

Supporting Information

Halogen Bonding versus Chalcogen and Pnicogen Bonding: A Combined Cambridge Structural Database and Theoretical Study

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Cartesian Coordinates

1.

C	-0.0664035	-0.0940528	0.0000000
F	-0.8472007	-0.1076629	1.0907062
F	0.6948415	-1.1984609	0.0000000
F	-0.8472007	-0.1076629	-1.0907062
Br	1.0659635	1.5078395	0.0000000

2.

C	-0.0899797	-0.1275799	0.0000000
F	-0.8742222	-0.1453648	1.0913272
F	0.6684022	-1.2370063	0.0000000
F	-0.8742222	-0.1453648	-1.0913272
I	1.1700220	1.6553159	0.0000000

3.

Se	-0.0176009	1.1115305	-0.8182690
C	1.4844190	0.1223806	0.0569444
C	-1.4854364	-0.0489201	-0.1110509
F	-1.5430415	-0.0553057	1.2348354
F	-1.3874471	-1.3272302	-0.5248330
F	-2.6401804	0.4688176	-0.5886330
F	1.3993619	0.1240157	1.4013018
F	1.5701009	-1.1597557	-0.3479663
F	2.6198245	0.7644674	-0.3023296

4.

C	1.5980388	0.1137857	0.0601515
C	-1.5983096	-0.0535826	-0.1042765

Te	-0.0173599	1.2584112	-0.9301741
F	-1.6509961	-0.0211174	1.2441994
F	-1.4540932	-1.3429186	-0.4767622
F	-2.7845482	0.3971018	-0.5848534
F	1.4879395	0.1152031	1.4055918
F	1.6454606	-1.1729937	-0.3440842
F	2.7738680	0.7061105	-0.2697923

5.

C	0.0000000	0.0000000	0.0477071
Se	0.0000000	0.0000000	-1.7108672
F	1.0696719	0.0000000	0.8315801
F	-1.0696719	0.0000000	0.8315801

6.

C	-0.0525132	-0.0910170	0.0000000
F	-1.3704937	-0.2327041	0.0000000
F	0.4848818	-1.3031150	0.0000000
Te	0.9381250	1.6268361	0.0000000

7.

Cl	0.9759942	1.6904715	-0.2558314
Cl	0.9759942	-1.6904715	-0.2558314
Cl	-1.9519884	0.0000000	-0.2558314
As	0.0000000	0.0000000	0.7674938

8.

Cl	1.0353180	1.7932233	-0.2874464
Cl	1.0353180	-1.7932233	-0.2874464
Cl	-2.0706359	0.0000000	-0.2874464
Sb	0.0000000	0.0000000	0.8623390

9.

N	0.0000000	0.0000000	0.9436404
C	-0.6996456	1.2118218	1.3621992
H	-0.1806081	2.0928901	0.9609432
H	-1.7221919	1.2028562	0.9609432
H	-0.7544178	1.3066900	2.4674659
C	-0.6996456	-1.2118218	1.3621992

H	-1.7221919	-1.2028562	0.9609432
H	-0.1806081	-2.0928901	0.9609432
H	-0.7544178	-1.3066900	2.4674659
C	1.3992913	0.0000000	1.3621992
H	1.9028000	-0.8900338	0.9609432
H	1.9028000	0.8900338	0.9609432
H	1.5088356	0.0000000	2.4674659
C	0.0000000	0.0000000	-3.7489389
F	0.6308586	-1.0926791	-4.2291423
F	0.6308586	1.0926791	-4.2291423
F	-1.2617172	0.0000000	-4.2291423
Br	0.0000000	0.0000000	-1.7619293

10.

N	0.0000000	0.0000000	1.0048713
C	-0.7001995	1.2127811	1.4342791
H	-0.1819620	2.0953997	1.0366254
H	-1.7236883	1.2052836	1.0366254
H	-0.7475600	1.2948119	2.5393688
C	-0.7001995	-1.2127811	1.4342791
H	-1.7236883	-1.2052836	1.0366254
H	-0.1819620	-2.0953997	1.0366254
H	-0.7475600	-1.2948119	2.5393688
C	1.4003990	0.0000000	1.4342791
H	1.9056504	-0.8901161	1.0366254
H	1.9056504	0.8901161	1.0366254
H	1.4951200	0.0000000	2.5393688
C	0.0000000	0.0000000	-3.9771352
F	0.6313790	-1.0935805	-4.4691165
F	0.6313790	1.0935805	-4.4691165
F	-1.2627580	0.0000000	-4.4691165
I	0.0000000	0.0000000	-1.7610829

11.

N	-1.5646484	0.0570499	0.0000000
C	-2.0052119	1.4455761	0.0000000
H	-1.6135176	1.9588046	0.8897145
H	-1.6135176	1.9588046	-0.8897145
H	-3.1134653	1.5481019	0.0000000
C	-1.9727901	-0.6479660	-1.2077402
H	-1.5889010	-0.1212526	-2.0932819
H	-1.5524723	-1.6637601	-1.2040445
H	-3.0782148	-0.7306192	-1.3078848
C	-1.9727901	-0.6479660	1.2077402

H	-1.5524723	-1.6637601	1.2040445
H	-1.5889010	-0.1212526	2.0932819
H	-3.0782148	-0.7306192	1.3078848
C	2.8763680	-0.0703236	-1.4817026
F	3.6516654	-1.1741330	-1.4751772
F	3.6938651	1.0029658	-1.4855328
F	2.1621751	-0.0621575	-2.6360648
C	2.8763680	-0.0703236	1.4817026
F	2.1621751	-0.0621575	2.6360648
F	3.6938651	1.0029658	1.4855328
F	3.6516654	-1.1741330	1.4751772
Se	1.5269699	-0.0338446	0.0000000

12.

N	-1.6402506	0.0565458	0.0000000
C	-2.0879312	1.4457116	0.0000000
H	-1.6983617	1.9602201	0.8895787
H	-1.6983617	1.9602201	-0.8895787
H	-3.1957072	1.5383747	0.0000000
C	-2.0539281	-0.6495736	-1.2084095
H	-1.6721875	-0.1233585	-2.0952361
H	-1.6360447	-1.6661622	-1.2047330
H	-3.1589398	-0.7272932	-1.3019203
C	-2.0539281	-0.6495736	1.2084095
H	-1.6360447	-1.6661622	1.2047330
H	-1.6721875	-0.1233585	2.0952361
H	-3.1589398	-0.7272932	1.3019203
C	3.0041046	-0.0693446	-1.6018974
F	3.7610665	-1.1892340	-1.5834410
F	3.8455082	0.9889491	-1.5678023
F	2.3412498	-0.0352524	-2.7927556
C	3.0041046	-0.0693446	1.6018974
F	2.3412498	-0.0352524	2.7927556
F	3.8455082	0.9889491	1.5678023
F	3.7610665	-1.1892340	1.5834410
Te	1.4589544	-0.0185337	0.0000000

13.

C	-2.1173356	-0.0186665	0.0000000
F	-2.9090190	-0.0068075	1.0696786
F	-2.9090190	-0.0068075	-1.0696786
N	2.5742279	0.0358345	0.0000000
C	3.0262104	0.7132103	1.2092457
H	2.6708925	1.7531853	1.2055217

H	2.6053988	0.2120620	2.0921580
H	4.1344784	0.7240353	1.3069331
C	3.0262104	0.7132103	-1.2092457
H	2.6053988	0.2120620	-2.0921580
H	2.6708925	1.7531853	-1.2055217
H	4.1344784	0.7240353	-1.3069331
C	2.9308546	-1.3774941	0.0000000
H	2.5088320	-1.8648104	0.8905010
H	2.5088320	-1.8648104	-0.8905010
H	4.0307307	-1.5447171	0.0000000
Se	-0.3422017	-0.0275468	0.0000000

14.

C	-4.1442250	-0.0961888	0.0000000
F	-4.9349257	-0.0925090	1.0697674
F	-4.9349257	-0.0925090	-1.0697674
N	0.7694274	0.0277887	0.0000000
C	1.2015420	0.7254869	1.2103486
H	0.8071747	1.7508299	1.2060162
H	0.8030450	0.2096776	2.0945302
H	2.3078651	0.7747456	1.2966735
C	1.2015420	0.7254869	-1.2103486
H	0.8030450	0.2096776	-2.0945302
H	0.8071747	1.7508299	-1.2060162
H	2.3078651	0.7747456	-1.2966735
C	1.2029472	-1.3684292	0.0000000
H	0.8086108	-1.8768352	0.8909512
H	0.8086108	-1.8768352	-0.8909512
H	2.3092889	-1.4680445	0.0000000
Te	-2.1240623	-0.0779181	0.0000000

15.

N	0.0000000	0.0000000	0.5503088
C	-0.6981604	1.2092493	0.9758448
H	-0.1809320	2.0955583	0.5821292
H	-1.7243407	1.2044709	0.5821292
H	-0.7519621	1.3024366	2.0827383
C	-0.6981604	-1.2092493	0.9758448
H	-1.7243407	-1.2044709	0.5821292
H	-0.1809320	-2.0955583	0.5821292
H	-0.7519621	-1.3024366	2.0827383
C	1.3963208	0.0000000	0.9758448
H	1.9052727	-0.8910874	0.5821292
H	1.9052727	0.8910874	0.5821292

H	1.5039242	0.0000000	2.0827383
As	0.0000000	0.0000000	-2.5334850
Cl	0.9888846	-1.7127983	-3.5617827
Cl	0.9888846	1.7127983	-3.5617827
Cl	-1.9777691	0.0000000	-3.5617827

16.

N	0.0000000	0.0000000	0.5926167
C	-0.6978868	1.2087754	1.0274105
H	-0.1816915	2.0975878	0.6378050
H	-1.7257186	1.2061434	0.6378050
H	-0.7475775	1.2948423	2.1343343
C	-0.6978868	-1.2087754	1.0274105
H	-1.7257186	-1.2061434	0.6378050
H	-0.1816915	-2.0975878	0.6378050
H	-0.7475775	-1.2948423	2.1343343
C	1.3957736	0.0000000	1.0274105
H	1.9074101	-0.8914445	0.6378050
H	1.9074101	0.8914445	0.6378050
H	1.4951550	0.0000000	2.1343343
Cl	1.0499141	-1.8185046	-3.7631712
Cl	1.0499141	1.8185046	-3.7631712
Cl	-2.0998282	0.0000000	-3.7631712
Sb	0.0000000	0.0000000	-2.6151673

17.

C	0.6993523	-1.2113137	-1.5295769
C	1.3986617	0.0000000	-1.5295375
C	0.6993523	1.2113137	-1.5295769
C	-0.6993309	1.2112766	-1.5295375
C	-1.3987046	0.0000000	-1.5295769
C	-0.6993309	-1.2112766	-1.5295375
H	1.2447605	-2.1559884	-1.5215436
H	2.4894829	0.0000000	-1.5213996
H	1.2447605	2.1559884	-1.5215436
H	-1.2447414	2.1559554	-1.5213996
H	-2.4895210	0.0000000	-1.5215436
H	-1.2447414	-2.1559554	-1.5213996
Br	0.0000000	0.0000000	1.8160759
C	0.0000000	0.0000000	3.7701698
F	1.2600798	0.0000000	4.2399756
F	-0.6300399	-1.0912611	4.2399756
F	-0.6300399	1.0912611	4.2399756

18.

C	0.6994916	-1.2115550	-1.6250716
C	1.3990123	0.0000000	-1.6237708
C	0.6994916	1.2115550	-1.6250716
C	-0.6995062	1.2115802	-1.6237708
C	-1.3989832	0.0000000	-1.6250716
C	-0.6995062	-1.2115802	-1.6237708
H	1.2448515	-2.1561460	-1.6155657
H	2.4897462	0.0000000	-1.6144064
H	1.2448515	2.1561460	-1.6155657
H	-1.2448731	2.1561835	-1.6144064
H	-2.4897030	0.0000000	-1.6155657
H	-1.2448731	-2.1561835	-1.6144064
C	0.0000000	0.0000000	4.0367616
F	1.2607656	0.0000000	4.5132928
F	-0.6303828	-1.0918551	4.5132928
F	-0.6303828	1.0918551	4.5132928
I	0.0000000	0.0000000	1.8598032

19.

Se	0.0000000	0.0000000	1.2903568
C	0.0000000	1.4857554	2.6244299
C	0.0000000	-1.4857554	2.6244299
F	-1.0882829	-1.4861432	3.4216764
F	1.0882829	-1.4861432	3.4216764
F	0.0000000	-2.6350774	1.9052038
F	-1.0882829	1.4861432	3.4216764
F	1.0882829	1.4861432	3.4216764
F	0.0000000	2.6350774	1.9052038
C	1.2118438	-0.6987500	-2.0081570
C	1.2118438	0.6987500	-2.0081570
C	0.0000000	1.3978363	-2.0059114
C	-1.2118438	0.6987500	-2.0081570
C	-1.2118438	-0.6987500	-2.0081570
C	0.0000000	-1.3978363	-2.0059114
H	2.1562897	-1.2444090	-1.9980125
H	2.1562897	1.2444090	-1.9980125
H	0.0000000	2.4886228	-1.9999143
H	-2.1562897	1.2444090	-1.9980125
H	-2.1562897	-1.2444090	-1.9980125
H	0.0000000	-2.4886228	-1.9999143

20.

C	0.0000000	1.6069652	2.8214960
C	0.0000000	-1.6069652	2.8214960
F	-1.0893653	-1.5856124	3.6215713
F	1.0893653	-1.5856124	3.6215713
F	0.0000000	-2.7889879	2.1463248
F	-1.0893653	1.5856124	3.6215713
F	1.0893653	1.5856124	3.6215713
F	0.0000000	2.7889879	2.1463248
C	1.2123514	-0.6988573	-2.1492231
C	1.2123514	0.6988573	-2.1492231
C	0.0000000	1.3980589	-2.1440080
C	-1.2123514	0.6988573	-2.1492231
C	-1.2123514	-0.6988573	-2.1492231
C	0.0000000	-1.3980589	-2.1440080
H	2.1567146	-1.2445866	-2.1412133
H	2.1567146	1.2445866	-2.1412133
H	0.0000000	2.4889001	-2.1364265
H	-2.1567146	1.2445866	-2.1412133
H	-2.1567146	-1.2445866	-2.1412133
H	0.0000000	-2.4889001	-2.1364265
Te	0.0000000	0.0000000	1.3006883

21.

C	-2.1173356	-0.0186665	0.0000000
F	-2.9090190	-0.0068075	1.0696786
F	-2.9090190	-0.0068075	-1.0696786
N	2.5742279	0.0358345	0.0000000
C	3.0262104	0.7132103	1.2092457
H	2.6708925	1.7531853	1.2055217
H	2.6053988	0.2120620	2.0921580
H	4.1344784	0.7240353	1.3069331
C	3.0262104	0.7132103	-1.2092457
H	2.6053988	0.2120620	-2.0921580
H	2.6708925	1.7531853	-1.2055217
H	4.1344784	0.7240353	-1.3069331
C	2.9308546	-1.3774941	0.0000000
H	2.5088320	-1.8648104	0.8905010
H	2.5088320	-1.8648104	-0.8905010
H	4.0307307	-1.5447171	0.0000000
Se	-0.3422017	-0.0275468	0.0000000

22.

C	-4.1442250	-0.0961888	0.0000000
F	-4.9349257	-0.0925090	1.0697674
F	-4.9349257	-0.0925090	-1.0697674
N	0.7694274	0.0277887	0.0000000
C	1.2015420	0.7254869	1.2103486
H	0.8071747	1.7508299	1.2060162
H	0.8030450	0.2096776	2.0945302
H	2.3078651	0.7747456	1.2966735
C	1.2015420	0.7254869	-1.2103486
H	0.8030450	0.2096776	-2.0945302
H	0.8071747	1.7508299	-1.2060162
H	2.3078651	0.7747456	-1.2966735
C	1.2029472	-1.3684292	0.0000000
H	0.8086108	-1.8768352	0.8909512
H	0.8086108	-1.8768352	-0.8909512
H	2.3092889	-1.4680445	0.0000000
Te	-2.1240623	-0.0779181	0.0000000

23.

As	0.0000000	0.0000000	2.2108352
Cl	0.9782933	1.6944538	3.2523150
Cl	0.9782933	-1.6944538	3.2523150
Cl	-1.9565867	0.0000000	3.2523150
C	-0.0002072	1.3990489	-0.9995218
C	-1.2115083	0.6997039	-0.9995218
C	-1.2115083	-0.6997039	-0.9995218
C	-0.0002072	-1.3990489	-0.9995218
C	1.2117155	-0.6993450	-0.9995218
C	1.2117155	0.6993450	-0.9995218
H	0.0001895	2.4897913	-0.9951082
H	-2.1563172	1.2447316	-0.9951082
H	-2.1563172	-1.2447316	-0.9951082
H	0.0001895	-2.4897913	-0.9951082
H	2.1561278	-1.2450597	-0.9951082
H	2.1561278	1.2450597	-0.9951082

24.

Cl	1.0354838	1.7935106	3.5383034
Cl	1.0354838	-1.7935106	3.5383034
Cl	-2.0709677	0.0000000	3.5383034
C	-0.0001472	1.3992964	-1.0815990
C	-1.2117526	0.6997757	-1.0815990

C	-1.2117526	-0.6997757	-1.0815990
C	-0.0001472	-1.3992964	-1.0815990
C	1.2118999	-0.6995207	-1.0815990
C	1.2118999	0.6995207	-1.0815990
H	0.0002093	2.4900869	-1.0816997
H	-2.1565832	1.2448622	-1.0816997
H	-2.1565832	-1.2448622	-1.0816997
H	0.0002093	-2.4900869	-1.0816997
H	2.1563739	-1.2452248	-1.0816997
H	2.1563739	1.2452248	-1.0816997
Sb	0.0000000	0.0000000	2.3648823