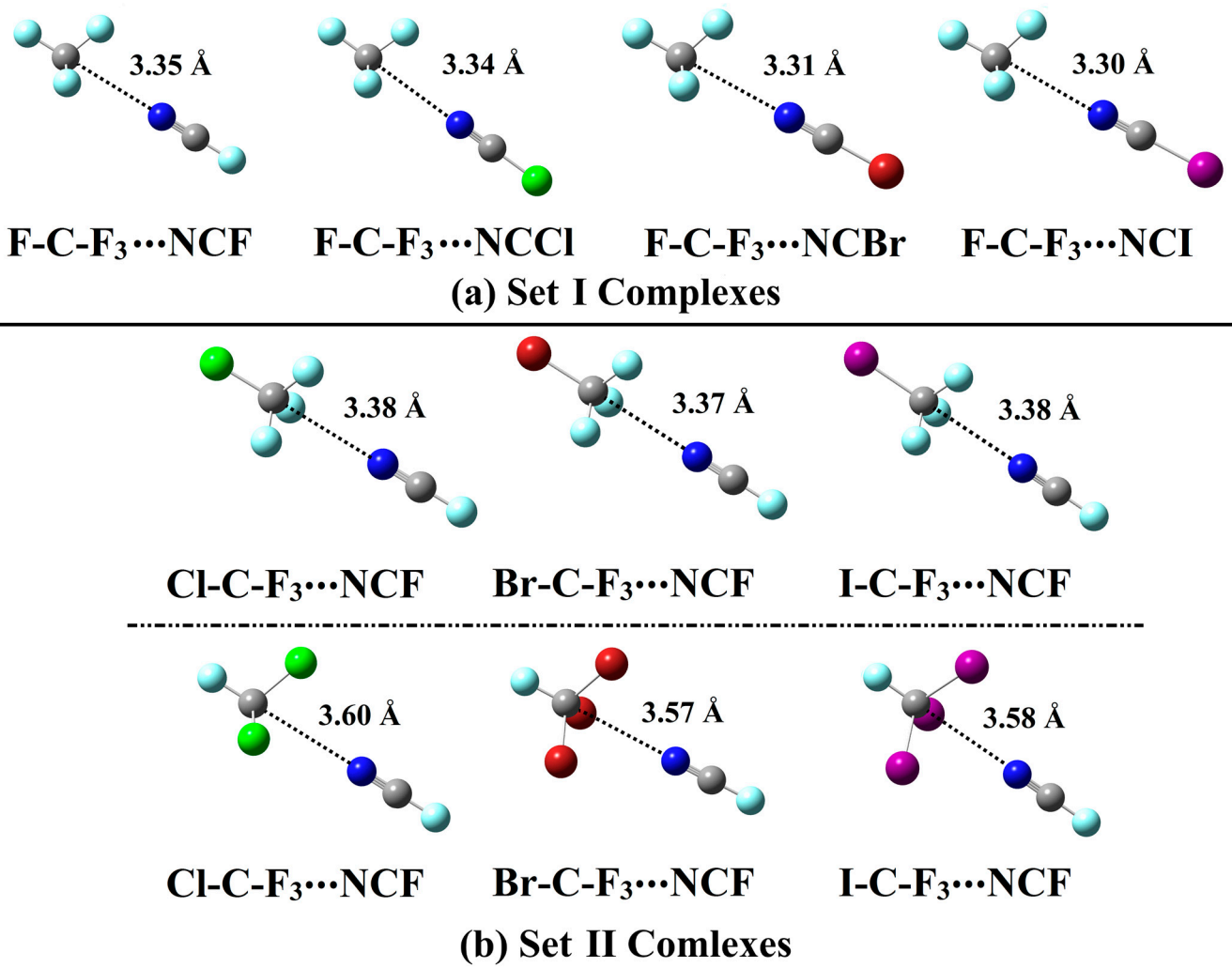

Figure S1. (**a**) Set I and (**b**) Set II complexes elucidating the Lewis basicity and acidity effects, respectively. The C···N distances are evaluated in Å.

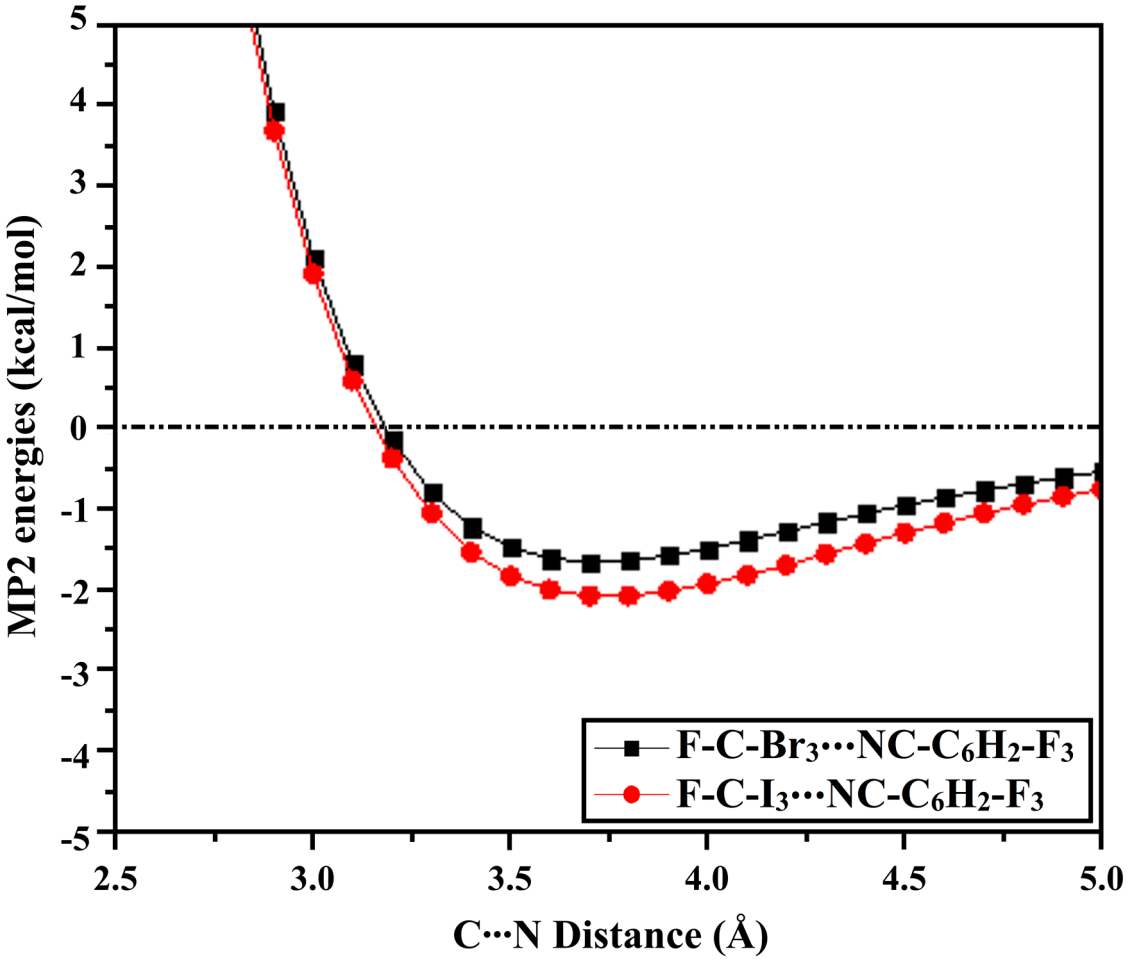

Figure S2. MP2 energies for the F-C-Br_3/ F-C-I_3···NC-C_6H_2-F_3 complexes. The C···N distances are evaluated in Å.

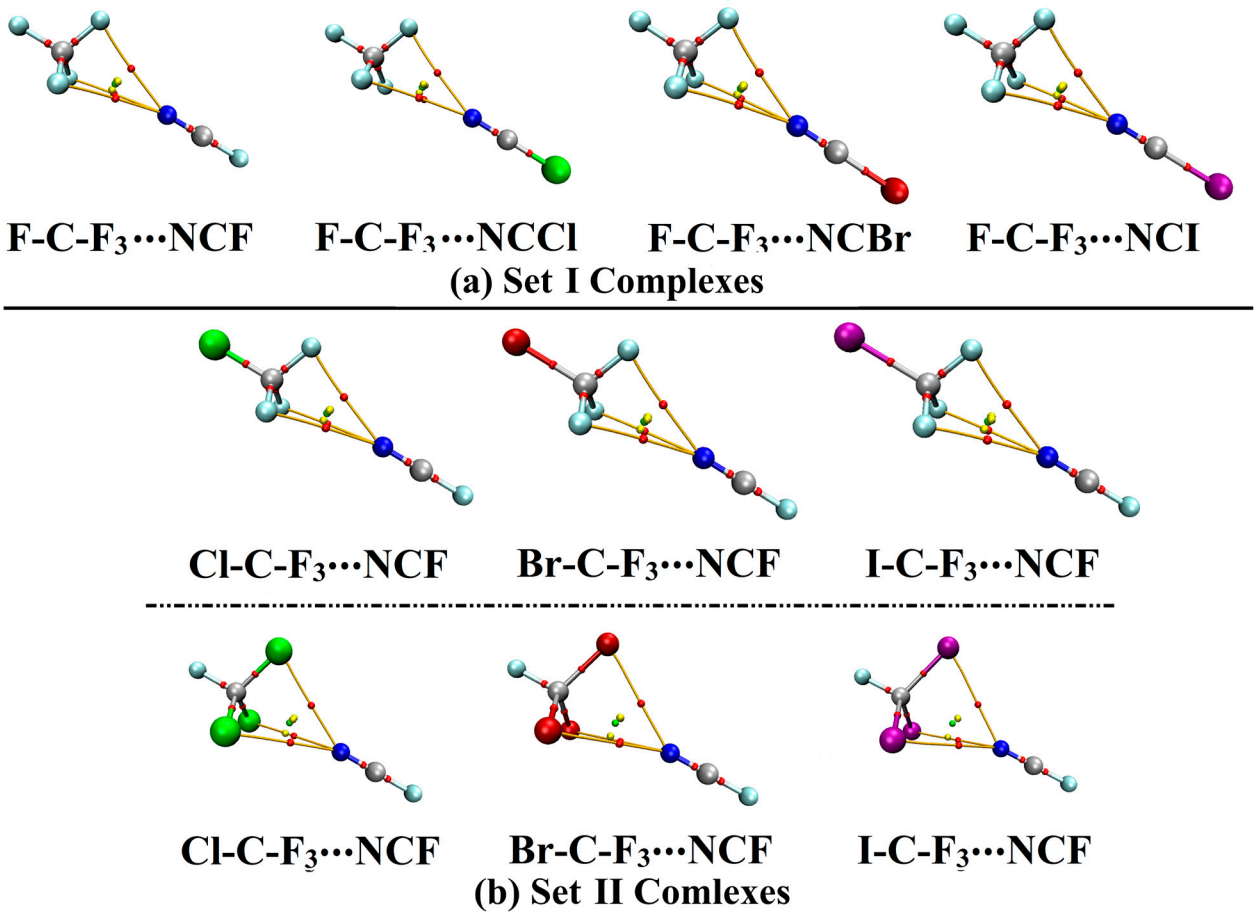

Figure S3. QTAIM diagrams of (**a**) Set I and (**b**) Set II complexes. Red dots point out the BCPs locations within the interacting species.

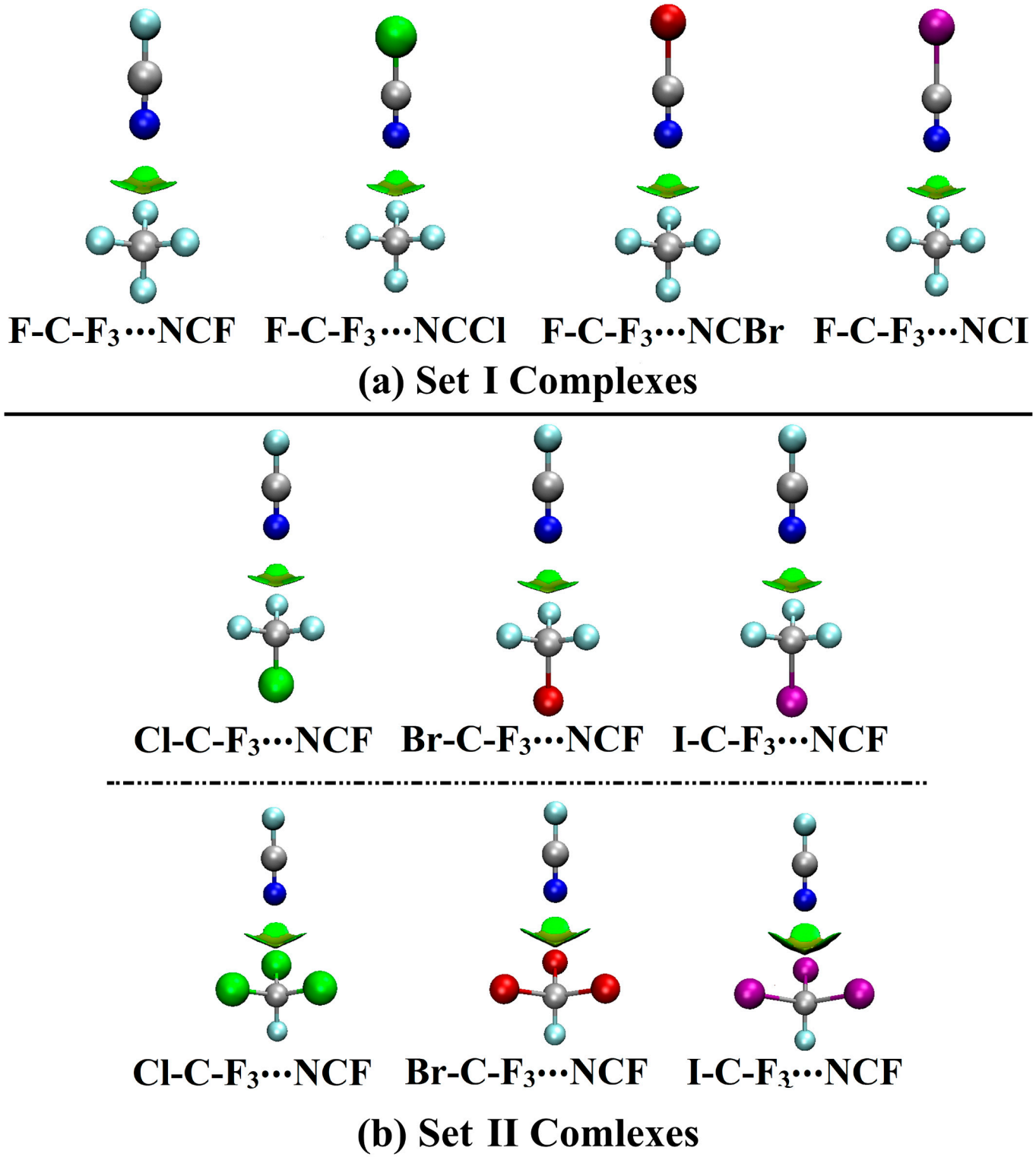

Figure S4. 3D NCI plots of the (**a**) Set I complexes and (**b**) Set II complexes. The color scope extended based on the sign(λ2)ϱ from −0.035 to 0.020 au (blue to red), where ϱ represents the electron density and λ2 refers to the second eigenvalue of the Hessian matrix based on the sign(λ2)ρ.

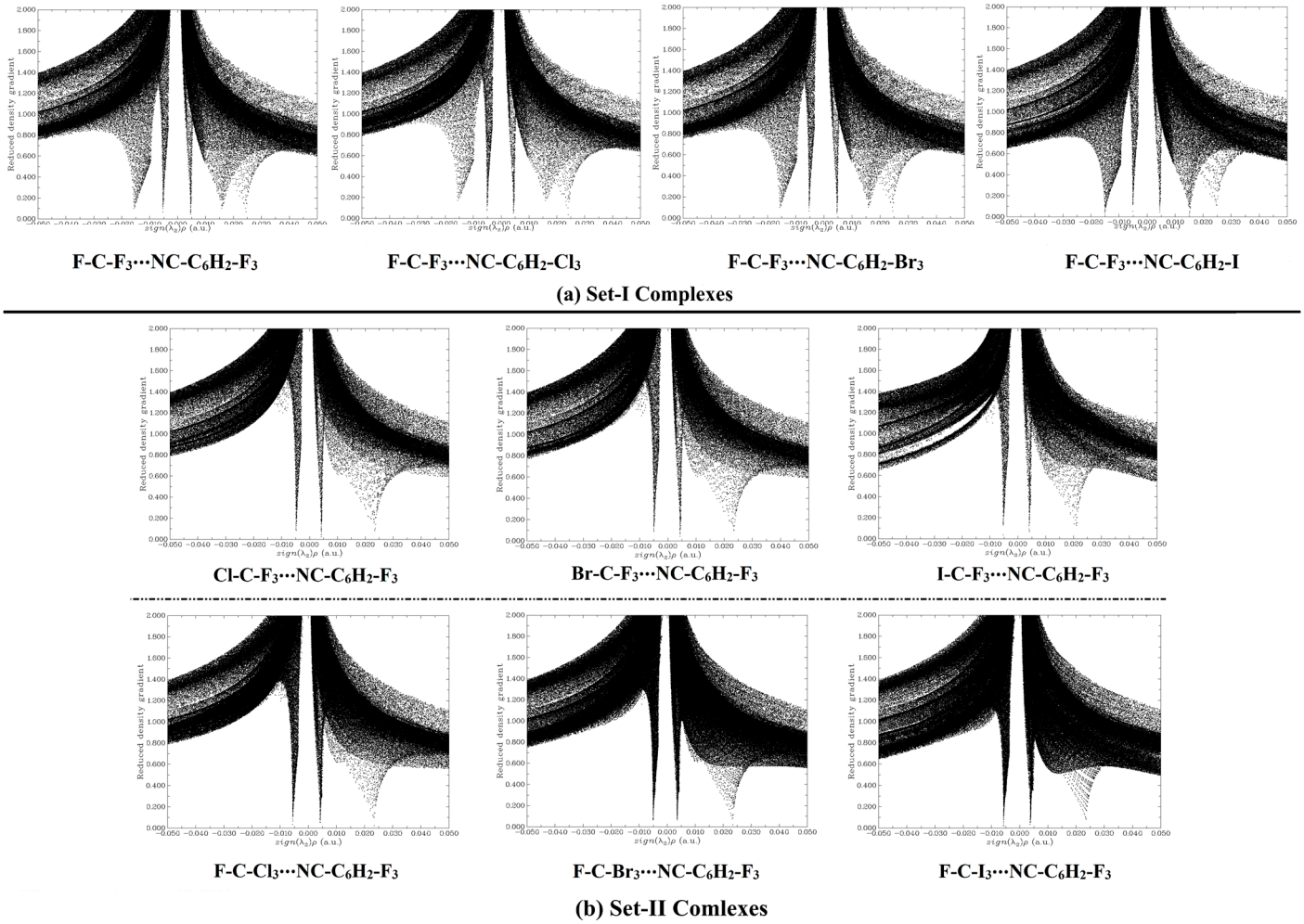

Figure S5. 2D noncovalent interaction (NCI) reduced density gradient (RDG) plots for the (**a**) Set I complexes and (**b**) Set II complexes.

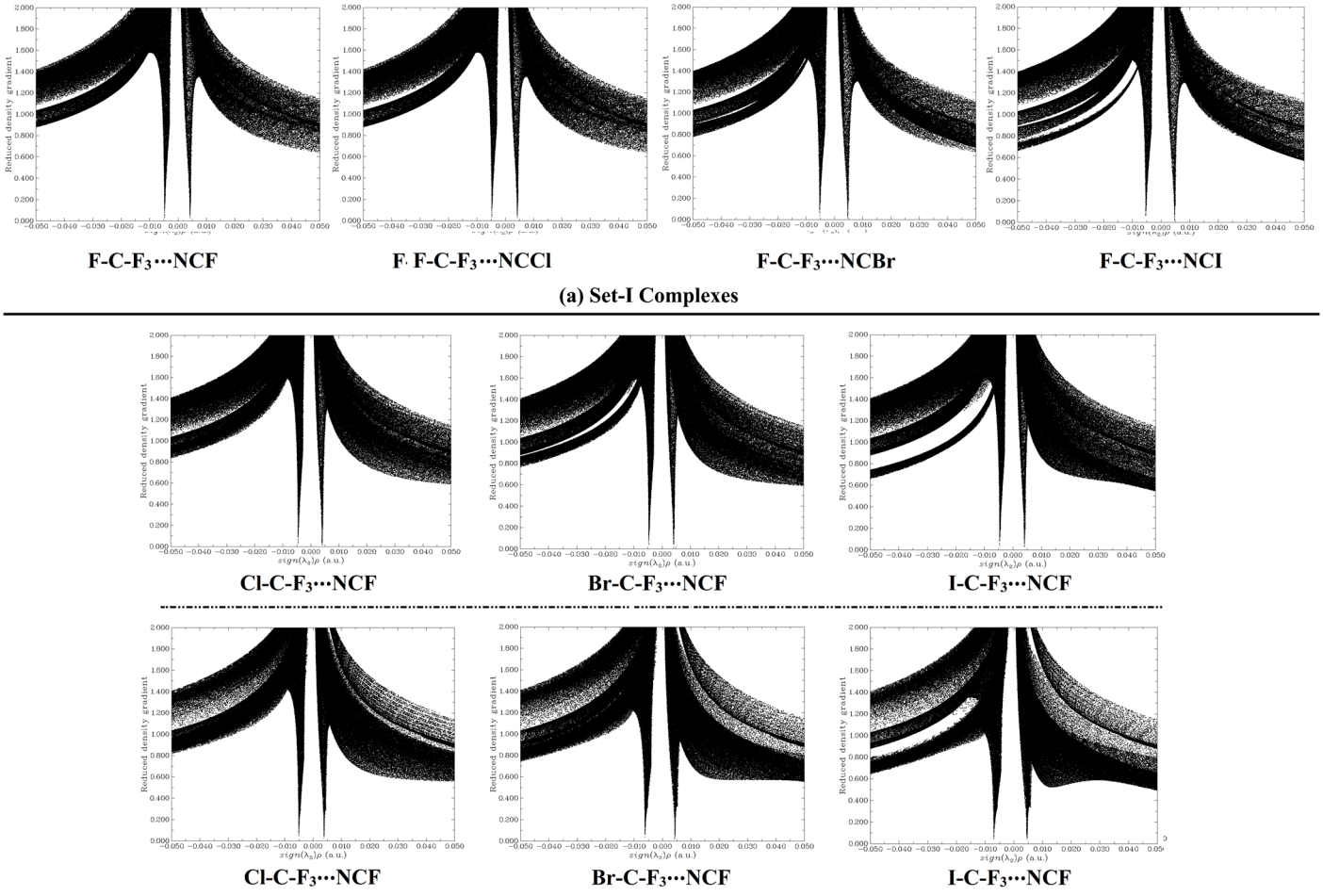

Figure S6. 2D noncovalent interaction (NCI) reduced density gradient (RDG) plots for the (**a**) Set I complexes and (**b**) Set II complexes.

Table S1. E_{elst}, E_{ind}, E_{disp}, and E_{exch}, along with total $E_{SAPT2+(3)dMP2}$ (in kcal/mol) of the F-C-F_3···NC-C_6H_2-X_3/NCX and W-C-F_3/F-C-X_3···NC-C_6H_2-F_3/NCF complexes.

W/X	Complexation parameters					Complexation parameters				
	E_{elst}	E_{ind}	E_{disp}	E_{exch}	$E_{SAPT2+(3)dMP2}$[a]	E_{elst}	E_{ind}	E_{disp}	E_{exch}	$E_{SAPT2+(3)dMP2}$[a]
	F-C-F_3···NC-C_6H_2-X_3					F-C-F_3···NCX				
F	-1.49	-0.05	-1.93	2.20	–1.28	-1.26	-0.03	-1.73	1.91	–1.10
Cl	-1.51	-0.05	-1.96	2.22	–1.30	-1.37	-0.03	-1.83	1.91	–1.18
Br	-1.59	-0.06	-2.03	2.38	–1.30	-1.52	-0.03	-1.97	2.05	–1.19
I	-1.55	-0.06	-2.00	2.28	–1.33	-1.57	-0.04	-2.01	2.34	–1.22
	W-C-F_3···NC-C_6H_2-F_3					W-C-F_3···NCF				
F	–1.49	–0.05	–1.93	2.20	–1.28	–1.26	–0.03	–1.73	1.91	–1.10
Cl	–1.14	–0.06	–1.97	2.08	–1.10	–0.95	–0.03	–1.74	1.81	–0.92
Br	–1.15	–0.07	–2.07	2.21	–1.08	–0.95	–0.04	–1.81	1.90	–0.90
I	–1.00	–0.08	–2.12	2.25	–0.95	–0.80	–0.05	–1.84	1.90	–0.79
	F-C-X_3···NC-C_6H_2-F_3					F-C-X_3···NCF				
F	–1.49	–0.05	–1.93	2.20	–1.28	–1.26	–0.03	–1.73	1.91	–1.10
Cl	–1.35	–0.28	–3.52	3.88	–1.27	–1.09	–0.20	–3.00	3.23	–1.05
Br	–0.99[b]	–0.40[b]	–3.64[b]	3.59[b]	–1.43[b]	–1.59	–0.42	–4.01	5.03	–0.99
I	–1.73[b]	–0.71[b]	–4.79[b]	5.44[b]	–1.79[b]	–2.66	–0.78	–5.24	7.53	–1.15

[a] $E_{\mathrm{SAPT2+(3)dMP2}} = E_{\mathrm{elst}} + E_{\mathrm{ind}} + E_{\mathrm{disp}} + E_{\mathrm{exch}}$.

[b] The SAPT results were recorded based on the PES scan depicted in Figure S2.

For Set I Complexes:

F-C-F_3···NC-C_6H_2-F_3

Molecule Name
18 17
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -1.2167 -0.3117 0.0109 C
2 F2 -0.7776 0.3101 -1.0665 F
3 F3 -0.7685 -1.5523 0.0273 F
4 F4 -0.7726 0.3234 1.0886 F
5 F5 -2.5358 -0.3105 0.0238 F
6 N6 -2.3306 -1.9038 -2.6864 N
7 C7 -2.7211 -2.4609 -3.6432 C
8 C8 -3.1957 -3.1387 -4.8082 C
9 C9 -2.4348 -4.1634 -5.3716 C
10 C10 -4.4167 -2.7713 -5.3743 C
11 C11 -2.8987 -4.8237 -6.5078 C
12 H12 -1.4897 -4.4426 -4.9274 H
13 C13 -4.8784 -3.4332 -6.5105 C
14 H14 -5.0008 -1.9764 -4.9322 H
15 C15 -4.1289 -4.4717 -7.0990 C
16 I16 -6.7093 -2.7918 -7.2551 I
17 I17 -4.8166 -5.4540 -8.7870 I
18 I18 -1.6729 -6.3294 -7.2482 I
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 Ar
7 8 9 Ar
8 8 10 Ar
9 9 11 Ar
10 9 12 1
11 10 13 Ar
12 10 14 1
13 11 15 Ar
14 11 18 1

15 13 15 Ar
16 13 16 1
17 15 17 1

$F\text{-}C\text{-}F_3\cdots NC\text{-}C_6H_2\text{-}Cl_3$

Molecule Name
18 17
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -1.2101 -0.3158 0.0261 C
2 F2 -0.7671 0.3111 -1.0468 F
3 F3 -0.7654 -1.5578 0.0359 F
4 F4 -0.7667 0.3115 1.1084 F
5 F5 -2.5293 -0.3112 0.0361 F
6 N6 -2.3248 -1.8927 -2.6881 N
7 C7 -2.7154 -2.4451 -3.6474 C
8 C8 -3.1905 -3.1175 -4.8159 C
9 C9 -2.4288 -4.1427 -5.3804 C
10 C10 -4.4112 -2.7420 -5.3804 C
11 C11 -2.8964 -4.7925 -6.5166 C
12 H12 -1.4837 -4.4350 -4.9451 H
13 C13 -4.8674 -3.3999 -6.5166 C
14 H14 -5.0024 -1.9488 -4.9452 H
15 C15 -4.1200 -4.4332 -7.1022 C
16 Cl16 -6.3723 -2.9238 -7.1973 Cl
17 Cl17 -4.6882 -5.2375 -8.5000 Cl
18 Cl18 -1.9450 -6.0520 -7.1971 Cl
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 Ar
7 8 9 Ar
8 8 10 Ar
9 9 11 Ar
10 9 12 1
11 10 13 Ar
12 10 14 1
13 11 15 Ar
14 11 18 1
15 13 15 Ar
16 13 16 1

17 15 17 1

F-C-F_3···NC-C_6H_2-Br_3

Molecule Name
18 17
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -1.2280 -0.3305 -0.0099 C
2 F2 -0.7938 0.2992 -1.0847 F
3 F3 -0.7723 -1.5685 0.0000 F
4 F4 -0.7865 0.3019 1.0704 F
5 F5 -2.5471 -0.3373 0.0045 F
6 N6 -2.3306 -1.9089 -2.7037 N
7 C7 -2.7201 -2.4642 -3.6617 C
8 C8 -3.1943 -3.1400 -4.8281 C
9 C9 -2.4275 -4.1580 -5.3974 C
10 C10 -4.4202 -2.7761 -5.3879 C
11 C11 -2.8939 -4.8124 -6.5326 C
12 H12 -1.4784 -4.4397 -4.9637 H
13 C13 -4.8768 -3.4372 -6.5232 C
14 H14 -5.0138 -1.9879 -4.9469 H
15 C15 -4.1239 -4.4647 -7.1147 C
16 Br16 -6.5234 -2.9091 -7.2290 Br
17 Br17 -4.7408 -5.3439 -8.6321 Br
18 Br18 -1.8267 -6.1662 -7.2514 Br
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 Ar
7 8 9 Ar
8 8 10 Ar
9 9 11 Ar
10 9 12 1
11 10 13 Ar
12 10 14 1
13 11 15 Ar
14 11 18 1
15 13 15 Ar
16 13 16 1

17 15 17 1

$F\text{-}C\text{-}F_3\cdots NC\text{-}C_6H_2\text{-}I_3$

```
  Molecule Name
18 17
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 C1       -1.2167      -0.3117       0.0109 C
2 F2       -0.7776       0.3101      -1.0665 F
3 F3       -0.7685      -1.5523       0.0273 F
4 F4       -0.7726       0.3234       1.0886 F
5 F5       -2.5358      -0.3105       0.0238 F
6 N6       -2.3306      -1.9038      -2.6864 N
7 C7       -2.7211      -2.4609      -3.6432 C
8 C8       -3.1957      -3.1387      -4.8082 C
9 C9       -2.4348      -4.1634      -5.3716 C
10 C10      -4.4167      -2.7713      -5.3743 C
11 C11      -2.8987      -4.8237      -6.5078 C
12 H12      -1.4897      -4.4426      -4.9274 H
13 C13      -4.8784      -3.4332      -6.5105 C
14 H14      -5.0008      -1.9764      -4.9322 H
15 C15      -4.1289      -4.4717      -7.0990 C
16 I16      -6.7093      -2.7918      -7.2551 I
17 I17      -4.8166      -5.4540      -8.7870 I
18 I18      -1.6729      -6.3294      -7.2482 I
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 Ar
7 8 9 Ar
8 8 10 Ar
9 9 11 Ar
10 9 12 1
11 10 13 Ar
12 10 14 1
13 11 15 Ar
14 11 18 1
15 13 15 Ar
16 13 16 1
```

17 15 17 1

F-C-F_3···NCF

Molecule Name
8 6
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -1.2066 -0.3112 0.0383 C
2 F2 -0.7627 0.3165 -1.0341 F
3 F3 -0.7628 -1.5538 0.0457 F
4 F4 -0.7645 0.3140 1.1213 F
5 F5 -2.5260 -0.3069 0.0457 F
6 N6 -2.3221 -1.8887 -2.6940 N
7 C7 -2.7125 -2.4409 -3.6505 C
8 F8 -3.1351 -3.0385 -4.6855 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1

F-C-F_3···NCCl

Molecule Name
8 6
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -1.2092 -0.3149 0.0319 C
2 F2 -0.7651 0.3132 -1.0400 F
3 F3 -0.7651 -1.5572 0.0399 F
4 F4 -0.7668 0.3107 1.1153 F
5 F5 -2.5284 -0.3102 0.0399 F
6 N6 -2.3224 -1.8892 -2.6948 N
7 C7 -2.7141 -2.4431 -3.6543 C
8 Cl8 -3.2578 -3.2119 -4.9858 Cl
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1

F-C-F_3···NCBr

Molecule Name
8 6
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -1.2138 -0.3214 0.0208 C
2 F2 -0.7694 0.3071 -1.0506 F
3 F3 -0.7694 -1.5635 0.0293 F
4 F4 -0.7714 0.3042 1.1046 F
5 F5 -2.5330 -0.3164 0.0293 F
6 N6 -2.3155 -1.8793 -2.6780 N
7 C7 -2.7073 -2.4335 -3.6378 C
8 Br8 -3.2992 -3.2707 -5.0878 Br
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1

F-C-F_3···NCI

Molecule Name
8 6
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -1.2134 -0.3208 0.0217 C
2 F2 -0.7689 0.3078 -1.0495 F
3 F3 -0.7689 -1.5628 0.0305 F
4 F4 -0.7708 0.3050 1.1056 F
5 F5 -2.5325 -0.3157 0.0305 F
6 N6 -2.3143 -1.8778 -2.6751 N
7 C7 -2.7065 -2.4325 -3.6358 C
8 I8 -3.3670 -3.3662 -5.2534 I
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1

For Set II Complexes (W-Effect)

$Cl\text{-}C\text{-}F_3\cdots NC\text{-}C_6H_2\text{-}F_3$

```
  Molecule Name
18 17
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 C1          5.3919         1.7202         8.7388 C
2 F2          5.0848         0.7658         9.6044 F
3 Cl3         6.5818         2.8085         9.4453 Cl
4 F4          4.2940         2.3935         8.4293 F
5 F5          5.8843         1.1666         7.6409 F
6 C6         -0.5329        -3.6603         5.1880 C
7 C7          0.7193        -4.1376         5.5647 C
8 C8          1.6681        -3.3022         6.1268 C
9 C9          1.3469        -1.9539         6.3135 C
10 C10        0.0960        -1.4495         5.9436 C
11 C11       -0.8280        -2.3142         5.3844 C
12 H12        2.6323        -3.6989         6.4101 H
13 H13       -0.1593        -0.4093         6.0848 H
14 F14       -2.0312        -1.8714         5.0188 F
15 F15       -1.4316        -4.4761         4.6499 F
16 F16        0.9877        -5.4291         5.3706 F
17 C17        2.3144        -1.0755         6.8929 C
18 N18        3.1087        -0.3541         7.3686 N
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 Ar
6 6 11 Ar
7 6 15 1
8 7 8 2
9 7 16 1
10 8 9 Ar
11 8 12 1
12 9 10 Ar
13 9 17 Ar
14 10 11 2
```

15 10 13 1
16 11 14 1
17 17 18 3

Br-C-F_3···NC-C_6H_2-F_3

Molecule Name
18 17
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 4.1438 2.9793 3.7664 C
2 F2 4.9925 2.0347 3.3890 F
3 F3 2.9816 2.4216 4.0712 F
4 F4 3.9679 3.8293 2.7658 F
5 Br5 4.8407 3.9077 5.2942 Br
6 N6 2.9259 1.3528 1.0922 N
7 C7 2.5004 0.7841 0.1576 C
8 C8 1.9824 0.0915 -0.9805 C
9 C9 2.7232 -0.9516 -1.5454 C
10 C10 0.7439 0.4691 -1.5091 C
11 C11 2.2063 -1.6107 -2.6465 C
12 H12 3.6806 -1.2489 -1.1425 H
13 C13 0.2582 -0.2124 -2.6108 C
14 H14 0.1661 1.2738 -1.0781 H
15 C15 0.9761 -1.2541 -3.1916 C
16 F16 -0.9184 0.1180 -3.1437 F
17 F17 0.4950 -1.8974 -4.2486 F
18 F18 2.8825 -2.6103 -3.2133 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 Ar
7 8 9 Ar
8 8 10 Ar
9 9 11 2
10 9 12 1
11 10 13 2
12 10 14 1
13 11 15 Ar
14 11 18 1
15 13 15 Ar
16 13 16 1

17 15 17 1

I-C-F_3···NC-C_6H_2-F_3

Molecule Name
18 17
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 2.9819 2.1457 2.7043 C
2 F2 3.8524 1.2186 2.3239 F
3 F3 1.8110 1.5655 2.9371 F
4 F4 2.8368 3.0270 1.7224 F
5 I5 3.6797 3.1258 4.4726 I
6 N6 1.8859 0.6036 -0.0764 N
7 C7 1.5045 0.0645 -1.0469 C
8 C8 1.0402 -0.5922 -2.2286 C
9 C9 1.8136 -1.6087 -2.7983 C
10 C10 -0.1793 -0.2068 -2.7945 C
11 C11 1.3486 -2.2332 -3.9419 C
12 H12 2.7566 -1.9118 -2.3668 H
13 C13 -0.6129 -0.8534 -3.9381 C
14 H14 -0.7821 0.5775 -2.3600 H
15 C15 0.1383 -1.8681 -4.5245 C
16 F16 -1.7700 -0.5145 -4.5072 F
17 F17 -0.2929 -2.4781 -5.6221 F
18 F18 2.0572 -3.2067 -4.5146 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 Ar
7 8 9 Ar
8 8 10 Ar
9 9 11 2
10 9 12 1
11 10 13 2
12 10 14 1
13 11 15 Ar
14 11 18 1
15 13 15 Ar
16 13 16 1

17 15 17 1

Cl-C-F_3···NCF

Molecule Name
8 6
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -0.9415 1.7501 -0.1572 C
2 F2 -1.4191 2.9769 -0.3053 F
3 F3 -1.4300 0.9780 -1.1165 F
4 F4 -1.3279 1.2754 1.0178 F
5 Cl5 0.8155 1.7761 -0.2449 Cl
6 N6 -4.3260 1.7000 0.0117 N
7 C7 -5.4959 1.6827 0.0701 C
8 F8 -6.7621 1.6644 0.1333 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1

Br-C-F_3···NCF

```
 Molecule Name
8 6
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 C1    -0.7555    1.6511    -0.1011 C
2 F2    -1.1883    2.8932    -0.2606 F
3 F3    -1.2483    0.8937    -1.0702 F
4 F4    -1.1817    1.1913     1.0662 F
5 Br5     1.1608     1.6158    -0.1559 Br
6 N6    -4.1309    1.7133    -0.0045 N
7 C7    -5.3017    1.7349     0.0290 C
8 F8    -6.5688    1.7575     0.0653 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1
```

I-C-F_3···NCF

Molecule Name
8 6
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -3.1508 1.3673 -0.0356 C
2 F2 -3.6807 2.5732 -0.2020 F
3 F3 -3.5729 0.5757 -1.0143 F
4 F4 -3.5674 0.8732 1.1242 F
5 I5 -1.0168 1.4918 -0.0584 I
6 N6 -6.5324 1.1697 0.0012 N
7 C7 -7.7019 1.1015 0.0139 C
8 F8 -8.9677 1.0278 0.0277 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1

For Set-II Complexes (X_3-Effect)
F-C-Cl_3···NC-C_6H_2-F_3

```
 Molecule Name
18 17
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 C1     1.8847     1.9057     3.4772 C
2 F2     2.2229     2.5755     4.5960 F
3 Cl3     2.5452     2.7750     2.0975 Cl
4 Cl4     0.1293     1.8374     3.3885 Cl
5 Cl5     2.5675     0.2878     3.5793 Cl
6 N6     0.9914     0.1362     0.5240 N
7 C7     0.6965    -0.4477    -0.4513 C
8 C8     0.3380    -1.1577    -1.6388 C
9 C9    -0.4159    -2.3312    -1.5362 C
10 C10     0.7474    -0.6666    -2.8827 C
11 C11    -0.7537    -3.0053    -2.6962 C
12 H12    -0.7357    -2.7167    -0.5789 H
13 C13     0.3912    -1.3669    -4.0215 C
14 H14     1.3299     0.2392    -2.9699 H
15 C15    -0.3586    -2.5373    -3.9462 C
16 F16     0.7625    -0.9308    -5.2254 F
17 F17    -0.6916    -3.1968    -5.0493 F
18 F18    -1.4714    -4.1274    -2.6397 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 Ar
7 8 9 Ar
8 8 10 Ar
9 9 11 2
10 9 12 1
11 10 13 2
12 10 14 1
13 11 15 Ar
14 11 18 1
15 13 15 Ar
```

```
16 13 16 1
17 15 17 1
```

F-C-Br_3···NC-C_6H_2-F_3

Molecule Name
18 17
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -0.0000 0.0000 0.0000 C
2 F2 -1.3447 -0.0000 -0.0000 F
3 Br3 0.6011 0.0000 1.8210 Br
4 Br4 0.6009 1.5773 -0.9101 Br
5 Br5 0.6006 -1.5770 -0.9108 Br
6 C6 8.3941 -1.0382 -0.5997 C
7 C7 7.0108 -1.0548 -0.6092 C
8 C8 6.3236 0.0001 -0.0000 C
9 C9 7.0107 1.0550 0.6091 C
10 C10 8.3940 1.0386 0.5995 C
11 C11 9.1010 0.0002 -0.0001 C
12 H12 6.4870 -1.8731 -1.0818 H
13 H13 6.4868 1.8733 1.0816 H
14 C14 4.8937 0.0000 0.0000 C
15 N15 3.7200 0.0000 0.0000 N
16 F16 9.0847 -2.0259 -1.1700 F
17 F17 10.4289 0.0003 -0.0001 F
18 F18 9.0845 2.0264 1.1699 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 1
6 6 11 1
7 6 16 1
8 7 8 1
9 7 12 1
10 8 9 1
11 8 14 1
12 9 10 1
13 9 13 1
14 10 11 1
15 10 18 1
16 11 17 1

17 14 15 1

F-C-I_3···NC-C_6H_2-F_3

Molecule Name
18 17
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -0.0000 0.0000 0.0000 C
2 F2 -1.3562 -0.0000 -0.0000 F
3 I3 0.6571 0.0000 2.0380 I
4 I4 0.6572 -1.7649 -1.0191 I
5 I5 0.6572 1.7650 -1.0189 I
6 C6 8.4241 0.0001 -1.1990 C
7 C7 7.0408 0.0001 -1.2181 C
8 C8 6.3536 0.0001 0.0000 C
9 C9 7.0407 0.0002 1.2182 C
10 C10 8.4240 0.0003 1.1992 C
11 C11 9.1310 0.0002 0.0001 C
12 H12 6.5170 0.0000 -2.1630 H
13 H13 6.5168 0.0002 2.1631 H
14 C14 4.9237 -0.0000 0.0000 C
15 N15 3.7500 -0.0000 0.0000 N
16 F16 9.1147 0.0001 -2.3395 F
17 F17 10.4589 0.0003 0.0002 F
18 F18 9.1145 0.0003 2.3398 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 1
6 6 11 1
7 6 16 1
8 7 8 1
9 7 12 1
10 8 9 1
11 8 14 1
12 9 10 1
13 9 13 1
14 10 11 1
15 10 18 1
16 11 17 1

17 14 15 1

F-C-Cl_3···NCF

Molecule Name
8 6
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -25.3146 0.0329 2.3815 C
2 F2 -23.9680 0.0268 2.4014 F
3 Cl3 -25.8529 1.6908 2.1432 Cl
4 Cl4 -25.8490 -0.9918 1.0551 Cl
5 Cl5 -25.8895 -0.5927 3.9220 Cl
6 N6 -28.9097 0.0492 2.3281 N
7 C7 -30.0818 0.0546 2.3107 C
8 F8 -31.3496 0.0604 2.2918 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1

F-C-Br_3···NCF

Molecule Name
8 6
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -10.6860 -0.1171 1.1796 C
2 F2 -9.3406 -0.1298 1.0908 F
3 Br3 -11.2372 -1.7532 2.0107 Br
4 Br4 -11.3925 0.0224 -0.5960 Br
5 Br5 -11.1925 1.3959 2.2404 Br
6 N6 -14.2439 -0.0838 1.4143 N
7 C7 -15.4138 -0.0730 1.4914 C
8 F8 -16.6791 -0.0614 1.5757 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1

F-C-I_3···NCF

Molecule Name
8 6
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -24.8447 -0.1174 2.2723 C
2 F2 -23.4882 -0.1891 2.2534 F
3 I3 -25.5704 -1.3357 0.6688 I
4 I4 -25.3787 1.9376 2.0009 I
5 I5 -25.4959 -0.8532 4.1741 I
6 N6 -28.4190 0.0718 2.3219 N
7 C7 -29.5900 0.1337 2.3380 C
8 F8 -30.8560 0.2008 2.3554 F
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 1 5 1
5 6 7 3
6 7 8 1