Supplementary Information for

A Cartography of the Van der Waals Territories

Santiago Alvarez

Departament de Química Inorgànica and Institut de Química Teòrica i Computacional, Universitat de Barcelona, Martí i Franquès 1-11, 08028 Barcelona, Spain.

Contents

Table S1. Main search results and characteristics of the histograms presented in Figures 4-7 from which van der Waals radii have been deduced. Probe elements other than oxygen are indicated in parentheses; n(k) is the number of atom pairs for the bin corresponding to the maximum of the van der Waals peak; d(vdW) is the element-probe distance that marks the half height of the van der Waals peak; the version of the CSD used for the data retrieval (including the number of updates) is given in the CSD column (for those elements for which only a single structure from the ICSD database could be used to get an estimate of the van der Waals radii, the collection code is given in that column); "contacts" indicates the total number of element-probe atom pairs for which intermolecular distances were obtained and plotted in the histogram, whereas "bonds" gives the number of bonding distances included in the bond peaks provided in the histograms for comparison.

Z	Elem.	n(k)	Bin width	d(vdW)	r(vdW)	Contacts	CSD	Bonds
1	H	231	0.10	2.40	1.20	9888	5.33 + 3 up.	55
2	He	6	0.05	2.93	1.43	12	72020 icsd	
3	Li	218	0.15	3.62	2.12	11067	5.33 + 4 up.	12848
4	Be	101	0.10	3.48	1.98	3515	5.34 + 1 up.	863
5	B	1589	0.10	3.41	1.91	152194	5.33 + 2 up.	9457
6	C	6419	0.05	3.27	1.77	385475	5.33 + 2 up.	20976
7	N (N)	7236	0.08	3.32	1.66	187967	5.33 + 2 up.	47564
8	O	7824	0.05	3.00	**1.50**	420207	5.33 + 2 up.	1853
9	F	6945	0.10	2.96	1.46	497497	5.33 + 3 up.	0
10	Ne				1.58	12	43427 icsd	
11	Na	330	0.10	4.00	2.50	16016	5.34 + 1 up.	10909
12	Mg	522	0.10	4.01	2.51	11581	5.33 + 4 up.	4094
13	Al	168	0.10	3.75	2.25	9877	5.33 + 2 up.	7391
14	Si	602	0.10	3.69	2.19	15077	5.33 + 3 up.	17409
15	P	1708	0.10	3.40	1.90	178077	5.33 + 3 up.	38845
16	S	3918	0.05	3.39	1.89	741158	5.33 + 2 up.	16721
17	Cl	9496	0.10	3.32	1.82	641448	5.33 + 4 up.	15062
18	Ar(C)	10	0.10	3.60	1.83	527	5.33 + 2 up.	117
19	K	1664	0.10	4.23	2.73	76013	5.34 + 1 up.	11682
20	Ca	278	0.15	4.12	2.62	5420	5.33 + 4 up.	2595
21	Sc	60	0.15	4.08	2.58	1287	5.33 + 2 up.	876
22	Ti	133	0.12	3.96	2.46	6685	5.33 + 3 up.	4773
23	V	198	0.10	3.92	2.42	17485	5.33 + 2 up.	21643
24	Cr	1386	0.10	3.95	2.45	60314	5.33 + 2 up.	6554
25	Mn	2118	0.10	3.95	2.45	81976	5.33 + 2 up.	17565
26	Fe	3859	0.10	3.94	2.44	207868	5.33 + 2 up.	18332
27	Co	4755	0.10	3.90	2.40	186046	5.33 + 2 up.	22165
28	Ni	2852	0.10	3.90	2.40	115164	5.33 + 2 up.	24402
29	Cu_cn6	1247	0.10	3.88	2.38	42451	5.33 + 2 up.	14639
30	Zn	1703	0.10	3.89	2.39	68186	5.33 + 2 up.	19306
31	Ga	69	0.10	3.82	2.32	6066	5.33 + 2 up.	1817
32	Ge	88	0.10	3.79	2.29	13207	5.33 + 2 up.	1660
33	As	169	0.10	3.38	1.88	22962	5.33 + 2 up.	2796
34	Se	401	0.10	3.32	1.82	36624	5.33 + 2 up.	340
35	Br	2756	0.10	3.36	1.86	172324	5.33 + 3 up.	22
36	Kr	18	0.15	3.75	2.25	131	5.33 + 2 up.	0
37	Rb	124	0.20	4.71	3.21	1960	5.33 + 4 up.	1110
38	Sr	98	0.15	4.34	2.84	2094	5.33 + 4 up.	3119
39	Y	180	0.15	4.25	2.75	3487	5.33 + 2 up.	2977
40	Zr	120	0.15	4.02	2.52	5523	5.34 + 1 up.	4529
41	Nb	65	0.15	4.06	2.56	3647	5.34 + 1 up.	1979
42	Mo	2409	0.10	3.95	2.45	138249	5.33 + 2 up.	47291
43	Tc	91	0.15	3.94	2.44	2880	5.33 + 2 up.	341
44	Ru	2811	0.10	3.96	2.46	165471	5.33 + 2 up.	6425
45	Rh	506	0.10	3.94	2.44	34854	5.33 + 2 up.	3890
46	Pd	806	0.15	3.65	2.15	35830	5.34 + 1 up.	4218
47	Ag	890	0.15	4.03	2.53	27221	5.33 + 3 up.	2426
48	Cd	538	0.10	3.99	2.49	21952	5.33 + 2 up.	17588
49	In	118	0.15	3.93	2.43	5230	5.34 + 1 up.	2237

50	Sn	591	0.15	3.92	2.42	30075	5.34 + 1 up.	10196
51	Sb	441	0.15	3.97	2.47	15850	5.34 + 1 up.	2625
52	Te	291	0.15	3.49	1.99	13772	5.33 + 2 up.	602
53	I	1373	0.15	3.54	2.04	56317	5.33 + 2 up.	396
54	Xe (C)	135	0.20	3.83	2.06	2264	5.34 + 1 up.	15
55	Cs	42	0.15	4.98	3.48	775	5.34 + 1 up.	2482
56	Ba	118	0.20	4.53	3.03	2402	5.33 + 2 up.	3778
57	La	251	0.10	4.48	2.98	6471	5.33 + 4 up.	4014
58	Ce	130	0.10	4.38	2.88	3681	5.33 + 4 up.	2604
59	Pr	168	0.15	4.42	2.92	3360	5.33 + 2 up.	2067
60	Nd	260	0.10	4.45	2.95	6346	5.33 + 2 up.	4212
62	Sm	173	0.10	4.40	2.90	4162	5.33 + 2 up.	3236
63	Eu	295	0.10	4.37	2.87	7042	5.33 + 2 up.	4804
64	Gd	267	0.10	4.33	2.83	6682	5.33 + 2 up.	7136
65	Tb	202	0.10	4.29	2.79	5538	5.34 + 1 up.	4969
66	Dy	164	0.10	4.37	2.87	3615	5.33 + 2 up.	3927
67	Ho	115	0.10	4.31	2.81	2493	5.33 + 2 up.	1993
68	Er	193	0.10	4.33	2.83	4246	5.33 + 2 up.	4361
69	Tm	75	0.15	4.29	2.79	1141	5.33 + 2 up.	558
70	Yb	178	0.10	4.30	2.80	4664	5.33 + 2 up.	3255
71	Lu	111	0.15	4.24	2.74	2018	5.33 + 2 up.	1163
72	Hf	57	0.10	4.13	2.63	936	5.33 + 2 up.	910
73	Ta	43	0.20	4.03	2.53	2793	5.34 + 1 up.	1584
74	W	1131	0.10	4.07	2.57	47936	5.33 + 2 up.	28376
75	Re	1481	0.10	3.99	2.49	61593	5.33 + 2 up.	3727
76	Os	1339	0.05	3.98	2.48	129040	5.33 + 2 up.	1239
77	Ir	358	0.15	3.91	2.41	18335	5.33 + 2 up.	1229
78	Pt	1162	0.10	3.79	2.29	55873	5.33 + 2 up.	3515
79	Au	180	0.20	3.82	2.32	5132	5.33 + 3 up.	262
80	Hg	821	0.15	3.95	2.45	30628	5.33 + 4 up.	1594
81	Tl	48	0.20	3.97	2.47	3486	5.33 + 4 up.	855
82	Pb	1653	0.20	4.10	2.60	36781	5.34 + 2 up.	2379
83	Bi	464	0.20	4.04	2.54	14030	5.34 + 2 up.	2232
89	Ac	6	0.50	4.63	2.8	33	31569 icsd	
90	Th	76	0.20	4.43	2.93	964	5.33 + 2 up.	738
91	Pa (C)	5	0.30	4.65	2.88	48	5.33 + 2 up.	1
92	U	891	0.10	4.21	2.71	35070	5.33 + 3 up.	5247
93	Np	48	0.20	4.32	2.82	830	5.34 + 1 up.	380
94	Pu	70	0.15	4.31	2.81	1299	5.32 + 3 up.	179
95	Am	14	0.25	4.33	2.83	128	5.33 + 2 up.	39
96	Cm	20	0.10	4.55	3.05	90	5.33 + 2 up.	4
97	Bk (Cl)	18	0.50	5.20	3.38		icsd 23165	6
98	Cf	3	0.10	4.55	3.05	14	5.33 + 2 up.	2

Table S2. Fitting parameters for the histograms of Figures 4-7 to equation 1. Probe elements other than oxygen are indicated in parentheses.

Z	Symbol	a	σ	d_{max}	b	thresh	ρ_{vdW} (%)
1	H	92.1	0.28	2.68	34.60	1.42	66.0
3	Li	108.7	0.28	4.03	19.25	2.67	76.3
4	Be	63.6	0.27	3.76	5.04	2.50	90.2
5	B	804.9	0.28	3.79	256.05	2.54	69.8
6	C	3254.4	0.25	3.58	675.15	2.39	82.2
7	N (N)	2986.5	0.32	3.74	477.97	1.82	52.3
8	O	3888.7	0.27	3.35	231.26	1.26	72.9
9	F	3182.4	0.27	3.34	798.46	1.90	66.4
11	Na	125.9	0.36	4.42	8.23	1.88	50.7
12	Mg	196.6	0.17	4.25	14.87	2.81	91.5
13	Al	44.4	0.13	3.99	6.76	2.13	75.2
14	Si	208.5	0.25	3.98	266.89	2.98	54.9
15	P	255.0	0.09	3.57	797.40	2.67	67.1
16	S	1659.1	0.31	3.71	701.68	2.42	58.3
17	Cl	5131.6	0.31	3.72	801.64	2.18	69.2
18	Ar(C)	3.1	0.13	3.80	1.71	3.06	93.1
19	K	265.5	0.27	4.69	23.82	1.20	28.3
20	Ca	130.5	0.25	4.51	6.44	2.42	78.3
21	Sc	26.1	0.18	4.36	3.50	3.27	92.8
22	Ti	14.1	0.17	4.19	17.39	2.70	36.1
23	V	30.9	0.19	4.21	18.16	2.39	36.8
24	Cr	818.0	0.35	4.41	154.26	3.06	71.2
25	Mn	1054.2	0.25	4.30	129.68	2.80	79.3
26	Fe	1621.4	0.28	4.33	407.34	2.91	66.6
27	Co	2263.2	0.24	4.22	236.38	2.65	80.6
28	Ni	1184.7	0.22	4.20	94.45	2.30	76.5
29	Cu_cn6	414.4	0.26	4.24	56.25	2.67	74.6
30	Zn	622.8	0.20	4.19	53.76	2.19	74.3
31	Ga	18.0	0.14	4.01	8.28	2.85	79.7
32	Ge	14.4	0.14	4.02	29.85	2.90	50.2
33	As	36.0	0.17	3.64	25.70	2.23	53.8
34	Se	95.0	0.20	3.68	11.77	1.06	46.5
35	Br	1662.8	0.36	3.79	180.11	2.12	68.4
36	Kr	8.3	0.18	3.91	0.07	2.12	97.9
37	Rb	26.7	0.28	5.31	1.97	1.94	33.3
38	Sr	62.2	0.32	4.76	6.23	3.42	83.9
39	Y	75.3	0.17	4.57	7.82	3.13	88.6
40	Zr	34.4	0.18	4.34	8.84	2.64	64.0
41	Nb	10.3	0.13	4.33	11.84	2.94	49.8
42	Mo	1257.9	0.37	4.38	212.43	2.83	63.1
43	Tc	54.2	0.34	4.36	8.39	3.10	79.4
44	Ru	1433.9	0.28	4.34	340.97	3.05	73.1
45	Rh	164.5	0.29	4.34	32.86	2.54	54.5
46	Pd	287.0	0.34	4.08	27.67	1.76	49.2
47	Ag	570.0	0.67	4.54	20.24	1.98	50.1
48	Cd	198.1	0.28	4.38	21.13	2.70	74.2
49	In	71.7	0.34	4.38	17.67	3.31	79.8
50	Sn	117.3	0.19	4.28	39.99	2.28	43.8
51	Sb	54.4	0.25	4.31	12.19	1.59	26.1
52	Te	96.3	0.21	3.73	9.73	1.65	67.4
53	I	419.1	0.23	3.93	56.17	1.67	52.7
54	Xe (C)	114.2	0.43	4.40	0.67	1.46	86.0
55	Cs	8.6	0.21	5.40	0.99	2.69	45.6
56	Ba	42.4	0.30	4.95	7.99	3.23	58.3
57	La	91.5	0.18	4.76	8.42	2.93	79.5
58	Ce	48.5	0.19	4.66	4.51	2.91	80.6
59	Pr	57.3	0.16	4.71	5.15	2.72	77.5
60	Nd	63.2	0.18	4.69	6.81	2.99	80.8

62	Sm	38.9	0.19	4.66	5.56	3.24	83.6
63	Eu	66.8	0.17	4.63	5.90	2.73	79.7
64	Gd	77.1	0.20	4.60	6.58	2.94	83.9
65	Tb	83.1	0.19	4.59	4.88	2.58	81.3
66	Dy	48.5	0.16	4.59	3.45	2.65	82.6
67	Ho	25.2	0.15	4.53	1.45	2.37	82.2
68	Er	64.7	0.18	4.54	4.55	2.78	85.5
69	Tm	12.1	0.16	4.54	0.88	2.68	84.4
70	Yb	46.0	0.19	4.54	4.39	2.89	83.4
71	Lu	21.2	0.19	4.51	2.47	3.09	86.4
72	Hf	10.4	0.12	4.32	0.99	2.57	86.3
73	Ta	14.6	0.19	4.29	38.10	3.69	79.7
74	W	496.2	0.30	4.52	45.36	2.45	61.5
75	Re	762.6	0.32	4.41	77.72	2.81	74.9
76	Os	983.8	0.31	4.37	170.67	3.42	89.5
77	Ir	172.3	0.26	4.28	67.57	3.16	73.1
78	Pt	616.6	0.34	4.20	38.30	2.11	67.4
79	Au	22.4	0.08	4.19	2.78	0.71	49.4
80	Hg	991.2	0.67	4.57	123.79	3.54	81.3
81	Tl	39.1	0.45	4.46	16.13	3.50	71.4
82	Pb	552.3	0.27	4.63	19.77	1.14	49.0
83	Bi	106.5	0.22	4.47	15.07	1.91	43.3
90	Th	11.9	0.15	4.70	1.31	2.99	82.8
91	Pa (C)	2.2	0.23	5.06	3.82	4.65	93.8
92	U	563.2	0.37	4.64	41.90	2.91	73.9
93	Np	8.3	0.12	4.67	0.73	1.57	55.0
94	Pu	26.3	0.19	4.64	1.37	2.34	76.8
95	Am	7.1	0.19	4.69	0.80	3.60	93.5
96	Cm	3.8	0.04	4.70	0.20	3.68	99.4
98	Cf	0.5	0.04	4.69	0.13	4.69	100.0

Table S3. Data for the sample of atom pairs whose histograms are shown in Figures S1 – S7: Position of the observed peak in the histogram, sum of the corresponding van der Waals radii, number of contacts and number of bond distances analyzed and indication of the presence or absence of a van der Waals gap.

E	X	Quality	Atom pairs	peak	sum	Gap?	Bonds
Ag	Ag	dubious	8466	5.8	5.06	no	2180
Ag	Cl	poor	2849	4.0	4.35	no	512
Ag	N	v.poor	23312	4.4	4.19	no	5629
Ag	S	fair	4547	3.6	4.42	no	3903
Al	C	no	167078		4.02	yes	9291
Al	H	no	265194		3.45	yes	1445
Al	S	v.poor	1001	4.4	4.14	yes	355
As	As	fair	11440	4.0	3.76	pseudo	945
Au	Au	poor	5114	4.4	4.64	no	2127
Au	Cl	v.good	9920	4.0	4.14	yes	2091
Au	N	poor	16699	3.8	3.98	yes	1871
Au	P	v.good	4605	4.3	4.22	yes	5886
Au	S	fair	6581	4.0	4.21	pseudo	2732
B	N	no	95174		3.57	yes	24809
Ba	Ba	v.poor	161	6.2	6.06	n.a.	0
Bi	Bi	v.good	758	4.6	5.08	no	116
Bi	C	v.poor	9959	4.1	4.04	yes	1338
Bi	Cl	fair	2364	3.2	4.36	no	1919
Bi	F	fair	2772	3.4	4.00	no	23
Bi	N	v.poor	4583	5.0	4.20	pseudo	1021
Bi	S	v.poor	1385	5.2	4.43	no	1141
Br	Br	v.good	193180	4.0	3.72	yes	350
Ca	S	no	598		4.51	yes	23
Cd	Cd	poor	1365	5.4	4.98	no	35
Cl	Cl	v.good	546424	3.8	3.64	yes	16
Co	P	good	4079	5.4	4.30	yes	5255
Cu	Cl	poor	157059	4.3	4.20	pseudo	7927
Cu	Cu	good	24431	5.3	4.76	no	2541
Cu	N	poor	157050	4.3	4.04	pseudo	53589
Dy	N	v.good	1545	4.6	4.53	yes	1049
Eu	S	v.poor	334	5.2	4.76	yes	151
Fe	N	v.poor	26942	4.6	4.10	yes	27769
Ga	Cl	v.poor	4973	4.4	4.14	yes	2415
Ga	N	v.poor	7669	4.2	3.98	yes	2415
Gd	N	good	1001	4.5	4.49	yes	1260
Ge	I	v.poor	309	4.6	4.33	no	119
Hg	Cl	v.good	9378	3.2	4.27	no	2099
Hg	F	v.poor	10000	3.4	3.91	pseudo	6
Hg	Hg	v.good	7122	4.1	4.90	no	99
Hg	I	no	1628		4.49	no	1437
Hg	N	v.poor	17497	4.1	4.11	no	1885
Hg	S	v.poor	9570	4.7	4.34	no	2039
I	I	v.good	59427	4.3	4.08	no	3160
In	In	dubious	1428	4.8	4.86	no	96
Ir	Ir	v.poor	2240	5.6	4.82	pseudo	1762
K	S	v.poor	5837	5.0	4.62	no	141
La	La	poor	391	6.4	5.96	yes	70

La	N	good	2463	4.7	4.64	yes	1940
Li	Li	fair	2314	4.2	4.24	no	599
Ln	Br	no	659		4.71	yes	297
Ln	Cl	v.good	5987	5.0	4.67	yes	3193
Ln	D	no	526		4.05	yes	1010
Ln	F	v.poor	5253	4.6	4.31	yes	162
Ln	Ln	fair	5728	6.0	5.70	no	101
Ln	N	v.good	21008	4.5	4.51	yes	17616
Ln	P	no	216		4.75	yes	222
Ln	Ph	no	9409		4.62	yes	687
Ln	S	fair	1425	5.3	4.74	yes	1143
Mg	Br	fair	528	4.6	4.37	pseudo	367
Mg	Cl	good	817	4.6	4.33	yes	494
Mg	N	v.good	3815	4.1	4.17	yes	2885
Mo	Mo	fair	17683	5.2	4.90	yes	4082
Mo	N	v.good	35658	4.2	4.11	yes	8821
Na	S	no	4289		4.39	no	199
Os	Os	no	17932		4.96	yes	9523
Os	S	fair	2395	5.2	4.37	yes	1944
P	P	poor	171114	4.7	3.80	yes	3963
Pb	B	no	249		4.51	no	42
Pb	C	v.poor	40793	4.1	4.37	yes	787
Pb	Cl	good	728	4.0	4.42	no	238
Pb	F	dubious	1290	3.8	4.06	no	19
Pb	I	poor	188	4.8	4.64	no	180
Pb	K	poor	125	5.6	5.33	no	25
Pb	N	poor	564	5.1	4.26	no	1685
Pb	P	poor	456	4.0	4.50	yes	76
Pb	Pb	poor	1321	4.1	4.10	no	445
Pb	S	v.poor	1230	5.6	4.49	no	806
Pb	Si	dubious	180	5.2	4.79	yes	25
Pd	Cl	dubious	24296	4.3	3.97	yes	8411
Pd	N	v.poor	35966	4.0	3.81	yes	13476
Pd	Pd	fair	9409	4.8	4.30	no	1322
Pd	S	fair	8283	4.4	4.04	pseudo	4986
Ph	Br	good	15135	3.9	3.63	yes	11630
Ph	Cl	v.good	31256	3.8	3.59	yes	24410
Ph	I	good	6996	4.1	3.81	yes	3095
Pt	Br	v.good	2012	4.6	4.15	pseudo	949
Pt	Cl	dubious	22600	4.6	4.11	yes	6614
Pt	H	dubious	407987	3.7	3.49	yes	398
Pt	N	fair	41198	3.8	3.95	yes	11221
Pt	P	poor	3970	5.3	4.19	yes	12331
Pt	Pt	dubious	10333	4.9	4.58	no	1594
Pt	S	no	7901		4.18	yes	4915
Rb	Br	v.poor	86	5.8	5.07	no	18
Rh	Cl	poor	9309	4.3	4.26	yes	3849
Rh	Rh	v.poor	5087	5.5	4.88	no	3190
S	S	v.good	126596	3.8	3.78	yes	5353
S	Se	v.good	10000	3.7	3.71	pseudo	259
S	Te	good	3244	4.0	3.88	no	1046
Sb	Sb	poor	5536	4.8	4.94	pseudo	370

Se	Se	v.good	51247	3.8	3.64	yes	1858
Se	Te	good	396	4.1	3.81	no	193
Si	F	v.good	22553	5.1	3.65	yes	1809
Si	N	v.good	46313	3.8	3.85	yes	18620
Sn	N	fair	20190	4.6	4.08	yes	5685
Sn	S	poor		4.6	4.31	no	3594
Sn	Sn	v.poor	9534	4.9	4.84	no	999
Sr	Cl	good	216	5.4	4.66	yes	2
Te	Te	good	9050	4.1	3.98	pseudo	576
Th	Th	good	155	6.4	5.86	yes	4
Tl	C	v.poor	46876	5.0	4.24	pseudo	398
Tl	Cl	v.good	1037	3.4	4.29	no	191
Tl	F	no	1387		3.93	no	13
Tl	N	v.poor	3560	4.6	4.13	no	914
Tl	Tl	fair	1457	4.0	3.97	no	43
U	F	v.poor	870	5.2	4.17	yes	179
U	N	fair	7374	4.6	4.37	yes	3174
Zn	Zn	v.poor	7196	5.6	4.78	no	70

Figure S1.- Chalcogen···Chalcogen Contacts

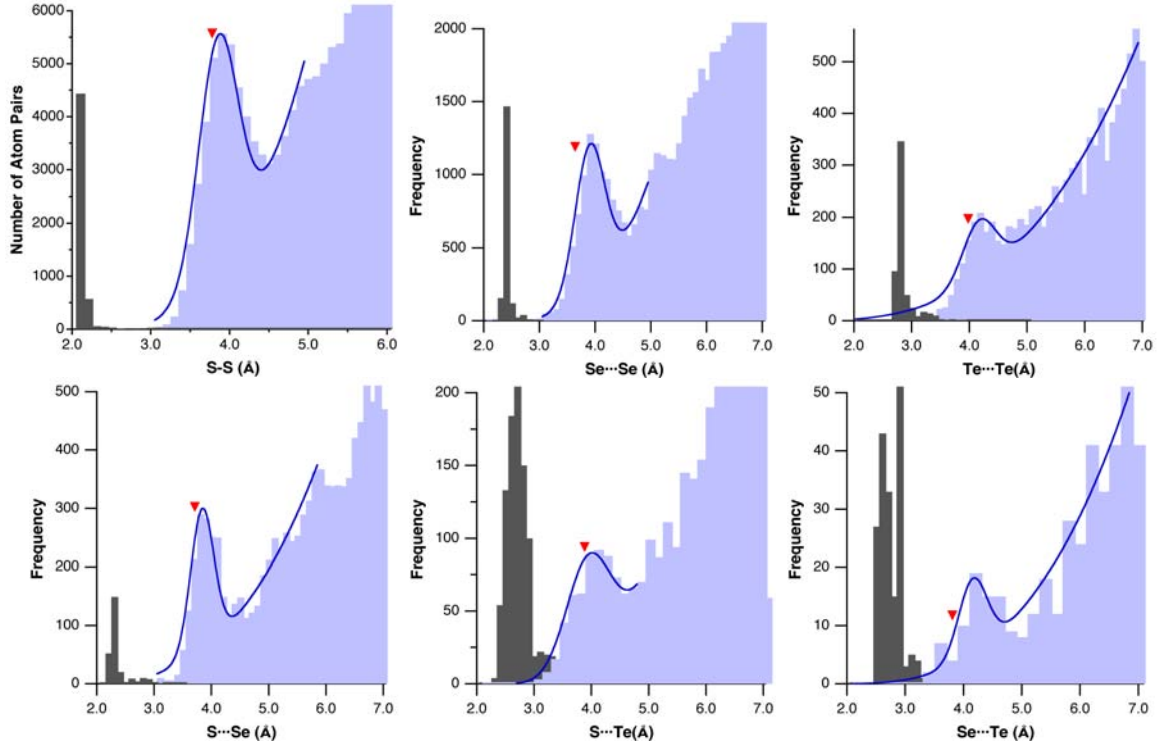
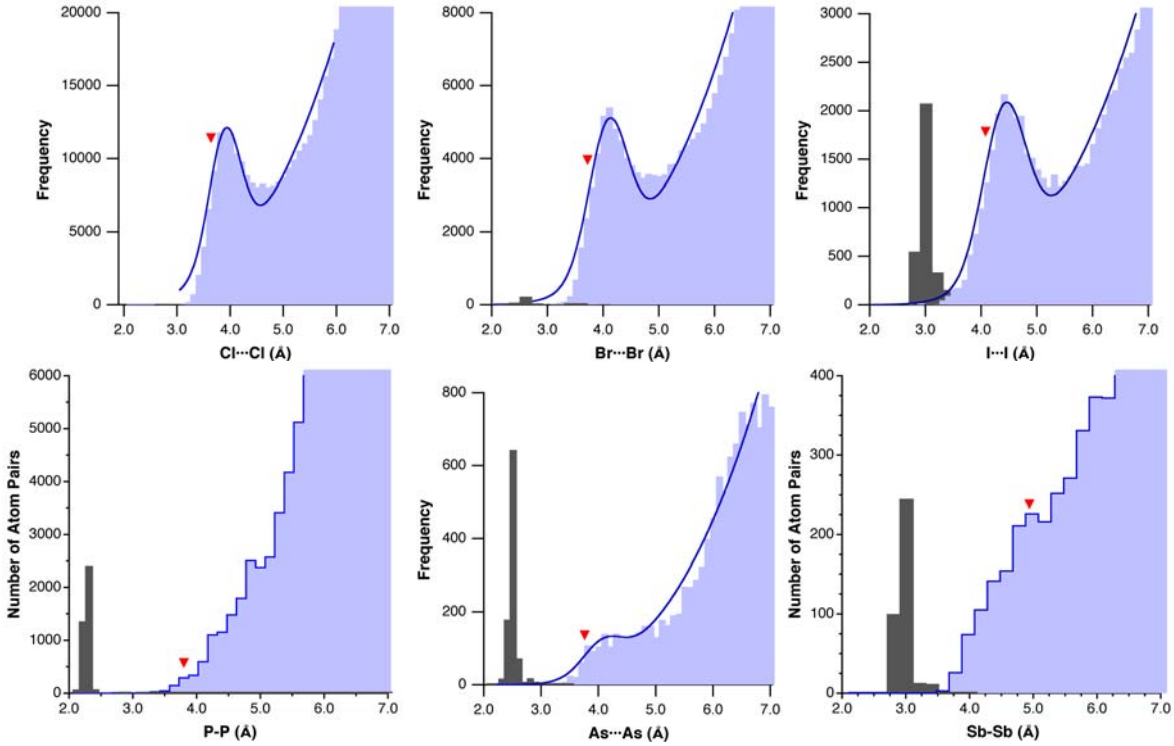


Figure S2.- E···E Contacts

For Li···Li and Ba···Ba contacts, zero- and mono-coordinated metals have been disregarded.



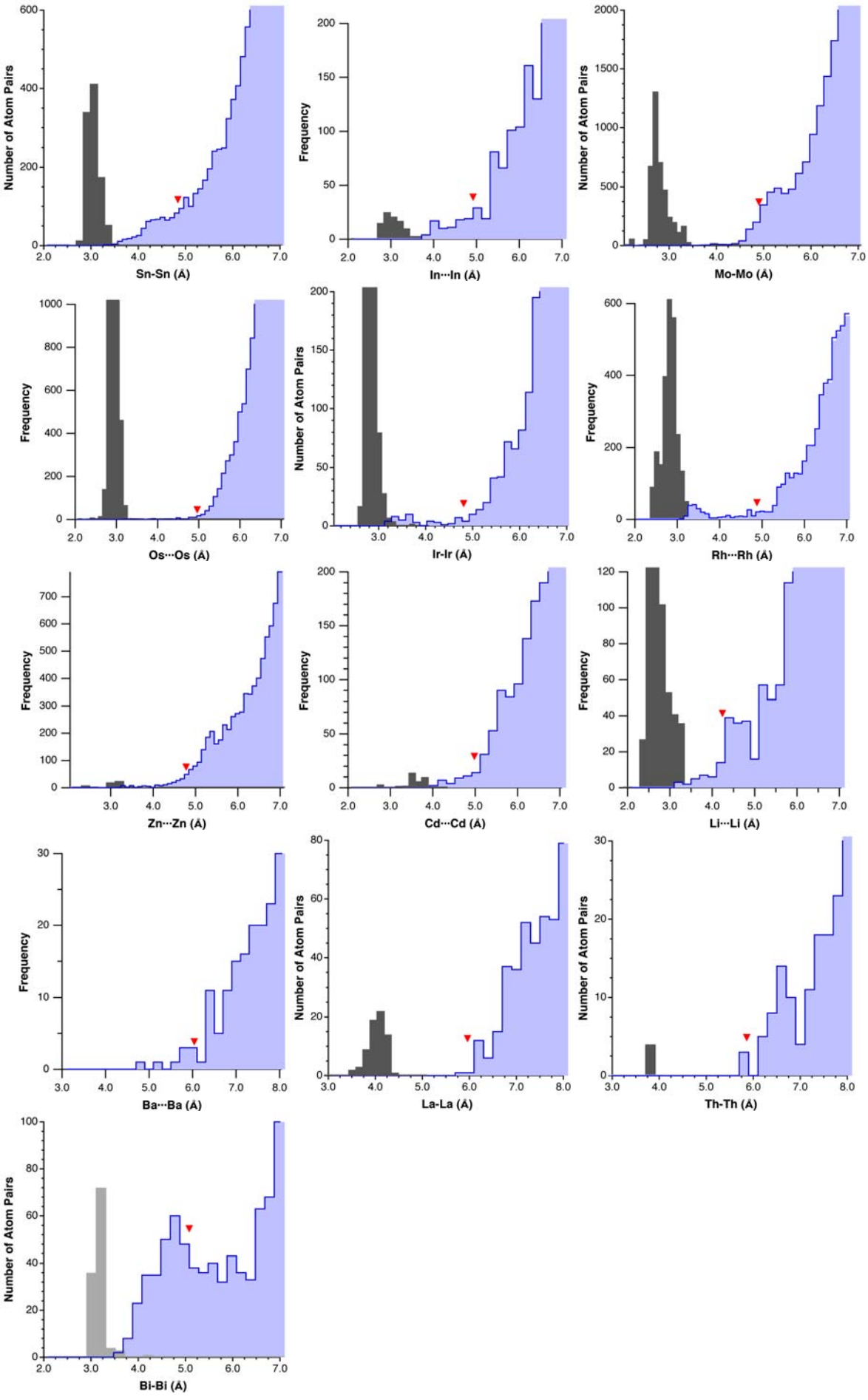
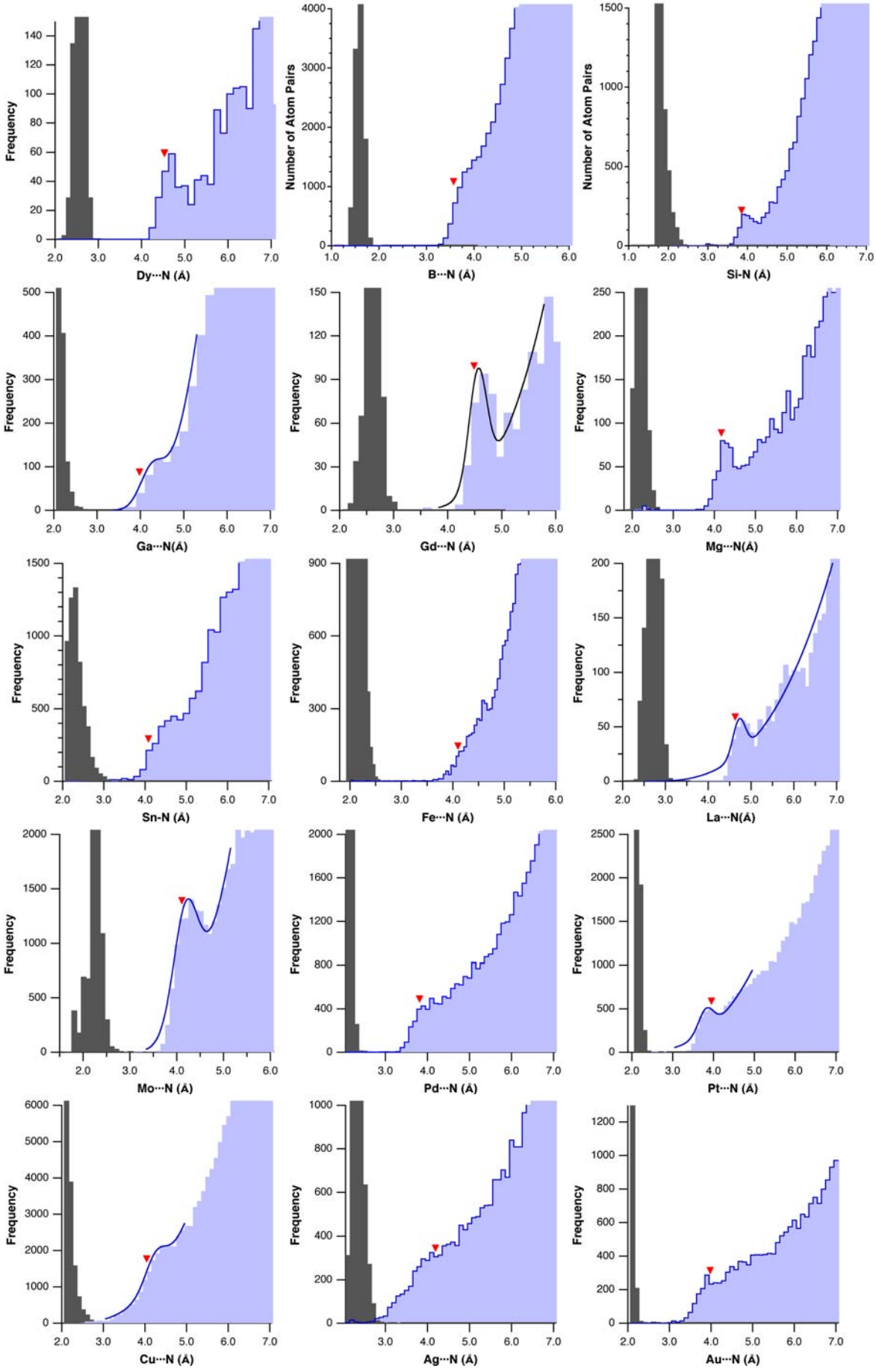

Number of Atom Pairs
Sn-Sn (Å)
Frequency
In···In (Å)
Number of Atom Pairs
Mo-Mo (Å)
Frequency
Os···Os (Å)
Number of Atom Pairs
Ir-Ir (Å)
Frequency
Rh···Rh (Å)
Frequency
Zn···Zn (Å)
Frequency
Cd···Cd (Å)
Frequency
Li···Li (Å)
Frequency
Ba···Ba (Å)
Number of Atom Pairs
La-La (Å)
Number of Atom Pairs
Th-Th (Å)
Number of Atom Pairs
Bi-Bi (Å)

Figure S3.- E···N and E···P Contacts



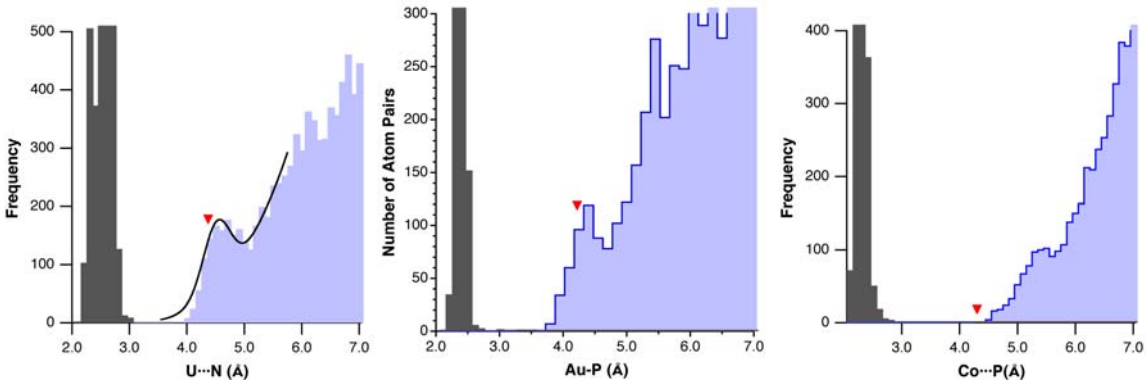
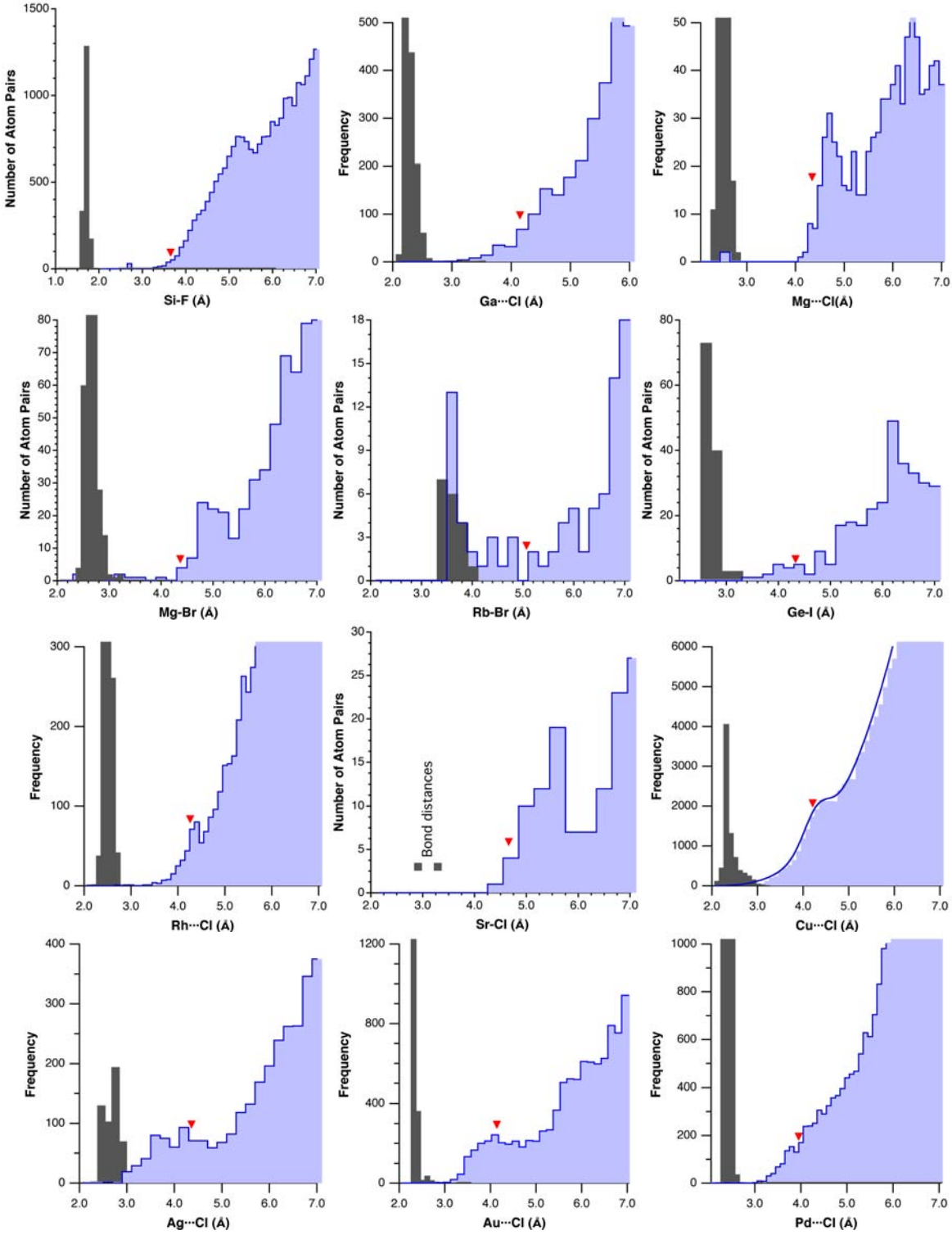


Figure S4.- M···Halogen Contacts



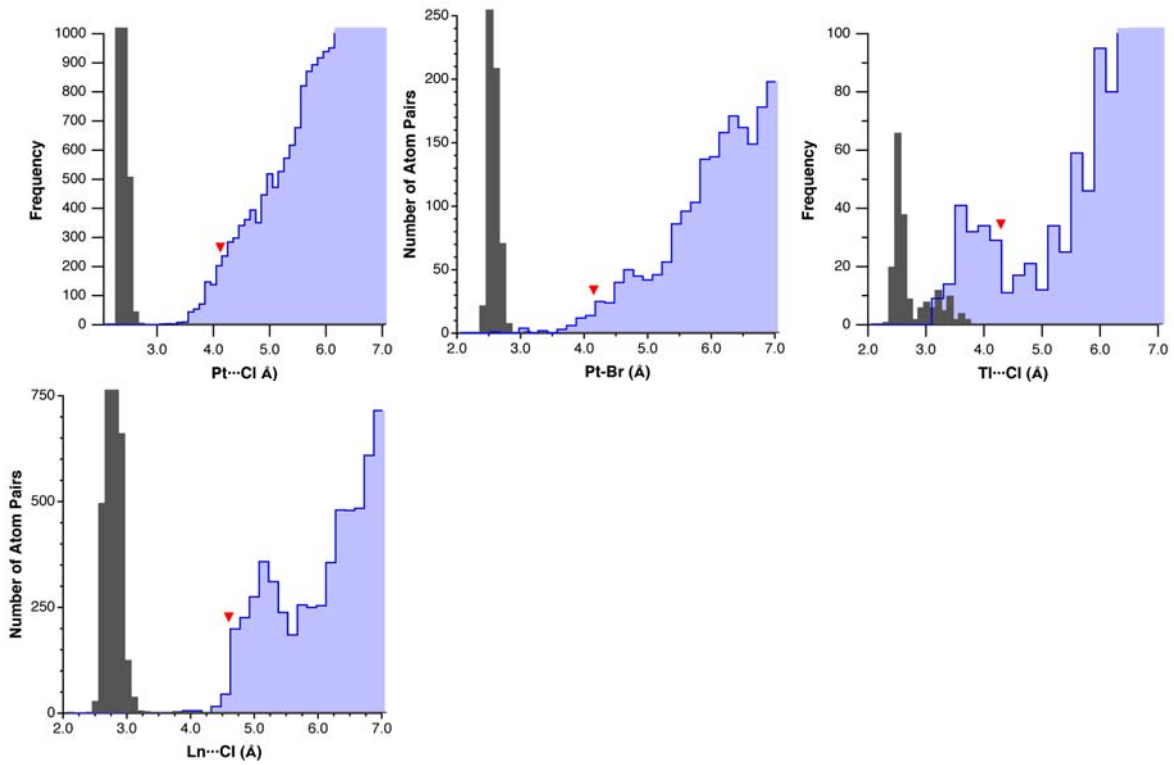
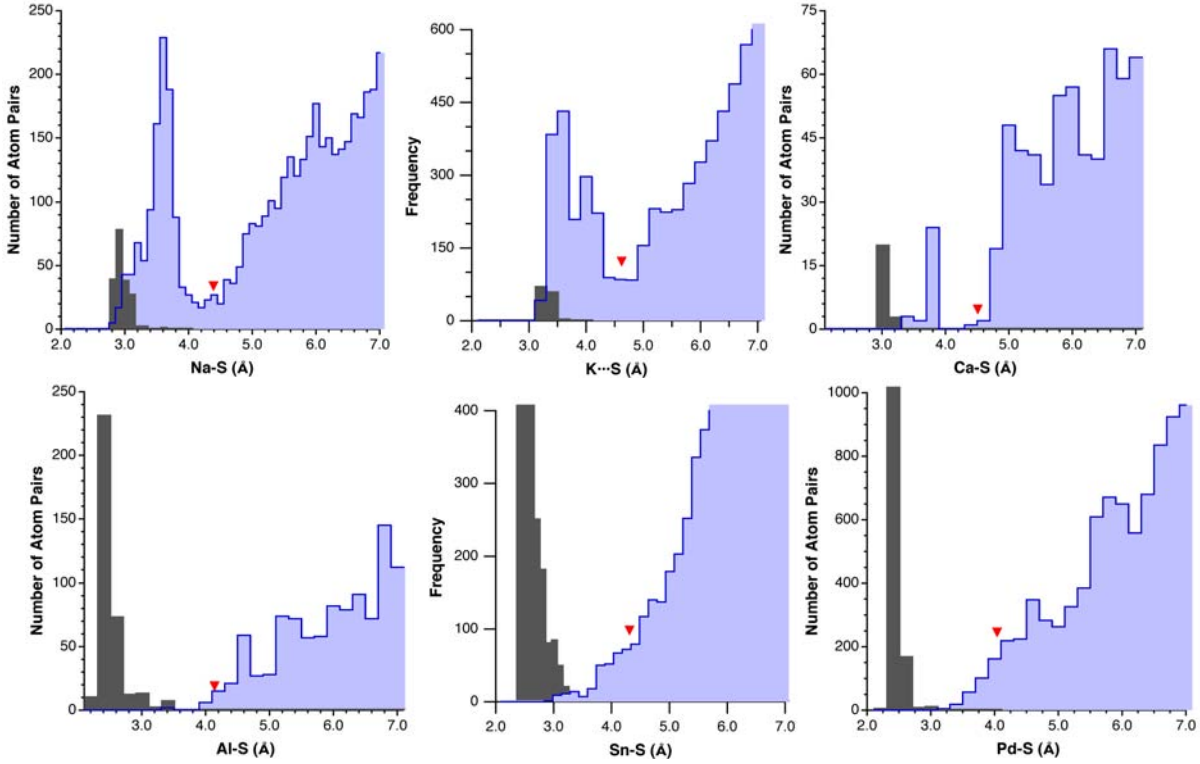


Figure S5.- M···S Contacts



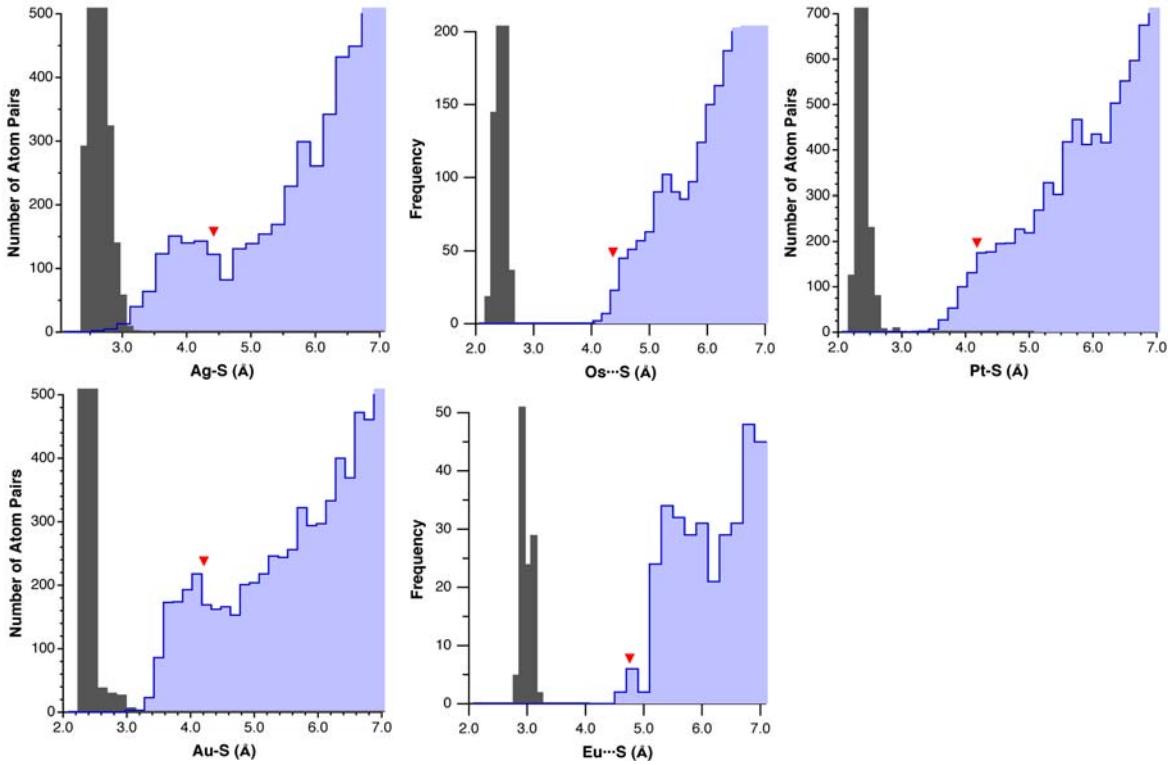


Figure S6.- M···H Contacts

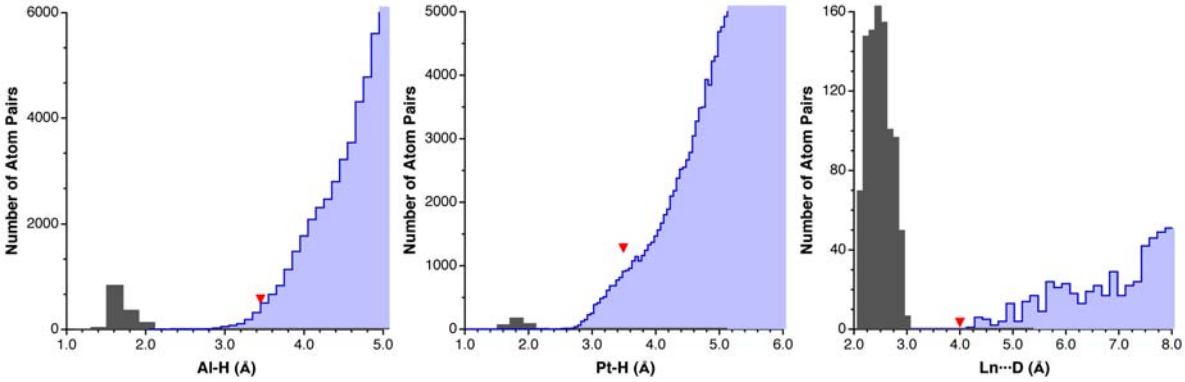


Figure S7.- E···C Contacts

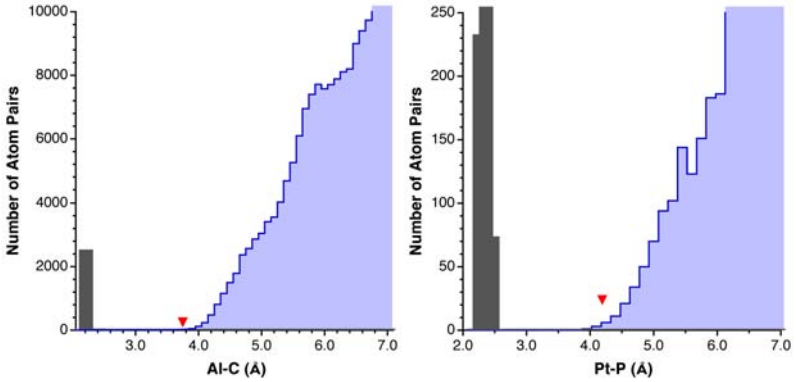


Figure S8.- Phenyl···Halogen Contacts

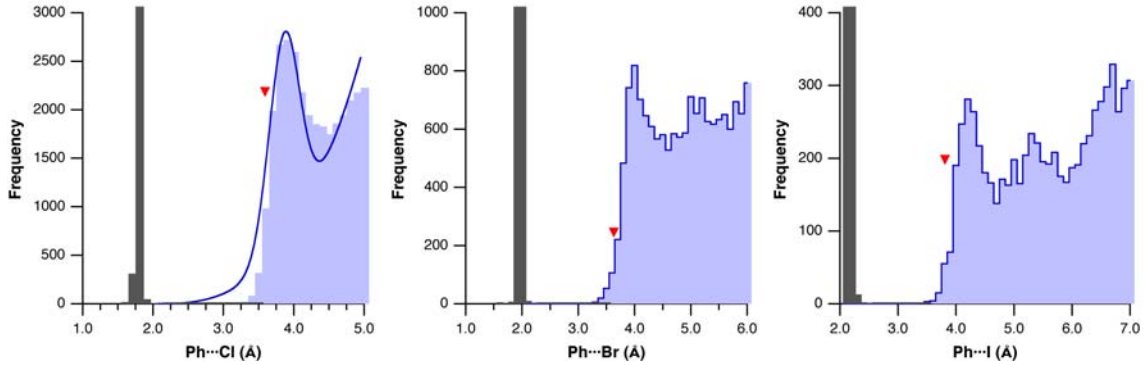


Figure S9.- Metallophilic Contacts

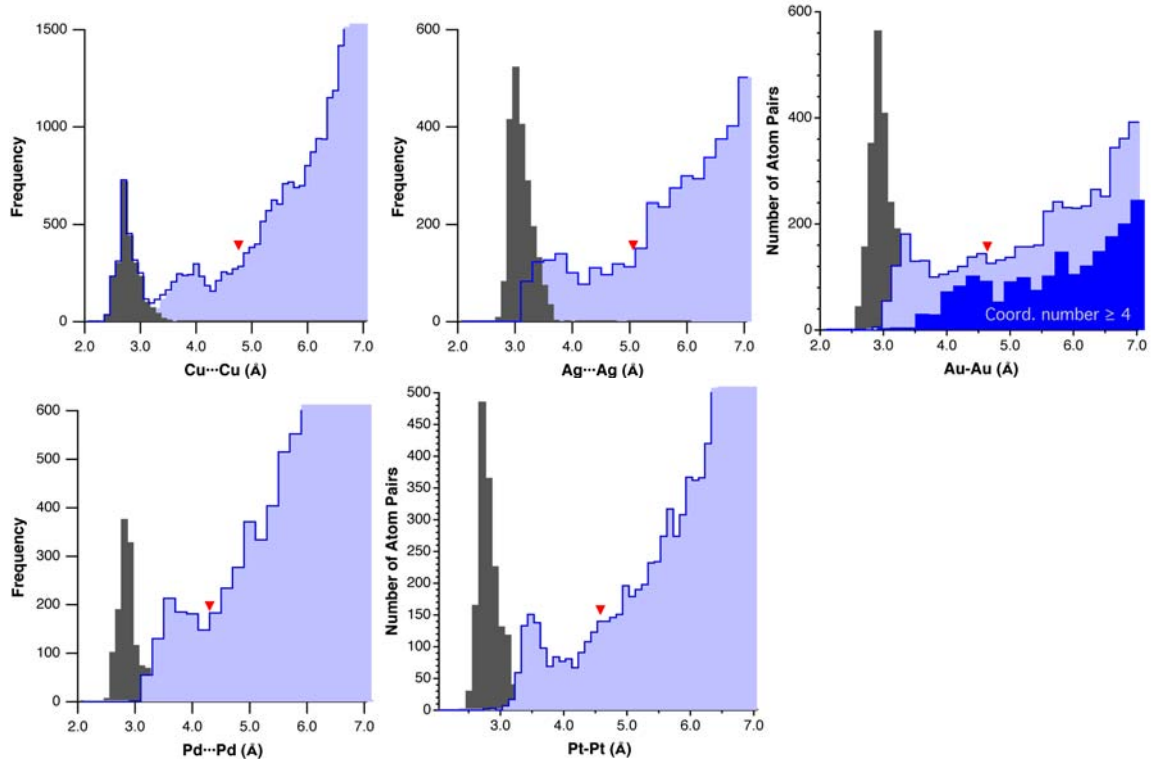
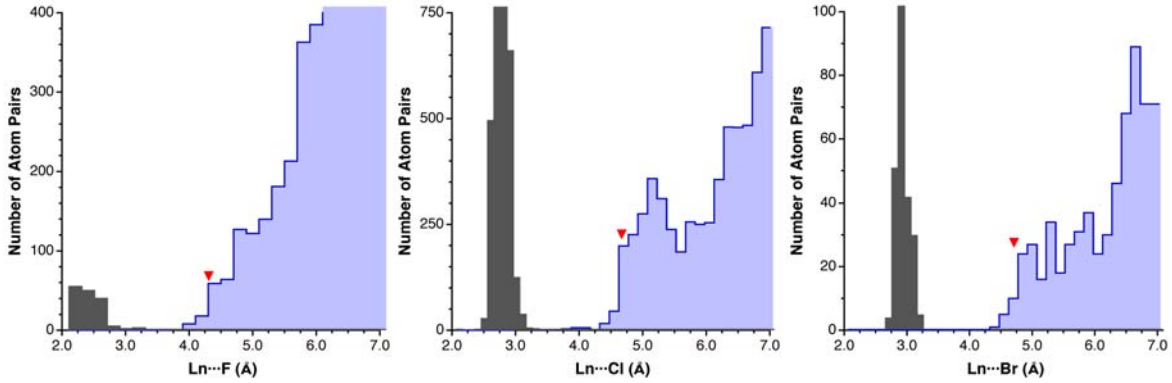


Figure S10.- Rare Earth···X Contacts



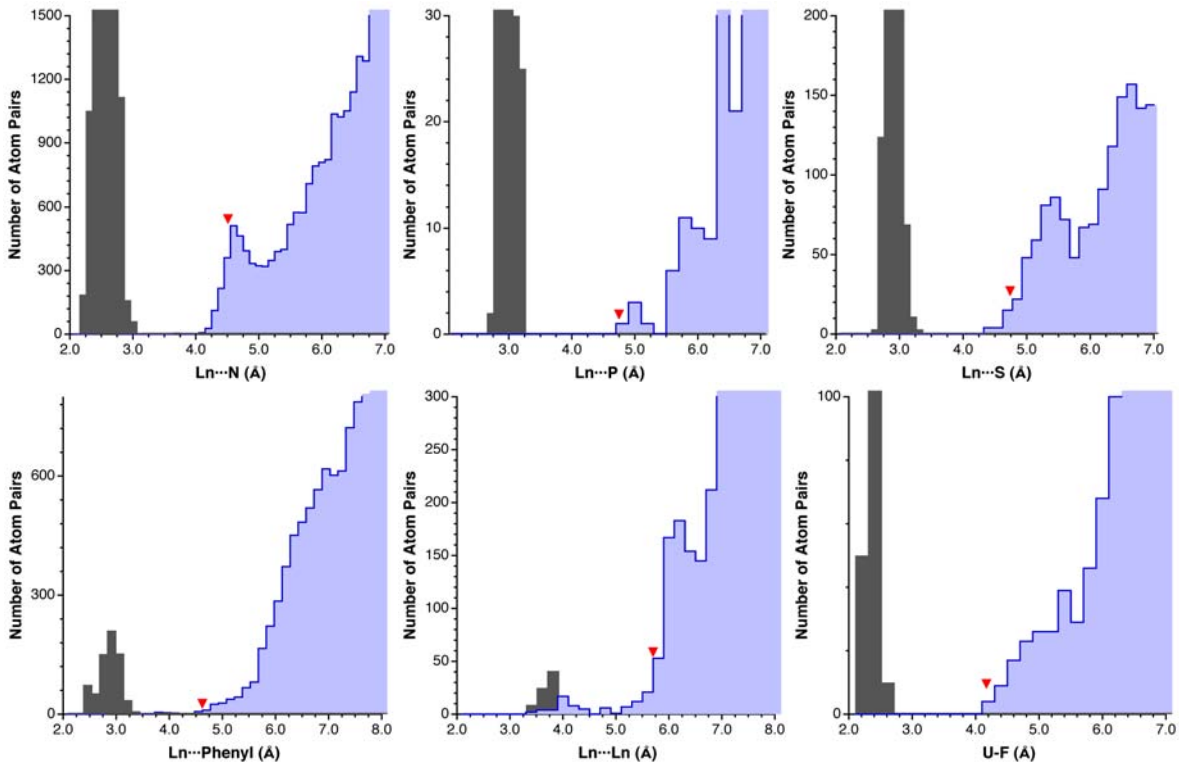
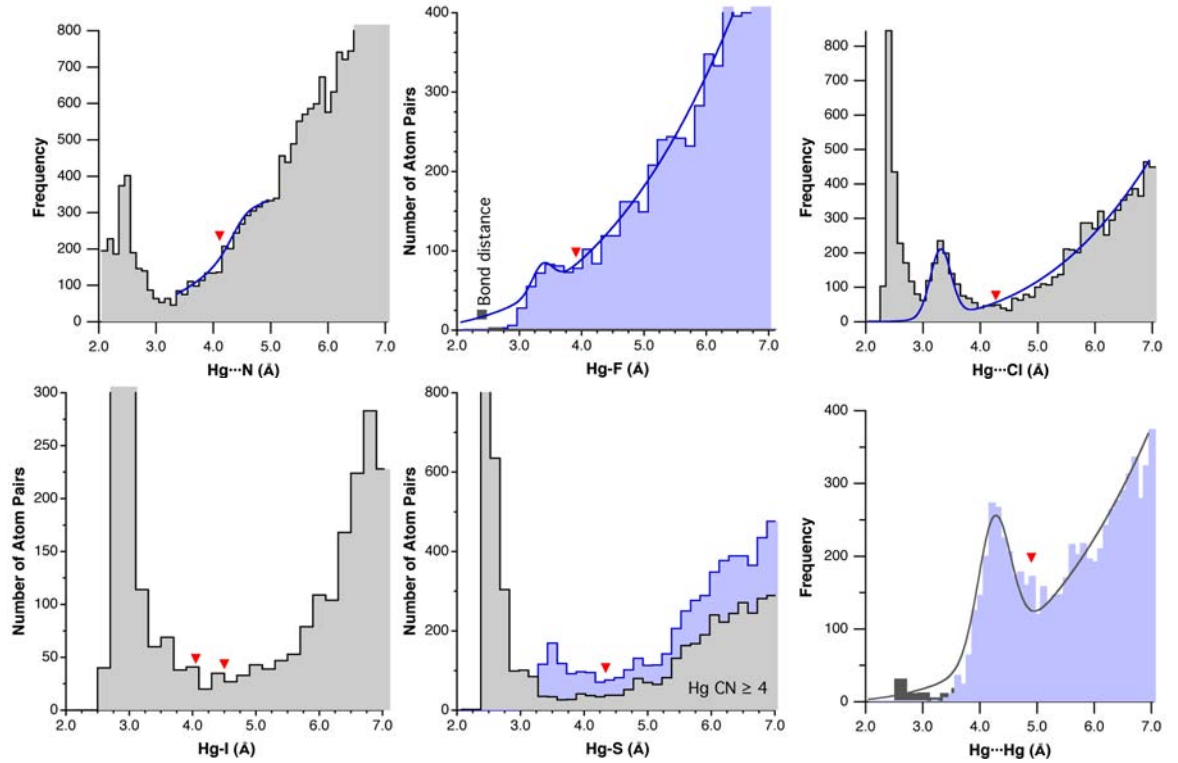
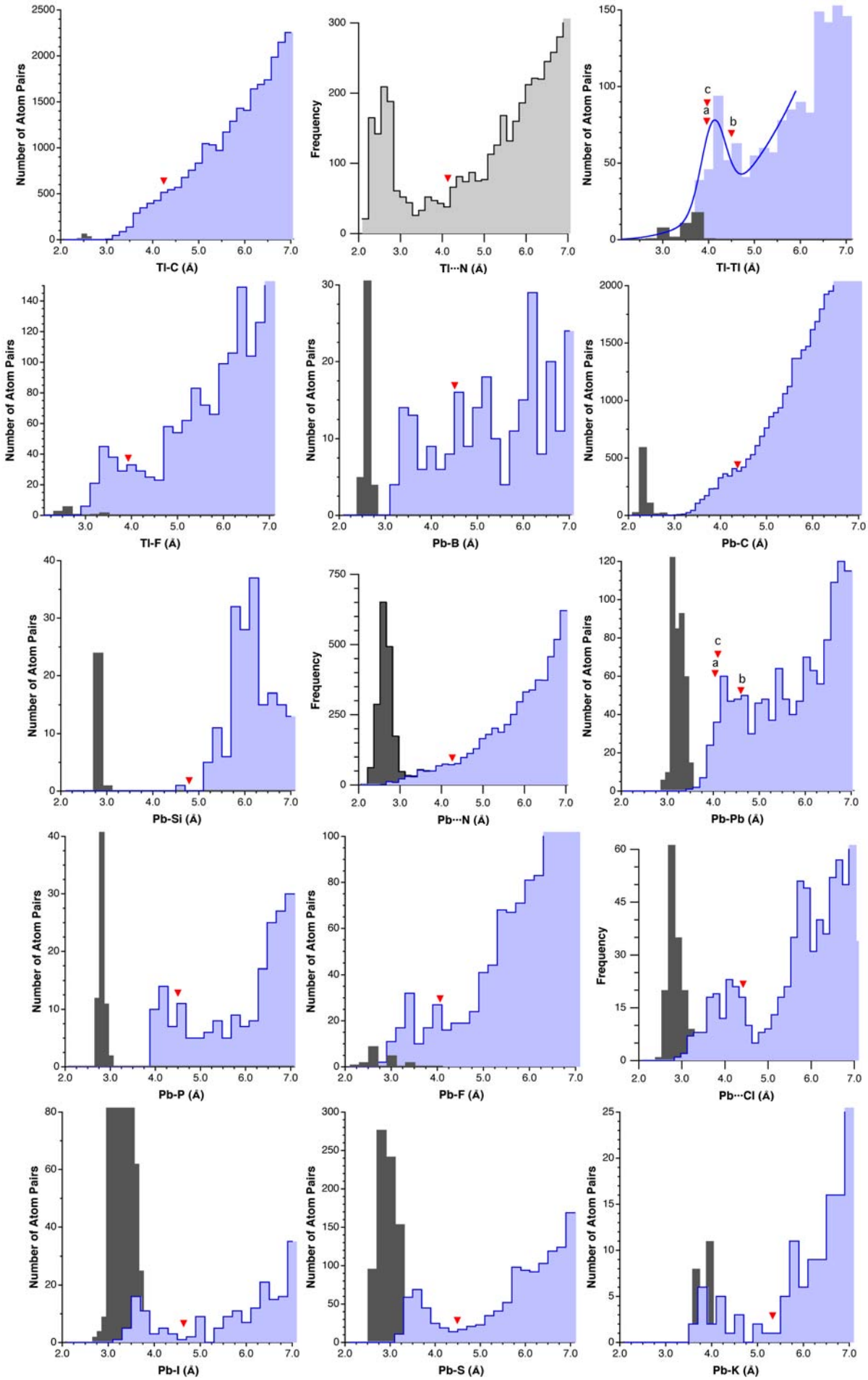
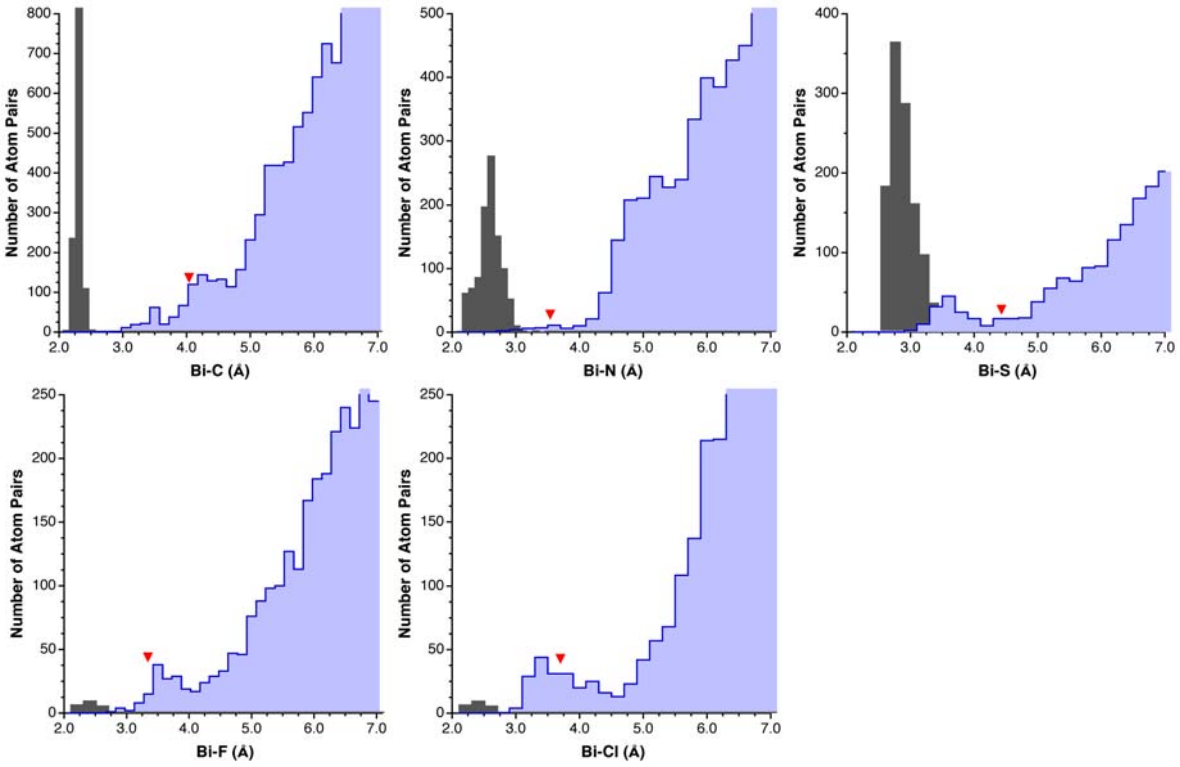


Figure S11.- M···X Contacts (M = Hg, Tl, Pb, Bi)

The red marks point to the van der Waals radii sum with the M radius deduced from M···O contacts (at longer M-X distance) and from the M···M contacts (at shorter distances when present). Dark gray bins represent bonded distances, light blue bins intermolecular distances, and light gray bins bonded and intermolecular distances combined.






Number of Atom Pairs
Bi-C (Å)
Bi-N (Å)
Bi-S (Å)
Bi-F (Å)
Bi-Cl (Å)