2.17394	0.70238	-4.12418
H	-0.74824	1.42925	-4.12373
C	-0.40094	-1.1141	-4.97537
H	0.09508	-0.45071	-5.49939

H	-1.26604	-1.28453	-5.39938
H	0.11296	-1.94817	-4.93407
C	0.70646	-0.405	-2.8599
C	1.99515	-0.71455	-3.26797
H	2.23496	-1.15341	-4.07498
N	-2.1158	-1.24547	-1.61358
H	-1.95382	-0.51285	-1.15501
N	-2.16942	-1.18795	1.68405
H	-2.04167	-0.44375	1.23154
N	0.81886	0.22708	-1.64045
H	0.14044	0.53003	-1.16911
C	0.69354	-0.38798	2.87199
C	1.9544	-0.73106	3.26984
H	2.18305	-1.18477	4.07292
C	2.86	-0.29347	2.27528
H	3.80534	-0.38931	2.29784
C	2.12637	0.29488	1.26803
C	-0.64387	-0.51213	3.58103
C	-1.3195	0.87663	3.6292
H	-1.51057	1.17959	2.71723
H	-2.15792	0.81502	4.13384
H	-0.72038	1.51672	4.06752
C	-0.41446	-0.99036	5.02631
H	0.207	-0.38193	5.47646
H	-1.268	-0.99914	5.50705
H	-0.03546	-1.89472	5.01568
C	-1.56875	-1.49959	2.89058
C	-2.0234	-2.74163	3.2695
H	-1.7793	-3.21117	4.05964
C	2.55833	1.03118	-0.00043
C	1.94597	2.45549	0.00394
H	0.96828	2.39007	0.01048
H	2.24689	2.93839	0.8011
H	2.23571	2.93858	-0.7992
C	2.14067	0.32044	-1.26203
C	2.8868	-0.26361	-2.27462
H	3.83237	-0.34539	-2.2952
N	0.80713	0.23306	1.64302
H	0.13342	0.54297	1.17053
F	-1.47035	0.93873	0.0486
C	-4.60764	-0.78299	0.04805
C	-5.9885	-0.5305	-0.05215
N	-3.96726	0.46365	0.06227
C	-6.18294	0.87827	-0.09385
C	-4.9235	1.48238	-0.03062
H	-2.95464	0.61581	0.01727
C	-4.59139	2.9127	0.018
O	-5.35609	3.85715	-0.05506
O	-3.24803	3.13817	0.12976
C	-2.77932	4.48311	0.09102
H	-3.28625	5.09441	0.87048
H	-3.02401	4.92764	-0.8925
C	-1.28046	4.42228	0.31683
H	-0.8519	5.4314	0.27356
H	-1.03142	3.99714	1.29793
H	-0.77278	3.81168	-0.44167
C	-7.50321	1.54643	-0.17106

H	-7.6272	2.2457	0.67867
H	-7.52663	2.17329	-1.09178
C	-7.12187	-1.4711	-0.13072
H	-6.91015	-2.30927	-0.81279
H	-7.36197	-1.89106	0.85598
H	-8.02457	-0.95393	-0.49844
C	4.10678	1.06632	-0.05879
C	5.0811	2.0813	-0.09331
N	4.79364	-0.15528	-0.04561
C	6.36484	1.46794	-0.09618
C	6.17337	0.08294	-0.07473
H	4.36552	-1.08259	-0.1313
C	7.18158	-0.98366	-0.00992
O	8.3931	-0.86468	-0.02923
O	6.62605	-2.23098	0.04822
C	7.49167	-3.36233	0.01806
H	8.24763	-3.29552	0.83183
H	8.03828	-3.3793	-0.94412
C	6.60702	-4.58442	0.17704
H	7.21473	-5.49696	0.13685
H	6.07424	-4.58175	1.13699
H	5.85019	-4.65268	-0.6158
C	4.92326	3.54684	-0.14268
H	4.13638	3.84893	-0.85129
H	4.6637	3.95442	0.84415
H	5.86664	4.02365	-0.45962
C	-8.6583	0.5284	-0.20145
H	-8.59392	-0.05746	-1.09449
H	-8.59046	-0.1136	0.65195
H	-9.59308	1.04884	-0.18285
C	7.70222	2.23137	-0.10168
H	8.26769	1.96662	0.76731
H	8.25646	1.97367	-0.97996
C	7.42841	3.74679	-0.09376
H	6.93042	4.02396	-0.99927
H	6.80917	3.99296	0.74351
H	8.35515	4.27639	-0.01981

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