

D1. Optimized position co-ordinates of Fe₂O₃

Fe	0	0	0.353772
Fe	0	0	0.646228
Fe	0	0	0.146228
Fe	0	0	0.853772
Fe	0.666667	0.333333	0.687105
Fe	0.666667	0.333333	0.979561
Fe	0.666667	0.333333	0.479561
Fe	0.666667	0.333333	0.187105
Fe	0.333333	0.666667	0.020439
Fe	0.333333	0.666667	0.312895
Fe	0.333333	0.666667	0.812895
Fe	0.333333	0.666667	0.520439
O	0.304508	0	0.25
O	0.695492	0	0.75
O	-2E-16	0.304508	0.25
O	2E-16	0.695492	0.75
O	0.695492	0.695492	0.25
O	0.304508	0.304508	0.75
O	0.971175	0.333333	0.583333
O	0.362158	0.333333	0.083333
O	0.666667	0.637842	0.583333
O	0.666667	0.028825	0.083333
O	0.362158	0.028825	0.583333
O	0.971175	0.637842	0.083333
O	0.637842	0.666667	0.916667
O	0.028825	0.666667	0.416667
O	0.333333	0.971175	0.916667
O	0.333333	0.362158	0.416667
O	0.028825	0.362158	0.916667
O	0.637842	0.971175	0.416667

D2. Gamma-point phonon vibrational frequency (in THz) of Fe₂O₃ with ⁵⁴Fe

18.94963	11.9118	8.785107	4.976733
18.94963	11.75395	8.785107	4.976733
18.88743	11.75395	8.785107	4.976733
18.88743	11.75395	8.785107	4.976658
18.86998	11.75395	8.498437	4.976658
16.73624	11.5265	8.498437	4.965504
16.4257	11.5265	8.132449	4.965504
16.4257	11.4599	8.132449	4.951535
16.20127	11.2064	8.132449	2.756525
16.20127	11.2064	8.132449	2.756525
15.90627	11.2064	8.030458	2.756525
15.90627	11.2064	8.030458	2.756525
15.90627	11.17155	7.904228	
15.90627	11.17155	7.904228	
15.03794	10.66844	7.904228	
15.03794	10.66844	7.904228	
14.70216	10.27276	7.654881	
14.70216	9.447885	6.785507	
14.70216	9.447885	6.785507	
14.70216	9.447885	6.624261	
14.22516	9.447885	6.612276	
14.22516	8.881463	6.612276	
14.11366	8.881463	6.148013	
13.61719	8.872957	6.148013	
11.9118	8.872957	4.976733	

D3. Gamma-point phonon vibrational frequency (in THz) of Fe₂O₃ with ⁵⁷Fe

18.92345	11.88186	8.693901	4.863411
18.92345	11.73414	8.693901	4.85763
18.87108	11.73414	8.691403	4.85763
18.81711	11.73414	8.691403	4.85763
18.81711	11.73414	8.44892	4.85763
16.7385	11.46975	8.44892	4.846601
16.43136	11.44673	8.037194	4.846601
16.43136	11.44673	8.037194	4.820013
16.2011	11.16018	8.037194	2.698535
16.2011	11.16018	8.037194	2.698535
15.90871	11.16018	8.021366	2.698535
15.90871	11.16018	8.021366	2.698535
15.90871	11.13055	7.751026	
15.90871	11.13055	7.751026	
15.03056	10.63011	7.751026	
15.03056	10.63011	7.751026	
14.69717	9.998558	7.599126	
14.69717	9.31046	6.6075	
14.69717	9.31046	6.6075	
14.69717	9.31046	6.448638	
14.22004	9.31046	6.443838	
14.22004	8.69875	6.443838	
14.11122	8.69875	5.994637	
13.60645	8.693901	5.994637	
11.88186	8.693901	4.863411	