



**Figure 14.** EFG  $V^*$  versus flattening angle for different bond lengths at  $T = 0$  K for different clusters. (a) FeO<sub>6</sub><sup>10-</sup>, squares,  $d = 2.06$  Å; circles,  $d = 2.11$  Å; triangles,  $d = 2.16$  Å;  $V^* = 0$  au at  $\psi_{\text{ideal}}$  (not shown) for all  $d$ ; (b) Fe(OH)<sub>6</sub><sup>4-</sup>, 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.