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1
2 #=====
3 # CRYSTAL DATA
4 #-----
5 data_VESTA_phase_1
6
7 _chemical_name_common          'POSCAR file written by OVITO Basic 3.6'
8 _cell_length_a                 13.338000
9 _cell_length_b                 13.338000
10 _cell_length_c                 13.338000
11 _cell_angle_alpha              90.000000
12 _cell_angle_beta               90.000000
13 _cell_angle_gamma              90.000000
14 _cell_volume                   2372.860289
15 _space_group_name_H-M_alt      'P 1'
16 _space_group_IT_number         1
17
18 loop_
19 _space_group_symop_operation_xyz
20   'x, y, z'
21
22 loop_
23   _atom_site_label
24   _atom_site_occupancy
25   _atom_site_fract_x
26   _atom_site_fract_y
27   _atom_site_fract_z
28   _atom_site_type_symbol
29   Ta1      1.0      0.296934      0.826793      0.594897      Ta
30   Ta2      1.0      0.597895      0.570562      0.978552      Ta
31   Ta3      1.0      0.598801      0.061667      0.248443      Ta
32   Ta4      1.0      0.012805      0.872078      0.150059      Ta
33   Ta5      1.0      0.700968      0.036971      0.795968      Ta
34   Ta6      1.0      0.272356      0.298860      0.832400      Ta
35   Ta7      1.0      0.395476      0.447736      0.390210      Ta
36   Ta8      1.0      0.158227      0.152499      0.382272      Ta
37   Ta9      1.0      0.161746      0.812442      0.008471      Ta
38   Ta10     1.0      0.258034      0.876377      0.808098      Ta
39   Ta11     1.0      0.864643      0.524740      0.584622      Ta
40   Ta12     1.0      0.846982      0.426626      0.035857      Ta
41   Cl1      1.0      0.168930      0.939500      0.658493      Cl
42   Cl2      1.0      0.632415      0.638553      0.142932      Cl
43   Cl3      1.0      0.213082      0.859961      0.434470      Cl
44   Cl4      1.0      0.441126      0.535197      0.042654      Cl
45   Cl5      1.0      0.558545      0.506225      0.823339      Cl
46   Cl6      1.0      0.196127      0.684564      0.607274      Cl
47   Cl7      1.0      0.575851      0.727422      0.916772      Cl
48   Cl8      1.0      0.431845      0.752283      0.513962      Cl
49   Cl9      1.0      0.386658      0.983420      0.578523      Cl
50   Cl10     1.0      0.777983      0.583861      0.948090      Cl
51   Cl11     1.0      0.664035      0.787103      0.403766      Cl
52   Cl12     1.0      0.825742      0.839118      0.183955      Cl
53   Cl13     1.0      0.611376      0.242473      0.235517      Cl
54   Cl14     1.0      0.604495      0.914549      0.124277      Cl
55   Cl15     1.0      0.006701      0.991567      0.310248      Cl
56   Cl16     1.0      0.408042      0.825607      0.262792      Cl
57   Cl17     1.0      0.427999      0.107469      0.144832      Cl
58   Cl18     1.0      0.433336      0.267085      0.901137      Cl
59   Cl19     1.0      0.913271      0.221636      0.332071      Cl
60   Cl20     1.0      0.890415      0.918598      0.510313      Cl
61   Cl21     1.0      0.724313      0.112165      0.959633      Cl
62   Cl22     1.0      0.268417      0.467335      0.801564      Cl
63   Cl23     1.0      0.613160      0.181476      0.745863      Cl
64   Cl24     1.0      0.797909      0.893326      0.854345      Cl
65   Cl25     1.0      0.334199      0.247348      0.677418      Cl
66   Cl26     1.0      0.560195      0.955993      0.862834      Cl
67   Cl27     1.0      0.217011      0.284162      0.992507      Cl
68   Cl28     1.0      0.658423      0.941913      0.648355      Cl
69   Cl29     1.0      0.846202      0.101178      0.722636      Cl
70   Cl30     1.0      0.122487      0.227722      0.785507      Cl
71   Cl31     1.0      0.221073      0.306884      0.442352      Cl

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72	C132	1.0	0.832492	0.520903	0.176977	C1
73	C133	1.0	0.367566	0.374385	0.233439	C1
74	C134	1.0	0.941501	0.648340	0.489251	C1
75	C135	1.0	0.127557	0.191268	0.216134	C1
76	C136	1.0	0.462549	0.293872	0.440040	C1
77	C137	1.0	0.054847	0.121656	0.520142	C1
78	C138	1.0	0.523127	0.543548	0.338777	C1
79	C139	1.0	0.258681	0.557788	0.369036	C1
80	C140	1.0	0.941936	0.021164	0.082274	C1
81	C141	1.0	0.179546	0.937532	0.150588	C1
82	C142	1.0	0.344361	0.840130	0.977662	C1
83	C143	1.0	0.994369	0.746570	0.012211	C1
84	C144	1.0	0.220502	0.669549	0.100976	C1
85	C145	1.0	0.408182	0.791367	0.742363	C1
86	C146	1.0	0.051948	0.743073	0.263641	C1
87	C147	1.0	0.170220	0.708709	0.843211	C1
88	C148	1.0	0.652389	0.407448	0.036605	C1
89	C149	1.0	0.115820	0.962502	0.901339	C1
90	C150	1.0	0.335732	0.037719	0.817864	C1
91	C151	1.0	0.992783	0.413213	0.568923	C1
92	C152	1.0	0.839180	0.361193	0.874289	C1
93	C153	1.0	0.747498	0.415207	0.647563	C1
94	C154	1.0	0.416602	0.492488	0.558791	C1
95	C155	1.0	0.738767	0.175105	0.509354	C1
96	C156	1.0	0.810470	0.470261	0.417597	C1
97	C157	1.0	0.010731	0.478221	0.020321	C1
98	C158	1.0	0.732561	0.653099	0.629451	C1
99	C159	1.0	0.942347	0.568153	0.730274	C1
100	C160	1.0	0.859345	0.274837	0.115865	C1
101	Li1	1.0	0.788800	0.782461	0.547514	Li
102	Li2	1.0	0.641361	0.032319	0.438063	Li
103	Li3	1.0	0.374985	0.017193	0.283112	Li
104	Li4	1.0	0.840362	0.315094	0.484541	Li
105	Li5	1.0	0.857426	0.060215	0.234857	Li
106	Li6	1.0	0.779141	0.898621	0.349163	Li
107	Li7	1.0	0.488879	0.884804	0.399669	Li
108	Li8	1.0	0.764204	0.947240	0.024886	Li
109	Li9	1.0	0.572534	0.767754	0.255196	Li
110	Li10	1.0	0.737988	0.222295	0.337613	Li
111	Li11	1.0	0.042803	0.868607	0.444653	Li
112	Li12	1.0	0.251240	0.737974	0.276908	Li
113	Li13	1.0	0.454542	0.066233	0.973808	Li
114	Li14	1.0	0.840769	0.075560	0.415167	Li
115	Li15	1.0	0.401164	0.095572	0.447609	Li
116	N1	1.0	0.273056	0.087703	0.378655	N
117	N2	1.0	0.727422	0.047645	0.307673	N
118	N3	1.0	0.039621	0.436094	0.287635	N
119	N4	1.0	0.096343	0.416815	0.227498	N
120	N5	1.0	0.513305	0.031448	0.354840	N
121						