



Figure 14. EFG V^* versus flattening angle for different bond lengths at $T = 0$ K for different clusters. (a) FeO₆¹⁰⁻, squares, $d = 2.06$ Å; circles, $d = 2.11$ Å; triangles, $d = 2.16$ Å; $V^* = 0$ au at ψ_{ideal} (not shown) for all d ; (b) Fe(OH)₆⁴⁻, squares, $d = 2.06$ Å; circles, $d = 2.11$ Å; triangles, $d = 2.16$ Å; (c) 7-oct., squares, $d_{\text{Fe}} = d_{\text{Mg}} = 2.06$ Å; circles, $d_{\text{Fe}} = d_{\text{Mg}} = 2.11$ Å; triangles, $d_{\text{Fe}} = 2.11$ Å and $d_{\text{Mg}} = 2.06$ Å.