INPUT FILES

EOS V1 - VX	SCELPHONO	SCELPHONO	...	SCELPHONO
EOS.out	V1_T.out	V2_T.out		VX_T.out

PROGRAM

QHA_master.py
blocking.sh
help_spacing.awk
temperature.sh

RESULTS

1) done_modes_sorted.dat

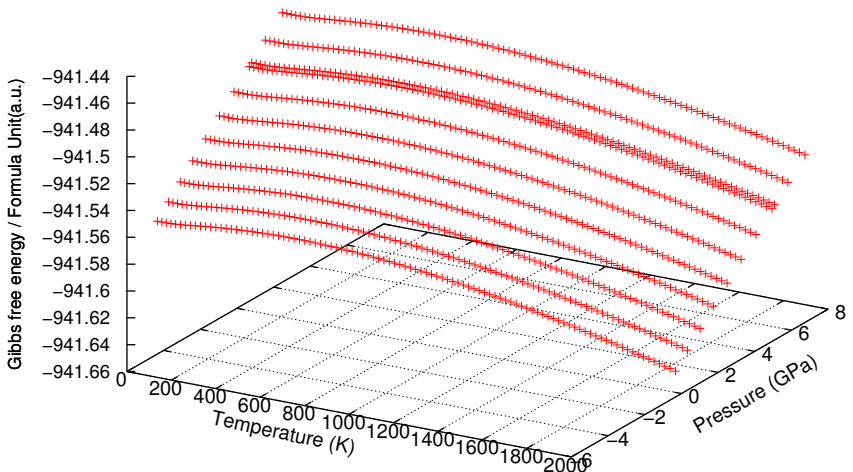
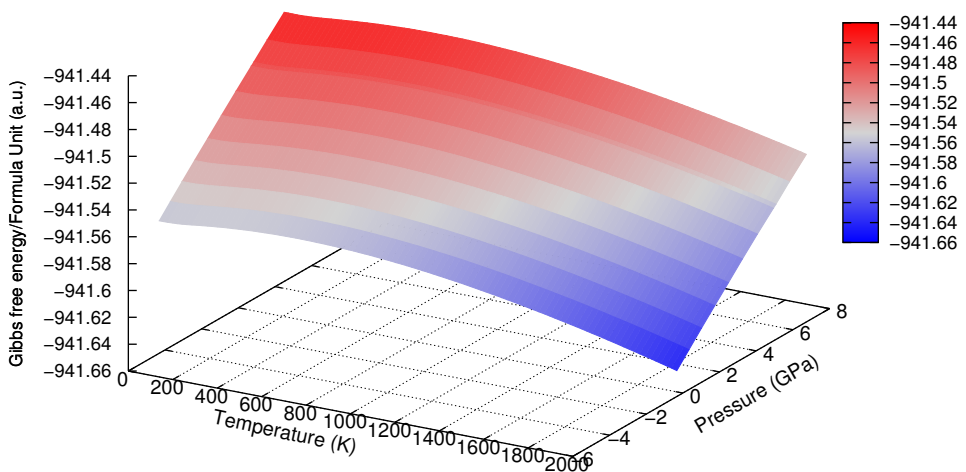
c	*d*	*f*	Mode number
-0.1078272675699	29.2742844676026	-1844.2472278933453	1
…	…	…	…

2) Thermo_with_header.dat

All per formula unit:

Volume	P(0K)	P	EL	E0	ET	S	TS	C_v	G	T
…	…	…	…	…	…	…	…	…	…	…

3) plot_scatter.eps



4) plot_palette.eps