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

Characterization of N...O non-covalent interactions involving σ-hole: "Electrostatics" or "dispersion"

Rahul Shukla[a] *and Deepak Chopra*[*a]

Crystallography and Crystal Chemistry Laboratory, Department of Chemistry,
Indian Institute of Science Education and Research Bhopal,
Bhopal By-pass Road, Bhauri
Bhopal-462066, Madhya Pradesh, India
Email: dchopra@iiserb.ac.in; Fax: +91 755 6692392

Coordinates of the optimized geometry

NO1

O 8.0 -1.76300 0.16710 -0.61940
F 9.0 -1.92550 -1.18470 -0.27840
F 9.0 -2.11770 0.83430 0.56310
N 7.0 1.23500 -0.20120 -0.25570
F 9.0 2.57340 -0.48180 -0.15960
F 9.0 1.24640 1.15970 -0.42250
F 9.0 0.82990 -0.31950 1.04690

NO2

O 8.0 -1.88930 0.26790 -0.59110
F 9.0 -2.23790 -1.08390 -0.45130
F 9.0 -2.23040 0.81170 0.65760
N 7.0 1.01330 -0.49550 -0.23770
F 9.0 2.26590 -1.09000 -0.21110
F 9.0 0.53760 -0.79980 1.02750
Cl 17.0 1.35320 1.22250 -0.16540

NO3

O 8.0 1.91570 0.47700 0.46700
F 9.0 2.26960 -0.79300 0.94830
F 9.0 2.62860 0.56510 -0.74030
N 7.0 -0.97490 -0.14790 0.48880
F 9.0 -2.25450 -0.52020 0.94550
Cl 17.0 -1.21900 1.45960 -0.17160
Cl 17.0 -0.68070 -1.22710 -0.86010

NO4

O 8.0 -2.07250 0.15220 -0.32430
F 9.0 -2.20780 -1.22620 -0.55930
F 9.0 -3.39600 0.55270 -0.05770
N 7.0 0.66920 -0.02660 -0.14630
Cl 17.0 0.80340 1.67670 0.29080
Cl 17.0 0.76930 -0.95170 1.34980

Cl 17.0 2.09380 -0.42920 -1.10110

NO5

O 8.0 1.36340 0.32070 -0.75900
N 7.0 -1.58460 0.22330 -0.21210
Cl 17.0 2.12260 -0.75340 0.28220
F 9.0 -1.10990 0.17240 1.07190
F 9.0 -1.39070 -1.06790 -0.63220
F 9.0 -2.94070 0.24770 -0.00700
F 9.0 1.45240 1.61220 -0.12610

NO6

O 8.0 1.49600 0.07710 0.83300
N 7.0 -1.47970 0.11910 0.52080
Cl 17.0 2.24340 0.63330 -0.56230
F 9.0 -1.10600 1.39280 0.11400
F 9.0 -2.86060 0.24380 0.57080
F 9.0 1.80060 -1.32970 0.90830
Cl 17.0 -1.19140 -0.88110 -0.88760

NO7

O 8.0 -1.57670 0.10390 -0.82120
N 7.0 1.35130 -0.20110 -0.47240
Cl 17.0 -2.42070 0.54610 0.56100
F 9.0 2.73690 -0.41950 -0.61280
F 9.0 -1.91240 -1.27660 -1.06160
Cl 17.0 0.92910 -1.11560 0.96280
Cl 17.0 1.24070 1.50140 -0.05640

NO8

O 8.0 -1.79540 -0.00330 -0.86370
F 9.0 -2.02190 -1.41290 -1.05920
N 7.0 1.08970 -0.10820 -0.29380
Cl 17.0 0.84170 1.61960 -0.02750
Cl 17.0 0.60620 -0.92750 1.19120
Cl 17.0 2.82930 -0.35130 -0.46860
Cl 17.0 -2.81060 0.45320 0.39310

NO9

O 8.0 1.18220 -0.02510 -0.72450
N 7.0 -1.71230 0.24720 -0.18020
Cl 17.0 1.77920 -1.29640 0.24700
Cl 17.0 1.58650 1.48500 -0.03670
F 9.0 -1.29230 -0.00780 1.09960
F 9.0 -1.73430 -1.01030 -0.72250
F 9.0 -3.04980 0.49180 0.01000

NO10

O 8.0 1.54420 0.02180 -0.72640
N 7.0 -1.34300 0.04420 -0.17910
Cl 17.0 -3.06240 0.32820 0.02860
Cl 17.0 2.28780 -1.16320 0.25270
Cl 17.0 1.74890 1.57110 -0.03800
F 9.0 -0.89170 -0.23980 1.10130
F 9.0 -1.27660 -1.20440 -0.77600

NO11

O 8.0 1.62970 -0.05620 -0.68390
N 7.0 -1.21760 0.21110 -0.08650
Cl 17.0 -1.30030 -1.47420 -0.56210
Cl 17.0 -2.86700 0.78030 0.10930
Cl 17.0 2.38530 -1.04490 0.48600
Cl 17.0 1.89920 1.59210 -0.32840
F 9.0 -0.72300 0.16290 1.23260

NO12

O 8.0 1.62970 -0.05620 -0.68390
N 7.0 -1.21760 0.21110 -0.08650
Cl 17.0 -1.30030 -1.47420 -0.56210
Cl 17.0 -2.86700 0.78030 0.10930
Cl 17.0 2.38530 -1.04490 0.48600
Cl 17.0 1.89920 1.59210 -0.32840
F 9.0 -0.72300 0.16290 1.23260

Table S1: Result of Energy Decomposition Analysis. All energies values are given in kcal/mol.

	E_{elec}	$E_{ex\text{-}rep}$	E_{pol}	E_{diso}	E_{total}
NO1	-0.38	1.21	-0.07	-1.3	-0.54
NO2	-0.58	1.76	-0.12	-1.8	-0.74
NO3	-1.07	2.57	-0.19	-2.3	-0.99
NO4	-1.63	3.5	-0.45	-2.81	-1.39
NO5	-0.86	1.75	-0.13	-1.65	-0.89
NO6	-1.31	2.87	-0.22	-2.51	-1.17
NO7	-1.58	3.97	-0.35	-3.48	-1.44
NO8	-1.6	4.17	-0.35	-3.73	-1.51
NO9	-1.15	2.37	-0.18	-2.18	-1.14
NO10	-1.12	2.74	-0.19	-2.65	-1.22
NO11	-1.64	3.97	-0.31	-3.69	-1.67
NO12	-2.32	5.58	-0.47	-4.96	-2.17

Table S2: Topological parameters of O…Cl contacts.

BPL (Å)	$\rho(e/Å^3)$	$\nabla^2\rho(e/Å^5)$	$\lvert V_b\rvert/G_b$
NO6			
3.340	0.043	0.615	0.774
NO7			
3.260	0.049	0.719	0.756
3.325	0.046	0.664	0.776
NO6			
3.232	0.051	0.772	0.756

Table S3: E(2) energies and charges of the interacting fragments.

	O(lp) to σ*(N-X) (kcal/mol)	N(lp) to σ*(O-Y) (kcal/mol)	OY_1Y_2	$NX_1X_2X_3$	Total
			Charges (au)		
NO1	0.28		0.00124	-0.00124	0.00
NO2	0.39		0.00175	-0.00175	0.00
NO3	0.47		0.00130	-0.00130	0.00
NO4	0.47	0.38	-0.00444	0.00444	0.00
NO5	0.53		0.00085	-0.00085	0.00
NO6	0.30		0.00125	-0.00125	0.00
NO7	0.36		0.00036	-0.00036	0.00
NO8	0.49		-0.00010	0.00010	0.00
NO9	0.35		0.00063	-0.00063	0.00
NO10	0.42		0.00198	-0.00198	0.00
NO11	0.54		0.00162	-0.00162	0.00
NO12	0.66		0.00110	-0.00110	0.00