

Synthetic Strategies for New Vanadium Oxyfluorides Containing Novel
Building Blocks: Structures of V(IV) and V(V) Containing $\text{Sr}_4\text{V}_3\text{O}_5\text{F}_{13}$,
 $\text{Pb}_7\text{V}_4\text{O}_8\text{F}_{18}$, $\text{Pb}_2\text{VO}_2\text{F}_5$, and Pb_2VOF_6

Jeongho Yeon,¹ Justin B. Felder,¹ Gregory Morrison,¹ and Hans-Conrad zur Loye,^{1}*

¹Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC 29208

Corresponding Authors: *E-mail: zurloye@mail.chem.sc.edu

Figure S1. The experimental and calculated powder X-ray diffraction data for $\text{Sr}_4\text{V}_3\text{O}_5\text{F}_{13}$

Figure S2. The experimental and calculated powder X-ray diffraction data for $\text{Pb}_7\text{V}_4\text{O}_8\text{F}_{18}$

Figure S3. The experimental and calculated powder X-ray diffraction data for $\text{Pb}_2\text{VO}_2\text{F}_5$

Figure S4. The experimental and calculated powder X-ray diffraction data for Pb_2VOF_6

Figure S5. UV-vis diffuse reflectance spectroscopy data for $\text{Sr}_4\text{V}_3\text{O}_5\text{F}_{13}$, $\text{Pb}_7\text{V}_4\text{O}_8\text{F}_{18}$, $\text{Pb}_2\text{VO}_2\text{F}_5$,
and Pb_2VOF_6

Table S1. Full bond valence sum calculation results

Figure S1. The experimental and calculated powder X-ray diffraction data for $\text{Sr}_4\text{V}_3\text{O}_5\text{F}_{13}$.

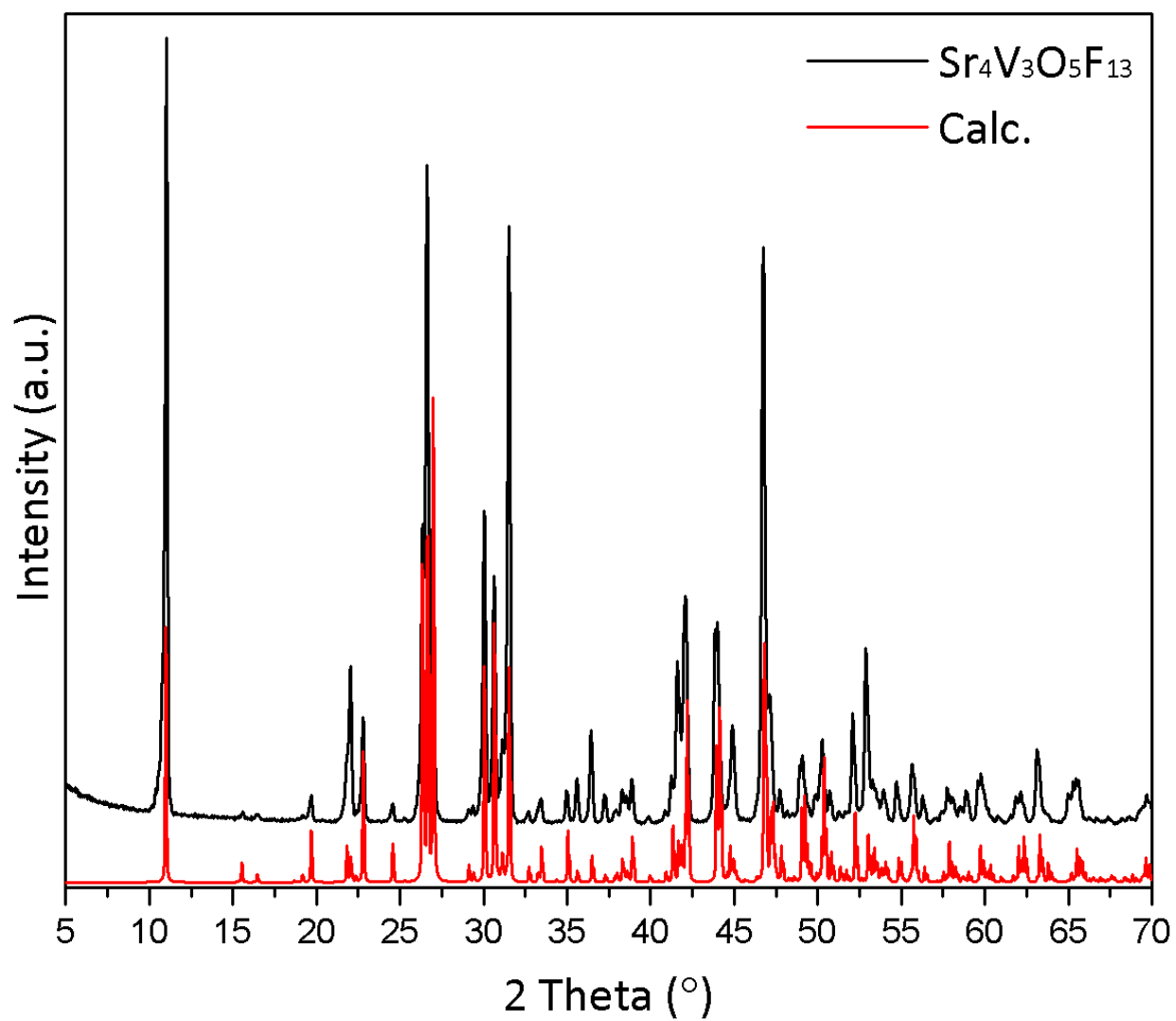


Figure S2. The experimental and calculated powder X-ray diffraction data for $\text{Pb}_7\text{V}_4\text{O}_8\text{F}_{18}$.

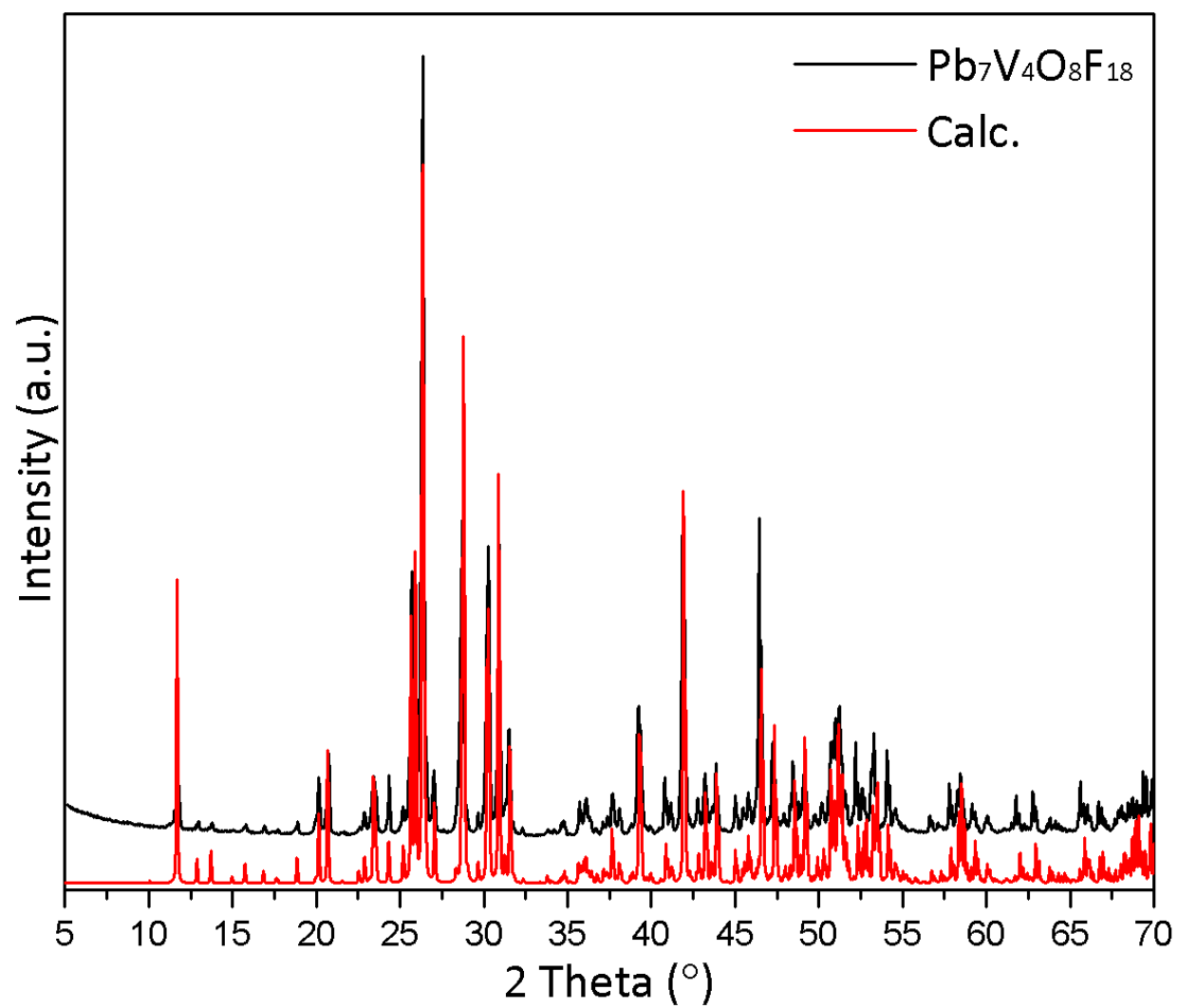


Figure S3. The experimental and calculated powder X-ray diffraction data for $\text{Pb}_2\text{VO}_2\text{F}_5$.

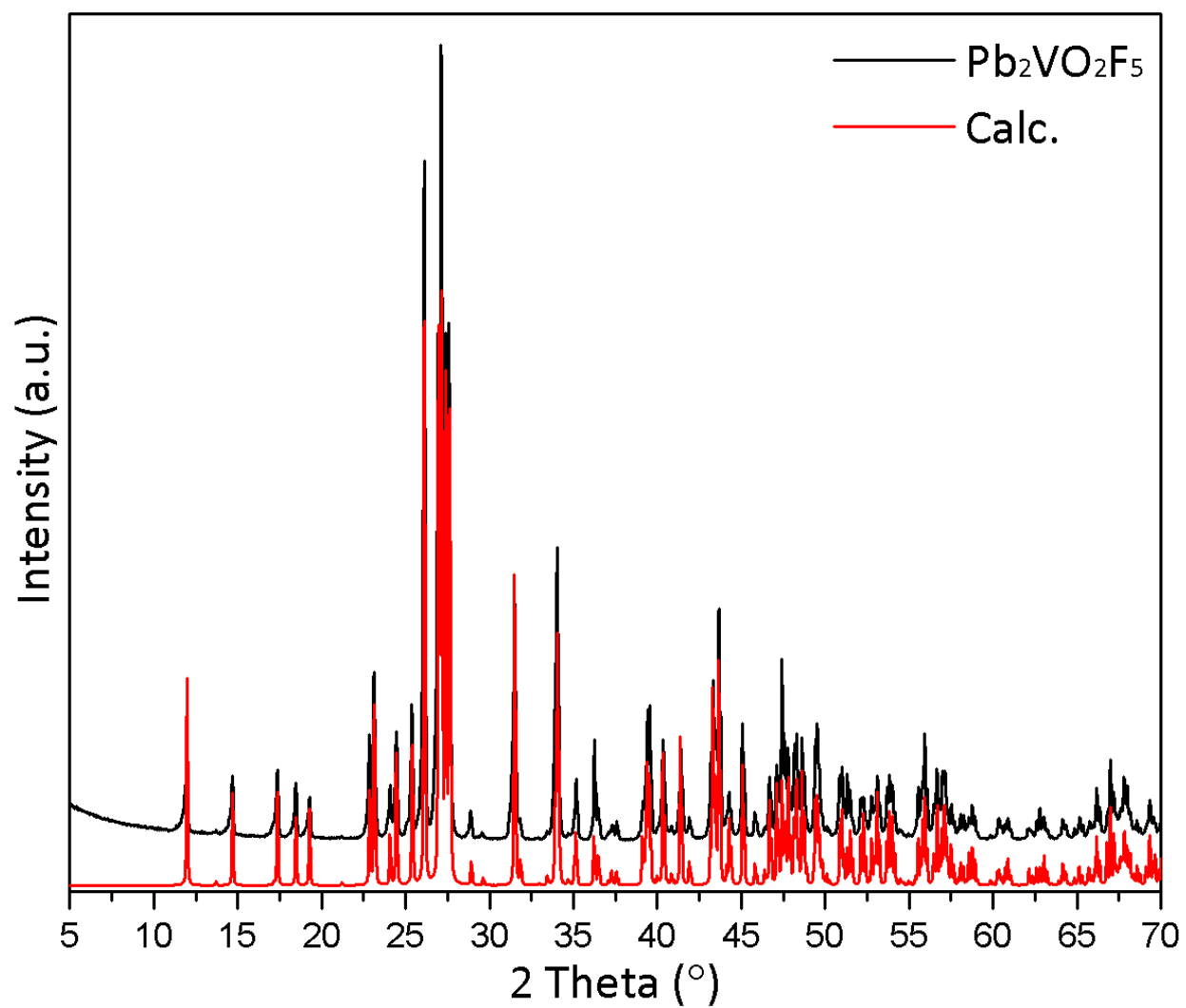


Figure S4. The experimental and calculated powder X-ray diffraction data for Pb_2VOF_6 .

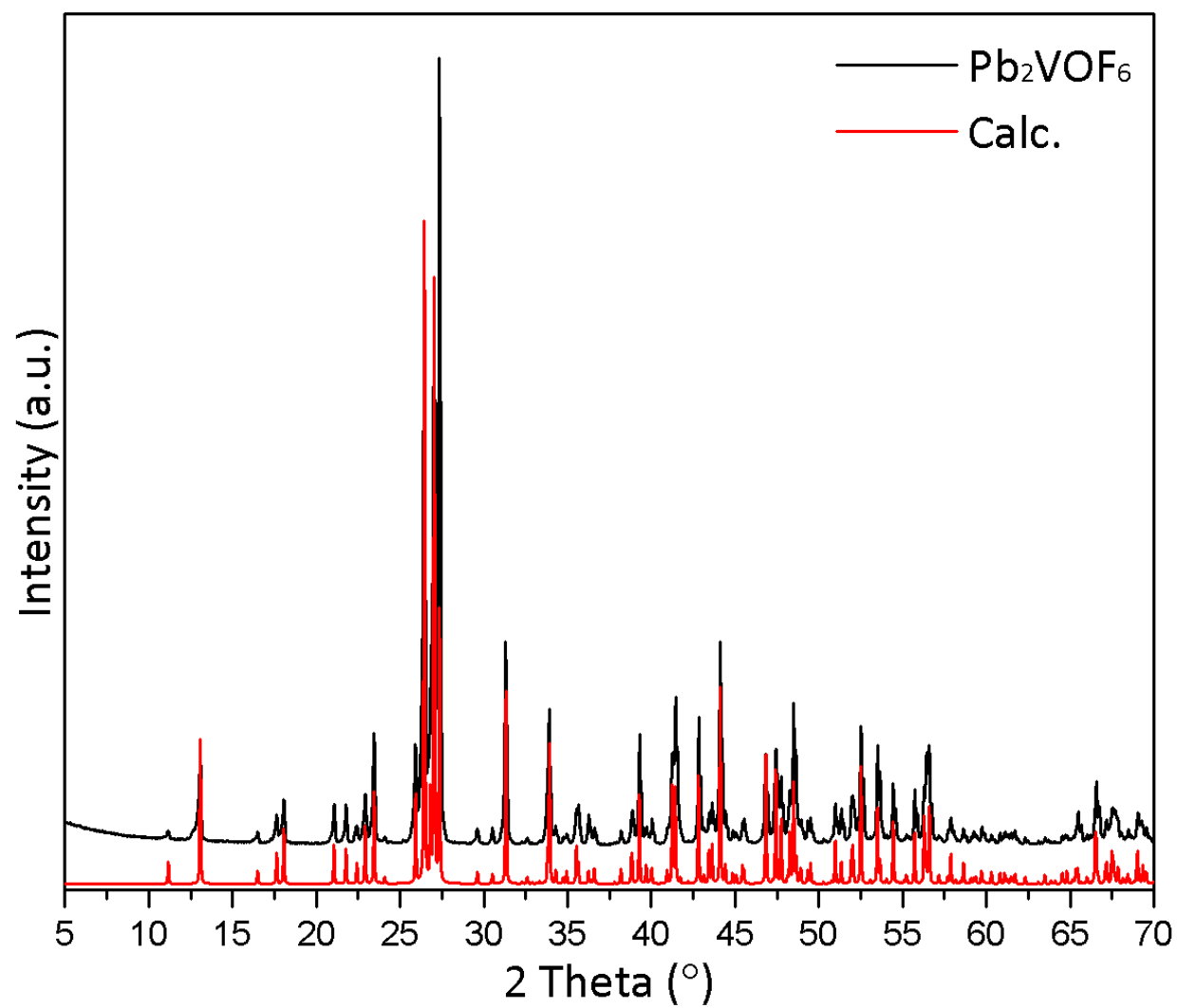


Figure S5. UV-vis diffuse reflectance spectroscopy data for $\text{Sr}_4\text{V}_3\text{O}_5\text{F}_{13}$, $\text{Pb}_7\text{V}_4\text{O}_8\text{F}_{18}$, $\text{Pb}_2\text{VO}_2\text{F}_5$, and Pb_2VOF_6 .

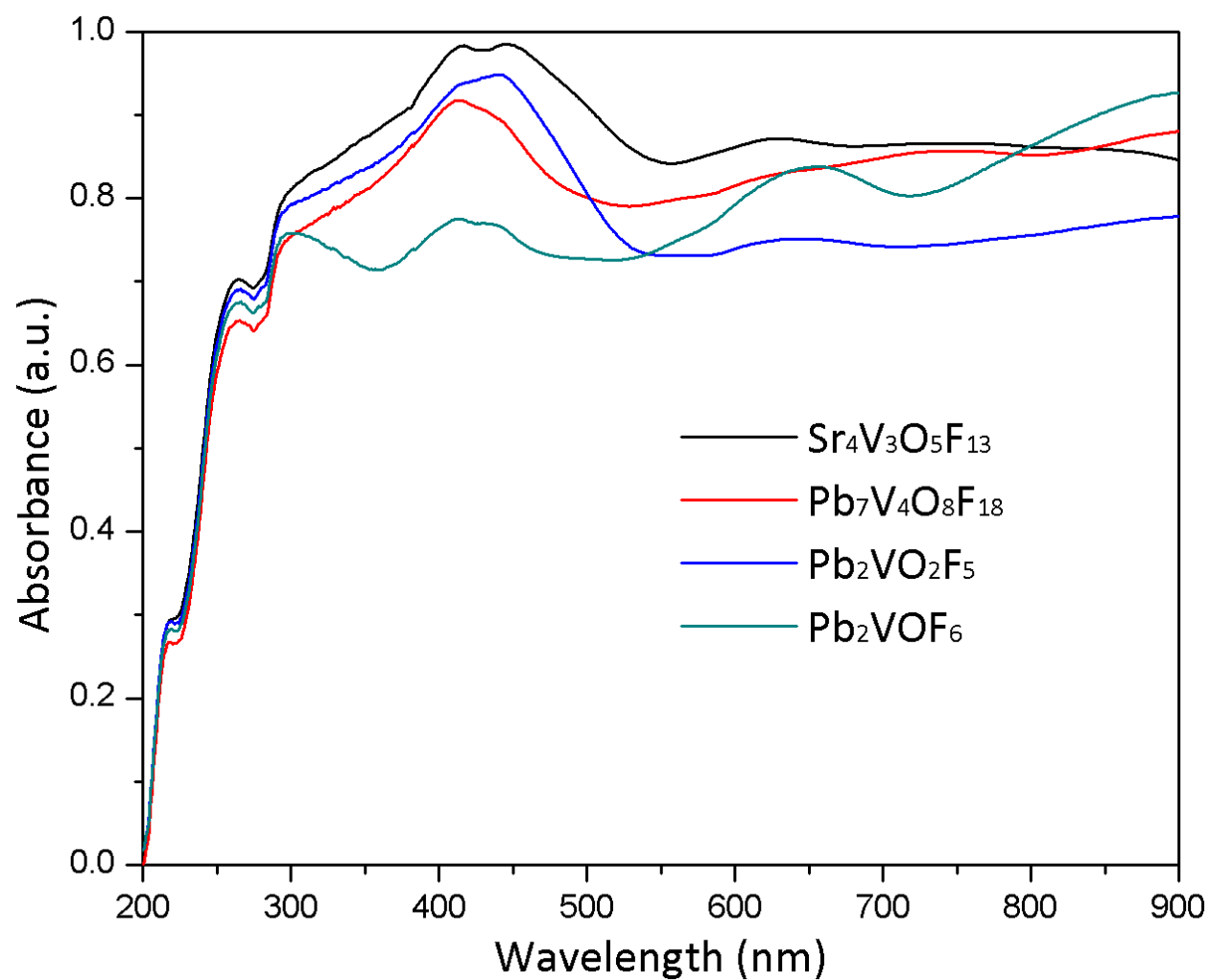


Table S1. Full bond valence sum calculation results.

Sr ₄ V ₃ O ₅ F ₁₃	Sr1	F1	2.447	-0.428	-1.157	0.315
		F2	2.505	-0.486	-1.314	0.269
		F5	2.515	-0.496	-1.341	0.262
		F1	2.556	-0.537	-1.451	0.234
		F4	2.578	-0.559	-1.511	0.221
		F3	2.579	-0.560	-1.514	0.220
		F7	2.618	-0.599	-1.619	0.198
		F6	2.625	-0.606	-1.638	0.194
		O2	2.695	-0.577	-1.559	0.210
	Sr2					2.12
		F2	2.447	-0.428	-1.157	0.315
		F2	2.489	-0.470	-1.270	0.281
		F1	2.49	-0.471	-1.273	0.280
		F4	2.584	-0.565	-1.527	0.217
		F6	2.6	-0.581	-1.570	0.208
		F3	2.625	-0.606	-1.638	0.194
		O1	2.626	-0.508	-1.373	0.253
		F5	2.628	-0.609	-1.646	0.193
		F4	2.67	-0.651	-1.759	0.172
		F1	2.743	-0.724	-1.957	0.141
	V1					2.11
		O2	1.6	0.203	0.549	1.731
		O1	1.724	0.079	0.214	1.238
		F3	1.887	-0.177	-0.478	0.620
		F5	1.904	-0.194	-0.524	0.592
		F4	1.97	-0.260	-0.703	0.495
	V2	F2	2.227	-0.517	-1.397	0.247
						4.92
		F7	1.63	0.173	0.468	1.596
		F6	1.784	-0.074	-0.200	0.819
		O1	1.937	-0.134	-0.362	0.696
		F6	1.956	-0.246	-0.665	0.514
		O1	1.973	-0.170	-0.459	0.632
		F7	2.262	-0.459	-1.241	0.289
						4.55

Pb ₇ V ₄ O ₈ F ₁₈	Pb1	F9	2.339	-0.309	-0.835	0.434
		F1	2.474	-0.444	-1.200	0.301
		F9	2.525	-0.495	-1.338	0.262
		F8	2.615	-0.585	-1.581	0.206
		F8	2.667	-0.637	-1.722	0.179
		F6	2.81	-0.780	-2.108	0.121
		F4	2.815	-0.785	-2.122	0.120
		O2	2.878	-0.766	-2.070	0.126
		O4	2.998	-0.886	-2.395	0.091
	Pb2					1.84
		F9	2.32	-0.290	-0.784	0.457
		F8	2.393	-0.363	-0.981	0.375
		F4	2.46	-0.430	-1.162	0.313
		F7	2.473	-0.443	-1.197	0.302
		O2	2.703	-0.591	-1.597	0.202
		O4	2.733	-0.621	-1.678	0.187
		O1	2.756	-0.644	-1.741	0.175
						2.01
	Pb3	F7	2.415	-0.385	-1.041	0.353
		F3	2.44	-0.410	-1.108	0.330
		F8	2.448	-0.418	-1.130	0.323
		F7	2.54	-0.510	-1.378	0.252
		F5	2.603	-0.573	-1.549	0.213
		O1	2.635	-0.523	-1.414	0.243
		F1	2.772	-0.742	-2.005	0.135
		O3	2.853	-0.741	-2.003	0.135
						1.85
	Pb4	F1	2.603	-0.573	-1.549	0.213
		F1	2.603	-0.573	-1.549	0.213
		F4	2.619	-0.589	-1.592	0.204
		F4	2.619	-0.589	-1.592	0.204
		F2	2.648	-0.618	-1.670	0.188
		F2	2.648	-0.618	-1.670	0.188
		F7	2.653	-0.623	-1.684	0.186
		F7	2.653	-0.623	-1.684	0.186
		F5	2.733	-0.703	-1.900	0.150
		F5	2.733	-0.703	-1.900	0.150
						1.73
	V1	O1	1.646	0.157	0.424	1.529
		O2	1.686	0.117	0.316	1.372
		F3	1.866	-0.156	-0.422	0.656

		O3	1.972	-0.169	-0.457	0.633
		F2	2.087	-0.377	-1.019	0.361
		F1	2.114	-0.404	-1.092	0.336
						4.89
	V2	O4	1.66	0.143	0.386	1.472
		O3	1.714	0.089	0.241	1.272
		F6	1.812	-0.102	-0.276	0.759
		F5	1.948	-0.238	-0.643	0.526
		F4	1.986	-0.276	-0.746	0.474
		F2	2.133	-0.423	-1.143	0.319
						4.82
Pb ₂ VO ₂ F ₅	Pb1	F1	2.402	-0.372	-1.005	0.366
		F1	2.437	-0.407	-1.100	0.333
		F2	2.551	-0.521	-1.408	0.245
		O2	2.553	-0.441	-1.192	0.304
		F4	2.567	-0.537	-1.451	0.234
		F2	2.612	-0.582	-1.573	0.207
		O1	2.649	-0.537	-1.451	0.234
		F3	2.662	-0.632	-1.708	0.181
						2.10
	Pb2	F1	2.313	-0.283	-0.765	0.465
		F2	2.408	-0.378	-1.022	0.360
		F2	2.528	-0.498	-1.346	0.260
		F4	2.56	-0.530	-1.432	0.239
		F5	2.728	-0.698	-1.886	0.152
		F3	2.729	-0.699	-1.889	0.151
		O1	2.796	-0.684	-1.849	0.157
		F5	2.857	-0.827	-2.235	0.107
		O2	2.904	-0.792	-2.141	0.118
						2.01
	V1	O2	1.663	0.140	0.378	1.460
		O1	1.71	0.093	0.251	1.286
		F3	1.884	-0.174	-0.470	0.625
		F4	1.927	-0.217	-0.586	0.556
		F5	2.024	-0.314	-0.849	0.428
		F5	2.214	-0.504	-1.362	0.256
						4.61
Pb ₂ VOF ₆	Pb1	F5	2.356	-0.326	-0.881	0.414
		F5	2.405	-0.375	-1.014	0.363
		F3	2.474	-0.444	-1.200	0.301

	F6	2.526	-0.496	-1.341	0.262
	O1	2.574	-0.462	-1.249	0.287
	F2	2.65	-0.620	-1.676	0.187
	F7	2.678	-0.648	-1.751	0.174
					1.99
Pb2	F5	2.373	-0.343	-0.927	0.396
	F7	2.436	-0.406	-1.097	0.334
	F1	2.493	-0.463	-1.251	0.286
	F6	2.497	-0.467	-1.262	0.283
	F3	2.613	-0.583	-1.576	0.207
	F2	2.721	-0.691	-1.868	0.154
	F4	2.783	-0.753	-2.035	0.131
	F4	2.827	-0.797	-2.154	0.116
	F1	2.892	-0.862	-2.330	0.097
					2.00
V1	O1	1.619	0.165	0.446	1.562
	F2	1.891	-0.181	-0.489	0.613
	F1	1.917	-0.207	-0.559	0.572
	F3	1.949	-0.239	-0.646	0.524
	F4	1.956	-0.246	-0.665	0.514
	F4	2.239	-0.529	-1.430	0.239
					4.02