

```

data_Conf9.cif
_audit_creation_method      'generated by CrystalMaker 6.3.7'
_cell_length_a              9.6007
_cell_length_b              10.2930
_cell_length_c              12.0497
_cell_angle_alpha           90.0000
_cell_angle_beta            90.0000
_cell_angle_gamma           90.0000

```

```

_symmetry_space_group_name_H-M  'P 1'
_symmetry_Int_Tables_number     1
_symmetry_cell_setting          triclinic
loop_
_symmetry_equiv_pos_as_xyz
' +x      +y      +z  '

```

```

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
H      112    0.2136  0.1465  0.0422
H      113    0.2070  0.9872  0.1232
H      114    0.3078  0.1280  0.1785
H      115    0.0332  0.2164  0.2864
Mg      1     0.0046  0.0012  0.0002
Mg      2     0.2493  0.4973 -0.0015
Mg      3     0.0039 -0.0043  0.2460
Mg      4     0.2488  0.4966  0.2496
Mg      5     0.4973  0.2766  0.1233
Mg      6     0.7458  0.2223  0.3754
Mg      7    -0.4960 -0.2774  0.3742
Mg      8    -0.2460  0.7764  0.1239
Mg     28     0.4958  0.0016  0.0016
Mg     29     0.7497  0.4995 -0.0013
Mg     30     0.5021 -0.0016  0.2502
Mg     31     0.7499  0.4989  0.2489
Mg     32     0.0030  0.2699  0.1137
Mg     33     0.2485  0.2229  0.3812
Mg     34     0.0040 -0.2769  0.3739
Mg     35     0.2536  0.7680  0.1244
Mg     56     0.0001 -0.0008  0.4983
Mg     57     0.2502  0.5017  0.4998
Mg     58    -0.0011 -0.0006  0.7497
Mg     59     0.2495  0.5024  0.7492
Mg     60     0.4965  0.2761  0.6245
Mg     61     0.7455  0.2227  0.8747
Mg     62    -0.4961 -0.2758  0.8748
Mg     63    -0.2459  0.7768  0.6247
Mg     84     0.4998 -0.0015  0.4998
Mg     85     0.7481  0.5006  0.4997
Mg     86     0.5000 -0.0002  0.7506

```

Mg	87	0.7492	0.5001	0.7490
Mg	88	0.9958	0.2764	0.6245
Mg	89	0.2443	0.2260	0.8664
Mg	90	0.0031	-0.2766	0.8749
Mg	91	0.2534	0.7769	0.6247
O	12	0.3838	0.0968	0.1305
O	13	0.6343	0.4072	0.3740
O	14	-0.3844	-0.0925	0.3746
O	15	-0.1347	0.5890	0.1241
O	16	0.1117	0.4416	0.1236
O	17	0.3607	0.0533	0.3736
O	18	-0.1142	-0.4445	0.3744
O	19	0.1270	0.9271	0.1236
O	20	0.1274	0.1678	0.0013
O	21	0.3872	0.3363	-0.0176
O	22	-0.1387	-0.1643	0.2649
O	23	0.1112	0.6575	0.2338
O	24	-0.1386	-0.1638	-0.0163
O	25	0.1116	0.6581	0.0144
O	26	0.1133	0.1675	0.2552
O	27	0.3869	0.3346	0.2659
O	40	0.8845	0.0911	0.1228
O	41	0.1336	0.4112	0.3772
O	42	0.1157	-0.0948	0.3746
O	43	0.3654	0.5887	0.1244
O	44	0.6114	0.4448	0.1244
O	45	0.8613	0.0534	0.3739
O	46	0.3889	-0.4469	0.3739
O	47	0.6373	0.9458	0.1244
O	48	0.6363	0.1628	0.0160
O	49	0.8869	0.3372	-0.0185
O	50	0.3615	-0.1642	0.2643
O	51	0.6115	0.6619	0.2336
O	52	0.3604	-0.1617	-0.0148
O	53	0.6111	0.6622	0.0154
O	54	0.6408	0.1628	0.2344
O	55	0.8925	0.3351	0.2675
O	68	0.3839	0.0910	0.6247
O	69	0.6338	0.4078	0.8739
O	70	-0.3853	-0.0909	0.8758
O	71	-0.1351	0.5918	0.6242
O	72	0.1112	0.4460	0.6246
O	73	0.3597	0.0552	0.8752
O	74	-0.1127	-0.4457	0.8734
O	75	0.1382	0.9449	0.6243
O	76	0.1375	0.1625	0.5161
O	77	0.3883	0.3366	0.4840
O	78	-0.1395	-0.1625	0.7656
O	79	0.1111	0.6637	0.7333
O	80	-0.1385	-0.1633	0.4835
O	81	0.1111	0.6628	0.5151
O	82	0.1364	0.1625	0.7322
O	83	0.3874	0.3376	0.7642
O	96	0.8841	0.0909	0.6241

O	97	0.1334	0.4103	0.8718
O	98	0.1150	-0.0929	0.8735
O	99	0.3650	0.5926	0.6244
O	100	0.6102	0.4459	0.6244
O	101	0.8610	0.0543	0.8749
O	102	0.3886	-0.4457	0.8743
O	103	0.6379	0.9452	0.6249
O	104	0.6376	0.1622	0.5156
O	105	0.8871	0.3388	0.4852
O	106	0.3618	-0.1626	0.7662
O	107	0.6113	0.6630	0.7338
O	108	0.3620	-0.1635	0.4832
O	109	0.6111	0.6628	0.5153
O	110	0.6377	0.1626	0.7337
O	111	0.8871	0.3372	0.7637
Si	9	0.4636	0.4056	0.3742
Si	10	-0.2134	-0.0938	0.3740
Si	11	0.0361	0.5893	0.1238
Si	36	0.7140	0.0930	0.1245
Si	37	0.9629	0.4098	0.3770
Si	38	0.2862	-0.0948	0.3736
Si	39	0.5362	0.5923	0.1245
Si	64	0.2132	0.0921	0.6245
Si	65	0.4632	0.4065	0.8739
Si	66	-0.2142	-0.0929	0.8754
Si	67	0.0357	0.5934	0.6244
Si	92	0.7135	0.0925	0.6247
Si	93	0.9627	0.4069	0.8725
Si	94	0.2855	-0.0929	0.8751
Si	95	0.5358	0.5938	0.6247