

	E _b	M	D	G		E _b	M	G	D
Ti ₁	N/A	2.00	N/A	R ₃	Fe ₁	N/A	4.00	N/A	R ₃
Ti ₂	1.39	1.00	1.94	D _{∞h}	Fe ₂	1.08	3.00	1.99	D _{∞h}
Ti ₃	1.86	1.33	2.34	D _{3h}	Fe ₃	1.42	2.67	2.16	D _{3h}
Ti ₄	2.38	1.00	2.49	D _{2d}	Fe ₄	1.98	3.50	2.25	D _{2d}
Ti ₅	2.72	0.04	2.52	D _{3h}	Fe ₅	2.30	3.60	2.38	C _{2v}

Table 1: The ground states structures of bare Ti_N and Fe_N (N=1-5). E_b: binding energy (eV), M: The average magnetic moment (μ_B) per atom, S: Symmetry Group, D: The average bond length in Å.