Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1998, 37(16), 4059-4065, DOI:10.1021/ic971608k

Ni2-N2'-N2	56.8(9)	F5-F4-F6	62.7(5)
Ni2-N2'-C6	102.4(10)	P-F5-F3	45.7(4)
Ni2-N2'-C20	104.4(11)	P-F5-F4	46.8(4)
N2-N2'-C6	62.8(11)	F3-F5-F4	60.6(4)
N2-N2'-C20	151.5(15)	P-F6-F1	45.7(4)
C6-N2'-C20	145.7(14)	P-F6-F2	46.0(4)
Ni2-N4'-N4	79.2(10)	P-F6-F4	45.2(4)
Ni2-N4'-N9	77.0(10)	F1-F6-F2	59.8(5)
Ni2-N4'-C10	110.4(9)	F1-F6-F4	90.9(5)
Ni2-N4'-C26	119.0(10)	F2-F6-F4	61.9(4)
N4-N4'-N9	143.9(15)	N12-C33-C34	177.0(17)
N4-N4'-C10	48.3(9)	N13-C35-C36	174.8(16)

Figure S1. Crystal structure of $[Ni_5(tpda)_4(CN)_2]$, (**2**). Atoms are shown as 20% thermal vibrational ellipsoids.

Figure S2. Crystal structure of $[Ni_5(tpda)_4(N_3)_2]$, (**3**). Atoms are shown as 20% thermal vibrational ellipsoids.

Figure S3. Crystal structure of $[Ni_5(tpda)_4(CH_3CN)_2]^{2+}$, (**5**). Atoms are shown as 30% thermal vibrational ellipsoids.

Figure S4 Molecular orbital diagram of Five Linear Ni_5 system for $[Ni_5(III)_4(NCS_2]$.

Figure S5. Magnetic data for $[Ni_5(\mu_5\text{-}tpda)_4(N_3)_2]$, (**3**). Solid line represents the result of theoretical simulation. O is the observed χ_M and □ the observed μ_{eff}.

Figure S6. Magnetic data for $[Ni_5(\mu_5\text{-}tpda)_4(NCS)_2]$, (**4**). Solid line represents the result of theoretical simulation. O is the observed χ_M and □ the observed μ_{eff}.

Figure S7. Magnetic data for $[Ni_5(\mu_5\text{-}tpda)_4(CH_3CN)_2]^{2+}$, (**5**). Solid line represents the result of theoretical simulation. O is the observed χ_M and □ the observed μ_{eff}.

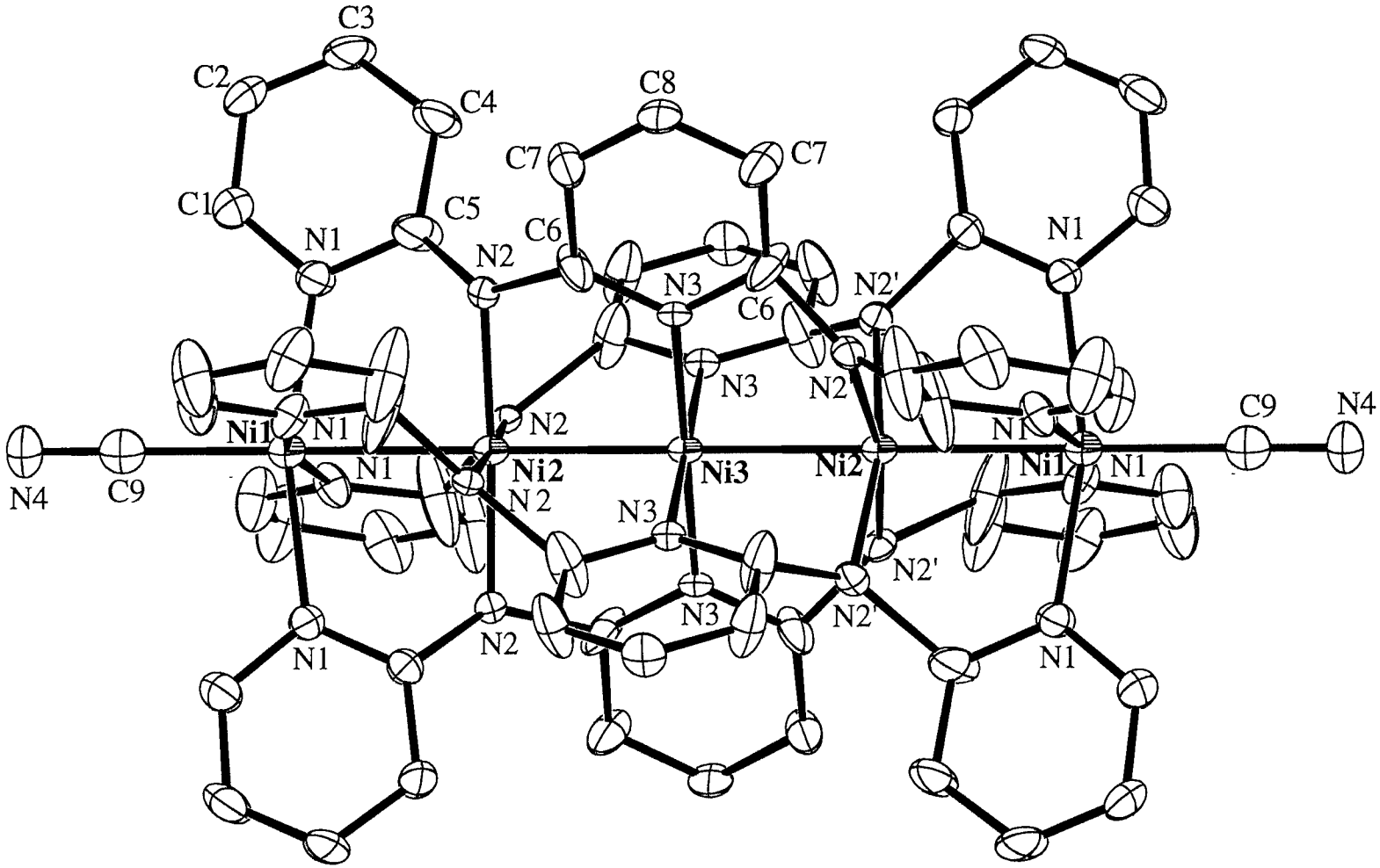
C3
C2
C4
C8
C7
C7
C1
C5
C6
N1
N2
N3
C6
N2'
N1
N3
N2'
C9
N4
Ni1
N1
N2
N1
Ni1
N1
N4
C9
N1
Ni2
Ni3
Ni2
N2
N3
N2'
N3
N2'
N2
N1
N1

Figure S1

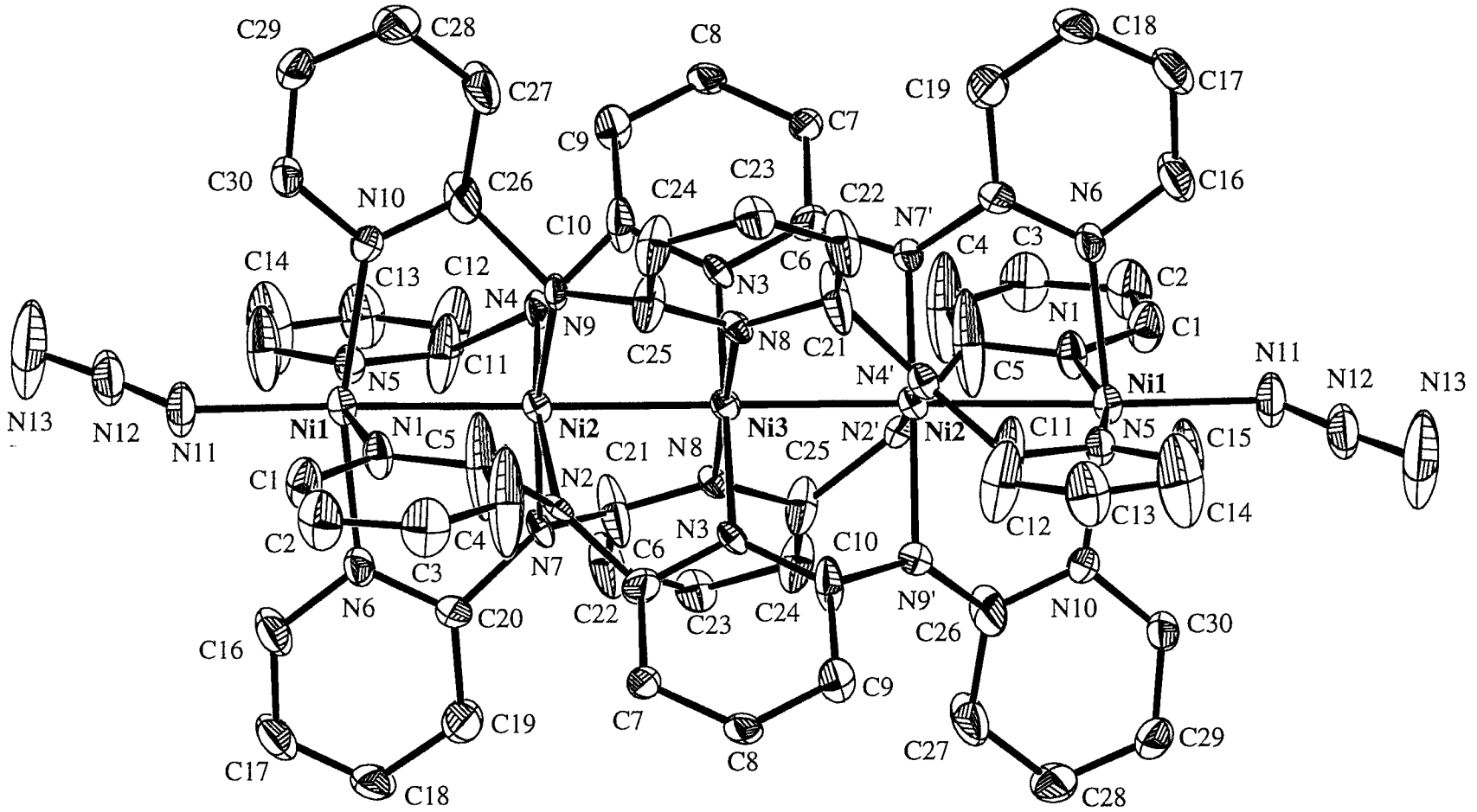
C29
C28
C27
C30
N10
C26
C14
C13
C12
N4
N5
C11
N13
N12
N11
Ni1
N1
C5
C1
C2
C4
C3
N6
C20
C16
C19
C17
C18
C8
C9
C7
C10
C24
C23
C22
N7'
C6
N3
N9
C25
N8
C21
N2
N7
C6
C22
C23
C24
C10
N9'
C26
C7
C8
C9
Ni2
Ni3
N2'
N4'
Ni2
C18
C19
C17
C16
N6
C4
C3
C2
N1
C1
C5
Ni1
N11
N12
N13
C11
N5
C15
C12
C13
C14
N10
C30
C27
C29
C28

Figure S2

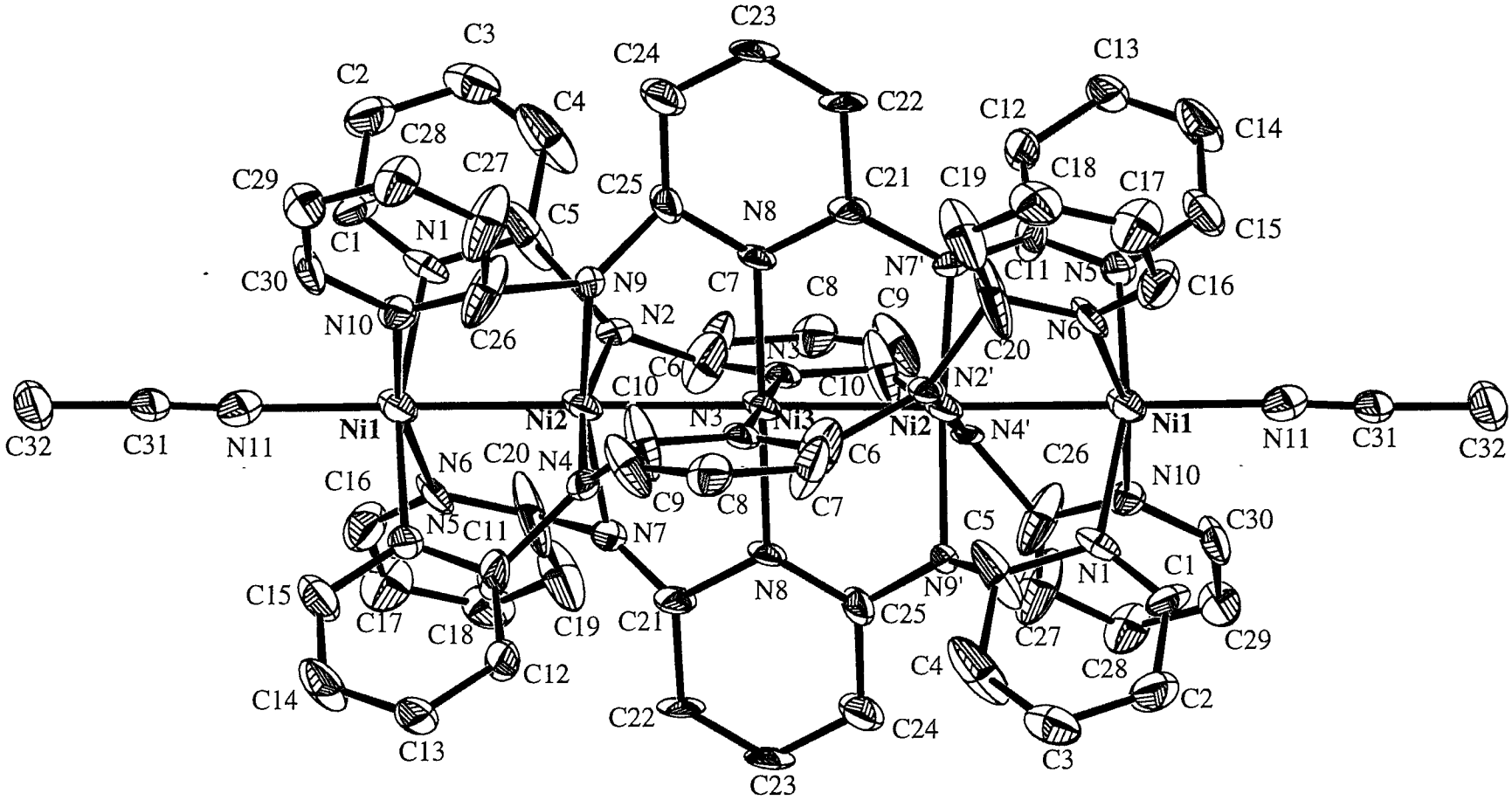
C23
C3
C24
C13
C2
C22
C4
C12
C14
C28
C27
C25
C21
C19
C18
C17
C29
N8
C5
C15
C1
N1
N7'
C11
N5
C30
N9
C7
C8
C9
C16
N10
N2
C26
N3
C20
N6
C6
C10
C10
N2'
C32
C31
N11
Ni1
Ni2
N3
Ni3
Ni2
N4'
Ni1
N11
C31
C32
C16
N6
C20
N4
C26
C6
N10
C9
C8
C7
C5
C30
N5
C11
N7
N1
C1
C15
N8
N9'
C17
C18
C19
C21
C25
C27
C29
C12
C4
C28
C14
C22
C24
C2
C13
C3
C23

Figure S3

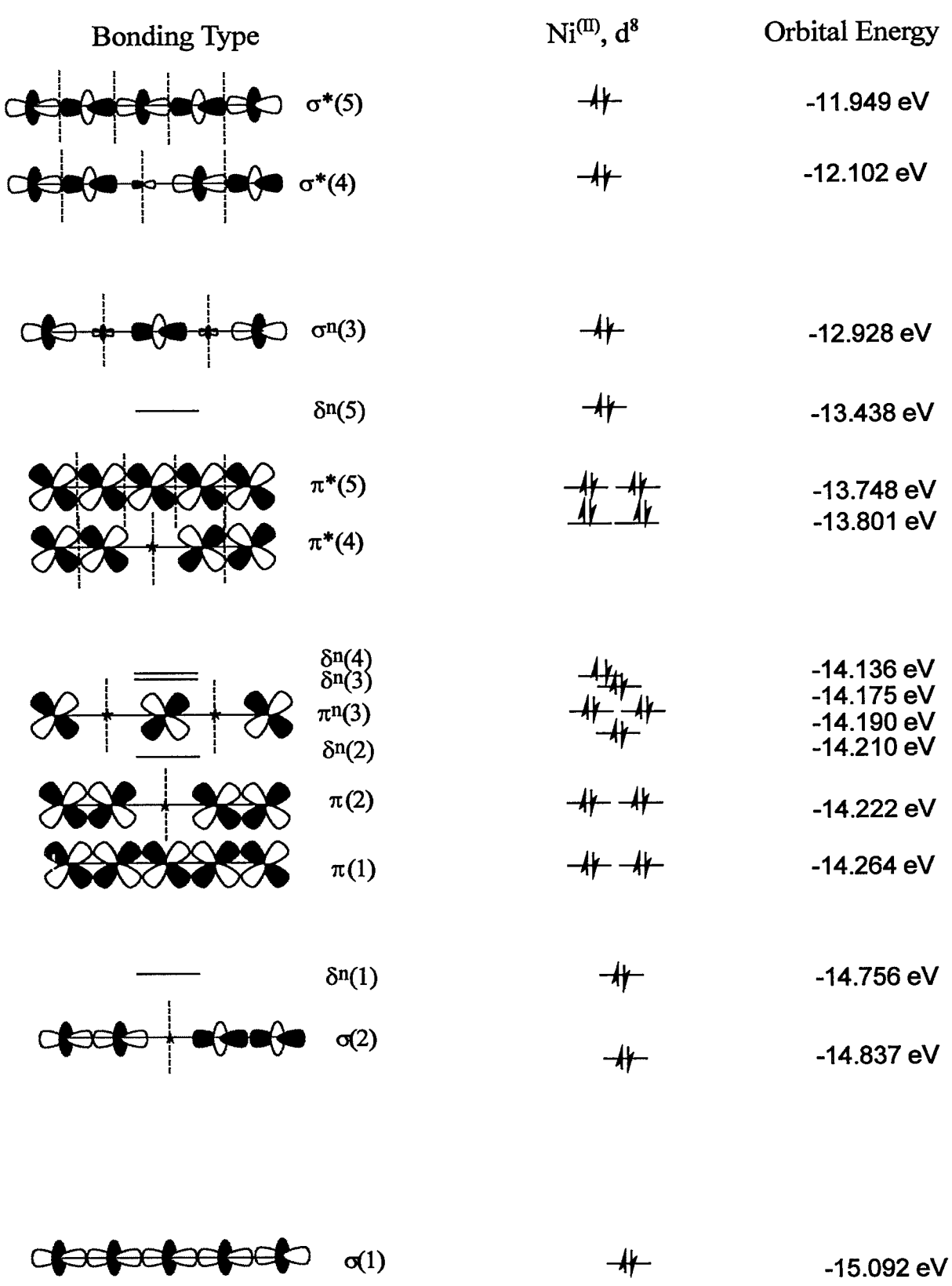

Figure S4: Molecular Orbital Diagram of Five Linear Ni_5 system for $[Ni_5(tpda)_4(NCS)_2]$ Complexes

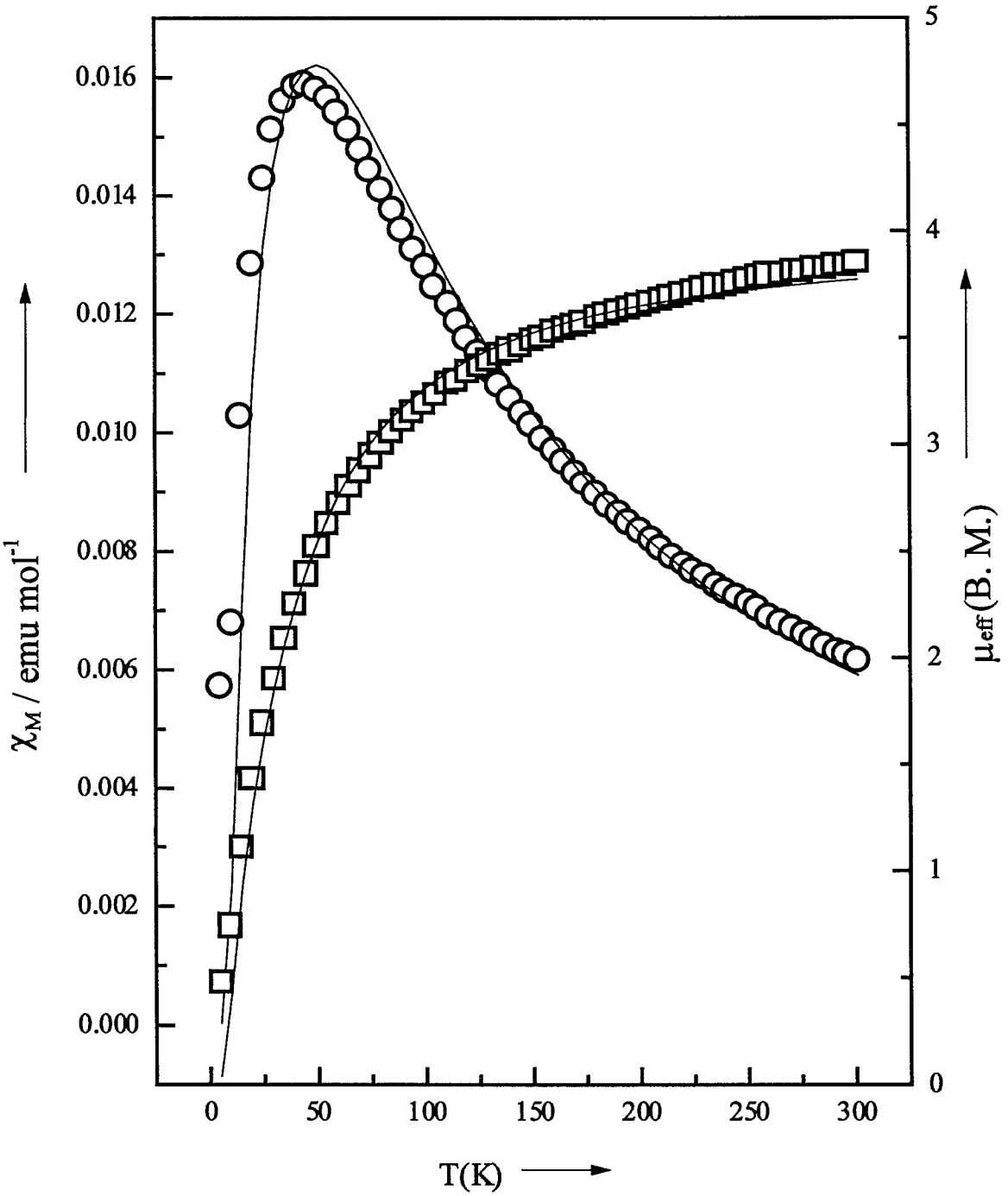
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
χ_M / emu mol^{-1}
0
50
100
150
200
250
300
T(K)
5
4
3
2
1
0
μ_{eff}(B. M.)

Figure S5

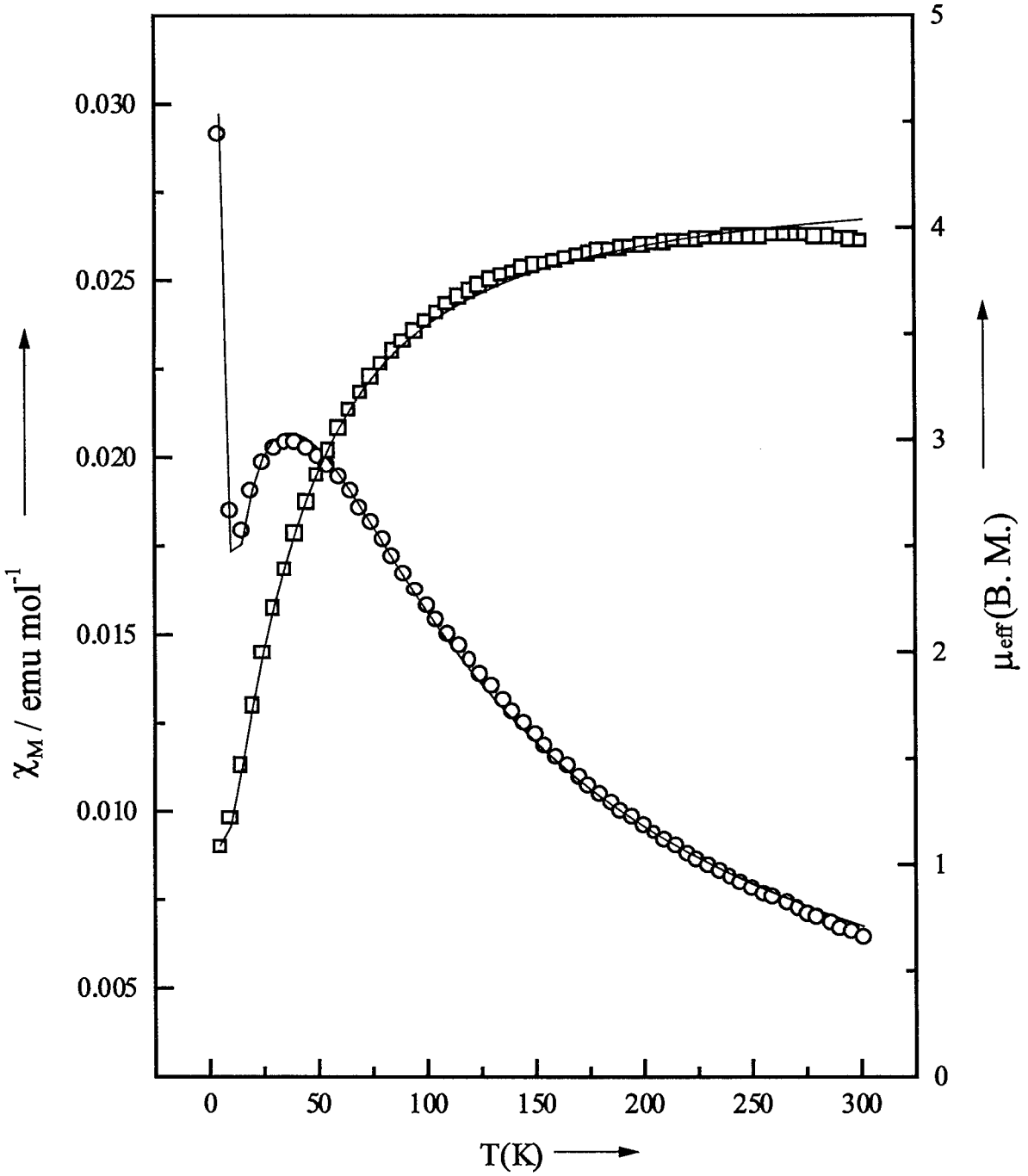
0.030
0.025
0.020
0.015
0.010
0.005
χ_M / emu mol^{-1}
5
4
3
2
1
0
μ_{eff}(B. M.)
0
50
100
150
200
250
300
T(K)

Figure S6

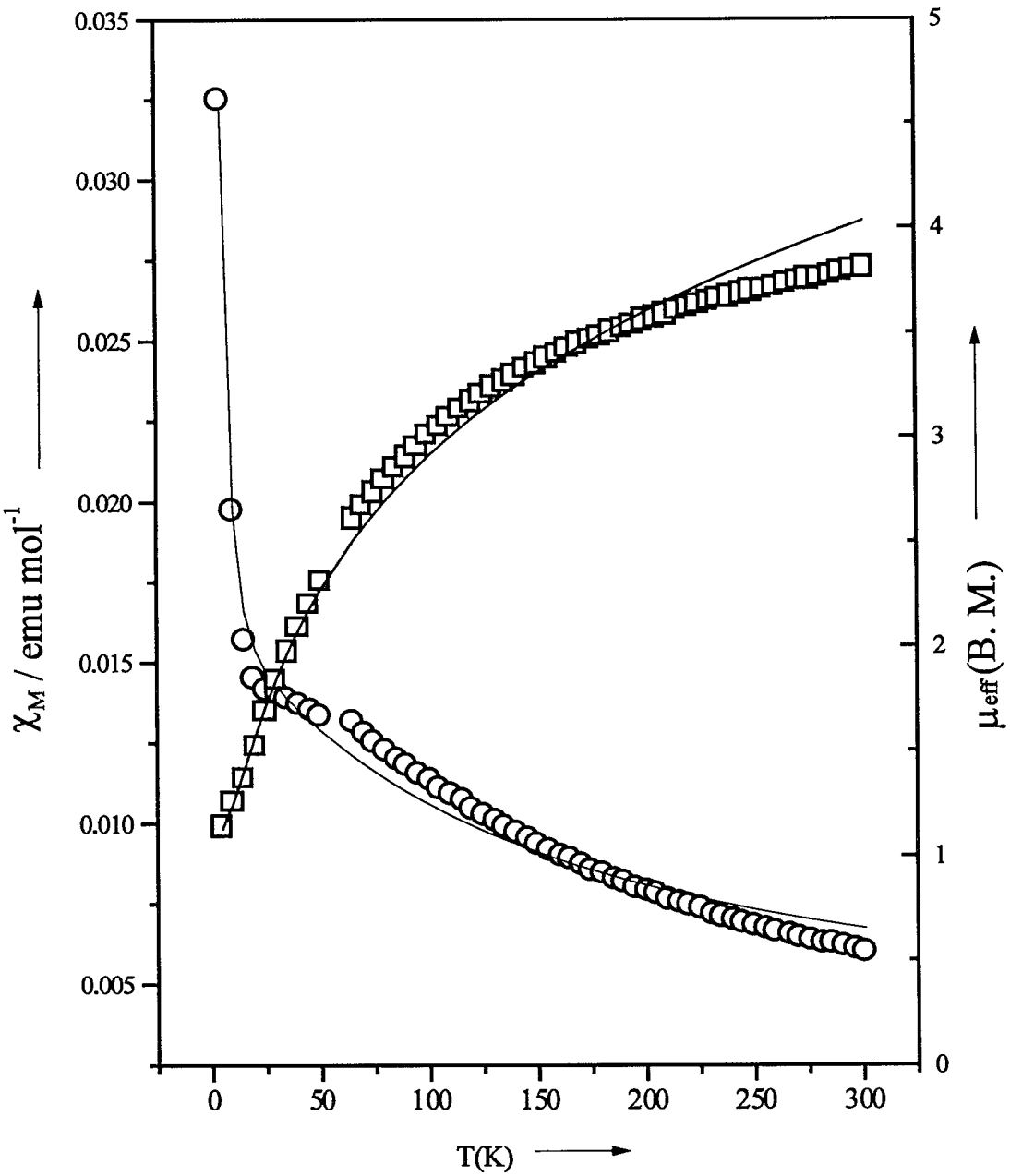
0.035
0.030
0.025
0.020
0.015
0.010
0.005
5
4
3
2
1
0
0
50
100
150
200
250
300
T(K)
χ_M / emu mol^{-1}
μ_{eff}(B. M.)

Figure S7