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

Supporting Information

for

Anion-π interaction with alkenes: persistent complexes vs irreversible reactions of anions with tetracyanoethylene

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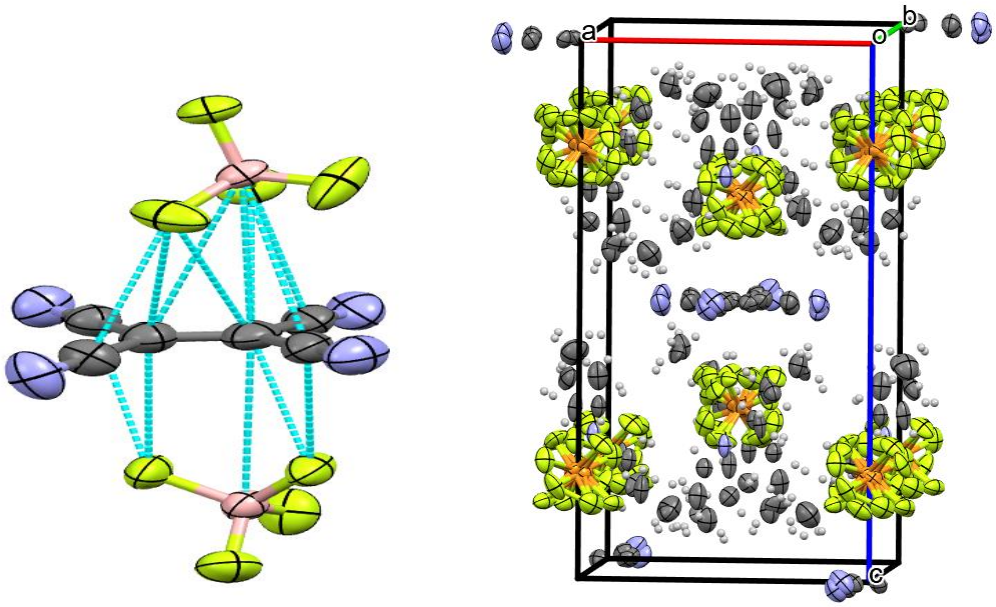

Figure S1. (Left) Fragments of the crystal structures showing 2:1 complexes in $((Pr_4N)BF_4)_2 \cdot TCNE$. Counter-ions are omitted for clarity. The blue lines show contacts shorter than the van der Waals separations. (Right) Crystal structures of $((Pr_4N)PF_6)_2 \cdot TCNE$.

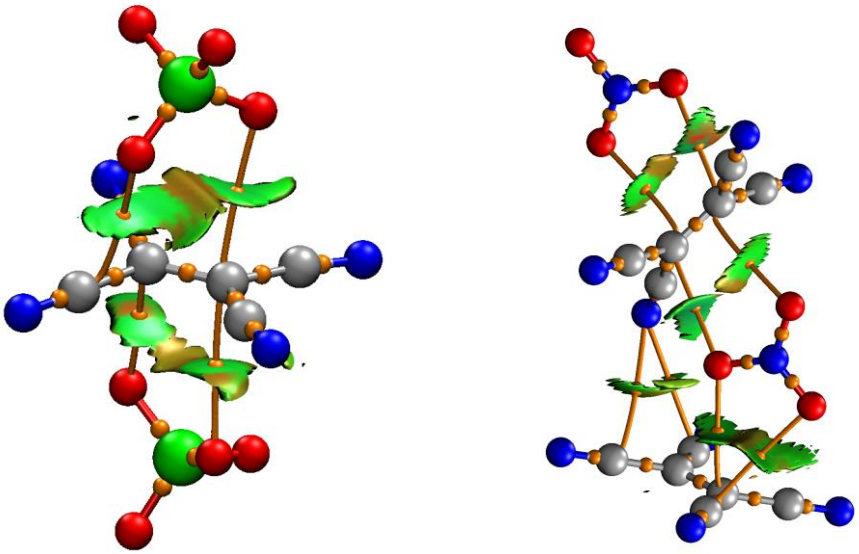

Figure S2. QTAIM and NCI analyses of the solid-state anion-π associations in $(Pr_4N)ClO_4 \cdot TCNE$ (left) and $(Pr_4N)NO_3 \cdot TCNE$ (right) (using atomic coordinates extracted from the X-ray structures). Orange lines and orange spheres show bond paths and BCPs and blue-green areas indicate bonding interactions

Table S1. Characteristics of the bond critical points (in a.u.) corresponding to short contacts in the co-crystals of TCNE with various anion.

Anion	$\rho(\mathbf{r})$	$G(\mathbf{r})$	$V(\mathbf{r})$	$H(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	ELF
ClO_4^-	0.01217	0.00997	-0.00817	0.00181	0.04711	0.03320
	0.01107	0.00845	-0.00685	0.00160	0.04017	0.03364
	0.01217	0.01025	-0.00840	0.00185	0.04841	0.03147
	0.01186	0.00927	-0.00760	0.00167	0.04375	0.03510
BF_4^-	0.01022	0.00885	-0.00679	0.00205	0.04360	0.02380
	0.00801	0.00639	-0.00482	0.00156	0.03181	0.02026
	0.00903	0.00732	-0.00560	0.00172	0.03615	0.02297
	0.00794	0.00657	-0.00497	0.00160	0.03269	0.01868
	0.00358	0.00266	-0.00191	0.00075	0.01363	0.00801
NO_3^-	0.00933	0.00678	-0.00543	0.00135	0.03252	0.02969
	0.01601	0.01341	-0.01129	0.00212	0.06210	0.04527
	0.00902	0.00687	-0.00539	0.00148	0.03337	0.02592
	0.00702	0.00516	-0.00397	0.00120	0.02544	0.01998
Br^-	0.01092	0.00686	-0.00609	0.00077	0.03051	0.04813
	0.01034	0.00632	-0.00538	0.00093	0.02901	0.04717

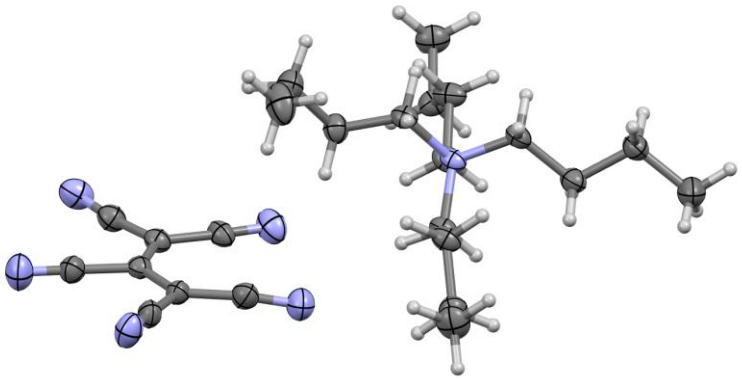

Figure S3. Crystal structure of tetrabutylammonium 1,1,2,3,3-pentacyanoprop-2-en-1-ide obtained from the reactions of the alkylammonium fluoride of chloride with TCNE.

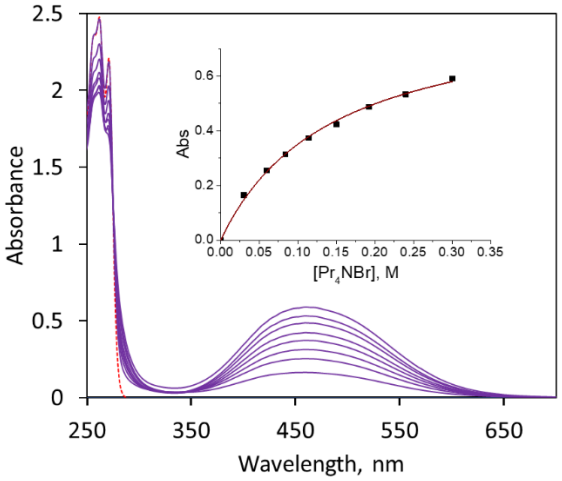

Figure S4. Spectra of solutions with variable concentrations (from 20 to 300 mM) of $(Pr_4N)Br$ and a constant concentration (1.5 mM) of TCNE in acetonitrile (purple lines). Dashed red and blue lines show spectra of the solutions of individual $(Pr_4N)Br$ and TCNE, respectively. Insert: Dependence of the intensity of absorption at 465 nm on the concentration of Br^- (the solid line shows a fit of the data to a 1:1 binding isotherm with formation constant of 7.0 ± 0.5 M^{-1}).

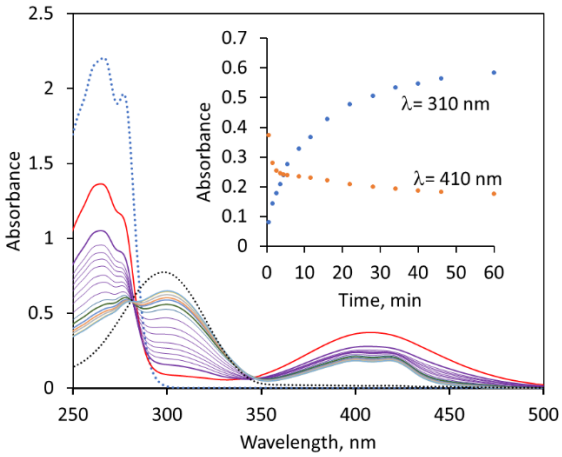

Figure S5. Time-dependence of the spectrum of the solutions of TCNE (1.5 mM) and 0.1 M Pr_4NCl in dichloromethane. Blue dotted line – spectrum individual TCNE, red line – spectrum immediate upon mixing, black dotted line – spectrum after 24 hours. Insert – changes of the intensity of absorbance with time at 310 and 410 nm.

Table S2. Energies of the (lowest-energy) absorption bands of the complexes of halide anions with different acceptors (for Mulliken correlation in Figure 7).

Acceptor, A	E_{red} (A),[a, b] V vs SCE	hν, eV [A,Br^-][a]	[A,I^-][a]	[A,Cl^-][a]	[A,NCS^-][c]
TCNE	0.17	2.668[d]	1.909[d]	3.063[d]	2.481
DDQ	0.52	2.182	-	2.820	2.409
oCA	0.15	2.660	-	-	2.496
pBA	0.02	2.272	1.859	3.181	2.558
pFA	-0.01	2.833	2.103	3.223	2.634
pCA	-0.02	2.733	2.001	3.094	-
$26Cl_2Q$	-0.18	2.885	2.195	3.300	-
$25Cl_2Q$	-0.20	2.885	2.204	3.317	-
TCP	-0.22	3.102	2.256	3.446	2.691
TNB	-0.42	3.446	2.697		3.181
TCB	-0.65	3.495	2.532		2.990

From: Kepler, S.; Zeller, M.; Rosokha, S.V. Anion–π complexes of halides with p-benzoquinones: structures, thermodynamics, and criteria of charge transfer to electron transfer transition *J. Am. Chem. Soc.*, **2019**, 141, 9338 – 9348. b) E_{ox} for I^-, Br^-, Cl^- and NCS^- are 1.06, 1.60, 2.03 and 1.52 V vs SCE, respectively. The value for I^-, Br^-, Cl^- are from and the value for NCS^- was calculated as described in: Isse, A.A.; Lin, C. Y.; Coote, M. L.; Gennaro, A. Estimation of standard reduction potentials of halogen atoms and alkyl halides. *J. Phys. Chem. B*, **2011**, 115, 678-684. c) From: Wilson, J.; Maxson, T.; Wright, I.; Zeller, M.; Rosokha, S.V. Diversity and uniformity in anion–π complexes of thiocyanate with aromatic, olefinic and quinoidal π-acceptors *Dalton Trans.*, **2020**, *49*, 8734-8743. d) Current work.

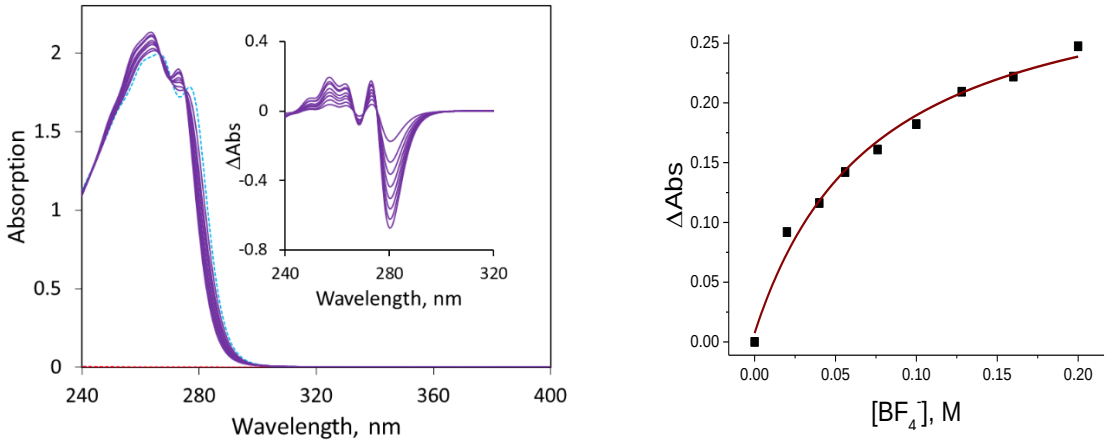

Figure S6. (Left) Spectra of the solutions (purple lines) containing variable (from 20 to 200 mM) concentrations of $(Bu_4N)BF_4$ and constant (1.5 mM) concentration of TCNE in CH_2Cl_2. Dashed red and blue lines show spectra of the individual solutions of $(Pr_4N)BF_4$ and TCNE, respectively. Insert: Differential spectra obtained by the subtraction of the absorption of individual components from the absorption of the mixture. (Right) Dependence of the absorption intensity at 270 nm on the concentration of BF_4^- (the solid line shows a fit of the data to the 1:1 binding isotherm).

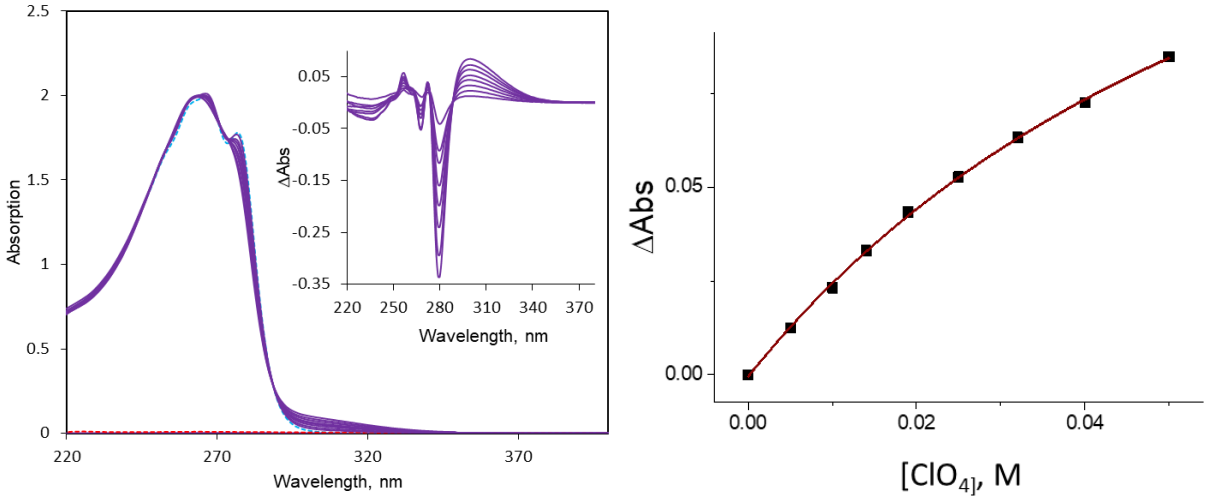

Figure S7. (Left) Spectra of the solutions (purple lines) containing variable (from 20 to 500 mM) concentrations of $(Pr_4N)ClO_4$ and constant (1.5 mM) concentration of TCNE in CH_2Cl_2. Dashed red and blue lines show spectra of the individual solutions of $(Pr_4N)ClO_4$ and TCNE, respectively. Insert: Differential spectra obtained by the subtraction of the absorption of individual components from the absorption of the mixture. (Right) Dependence of the absorption intensity at 310 nm on the concentration of ClO_4^- (the solid line shows a fit of the data to the 1:1 binding isotherm).

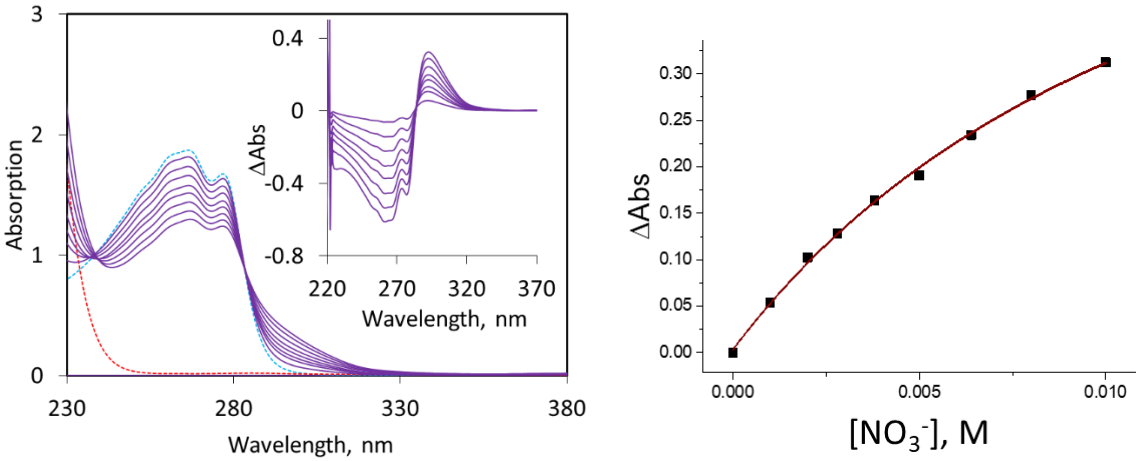

Figure S8. (Left) Spectra of the solutions (purple lines) containing variable (from 20 to 100 mM) concentrations of $(Pr_4N)NO_3$ and constant (1.5 mM) concentration of TCNE in CH_2Cl_2. Dashed red and blue lines show spectra of the individual solutions of $(Pr_4N)NO_3$ and TCNE, respectively. Insert: Differential spectra obtained by the subtraction of the absorption of individual components from the absorption of the mixture. (Right) Dependence of the absorption intensity at 290 nm on the concentration of NO_3^- (the solid line shows a fit of the data to the 1:1 binding isotherm).

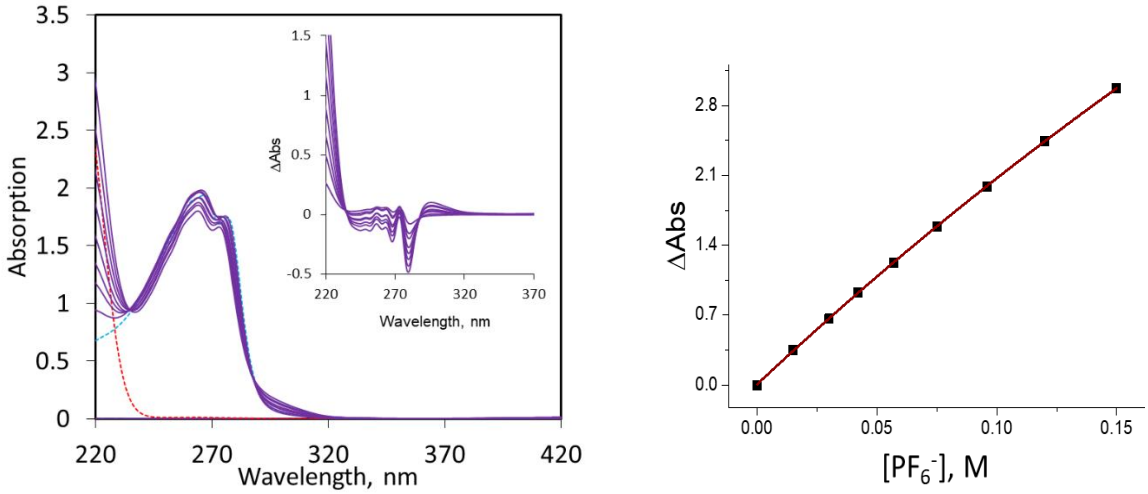

Figure S9. (Left) Spectra of the solutions (purple lines) containing variable (from 20 to 100 mM) concentrations of $(Pr_4N)PF_6$ and constant (1.5 mM) concentration of TCNE in CH_2Cl_2. Dashed red and blue lines show spectra of the individual solutions of $(Pr_4N)PF_6$ and TCNE, respectively. Insert: Differential spectra obtained by the subtraction of the absorption of individual components from the absorption of the mixture. (Right) Dependence of the absorption intensity at 290 nm on the concentration of PF_6^- (the solid line shows a fit of the data to the 1:1 binding isotherm).

Calculation of the equilibria constants

Formation constants of the complexes, [TCNE, X^-], between anions, X^- and TCNE were established via UV-Vis measurements of the dichloromethane solutions containing constant concentrations (from 1 to 5 mM) of TCNE and variable concentrations (from 0 to ~ 0.5M) of tetrapropylammonium or tetrabutyl-ammonium salts of anions. The formation constants and spectral characteristics represent average values from 3-5 series of UV-Vis experiments for each TCNE/X^- pair. Each such series typically included 8 -10 points (each measured immediately after mixing of reactants). The measurements were carried out at 22 ^oC in capped quartz spectroscopic cuvettes (1.0 mm path length) equipped with a sidearm under argon atmosphere immediately on a CARY 500 spectrophotometer.

Apparent equilibrium constants of the complex formation, Kwere calculated via regression analysis of the dependence of the differential intensity of absorption (obtained by subtraction of absorption of components from the absorption of their mixtures) of solutions containing constant concentrations of TCNE and variable concentrations of anions:

$$\text{TCNE} + X^- \overset{K}{\rightleftharpoons} [\text{TCNE}, X^-] \qquad \text{(S1)}$$

The formation constant of the complex is expressed as

$$K = C_{com} / ((C^o_D - C_{com})(C^o_A - C_{com})) \qquad \text{(S2)}$$

where C_{com} is the concentartion of the complex, and C^o_D and C^o_A are initial concentrations of X^- and TCNE, respectively. From eq. S2, concentration of complex is expressed as:

$$C_{com} = (C^o_A + C^o_D + 1/K_{eff}) +/- (((C^o_A + C^o_D + 1/K_{eff})^2 - 4C^o_A C^o_D)^{0.5}\}/2 \qquad \text{(S3)}$$

So, changes in the UV-Vis absorption intensity can be expressed as:

$$\Delta Abs = \varepsilon l \times C_{com} = \varepsilon l \times \{(C^o_A + C^o_D + 1/K_{eff}) - ((C^o_A + C^o_D + 1/K_{eff})^2 - 4C^o_A C^o_D)^{0.5}\}/2 \qquad \text{(S4)}$$

where ε and l are the difference between the extrtinction coefficients of TCNE and complex at certain wabvelength and the length of the cell. The fitting of the results of the UV-Vis titrations to eqs S4 (with ε and K as the ajustable parameters) using the Origin Pro 2016 is illustrated in Figures S4 and S6 – S9. Such fits produced values of K in Table S3.

Table S3. Apparent equilibria constants, K, of complex formation between various π-acceptors and anions.

	TCNE	TCP[a]	pFA[b]	DDQ[c]
PF_6^-	8	14	7	15
BF_4^-	12	15	3	20
ClO_4^-	13	40	6	35
NO_3^-	76	-	-	-
Cl^-	d	8	3	350
Br^-	31	7	2.3	d
I^-	e	4	e	e

a) Tetracyanopyrazine; b) Tetrafluoro-p-benzoquinone; c) Dichlorodicyano-p-benzoquinone; d) Formation of PCP^- anion hindered quantitative measurements of anion-π complexes. e) Redution of TCNE hindered quantitative measurements of anion-π complexes.

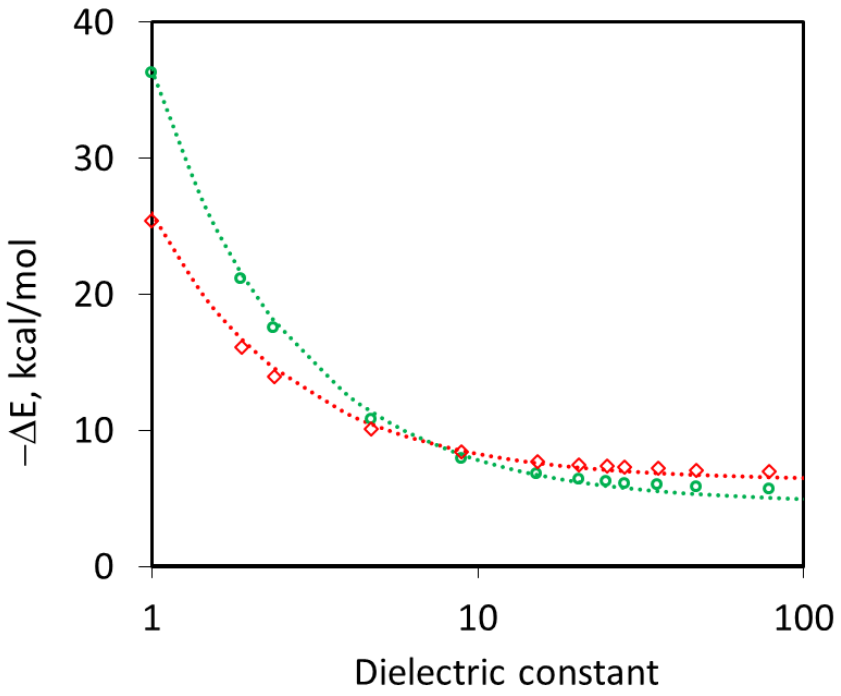

Figure S10. Dependencies of ΔE for TCNE·Br^- (○) and TCNE·BF_4^- (Δ) pairs on the dielectric constant (see details in Table S2 below), note that dashed lines represent fit of variations of interaction energies with ε_r using Born model, $\Delta E = \Delta E^v - N_A e^2/(8\varepsilon_0) \times (1-1/\varepsilon_r)\,(1/r_\pi - 1/r_X)$), where N_A is Avogadro number, e is the charge of an ion (the elementary charge), ε_0 is permittivity of vacuum, r is an effective radius of the ion (r_X - individual ion, r_π ion in the anion-π complex) and ε_r is a dielectric constant of the solvent. The good fit obtained with r_X = 2.00 Å and r_π = 2.5 Å for TCNE/Br^- pair and r_X = 3.1 Å and r_π = 3.8 Å for TCNE/BF_4^- (see F.E. Odubo, M. Zeller and S. Rosokha *J. Phys. Chem. A*, 2023, **127**, 5851. For similar dependencies with p-benzoquinone acceptors and details of calculations).

Table S4. Sum of electronic and zero-point energies, E (in Hartree) and binding energies, ΔE (in kcal/mol) for the TCNE·Br^- , TCNE· BF_4^- (and their components) in optimized in various solvents

Solvent	ε_r[a]	E					ΔE	
		TCNE	Br^-	BF_4^-	TCNE·Br^-	TCNE·BF_4^-	TCNE·Br^-	TCNE·BF_4^-
Vacuum	1	-447.47792	-2574.27094	-424.58251	-3021.80661	-872.10087	-36.2	-25.4
n-Hexane	1.88	-447.48202	-2574.32195	-424.62710	-3021.83762	-872.13473	-21.1	-16.1
Toluene	2.37	-447.48336	-2574.33394	-424.63763	-3021.84519	-872.14319	-17.5	-13.9
Chloroform	4.71	-447.48654	-2574.35671	-424.65753	-3021.86038	-872.16016	-10.8	-10.1
Dichloromethane	8.93	-447.48845	-2574.36763	-424.66709	-3021.86869	-872.16898	-7.9	-8.4
2-Pentanone	15.20	-447.48945	-2574.37267	-424.67149	-3021.87292	-872.17320	-6.8	-7.7
Acetone	20.49	-447.48984	-2574.37452	-424.67311	-3021.87454	-872.17479	-6.4	-7.4
Ethanol	24.85	-447.49004	-2574.37545	-424.67395	-3021.87537	-872.17570	-6.2	-7.4
Nitroethane	28.29	-447.49015	-2574.37598	-424.67441	-3021.87585	-872.17617	-6.1	-7.3
Acetonitrile	35.69	-447.49033	-2574.37678	-424.67510	-3021.87658	-872.17689	-5.9	-7.2
DMSO	46.83	-447.49049	-2574.37751	-424.67574	-3021.87725	-872.17753	-5.8	-7.1
Water	78.36	-447.49070	-2574.37845	-424.67655	-3021.87811	-872.17837	-5.6	-7.0

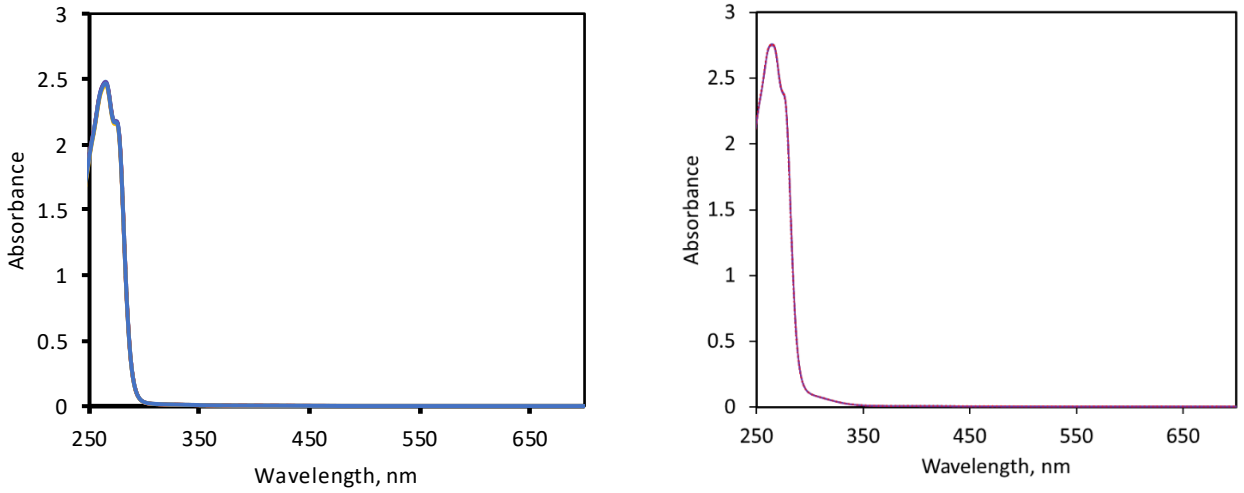

Figure S10. Time-independent spectrum of the solutions of TCNE (1.5 mM) and 0.1 M of Bu_4NPF_6 (left) or 0.05 M Pr_4NClO_4 (right) in dichloromethane showing that intensity of absorbance at absorption band maximum, 265 nm, for 5 spectra taken during 3 hours is 2.65 ± 0.01 (i.e. within accuracy of the measurements).

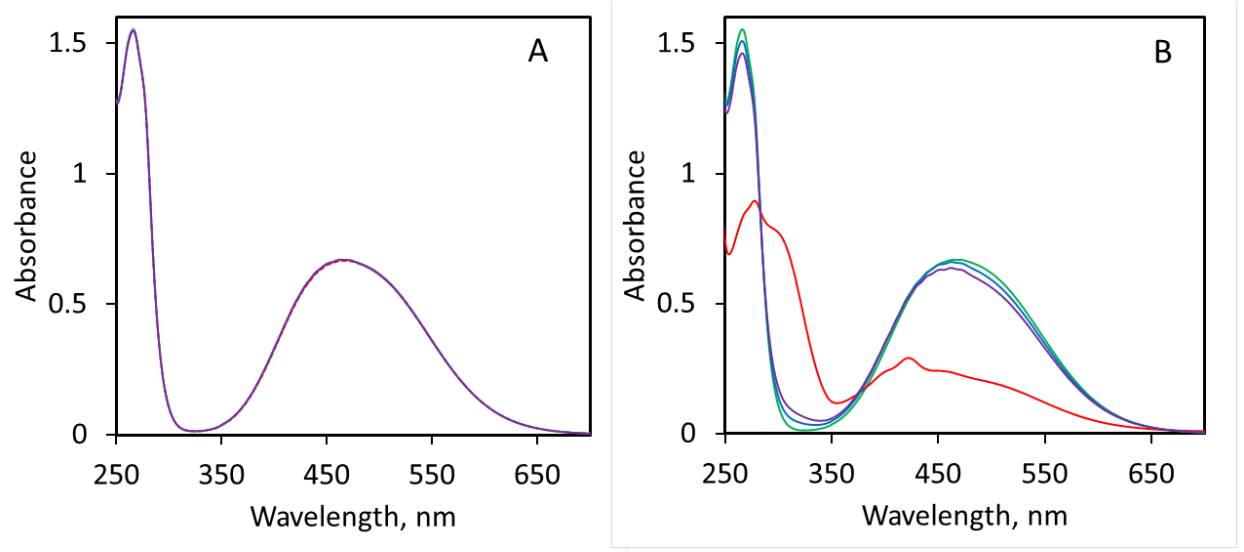

Figure S11. Spectra of solution of a mixture of TCNE (1.5 mM) and Bu_4NBr (0.2 M) in dichloromethane (at 22 °C) showing (A) essentially time-independent spectra of the anion-π complex measured at 1 min, 4 min, and 14 min after mixing of reactants and (B) some small decrease of absorbance of the complex and increase of absorption around 300-350 nm during longer time (spectra measured at 1 min (green),123 min (blue), 188 min (violet) and 24 h (red) after mixing of reactants).

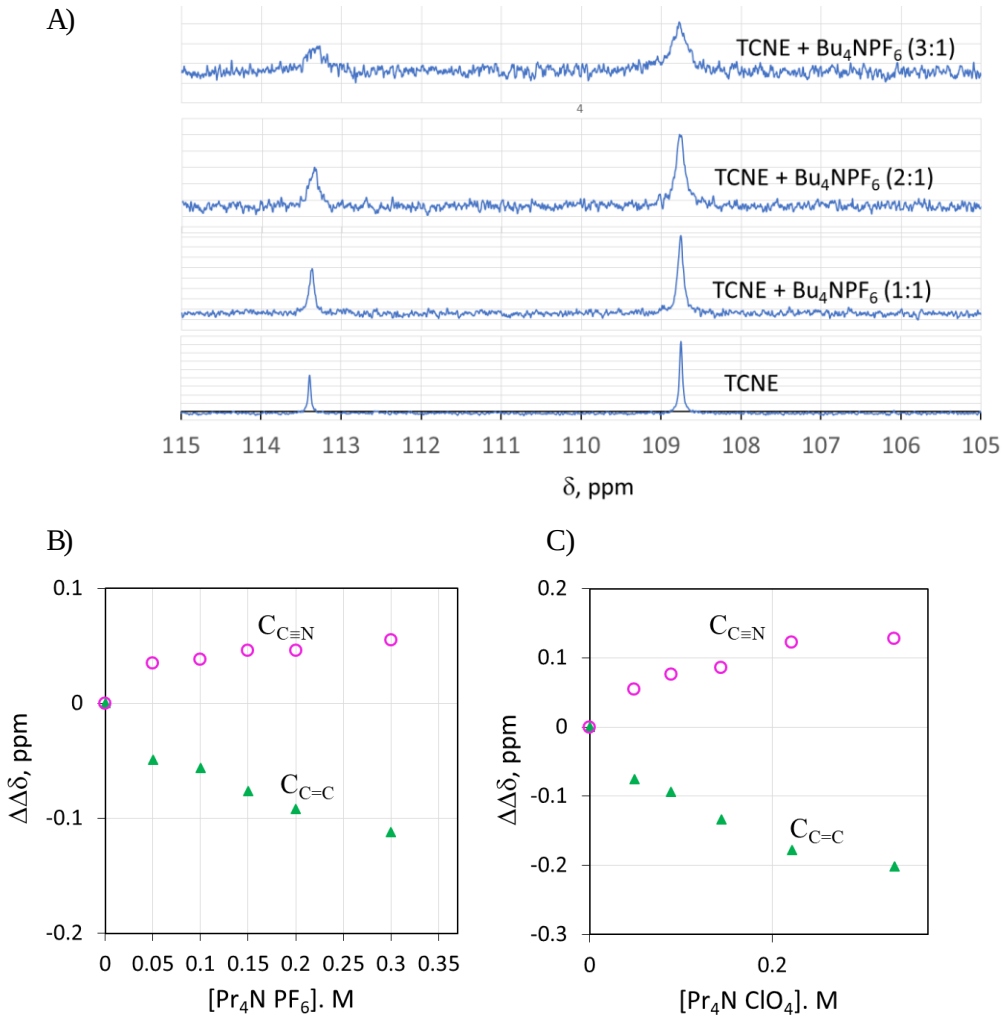

Figure S12. (A) Fragment of ^{13}C NMR spectra showing broadening and slight shifts of the signals of sp^2 (C=C) and sp^3 (C≡N) carbons of TCNE in the presence of Bu_4NPF_6. (B) and (C) Shifts of the signals of sp^2 (C=C) and sp^3 (C≡N) carbons in ^{13}C NMR spectra of TCNE (relative to the values in the individual π-acceptors) with increase of the concentration of anions (CD_3CN, concentration of TCNE is constant, 0.1 M, in all solutions).

Table S5. Characteristics of the bond critical points (in a.u.) in the optimized complexes of TCNE with various anion.

Anion	$\rho(\mathbf{r})$	$G(\mathbf{r})$	$V(\mathbf{r})$	$H(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$
Br^-	0.02067	0.01190	-0.01143	0.00047	0.04947
Cl^-	0.02823	0.01748	-0.01751	-0.00003	0.06980
F^-	0.23372	0.20887	-0.51299	-0.30412	-0.38101
BF_4^-	0.01245	0.01119	-0.00874	0.00245	0.05454
	0.01110	0.00943	-0.00738	0.00206	0.04596
PF_6^-	0.00813	0.00707	-0.00535	0.00172	0.03518
	0.00827	0.00721	-0.00545	0.00176	0.03587
	0.01141	0.01011	-0.00782	0.00228	0.04957
	0.01118	0.00983	-0.00759	0.00223	0.04823
ClO_4^-	0.01240	0.01007	-0.00808	0.00199	0.04823
	0.00960	0.00745	-0.00583	0.00161	0.03625
	0.00983	0.00762	-0.00599	0.00164	0.03704
N_3^-	0.01421	0.00864	-0.00741	0.00123	0.03947
	0.01438	0.00875	-0.00753	0.00122	0.03988
NCS^-	0.01566	0.01086	-0.00953	0.00132	0.04871
	0.01789	0.00971	-0.00916	0.00055	0.04106
NO_3^-	0.01603	0.01282	-0.01069	0.00212	0.05975
	0.01586	0.01266	-0.01055	0.00211	0.05907

Table S6. Interaction energies and their components (in kcal/mol) from the EDA analysis of the complexes of TCNE with various anions.

Anion	E_{Pauli}	E_{elstat}	E_{oi}	E_{disp}	E_{int}
PF_6^-	0.6	-7.2	-2.0	-1.7	-10.3
BF_4^-	16.5	-24.9	-9.6	-5.8	-23.7
ClO_4^-	16.9	-23.6	-10.2	-7.7	-24.6
NO_3^-	21.1	-27.1	-16.1	-6.3	-28.5
Cl^-	36.3	-39.9	-33.5	-2.7	-39.8
Br^-	29.1	-33.8	-26.9	-3.3	-34.9
I^-	27.6	-30.8	-24.2	-3.8	-31.1
NCS^-	31.5	-33.5	-25.8	-6.0	-33.8
N_3^-	50.6	-48.1	-46.8	-5.0	-49.3
F^-	387.5	-236.6	-249.3	-1.1	-99.5

Table S7. Crystallographic, data collection and structure refinement details

	TCNE·NO_3^-	TCNE·$2PF_6^-$	TCNE·$2BF_4^-$
Chemical formula	$C_{12}H_{28}N·C_6N_4·NO_3$	$C_{15}H_{28}F_6N_3P$	$2(C_{16}H_{36}N)·(C_6N_4)·2(BF_4)$
M_r	376.46	395.37	786.63
Crystal system,	Triclinic	Tetragonal	Triclinic
space group	*P*1	*I*4	*P*1
Temperature (K)	150	150	150
a, *b*, *c* (Å)	10.4139 (4), 10.7266 (4), 10.9100 (4)	10.3526 (8), 19.1311 (17)	12.847 (4), 17.517 (5), 20.811 (6)
α, β, γ (°)	80.179 (2), 84.466 (2), 61.796 (2)		94.897 (11), 90.015(16) 97.384 (14)
V (Å^3)	1058.10 (7)	2050.4 (4)	4627 (2)
Z	2	4	4
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α
μ (mm^{-1})	0.08	0.19	0.09
Crystal size (mm)	0.35 × 0.32 × 0.27	0.31 × 0.27 × 0.25	0.45 × 0.42 × 0.32
T_{min}, T_{max}	0.668, 0.747	0.656, 0.747	0.600, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25778, 8059, 5437	27133, 3898, 2697	107575, 27265, 21911
R_{int}	0.037	0.082	0.047
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.771	0.770	0.670
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.049, 0.133, 1.02	0.053, 0.156, 1.06	0.060, 0.185, 1.04
No. of reflections	8059	3898	27265
No. of parameters	274	301	1143
No. of restraints	27	829	564
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.52, −0.60	0.19, −0.28	0.68, −0.28

Table S7 (cont). Crystallographic, data collection and structure refinement details

	$TCNE{\cdot}Br^-$	PCP^-	$TCNE{\cdot}2ClO_4^-$
Chemical formula	$C_{19}H_{18}P{\cdot}C_6N_4{\cdot}Br$	$C_{16}H_{36}N{\cdot}C_8N_5$	$2(C_{12}H_{28}N){\cdot}C_6N_4{\cdot}2(ClO_4)$
M_r	485.31	408.53	699.70
Crystal system,	Triclinic	Monoclinic	Tetragonal
space group	$P1$	$C2/c$	$P42_1c$
Temperature (K)	150	150	150
a, b, c (Å)	10.8503 (4), 11.6951 (4), 12.0077 (4)	22.2957 (9), 10.8914 (4), 21.7156 (9)	10.2231 (5), 18.5008 (14)
α, β, γ (°)	118.266 (2), 90.146 (2), 115.285 (2)	108.2977 (15)	
V (Å^3)	1172.64 (8)0	5006.6 (3)	1933.6 (2)
Z	2	8	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.84	0.07	0.22
Crystal size (mm)	0.38 × 0.21 × 0.13	0.35 × 0.22 × 0.08	0.45 × 0.45 × 0.42
T_{min}, T_{max}	0.594, 0.747	0.654, 0.746	0.690, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	67705, 8967, 7045	66277, 7658, 6237	42157, 3696, 3090
R_{int}	0.056	0.034	0.047
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.770	0.715	0.770
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.068, 1.03	0.036, 0.106, 1.04	0.045, 0.136, 1.07
No. of reflections	8967	7658	3696
No. of parameters	281	469	189
No. of restraints		655	312
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.67, −0.64	0.25, −0.16	0.33, −0.34

Table S8. Interaction energies (in a.u.) of the complexes and their components[a]

	TCNE ·X⁻		X⁻	
X⁻	E	ZPE	E	ZPE
PF_6^-	-1388.42971	0.06818	-940.88100	0.01950
BF_4^-	-872.23220	0.06322	-424.68149	0.01442
ClO_4^-	-1208.55166	0.06538	-761.00086	0.01659
NO_3^-	-728.01549	0.06390	-280.46210	0.01455
Cl^-	-907.91248	0.04818	-460.36041	0.00000
Br^-	-3021.91676	0.04808	-2574.36763	0.00000
I^-	-745.35692	0.04793	-297.81008	0.00000
NCS^-	-938.74798	0.05775	-491.19191	0.00893
N_3^-	-611.89808	0.06085	-164.32104	0.01130
F^-	-547.56078	0.04976	-205.24869	0.00830

a) From M062X/def2tzvpp calculation, PCM model, CH_2Cl_2. For individual TCNE: E = -447.53604 ZPE= 0.04759

Atomic coordinates of the optimized complexes *TCNE ·X⁻*

Anion				
	C	1.86580500	0.67706400	-0.00203400
	C	1.84633100	-0.64177000	-0.27026600
	C	2.07072400	-1.60931500	0.76146800
	C	1.61491400	-1.13743200	-1.59309500
	C	1.65562100	1.65639300	-1.02479900
	C	2.11205600	1.15828200	1.32414900
	N	2.27354100	-2.38249100	1.58179200
	N	1.46615600	-1.54746200	-2.65215200
	N	1.52228800	2.45264000	-1.83726700
PF_6^-	N	2.33081700	1.54412800	2.38014300
	P	-1.75418100	-0.01545700	0.12353600
	F	-2.70506200	1.23743400	-0.18204000
	F	-2.72910100	-0.98142100	-0.70341800
	F	-2.56197000	-0.32382100	1.47212800
	F	-0.77141200	-1.26788100	0.42673200
	F	-0.74723700	0.94936700	0.94817700
	F	-0.91073000	0.29130100	-1.22082300
	C	-1.36265800	0.32103000	-0.33078000
	C	-0.99044500	-0.20775300	0.84971700
	C	-1.02377800	-1.62252900	1.06842000
	C	-0.56239700	0.62030800	1.93632800
	C	-1.34856200	1.73481500	-0.55619500
	C	-1.80822100	-0.50963300	-1.40891500
	N	-1.08646400	-2.75170300	1.24964300
BF_4^-	N	-0.25973300	1.28171600	2.82098300
	N	-1.37816900	2.86501300	-0.73990200
	N	-2.19502900	-1.16533900	-2.26465900
	B	1.89319400	-0.08740300	-0.41554500
	F	1.08606800	-0.62447400	-1.43143400
	F	3.22923000	-0.13609600	-0.78706300
	F	1.69078000	-0.83110900	0.76086900
	F	1.49905100	1.23743200	-0.17972400

	C	1.54887500	0.02479300	-0.45707600
	C	1.21216800	-0.01161600	0.84633400
	C	1.01694800	1.19353600	1.59430100
	C	1.05352500	-1.25782600	1.53323600
	C	1.76062900	-1.17774200	-1.20495500
	C	1.72830600	1.26642400	-1.14720600
	N	0.90053800	2.16068000	2.19675300
	N	0.96686700	-2.25786200	2.08487700
ClO_4^-	N	1.96365700	-2.13249600	-1.80434400
	N	1.90820100	2.25281900	-1.70105900
	Cl	-1.84640200	-0.00781600	-0.25652100
	O	-1.21427600	-1.14245300	-0.88778800
	O	-3.25429900	-0.01428000	-0.52801800
	O	-1.24921300	1.20555100	-0.76238200
	O	-1.62080100	-0.08063500	1.17062200
	C	0.49128100	-0.67135600	-0.70868100
	C	0.51881000	0.67721900	-0.68981400
	C	1.63285300	1.38631400	-0.13404500
	C	-0.53479500	1.45772800	-1.26730300
	C	-0.59257200	-1.39087700	-1.30841500
	C	1.57400400	-1.44047700	-0.17126300
	N	2.54284300	1.95253700	0.27004000
NO_3^-	N	-1.34642100	2.09225700	-1.76816600
	N	-1.42877200	-1.97554900	-1.82913300
	N	2.45915800	-2.05318700	0.22001300
	O	-2.22248100	0.04396800	1.00090000
	N	-1.11250300	-0.00695100	1.54327800
	O	-0.57097800	-1.10759200	1.76033100
	O	-0.49874200	1.04174200	1.81688300
	C	1.09298000	0.00044000	-0.11030000
	C	-0.18817300	-0.00010100	-0.55672600
	C	-0.82556700	-1.22755700	-0.94293200
	C	-0.82681000	1.22655800	-0.94334900
	C	1.77608700	1.22225800	0.16873000
	C	1.77707100	-1.22080800	0.16881000
Cl^-	N	-1.26930000	-2.21123900	-1.32796300
	N	-1.27171400	2.20954600	-1.32880000
	N	2.32854100	2.20262200	0.39035500
	N	2.33042300	-2.20066300	0.39044700
	Cl	-1.86230500	-0.00038800	1.55449000
	C	1.55310700	0.00108600	-0.06733300
	C	0.51437000	-0.00101500	0.80197800
	C	0.03025300	1.22522000	1.36817800
	C	0.03252200	-1.22952200	1.36518400
	C	2.10117900	-1.21953500	-0.56694100
	C	2.09748000	1.22425200	-0.56486400
Br^-	N	-0.26833300	2.21025200	1.87173900
	N	-0.26456500	-2.21638500	1.86603700
	N	2.54557400	-2.19794300	-0.96680400
	N	2.53771700	2.20506300	-0.96343900
	Br	-1.99503500	-0.00028100	-0.76199800

	C	-1.93557300	0.00095300	-0.20301400
	C	-1.05822800	-0.00051200	0.83008000
	C	-0.67856900	-1.22801300	1.46775000
	C	-0.67693300	1.22524700	1.47017100
	C	-2.39055700	1.22343000	-0.78384500
	C	-2.39235200	-1.22012200	-0.78547200
I^-	N	-0.46871300	-2.21315000	2.01439000
	N	-0.46545800	2.20894400	2.01879400
	N	-2.75821700	2.20453400	-1.24962400
	N	-2.76157600	-2.20018400	-1.25223500
	I	1.88624600	-0.00013000	-0.42817500
	C	-1.04823500	-0.03855900	-0.45260000
	C	0.19517400	-0.10482300	-0.99210300
	C	0.82628800	-1.36734100	-1.23850000
	C	0.84898900	1.06995700	-1.48753000
	C	-1.72342700	1.21346000	-0.30636600
	C	-1.74674600	-1.22366500	-0.06212300
	N	1.29296500	-2.38434100	-1.48751400
NCS^-	N	1.33463600	2.00697500	-1.93500700
	N	-2.26924000	2.21907900	-0.23427000
	N	-2.31153900	-2.18445100	0.20676000
	C	0.44510200	0.20502900	2.02134400
	N	-0.67389300	0.24462200	2.34936200
	S	1.97541400	0.13515400	1.42574700
	C	0.54645300	0.11321900	-0.69139200
	C	-0.70236400	-0.07644100	0.09946800
	C	-1.66179600	1.01623800	-0.18006000
	C	-1.35314500	-1.35564600	-0.26490300
	C	1.31095700	-0.99849000	-1.06580000
	C	1.02740400	1.40815200	-0.92208600
	N	-2.39155900	1.87069500	-0.39714000
N_3^-	N	-1.84280900	-2.35250800	-0.54128900
	N	1.92697300	-1.92769400	-1.37568300
	N	1.40457200	2.48559000	-1.11071500
	N	0.58091300	-0.05485300	2.00015300
	N	-0.58776100	-0.10646300	1.62354400
	N	1.62323400	-0.00651000	2.39379200
	C	-0.03647300	0.81967800	0.03872800
	C	0.02732700	-0.61057800	-0.27282900
	C	-1.14702800	-1.33641100	0.26538000
	C	1.26078900	-1.22999500	0.26613400
	C	1.14537900	1.57403800	0.10091900
F^-	C	-1.28070700	1.46586800	0.10080800
	N	-2.05632900	-1.88670200	0.68924100
	N	2.21497400	-1.69851200	0.68962700
	N	2.12450300	2.18514300	0.16284100
	N	-2.31015000	1.98781200	0.16242900
	F	0.04147600	-0.91219900	-1.65820100