Atomic coordinates for CsNaMgP2O7

	x	y	z	x	y	z
P2	0	0.06	0.721	0	0.9	6.991
O4	0.236	0.092	0.797	1.236	1.377	7.729
O5	0	0.113	0.574	0	1.689	5.563
O2	0	-0.036	0.684	0	-0.537	6.638
O4iv	-0.236	0.092	0.797	-1.236	1.377	7.729
P1	0	0.221	0.565	0	3.307	5.484
O5	0	0.113	0.574	0	1.689	5.563
O1	0.239	0.253	0.633	1.254	3.778	6.139
O3	0	0.24	0.416	0	3.597	4.037
O1iv	-0.239	0.253	0.633	-1.254	3.778	6.139

Bond valence calculation for CsNaMgP2O7

	bond distances	bond valence
O4	1.516	1.26
O5	1.631	0.968
O2	1.479	1.371
O4iv	1.516	1.26
P2		4.86
O5	1.619	0.995
O1	1.491	1.334
O3	1.476	1.381
O1iv	1.491	1.334
P1		5.045

	CsNaMgP2O7			Cart. Coord.		
Z		charges	x	y	z	distance
15	P2	4.86	0	0.9	6.991	
8	O4	-1.26	1.236	1.377	7.729	1.516
8	O5	-0.968	0	1.689	5.563	1.631
8	O2	-1.371	0	-0.537	6.638	1.479
8	O4iv	-1.26	-1.236	1.377	7.729	1.516

x	y	z	unitized	C_grav	C_charge	u_debye
0.815	0.315	0.487	1	0.348	0.477	15.906
0	0.484	-0.875	1.001	0.348	0.469	16.336
0	-0.972	-0.239	1.001	0.348	0.48	15.77
-0.815	0.315	0.487	1	0.348	0.477	15.906

	Dipole Moment		Magnitude	
x	y	z		
0	2.594	-2.576	3.656	esu*cm
	Cell Volume		760.05	
	Z		4	
	Dipole Moment =		0.019	esu*cm/A^3
		pm/V	4.59E+07	conversion to pm/V cm/A^3

			Cart. Coord.			
Z		charges	x	y	z	distance
15	P1	5.045	0	3.307	5.484	
8	O5	-0.995	0	1.689	5.563	1.619
8	O1	-1.334	1.254	3.778	6.139	1.491
8	O3	-1.381	0	3.597	4.037	1.476
8	O1iv	-1.334	-1.254	3.778	6.139	1.491

x	y	z	unitized	C_grav	C_charge	u_debye
0	-0.999	0.049	1	0.348	0.475	16.718
0.841	0.316	0.439	1	0.348	0.484	16.186
0	0.197	-0.981	1	0.348	0.485	16.125
-0.841	0.316	0.439	1	0.348	0.484	16.186

	Dipole Moment		Magnitude	
x	y	z		
0	-3.285	-0.783	3.377	esu*cm
	Cell Volume		760.05	
	Z		4	
	Dipole Moment =		0.018	esu*cm/A^3
		pm/V	4.24E+07	conversion to pm/V cm/A^3

Total Dipole Moment for P2O7 =

	Dipole Moment		**Magnitude**	
x	**y**	**z**		
0	**0.691**	**-3.359**	**3.43**	
	Cell Volume		**760.05**	
	Z		**4**	
	Total Dipole Moment for P2O7 =		**0.018**	
		pm/V	**4.31E+07**	**conversion to pm/V cm/A^3**