

Chapter 1

Results

For Cr_2O_3 we determine the parameters of the effective Heisenberg model introduced in Chapter.2

1.1 Table

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Chapter reference Fig??.

	A_{2u} modes		E_u modes			
LDA+U (this work)	407	574	311	447	562	635
PBE (Ref. [?])	388	522	297	427	510	610
Expt. (Ref. [?])	402	533	305	440	538	609

Table1.1: Phonon frequencies (cm^{-1})