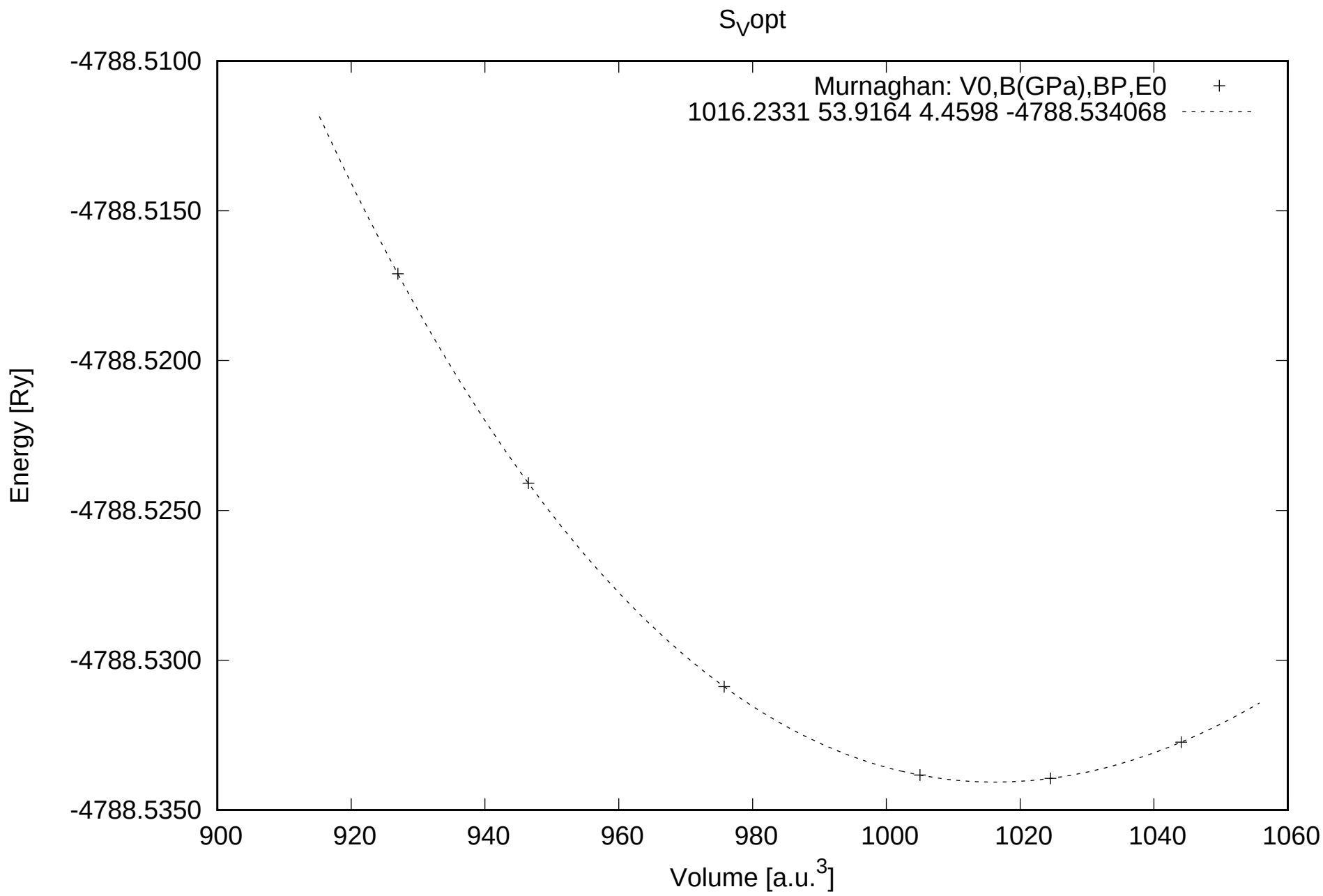
S_Vopt
Murnaghan: V0,B(GPa),BP,E0
1016.2331 53.9164 4.4598 -4788.534068
-4788.5100
-4788.5150
-4788.5200
-4788.5250
-4788.5300
-4788.5350
Energy [Ry]
900
920
940
960
980
1000
1020
1040
1060
Volume [a.u.^3]