DCoupry / **AuToGraFS**

Branch: **master** **AuToGraFS** / libraries / **uff4mof.csv** Find file Copy path

DCoupry added the AtomTyper libraries directory `2620b4a` on Oct 17, 2016

1 contributor

230 lines (229 sloc) 4.05 KB

Search this file…

	symbol	radius	angle	coordination
2	H_	0.354	180	1
3	H_b	0.46	83.5	2
4	He4+4	0.849	90	4
5	Li	1.336	180	1
6	Li3f2	1.28	109.4712	4
7	Be3+2	1.074	109.4712	4
8	B_3	0.838	109.4712	4
9	B_2	0.828	120	3
10	C_3	0.757	109.4712	4
11	C_R	0.729	120	3
12	C_2	0.732	120	3
13	C_1	0.706	180	2
14	N_3	0.7	106.7	3
15	N_R	0.699	120	2
16	N_2	0.685	111.3	2
17	N_1	0.656	180	1
18	N_3+4	0.7	106.7	4
19	O_3	0.658	104.51	3
20	O_3_z	0.528	145.5	3
21	O_R	0.68	110.3	2
22	O_2	0.634	120	2
23	O_1	0.639	180	1
24	O_3_f	0.634	109.4712	4
25	O_2_z	0.528	120	3
26	F_	0.668	180	1
27	Ne4+4	0.92	90	4
28	Na	1.539	180	1
29	Na3f2	1.623	109.4712	4
30	Na4f2	1.79	90	4
31	Mg3+2	1.421	109.4712	4
32	Mg6f3	1.525	90	6
33	Al3	1.244	109.4712	4
34	Al6+3	1.22	90	6

symbol	radius	angle	coordination
Al3f2	1.28	109.4712	4
Si3	1.117	109.4712	4
P_3+3	1.101	93.8	3
P_3+5	1.056	109.4712	3
P_3+q	1.056	109.4712	3
S_3+2	1.064	92.1	3
S_3+4	1.049	103.2	3
S_3+6	1.027	109.4712	3
S_R	1.077	92.2	2
S_2	0.854	120	2
S_3_f	0.854	109.4712	3
Cl	1.044	180	1
Ar4+4	1.032	90	4
K	1.953	180	1
K_3f2	2.38	109.4712	4
K_4f2	2.01	90	4
Ca6+2	1.761	90	6
Ca1f1	1.56	180	2
Ca3f2	1.705	109.4712	4
Sc3+3	1.513	109.4712	4
Sc6+3	1.44	90	6
Ti3+4	1.412	109.4712	4
Ti4+2	1.38	90	4
Ti6+4	1.412	90	6
Ti8f4	1.46	72.4	8
V_3+5	1.402	109.4712	4
V_4+2	1.18	90	4
V_6+3	1.3	90	6
V_3f2	1.12	109.4712	4
Cr6+3	1.345	90	6
Cr4+2	1.1	90	4
Cr6f3	1.28	90	6
Mn6+2	1.382	90	6
Mn6+3	1.34	90	6
Mn4+2	1.26	90	4
Mn1f1	1.38	180	2
Mn3f2	1.18	109.4712	4
Mn8f4	1.52	72.4	8
Fe3+2	1.27	109.4712	4
Fe6+2	1.335	90	6
Fe6+3	1.32	90	6
Fe4+2	1.1	90	4

symbol	radius	angle	coordination
Fe1f1	1.38	180	2
Co6+2	1.241	90	6
Co3+2	1.24	109.4712	4
Co4+2	1.16	90	4
Co1f1	1.28	180	2
Co2f2	1.25	120	3
Ni4+2	1.164	90	4
Cu3+1	1.302	109.4712	4
Cu4+2	1.28	90	4
Cu1f1	1.24	180	2
Cu2f2	1.11	120	3
Cu3f2	1.19	109.4712	4
Zn3+2	1.193	109.4712	4
Zn4+2	1.34	90	4
Zn3f2	1.24	109.4712	4
Zn1f1	1.3	180	2
Zn2f2	1.3	120	3
Ga3+3	1.26	109.4712	4
Ga3f2	1.15	109.4712	4
Ga6f3	1.48	90	6
Ge3	1.197	109.4712	4
As3+3	1.211	92.1	4
Se3+2	1.19	90.6	4
Br	1.192	180	1
Kr4+4	1.147	90	4
Rb	2.26	180	1
Sr6+2	2.052	90	6
Sr8f4	1.82	72.4	8
Y_3+3	1.698	109.4712	4
Y_6f3	1.6	90	6
Y_8f4	1.68	72.4	8
Zr3+4	1.564	109.4712	4
Zr6f3	1.25	90	6
Zr8f4	1.68	72.4	8
Nb3+5	1.473	109.4712	4
Nb8f4	1.37	72.4	8
Mo6+6	1.467	90	6
Mo3+6	1.484	109.4712	4
Mo3f2	1.24	109.4712	4
Mo4f2	1.4	90	4
Mo8f4	1.28	72.4	8
Tc6+5	1.322	90	6

symbol	radius	angle	coordination
Ru6+2	1.478	90	6
Ru4f2	1.32	90	4
Rh6+3	1.332	90	6
Rh4f2	1.22	90	4
Pd4+2	1.338	90	4
Pd6f3	1.19	90	6
Ag1+1	1.386	180	2
Ag1f1	1.22	180	2
Ag2f2	1.34	120	3
Ag3f2	1.48	109.4712	4
Ag4f2	1.51	90	4
Cd3+2	1.403	109.4712	4
Cd1f1	1.4	180	2
Cd3f2	1.29	109.4712	4
Cd4f2	1.46	90	4
Cd8f4	1.64	72.4	8
In3+3	1.459	109.4712	4
In3f2	1.33	109.4712	4
In6f3	1.53	90	6
In8f4	1.53	72.4	8
Sn3	1.398	109.4712	4
Sb3+3	1.407	91.6	4
Te3+2	1.386	90.25	4
I_	1.382	180	1
Xe4+4	1.267	90	4
Cs	2.57	180	1
Ba6+2	2.277	90	4
Ba3f2	2.04	109.4712	4
La3+3	1.943	109.4712	4
La2f2	1.86	120	3
La8f4	1.66	72.4	8
Ce6+3	1.841	90	6
Ce8f4	1.76	72.4	8
Pr6+3	1.823	90	6
Pr8f4	1.83	72.4	8
Nd6+3	1.816	90	6
Nd8f4	1.78	72.4	8
Pm6+3	1.801	90	6
Sm6+3	1.78	90	6
Sm8f4	1.78	72.4	8
Eu6+3	1.771	90	6
Eu6f3	1.6	90	6

1	symbol	radius	angle	coordination
161	Eu8f4	1.74	72.4	8
162	Gd6+3	1.735	90	6
163	Gd6f3	1.55	90	6
164	Gd8f4	1.7	72.4	8
165	Tb6+3	1.732	90	6
166	Tb8f4	1.64	72.4	8
167	Dy6+3	1.71	90	6
168	Dy6f3	1.58	90	6
169	Dy8f4	1.7	72.4	8
170	Ho6+3	1.696	90	6
171	Ho8f4	1.7	72.4	8
172	Er6+3	1.673	90	6
173	Er8f4	1.64	72.4	8
174	Tm6+3	1.66	90	6
175	Tm8f4	1.67	72.4	8
176	Yb6+3	1.637	90	6
177	Yb6f3	1.45	90	6
178	Yb8f4	1.62	72.4	8
179	Lu6+3	1.671	90	6
180	Lu1f1	1.65	180	2
181	Lu8f4	1.66	72.4	8
182	Hf3+4	1.611	109.4712	4
183	Hf8f4	1.46	72.4	8
184	Ta3+5	1.511	109.4712	4
185	W_6+6	1.392	90	6
186	W_3+4	1.526	109.4712	4
187	W_3+6	1.38	109.4712	4
188	W_3f4	1.16	109.4712	4
189	W_4f2	1.345	90	4
190	W_8f4	1.27	72.4	8
191	Re6+5	1.372	90	6
192	Re3+7	1.314	109.4712	4
193	Re6f3	1.23	90	6
194	Os6+6	1.372	90	6
195	Ir6+3	1.371	90	6
196	Pt4+2	1.364	90	4
197	Pt4f2	1.125	90	4
198	Au4+3	1.262	90	4
199	Au1f1	1.11	180	2
200	Hg1+2	1.34	180	1
201	Hg3f2	1.248	109.4712	4
202	Tl3+3	1.518	120	3

1	symbol	radius	angle	coordination
203	Pb3	1.459	109.4712	4
204	Pb4f2	1.67	90	4
205	Bi3+3	1.512	90	4
206	Po3+2	1.5	90	4
207	At	1.545	180	1
208	Rn4+4	1.42	90	4
209	Fr	2.88	180	1
210	Ra6+2	2.512	90	6
211	Ac6+3	1.983	90	6
212	Th6+4	1.721	90	6
213	Pa6+4	1.711	90	6
214	U_6+4	1.684	90	6
215	U_6f3	1.65	90	6
216	U_8f4	1.73	72.4	8
217	Np6+4	1.666	90	6
218	Pu6+4	1.657	90	6
219	Am6+4	1.66	90	6
220	Cm6+3	1.801	90	6
221	Bk6+3	1.761	90	6
222	Cf6+3	1.75	90	6
223	Es6+3	1.724	90	6
224	Fm6+3	1.712	90	6
225	Md6+3	1.689	90	6
226	No6+3	1.679	90	6
227	Lr6+3	1.698	90	6
228	H_OH	0.354	180	1
229	O_HH	0.658	104.51	2