Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Breaking bonds with electrons: stepwise and concerted cleavage of C-S, C-Se and Se-CN bonds in phenacylthiocyanates and phenacylselenocyanates

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Reduced *p*-methoxylphenacylthiocyanate (1c + e^-) in DMF **21**

Reduced *p*-cyanophenacylthiocyanate ($1d^{\bullet -}$) in DMF **21**

Reduced *p*-nitrophenacylthiocyanate ($1e^{\bullet -}$) in DMF **22**

Reduced phenacylselenocyanate (2a + e^-) in DMF **22**

Reduced *p*-methylphenacylselenocyanate (2b + e^-) in DMF **23**

Reduced *p*-methoxylphenacylselenocyanate (2c + e^-) in DMF **23**

Reduced *p*-cyanophenacylselenocyanate ($2d^{\bullet -}$) in DMF **24**

Reduced *p*-nitrophenacylselenocyanate ($2e^{\bullet -}$) in DMF **24**

Electrochemical characteristics of phenacylthiocyanates (1b-e)

a- Cyclic voltammetry

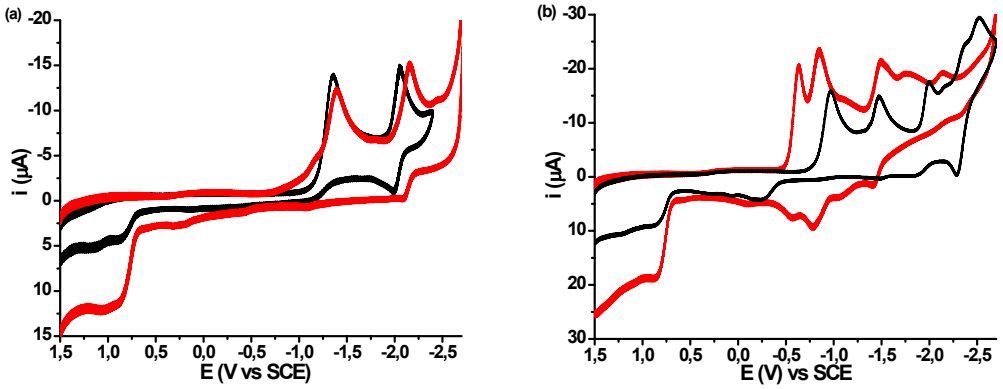


Figure S1. CVs of (a)**1b** (–) and **1c** (–); (b) **1d** (–) and **1e** (–)*C* = 1mM, in DMF/TBAF (0.1M) at a glassy carbon electrode, $v = 0.1 Vs^{-1}$.

b- Variation of peak potential $E_p$with log v,1st reduction wave

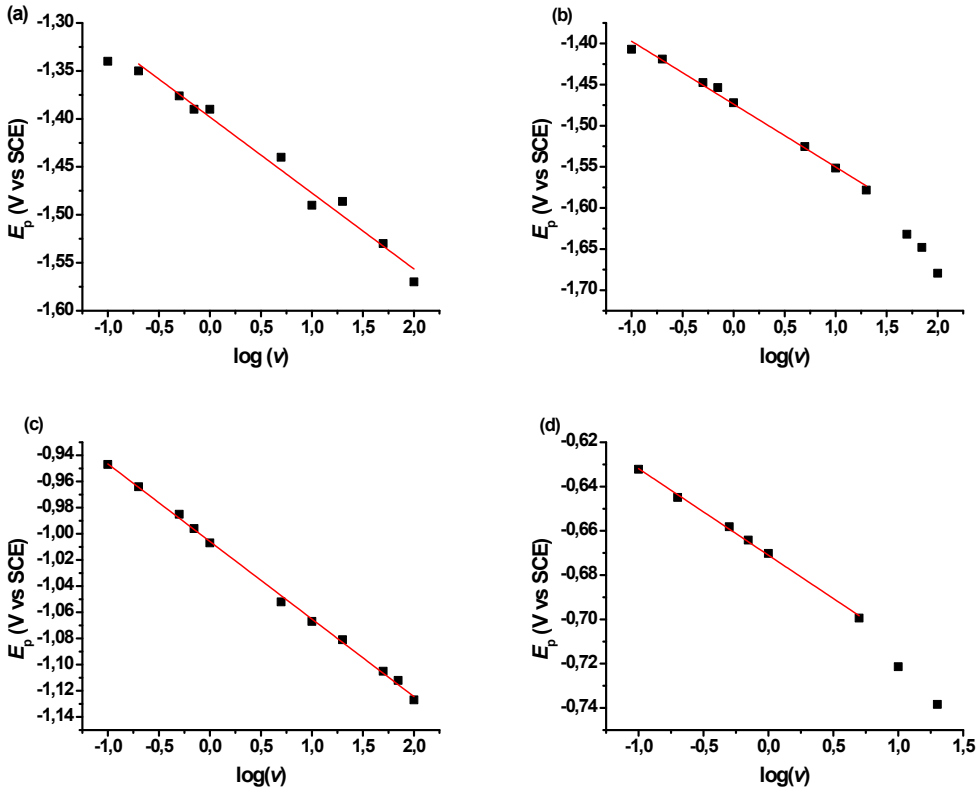


Figure S2. E_p vs log$v$for (a)**1b**;(b) **1c**; (c) **1d** and (d)**1e**, in DMF/TBAF (0.1M) at a glassy carbon electrode, $C_{substrate}$ = 1mM.

Electrochemical characteristics of phenacylselenocyanates (2b-e)

a- Cyclic voltammetry

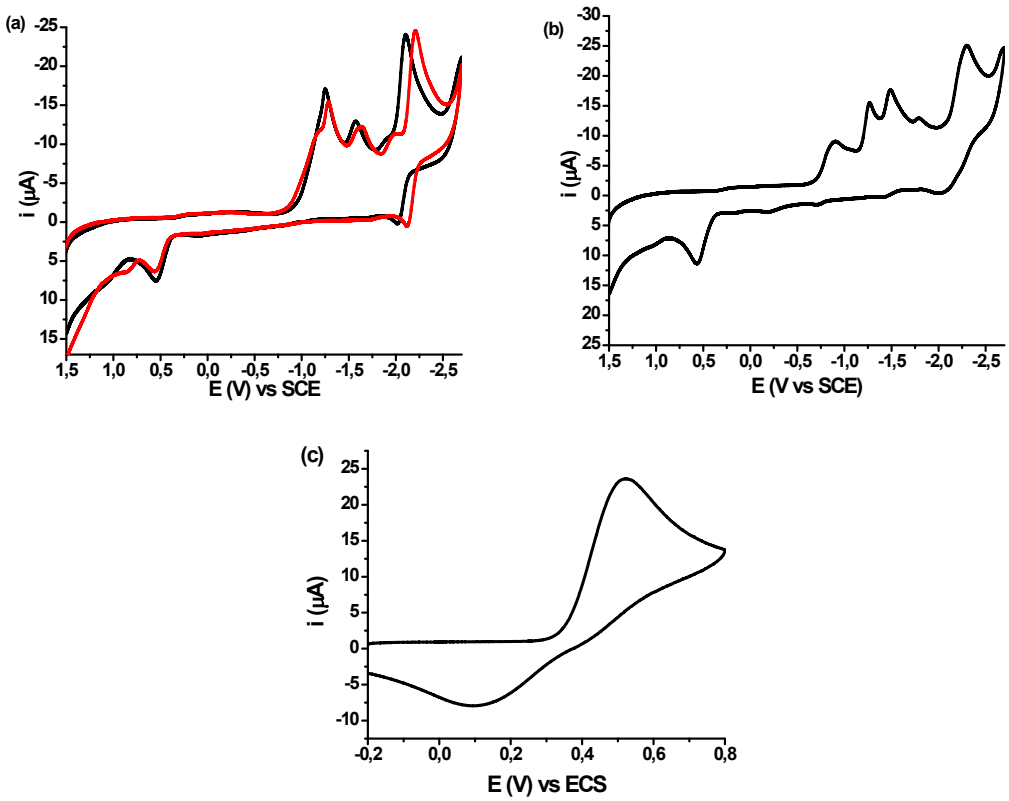
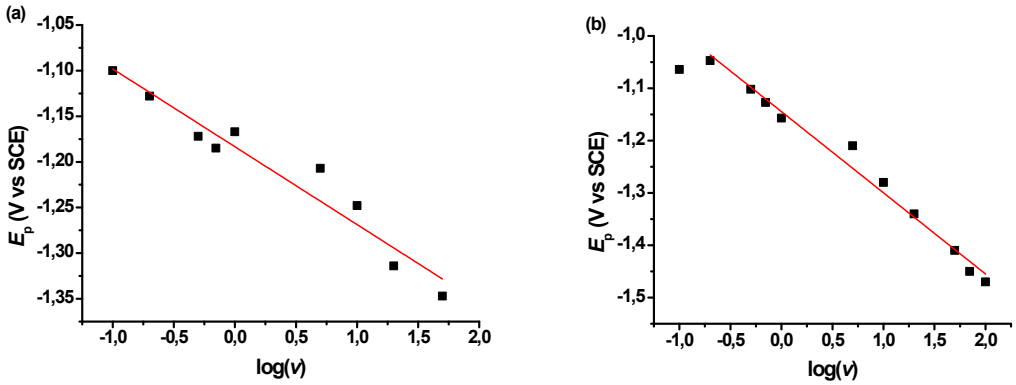


Figure S3. CVs of (a)**2b** (–) and **2c** (–); (b) **2d** (–); (c) KSeCN, in DMF/TBAF (0.1M) at a glassy carbon electrode, v = 0.1V s^{-1}, $C_{substrate}$ = 1mM.

b- Variation of peak potential E_p with log v, 1st reduction wave



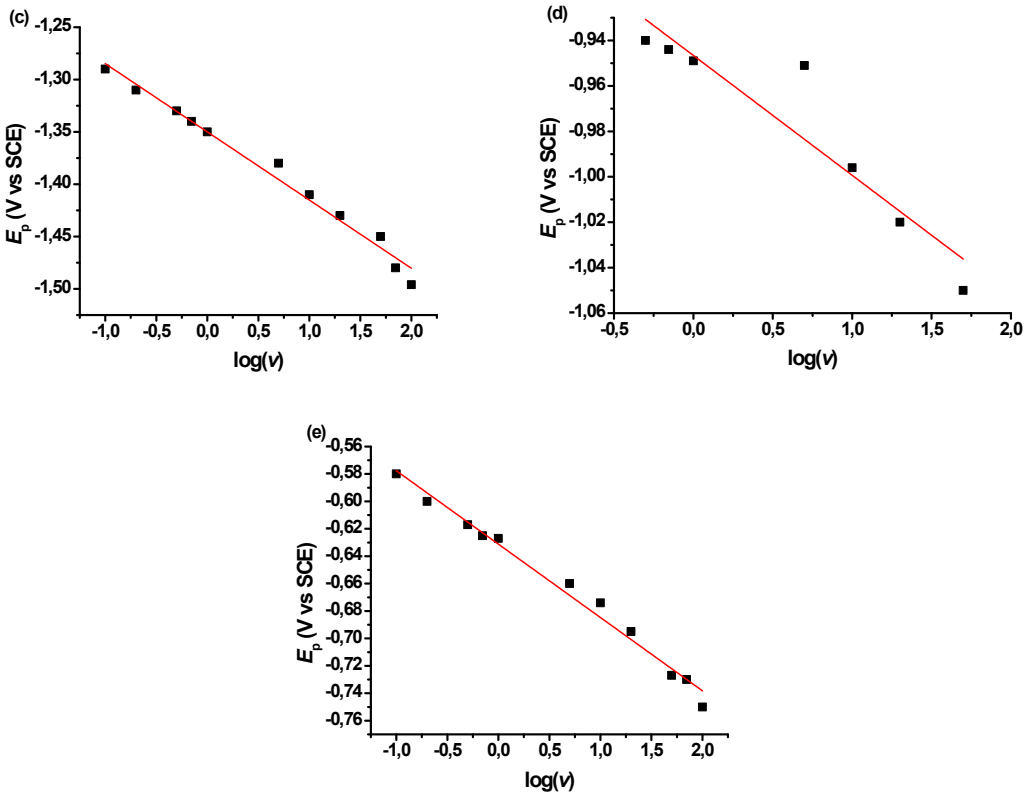


Figure S4. E_p vs log v for (a)**2a**;(b) **2b**; (c) **2c**; (d) **2d**and (e) **2e** in DMF/TBAF (0.1M) at a glassy carbon electrode, $C_{substrate}$ = 1mM.

Electrochemical characteristics of 4a and 5a

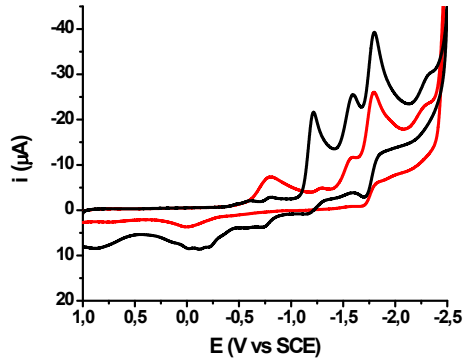
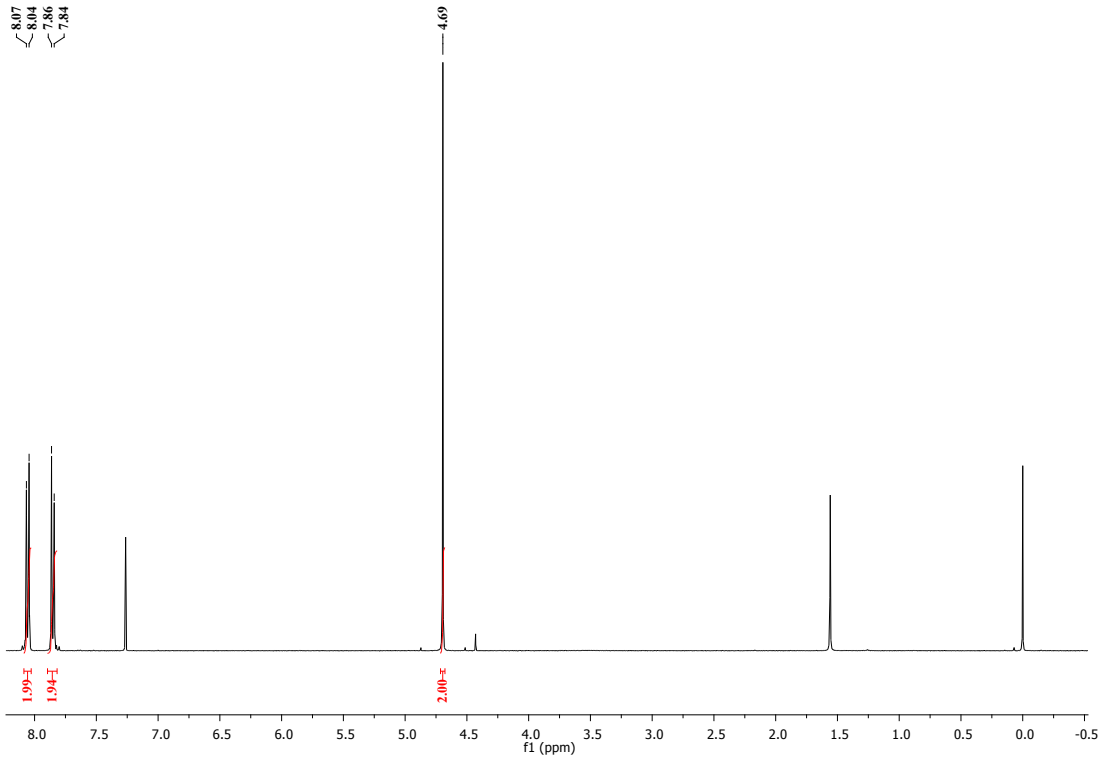
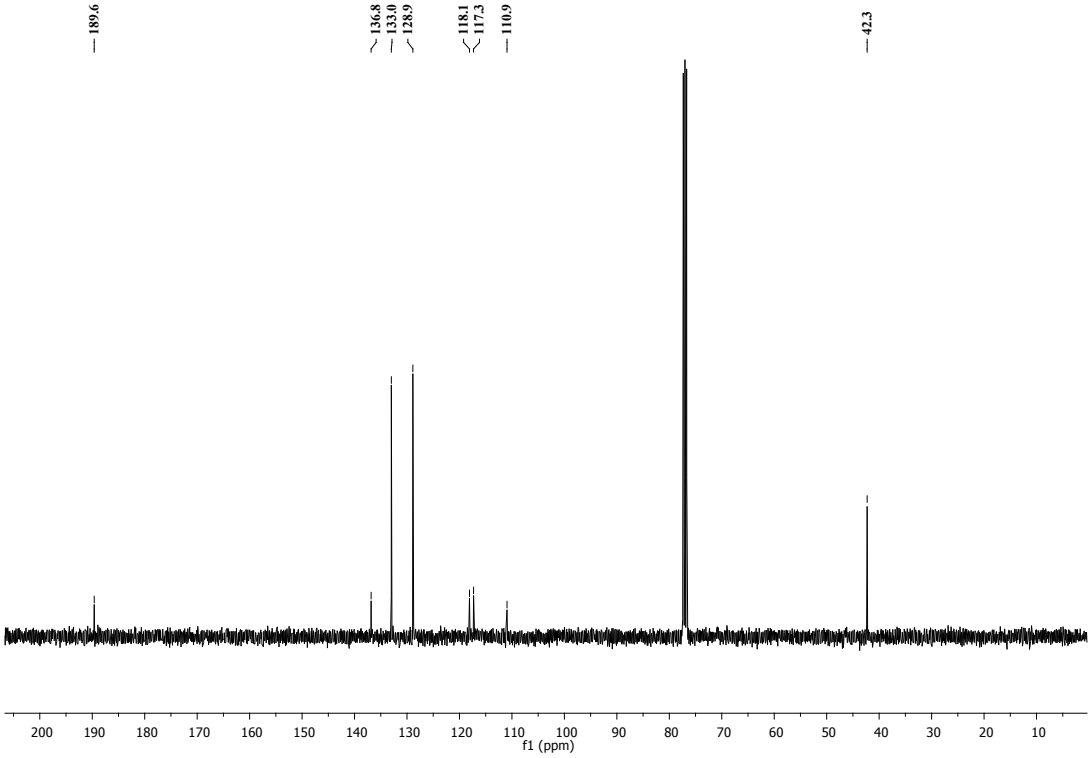


Figure S5. CVs of **4a** (–) and **5a** (–), in DMF/TBAF (0.1M) at a glassy carbon electrode, v = 0.1Vs^{-1}, $C_{substrate}$ = 1mM.

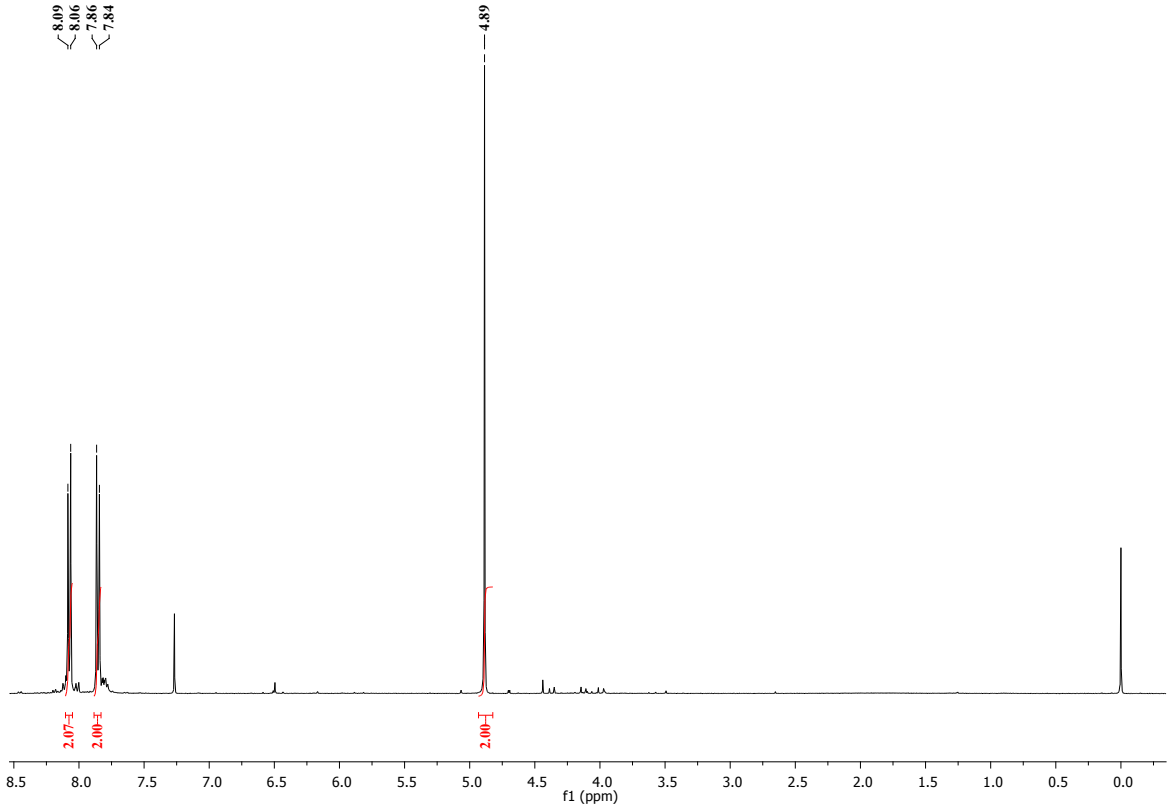
^{1}H NMR. 4-Cyanophenacyl thiocyanate (1d)



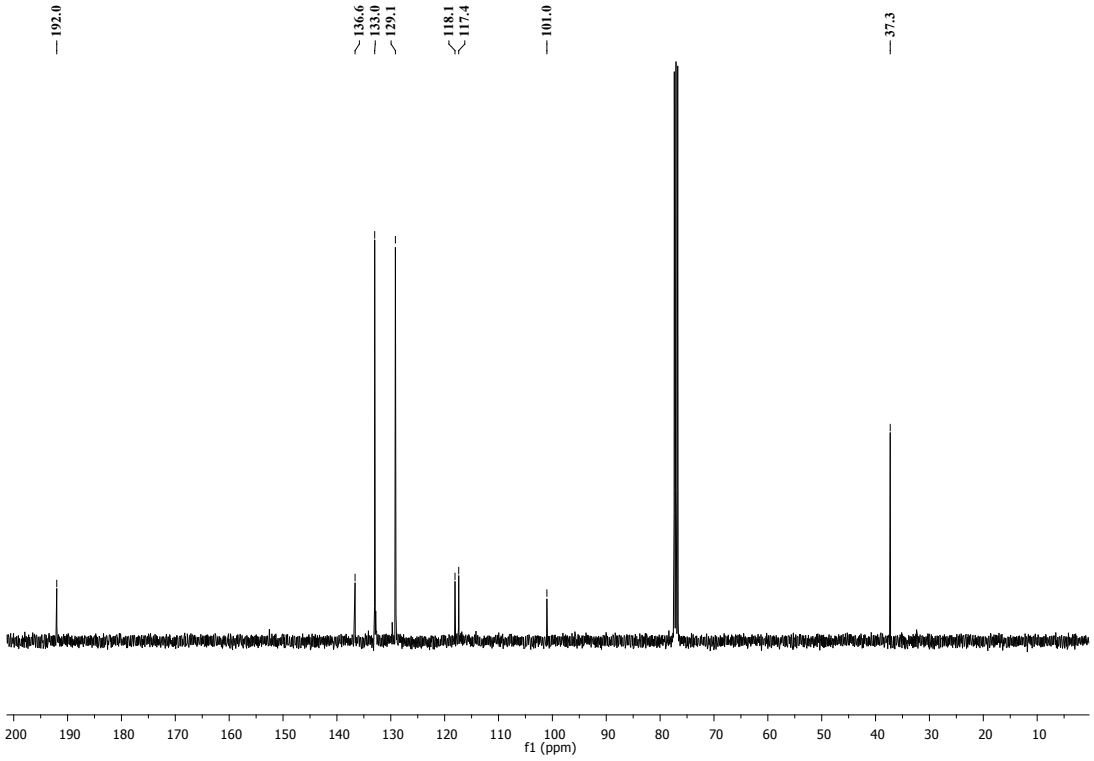
^{13}C NMR. 4-Cyanophenacyl thiocyanate (1d)



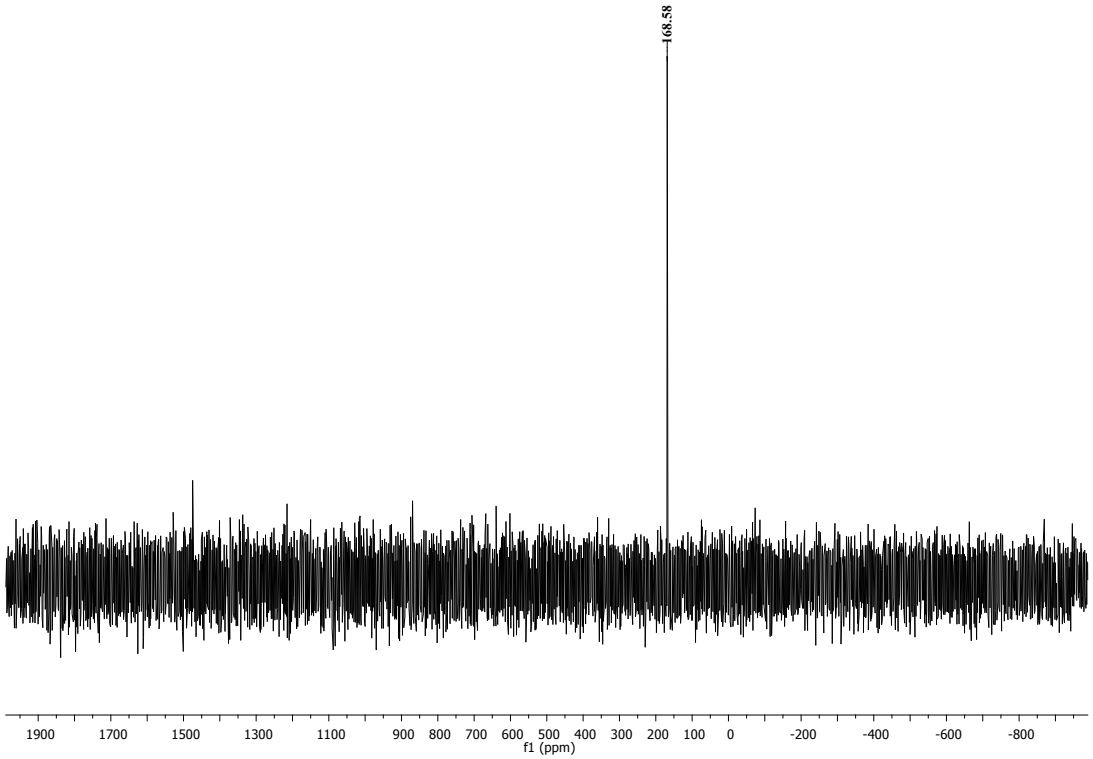
^{1}H NMR. 4-Cyanophenacyl selenocyanate (2d)



^{13}C NMR. 4-Cyanophenacyl selenocyanate (2d)



^{77}Se NMR. 4-Cyanophenacyl selenocyanate (2d)

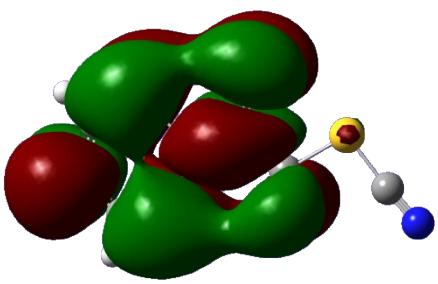


Computational calculations

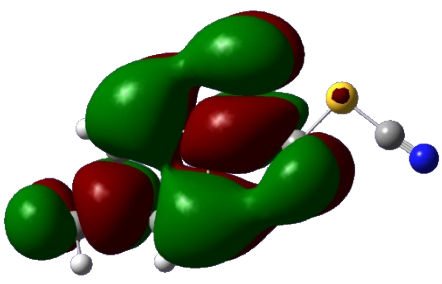
The calculations were performed using the Gaussian 09 package.[1]Optimizationswere carried out using DFT at the B3LYP/6-31+G(d,p) and B3LYP/6-311+G(d,p) level for the sulphur and selenium atoms. We checked that the conformations obtained were minima by running frequency calculations. No imaginary vibrational frequencies were found. All energy values include zero point correction. LUMO calculation, geometries for one electron reduced compounds were calculated in DMF by using the PCM model.

LUMOs for neutral compounds 1 and 2 (in DMF)

a



b



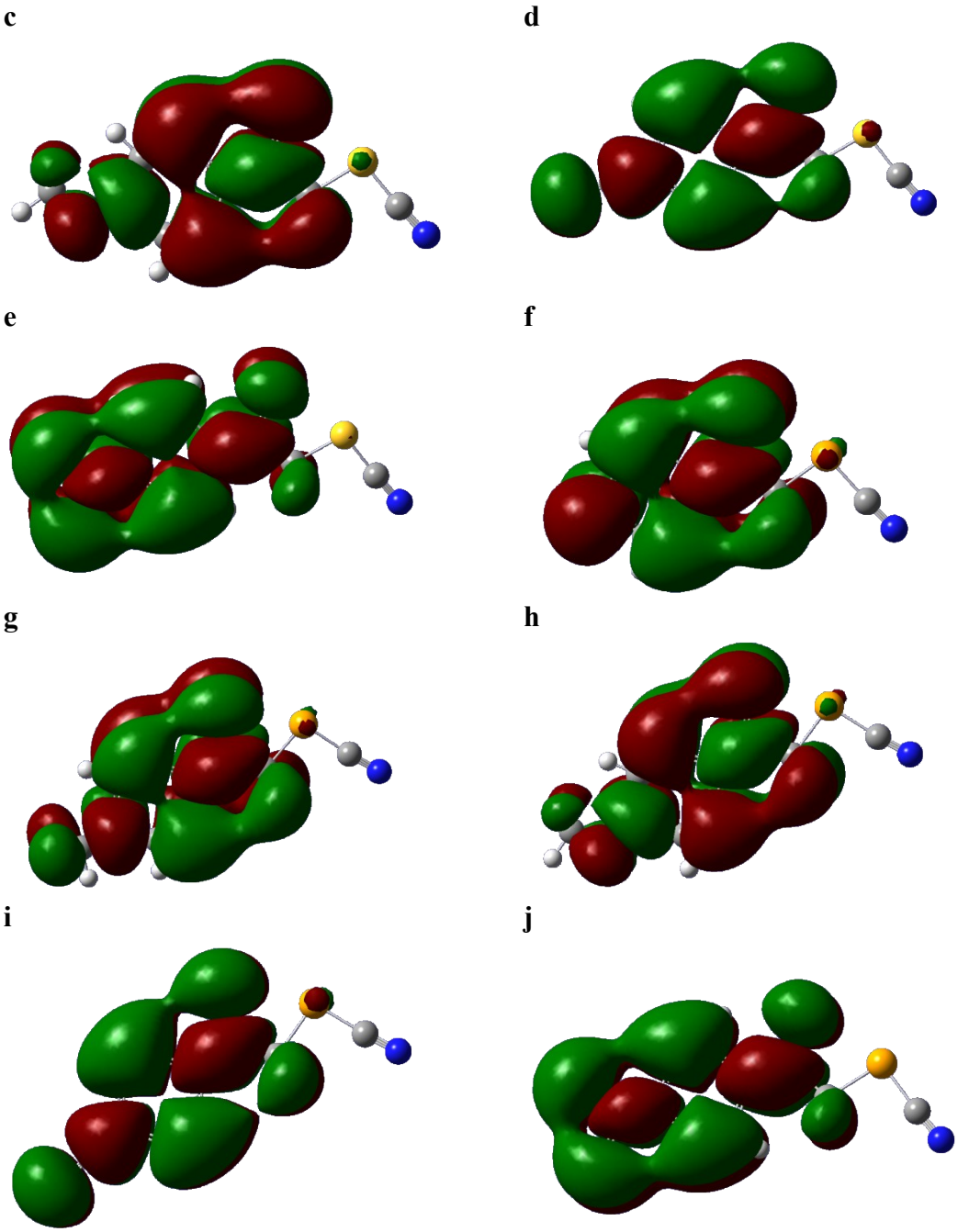


Figure S6. LUMOs of (a) **1a**; (b) **1b**; (c) **1c**; (d) **1d**; (e) **1e**; (f) **2a**; (g) **2b**; (h) **2c**; (i) **2d** and (j) **2e**.

Optimized geometries for one electron reduced compounds 1 and 2.

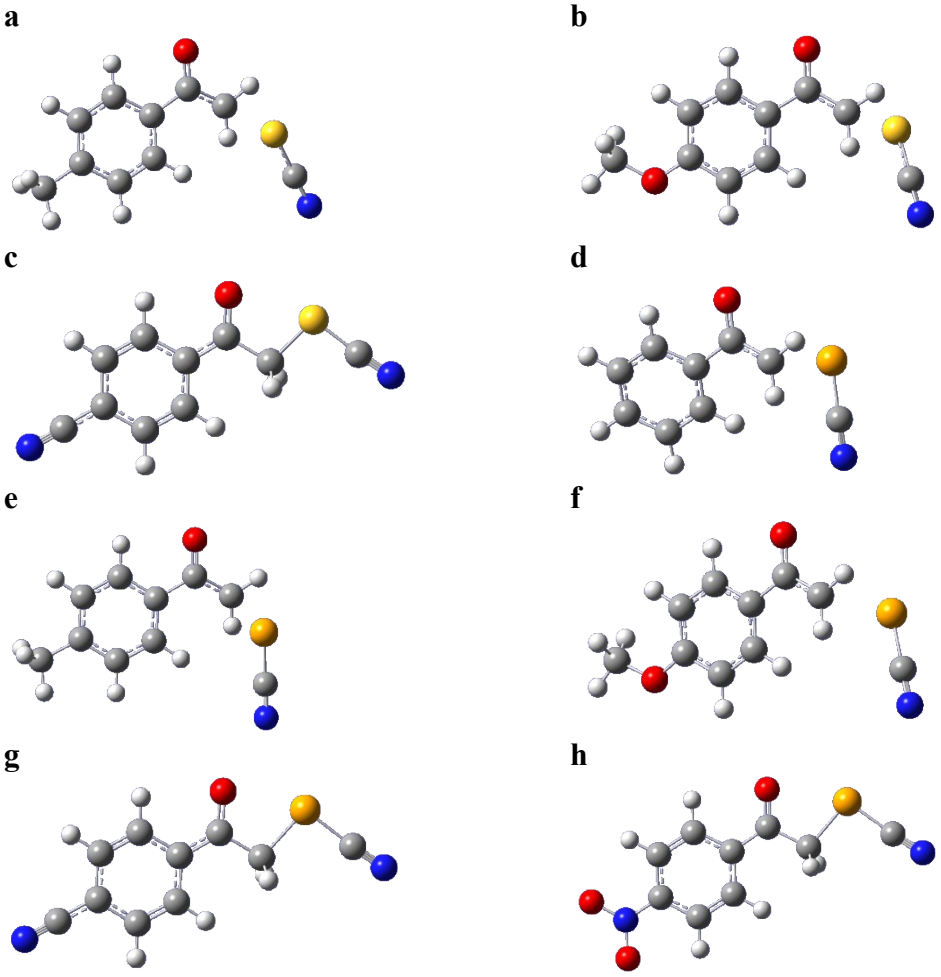


Figure S7. Optimized structures for (a) **1b** + e^-; (b) **1c** + e^-; (c) $\mathbf{1d}^{\bullet-}$; (d) **2a** +e^-; (e) **2b** + e^-; (f) **2c** + e^-; (g) $\mathbf{2d}^{\bullet-}$; (h) $\mathbf{2e}^{\bullet-}$

Table S1: LUMO coefficient for neutral 1a-e and 2a-e, and C-X (X = S, Se)bond distance in1a-e and 2a-e after one electron reduction.[a]

Compound	LUMO coefficient for neutral molecule	Distance CH_2-X (X= S or Se) in $\bullet^-$ (Å)
1a	$C(H_2)$ =0.40 ; S = 0.61	3.15
1b	$C(H_2)$ = 0.23 ; S = 0.58	3.22
1c	$C(H_2)$ = 0.19 ; S = 0.60	3.38
1d	$C(H_2)$ = 0.25 ; S = 0.51	1.85
1e	$C(H_2)$ = 0 ; S = 0	1.85
2a	$C(H_2)$ = 0.15 ; Se = 0.40	3.07
2b	$C(H_2)$ = 0.17 ; Se = 0.41	3.12
2c	$C(H_2)$ = 0.16 ; Se = 0.40	3.17
2d	$C(H_2)$ = 0.20 ; Se = 0.41	1.99
2e	$C(H_2)$ = 0 ; Se = 0	1.99

a Calculations performed with B3LYP/6-311+G(p,d) (in DMF).

Z-Matrix for optimized geometries

Phenacylthiocyanate (1a) in gas phase

Energy:-875.345193 a.u. ZPVC:0.138300 a.u. Total energy: -875.206893 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000013589	-0.000008852	0.000014531
2	6	-0.000022330	-0.000008302	-0.000014528
3	6	0.000005621	0.000036529	-0.000001463
4	6	0.000010327	0.000017078	0.000011375
5	6	-0.000007526	0.000006839	-0.000005067
6	1	0.000000590	-0.000002620	0.000005057
7	1	-0.000000254	-0.000002718	0.000001819
8	1	-0.000002065	-0.000005575	0.000000471
9	1	-0.000002088	-0.000009155	-0.000000216
10	1	0.000000595	-0.000003551	0.000004990
11	6	0.000015952	-0.000009657	-0.000000159
12	6	0.000000888	-0.000017937	0.000007629
13	6	0.000017957	-0.000000095	0.000023484
14	1	-0.000007154	0.000000225	-0.000009149
15	1	-0.000007593	-0.000003010	-0.000007397
16	8	-0.000010955	0.000016844	-0.000013625
17	16	0.000026181	-0.000006778	0.000016002
18	6	-0.000048162	-0.000010748	-0.000039519
19	7	0.000016424	0.000011483	0.000005763

***p*-Methylphenacylthiocyanate (1b) in gas phase**

Energy:-914.664280 a.u. ZPVC:0.165673 a.u. Total energy: -914.4986069 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000012581	-0.000001601	0.000011053
2	6	-0.000018807	-0.000009464	-0.000013930
3	6	0.000002772	0.000042056	-0.000003888
4	6	0.000007816	0.000018741	0.000005520
5	6	-0.000007433	0.000005321	-0.000002906
6	1	-0.000000461	-0.000001555	0.000001367
7	1	-0.000000672	-0.000006176	0.000000442
8	1	0.000000310	-0.000005771	0.000000472
9	1	0.000000303	-0.000002794	0.000003156
10	6	-0.000005605	0.000074755	-0.000016466
11	6	0.000007495	-0.000060898	0.000013948
12	6	0.000020368	0.000011081	0.000012796
13	1	-0.000006458	-0.000004318	-0.000007801
14	1	-0.000009080	-0.000005974	-0.000006000
15	8	0.000011932	-0.000027701	0.000009859
16	16	0.000013766	-0.000017518	0.000004142
17	6	-0.000031763	-0.000011887	-0.000022015
18	7	0.000008669	0.000009021	-0.000000331
19	6	0.000001100	-0.000010419	0.000007047
20	1	-0.000002960	0.000003199	0.000002116
21	1	-0.000002573	0.000001744	0.000000111
22	1	-0.000001302	0.000000160	0.000001308

***p*-Methoxyphenacylthiocyanate (1c) in gas phase**

Energy:-989.8734602a.u. ZPVC:0.170927 a.u. Total energy:-989.7025332a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000014330	0.000021485	0.000003899
2	6	-0.000001425	-0.000006245	-0.000005921
3	6	0.000001395	0.000002194	-0.000001776
4	6	-0.000003313	-0.000001621	0.000002081
5	6	-0.000005871	0.000004358	-0.000002032
6	1	0.000004850	0.000000018	-0.000004473
7	1	0.000003674	-0.000002438	-0.000002702
8	1	-0.000004395	0.000001316	0.000004095
9	1	-0.000001197	0.000004413	0.000004412
10	6	-0.000006124	-0.000003267	-0.000003132
11	6	-0.000002996	-0.000001334	-0.000000628
12	6	0.000000734	0.000009383	0.000005127
13	1	0.000000202	-0.000000037	-0.000004225
14	1	0.000002505	-0.000002717	0.000000222
15	8	0.000001110	-0.000001558	0.000008905
16	16	0.000009471	-0.000011270	0.000013581
17	6	-0.000005916	0.000012749	-0.000007790
18	7	0.000004482	-0.000008395	0.000001500
19	8	-0.000013109	-0.000018006	-0.000008597
20	6	0.000014105	0.000001540	0.000010252
21	1	-0.000001924	0.000000842	-0.000005819
22	1	-0.000004484	-0.000002586	-0.000001873
23	1	-0.000006105	0.000001174	-0.000005106

Thiocyanate radical (•SCN) in gas phase

Energy:-491.0146638 a.u. ZPVC:0.007963 a.u. Total energy: -491.0067008 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000075243	0.000001306	0.000000000
2	7	0.000095848	-0.000000755	0.000000000
3	16	-0.000020605	-0.000000551	0.000000000

$C_6H_4COCH_2$• in gas phase

Energy:-384.251522 a.u. ZPVC:0.124577 a.u. Total energy: -384.126945 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000004079	0.000006456	-0.000004022
2	6	-0.000000853	0.000000469	0.000012595
3	6	0.000003666	-0.000031572	0.000028381
4	6	-0.000000861	0.000000860	0.000001721
5	6	0.000008510	-0.000006850	0.000002487
6	1	-0.000000319	0.000001190	0.000006551
7	1	-0.000001465	-0.000002214	-0.000003705
8	1	-0.000032387	-0.000010224	-0.000030468
9	1	-0.000007800	0.000003196	0.000003265
10	1	-0.000001742	0.000004932	0.000003749

11	6	-0.000009838	-0.000141482	0.000049654
12	6	0.000013717	0.000085855	-0.000013731
13	6	0.000014045	0.000072770	-0.000025042
14	1	-0.000003229	-0.000032800	0.000000127
15	1	0.000000481	0.000007889	-0.000003804
16	8	0.000013996	0.000041525	-0.000027758

$CH_3C_6H_4COCH_2^{\bullet}$ in gas phase

Energy:-423.570720 a.u. ZPVC:0.151935 a.u. Total energy: -423.418785 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000001254	0.000000071	0.000001050
2	6	0.000001746	0.000000793	0.000000628
3	6	0.000001235	-0.000000912	-0.000001004
4	6	0.000000149	0.000000778	0.000000981
5	6	-0.000001249	-0.000002091	0.000002276
6	1	0.000001696	0.000000399	0.000000132
7	1	0.000001709	0.000001281	-0.000002527
8	1	-0.000002303	-0.000000933	0.000000628
9	1	-0.000002107	-0.000001110	0.000003356
10	6	0.000000210	-0.000000820	-0.000002458
11	6	-0.000002263	0.000000468	-0.000002176
12	6	0.000001486	0.000001568	-0.000003807
13	1	0.000000817	0.000001250	-0.000005380
14	1	0.000002027	0.000001438	-0.000004562
15	8	-0.000001642	0.000000881	-0.000002857
16	6	0.000000242	-0.000000619	0.000003639
17	1	0.000000774	-0.000000568	0.000003282
18	1	0.000000358	-0.000000764	0.000005048
19	1	-0.000001629	-0.000001111	0.000003752

$CH_3OC_6H_4COCH_2^{\bullet}$ in gas phase

Energy:-498.780122 a.u. ZPVC:0.157157 a.u. Total energy: -498.622965 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000015320	0.000019170	0.000022786
2	6	-0.000015287	-0.000021635	-0.000019125
3	6	0.000013597	0.000007771	0.000001137
4	6	0.000014568	0.000002285	0.000015192
5	6	-0.000019714	0.000008062	-0.000017432
6	1	0.000007492	0.000003066	-0.000003206
7	1	0.000000745	-0.000006459	-0.000004294
8	1	-0.000009573	-0.000003896	0.000001744
9	1	0.000000757	0.000000706	0.000008404
10	6	-0.000005200	-0.000027010	0.000005413
11	6	0.000000334	0.000014243	0.000006065
12	6	0.000012637	0.000005423	-0.000012344
13	1	-0.000001342	-0.000004553	-0.000002252
14	1	0.000001443	-0.000003814	0.000011295
15	8	-0.000007402	0.000014416	-0.000001169
16	8	-0.000002828	-0.000017765	-0.000015424
17	6	0.000000443	0.000006472	0.000004677

18	1	0.000000159	0.000002203	-0.000000604
19	1	-0.000001412	-0.000000390	0.000001433
20	1	-0.000004737	0.000001704	-0.000002297

Phenacylselenocyanate (2a) in gas phase

Energy:-2878.680517 a.u. ZPVC:0.137028 a.u. Total energy: -2878.543489 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000000062	-0.000001230	0.000004437
2	6	-0.000004042	-0.000000968	0.000002987
3	6	-0.000001553	0.000003488	0.000000392
4	6	-0.000001652	-0.000004726	-0.000001069
5	6	-0.000000105	0.000004404	-0.000000154
6	1	-0.000002857	0.000000672	0.000004388
7	1	-0.000002587	0.000001297	0.000006187
8	1	-0.000000601	0.000000090	0.000003721
9	1	0.000001334	-0.000000622	-0.000003576
10	1	-0.000000345	0.000000137	0.000000134
11	6	-0.000000715	-0.000004755	-0.000003909
12	6	0.000000306	0.000003349	0.000000067
13	6	0.000005120	-0.000000086	0.000004023
14	1	0.000000471	-0.000000856	-0.000000729
15	1	-0.000000795	0.000001625	-0.000001522
16	8	0.000002157	-0.000002262	-0.000005508
17	6	0.000003412	-0.000000294	-0.000001089
18	7	0.000000928	0.000000100	-0.000002445
19	34	0.000001586	0.000000637	-0.000006336

$C_6H_4COCH_2Se^{\bullet}$ in gas phase

Energy:-2785.8147225a.u. ZPVC: 0.128000a.u. Total energy:-2785.686723a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000007279	-0.000003942	0.000013540
2	6	-0.000009763	-0.000006282	0.000003238
3	6	-0.000002805	0.000009252	-0.000000598
4	6	-0.000008835	-0.000019917	-0.000004419
5	6	-0.000001514	0.000017781	-0.000001574
6	1	-0.000000429	-0.000001083	0.000011159
7	1	-0.000002562	0.000000913	0.000010301
8	1	-0.000000558	0.000001366	0.000004077
9	1	0.000000665	-0.000000249	-0.000004563
10	1	0.000000571	0.000000299	0.000002473
11	6	-0.000024871	0.000051713	-0.000022759
12	6	0.000002249	-0.000019942	-0.000003999
13	6	0.000030143	-0.000051229	0.000008219
14	1	-0.000007230	0.000014995	-0.000006251
15	1	-0.000015094	0.000017335	-0.000014218
16	8	0.000019687	-0.000034466	0.000016356
17	34	0.000013067	0.000023457	-0.000010983

Selenocyanate radical (•SeCN) in gas phase

Energy:-2494.353982 a.u. ZPVC:0.007583a.u. Total energy: -2494.346399 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000304265	-0.000000449	-0.000000518
2	7	0.000282085	0.000000268	0.000000308
3	34	0.000022181	0.000000182	0.000000210

Cyano radical (•CN) in gas phase

Energy:-92.7171831a.u. ZPVC:0.004901a.u. Total energy: -92.7122821a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000001193	0.000000000	-0.000000002
2	7	-0.000001193	0.000000000	0.000000002

Phenacylthiocyanate (1a) in DMF

Energy:−875.358638a.u. ZPVC:0.138322a.u. Total energy: -875.220316 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000005149	-0.000001412	0.000004621
2	6	0.000000330	-0.000000383	0.000003767
3	6	-0.000002422	0.000000732	0.000003044
4	6	-0.000004000	0.000000587	0.000002948
5	6	-0.000005719	0.000000036	0.000003889
6	1	-0.000004564	0.000000599	0.000007082
7	1	-0.000001080	0.000000995	0.000003834
8	1	0.000001168	-0.000000301	0.000000065
9	1	-0.000002815	0.000000169	0.000002347
10	1	-0.000004983	0.000000329	0.000006501
11	6	-0.000002866	0.000012576	-0.000001006
12	6	0.000004485	-0.000002613	0.000001578
13	6	0.000009212	-0.000000159	-0.000011917
14	1	0.000000887	-0.000000946	-0.000000139
15	1	0.000001521	-0.000000115	-0.000001376
16	8	0.000001719	-0.000006561	0.000000745
17	16	-0.000008540	-0.000001140	-0.000014348
18	6	0.000019590	-0.000001636	0.000001017
19	7	0.000003227	-0.000000758	-0.000012652

***p*-Methylphenacylthiocyanate (1b) in DMF**

Energy:-914.6778458a.u. ZPVC:0.165669 a.u. Total energy:-914.5121768a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000001517	-0.000002060	0.000001761
2	6	0.000003343	0.000000888	-0.000001892
3	6	-0.000004470	0.000000184	0.000002927
4	6	-0.000004654	-0.000001653	0.000003431

5	6	-0.000001041	-0.000000299	0.000002420
6	1	0.000002223	0.000000314	0.000001194
7	1	0.000001026	0.000000355	0.000000560
8	1	-0.000002738	-0.000000519	0.000001573
9	1	-0.000002756	-0.000001433	0.000003243
10	6	0.000054927	0.000005579	-0.000087207
11	6	-0.000010317	-0.000000702	0.000025037
12	6	-0.000017491	0.000006585	0.000020020
13	1	-0.000003555	-0.000000226	-0.000005093
14	1	0.000007157	-0.000000385	0.000001985
15	8	-0.000019564	-0.000004065	0.000031163
16	16	-0.000016340	-0.000001556	-0.000014329
17	6	0.000021277	0.000000747	0.000007145
18	7	-0.000003065	0.000002059	-0.000011330
19	6	-0.000002130	-0.000000456	0.000005074
20	1	0.000000039	-0.000000610	0.000003954
21	1	0.000000085	-0.000000986	0.000004233
22	1	-0.000000438	-0.000001759	0.000004131

_p_-Methoxyphenacylthiocyanate (1c) in DMF

Energy:-989.888932a.u. ZPVC:0.170890 a.u. Total energy: -989.718042 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000000334	-0.000000343	-0.000002515
2	6	0.000003703	0.000001080	-0.000001769
3	6	0.000001609	-0.000002806	-0.000004679
4	6	-0.000000339	-0.000000626	-0.000000653
5	6	-0.000001496	0.000001204	-0.000000269
6	1	0.000004045	-0.000000981	-0.000004599
7	1	0.000002941	-0.000001423	-0.000001110
8	1	-0.000004372	0.000001669	0.000003562
9	1	-0.000001999	0.000000637	0.000000558
10	6	-0.000004167	0.000015806	-0.000003609
11	6	0.000001066	-0.000000537	0.000007325
12	6	-0.000000011	0.000002695	0.000000777
13	1	-0.000000768	-0.000000764	0.000001574
14	1	0.000001574	-0.000003837	0.000003615
15	8	-0.000003811	-0.000007386	0.000010641
16	16	-0.000013938	-0.000003723	-0.000007316
17	6	0.000011972	-0.000001561	0.000018683
18	7	-0.000004145	-0.000001300	-0.000001778
19	8	0.000000224	-0.000001636	-0.000006680
20	6	0.000004352	0.000001514	-0.000001008
21	1	0.000003134	0.000000471	-0.000005190
22	1	0.000001080	-0.000000868	-0.000001713
23	1	-0.000000318	0.000002715	-0.000003848

_p_-Cyanophenacylthiocyanate (1d) in DMF

Energy:-967.6033244a.u. ZPVC:0.136700 a.u. Total energy: -967.4666244 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000003232	-0.000000961	0.000003818
2	6	0.000000375	0.000002004	0.000002049
3	6	-0.000003931	-0.000001081	0.000002445
4	6	-0.000003793	-0.000001142	0.000002865
5	6	-0.000002908	-0.000000196	0.000004560

6	1	-0.000000916	0.000000782	0.000004218
7	1	0.000000196	0.000000213	0.000001150
8	1	-0.000002726	-0.000000030	0.000002281
9	1	-0.000005049	0.000000175	0.000006341
10	6	0.000030758	0.000006328	-0.000047382
11	6	-0.000004944	-0.000000646	0.000014685
12	6	0.000000429	0.000001667	-0.000004187
13	1	-0.000001205	-0.000001218	-0.000000449
14	1	0.000003029	0.000000098	0.000002662
15	8	-0.000010650	-0.000004207	0.000017851
16	16	-0.000010993	-0.000000699	-0.000019642
17	6	0.000024996	-0.000002405	0.000004317
18	7	0.000002082	0.000000183	-0.000015453
19	6	-0.000007554	-0.000000358	0.000007736
20	7	-0.000003966	0.000001495	0.000010135

_p_-Nitrophenacylthiocyanate (1e) in DMF

Energy:-1079.8659199a.u. ZPVC:0.140411 a.u. Total energy: -1079.725509 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000007497	-0.000005636	0.000003704
2	6	0.000003160	0.000001215	0.000000926
3	6	-0.000003419	-0.000002164	0.000003458
4	6	-0.000006872	0.000000882	0.000003462
5	6	-0.000002950	0.000001634	0.000002334
6	1	0.000000022	-0.000000378	0.000002677
7	1	0.000000696	-0.000000210	0.000001245
8	1	-0.000003850	0.000000652	0.000002855
9	1	-0.000006399	0.000000758	0.000005914
10	6	0.000087604	0.000002148	-0.000119376
11	6	-0.000018433	0.000003185	0.000036925
12	6	-0.000022231	0.000001576	0.000026053
13	1	-0.000003724	-0.000000092	-0.000004912
14	1	0.000011665	0.000000585	0.000004185
15	8	-0.000026499	0.000000199	0.000040576
16	16	-0.000027073	-0.000001082	-0.000022028
17	6	0.000040173	-0.000005969	0.000007772
18	7	-0.000000775	-0.000001815	-0.000017377
19	7	-0.000005566	-0.000007212	0.000001872
20	8	-0.000005803	0.000006325	0.000010356
21	8	-0.000002227	0.000005399	0.000009377

Phenacylselenocyanate (2a) in DMF

Energy: -2878.693797 a.u. ZPVC:0.137099 a.u. Total energy: -2878.830896 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000001592	-0.000006551	0.000011304
2	6	-0.000009572	-0.000004306	0.000005754
3	6	0.000001077	-0.000009242	0.000009258
4	6	-0.000008944	0.000004141	-0.000008288
5	6	-0.000005304	0.000004274	0.000003014
6	1	-0.000005202	0.000002040	0.000011483
7	1	-0.000009114	-0.000003923	0.000009018
8	1	-0.000004171	0.000000526	-0.000000920
9	1	0.000006189	-0.000002808	0.000000435
10	1	-0.000003561	0.000000726	0.000003501

11	6	-0.000042914	-0.000004737	0.000064801
12	6	0.000005494	0.000005365	-0.000025304
13	6	0.000014130	0.000007085	-0.000045089
14	1	0.000019963	0.000004968	0.000007687
15	1	0.000004094	0.000011580	0.000006527
16	8	-0.000004013	0.000028890	-0.000048703
17	6	0.000001740	0.000016416	-0.000020967
18	7	0.000064334	-0.000008304	0.000043456
19	34	-0.000022636	-0.000046142	-0.000026966

_p_-Methylphenacylselenocyanate (2b) in DMF

Energy:-2918.0130114a.u. ZPVC:0.164408 a.u. Total energy: -2917.848603 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000003629	-0.000002621	0.000007775
2	6	-0.000006024	-0.000010410	0.000001019
3	6	-0.000001087	-0.000000512	0.000005617
4	6	-0.000003120	0.000005450	-0.000001361
5	6	-0.000002629	-0.000004486	-0.000002065
6	1	-0.000002755	-0.000001885	0.000004416
7	1	-0.000003234	-0.000000152	0.000000224
8	1	0.000002986	-0.000003351	-0.000001760
9	1	0.000000438	0.000000064	0.000000970
10	6	0.000026173	0.000010061	-0.000026428
11	6	-0.000010947	-0.000003816	0.000000663
12	6	-0.000006630	-0.000021003	-0.000007487
13	1	0.000011090	0.000015298	0.000000285
14	1	0.000004101	0.000019599	0.000007753
15	8	-0.000016349	0.000018965	-0.000004385
16	6	0.000008257	0.000002140	-0.000005139
17	7	0.000036097	-0.000002753	0.000020836
18	6	-0.000002443	-0.000002378	0.000005284
19	1	-0.000004004	-0.000000283	0.000006659
20	1	-0.000003304	0.000001715	0.000006213
21	1	-0.000003364	-0.000000909	0.000005783
22	34	-0.000026882	-0.000018733	-0.000024873

_p_-Methoxylphenacylselenocyanate (2c) in DMF

Energy:-2993.2241333a.u. ZPVC:0.169615 a.u. Total energy: -2993.054518 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000002525	-0.000001549	-0.000004306
2	6	-0.000006107	-0.000013884	-0.000006939
3	6	0.000004693	0.000001919	0.000000762
4	6	-0.000001941	0.000008969	0.000001393
5	6	0.000001072	-0.000019989	-0.000001928
6	1	0.000000549	-0.000002605	-0.000001308
7	1	-0.000001648	-0.000001260	0.000000647
8	1	0.000001455	-0.000003394	0.000001188
9	1	-0.000006348	-0.000005318	-0.000005576
10	6	0.000024956	0.000010804	-0.000009806
11	6	-0.000018962	-0.000013416	-0.000000770
12	6	-0.000008532	-0.000019966	-0.000006707
13	1	0.000004704	0.000014188	0.000010726
14	1	-0.000001304	0.000007638	0.000010754

15	8	-0.000023513	0.000009977	-0.000011264
16	6	0.000003323	0.000022543	0.000001565
17	7	0.000031725	-0.000008972	0.000044090
18	8	-0.000006106	-0.000000228	-0.000008933
19	6	0.000017463	0.000018200	0.000010542
20	1	0.000002530	0.000000281	-0.000004186
21	1	-0.000000710	0.000004192	-0.000004823
22	1	0.000002844	0.000007404	-0.000006567
23	34	-0.000017617	-0.000015536	-0.000008554

_p_-Cyanophenacylselenocyanate (2d) in DMF

Energy:-2970.9384605 a.u. ZPVC:0.135489 a.u. Total energy: -2970.802972 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000010912	0.000005844	-0.000000442
2	6	-0.000003903	0.000000039	0.000006481
3	6	-0.000002012	-0.000002291	0.000003238
4	6	-0.000002649	-0.000002140	-0.000003060
5	6	-0.000000143	0.000006221	0.000003205
6	1	-0.000007983	0.000000752	0.000006871
7	1	-0.000002345	0.000000680	0.000001489
8	1	0.000003521	0.000001289	-0.000002168
9	1	-0.000002453	0.000001107	0.000002391
10	6	-0.000001649	-0.000009706	-0.000006619
11	6	0.000002251	0.000002452	0.000000525
12	6	0.000005930	0.000012324	-0.000010824
13	1	-0.000001891	-0.000010140	-0.000000153
14	1	0.000000805	-0.000003778	-0.000004166
15	8	0.000009888	0.000000829	0.000000804
16	6	-0.000002636	0.000002126	-0.000006473
17	7	0.000015294	-0.000003831	-0.000006040
18	6	0.000001070	-0.000003266	0.000016362
19	7	-0.000013970	0.000005510	0.000007016
20	34	0.000013787	-0.000004018	-0.000008436

_p_-Nitrophenacylselenocyanate (2e) in DMF

Energy:-3083.2010531 a.u. ZPVC:0.139207 a.u. Total energy: -3083.061846 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000004272	-0.000000939	0.000005143
2	6	-0.000002048	-0.000000292	0.000003322
3	6	-0.000002868	-0.000002957	0.000004188
4	6	-0.000002576	0.000000373	-0.000000011
5	6	0.000000489	0.000005167	0.000001448
6	1	-0.000005949	-0.000000026	0.000004103
7	1	-0.000003331	-0.000001037	0.000000451
8	1	0.000001828	0.000001575	-0.000001556
9	1	-0.000002654	0.000003187	0.000001971
10	6	0.000038465	0.000005650	-0.000056125
11	6	-0.000009692	-0.000002294	0.000013860
12	6	-0.000004945	0.000003247	0.000003711
13	1	0.000001294	-0.000000402	-0.000002624
14	1	0.000004579	0.000004994	0.000003225
15	8	-0.000003126	0.000001237	0.000017617
16	6	0.000003009	-0.000007296	-0.000012766
17	7	0.000017698	-0.000003722	0.000001284

18	7	-0.000003047	0.000005055	0.000004175
19	8	-0.000010084	0.000003419	0.000006350
20	8	-0.000009161	0.000001483	0.000007362
21	34	-0.000003610	-0.000016422	-0.000005129

Reduced phenacylthiocyanate (1a + e^-) in DMF

Energy:-875.4858897 a.u. ZPVC:0.134163 a.u. Total energy: -875.3517267 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000010096	0.000001819	-0.000008668
2	6	0.000006842	0.000008999	0.000004049
3	6	-0.000000918	-0.000011242	0.000008102
4	6	0.000008409	0.000007787	-0.000002490
5	6	-0.000000756	-0.000010557	0.000001646
6	1	-0.000001508	0.000001026	0.000000215
7	1	-0.000005499	0.000000395	0.000002282
8	1	-0.000001298	0.000001758	0.000002878
9	1	0.000004299	-0.000001980	-0.000005272
10	1	0.000002627	0.000002103	-0.000005821
11	6	0.000000662	-0.000012595	0.000003149
12	6	-0.000000339	0.000008623	-0.000007641
13	6	0.000008048	0.000003834	-0.000000484
14	1	0.000003394	-0.000003078	0.000002009
15	1	-0.000001624	-0.000003366	0.000005483
16	8	0.000002972	0.000003868	-0.000007776
17	16	-0.000000896	-0.000002010	0.000000390
18	6	-0.000007648	0.000003262	0.000001436
19	7	-0.000006672	0.000001353	0.000006512

Reduced *p*-methylphenacylthiocyanate (1b + e^-) in DMF

Energy:-914.8043289 a.u. ZPVC:0.161354 a.u. Total energy: -914.6429749 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000003522	0.000002827	-0.000008531
2	6	0.000003308	0.000005097	0.000006032
3	6	0.000002020	-0.000009129	0.000001530
4	6	0.000002904	0.000004730	-0.000000074
5	6	0.000001833	-0.000009711	0.000000139
6	1	-0.000000434	0.000000738	0.000001484
7	1	-0.000002198	0.000001635	0.000003581
8	1	0.000000202	-0.000002370	-0.000001066
9	1	0.000002545	-0.000000754	-0.000002639
10	6	-0.000002751	0.000001071	0.000001591
11	6	0.000000462	0.000004562	-0.000007248
12	6	0.000001509	-0.000003070	-0.000000343
13	1	-0.000003565	0.000002711	-0.000000834
14	1	-0.000003176	0.000001876	0.000000327
15	8	0.000008849	-0.000003342	0.000001287
16	16	-0.000003999	0.000000245	0.000005827
17	6	-0.000004710	0.000007059	-0.000008392
18	7	-0.000006061	0.000000886	0.000008655
19	6	0.000000202	-0.000003074	0.000000238
20	1	0.000001282	-0.000000456	0.000000234
21	1	0.000002350	-0.000000130	-0.000002250
22	1	0.000002949	-0.000001401	0.000000453

Reduced *p*-methoxylphenacylthiocyanate (1c + e^-) in DMF

Energy:-990.0146738 a.u. ZPVC:0.166626 a.u. Total energy: -989.8480478 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000003615	0.000002616	-0.000003105
2	6	0.000008228	0.000006416	0.000001974
3	6	0.000006815	-0.000018895	0.000005874
4	6	0.000001638	0.000003200	0.000007329
5	6	0.000000442	-0.000008610	0.000004554
6	1	0.000005885	0.000000551	-0.000005703
7	1	0.000004791	0.000013087	-0.000011466
8	1	-0.000007073	-0.000004210	0.000006325
9	1	-0.000003057	-0.000002542	0.000005810
10	6	-0.000000506	-0.000020394	0.000007673
11	6	-0.000012610	0.000010093	-0.000004873
12	6	-0.000001579	-0.000000341	-0.000002863
13	1	0.000002403	0.000000452	0.000004731
14	1	-0.000005213	0.000002781	-0.000002908
15	8	-0.000004408	0.000005720	0.000004560
16	16	-0.000007410	0.000008927	-0.000008387
17	6	-0.000017057	-0.000001260	0.000000225
18	7	0.000020918	0.000012187	-0.000017091
19	8	0.000003291	-0.000000760	-0.000000011
20	6	0.000003411	-0.000002477	0.000000584
21	1	0.000003857	-0.000001543	-0.000000125
22	1	0.000002845	-0.000004249	0.000005065
23	1	-0.000001997	-0.000000750	0.000001829

Reduced *p*-cyanophenacylthiocyanate ($1d^{\bullet-}$) in DMF

Energy: -967.722426a.u. ZPVC:0.134150 a.u. Total energy: -967.588276 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000000437	-0.000003437	0.000003725
2	6	0.000004708	0.000007324	0.000000848
3	6	-0.000002554	-0.000004482	0.000000422
4	6	-0.000000951	-0.000004499	0.000001781
5	6	-0.000004131	0.000002032	0.000004719
6	1	0.000002978	-0.000001507	-0.000003083
7	1	0.000006688	0.000000822	-0.000002767
8	1	-0.000006541	0.000003191	0.000004186
9	1	-0.000004996	0.000002434	0.000006962
10	6	-0.000001476	-0.000007536	0.000005272
11	6	0.000000856	0.000011786	0.000005001
12	6	-0.000004989	-0.000001427	0.000001365
13	1	0.000005533	0.000000571	-0.000006162
14	1	0.000008838	-0.000006069	-0.000003444
15	8	-0.000006132	0.000002205	-0.000003919
16	16	0.000004017	0.000000302	-0.000001391
17	6	-0.000002139	-0.000001757	-0.000008240
18	7	0.000008032	-0.000001307	-0.000006847
19	6	-0.000010345	0.000002117	-0.000004756
20	7	0.000002170	-0.000000761	0.000006329

Reduced *p*-nitrophenacylthiocyanate (1e$^{\bullet-}$) in DMF

Energy:-1080.0089554 a.u. ZPVC:0.138318a.u. Total energy: -1079.870637 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	0.000009159	0.000041967	0.000000306
2	6	0.000023906	0.000028214	0.000014443
3	6	-0.000012494	-0.000021250	0.000002171
4	6	-0.000024223	-0.000018504	-0.000017949
5	6	-0.000003742	0.000031791	-0.000001092
6	1	0.000003863	0.000004603	0.000000785
7	1	0.000009334	0.000001084	-0.000000440
8	1	-0.000002092	-0.000000470	0.000004545
9	1	-0.000002738	0.000003926	0.000008206
10	6	-0.000041826	0.000040829	-0.000016579
11	6	0.000034918	-0.000010662	0.000026121
12	6	0.000017152	-0.000007921	0.000005571
13	1	0.000005513	-0.000001083	-0.000004375
14	1	0.000004829	-0.000003854	-0.000002237
15	8	0.000015528	0.000004647	-0.000002160
16	16	0.000017285	-0.000003766	0.000013916
17	6	-0.000017990	-0.000000428	-0.000033032
18	7	0.000011593	-0.000000270	-0.000004281
19	7	-0.000043654	-0.000085340	-0.000003289
20	8	-0.000011104	0.000005939	-0.000001054
21	8	0.000006784	-0.000009451	0.000010423

Reduced phenacylselenocyanate (2a + e^{-}) in DMF

Energy:-2878.8205495a.u. ZPVC:0.133723 a.u. Total energy:-2878.686827a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000038939	0.000006820	-0.000001203
2	6	0.000013971	0.000023512	0.000019792
3	6	0.000023015	-0.000029266	-0.000007372
4	6	0.000013943	0.000029713	0.000014585
5	6	0.000022827	-0.000028559	-0.000010788
6	1	0.000005015	-0.000001748	0.000008779
7	1	-0.000005982	-0.000006217	0.000001380
8	1	-0.000005428	0.000003896	0.000007042
9	1	0.000004287	-0.000002111	-0.000006538
10	1	-0.000004894	0.000003440	0.000004155
11	6	0.000008903	-0.000013292	-0.000035527
12	6	-0.000044274	0.000020717	-0.000008676
13	6	0.000020860	-0.000011440	0.000050377
14	1	-0.000007786	0.000007613	-0.000014734
15	1	-0.000026071	0.000009160	-0.000030999
16	8	0.000008968	-0.000006689	0.000010233
17	6	-0.000017740	0.000017072	-0.000023670
18	7	-0.000002217	-0.000001165	0.000011205
19	34	0.000031541	-0.000021455	0.000011957

Reduced *p*-methylphenacylselenocyanate (2b + e^-) in DMF

Energy:-2918.1388616 a.u. ZPVC:0.160995 a.u. Total energy: -2917.977867 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000000649	0.000001312	-0.000000712
2	6	0.000000048	-0.000001201	-0.000003143
3	6	-0.000004958	0.000007092	0.000000977
4	6	0.000003453	-0.000004089	-0.000003445
5	6	-0.000000269	0.000001034	0.000000374
6	1	-0.000002602	0.000000541	0.000001204
7	1	0.000001115	-0.000006975	0.000002989
8	1	0.000001281	0.000001133	-0.000000040
9	1	-0.000000320	0.000001418	-0.000000746
10	6	0.000004367	-0.000001188	-0.000001632
11	6	-0.000003117	0.000004502	0.000005248
12	6	-0.000000909	0.000001156	0.000000463
13	1	0.000003260	0.000000338	0.000001285
14	1	0.000003030	-0.000002722	-0.000003359
15	8	0.000001264	-0.000000383	0.000001069
16	6	0.000004236	-0.000003937	0.000005470
17	7	-0.000004991	0.000006028	-0.000002542
18	6	-0.000002537	0.000001772	0.000000772
19	1	-0.000002994	0.000001315	0.000000126
20	1	-0.000002423	0.000001781	-0.000001413
21	1	-0.000001843	0.000000918	-0.000000385
22	34	0.000005560	-0.000009847	-0.000002562

Reduced *p*-methoxylphenacylselenocyanate (2c + e^-) in DMF

Energy:-2993.3490693 a.u. ZPVC:0.166160 a.u. Total energy: -2993.182909 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000003458	0.000002922	-0.000000836
2	6	0.000002955	0.000003789	0.000002092
3	6	-0.000000065	0.000001689	-0.000002158
4	6	-0.000001383	0.000002138	-0.000001838
5	6	0.000003995	-0.000000983	0.000005178
6	1	0.000000583	0.000000323	0.000001482
7	1	-0.000001245	-0.000000268	-0.000001550
8	1	0.000000698	-0.000000872	-0.000000065
9	1	-0.000000303	-0.000004848	-0.000000028
10	6	0.000001236	-0.000004832	0.000003163
11	6	0.000000579	-0.000005221	0.000001444
12	6	-0.000008749	0.000012708	-0.000011608
13	1	0.000003390	-0.000000322	-0.000008069
14	1	-0.000004428	0.000000275	-0.000002488
15	8	0.000003434	0.000000609	0.000000175
16	6	0.000000646	0.000001925	-0.000006701
17	7	-0.000000180	0.000003873	-0.000000580
18	8	-0.000005639	-0.000008100	0.000005548
19	6	0.000008607	0.000003714	0.000004470
20	1	0.000001270	-0.000001906	0.000004015
21	1	-0.000000267	-0.000002374	0.000003604
22	1	-0.000001224	-0.000002244	0.000001958
23	34	-0.000000453	-0.000001994	0.000002794

Reduced *p*-cyanophenacylselenocyanate ($2d^{\bullet-}$) in DMF

Energy:-2971.0586597 a.u. ZPVC:0.132905 a.u. Total energy:-2970.925755 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000002290	-0.000005874	0.000002400
2	6	0.000007046	0.000008083	0.000000262
3	6	-0.000001660	-0.000007984	-0.000002798
4	6	-0.000008205	-0.000007173	0.000003688
5	6	-0.000002918	0.000004586	0.000006495
6	1	0.000004722	-0.000002231	-0.000004619
7	1	0.000007210	0.000000852	-0.000003596
8	1	-0.000008388	0.000003457	0.000007321
9	1	-0.000006301	0.000001671	0.000009397
10	6	0.000007794	0.000017739	-0.000001496
11	6	-0.000001899	-0.000007814	0.000005765
12	6	-0.000002969	-0.000003380	0.000000244
13	1	0.000001868	0.000002971	-0.000007857
14	1	0.000007821	-0.000001882	-0.000003208
15	8	-0.000007789	0.000002269	0.000003158
16	6	-0.000002670	-0.000000779	-0.000010061
17	7	0.000007583	-0.000000092	-0.000010800
18	6	-0.000007190	-0.000002125	-0.000001870
19	7	0.000002923	0.000000284	0.000005486
20	34	0.000005314	-0.000002578	0.000002092

Reduced *p*-nitrophenacylselenocyanate ($2e^{\bullet-}$) in DMF

Energy:-3083.3444004 a.u. ZPVC:0.137080 a.u. Total energy: -3083.20732 a.u.

Center Number	Atomic Number	X	Y	Z
1	6	-0.000002095	0.000005185	0.000002342
2	6	-0.000001167	0.000000301	0.000001325
3	6	-0.000000327	-0.000001133	-0.000001469
4	6	-0.000003449	-0.000000893	0.000000986
5	6	-0.000002623	-0.000000642	0.000002415
6	1	0.000000663	-0.000000238	0.000001459
7	1	0.000001139	-0.000001454	-0.000001034
8	1	-0.000002377	0.000000723	0.000002031
9	1	-0.000004005	0.000001846	0.000003992
10	6	-0.000016546	0.000024618	-0.000017527
11	6	0.000007893	-0.000003941	0.000007675
12	6	0.000003791	-0.000007027	0.000002179
13	1	0.000001429	0.000000188	-0.000004541
14	1	0.000004005	0.000000140	-0.000003107
15	8	0.000007912	-0.000015634	0.000007068
16	6	0.000000608	0.000002726	-0.000009621
17	7	0.000006429	-0.000002469	-0.000005917
18	7	-0.000001946	-0.000002345	0.000002612
19	8	-0.000008493	0.000003356	0.000002342
20	8	0.000001028	-0.000002522	0.000007134
21	34	0.000008132	-0.000000784	-0.000000342

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