Unsymmetrical 1λ³-1,2,4,6-thiatriazinyls with aryl and trifluoromethyl substituents: synthesis, crystal structures, EPR spectroscopy and voltammetry

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Supplementary Information

Crystallographic characterization of benzamidine 1a

Hydrogen bonding in the crystal structures of imidoylamidines 2a-e

Infra-red spectra of 2a-e and 3a-e

Crystallographic Characterization of *para*-substituted benzamidine 1a

Amidine chemistry is of interest due to the multifaceted bonding modes of these compounds as complex-ligands and their widespread use as synthons for subsequent chemical transformations.[1] This compound was characterized by X-ray crystallography as an example of an aryl benzamidine. No structure of this derivative has yet been reported in the Cambridge Crystallographic Database (2010 edition.) Plate shaped X-ray quality crystals of **1a** were collected on a cold finger following vacuum sublimation and its structure was determined by crystallography (Figure 1). The unit cell contains two independent hydrogen-bonded centrosymmetric dimers of a type previously determined for amidines.[2] The C–N distances in the amidine unit are indicative of partial single (C1–N1 = 1.358(3) Å) and partial double bond (C1–N2 = 1.294(3) Å) character, and are consistent with previously known values for aryl amidines.[3]

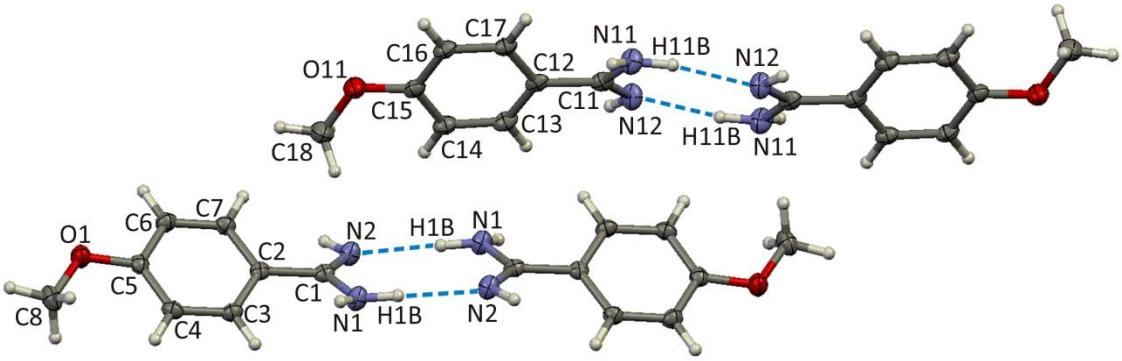
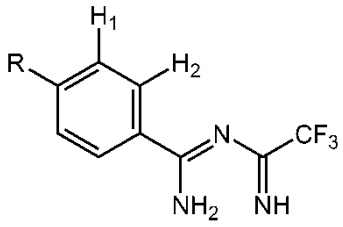


Figure S1. Thermal ellipsoids (30%) plot showing the two independent hydrogen-bonded dimers of **1a** found within the crystal lattice at −100(2) °C. Each dimeric pair is connected in ribbons to adjacent dimers of the same type through additional H bonding between N2 and H1A.The molecules that are fully-labelled comprise the asymmetric unit of the cells, each related to another molecule of the same type by inversion symmetry as required by the $P\bar{1}$ space group.

Table S1. ^{1}H NMR spectral data for the aryl N-imidoylamidines **2a–e**.[a]



cmpd	R	H_1	H_2	J_{AB} (Hz)	R	NH	NH	NH
2a	CH_3O	6.93	7.87	9.0	3.85	11.0	9.0	6.7
2b	CH_3	7.26	7.81	8.1	2.41	11.0	9.1	6.7
2c	H	m 7.38– 7.54	m 7.83 – 7.88	—	m 7.38 – 7.54	11.0	9.1	6.8
2d	Cl	7.42	7.84	8.8	—	11.0	9.2	6.7
2e	CF_3	7.73	8.02	8.1	—	11.1	9.3	6.8

[a] All values are in ppm, with reference to TMS.

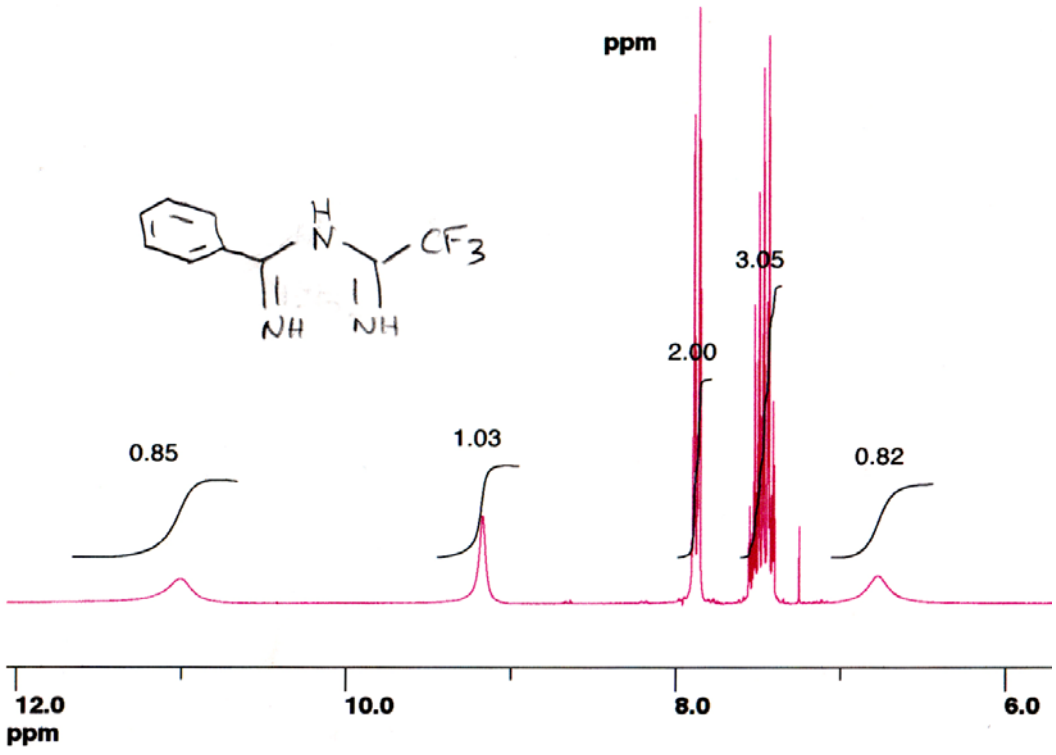
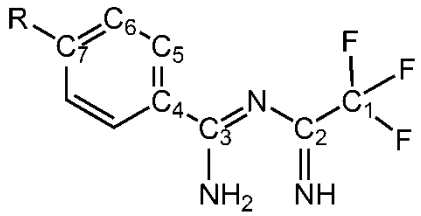


Figure S2. ^{1}H NMR Spectrum (250MHz, $CDCl_3$) of compound **2c** which is entirely typical of all the imidoylamidines prepared in this work. The three kinds of NH peaks have very distinct chemical shifts and linewidths.

Table S2. ^{13}C NMR of aryl imidoylamidines **2a–e**.[a]



cmpd	C_1	C_2	C_3	C_4	C_5	C_6	C_7	R
2a	117.86[b]	163.41[c]	165.33	127.33	129.25	114.32	163.09	55.66
2b	117.84[b]	163.55[c]	165.83	132.37	127.64	129.70	142.84	21.65
2c	117.80[b]	163.51[c]	165.92	135.22	127.44	129.02	132.20	—
2d	117.70[b]	163.31[c]	164.76	133.60	128.83	129.28	138.62	—
2e	117.67[b]	163.23[c]	164.65	138.55	127.91	125.98[d]	133.91[c]	123.91[e]

[a] All values are in ppm, with reference to TMS. [b] q, $^3J_{(F,C)}$ = 281 Hz [c] q, $^3J_{(F,C)}$ = 33 Hz. [d] q, $^3J_{(F,C)}$ = 3.9 Hz. [e] q, $^3J_{(F,C)}$ = 273 Hz.

Hydrogen bonding in the crystal structures of imidoylamidines 2a-e

Strong intramolecular hydrogen bonding (Table S3) is found from N3 to H1A and N6 to H4A in all cases, leading to *pseudo* six-membered rings with N··N distances in the range 2.6350(18) – 2.6928(18) Å. There are also weaker (2.9765(15) – 3.1934(16) Å) intermolecular H-bonds which link N1 and N4 to the backbone nitrogen atoms (N2, N5) of the next molecule in **2c** and **2e** (compared to the typical N··N distance range 2.94 – 3.15 Å for H-bonding between nitrogen.)[4] However, **2a** differs from the others by having additional short contacts between both N3 and H4A and N6 and H3A. In this case all the intermolecular N··N distances are rather long, ranging from 3.1832(16) to 3.2342(17) Å. The N–H···N angles range between 124.9(13) and 175.1(14)°, normal for this class.[4] Interestingly, in the case of **2c** and **2e** one NH atom from each imidoylamidine is not involved in any H-bonding (H3A, H6A).

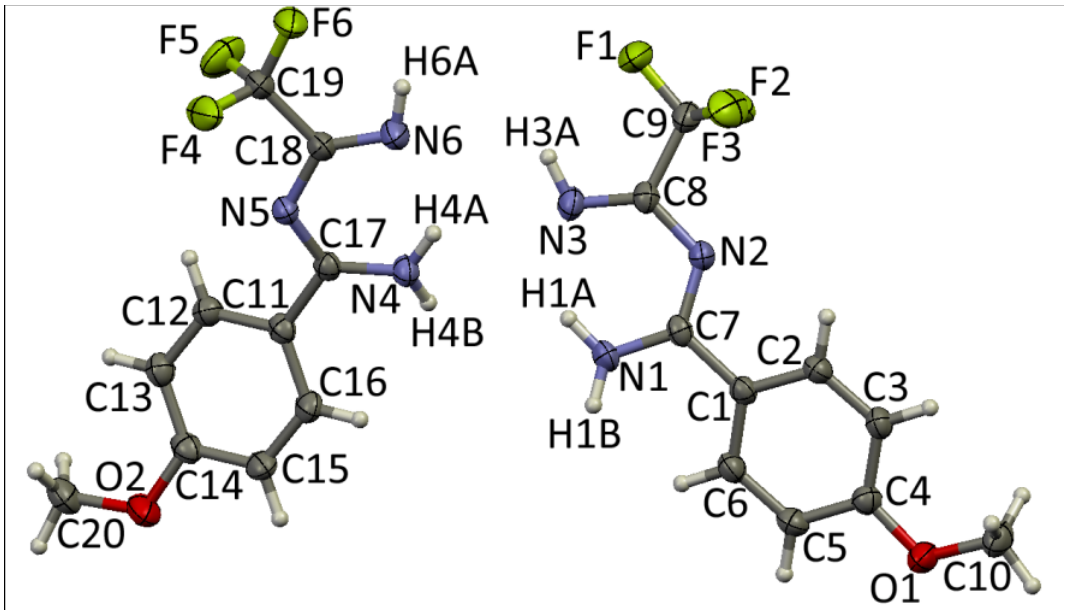


Figure S3. Thermal ellipsoids (30%) plot showing the two independent molecules of **2a** found within the crystal lattice at −100(2) °C. There are short contacts between both N4 and N6 with N3, but N4 to N6 is slightly beyond the range of a normal H-bond at −100(2) °C.

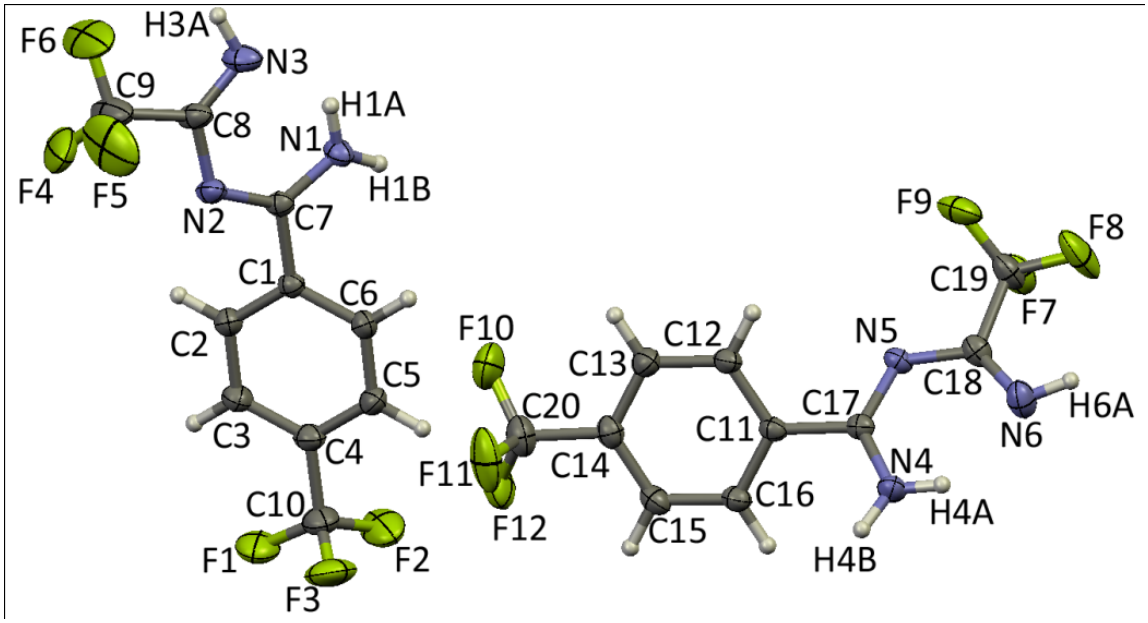


Figure S4. Thermal ellipsoids (30%) plot showing the two independent hydrogen-bonded molecules of **2e** found within the crystal lattice at −100(2) °C.

Table S3. Hydrogen bonds [Å] and angles [°] for imidoylamidines **2a**, **2c**, and **2e**.

Bond Type	D–H...A	Cmpd	d(D...A)	<(DHA)
Inter	N1–H1B...N5	**2a**	3.1832(16)	139.2(14)
		2c	3.0868(16)	175.1(14)
		2e	2.994(2)	170.2(19)
Inter	N4–H4B...N2	**2a**	3.1869(16)	136.3(14)
		2c	2.9765(15)	153.3(13)
		2e	3.099(2)	172(2)
Intra	N1–H1A...N3	**2a**	2.6448(18)	133.9(14)
		2c	2.6712(17)	131.4(13)
		2e	2.660(2)	134.5(18)
Intra	N4–H4A...N6	**2a**	2.6928(18)	129.3(14)
		2c	2.6350(18)	133.5(13)
		2e	2.643(2)	132.0(18)
Inter	N4–H4A...N3	**2a**	3.1934(16)	139.5(13)
Inter	N3–H3A...N6	**2a**	3.2342(17)	124.9(13)

Infra-red spectra of 2a-e and 3a-e

(KBr pellets; recorded on a Bomem MB102 FTIR spectrometer)

2a: 3383 (m), 3325 (m), 3178 (w), 1601 (s), 1572 (s), 1485 (s), 1466 (sh), 1438 (m), 1423 (m), 1399 (m), 1311 (m), 1261 (s), 1233 (s), 1221 (s), 1174 (vs), 1141 (vs), 1113 (sh), 1094 (m), 1029 (m), 998 (m), 837 (s), 815 (w), 786 (m), 758 (w), 745 (w), 729 (w), 708 (w), 689 (w), 642 (w), 614 (w), 588 (w), 563 (m), 514 (w), 479 (w), 433 (w) cm^{-1}.

2b: 3455 (m), 3345 (m), 3330 (m), 1612 (s), 1571 (m), 1524 (m), 1486 (s), 1400 (m), 1289 (w), 1231 (s), 1175 (s), 1154 (vs), 1111 (sh), 1019 (m), 998 (m), 954 (w), 867 (w), 842 (m), 831 (m), 820 (m), 781 (m), 734 (m), 687 (m), 670 (w), 593 (w), 543 (m), 513 (m), 466 (w), 441 (w) cm^{-1}.

2c: 3330 (m), 3118 (w), 1631 (s), 1600 (s), 1579 (s), 1513 (s), 1481 (s), 1449 (s), 1420 (m), 1320 (w), 1300 (w), 1224 (s), 1164 (s), 1144 (vs), 1076 (w), 1031 (m), 1000 (s), 932 (w), 878 (m), 826 (m), 800 (w), 775 (m), 715 (m), 695 (s), 614 (w), 602 (w), 583 (m), 516 (w), 448 (w), 421 (w) cm^{-1}.

2d: 3333 (s), 3257 (m), 3102 (m), 1644 (s), 1600 (s), 1572 (w), 1515 (m), 1475 (m), 1428 (w), 1395 (w), 1300 (w), 1226 (s), 1194 (s), 1179 (m), 1160 (sh), 1146 (vs), 1089 (m), 1017 (s), 884 (w), 844 (m), 836 (w), 794 (w), 732 (m), 675 (w), 647 (w), 625 (w), 592 (w), 519 (w), 485 (w), 458 (w), 428 (w) cm^{-1}.

2e: 3330 (m), 3249 (m), 3083 (m), 1636 (m), 1607 (s), 1582 (m), 1527 (s), 1493 (s), 1436 (w), 1406 (m), 1326 (vs), 1299 (sh), 1229 (s), 1202 (s), 1152 (s), 1130 (s), 1112 (sh), 1067 (s), 1019 (s), 962 (w), 886 (w), 852 (s), 830 (w), 801 (w), 761 (m), 713 (s), 692 (w), 630 (w), 601 (w), 590 (sh), 519 (w), 408 (w) cm^{-1}.

3a: 3199 (s), 3123 (s), 3027 (s), 2846 (w), 1705 (s), 1675 (m), 1641 (w), 1604 (s), 1584 (m), 1509 (m), 1457 (m), 1430 (m), 1408 (s), 1317 (m), 1266 (s), 1210 (vs), 1186 (m), 1158 (s), 1030 (m), 989 (w), 852 (w), 835 (m), 751 (w), 723 (w), 689 (w), 651 (m), 631 (w), 573 (m), 518 (w), 505 (w), 415 (w) cm^{-1}.

3b: 3185 (m), 3085 (m), 2960 (m), 2925 (m), 2854 (w), 1698 (s), 1637 (m), 1609 (m), 1528 (w), 1515 (w), 1428 (m), 1399 (m), 1316 (w), 1292 (w), 1213 (s), 1193 (sh), 1158 (vs), 1122 (w), 1037 (w), 1019 (w), 998 (w), 848 (w), 827 (m), 731 (m), 674 (w), 652 (w), 637 (w), 594 (w), 567 (w), 516 (w), 498 (w), 468 (w), 420 (w) cm^{-1}.

3c: IR 3203 (s), 3098 (s), 1694 (vs), 1637 (m), 1602 (w), 1528 (w), 1499 (w), 1450 (m), 1415 (m), 1305 (w), 1212 (s), 1193 (m), 1154 (s), 1028 (w), 1002 (w), 933 (w), 843 (w), 795 (w), 783 (w), 724 (w), 696 (m), 659 (w), 603 (w), 591 (m), 515 (w), 502 (w), 426 (w) cm^{-1}.

3d: 3199 (s), 3103 (s), 3020 (m), 1697 (s), 1637 (m), 1593 (m), 1523 (w), 1491 (w), 1459 (w), 1421 (m), 1394 (m), 1310 (w), 1282 (w), 1223 (s), 1210 (vs), 1190 (m), 1162 (s), 1091 (m), 1013 (w), 848 (w), 805 (w), 738 (w), 697 (w), 661 (w), 637 (m), 593 (w), 519 (w), 493 (w), 470 (w), 412 (w) cm^{-1}.

3e: 3187 (s), 3105 (s), 3021 (s), 1705 (s), 1643 (m), 1541 (w), 1517 (w), 1429 (m), 1402 (w), 1327 (vs), 1302 (w), 1226 (s), 1212 (s), 1191 (m), 1164 (s), 1131 (s), 1120 (s), 1068 (s), 1016 (m), 858 (m), 812 (w), 761 (w), 699 (m), 668 (w), 624 (m), 595 (w), 514 (w), 463 (w), 415 (w) cm^{-1}.

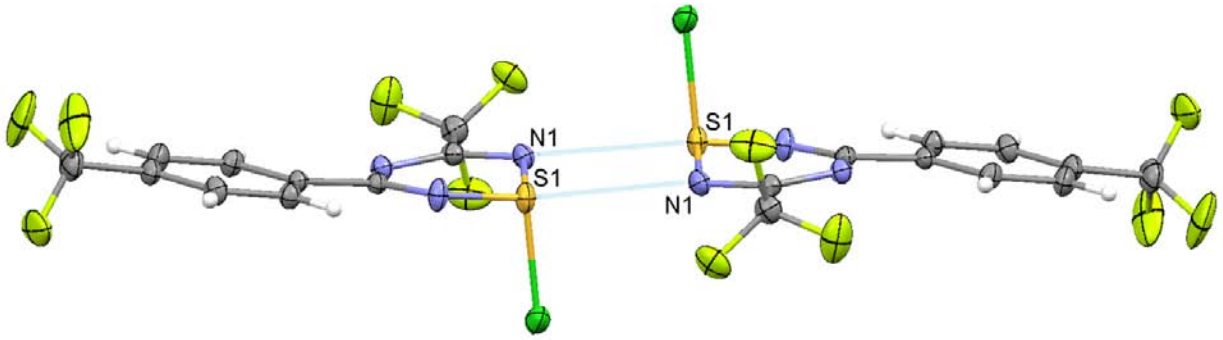
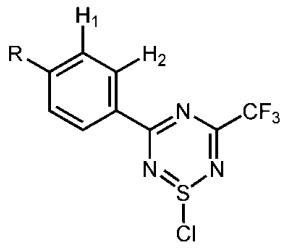


Figure S5: Thermal ellipsoids (30%) plot showing the short intermolecular S(δ^+)–N(δ^-) interactions in **4e** within the crystal lattice at −100(2) °C. The S1···N1 distance is 3.043(1) Å. Intermolecular short-contacts of this type are very common in thiazyl chemistry. Interestingly, the strength of such interactions - as measured from the interatomic distances - are very similar for the S(IV) chlorothiatriazines and the S(III) thiatriazinyls (see main text and figures below.)

Table S4. ^{1}H NMR spectral data for the 1-chlorothiatriazines

	cmpd	H_1	H_2	J_{AB} (Hz)	R
	**4a**	7.02	8.45	9.0	3.94
	4b	7.35	8.37	8.2	2.49
	4c	m 7.52 – 7.58	m 8.45 – 8.48	—	m 7.67 – 7.74
	4d	7.53	8.41	8.9	—
	4e	7.82	8.59	8.5	—

Crystal structure of N-Sulfurylchloride-N,N'-benzamidine

Hydrolysis product **6** was obtained as colorless blocks suitable for X-ray analysis (Figure S6). This is the first chlorosulfonyl derivative of a primary amidine to have been structurally characterized. In all, fifteen structures with chlorosulfonyl groups attached to nitrogen have been reported.[5] The structure of **6** is stabilized by a complex network of H-bonding involving all the nitrogen and oxygen atoms (see Figures S7, S8 and Table S5). The structure of $[ClSO_2NPCl_2NH]_2BCl$ is the most comparable reported in the literature.[5c]

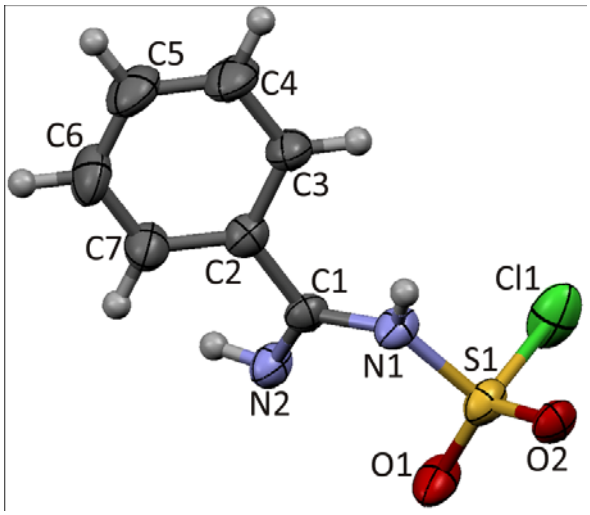


Figure S6. Thermal ellipsoids (30%) plot with atom numbering scheme showing the molecular structure of **6** as found within the crystal lattice at −100(2) °C.

Table S5. Hydrogen bonds and short contacts [Å] and angles [°] for **6**.

Bond Type	D–H...A	d(D...A)	<(DHA)
Inter	N2–H2...O2#1	2.763(3)	153(4)
Inter	N1–H1...O1#2	2.675(4)	151(4)
Intra	O1...N2	2.762(4)	
Intra	N2...O2#3	2.930(3)	

Symmetry transformations used to generate equivalent atoms:
#1 -y+1/2,x-1/2,z+1/4 #2 -x+1/2,y+1/2,-z+1/4 #3 -x+1/2,-y+1/2,-z+1/4

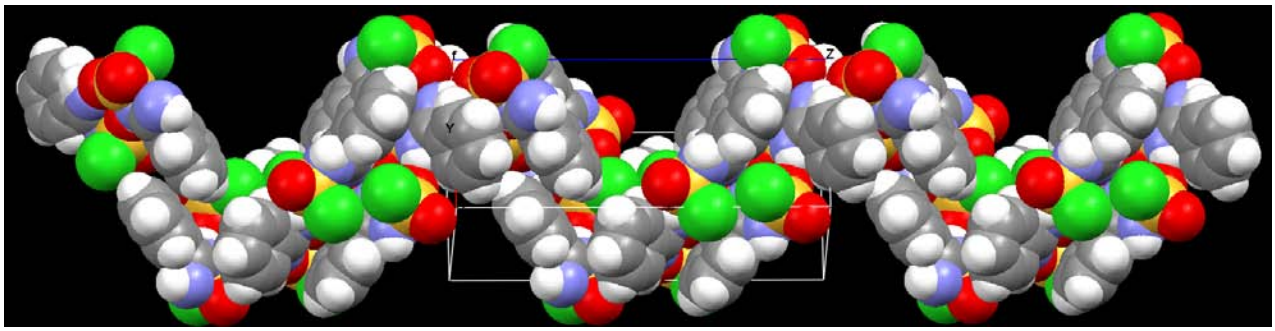


Figure S7. A packing diagram for **6** showing the double-layer "W"-shaped chain of molecules along the four-fold *c* axis of the tetragonal unit cell. The sheets defined by H-bonding as discussed in Figure S6 are clearly visible.

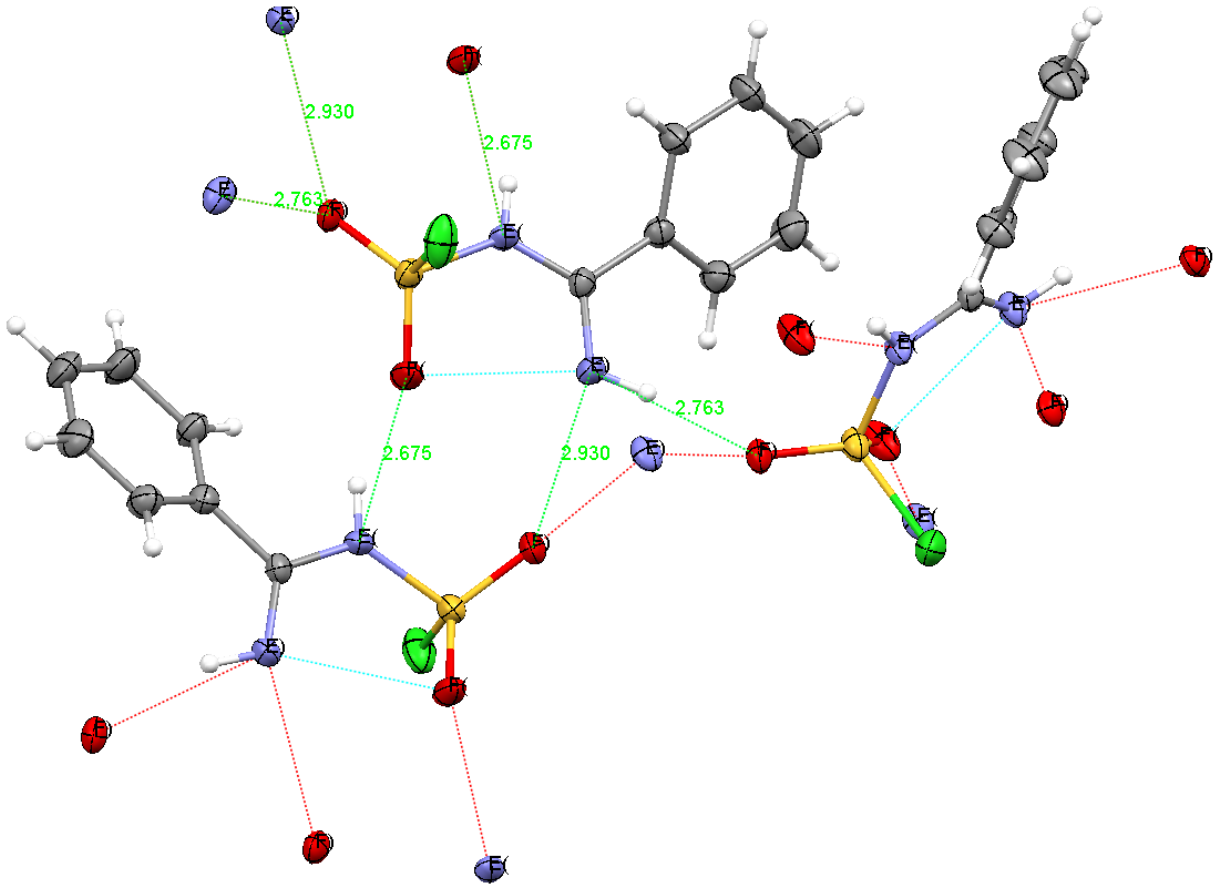


Figure S8. The complex network of hydrogen bonds in the crystal structure of **6** and short contacts that form (a) through N1-H1...O1 a chain of face-to-tail chelates vertically in the page at the l.h.s. and (b) through N2-H2...O2 a second direction directed out of the page at the r.h.s. Short contacts are also induced intra-molecularly between O1...N2 and inter-molecularly between N2...O3. The two intertwined H-bonded sheets define planes with approximate Miller indices of (24 2 -42) and (-1 12 -20). The view is approximately perpendicular to the former. The lattice contains two further sheets of molecules with approximate Miller indices of (9 0 15) and (0 16 28). Only two other known sulfonylchlorides bonded to N have been reported which also contain H-bond donors. Refcode GIVWEN contains a single type of N-H...O=S contact of 2.858(4) Å.[6] Refcode GIVXAK is the most comparable structure, containing a U-shaped chelate ring bridged by an H-bond (N-H...H 2.81(1) Å) and chain forming link between the backbone N and a neighboring chlorosulfonyl oxygen (N-H...O=S 2.96(1) Å).[7]

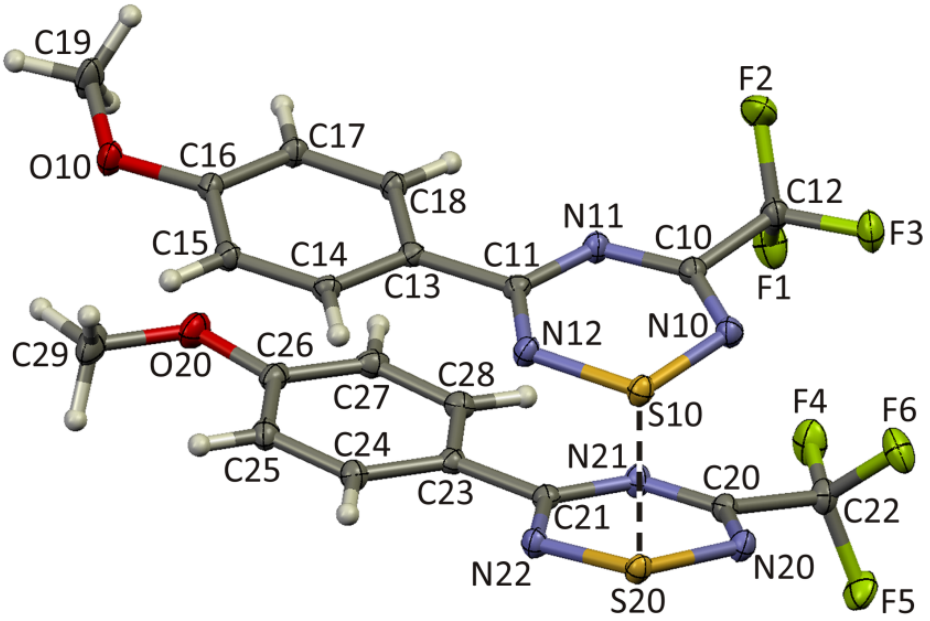


Figure S9: Thermal ellipsoids (30%) plot with atom numbering scheme showing the molecule **5a** found within the crystal lattice at −100(2) °C. The S10···S20 distance is 2.6370(3) Å.

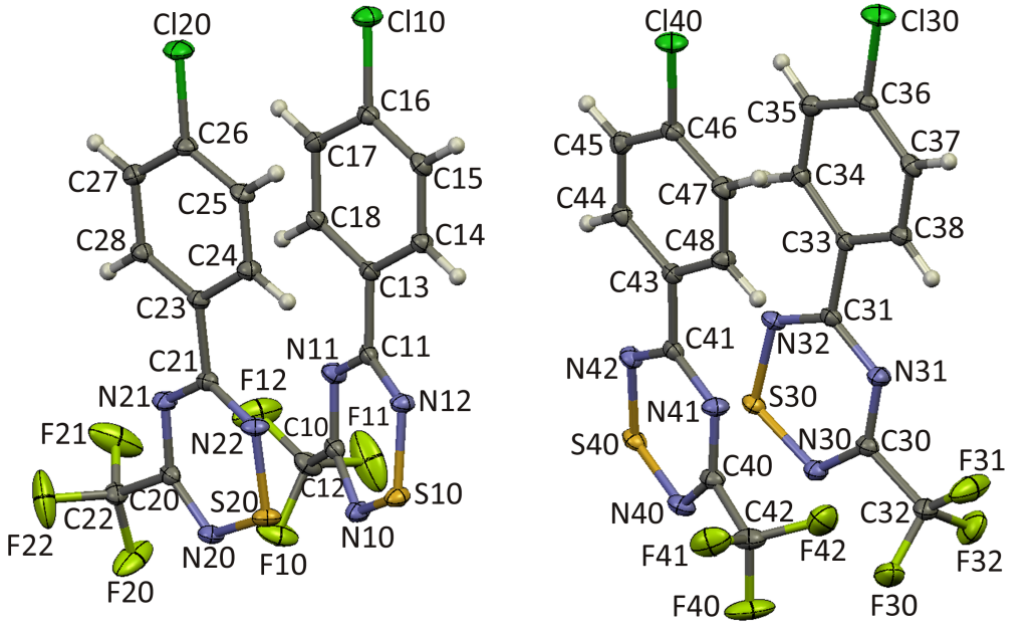


Figure S10: Thermal ellipsoids (30%) plot with atom numbering scheme showing the molecule **5d** found within the crystal lattice at −100(2) °C. The S10···S20 distance is 2.659(1) Å and the S30···S40 distance is 2.635(1) Å.

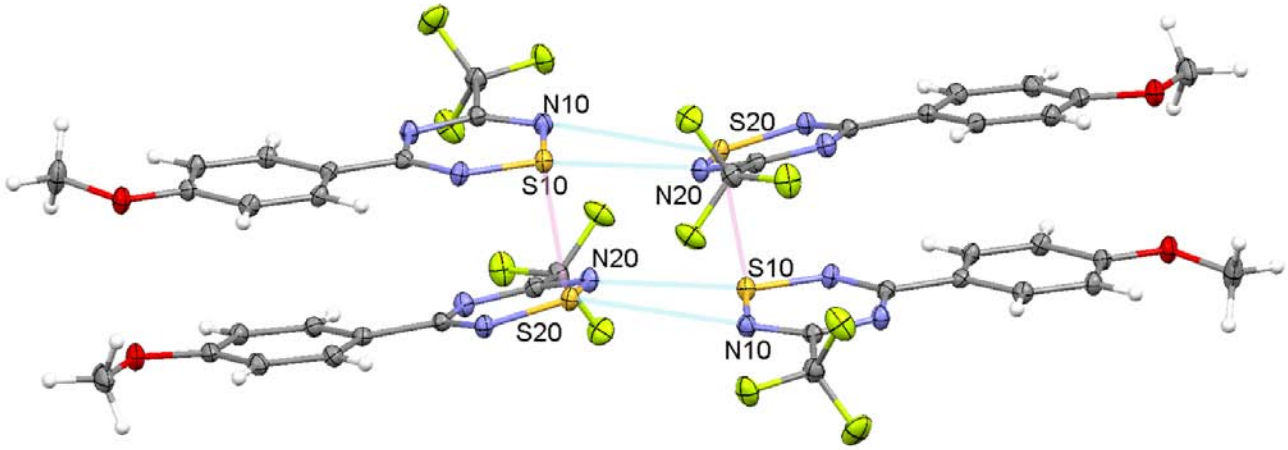


Figure S11: Thermal ellipsoids (30%) plot showing the short intermolecular and inter-dimer contacts in **5a** within the crystal lattice at −100(2) °C. The S10···N20 distance is 2.941(1) Å and the S20···N10 distance is 3.341(1) Å. Thus the shortest contacts are between the two "top" and "bottom" rings of approximately co-planar dimers of thiatriazinyls. The dimers are centrosymetrically arranged.

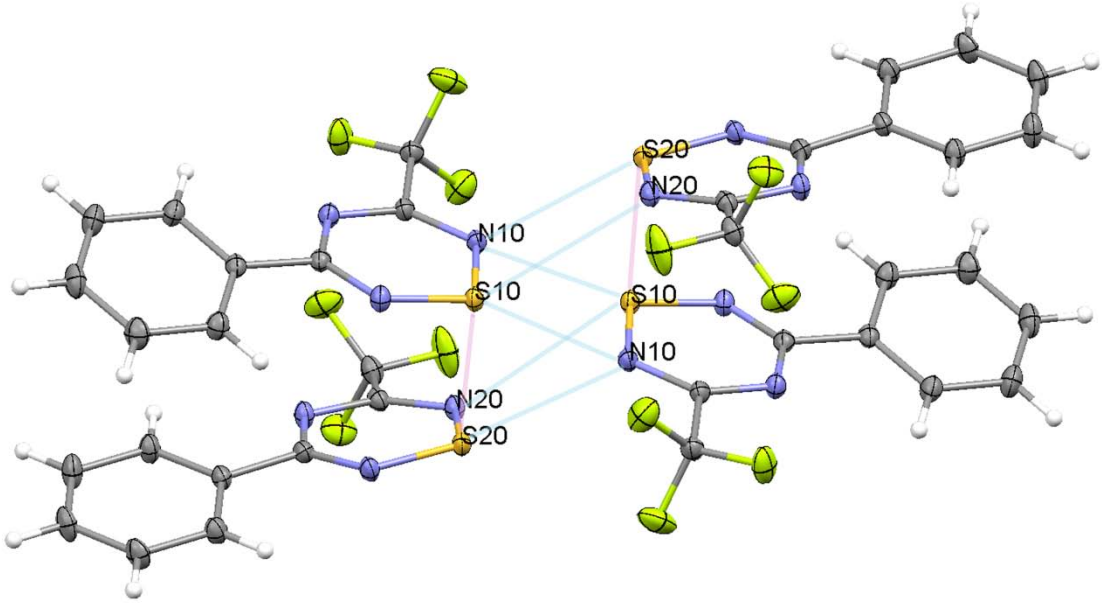


Figure S12. Thermal ellipsoids (30%) plot showing the short intermolecular and inter-dimer contacts in **5c** within the crystal lattice at −100(2) °C. The S10···N20 distance is 3.297(2) Å, the S20····N10 distance is 3.025(2) S Å and the S10···N10 distance is 3.108(2) S Å. Thus the two pairs of thiatriazinyl dimers are almost equally out of register and, though still centrosymmetrical, form a less-compact pair than that found in **5a** (Figure S9).

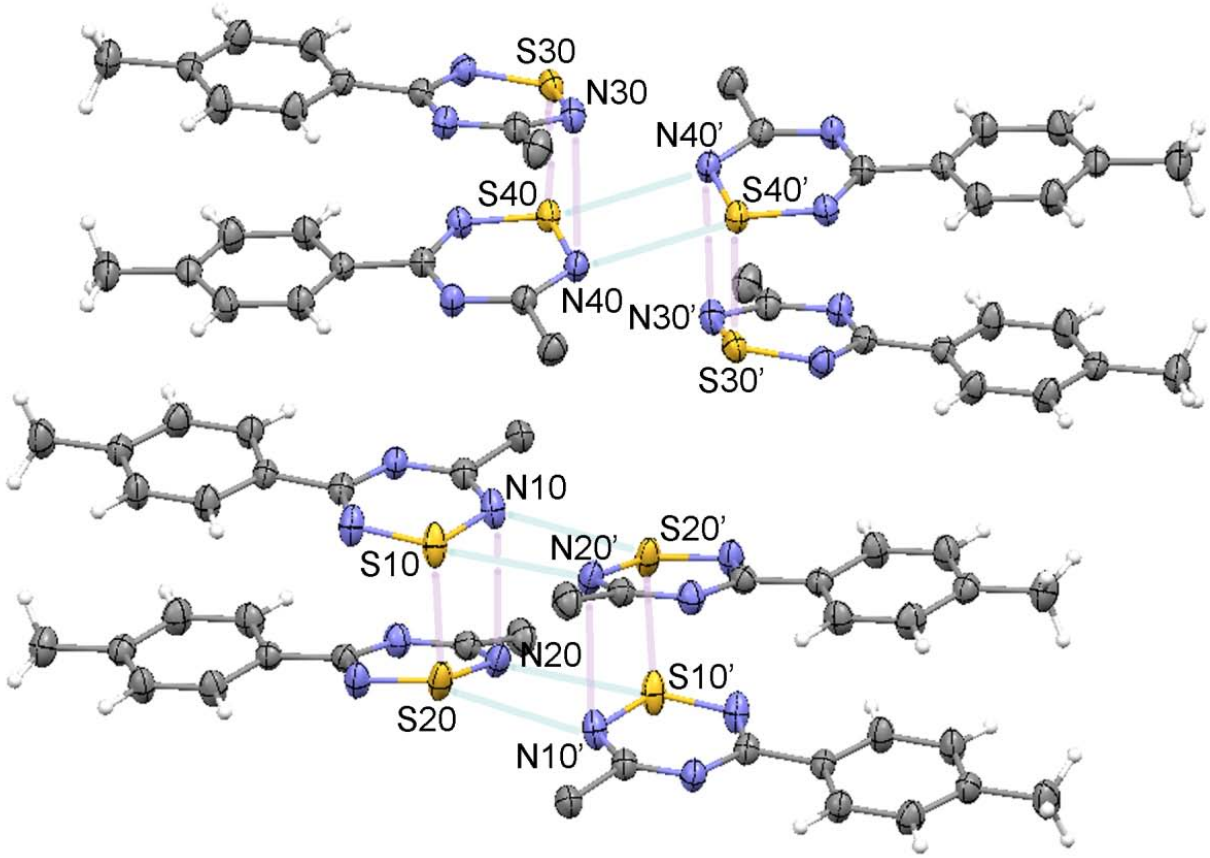
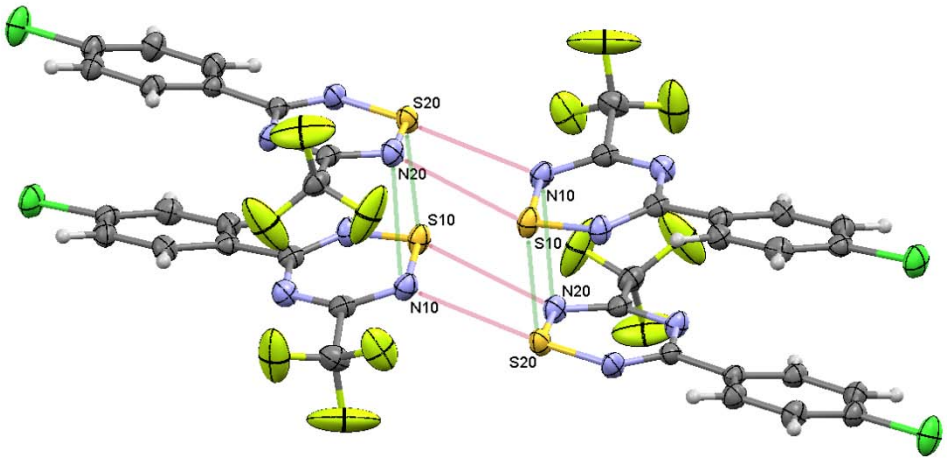
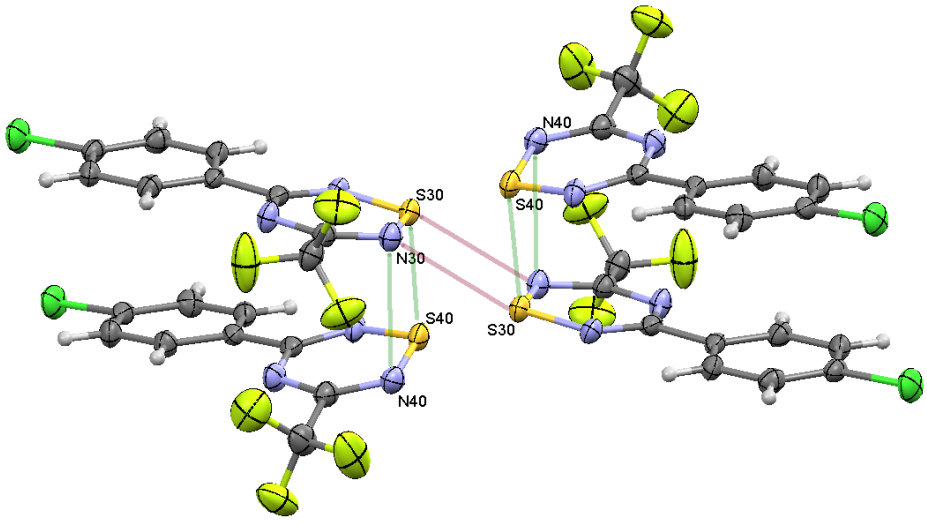


Figure S13. Thermal ellipsoids (30%) plot showing the short intermolecular and inter-dimer contacts in **5b** within the crystal lattice at 23(2) ℃ (fluorine atoms omitted for clarity). Here are found two distinct arrangements for the two pairs of dimers. That relating the S10,N10-S20,N20 pair forms approximately co-planar arrangements very similar to that observed for **5a**. (The S10···N20' distance is 3.085(2) Å and the S20···N10' distance is 3.088 (2) Å.) The second dimer pair is out of register in an arrangement very similar to that found in the structure of **4c** with S40···N40' at 3.108(1) Å and S30···N40' at 3.277 (2) Å.



(a)



(b)

Figure S14. Thermal ellipsoids (30%) plot showing the short intermolecular and inter-dimer contacts in **5d** within the crystal lattice at −100(2) °C. Like **5b**, there are two distinct arrangements for the two pairs of dimers. (a) The S10,N10-S20,N20 pair forms an intermediate arrangment between that of **5a** and **5c**, with the S10···N20' distance at 3.123(2) Å and S20···N10' at 3.035(2) Å.) (b) The second dimer pair is strongly out of register in an arrangement very similar to that found in the structure of **4c** with S30···N30' at 3.087(2) Å. Here the S40···N30' and S30···N40' distances are very long at 3.407(3) and 3.756(3) Å, respectively.

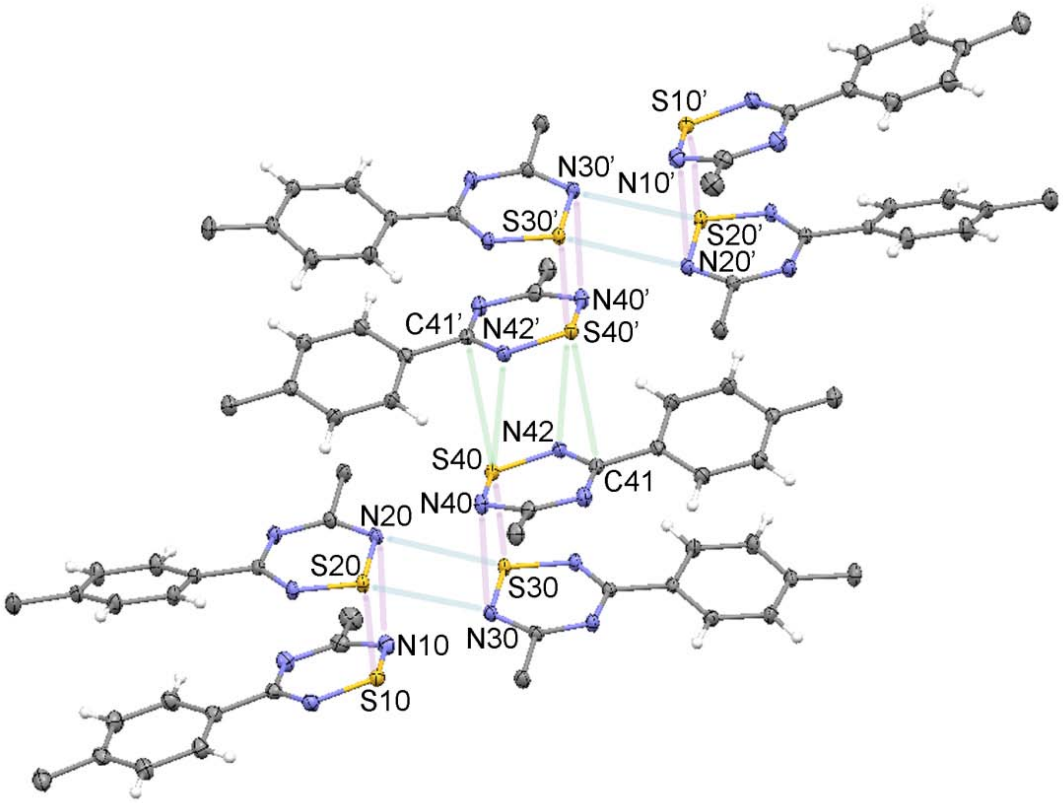


Figure S15. Thermal ellipsoids (30%) plot showing the short intermolecular and inter-dimer contacts in **5e** within the crystal lattice at −100(2) °C. Apart from the interactions within the tetramer shown in Figure 8, there are short "stacking" interactions between S40 with C41' and C41 with S40' of 3.447(2) Å.

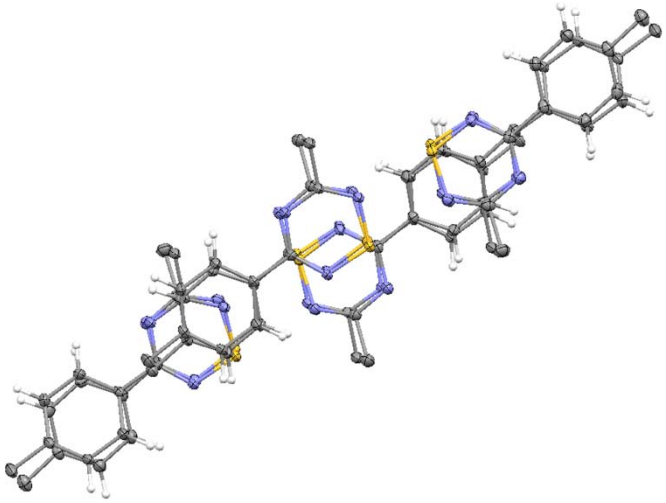


Figure S16. Stacking between two layers of thiatriazinyl dimers in **5e** leading to short S40 with C41' and C41 with S40' of 3.447(2) Å. This is the strongest interaction ever detected among multiple thiatriazinyl rings, but the stacking does not extend beyond the eight associated monomers shown in this bird's eye view approximately down the crystallographic *c* axis.

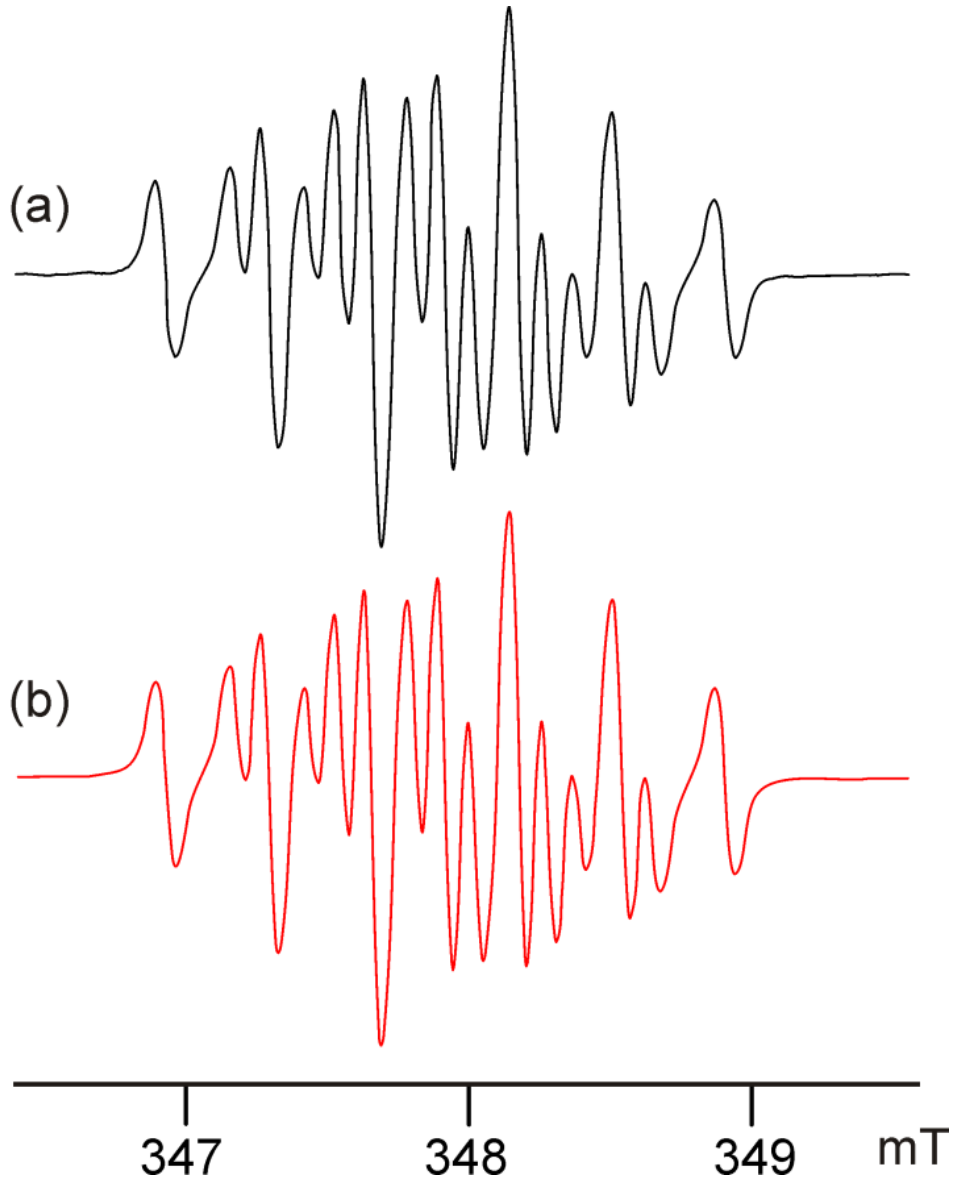


Figure S17. (a) Experimental and (b) simulated EPR spectra of **5a** in CH_2Cl_2 at 18 °C, modulation amplitude 0.005 mT, modulation frequency 100 kHz, 100% Lorentzian lineshape.

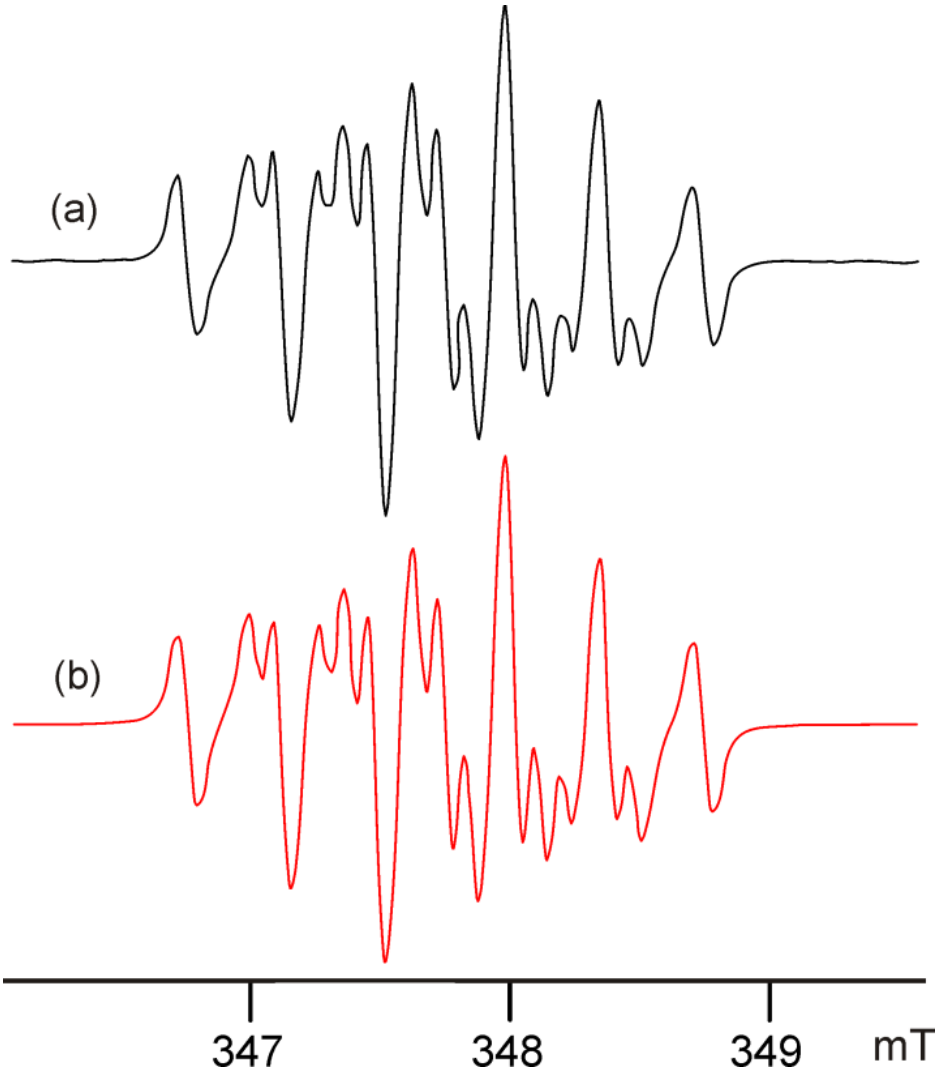


Figure S18 (a) Experimental and (b) simulated EPR spectra of **5b** in CH_2Cl_2 at 18 °C, modulation amplitude 0.01 mT, modulation frequency 100 kHz, 100% Lorentzian lineshape.

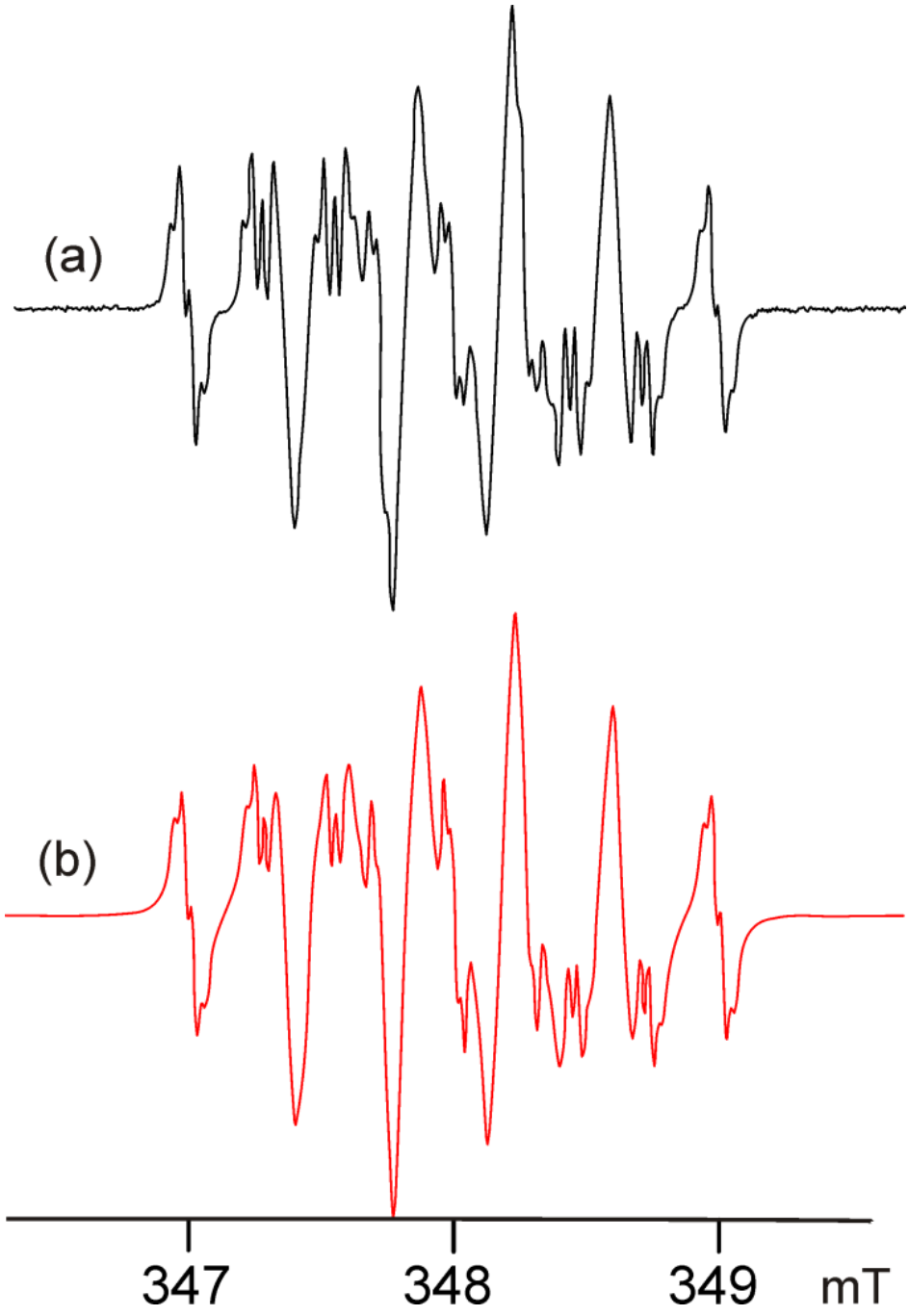


Figure S19. (a) Experimental and (b) simulated EPR spectra of **5c** in CH_2Cl_2 at 18 °C, modulation amplitude 0.01 mT, modulation frequency 100 kHz, 100% Lorentzian lineshape.

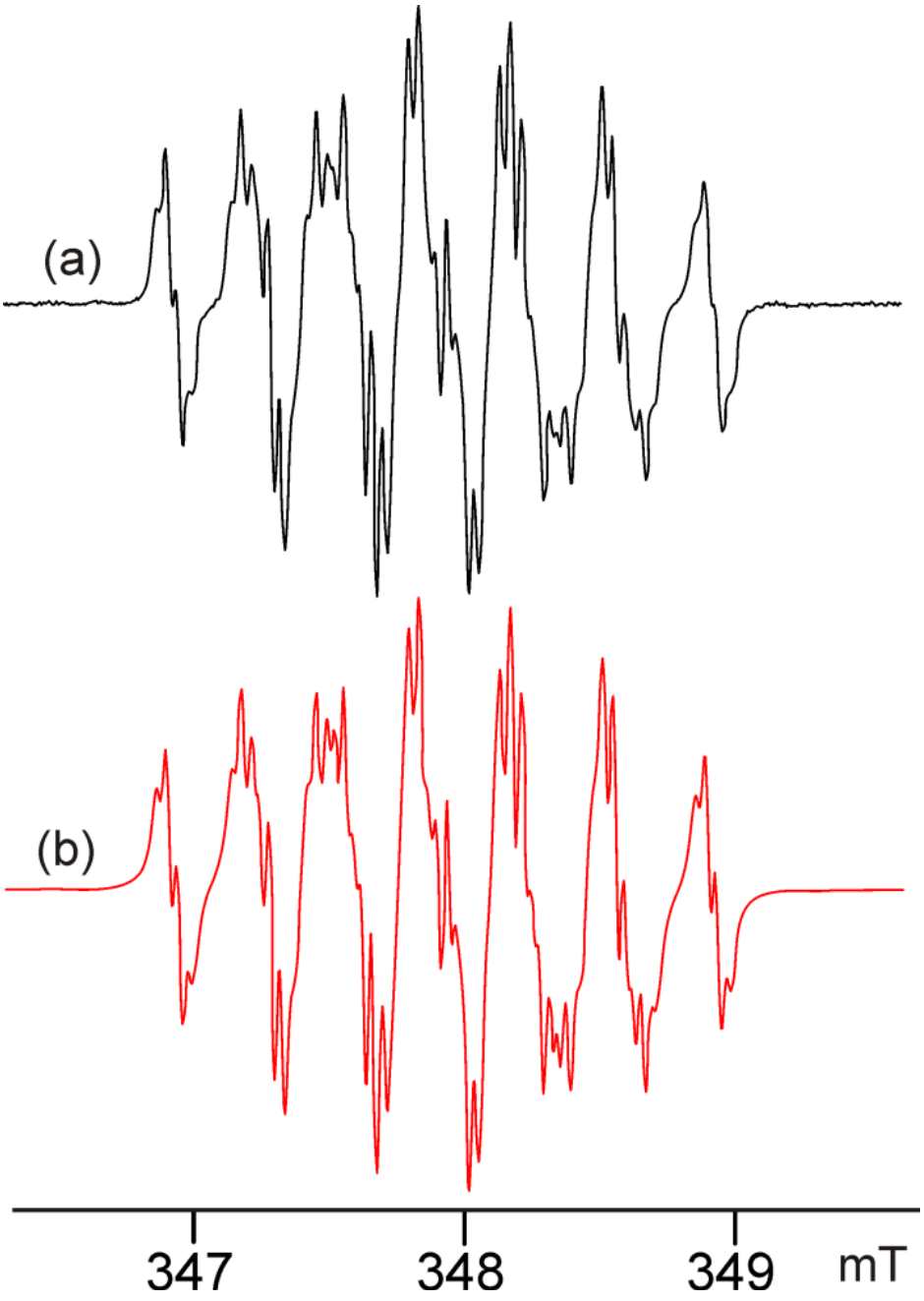


Figure S20. (a) Experimental and (b) simulated EPR spectra of **5e** in CH_2Cl_2 at 18 °C, modulation amplitude 0.01 mT, modulation frequency 100 kHz, 100% Lorentzian lineshape.

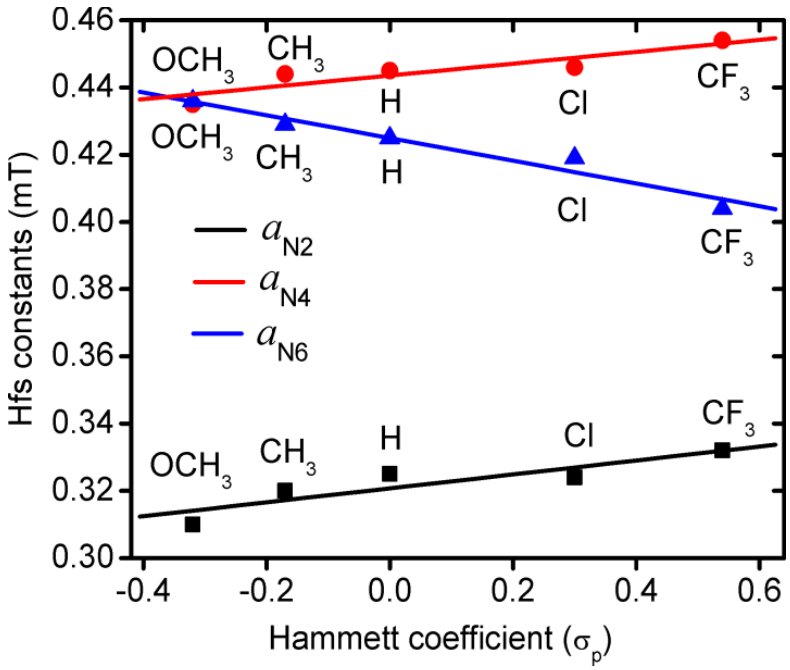


Figure S21. Plot of the Hammett coefficients (σ_p) versus the hyperfine splitting constants (mT) of **5a–e** as measured by EPR spectroscopy in CH_2Cl_2. More strongly electron donating substituents appear to increase spin density on the NSN portion of the ring, in particular on N6, but that increase is almost exactly compensated-for by decreased spin density on N2,4. Blue line (N6) R= 0.976, red line (N4) R= 0.910, black line (N2) R= 0.896.

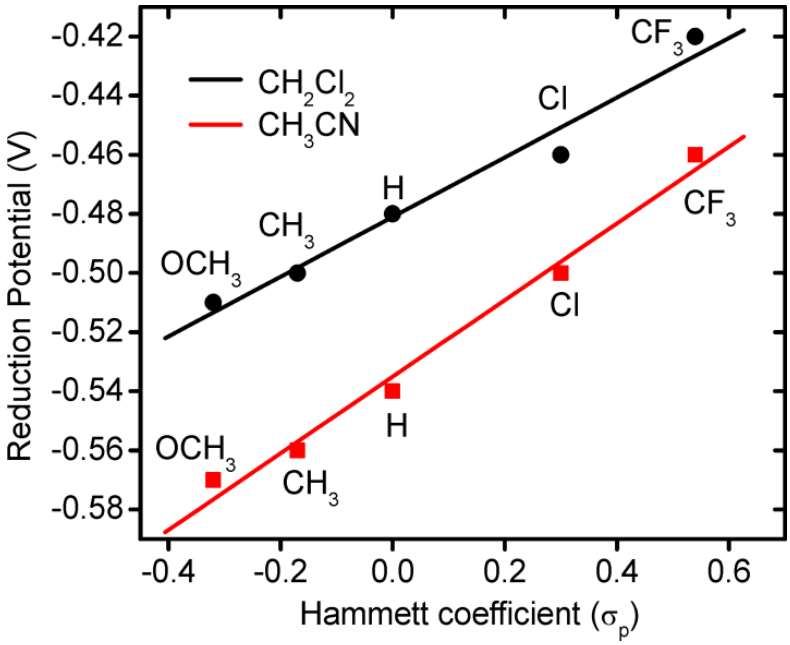


Figure S22. Plot of the Hammett coefficients (σ_p) versus the reduction peak potentials (V) at low concentrations of **5a–e** as measured by CV in both CH_2Cl_2 (black line, R = 0.993) and CH_3CN (red line, R = 0.986).

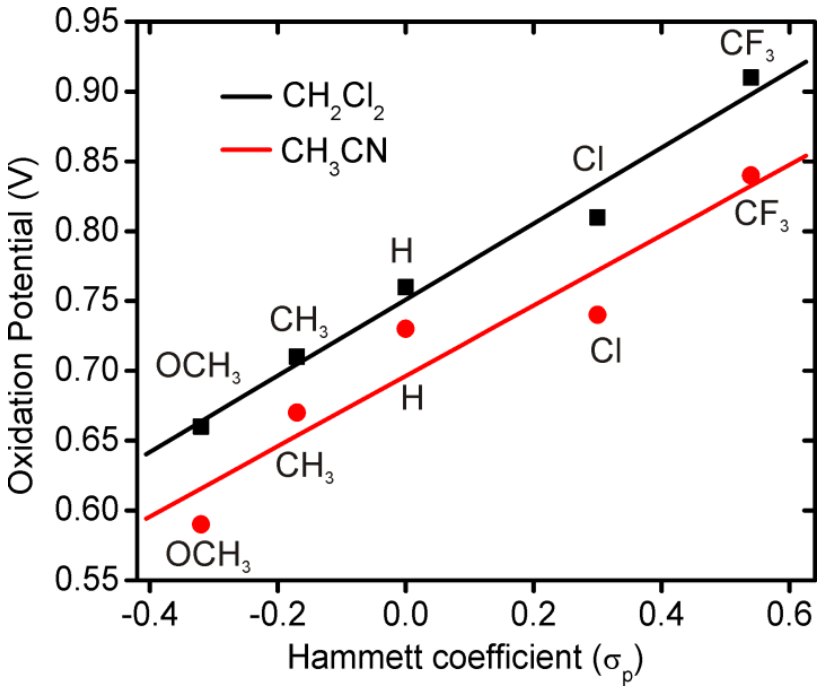


Figure S23. Plot of the Hammett coefficients (σ_p) versus the oxidation peak potentials (V) at low concentrations of **5a–e** as measured by CV in both CH_2Cl_2 (black line, R = 0.989) and CH_3CN (red line, R = 0.953).

References

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2. (a) Barker, J.; Phillips, P. R.; Wallbridge, M. G. H.; Powell, H. R. *Acta Cryst.* **1996**, *C52*, 2617–2619. (b) Jokić, M.; Bajić, M.; Žinić, M.; Perić, B.; Kojić-Prodić, B. *Acta Cryst.* **2001**, *C57*, 1354–1355.

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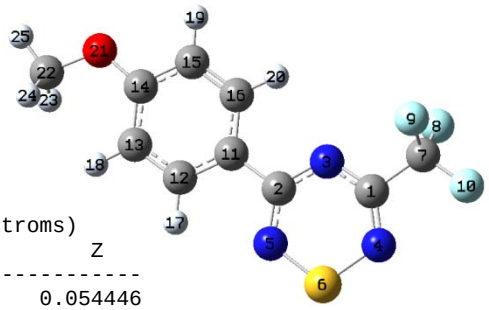
7. Novotny, D.; Prihoda, J.; Zak, Z.; Marek, J. *Main Group Chem*. **1997**, *2*, 117–122.

Gaussian 98 Calculations output, by compound and charge

MeO CF_3 radical 5a



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	7	0	-1.290232	-0.112908	-0.176238
5	7	0	-1.299921	-0.228323	2.536393
6	16	0	-2.251715	-0.292894	1.179445
7	6	0	0.879630	0.208285	-1.186422
8	9	0	1.518050	1.392861	-1.139588
9	9	0	1.812032	-0.761941	-1.226657
10	9	0	0.171974	0.157682	-2.320817
11	6	0	0.829868	-0.007433	3.610141
12	6	0	0.234187	-0.127123	4.875172
13	6	0	0.997381	-0.081274	6.036529
14	6	0	2.388422	0.086874	5.945852
15	6	0	2.995595	0.207991	4.683477
16	6	0	2.227028	0.161886	3.534056
17	1	0	-0.840427	-0.257176	4.941646
18	1	0	0.508282	-0.176020	6.998910
19	1	0	4.072099	0.337182	4.637580
20	1	0	2.691482	0.255354	2.559319
21	8	0	3.227860	0.144311	7.009396
22	6	0	2.682552	0.030845	8.318333
23	1	0	1.975710	0.843030	8.529233
24	1	0	2.181543	-0.934753	8.461041
25	1	0	3.531289	0.102901	8.999973

Isotropic Fermi Contact Couplings

Atom		a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.01482	-16.65818	-5.94405	-5.55657
2	C(13)	-0.01706	-19.18077	-6.84418	-6.39802
3	N(14)	0.04375	14.13567	5.04396	4.71515
4	N(14)	0.03175	10.25948	3.66084	3.42220
5	N(14)	0.04930	15.93020	5.68429	5.31374
6	S(33)	0.05592	19.20841	6.85404	6.40724
7	C(13)	0.00008	0.08493	0.03031	0.02833
8	F(19)	-0.00078	-3.26301	-1.16432	-1.08842
9	F(19)	-0.00076	-3.20770	-1.14459	-1.06998
10	F(19)	-0.00003	-0.11743	-0.04190	-0.03917
11	C(13)	0.00118	1.32394	0.47241	0.44162
12	C(13)	-0.00188	-2.11816	-0.75581	-0.70654
13	C(13)	0.00081	0.90688	0.32360	0.30250
14	C(13)	-0.00132	-1.48193	-0.52879	-0.49432
15	C(13)	0.00144	1.61817	0.57740	0.53976
16	C(13)	-0.00219	-2.45986	-0.87774	-0.82052
17	H	0.00024	1.05894	0.37786	0.35323
18	H	-0.00006	-0.28718	-0.10247	-0.09579
19	H	-0.00018	-0.78459	-0.27996	-0.26171
20	H	0.00022	0.99449	0.35486	0.33173
21	O(17)	-0.00052	0.31665	0.11299	0.10562
22	C(13)	0.00004	0.04078	0.01455	0.01360
23	H	-0.00002	-0.09740	-0.03475	-0.03249
24	H	-0.00002	-0.09743	-0.03477	-0.03250
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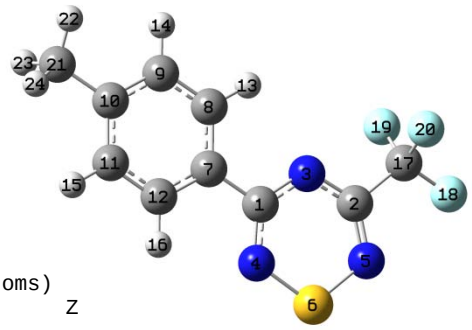
Tolyl CF_3 radical 5b



Geometry

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5	7	0	-1.929371	-0.293989	2.181382
6	16	0	-2.880621	-0.392743	0.810071
7	6	0	0.220278	0.051716	-1.578087
8	6	0	1.610737	0.218605	-1.477973
9	6	0	2.386710	0.332068	-2.626864
10	6	0	1.807806	0.281313	-3.902718
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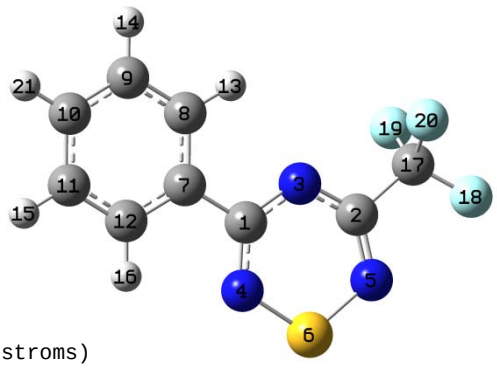
15	1	0	-0.055353	0.084811	-4.972046
16	1	0	-1.443564	-0.119680	-2.935220
17	6	0	0.226737	-0.002815	3.229108
18	9	0	-0.470092	-0.239651	4.346260
19	9	0	1.245404	-0.879320	3.172001
20	9	0	0.750135	1.235699	3.311804
21	6	0	2.657253	0.372188	-5.146593
22	1	0	3.596712	0.899975	-4.953971
23	1	0	2.914958	-0.628396	-5.519211
24	1	0	2.131597	0.892132	-5.954590

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.01711	-19.22983	-6.86168	-6.41438
2	C(13)	-0.01556	-17.49585	-6.24296	-5.83599
3	N(14)	0.04480	14.47509	5.16507	4.82837
4	N(14)	0.04743	15.32518	5.46841	5.11193
5	N(14)	0.03313	10.70340	3.81924	3.57027
6	S(33)	0.05588	19.19410	6.84894	6.40246
7	C(13)	0.00121	1.35546	0.48366	0.45213
8	C(13)	-0.00232	-2.61307	-0.93241	-0.87163
9	C(13)	0.00140	1.57425	0.56173	0.52511
10	C(13)	-0.00160	-1.80212	-0.64304	-0.60112
11	C(13)	0.00105	1.18395	0.42246	0.39492
12	C(13)	-0.00183	-2.05461	-0.73314	-0.68535
13	H	0.00025	1.10103	0.39288	0.36726
14	H	-0.00016	-0.70408	-0.25123	-0.23486
15	H	-0.00010	-0.45637	-0.16284	-0.15223
16	H	0.00022	0.98920	0.35297	0.32996
17	C(13)	0.00020	0.22511	0.08032	0.07509
18	F(19)	-0.00003	-0.12090	-0.04314	-0.04033
19	F(19)	-0.00077	-3.24140	-1.15661	-1.08121
20	F(19)	-0.00087	-3.67655	-1.31188	-1.22636
21	C(13)	0.00036	0.40007	0.14276	0.13345
22	H	-0.00007	-0.33445	-0.11934	-0.11156
23	H	-0.00038	-1.67757	-0.59860	-0.55958
24	H	-0.00012	-0.55250	-0.19715	-0.18429

Ph CF_3 radical 5c



Geometry

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5	7	0	2.186018	1.309151	-0.017225
6	16	0	1.065772	2.550321	-0.009308
7	6	0	-1.970016	0.036038	0.001305
8	6	0	-2.181156	-1.352355	-0.018059
9	6	0	-3.477460	-1.861343	-0.019644
10	6	0	-4.572058	-0.993929	-0.000925
11	6	0	-4.367440	0.388960	0.019183
12	6	0	-3.075029	0.903933	0.019892
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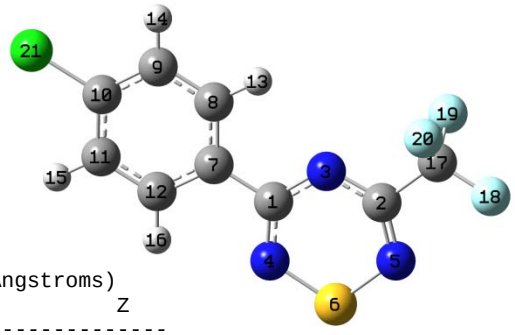
14	1	0	-3.633650	-2.936244	-0.035748
15	1	0	-5.217382	1.065367	0.034134
16	1	0	-2.906367	1.974964	0.034817
17	6	0	2.716112	-1.047006	0.003298
18	9	0	3.969271	-0.595923	-0.120027
19	9	0	2.623621	-1.728719	1.161234
20	9	0	2.473903	-1.905567	-1.003209
21	1	0	-5.582711	-1.393384	-0.002083

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.01720	-19.34019	-6.90106	-6.45119
2	C(13)	-0.01578	-17.73903	-6.32973	-5.91710
3	N(14)	0.04521	14.60825	5.21259	4.87279
4	N(14)	0.04683	15.13081	5.39905	5.04710
5	N(14)	0.03350	10.82333	3.86203	3.61027
6	S(33)	0.05593	19.21119	6.85503	6.40816
7	C(13)	0.00123	1.38184	0.49308	0.46093
8	C(13)	-0.00233	-2.61787	-0.93412	-0.87323
9	C(13)	0.00134	1.50116	0.53565	0.50073
10	C(13)	-0.00156	-1.75230	-0.62527	-0.58451
11	C(13)	0.00109	1.23028	0.43899	0.41038
12	C(13)	-0.00186	-2.09347	-0.74700	-0.69831
13	H	0.00025	1.10995	0.39606	0.37024
14	H	-0.00015	-0.67969	-0.24253	-0.22672
15	H	-0.00011	-0.50105	-0.17879	-0.16713
16	H	0.00023	1.00688	0.35928	0.33586
17	C(13)	0.00024	0.26497	0.09455	0.08839
18	F(19)	-0.00003	-0.11427	-0.04078	-0.03812
19	F(19)	-0.00089	-3.75477	-1.33980	-1.25246
20	F(19)	-0.00079	-3.31083	-1.18139	-1.10437
21	H	0.00019	0.86439	0.30844	0.28833

Cl CF_3 radical 5d



Geometry

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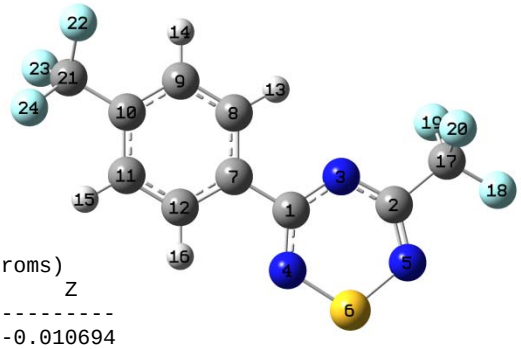
4	7	0	0.517156	2.042438	-0.000400
5	7	0	3.067257	1.117231	-0.017680
6	16	0	2.116025	2.491577	-0.008392
7	6	0	-1.212659	0.384198	0.002826
8	6	0	-1.600637	-0.965019	-0.012837
9	6	0	-2.947555	-1.313482	-0.014691
10	6	0	-3.911507	-0.304351	0.000113
11	6	0	-3.548573	1.044575	0.016611
12	6	0	-2.200444	1.382753	0.017502
13	1	0	-0.836497	-1.733356	-0.024671
14	1	0	-3.250275	-2.354831	-0.027886
15	1	0	-4.313453	1.813347	0.028292
16	1	0	-1.901718	2.424955	0.029662
17	6	0	3.295075	-1.287764	0.002028
18	9	0	4.594558	-0.999297	-0.124541
19	9	0	3.118288	-1.951124	1.160605
20	9	0	2.942120	-2.107920	-1.003546
21	17	0	-5.610396	-0.736472	-0.002480

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.01724	-19.37533	-6.91360	-6.46291
2	C(13)	-0.01565	-17.59287	-6.27758	-5.86835
3	N(14)	0.04523	14.61526	5.21509	4.87512
4	N(14)	0.04639	14.98858	5.34830	4.99965
5	N(14)	0.03350	10.82271	3.86181	3.61007
6	S(33)	0.05620	19.30454	6.88834	6.43930
7	C(13)	0.00123	1.38231	0.49324	0.46109
8	C(13)	-0.00227	-2.55031	-0.91002	-0.85069
9	C(13)	0.00135	1.51847	0.54183	0.50651
10	C(13)	-0.00173	-1.94651	-0.69456	-0.64928
11	C(13)	0.00109	1.22525	0.43720	0.40870
12	C(13)	-0.00190	-2.13801	-0.76289	-0.71316
13	H	0.00024	1.06877	0.38136	0.35650
14	H	-0.00016	-0.70500	-0.25156	-0.23516
15	H	-0.00011	-0.49685	-0.17729	-0.16573
16	H	0.00023	1.04075	0.37137	0.34716
17	C(13)	0.00020	0.22597	0.08063	0.07538
18	F(19)	-0.00002	-0.10040	-0.03582	-0.03349
19	F(19)	-0.00087	-3.66492	-1.30774	-1.22249
20	F(19)	-0.00078	-3.26254	-1.16416	-1.08827
21	Cl(35)	-0.00028	-0.12442	-0.04440	-0.04150

CF_3 CF_3 radical 5e



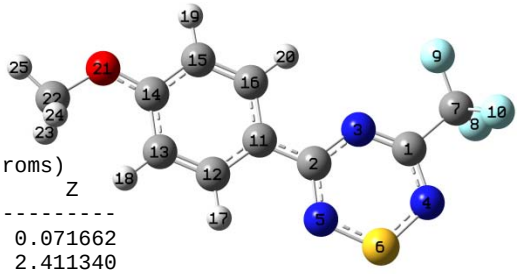
Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.871536	0.793984	-0.010694
2	6	0	3.036831	-0.064302	0.014311
3	7	0	1.709816	-0.273089	-0.007905
4	7	0	1.216272	2.079517	-0.000718
5	7	0	3.726865	1.053638	0.030849
6	16	0	2.832103	2.465744	0.021412
7	6	0	-0.580882	0.492636	-0.023650
8	6	0	-1.019868	-0.840313	-0.018857
9	6	0	-2.380824	-1.128744	-0.027374
10	6	0	-3.314104	-0.088723	-0.041590
11	6	0	-2.884381	1.242053	-0.049844
12	6	0	-1.524962	1.531570	-0.040983
13	1	0	-0.285834	-1.637171	-0.009722
14	1	0	-2.718830	-2.159581	-0.029685
15	1	0	-3.613116	2.045137	-0.070418
16	1	0	-1.182833	2.560142	-0.049654
17	6	0	3.859168	-1.358917	0.002099
18	9	0	5.168480	-1.122769	0.132792
19	9	0	3.469702	-2.163922	1.006131
20	9	0	3.658491	-2.012933	-1.157556
21	6	0	-4.787374	-0.401752	0.010850
22	9	0	-5.074848	-1.566040	-0.609751
23	9	0	-5.220798	-0.516458	1.287136
24	9	0	-5.527086	0.565917	-0.572565

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.01736	-19.51666	-6.96403	-6.51006
2	C(13)	-0.01603	-18.01733	-6.42903	-6.00993
3	N(14)	0.04586	14.81752	5.28726	4.94259
4	N(14)	0.04533	14.64676	5.22633	4.88563
5	N(14)	0.03417	11.03962	3.93921	3.68242
6	S(33)	0.05617	19.29405	6.88460	6.43580
7	C(13)	0.00128	1.43593	0.51238	0.47897
8	C(13)	-0.00227	-2.54731	-0.90894	-0.84969
9	C(13)	0.00127	1.42988	0.51022	0.47696
10	C(13)	-0.00155	-1.74434	-0.62242	-0.58185
11	C(13)	0.00119	1.33839	0.47757	0.44644
12	C(13)	-0.00193	-2.16447	-0.77234	-0.72199
13	H	0.00024	1.07337	0.38300	0.35804
14	H	-0.00014	-0.64378	-0.22972	-0.21474
15	H	-0.00012	-0.55495	-0.19802	-0.18511
16	H	0.00023	1.03450	0.36914	0.34507
17	C(13)	0.00026	0.29547	0.10543	0.09856
18	F(19)	-0.00002	-0.08337	-0.02975	-0.02781
19	F(19)	-0.00080	-3.38069	-1.20632	-1.12768
20	F(19)	-0.00090	-3.79826	-1.35531	-1.26696
21	C(13)	0.00038	0.42429	0.15140	0.14153
22	F(19)	-0.00007	-0.31323	-0.11177	-0.10448
23	F(19)	-0.00040	-1.68151	-0.60000	-0.56089
24	F(19)	-0.00008	-0.32978	-0.11767	-0.11000

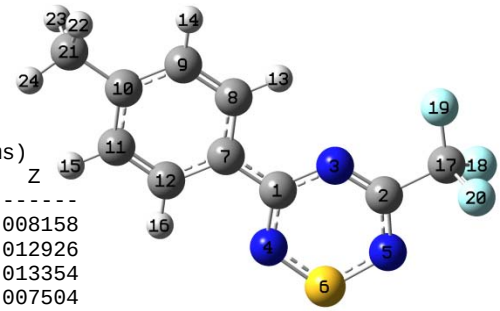
MeO CF_3 cation 5a



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.066438	0.092940	0.071662
2	6	0	0.085435	0.005010	2.411340
3	7	0	0.726788	0.085279	1.194180
4	7	0	-1.292384	0.033473	-0.113135
5	7	0	-1.284748	-0.080017	2.512457
6	16	0	-2.170640	-0.071367	1.205418
7	6	0	0.859192	0.201947	-1.243829
8	9	0	0.589004	1.387546	-1.804135
9	9	0	2.165417	0.102933	-1.017505
10	9	0	0.470864	-0.773822	-2.070131
11	6	0	0.852837	0.008770	3.605188
12	6	0	0.222106	-0.072926	4.879565
13	6	0	0.964258	-0.065421	6.037902
14	6	0	2.377949	0.025438	5.960693
15	6	0	3.019896	0.106668	4.694419
16	6	0	2.276143	0.098468	3.543641
17	1	0	-0.858431	-0.141662	4.935810
18	1	0	0.466115	-0.128299	6.997404
19	1	0	4.102060	0.174355	4.672972
20	1	0	2.761692	0.160158	2.576798
21	8	0	3.187452	0.041862	7.006689
22	6	0	2.665879	-0.033555	8.348944
23	1	0	2.015516	0.821781	8.554011
24	1	0	2.127546	-0.974301	8.496721
25	1	0	3.541533	0.000575	8.994845

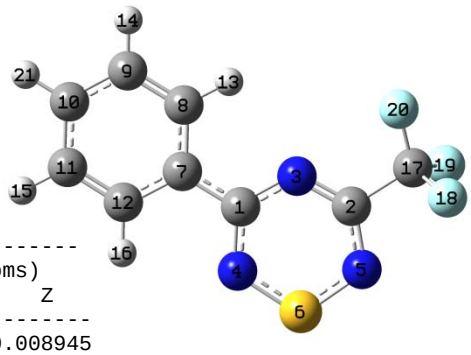
Tolyl CF_3 cation 5b



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.207739	0.629363	-0.008158
2	6	0	-2.035390	-0.037213	-0.012926
3	7	0	-0.764612	-0.338332	-0.013354
4	7	0	-0.093756	1.971744	-0.007504
5	7	0	-2.605219	1.207118	-0.002914
6	16	0	-1.602995	2.438779	-0.001462
7	6	0	1.581865	0.244092	-0.004053
8	6	0	1.932968	-1.132803	-0.005531
9	6	0	3.262534	-1.502336	0.003782
10	6	0	4.290994	-0.532487	0.012316
11	6	0	3.934847	0.833665	0.015508
12	6	0	2.611010	1.224531	0.006062
13	1	0	1.150950	-1.883163	-0.011553
14	1	0	3.526301	-2.555731	0.005978
15	1	0	4.716791	1.586712	0.027223
16	1	0	2.352165	2.277288	0.009669
17	6	0	-3.061862	-1.186596	-0.000605
18	9	0	-3.937718	-0.997369	-0.991052
19	9	0	-2.456125	-2.359117	-0.153824
20	9	0	-3.706683	-1.161506	1.171577
21	6	0	5.730516	-0.951264	-0.005749
22	1	0	5.890255	-1.863247	0.577917
23	1	0	6.041260	-1.172631	-1.036990
24	1	0	6.388712	-0.165183	0.373365

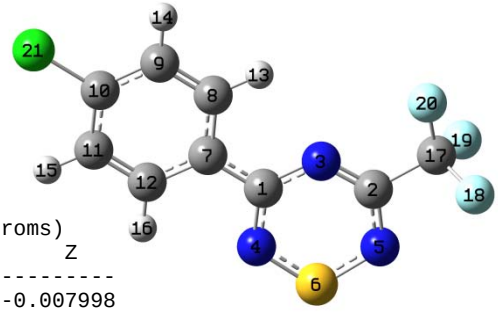
Ph CF_3 cation 5c



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.636275	0.513189	-0.008945
2	6	0	1.653409	0.033018	-0.013833
3	7	0	0.408602	-0.370053	-0.014005
4	7	0	-0.447232	1.874677	-0.007625
5	7	0	2.117031	1.317930	-0.001359
6	16	0	1.019060	2.465467	0.001012
7	6	0	-1.979888	0.014613	-0.005419
8	6	0	-2.209211	-1.385925	-0.007622
9	6	0	-3.508001	-1.866425	-0.001373
10	6	0	-4.587193	-0.969115	0.006680
11	6	0	-4.371389	0.416997	0.008234
12	6	0	-3.079224	0.914014	0.002232
13	1	0	-1.365581	-2.066112	-0.014584
14	1	0	-3.690389	-2.935944	-0.002939
15	1	0	-5.215207	1.098897	0.014229
16	1	0	-2.901805	1.983357	0.003566
17	6	0	2.769100	-1.031503	-0.001039
18	9	0	3.647624	-0.750859	-0.966031
19	9	0	3.382047	-0.979514	1.186843
20	9	0	2.260820	-2.243588	-0.191992
21	1	0	-5.603172	-1.353106	0.011589

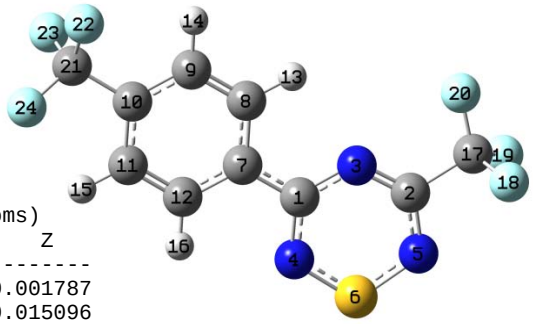
Cl CF_3 cation 5d



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.163776	0.684306	-0.007998
2	6	0	2.376948	-0.072665	-0.011617
3	7	0	1.094022	-0.321905	-0.012380
4	7	0	0.516107	2.012244	-0.004998
5	7	0	2.994369	1.147923	-0.002314
6	16	0	2.043745	2.419957	0.000853
7	6	0	-1.227484	0.352398	-0.006390
8	6	0	-1.627587	-1.010093	-0.011471
9	6	0	-2.968237	-1.339995	-0.007914
10	6	0	-3.931830	-0.313656	0.000860
11	6	0	-3.556403	1.042641	0.005627
12	6	0	-2.216223	1.372818	0.001879
13	1	0	-0.874320	-1.789233	-0.018524
14	1	0	-3.285257	-2.376798	-0.011860
15	1	0	-4.318892	1.813304	0.012309
16	1	0	-1.917435	2.414846	0.005711
17	6	0	3.356748	-1.262806	0.000471
18	9	0	4.230418	-1.114027	-0.998186
19	9	0	4.010445	-1.255503	1.167420
20	9	0	2.702013	-2.409981	-0.140483
21	17	0	-5.602331	-0.726550	0.005713

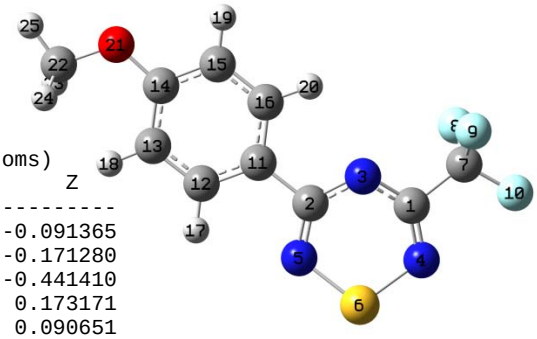
CF_3 CF_3 cation 5e



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.813607	0.737777	-0.001787
2	6	0	2.994512	-0.105376	0.015096
3	7	0	1.699329	-0.301790	0.004208
4	7	0	1.216243	2.050035	0.004888
5	7	0	3.656442	1.088065	0.015773
6	16	0	2.759555	2.398946	0.011597
7	6	0	-0.596469	0.459514	-0.014549
8	6	0	-1.045461	-0.884606	-0.018635
9	6	0	-2.403318	-1.154671	-0.032177
10	6	0	-3.325234	-0.096886	-0.039694
11	6	0	-2.892853	1.236739	-0.040329
12	6	0	-1.537596	1.519966	-0.026959
13	1	0	-0.323596	-1.692680	-0.012325
14	1	0	-2.757073	-2.179596	-0.042753
15	1	0	-3.620354	2.040236	-0.057389
16	1	0	-1.196334	2.548712	-0.028139
17	6	0	3.924939	-1.336057	0.003529
18	9	0	4.568472	-1.359770	-1.168247
19	9	0	4.809992	-1.216831	0.995165
20	9	0	3.222731	-2.452530	0.155216
21	6	0	-4.812395	-0.404125	0.006735
22	9	0	-5.086346	-1.547617	-0.641333
23	9	0	-5.206567	-0.540601	1.284975
24	9	0	-5.528062	0.585391	-0.550932

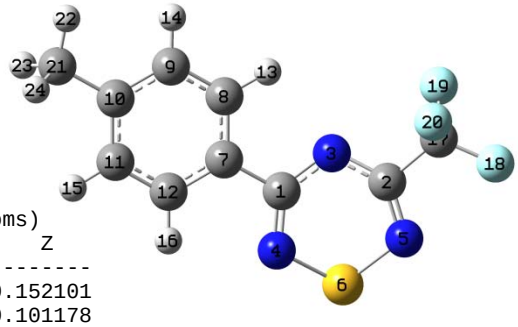
MeO CF_3 anion 5a



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.452266	0.036891	-0.091365
2	6	0	0.265317	0.779439	-0.171280
3	7	0	1.166236	-0.218780	-0.441410
4	7	0	3.102907	1.128255	0.173171
5	7	0	0.465603	2.043017	0.090651
6	16	0	2.124462	2.556368	-0.121420
7	6	0	3.259006	-1.245638	0.108062
8	9	0	2.824602	-1.952353	1.184346
9	9	0	3.149755	-2.072351	-0.962225
10	9	0	4.578749	-1.030707	0.295662
11	6	0	-1.164114	0.327861	-0.116732
12	6	0	-2.204735	1.231467	0.124935
13	6	0	-3.536665	0.815104	0.172656
14	6	0	-3.845650	-0.535139	-0.031182
15	6	0	-2.816892	-1.450913	-0.279657
16	6	0	-1.494252	-1.022123	-0.318331
17	1	0	-1.949576	2.274988	0.278255
18	1	0	-4.315972	1.545288	0.366011
19	1	0	-3.077021	-2.494699	-0.435145
20	1	0	-0.680985	-1.715635	-0.501521
21	8	0	-5.123663	-1.056109	-0.007588
22	6	0	-6.188042	-0.168493	0.254536
23	1	0	-6.092048	0.309263	1.240558
24	1	0	-6.264932	0.619823	-0.508711
25	1	0	-7.100171	-0.771521	0.237190

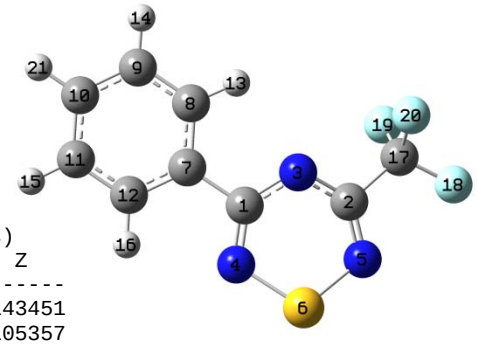
Tolyl CF_3 anion 5b



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.106855	0.776627	-0.152101
2	6	0	-2.081004	0.034351	-0.101178
3	7	0	-0.790375	-0.222081	-0.432155
4	7	0	-0.096681	2.041188	0.102000
5	7	0	-2.735074	1.125924	0.154169
6	16	0	-1.752365	2.554314	-0.127374
7	6	0	1.537051	0.327893	-0.076515
8	6	0	1.869936	-1.018498	-0.267776
9	6	0	3.200221	-1.438930	-0.208916
10	6	0	4.237397	-0.535851	0.045697
11	6	0	3.897688	0.813337	0.239140
12	6	0	2.575168	1.239344	0.176417
13	1	0	1.060613	-1.715106	-0.456988
14	1	0	3.436182	-2.491856	-0.360195
15	1	0	4.685873	1.538439	0.441519
16	1	0	2.314609	2.282299	0.324302
17	6	0	-2.891592	-1.247896	0.085065
18	9	0	-4.212910	-1.031931	0.259568
19	9	0	-2.772006	-2.070375	-0.987400
20	9	0	-2.469372	-1.959288	1.162967
21	6	0	5.679408	-0.987753	0.102501
22	1	0	5.757907	-2.078938	0.037973
23	1	0	6.271935	-0.566516	-0.721954
24	1	0	6.167456	-0.673951	1.035018

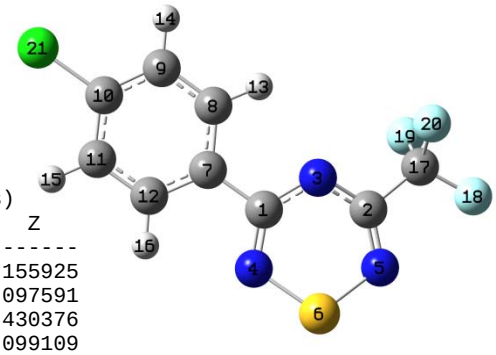
Ph CF_3 anion 5c



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.554889	0.659572	-0.143451
2	6	0	1.692311	0.121939	-0.105357
3	7	0	0.428223	-0.253960	-0.424946
4	7	0	-0.466830	1.938795	0.102030
5	7	0	2.244969	1.270581	0.138717
6	16	0	1.132808	2.601108	-0.142488
7	6	0	-1.938408	0.081145	-0.054923
8	6	0	-2.141030	-1.294262	-0.237488
9	6	0	-3.424649	-1.839076	-0.169825
10	6	0	-4.526203	-1.020399	0.086172
11	6	0	-4.331871	0.352905	0.270365
12	6	0	-3.051747	0.898051	0.197870
13	1	0	-1.267933	-1.908512	-0.428357
14	1	0	-3.564362	-2.909061	-0.314345
15	1	0	-5.183969	1.000421	0.470314
16	1	0	-2.883596	1.961187	0.335155
17	6	0	2.619011	-1.079144	0.081219
18	9	0	3.916111	-0.741225	0.243112
19	9	0	2.272614	-1.819429	1.166641
20	9	0	2.567066	-1.915872	-0.985586
21	1	0	-5.526880	-1.445337	0.141446

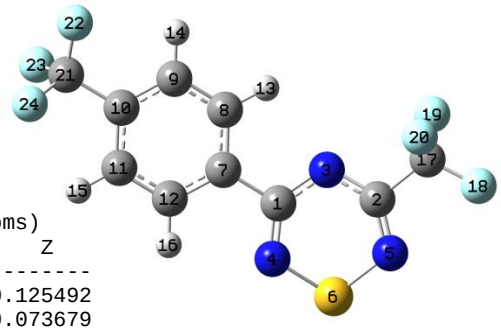
Cl CF_3 anion 5d



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.273251	0.827460	-0.155925
2	6	0	2.424112	-0.012044	-0.097591
3	7	0	1.122383	-0.211506	-0.430376
4	7	0	0.528512	2.081860	0.099109
5	7	0	3.122164	1.049903	0.161025
6	16	0	2.206265	2.523408	-0.111989
7	6	0	-1.176059	0.444246	-0.088733
8	6	0	-1.562555	-0.889383	-0.279399
9	6	0	-2.906478	-1.263495	-0.229673
10	6	0	-3.868339	-0.288532	0.018259
11	6	0	-3.515758	1.047313	0.212426
12	6	0	-2.170496	1.403598	0.154374
13	1	0	-0.780826	-1.618176	-0.462846
14	1	0	-3.202663	-2.297544	-0.377610
15	1	0	-4.282606	1.791549	0.404204
16	1	0	-1.863397	2.434007	0.298939
17	6	0	3.178037	-1.328564	0.085937
18	9	0	4.506881	-1.169591	0.257513
19	9	0	2.725847	-2.019907	1.164167
20	9	0	3.018793	-2.142960	-0.987016
21	17	0	-5.582361	-0.751626	0.087694

CF3 CF3 anion 5e



Geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.917932	0.838595	0.125492
2	6	0	3.018330	-0.042112	0.073679
3	7	0	1.717985	-0.224187	0.363710
4	7	0	1.221373	2.060940	-0.092459
5	7	0	3.711843	0.997351	-0.141207
6	16	0	2.870983	2.470484	0.105703
7	6	0	-0.551933	0.512039	0.069725
8	6	0	-0.989249	-0.795934	0.224642
9	6	0	-2.341659	-1.099707	0.180573
10	6	0	-3.270036	-0.094768	-0.023269
11	6	0	-2.842617	1.218857	-0.179448
12	6	0	-1.496730	1.517124	-0.131669
13	1	0	-0.258246	-1.564428	0.375698
14	1	0	-2.664257	-2.117430	0.298257
15	1	0	-3.560822	2.002256	-0.342561
16	1	0	-1.154545	2.525882	-0.252165
17	6	0	3.759528	-1.363565	-0.072681
18	9	0	5.059065	-1.224236	-0.264475
19	9	0	3.614103	-2.120213	1.008601
20	9	0	3.296045	-2.069001	-1.098950
21	6	0	-4.737277	-0.395225	-0.032846
22	9	0	-4.996246	-1.677838	-0.253954
23	9	0	-5.325828	-0.089103	1.121241
24	9	0	-5.386472	0.293216	-0.966459