

**ESI for Manuscript:**

**On the energetic stability of halogen bonds involving metals: implications in  
crystal engineering**

Ismael Benito,<sup>a</sup> Rosa M. Gomila<sup>a</sup> and Antonio Frontera\*<sup>a</sup>

*Departament de Química, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5,  
07122 Palma, Spain.*

**Cartesian Coordinates**

**7**

6	1.206984	2.501141	2.986661
1	2.135651	3.083113	2.967357
6	-0.000000	3.187369	2.948119
1	-0.000000	4.266689	2.895773
6	-1.206984	2.501141	2.986661
1	-2.135651	3.083113	2.967357
8	1.365699	1.253172	3.045664
8	-1.365699	1.253172	3.045664
6	1.206984	-2.501141	2.986661
1	2.135651	-3.083113	2.967357
6	-0.000000	-3.187369	2.948119
1	-0.000000	-4.266689	2.895773
6	-1.206984	-2.501141	2.986661
1	-2.135651	-3.083113	2.967357
8	1.365699	-1.253172	3.045664
8	-1.365699	-1.253172	3.045664
6	0.000000	0.000000	-4.814305
6	-0.000000	1.199446	-4.120472
6	-0.000000	1.195523	-2.735375
6	0.000000	0.000000	-2.027503
6	-0.000000	-1.195523	-2.735375
6	-0.000000	-1.199446	-4.120472
9	0.000000	-2.351958	-2.094865
9	0.000000	-2.344990	-4.782999
9	0.000000	0.000000	-6.135859
9	0.000000	2.344990	-4.782999
9	0.000000	2.351958	-2.094865
17	0.000000	0.000000	-0.323203
28	0.000000	-0.000000	3.059294

**8**

6	-1.206425	2.496711	-3.041018
1	-2.135621	3.077528	-3.020354
6	0.000000	3.183144	-2.999670
1	0.000000	4.262221	-2.943521
6	1.206425	2.496711	-3.041018
1	2.135621	3.077528	-3.020354
8	-1.364027	1.248763	-3.104037
8	1.364027	1.248763	-3.104037
6	-1.206425	-2.496711	-3.041018

1	-2.135621	-3.077528	-3.020354
6	-0.000000	-3.183144	-2.999670
1	-0.000000	-4.262221	-2.943521
6	1.206425	-2.496711	-3.041018
1	2.135621	-3.077528	-3.020354
8	-1.364027	-1.248763	-3.104037
8	1.364027	-1.248763	-3.104037
6	0.000000	0.000000	4.861604
6	0.000000	1.199471	4.167974
6	0.000000	1.194525	2.782621
6	0.000000	0.000000	2.075754
6	-0.000000	-1.194525	2.782621
6	-0.000000	-1.199471	4.167974
35	0.000000	0.000000	0.208112
9	-0.000000	-2.354662	2.147504
9	-0.000000	-2.344825	4.831287
9	0.000000	0.000000	6.183068
9	0.000000	2.344825	4.831287
9	0.000000	2.354662	2.147504
28	0.000000	-0.000000	-3.117962

**9**

6	-1.206054	2.495472	-3.112579
1	-2.135698	3.075038	-3.090232
6	0.000000	3.181596	-3.066016
1	0.000000	4.260238	-3.003293
6	1.206054	2.495472	-3.112579
1	2.135698	3.075038	-3.090232
8	-1.363035	1.247392	-3.182463
8	1.363035	1.247392	-3.182463
6	-1.206054	-2.495472	-3.112579
1	-2.135698	-3.075038	-3.090232
6	-0.000000	-3.181596	-3.066016
1	-0.000000	-4.260238	-3.003293
6	1.206054	-2.495472	-3.112579
1	2.135698	-3.075038	-3.090232
8	-1.363035	-1.247392	-3.182463
8	1.363035	-1.247392	-3.182463
6	0.000000	0.000000	4.973075
6	0.000000	1.199254	4.279264
6	0.000000	1.191457	2.893899
6	0.000000	0.000000	2.183270
6	-0.000000	-1.191457	2.893899
6	-0.000000	-1.199254	4.279264
9	0.000000	-2.357147	2.264407
9	0.000000	-2.344744	4.943653
9	0.000000	0.000000	6.294738
9	0.000000	2.344744	4.943653
9	0.000000	2.357147	2.264407
53	0.000000	0.000000	0.108365
28	0.000000	0.000000	-3.194881

**10**

6	1.228983	2.582948	2.746108
1	2.128677	3.208989	2.726316
6	-0.000000	3.234549	2.713441
1	-0.000000	4.314939	2.667399
6	-1.228983	2.582948	2.746108
1	-2.128677	3.208989	2.726316
8	1.458552	1.346506	2.798342
8	-1.458552	1.346506	2.798342

6	1.228983	-2.582948	2.746108
1	2.128677	-3.208989	2.726316
6	-0.000000	-3.234549	2.713441
1	-0.000000	-4.314939	2.667399
6	-1.228983	-2.582948	2.746108
1	-2.128677	-3.208989	2.726316
8	1.458552	-1.346506	2.798342
8	-1.458552	-1.346506	2.798342
6	0.000000	0.000000	-5.076991
6	0.000000	1.199404	-4.383109
6	0.000000	1.195293	-2.998022
6	0.000000	0.000000	-2.289853
6	-0.000000	-1.195293	-2.998022
6	-0.000000	-1.199404	-4.383109
9	0.000000	-2.352045	-2.357662
9	0.000000	-2.345037	-5.045687
9	0.000000	0.000000	-6.398655
9	0.000000	2.345037	-5.045687
9	0.000000	2.352045	-2.357662
46	-0.000000	0.000000	2.811059
17	0.000000	0.000000	-0.584751

**11**

6	1.228884	2.581999	2.851035
1	2.128747	3.207493	2.829116
6	0.000000	3.233286	2.815339
1	0.000000	4.313420	2.764038
6	-1.228884	2.581999	2.851035
1	-2.128747	3.207493	2.829116
8	1.458414	1.345521	2.908573
8	-1.458414	1.345521	2.908573
6	1.228884	-2.581999	2.851035
1	2.128747	-3.207493	2.829116
6	-0.000000	-3.233286	2.815339
1	-0.000000	-4.313420	2.764038
6	-1.228884	-2.581999	2.851035
1	-2.128747	-3.207493	2.829116
8	1.458414	-1.345521	2.908573
8	-1.458414	-1.345521	2.908573
6	0.000000	0.000000	-5.146279
6	0.000000	1.199429	-4.452577
6	0.000000	1.194251	-3.067227
6	0.000000	0.000000	-2.359998
6	-0.000000	-1.194251	-3.067227
6	-0.000000	-1.199429	-4.452577
35	0.000000	0.000000	-0.491387
9	0.000000	-2.354726	-2.432318
9	0.000000	-2.344863	-5.115914
9	0.000000	0.000000	-6.467817
9	0.000000	2.344863	-5.115914
9	0.000000	2.354726	-2.432318
46	0.000000	-0.000000	2.922273

**12**

6	-1.228521	2.581894	-2.932070
1	-2.128867	3.206218	-2.907140
6	0.000000	3.232920	-2.890174
1	0.000000	4.312518	-2.830168
6	1.228521	2.581894	-2.932070
1	2.128867	3.206218	-2.907140
8	-1.457699	1.345420	-2.998841

8	1.457699	1.345420	-2.998841
6	-1.228521	-2.581894	-2.932070
1	-2.128867	-3.206218	-2.907140
6	-0.000000	-3.232920	-2.890174
1	-0.000000	-4.312518	-2.830168
6	1.228521	-2.581894	-2.932070
1	2.128867	-3.206218	-2.907140
8	-1.457699	-1.345420	-2.998841
8	1.457699	-1.345420	-2.998841
6	0.000000	0.000000	5.240793
6	0.000000	1.199204	4.546928
6	0.000000	1.191068	3.161559
6	0.000000	0.000000	2.450535
6	-0.000000	-1.191068	3.161559
6	-0.000000	-1.199204	4.546928
9	-0.000000	-2.357194	2.532272
9	-0.000000	-2.344785	5.211425
9	0.000000	0.000000	6.562581
9	0.000000	2.344785	5.211425
9	0.000000	2.357194	2.532272
53	0.000000	0.000000	0.372898
46	0.000000	-0.000000	-3.012165

**13**

6	1.232195	2.579161	2.421225
1	2.131435	3.202563	2.407550
6	0.000000	3.223250	2.398830
1	0.000000	4.304320	2.366668
6	-1.232195	2.579161	2.421225
1	-2.131435	3.202563	2.407550
8	1.466916	1.338652	2.457409
8	-1.466916	1.338652	2.457409
6	1.232195	-2.579161	2.421225
1	2.131435	-3.202563	2.407550
6	-0.000000	-3.223250	2.398830
1	-0.000000	-4.304320	2.366668
6	-1.232195	-2.579161	2.421225
1	-2.131435	-3.202563	2.407550
8	1.466916	-1.338652	2.457409
8	-1.466916	-1.338652	2.457409
6	-0.000000	-0.000000	-5.471178
6	0.000000	1.199239	-4.777094
6	0.000000	1.194825	-3.392018
6	-0.000000	-0.000000	-2.683008
6	-0.000000	-1.194825	-3.392018
6	-0.000000	-1.199239	-4.777094
9	-0.000000	-2.352136	-2.752081
9	-0.000000	-2.345085	-5.439681
9	-0.000000	-0.000000	-6.793036
9	0.000000	2.345085	-5.439681
9	0.000000	2.352136	-2.752081
78	0.000000	0.000000	2.464911
17	-0.000000	-0.000000	-0.977387

**14**

6	1.232000	2.578759	2.516786
1	2.131454	3.201635	2.501502
6	0.000000	3.222747	2.490853
1	0.000000	4.303582	2.453270
6	-1.232000	2.578759	2.516786
1	-2.131454	3.201635	2.501502

8	1.466606	1.338274	2.558511
8	-1.466606	1.338274	2.558511
6	1.232000	-2.578759	2.516786
1	2.131454	-3.201635	2.501502
6	-0.000000	-3.222747	2.490853
1	-0.000000	-4.303582	2.453270
6	-1.232000	-2.578759	2.516786
1	-2.131454	-3.201635	2.501502
8	1.466606	-1.338274	2.558511
8	-1.466606	-1.338274	2.558511
6	0.000000	0.000000	-5.497818
6	0.000000	1.199252	-4.803964
6	0.000000	1.193629	-3.418621
6	0.000000	0.000000	-2.710594
6	-0.000000	-1.193629	-3.418621
6	-0.000000	-1.199252	-4.803964
35	0.000000	0.000000	-0.838883
9	0.000000	-2.354831	-2.784104
9	0.000000	-2.344928	-5.467555
9	0.000000	0.000000	-6.819689
9	0.000000	2.344928	-5.467555
9	0.000000	2.354831	-2.784104
78	0.000000	-0.000000	2.565532

**15**

6	1.231696	2.578994	2.582183
1	2.131494	3.200899	2.564902
6	0.000000	3.222523	2.549275
1	0.000000	4.302904	2.502370
6	-1.231696	2.578994	2.582183
1	-2.131494	3.200899	2.564902
8	1.466386	1.338435	2.633525
8	-1.466386	1.338435	2.633525
6	1.231696	-2.578994	2.582183
1	2.131494	-3.200899	2.564902
6	-0.000000	-3.222523	2.549275
1	-0.000000	-4.302904	2.502370
6	-1.231696	-2.578994	2.582183
1	-2.131494	-3.200899	2.564902
8	1.466386	-1.338435	2.633525
8	-1.466386	-1.338435	2.633525
6	0.000000	0.000000	-5.550010
6	0.000000	1.199018	-4.855959
6	0.000000	1.189908	-3.470577
6	0.000000	0.000000	-2.758471
6	-0.000000	-1.189908	-3.470577
6	-0.000000	-1.199018	-4.855959
9	0.000000	-2.357333	-2.841718
9	0.000000	-2.344960	-5.520939
9	0.000000	0.000000	-6.872326
9	0.000000	2.344960	-5.520939
9	0.000000	2.357333	-2.841718
53	0.000000	0.000000	-0.672233
78	0.000000	-0.000000	2.636866