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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      0.253560      0.828990      0.685220      Ta
30 Ta2      1.0      0.534430      0.737080      0.713930      Ta
31 Ta3      1.0      0.672050      0.952020      0.274650      Ta
32 Ta4      1.0      0.962390      0.893110      0.255000      Ta
33 Ta5      1.0      0.685200      0.228500      0.797370      Ta
34 Ta6      1.0      0.981140      0.204710      0.794190      Ta
35 Ta7      1.0      0.727710      0.362690      0.427540      Ta
36 Ta8      1.0      0.975300      0.234870      0.325010      Ta
37 Ta9      1.0      0.981140      0.735240      0.034120      Ta
38 Ta10     1.0      0.149570      0.798520      0.797940      Ta
39 Ta11     1.0      0.879710      0.526620      0.542060      Ta
40 Ta12     1.0      0.901390      0.453100      0.255220      Ta
41 Cl1      1.0      0.271360      0.880780      0.849720      Cl
42 Cl2      1.0      0.520600      0.799220      0.875210      Cl
43 Cl3      1.0      0.194310      0.979280      0.633110      Cl
44 Cl4      1.0      0.354680      0.674970      0.738170      Cl
45 Cl5      1.0      0.593850      0.586780      0.765830      Cl
46 Cl6      1.0      0.109120      0.745410      0.716260      Cl
47 Cl7      1.0      0.516260      0.685180      0.549530      Cl
48 Cl8      1.0      0.267590      0.766560      0.524100      Cl
49 Cl9      1.0      0.433290      0.891190      0.661370      Cl
50 Cl10     1.0      0.678760      0.820740      0.682650      Cl
51 Cl11     1.0      0.671990      0.827320      0.395110      Cl
52 Cl12     1.0      0.929640      0.775040      0.377670      Cl
53 Cl13     1.0      0.591300      0.063150      0.374360      Cl
54 Cl14     1.0      0.794590      0.839560      0.179320      Cl
55 Cl15     1.0      0.043330      0.782170      0.155220      Cl
56 Cl16     1.0      0.542230      0.883850      0.189130      Cl
57 Cl17     1.0      0.962110      0.017660      0.134430      Cl
58 Cl18     1.0      0.705040      0.069820      0.151820      Cl
59 Cl19     1.0      0.839800      0.005260      0.350570      Cl
60 Cl20     1.0      0.092100      0.961530      0.340470      Cl
61 Cl21     1.0      0.711190      0.324080      0.939680      Cl
62 Cl22     1.0      0.973800      0.302970      0.936860      Cl
63 Cl23     1.0      0.585830      0.345080      0.724270      Cl
64 Cl24     1.0      0.825890      0.116890      0.864460      Cl
65 Cl25     1.0      0.080660      0.088090      0.867070      Cl
66 Cl26     1.0      0.569910      0.129160      0.872560      Cl
67 Cl27     1.0      0.954840      0.108980      0.652080      Cl
68 Cl28     1.0      0.692830      0.130040      0.654900      Cl
69 Cl29     1.0      0.840470      0.316500      0.727460      Cl
70 Cl30     1.0      0.096280      0.304040      0.718780      Cl
71 Cl31     1.0      0.749860      0.472750      0.295410      Cl

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72	C132	1.0	0.969570	0.359320	0.204420	C1
73	C133	1.0	0.565780	0.330850	0.387830	C1
74	C134	1.0	0.918220	0.371060	0.447260	C1
75	C135	1.0	0.137290	0.266440	0.364750	C1
76	C136	1.0	0.709970	0.487050	0.541710	C1
77	C137	1.0	0.953050	0.125130	0.457350	C1
78	C138	1.0	0.733840	0.238300	0.548130	C1
79	C139	1.0	0.784840	0.226800	0.305030	C1
80	C140	1.0	0.992850	0.110370	0.210970	C1
81	C141	1.0	0.031810	0.891000	0.090980	C1
82	C142	1.0	0.181280	0.947160	0.881390	C1
83	C143	1.0	0.816570	0.767280	0.060620	C1
84	C144	1.0	0.161030	0.716150	0.970670	C1
85	C145	1.0	0.314090	0.766390	0.771190	C1
86	C146	1.0	0.023390	0.657180	0.178810	C1
87	C147	1.0	0.098940	0.642650	0.741460	C1
88	C148	1.0	0.949810	0.586620	0.950560	C1
89	C149	1.0	0.969820	0.817940	0.861570	C1
90	C150	1.0	0.107100	0.876430	0.653240	C1
91	C151	1.0	0.997910	0.401980	0.565640	C1
92	C152	1.0	0.017140	0.336740	0.311090	C1
93	C153	1.0	0.967720	0.641610	0.630630	C1
94	C154	1.0	0.802020	0.408180	0.412890	C1
95	C155	1.0	0.813340	0.338290	0.166450	C1
96	C156	1.0	0.775930	0.465170	0.661510	C1
97	C157	1.0	0.783030	0.577610	0.231980	C1
98	C158	1.0	0.763840	0.642700	0.485940	C1
99	C159	1.0	0.979320	0.571230	0.384490	C1
100	C160	1.0	0.005100	0.514800	0.135860	C1
101	Li1	1.0	0.123470	0.893850	0.463120	Li
102	Li2	1.0	0.356100	0.791640	0.369930	Li
103	Li3	1.0	0.323070	0.059750	0.386420	Li
104	Li4	1.0	0.832600	0.091260	0.533640	Li
105	Li5	1.0	0.770020	0.829660	0.503700	Li
106	Li6	1.0	0.021320	0.915510	0.451560	Li
107	Li7	1.0	0.413140	0.613790	0.040770	Li
108	Li8	1.0	0.366230	0.389190	0.184290	Li
109	Li9	1.0	0.580460	0.402150	0.019430	Li
110	Li10	1.0	0.220200	0.146880	0.718400	Li
111	Li11	1.0	0.488700	0.130780	0.688510	Li
112	Li12	1.0	0.342560	0.282980	0.519030	Li
113	Li13	1.0	0.016750	0.747080	0.442320	Li
114	Li14	1.0	0.181330	0.759050	0.227810	Li
115	Li15	1.0	0.184830	0.541750	0.389080	Li
116	N1	1.0	0.267540	0.915080	0.406490	N
117	N2	1.0	0.874650	0.945480	0.496300	N
118	N3	1.0	0.453280	0.468380	0.081500	N
119	N4	1.0	0.350490	0.186880	0.641980	N
120	N5	1.0	0.127640	0.682630	0.353070	N
121						