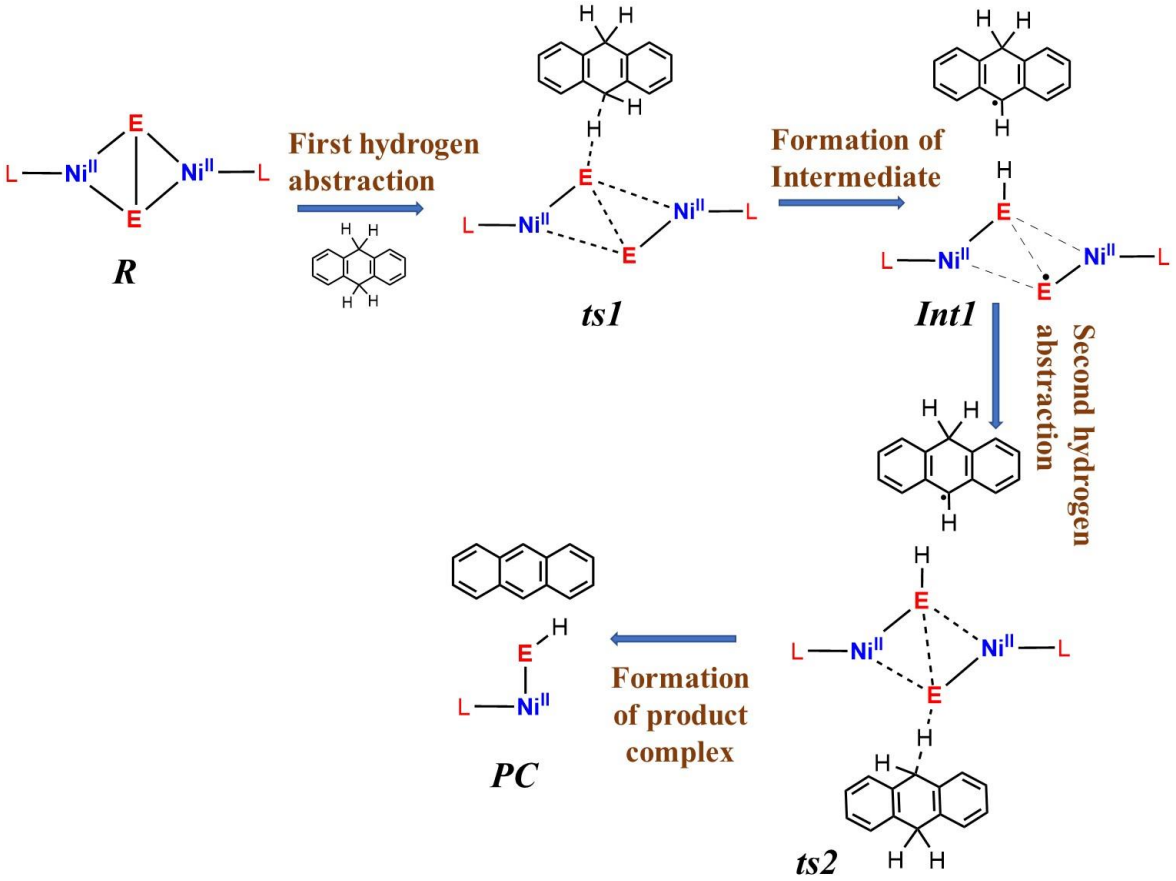
Supporting Information on

The Interplay of Covalency, Cooperativity, and Coupling Strength in Governing C–H Bond Activation in Ni_2E_2 (E = O, S, Se, Te) Complexes

Sunita Sharma,[a] Bhawana Pandey,[a] and Gopalan Rajaraman*[a]

[a] Department of Chemistry, Indian Institute of Technology Bombay, Mumbai-400076, India. E-mail: rajaraman@chem.iitb.ac.in

Table of Contents



Scheme 1. The proposed mechanism for the reactivity of complexes **1-4** towards the DHA molecule.

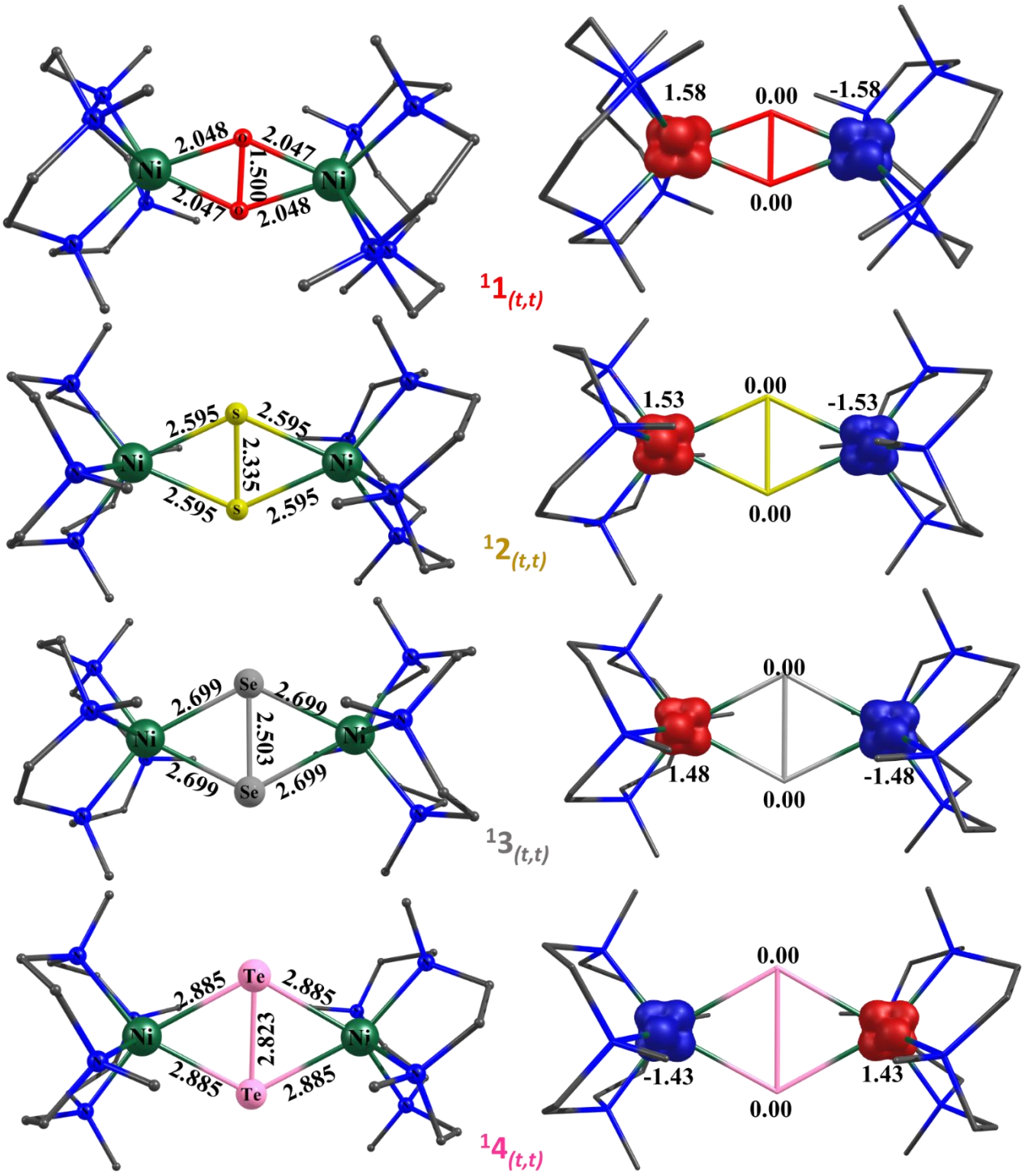


Figure S1. The optimized structures and its corresponding spin density plot for complexes ^{1}**1-4**$_{(t,t)}$ ground state reactant.

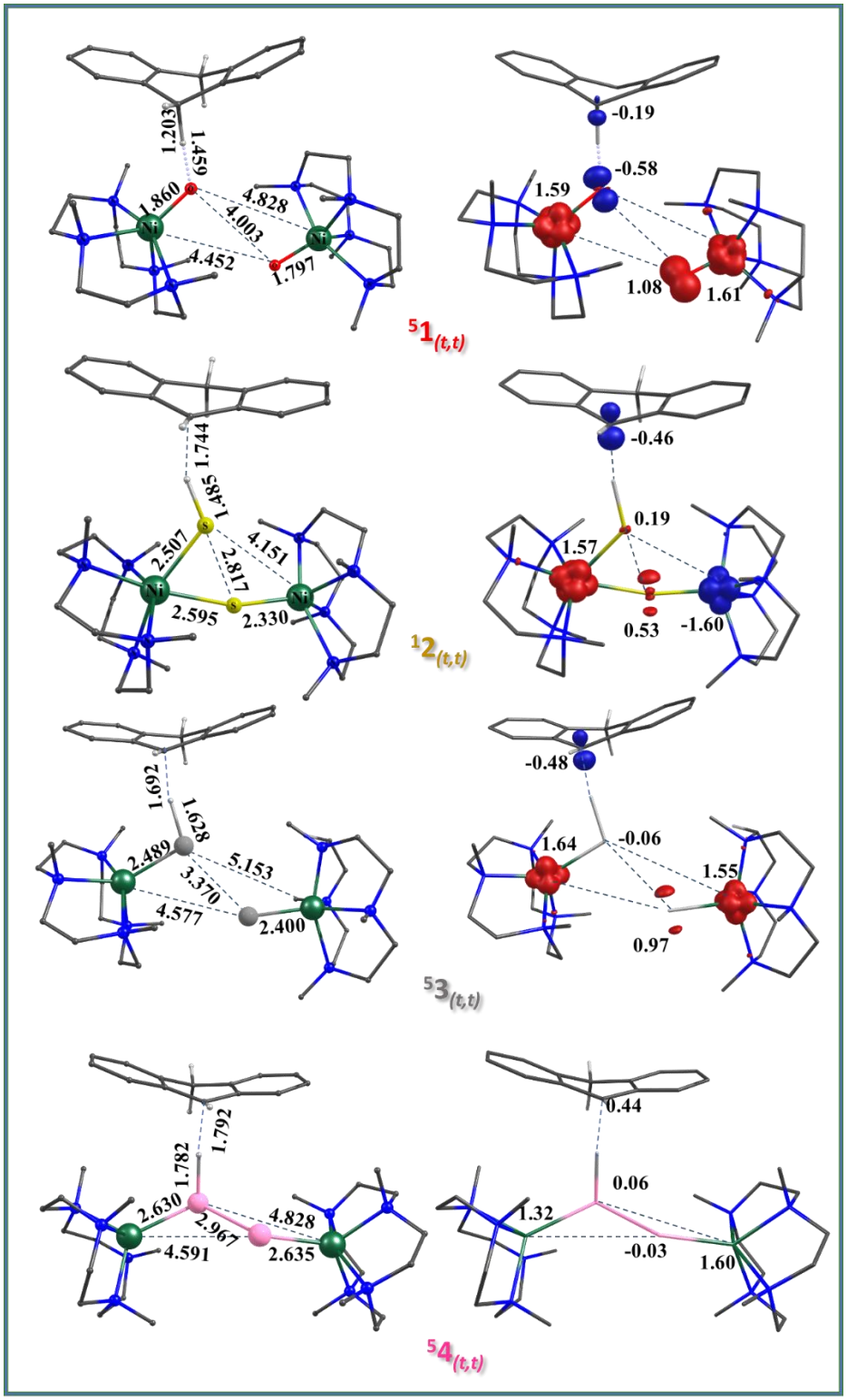


Figure S2. The optimized structures and its corresponding spin density plot of the ground state of first hydrogen abstraction transition state (**ts1**) for complexes **1**-**4**.

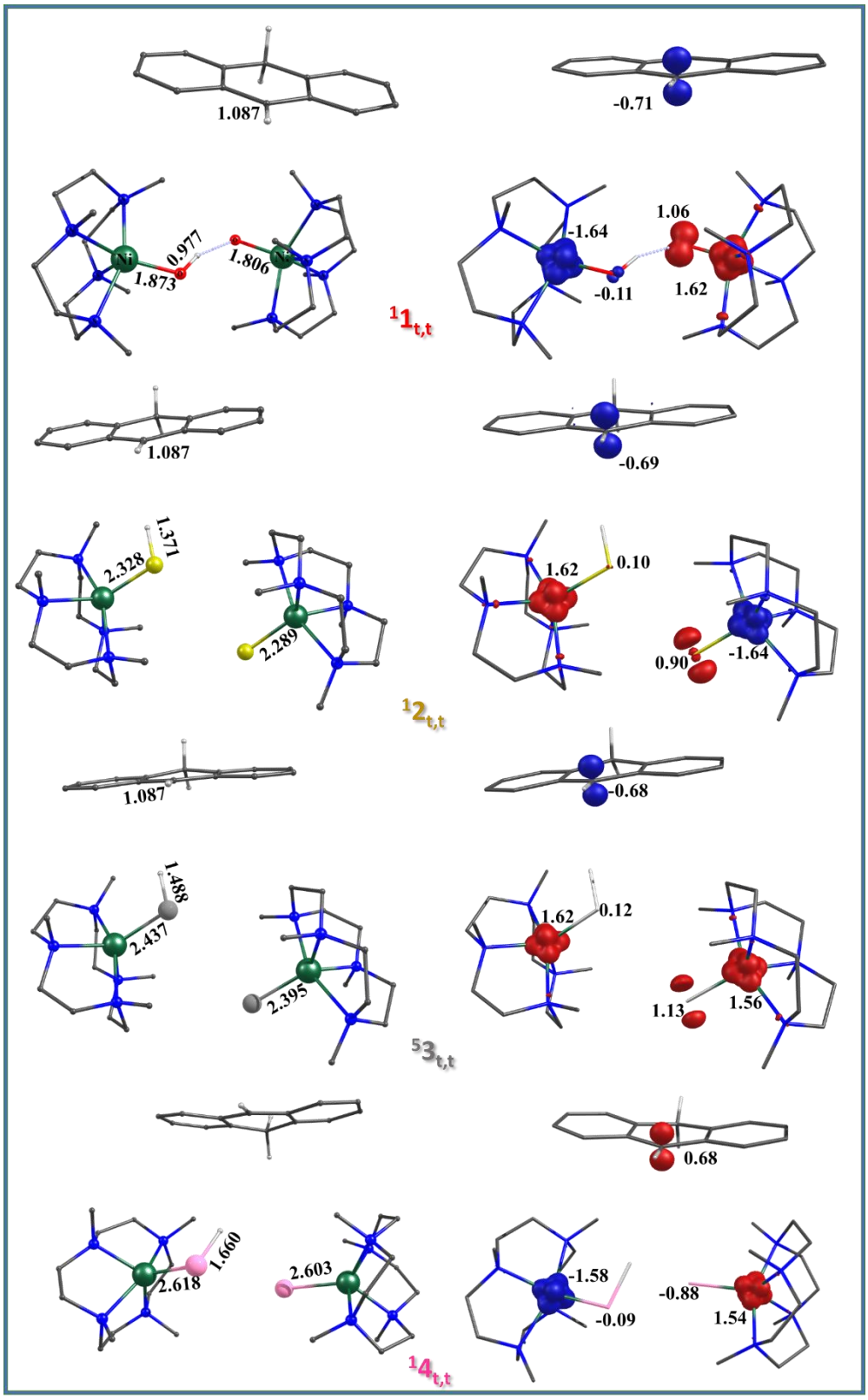


Figure S3. The optimized structures and its corresponding spin density plot of the ground state of intermediate species (**Int1**) for complexes **1-4.**

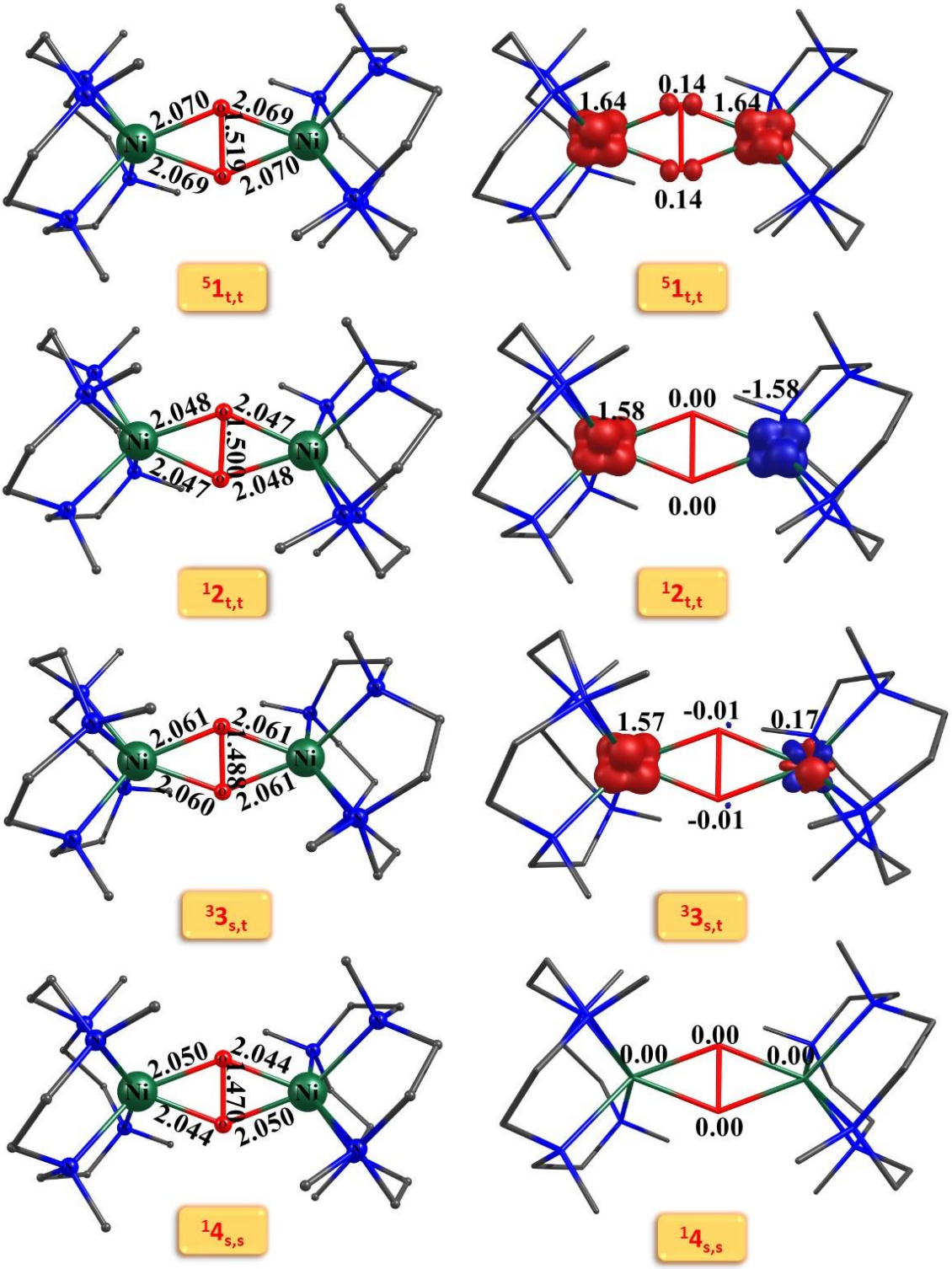


Figure S4. The optimized structures of reactant **1** and its corresponding spin density plot. Here all the hydrogen atoms are omitted for clarity.

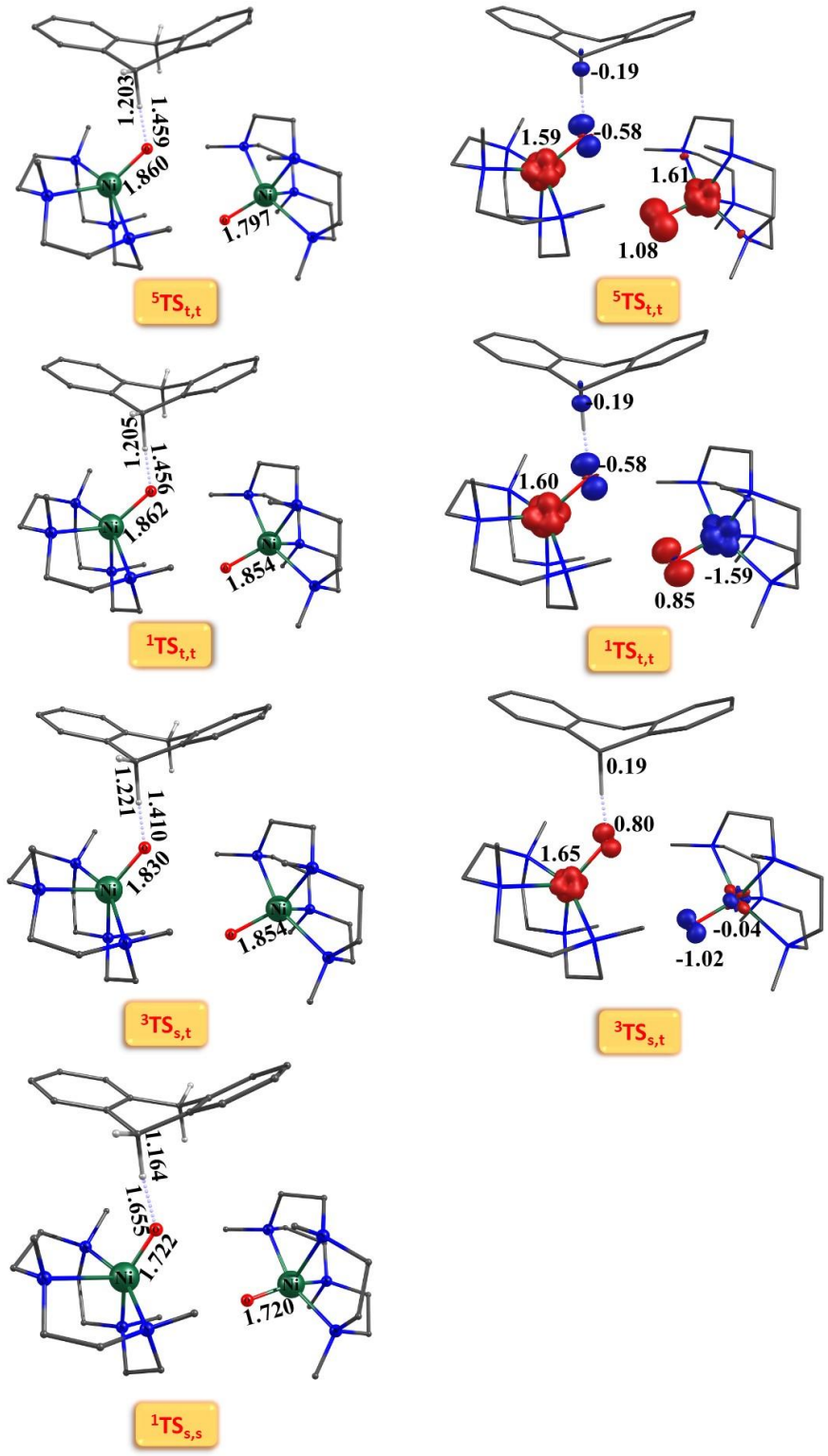


Figure S5. The optimized structures of the first hydrogen abstraction transition state (***ts1***) of complex **1**, and its corresponding spin density plot. Here all the hydrogen atoms (except alpha position hydrogens of the middle ring of the DHA substrate) are omitted for clarity.

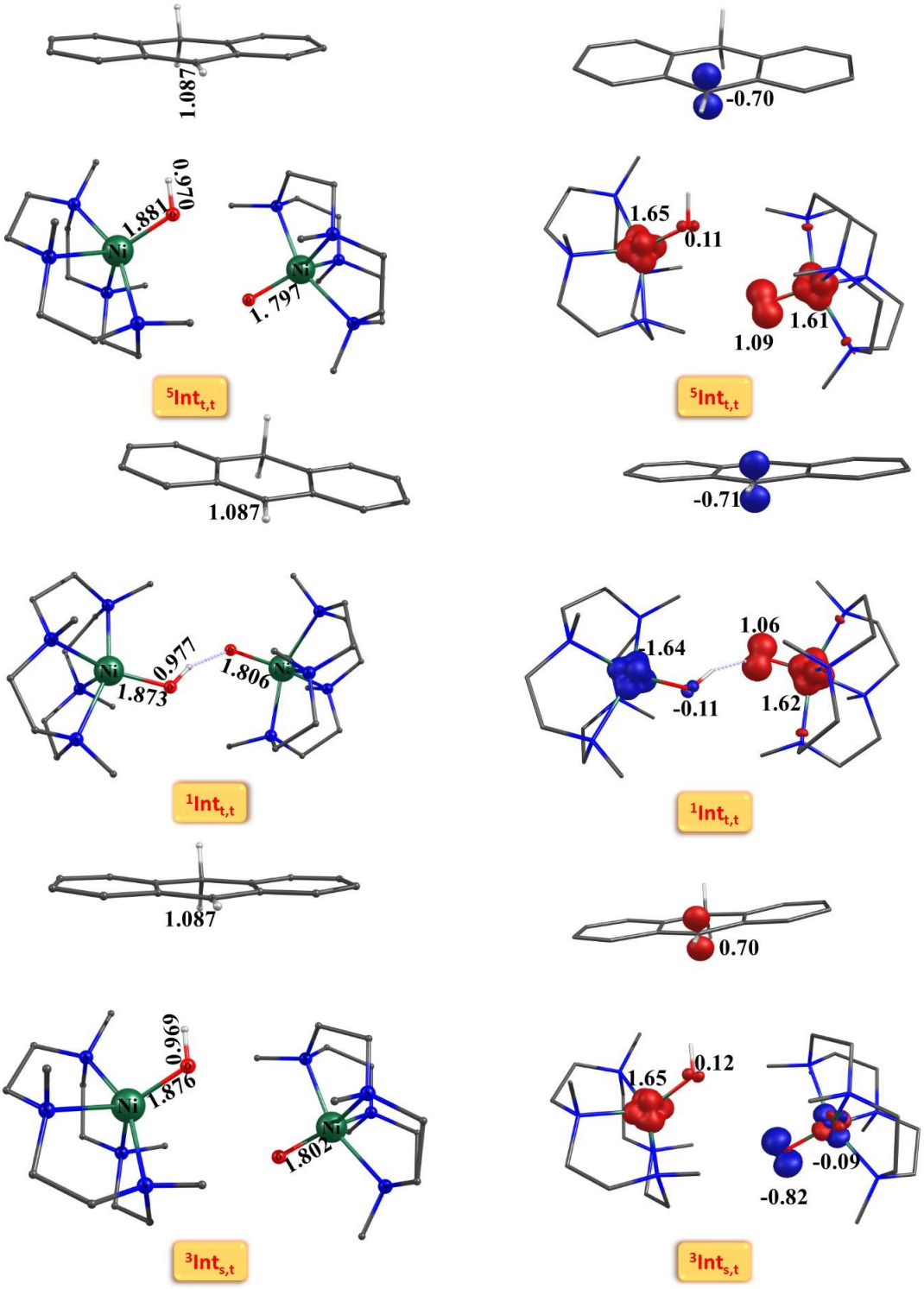


Figure S6. The optimized structure of intermediates of complex **1** and its corresponding spin density plot. Here all the hydrogen atoms (except alpha position hydrogens of the middle ring of the DHA substrate and abstracted hydrogen atom by the chalcogenide group) are omitted for clarity.

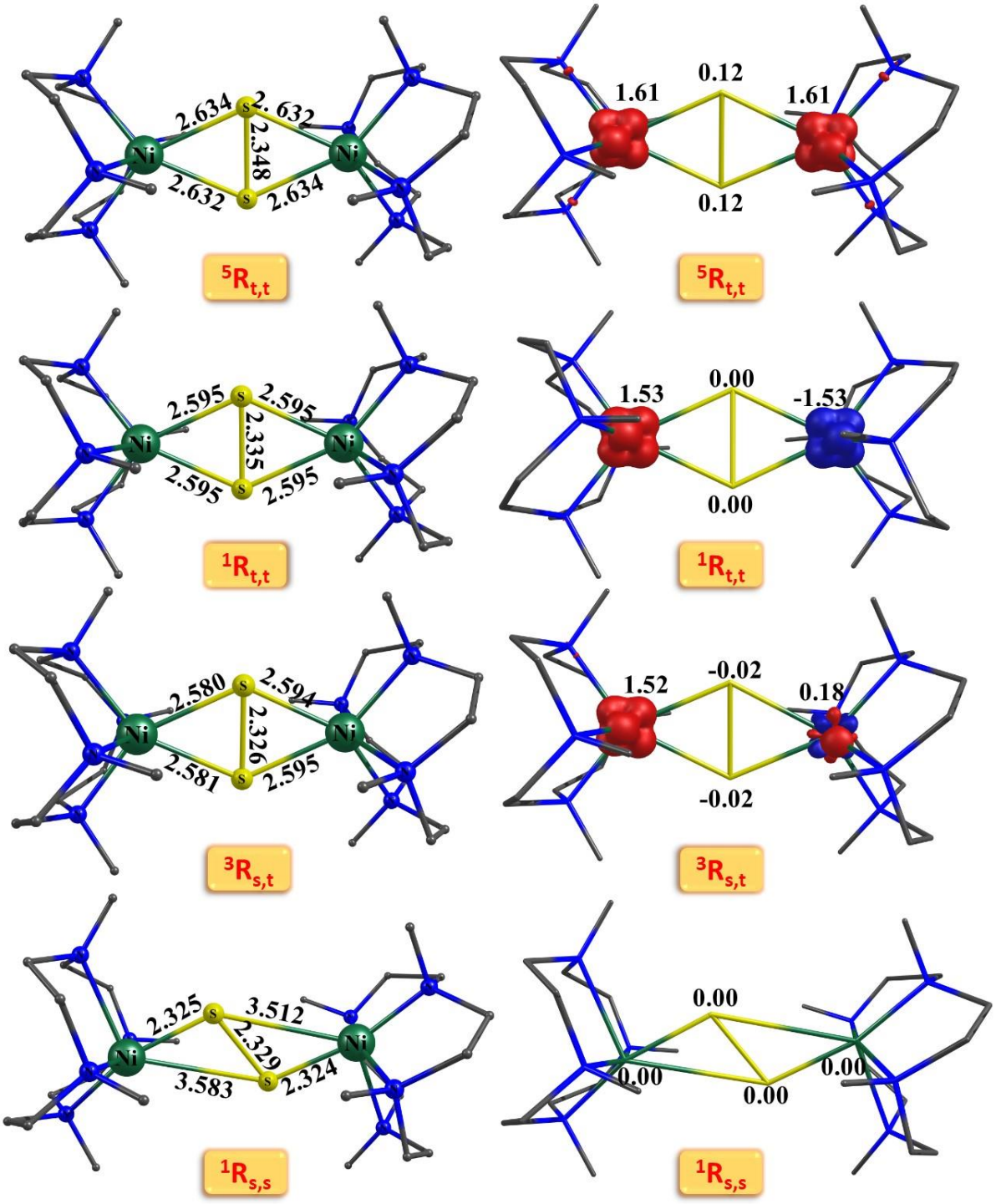


Figure S7. The optimized structure of reactant **2** and its corresponding spin density plot. Here all the hydrogen atoms are omitted for clarity.

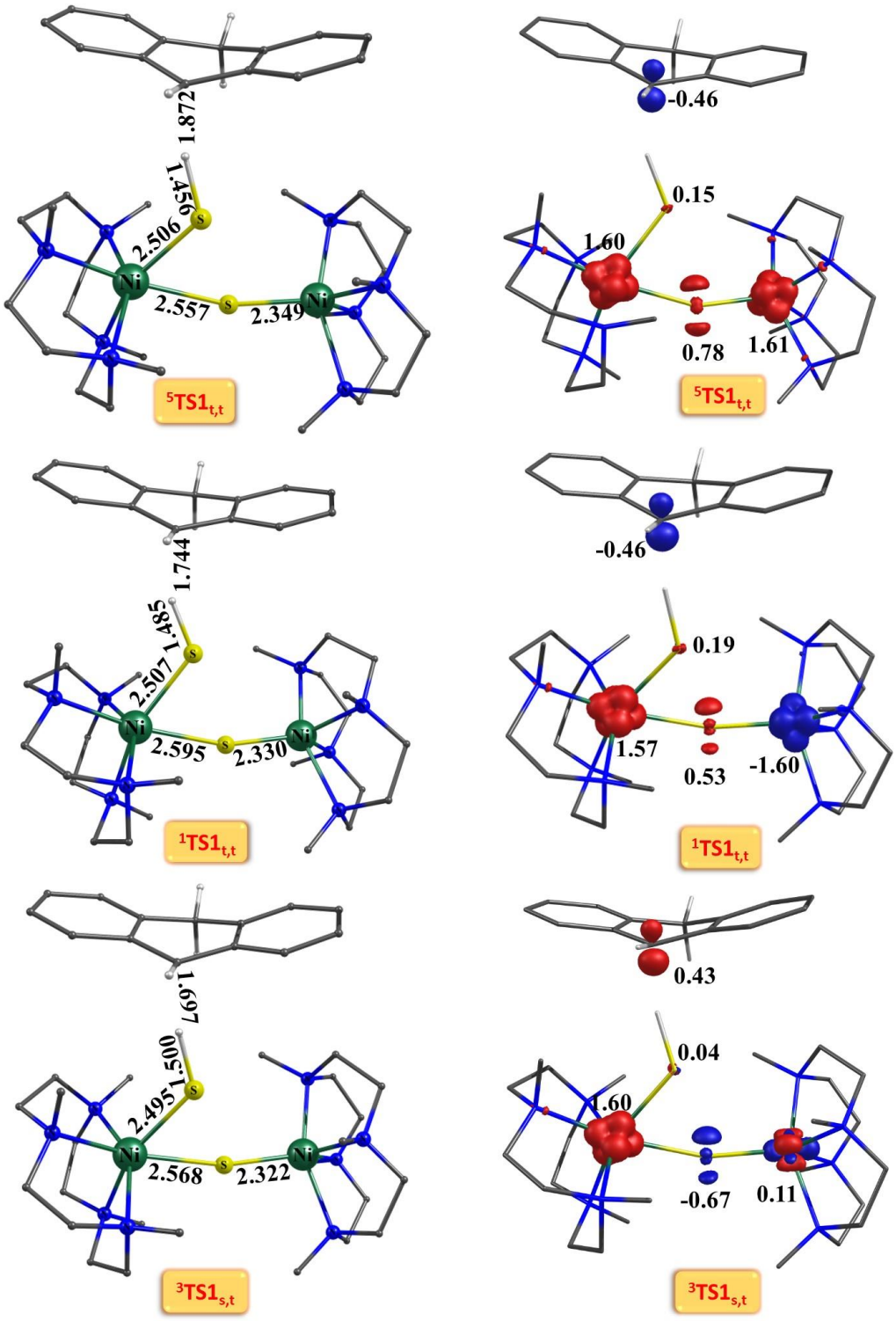


Figure S8. The optimized structure of the first hydrogen abstraction transition state (***ts1***) of complex **2** and its corresponding spin density plot. Here all the hydrogen atoms (except alpha position hydrogens of the middle ring of the DHA substrate) are omitted for clarity.

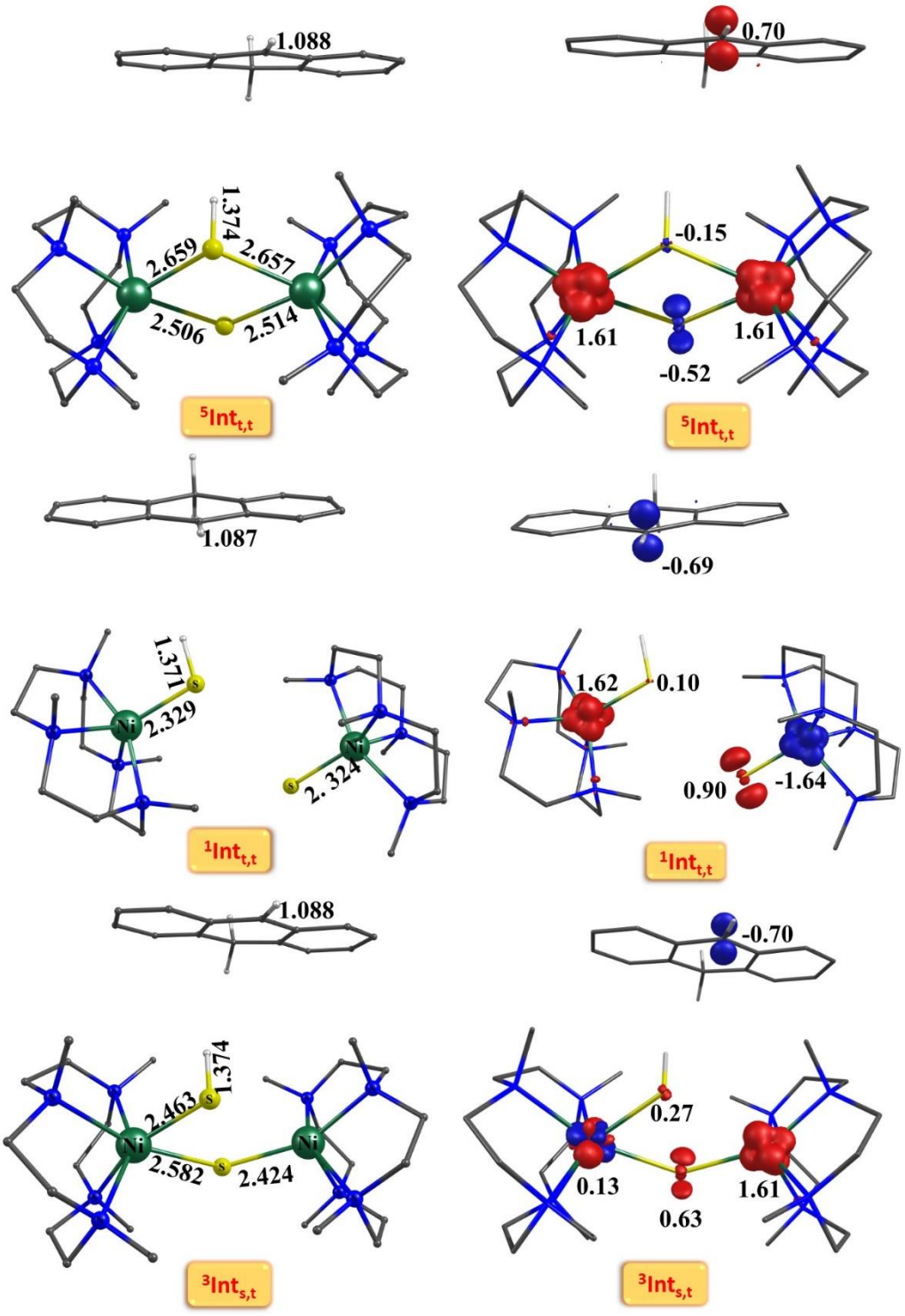


Figure S9. The optimized structure of intermediates of complex **2** and its corresponding spin density plot. Here all the hydrogen atoms (except alpha position hydrogens of the middle ring of the DHA substrate and abstracted hydrogen atom by the chalcogenide group) are omitted for clarity.

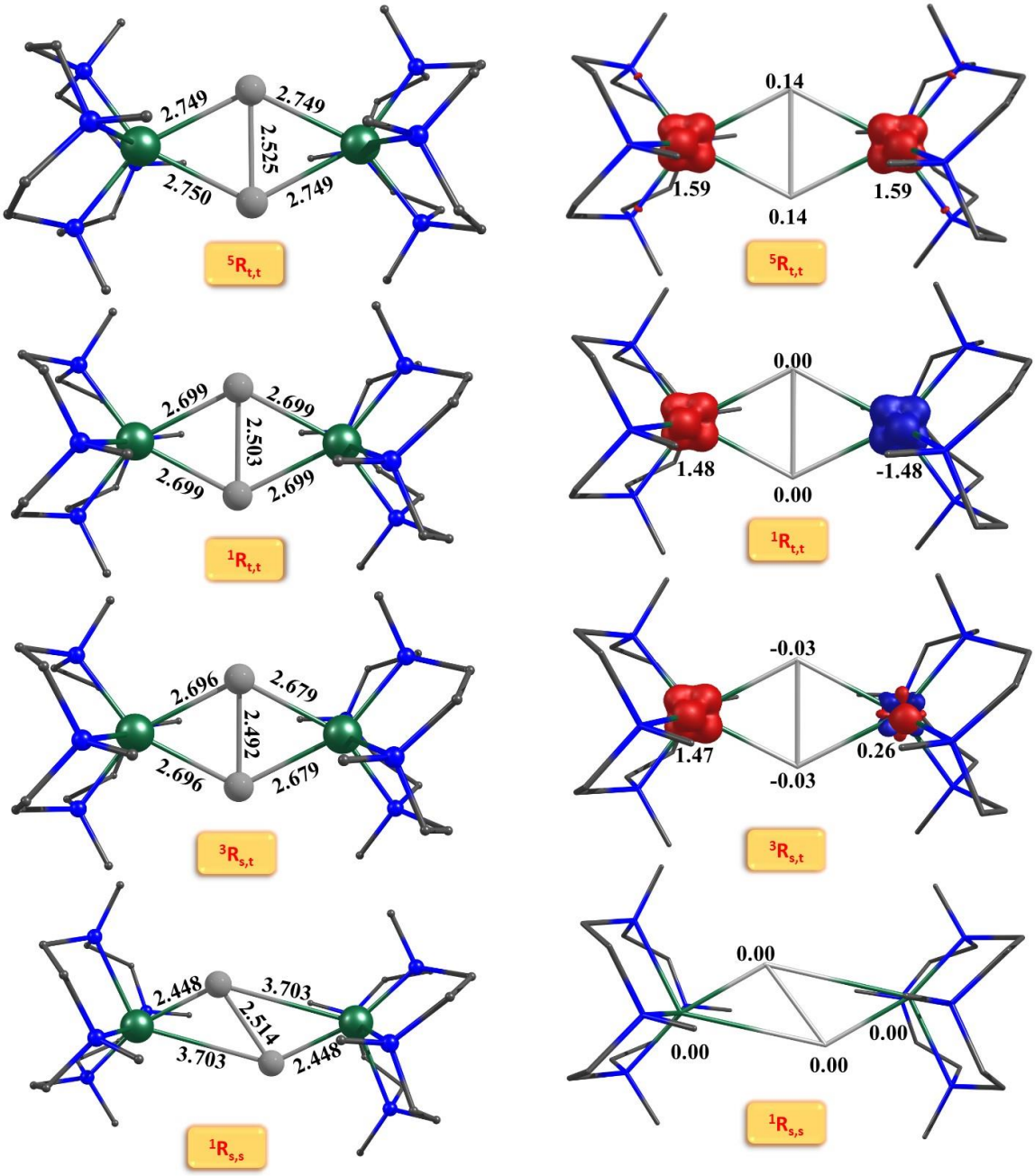


Figure S10. The optimized structure of reactant **3** and its corresponding spin density plot. Here all the hydrogen atoms are omitted for clarity.

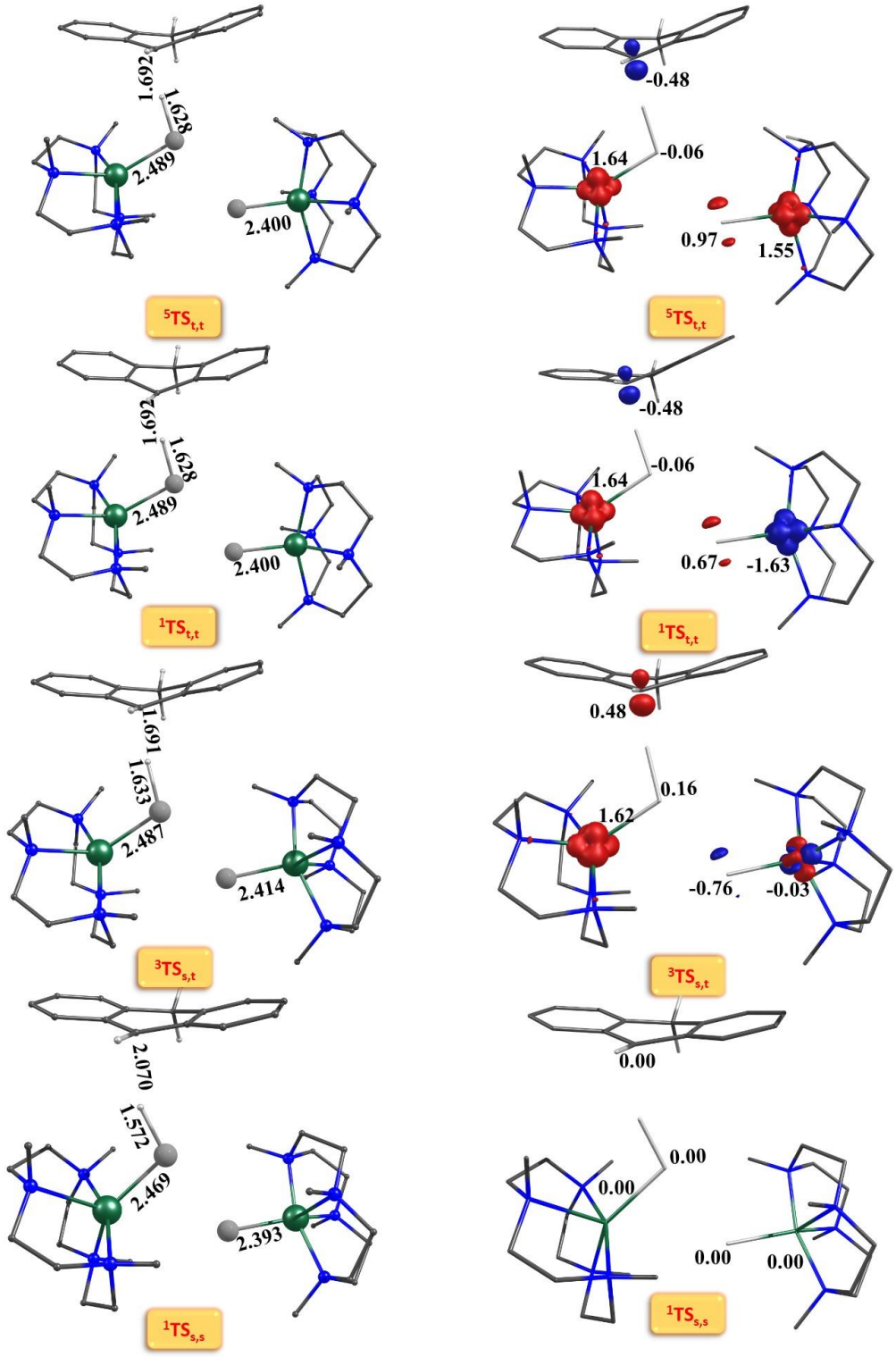


Figure S11. The optimized structure of the first hydrogen abstraction transition state (***ts1***) of complex **3** and its corresponding spin density plot. Here all the hydrogen atoms (except alpha position hydrogens of the middle ring of the DHA substrate) are omitted for clarity.

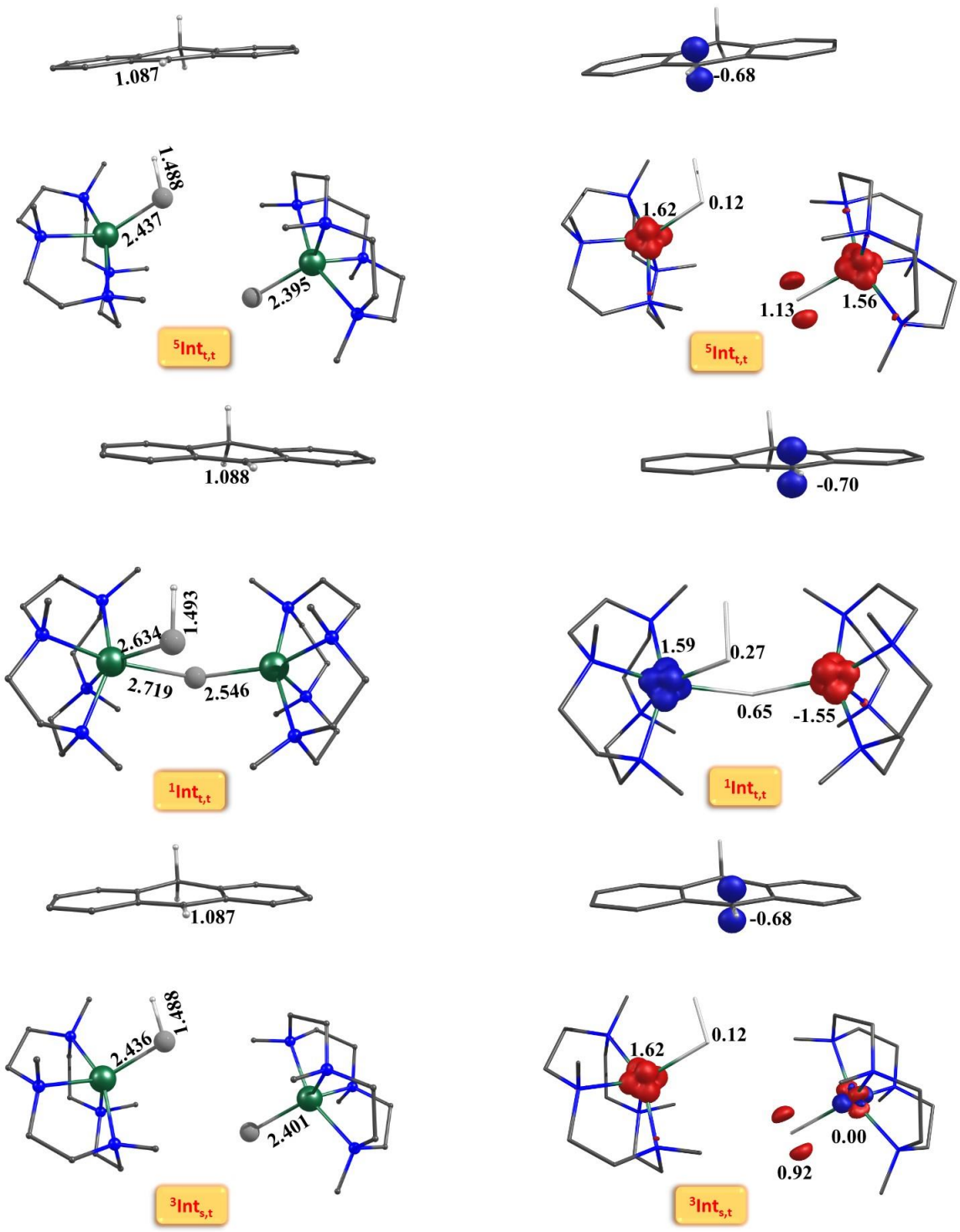
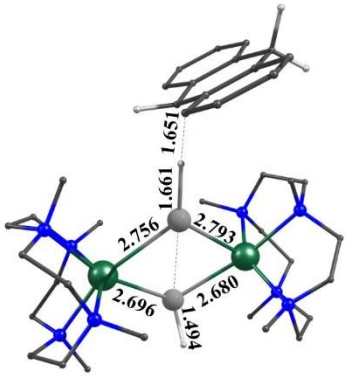
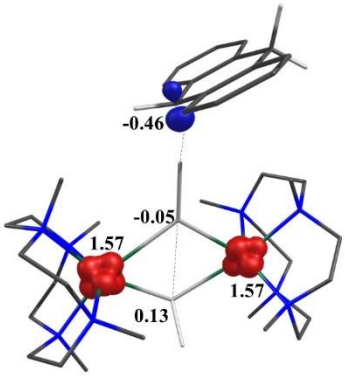
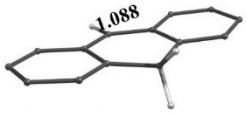


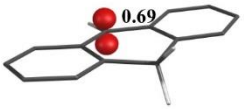
Figure S12. The optimized structure of intermediates of complex **3** and its corresponding spin density plot. Here all the hydrogen atoms (except alpha position hydrogens of the middle ring of the DHA substrate and abstracted hydrogen atom by the chalcogenide group) are omitted for clarity.



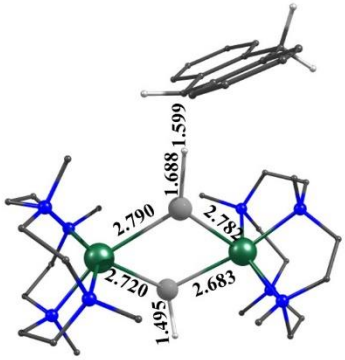


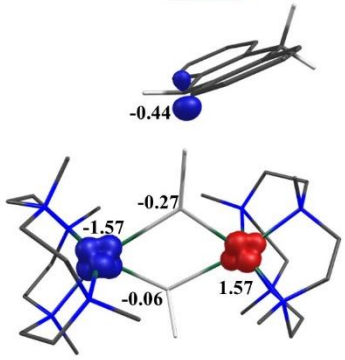


$^5TS2_{t,t}$

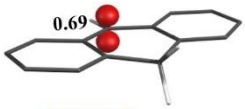


$^5TS2_{t,t}$

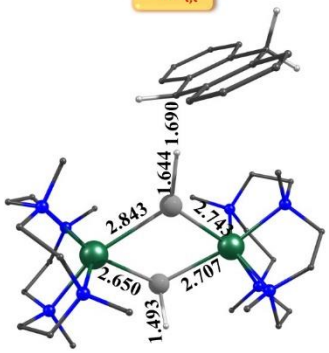


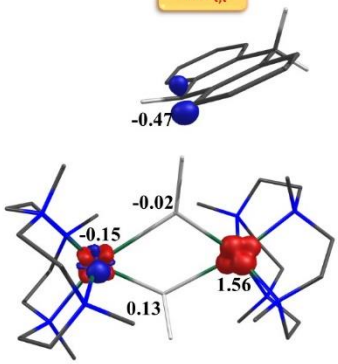


$^1TS2_{t,t}$



$^1TS2_{t,t}$





$^3TS2_{s,t}$

$^3TS2_{s,t}$

Figure S13. The optimized structure of the second hydrogen abstraction transition state (***ts2***) of complex **3** and its corresponding spin density plot. Here all the hydrogen atoms (except alpha position hydrogens of the middle ring of the DHA substrate and abstracted hydrogen atom by the chalcogenide group) are omitted for clarity.

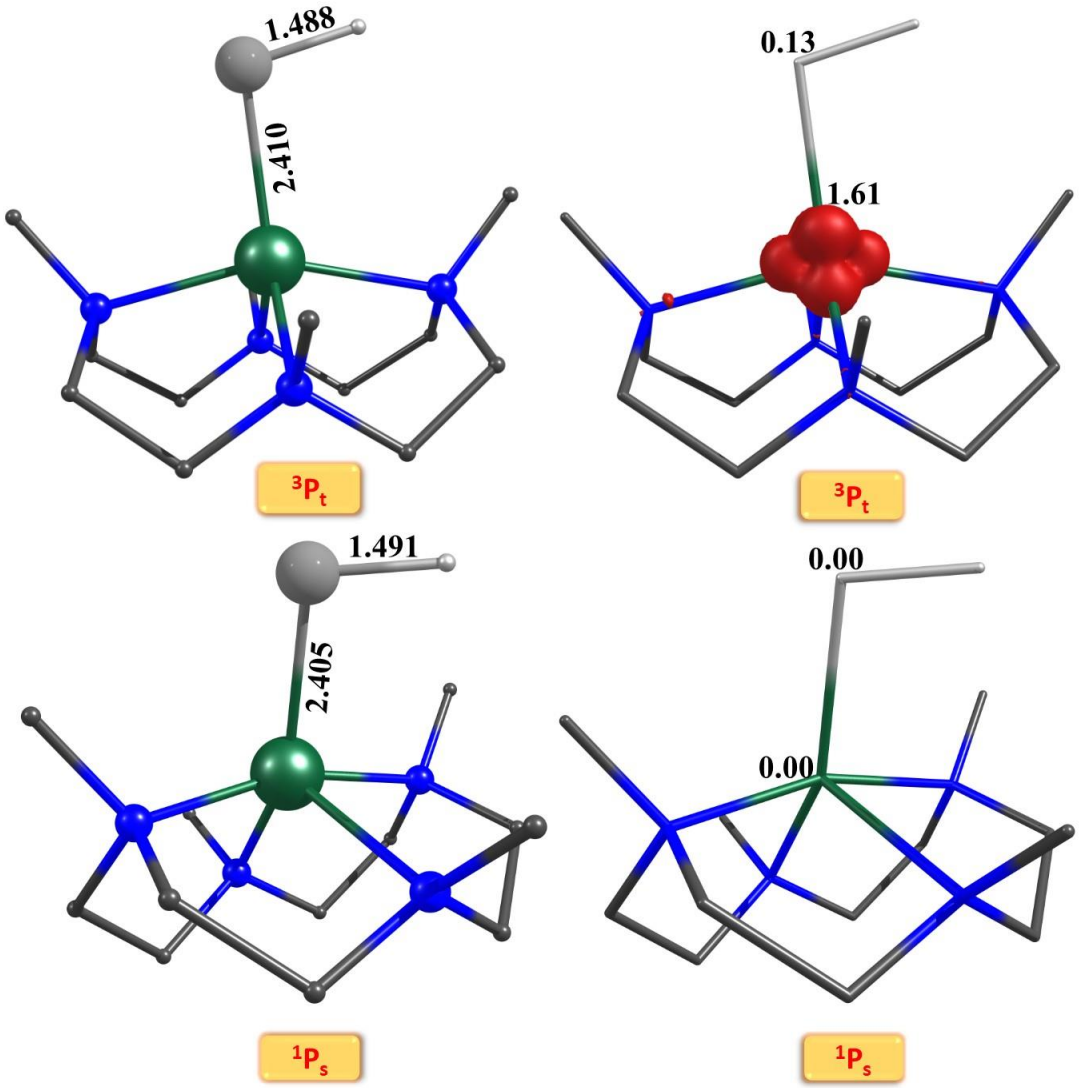
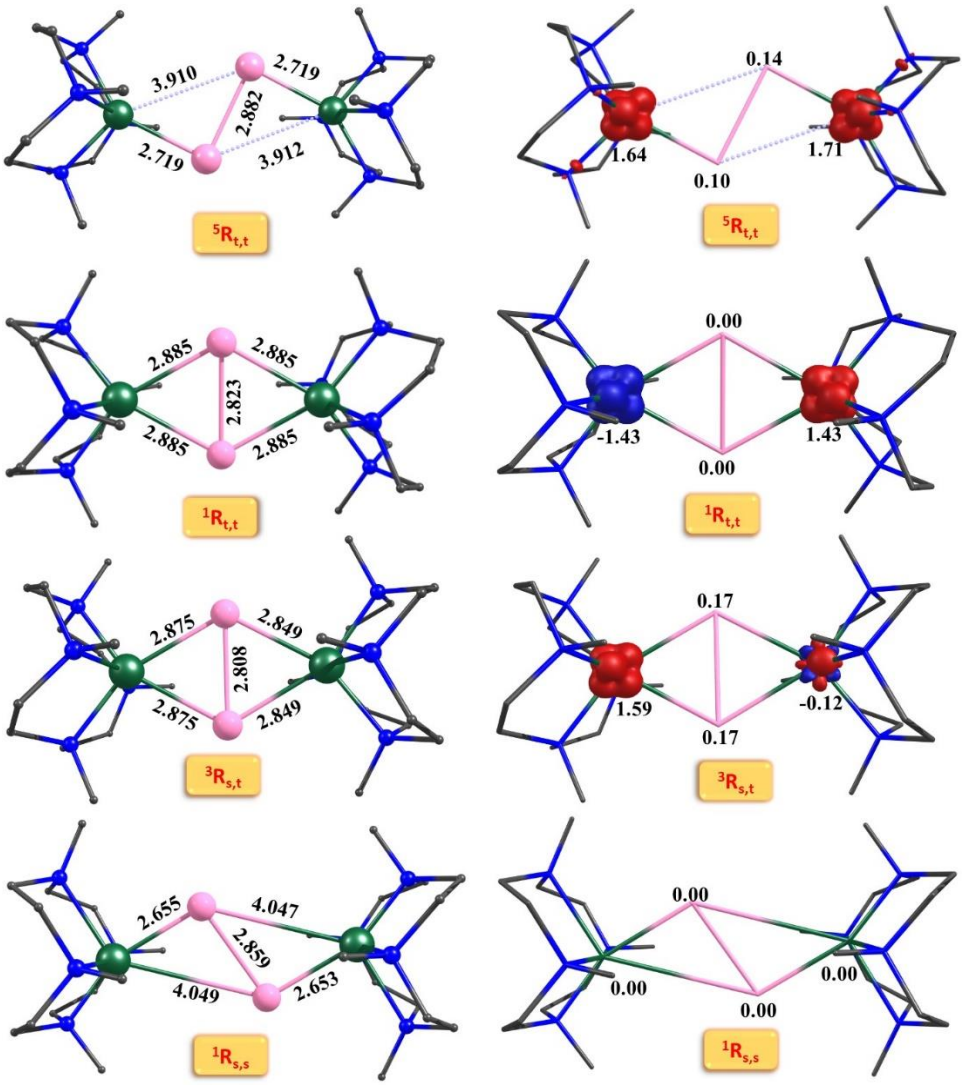
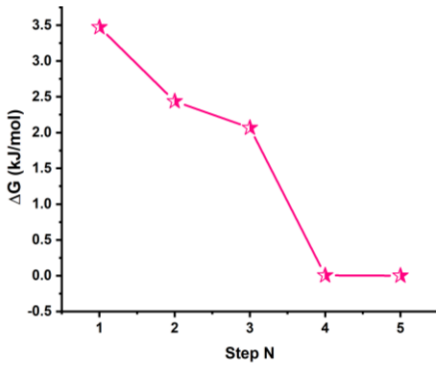


Figure S14. The optimized structure of monomer Nickel selenide complex (***PC***) of complex **3** and its corresponding spin density plot. Here all the hydrogen atoms (abstracted hydrogen atoms by the chalcogenide group) are omitted for clarity.



AIM analysis of excited state reactant species $^5\mathbf{R}_{(t,t)}$ for complex **4**, shows V(r)/G(r) value 0.76 for one of the Ni1-E1 bond and 1.23 for other Ni2-E2 bond.



This change in symmetry occurred during the SCF convergence cycle, resulting in a high energy gap of 71.5 kJ between the singlet ground state ($^1\mathbf{4}_{t,t}$) and the quintet excited state ($^5\mathbf{4}_{t,t}$). Additionally, the SCF convergence graph shows that the side-on quintet geometry is only 3.5 kJ/mol higher in energy than the trans-end-on quintet geometry, which occurs only in the case of the quintet state of complex **4.** This results in a higher energy singlet-quintet gap compared to other complexes.

Figure S15. The optimized structure of reactant **4** and its corresponding spin density plot. Here all the hydrogen atoms are omitted for clarity. The bottom graph corresponds to SCF cycle progress of quintet state optimization on **4**.

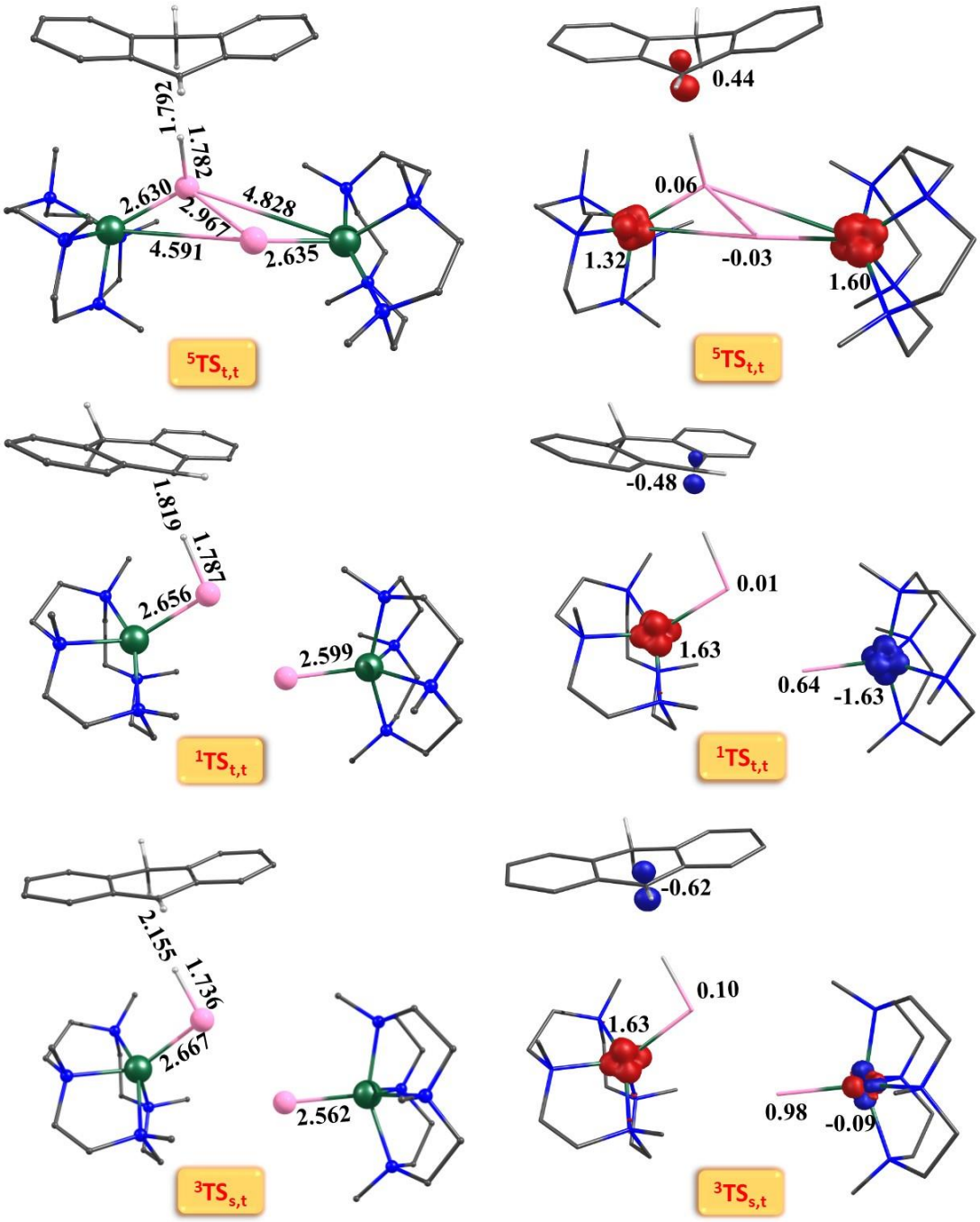


Figure S16. The optimized structure of the first hydrogen abstraction transition state (***ts1***) of complex **4** and its corresponding spin density plot. Here all the hydrogen atoms (except alpha position hydrogens of the middle ring of the DHA substrate) are omitted for clarity.

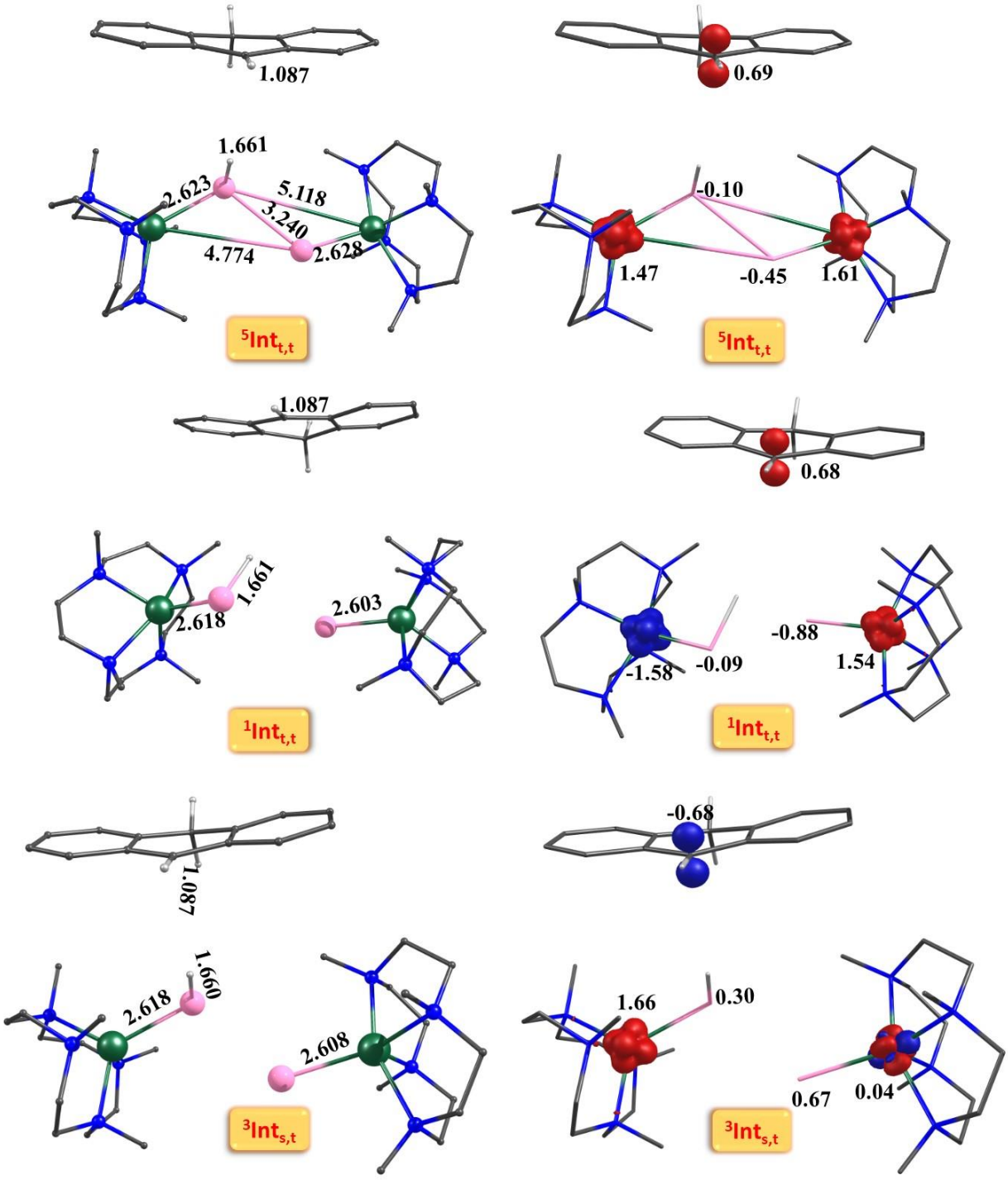


Figure S17. The optimized structure of the intermediates of complex **4** and its corresponding spin density plot. Here all the hydrogen atoms (except alpha position hydrogens of the middle ring of the DHA substrate) are omitted for clarity.

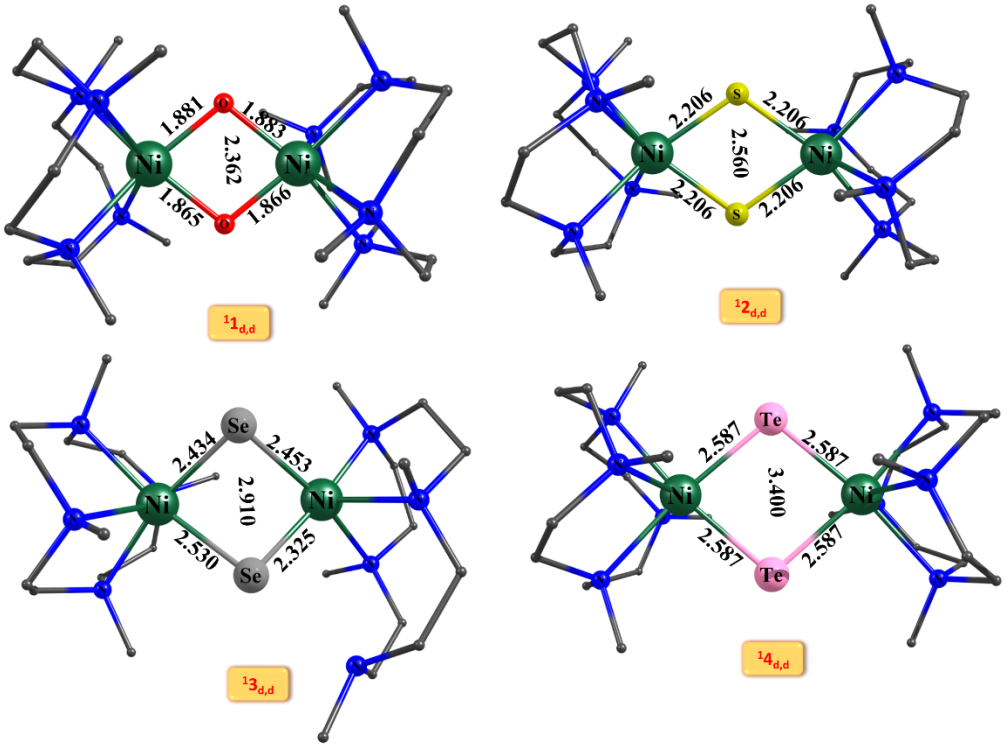


Figure S18. Optimized geometries of bis(μ-oxo) $\{Ni_2(III)E_2\}$ type complexes. (For optimization, fixed Ni_1-Ni_2 and E_1-E_2 distances on the basis of previous literature data).

Table S1. DLPNO-CCSD(T) calculated values –

Complex	**Amplitude (T1)**
^{5}**1**$_{(t,t)}$ (T1)	0.015
^{1}**1**$_{(t,t)}$ (T2)	0.010

Table S2. The spin configurations are computed for **1-4**, along with its energetics. The value in the parenthesis is computed using DLPNO-CCSD(T) methods (see computational details).

Spin States	Ni1	Ni2	Energy (kJ/mol)			
			1	**2**	**3**	**4**
$[Ni(II)_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}E_2)(L)_2]^{2+}$						
$^5R_{(t,t)}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	12.3 (2.6)	16.1	12.4	71.5
$^1R_{(t,t)}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	0.0 (0.0)	0.0	0.0	0.0
$^3R_{(s,t)}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	53.6	47.7	46.0	81.9
$^1R_{(s,s)}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	336.5 (380)	156.4	159.8	180.8
$[Ni(III)_2(\mu\text{-}E)_2(L)_2]^{2+}$						
$^1R_{(d,d)}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	$\delta_{xy}\ \pi^*_{yz}\ \pi^*_{xz}\ \sigma^*_{x^2-y^2}\ \sigma^*_{z^2}$	61.6	72.5	144.4	102.1

Table S3. Selected structural parameters reported for structurally analogue complexes (X-ray) along with DFT computed ground state geometries for **1-4**.

a

Complexes	Ni-E (Å)	Ni1-Ni2 (Å)	E1-E2 (Å)	Ni-E-Ni (˚)	E-Ni-E (˚)	Ref.
$^1\mathbf{1}_{t,t}$	2.047	3.810	1.500	137	43	This work
$[(L)Ni]_2(\mu\text{-}O)_2]^a$	1.841-1.870	2.882-3.130	1.820-2.390	105	75	[1-3]
$/[LNi^{III}(\mu\text{-}O)_2Ni^{III}L]^b$						
$^1\mathbf{2}_{t,t}$	2.595	4.635	2.335	126	53	This work
$[(L)Ni(\mu\text{-}S_2)\text{-}Ni(L)]^{+\ c}$	2.217-2.234	3.865-3.926	2.208-2.177	120-122	58-59	[4-6]
$/[(L)Ni]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}S_2)]^d$						
$^1\mathbf{3}_{t,t}$	2.699	4.781	2.503	125	55	This work
$[[(L)Ni]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}Se_2)]^e$	2.557-2.566	3.438	2.379-2.479	125	55	[5, 7, 8,]
$/[[(Ni(L)]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}Se_2)]^f$						
$^1\mathbf{4}_{t,t}$	2.885	5.033	2.823	121	59	This work
$[(L)\ Ni(Te2)Ni(L)]^g$	2.576-2.596	3.771	2.802	-	66	[5, 9]
$/[(LNi^{II})_2Te_2]^h$						

(L=($PhTt^{tBu}$)), b (L= Tp^{Me3}), c (L= triphos), d (L= $PhTt^{tBu}$), e (L=($PhTt^{tBu}$)), f L=(Me_4[12]aneN$_4$), g (L=$MeC(CH_2PPh_2)_3$), h (L=β-diketiminiate, $CH(CMeNR)_2$).

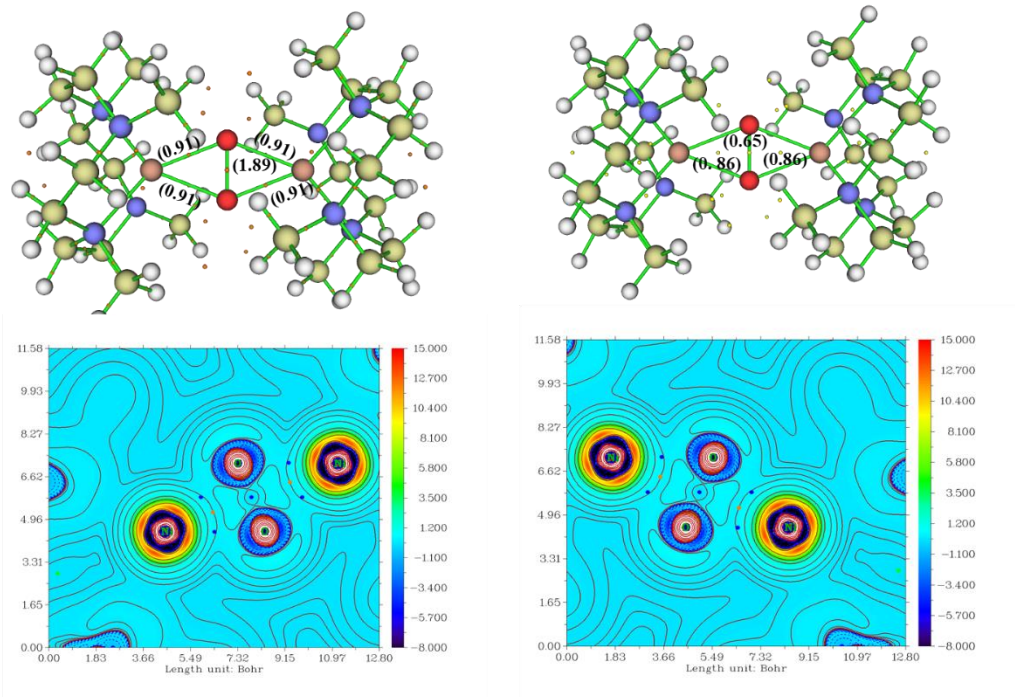


Figure S19. AIM plots for complex **1** (For ground state $^{1}\mathbf{R}_{(t,t)}$).

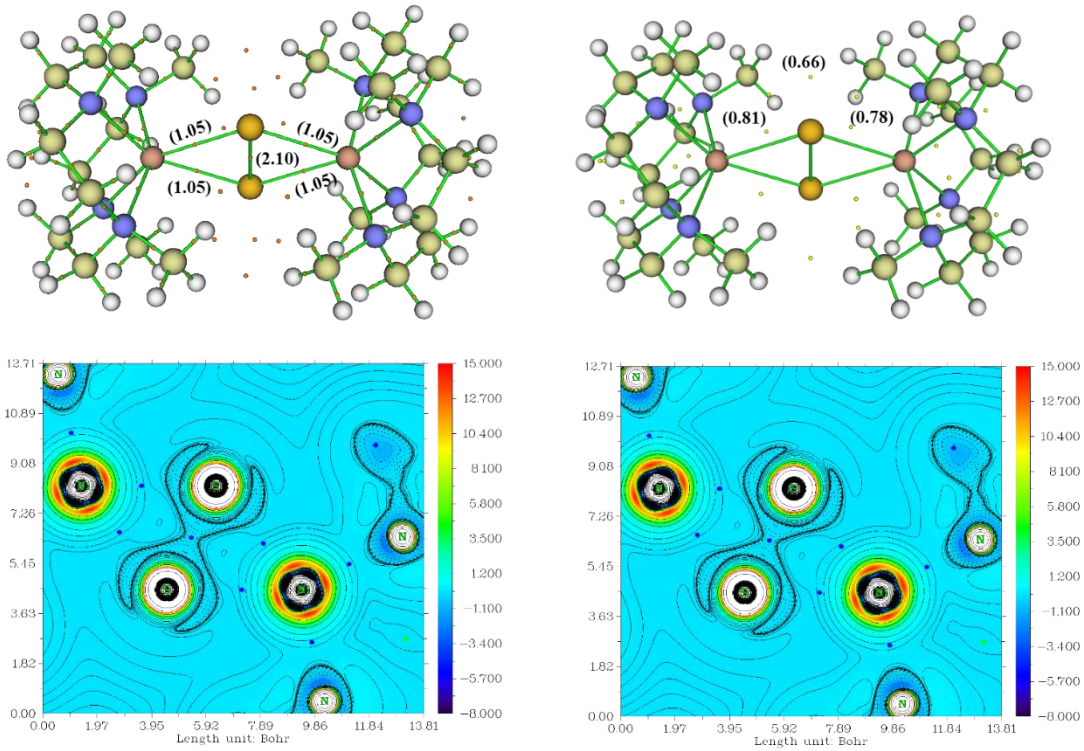


Figure S20. AIM plots for complex **2** (For ground state $^{1}\mathbf{R}_{(t,t)}$).

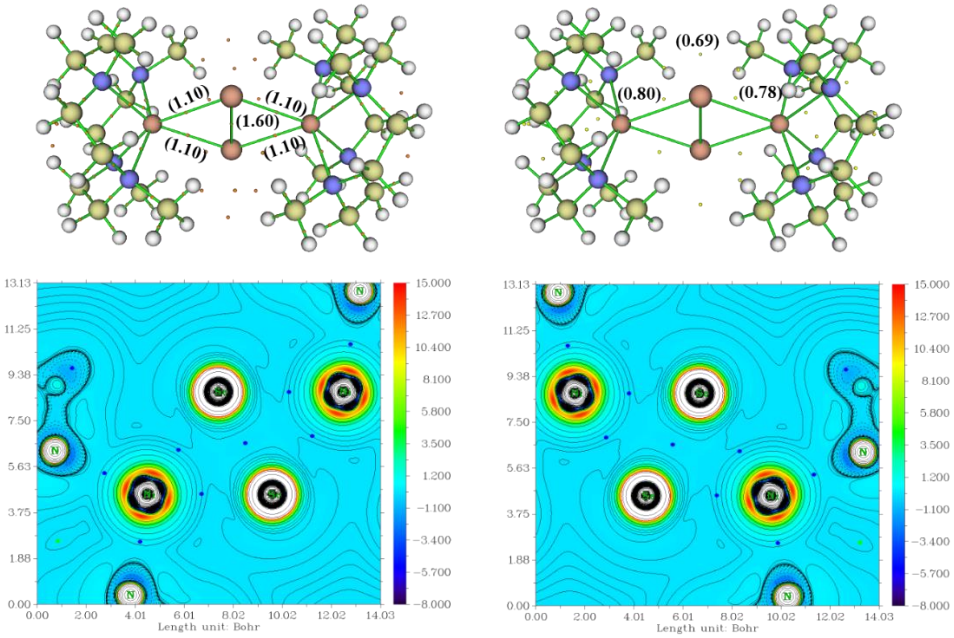


Figure S21. AIM plots for complex **3** (For ground state $^{1}\mathbf{R}_{(t,t)}$).

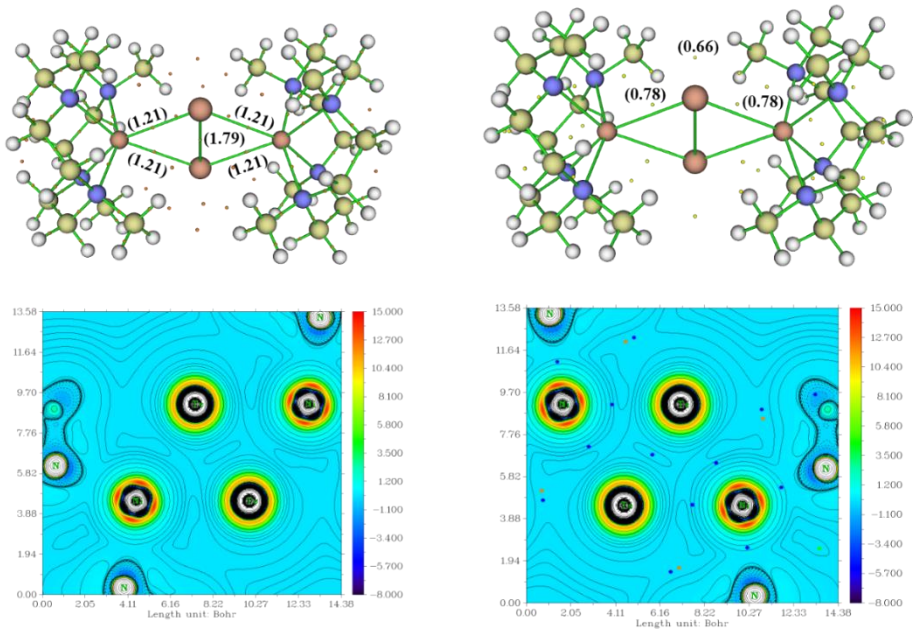


Figure S22. AIM plots for complex **4** (For ground state $^{1}\mathbf{R}_{(t,t)}$).

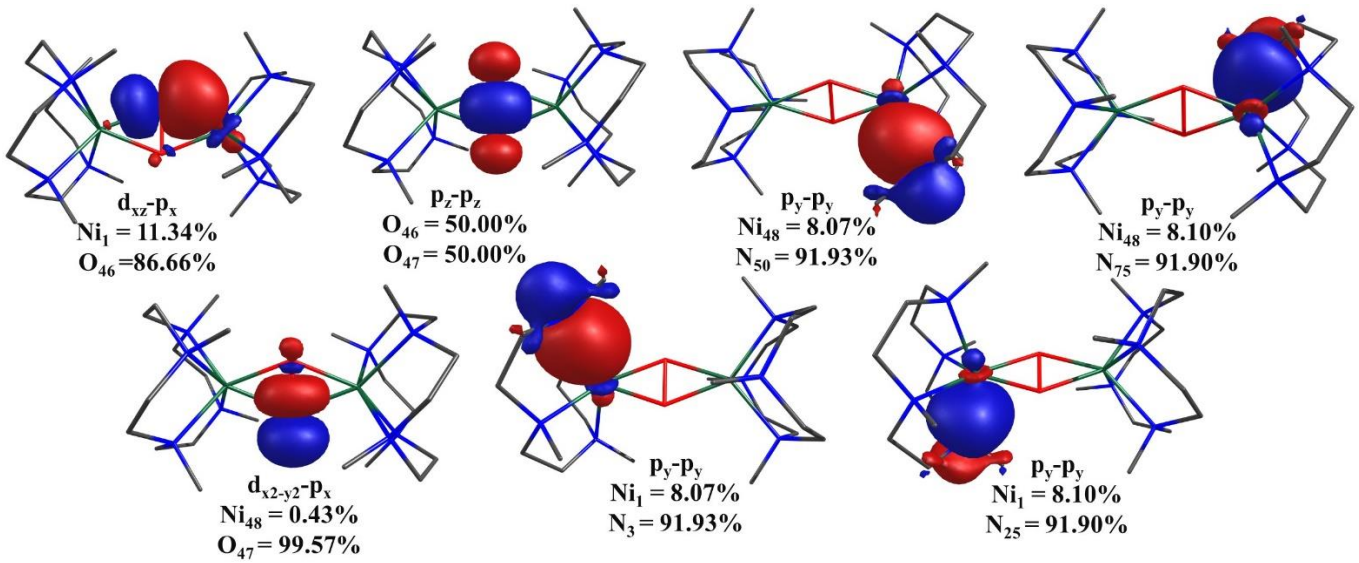


Figure S23. Computed NBO plots for complex **1** (for the ground state $^1\mathbf{R}_{(t,t)}$).

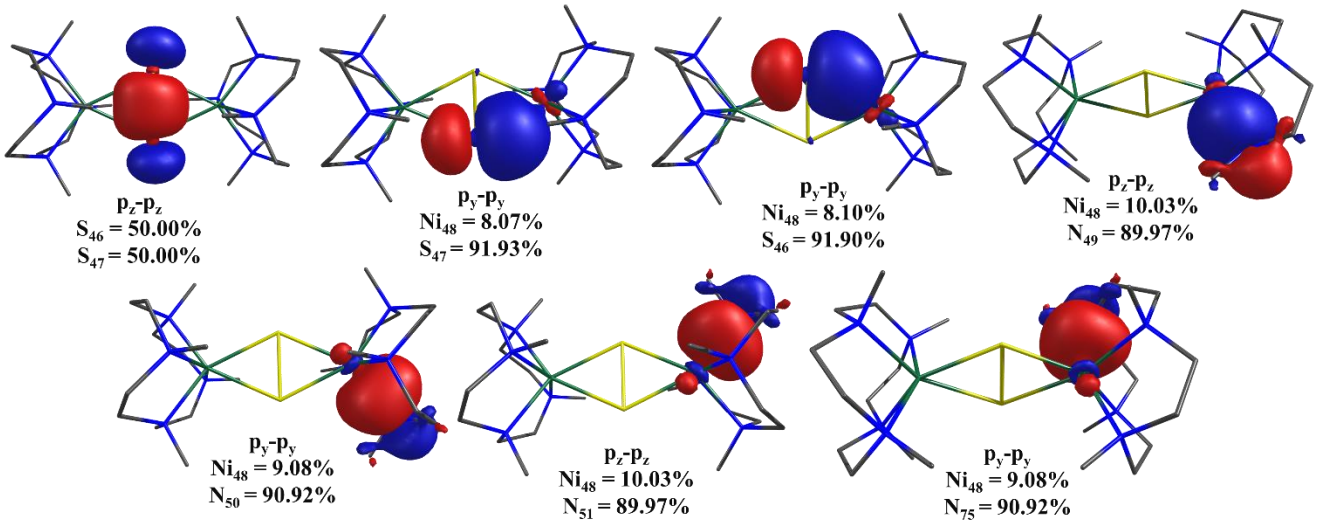


Figure S24. Computed NBO plots for complex **2** (for the ground state $^1\mathbf{R}_{(t,t)}$).

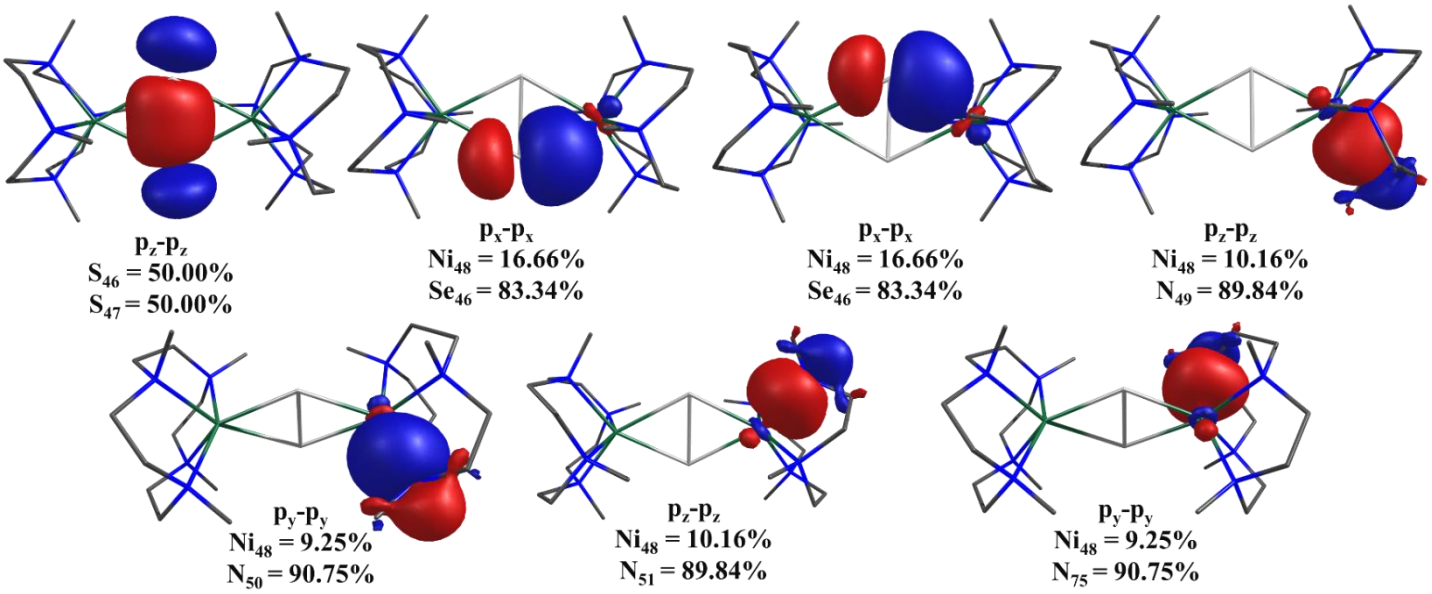


Figure S25. Computed NBO plots for complex **3** (for the ground state $^1\mathbf{R}_{(t,t)}$).

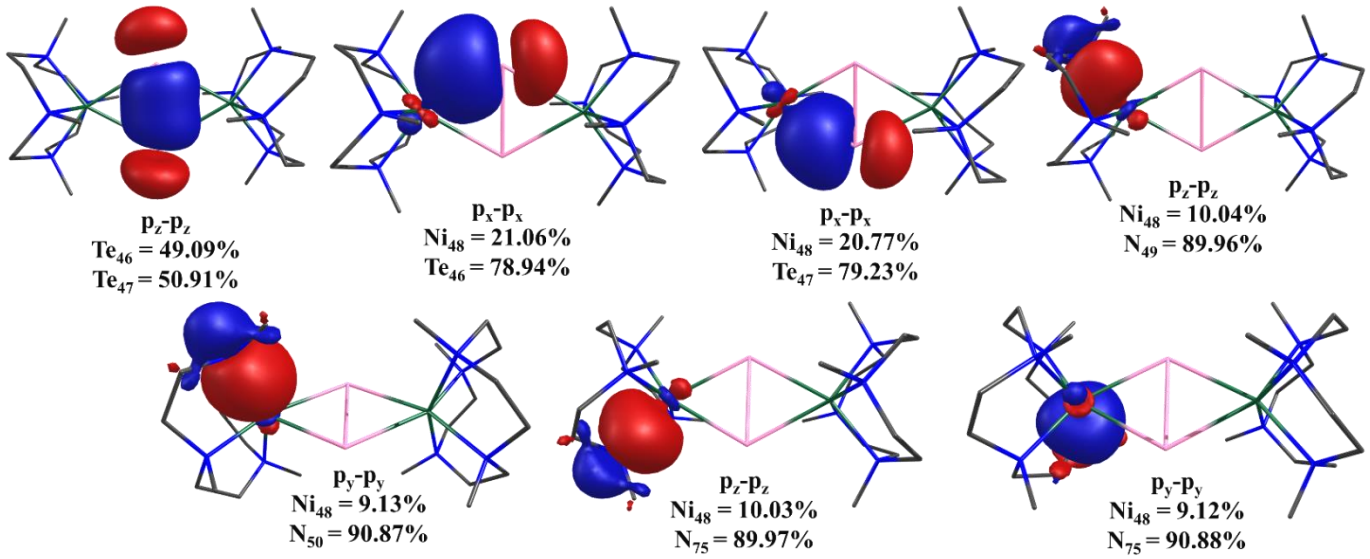


Figure S26. Computed NBO plots for complex **4** (for the ground state $^1\mathbf{R}_{(t,t)}$).

Table S4- WBI values for ground state only of complexes ^{1}**1-4**$_{(t,t)}$.

WBI (GS)	Ni-E1	Ni1-E2	E1-E2	Ni2-E1	Ni2-E2	Ni1-Ni2
^{1}**1**$_{(hs, bs)}$	0.261	0.261	1.032	0.261	0.261	0.040
^{1}**2**$_{(hs, bs)}$	0.363	0.363	1.013	0.363	0.363	0.026
^{1}**3**$_{(hs, bs)}$	0.376	0.376	0.922	0.376	0.376	0.016
^{1}**4**$_{(hs, bs)}$	0.478	0.478	0.932	0.478	0.478	0.024

Table S5- The second-order perturbation analysis of donor (i) and accepter (j) orbital with their stabilization energies (E_2) (in kcal/mol).

Donar (i)	Acceptor (j)	Stabilization Energy (E_2)
BD O_{46}-O_{47}	LP* Ni_{48}	9.3
BD S_{46}-S_{47}	LP* Ni_{48}	11.7
BD Se_{46}-Se_{47}	LP* Ni_{48}	13.2
BD Te_{46}-Te_{47}	LP* Ni_{48}	16.8
LP O_{47}	LP* Ni_{48}	13.8
LP S_{47}	LP* Ni_{48}	19.4
LP Se_{47}	LP* Ni_{48}	22.0
LP Te_{47}	LP* Ni_{48}	23.0

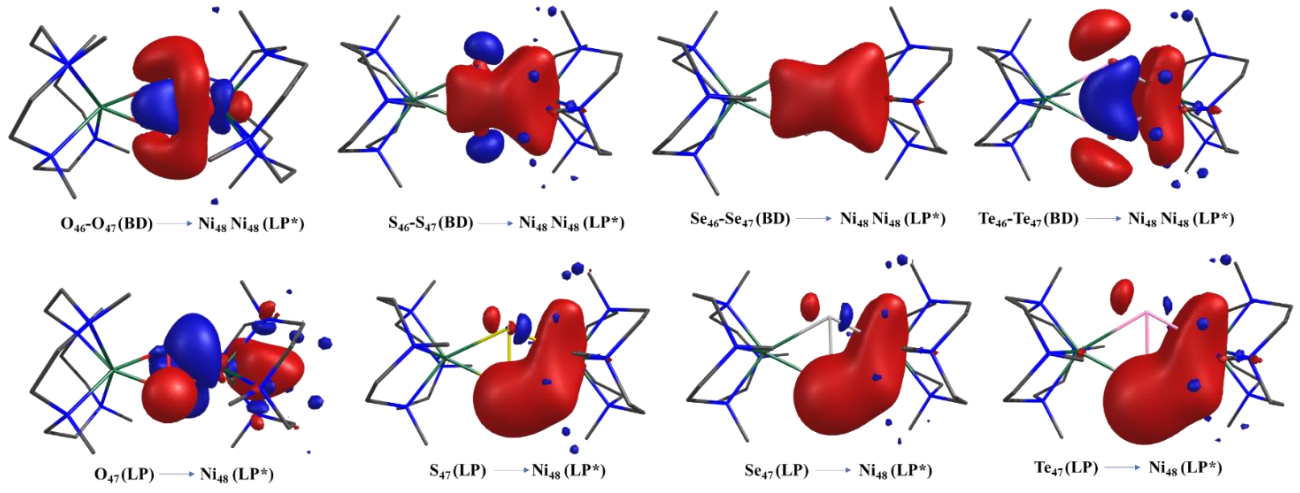


Figure S27. Computed NBO plots for complex ^{1}**1-4**$_{(t,t)}$.

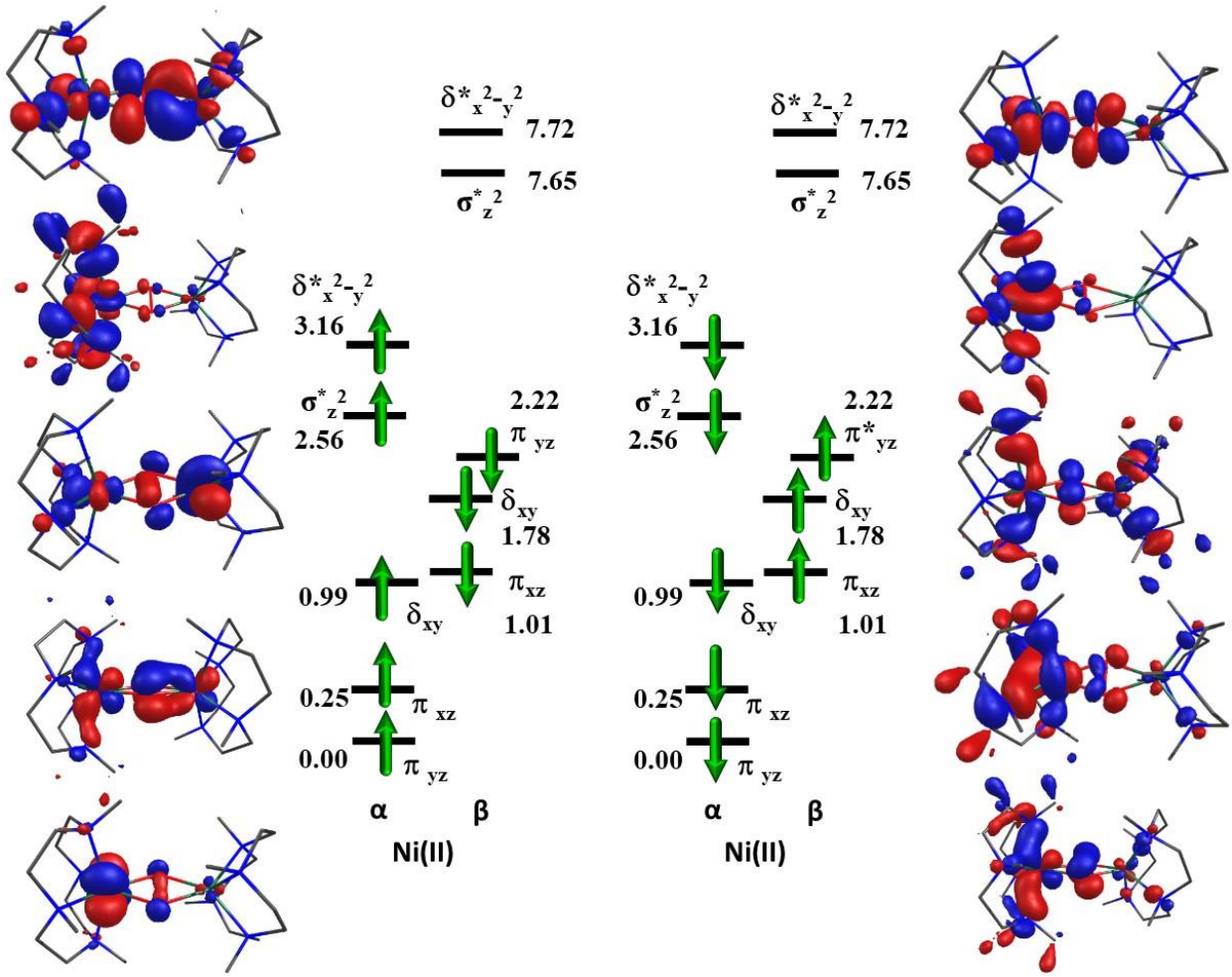


Figure S28. Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the ground state $^{1}\mathbf{R}_{(t,t)}$ of the complex **1** (energies are given in eV)

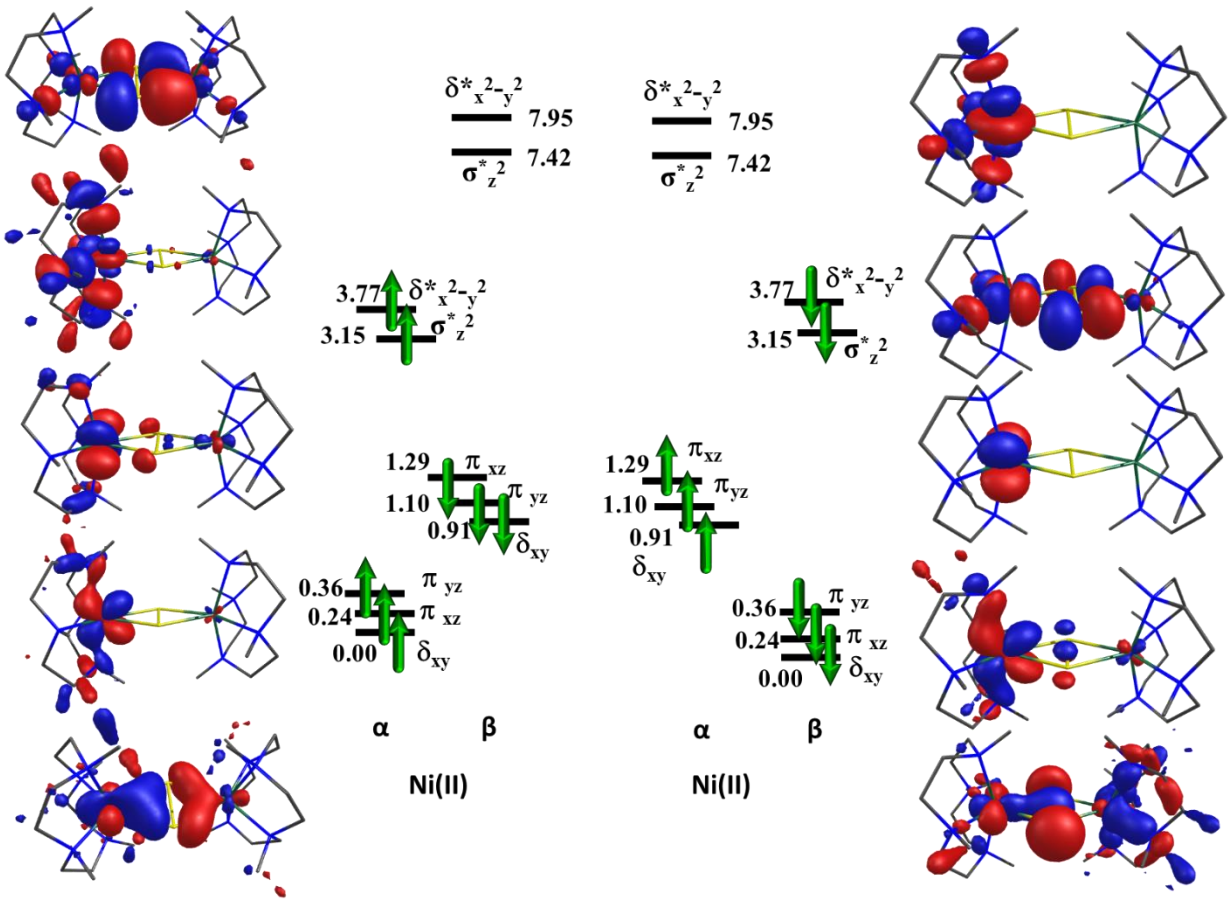


Figure S29. Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the ground state $^{1}\mathbf{R}_{(t,t)}$ of the complex **2** (energies are given in eV)

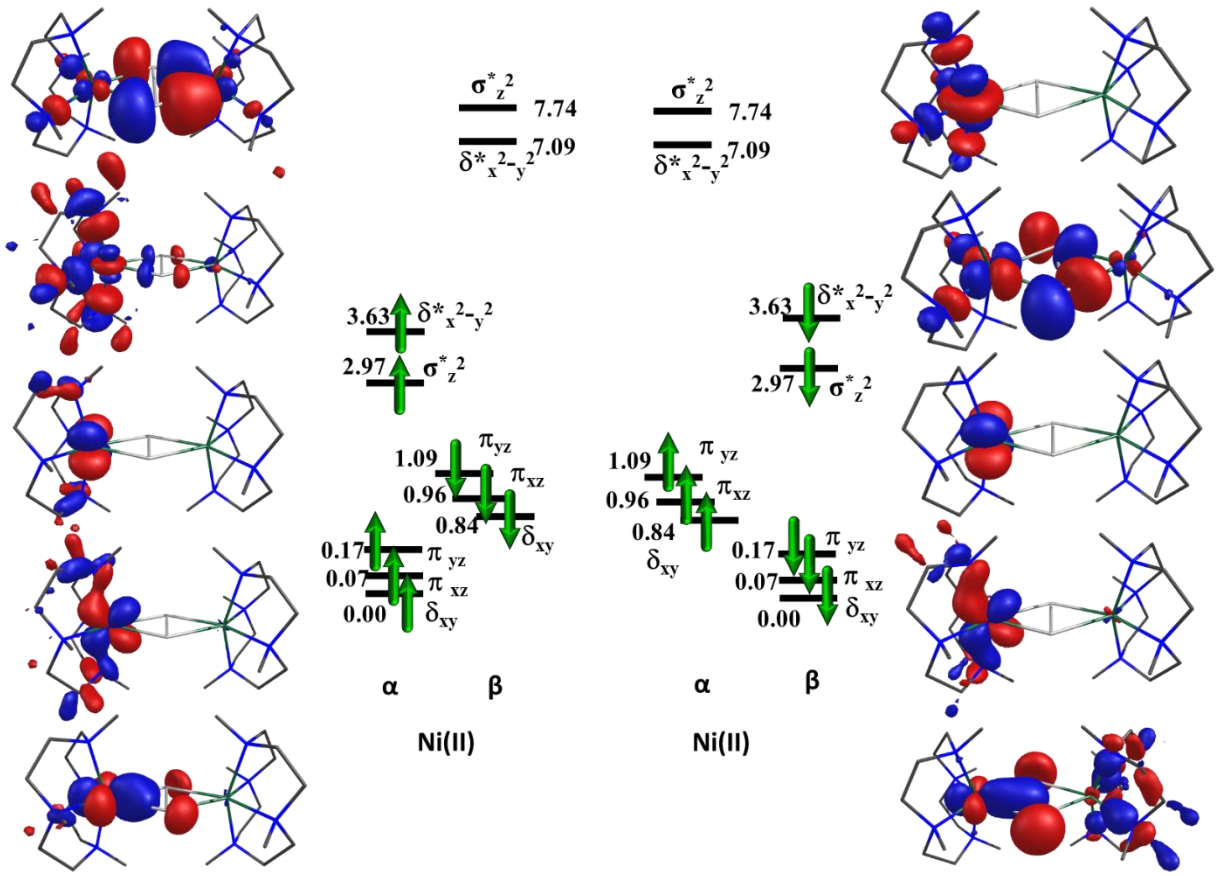


Figure S30. Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the ground state $^{1}\mathbf{R}_{(t,t)}$ of the complex **3** (energies are given in eV)

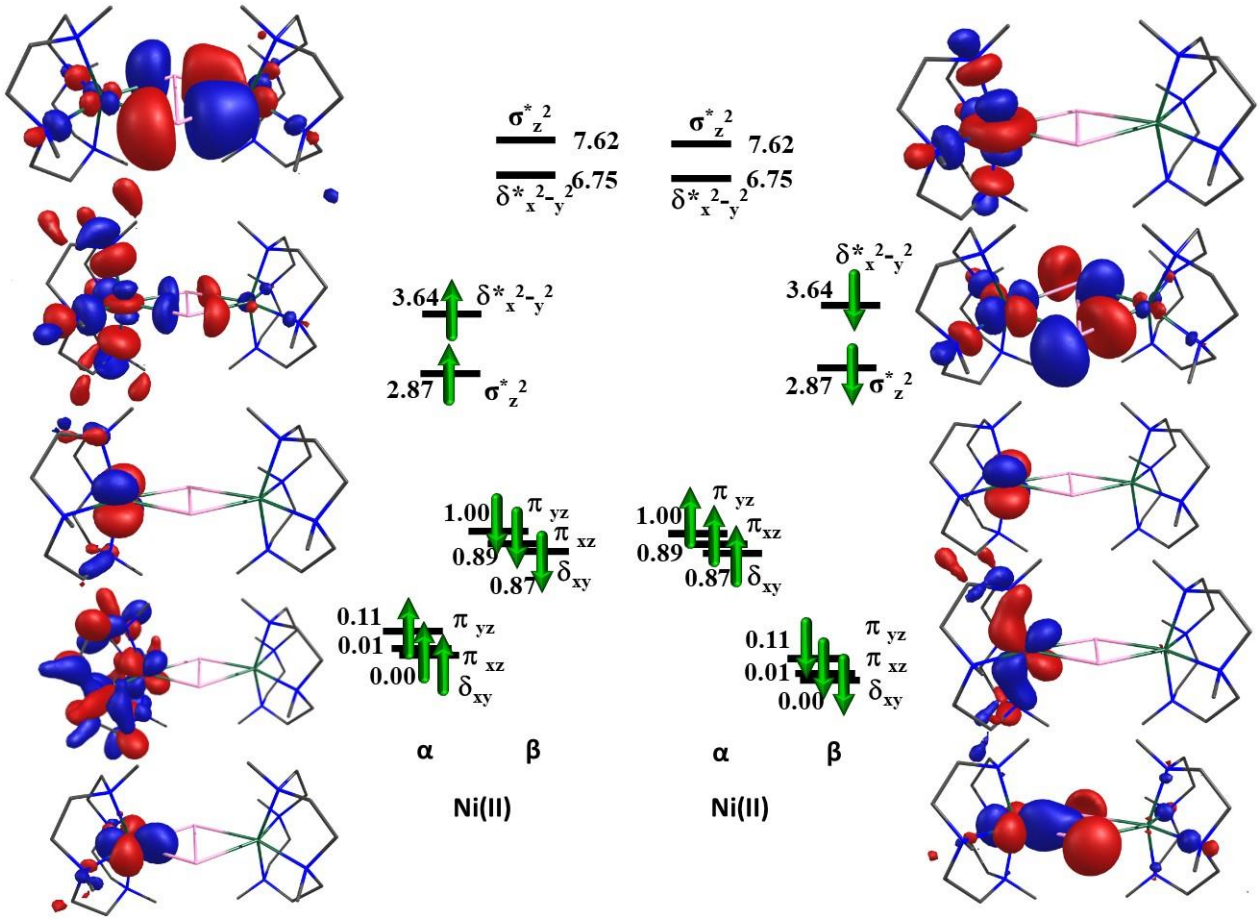


Figure S31. Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the ground state $^{1}\mathbf{R}_{(t,t)}$ of the complex **4** (energies are given in eV)

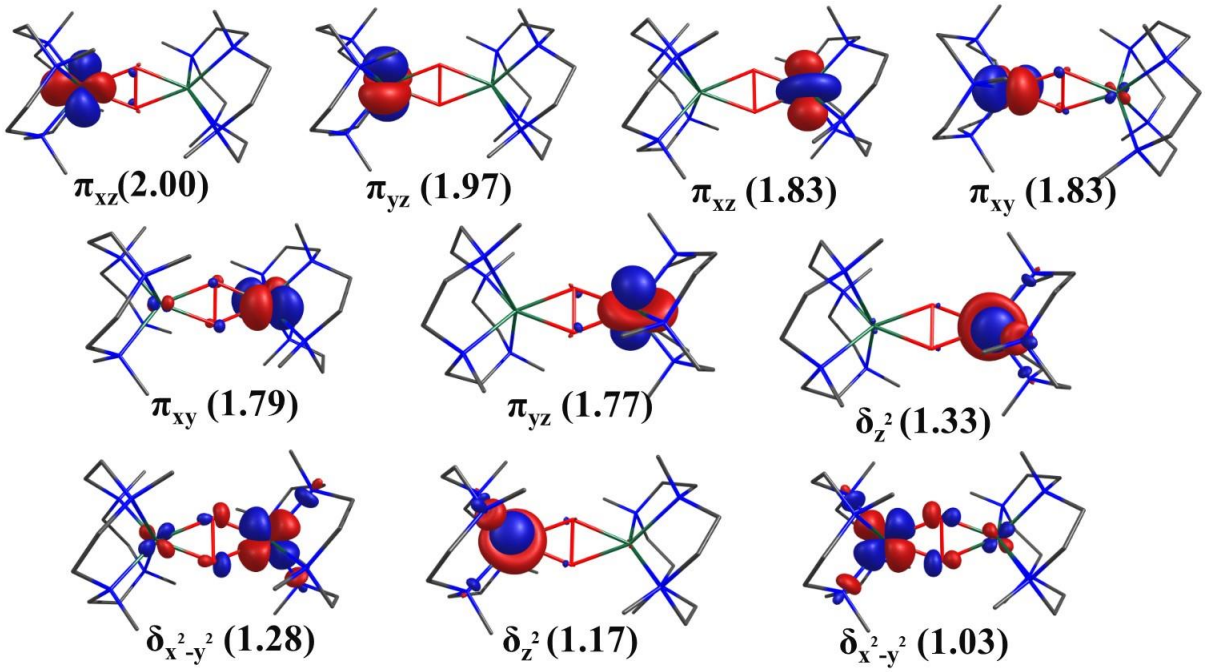


Figure S32. SA-CASSCF plots for the Ni orbitals for the complex **1** for active space CAS(16,10).

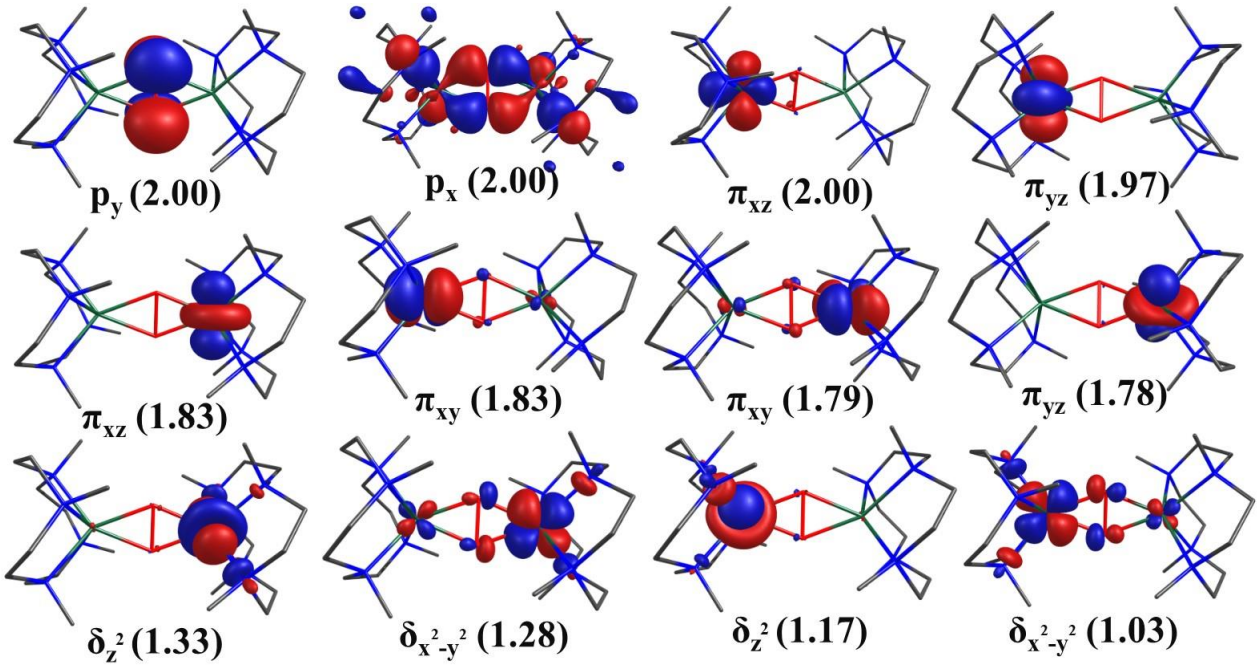


Figure S33. SA-CASSCF plots for the Ni and O orbitals for the complex **1** for active space CAS(20,12).

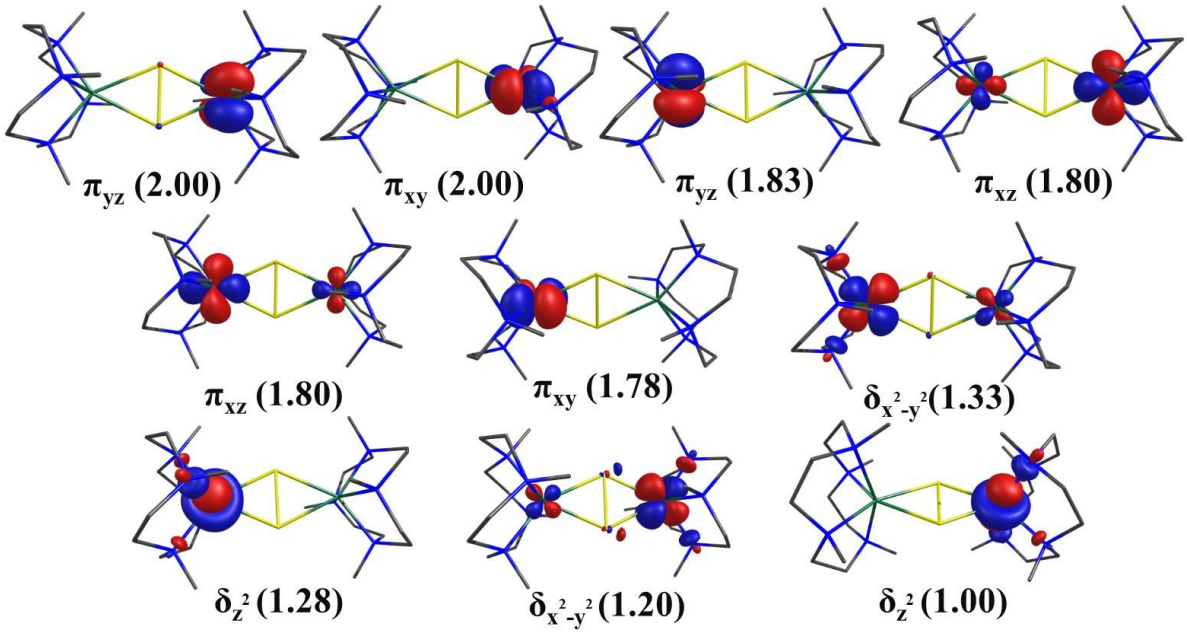


Figure S34. SA-CASSCF plots for the Ni orbitals for the complex **2** for active space CAS(16,10).

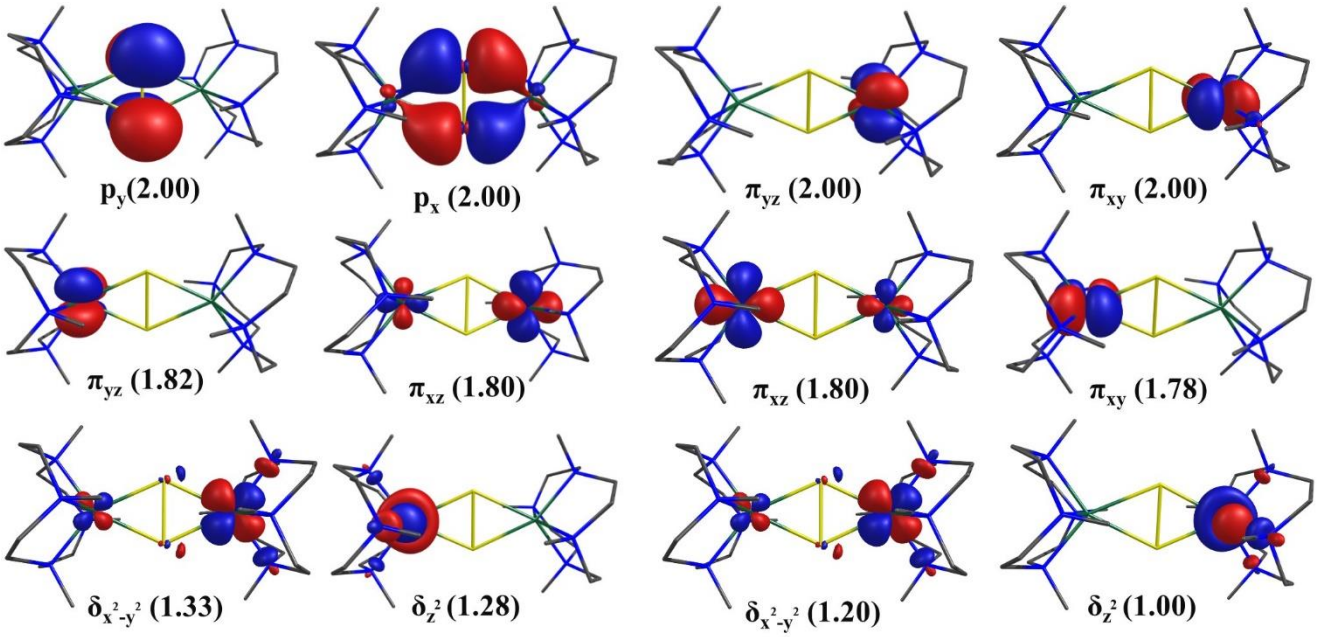


Figure S35. SA-CASSCF plots for the Ni and S orbitals for complex **2** for active space CAS(20,12).

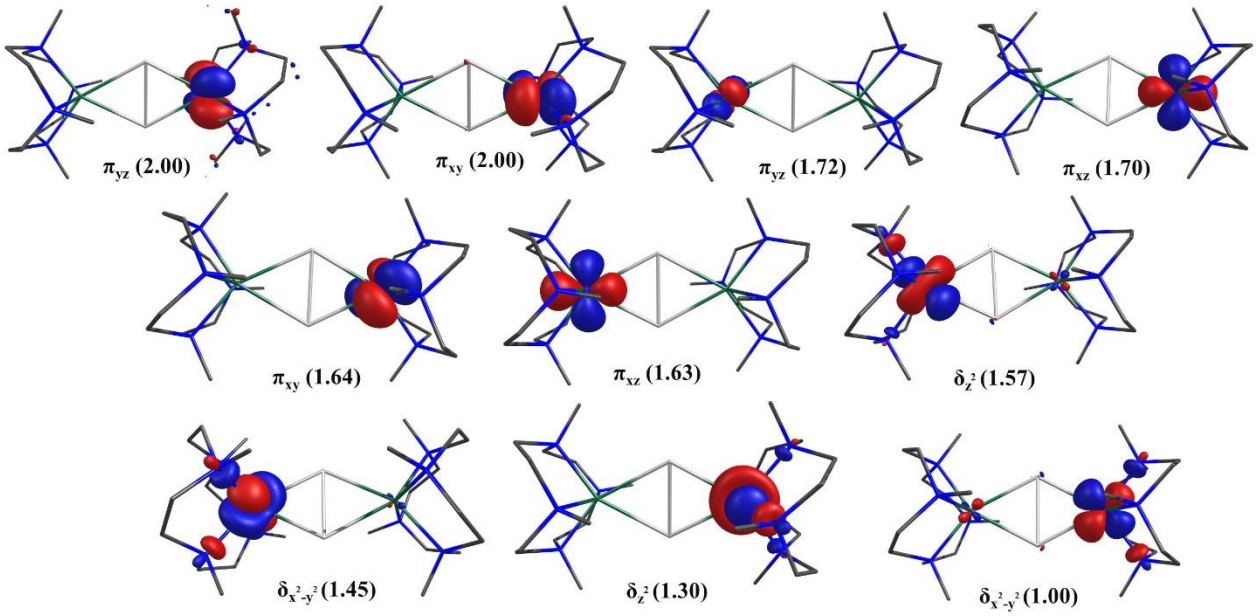


Figure S36. SA-CASSCF plots for the Ni orbitals for the complex **3** for active space CAS(16,10).

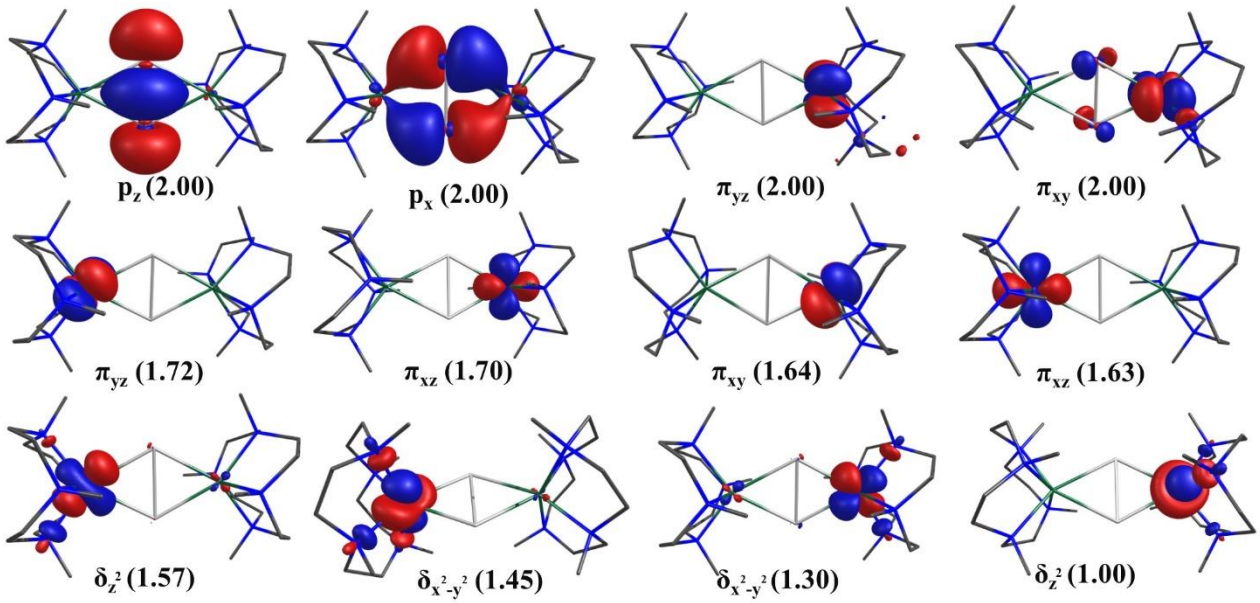


Figure S37. SA-CASSCF plots for the Ni and Se orbitals for complex **3** for active space CAS(20,12).

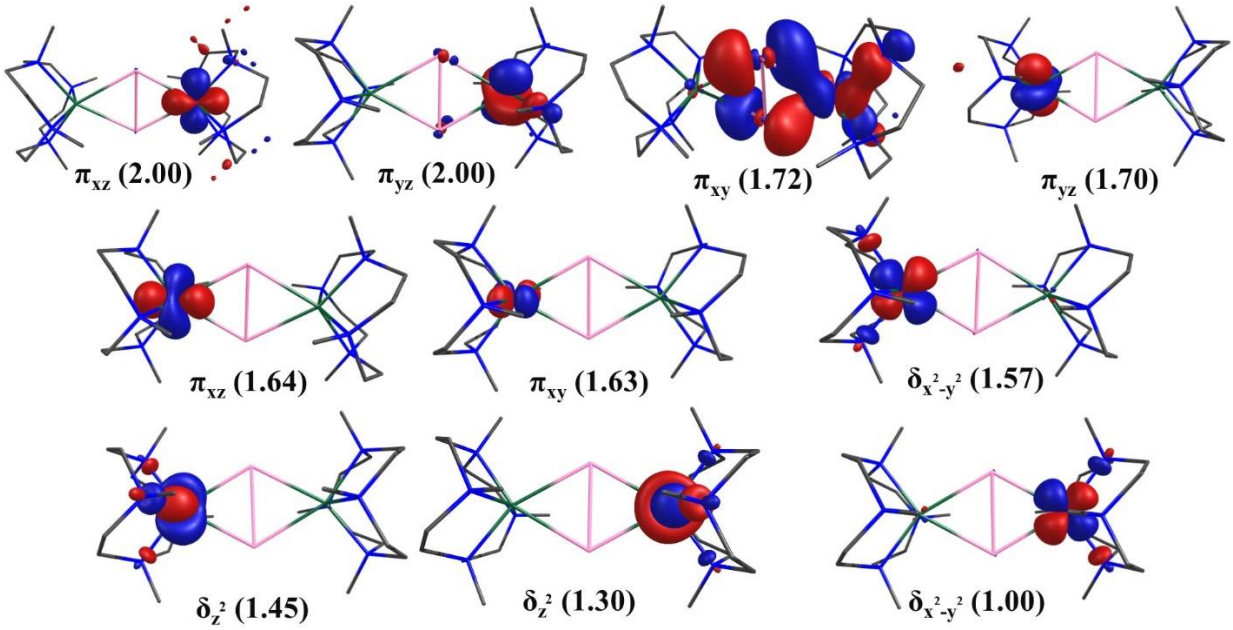


Figure S38. SA-CASSCF plots for the Ni orbitals for the complex **4** for active space CAS(16,10).

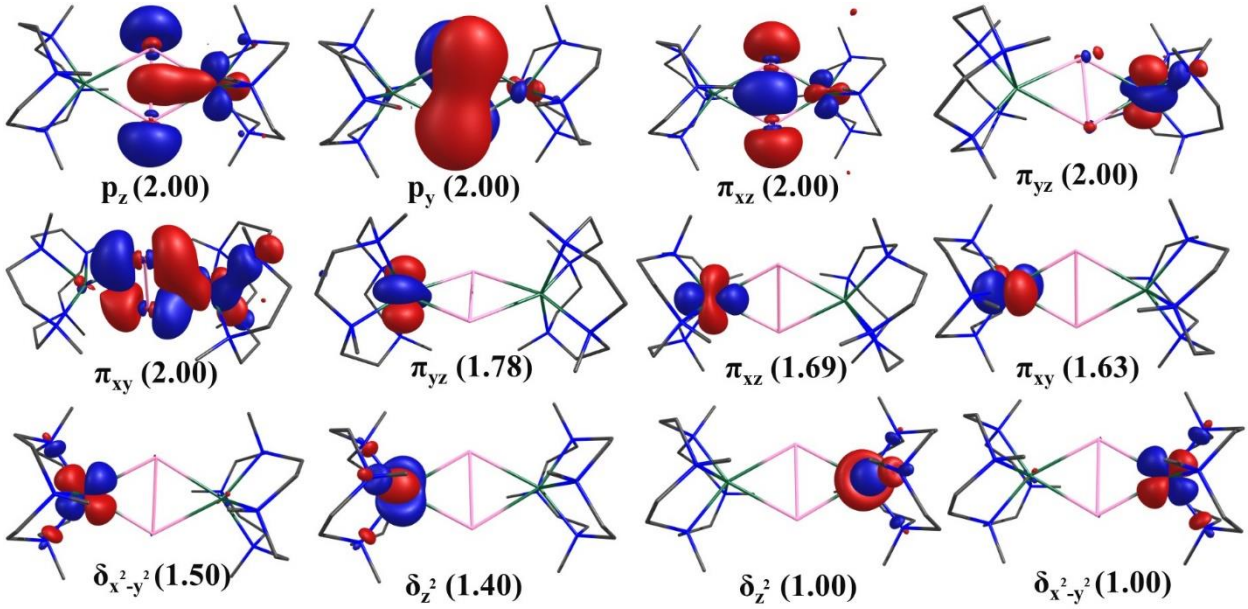


Figure S39. SA-CASSCF plots for the Ni and Te orbitals for the complex **4** for active space CAS(20,12).

Table S6- CASSCF orbitals for root0 of complexes ^{1}**1-4**$_{(t,t)}$ for active space (16,10) and (20,12).

CASSCF	CAS(16,10)(root 0)	CAS(20,12)(root 0)
1	$d_{xz}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{yz}^2d_{y^2}^1d_{x^2-y^2}^1d_{z}^1d_{x^2-y^2}^1$ (94.3%)(GS)+$d_{xz}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{xy}^2d_{yz}^2d_{z^2}^1d_{x^2-y^2}^2d_{z^2}^1d_{x^2-y^2}^0$ (3.2%)(ES_1)	$p_y^2p_x^2d_{xz}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{xy}^2d_{yz}^2d_{z^2}^1d_{x^2-y^2}^1d_{z^2}^1d_{x^2-y^2}^1$ (94.2%)(GS)+ $p_y^2p_x^2d_{xz}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{xy}^2d_{yz}^2d_{z^2}^1d_{x^2-y^2}^2d_{z^2}^1d_{x^2-y^2}^0$ (3.3%)(ES_1)
2	$d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xz}^2d_{xy}^2d_{x^2-y^2}^1d_{z^2}^1d_{x^2-y^2}^1d_{z^2}^1$ (90.0%)(GS)+ d_{yz}^2 d_{xy}^2 d_{yz}^2 d_{xz}^2 $d_{xz}^2d_{xy}^2d_{x^2-y^2}^2d_{z^2}^1$ $d_{x^2-y^2}^0d_{z^2}^1$(5.9%)(ES_1)	$p_y^2p_x^2d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xz}^2d_{xy}^2d_{x^2-y^2}^1d_{z^2}^1d_{x^2-y^1}^1d_{z^2}^1$(90.0%)(GS)+ $p_y^2p_x^2d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xz}^2d_{xy}^2d_{x^2-y^2}^2d_{z^2}^1d_{x^2-y^2}^0d_{z^2}^1$(5.8%)($ES_1$)
3	$d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{xz}^2d_{z^2}^1d_{x^2-y^2}^1d_{z^2}^1d_{x^2-y^2}^1$(93.8%)(GS)+ $d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xz}^2d_{xy}^2d_{x^2-y^2}^2d_{z^2}^1d_{x^2-y^2}^0d_{z^2}^1$ (3.6%)(ES_1)	$P_z^2p_x^2d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{xz}^2d_{z^2}^1d_{x^2-y^2}^1d_{x^2-y^2}^1d_{z^2}^1$ (93.8%)(GS)+ $P_z^2p_x^2d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{xz}^2d_{z^2}^2d_{x^2-y^2}^1d_{x^2-y^2}^0d_{z^2}^1$ 3.6%)(ES_1)
4	$d_{xz}^2d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{x^2-y^2}^1d_{z^2}^1d_{z^2}^1d_{x^2-y^2}^1$(88.9%)(GS)+$d_{xz}^2d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{x^2-y^2}^2d_{z^2}^0d_{z^2}^1d_{x^2-y^2}^1$(7.1%)($ES_1$)	$P_z^2p_y^2d_{xz}^2d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{x^2-y^2}^1d_{z^2}^1d_{z^2}^1d_{x^2-y^2}^1$(88.9%)(GS)+ $P_z^2p_y^2d_{xz}^2d_{yz}^2d_{xy}^2d_{yz}^2d_{xz}^2d_{xy}^2d_{x^2-y^2}^2d_{z^2}^0d_{z^2}^1d_{x^2-y^2}^1$(7.1%)($ES_1$)

Table S7- Overlap integral for the ground state of complexes ^{1}**1-4**$_{(t,t)}$.

^{1}**1**$_{t,t}$		
Ni^{II}/Ni^{II}	**d_z^2**	**$d_{x^2-y^2}$**
d_z^2	0.06	0.00
$d_{x^2-y^2}$	0.00	0.44
^{1}**2**$_{t,t}$		
Ni^{II}/Ni^{II}	**d_z^2**	**$d_{x^2-y^2}$**
d_z^2	0.05	0.07
$d_{x^2-y^2}$	0.07	-0.32
^{1}**3**$_{t,t}$		
Ni^{II}/Ni^{II}	**d_z^2**	**$d_{x^2-y^2}$**
d_z^2	-0.27	0.01
$d_{x^2-y^2}$	0.01	0.97
^{1}**4**$_{t,t}$		
Ni^{II}/Ni^{II}	**d_z^2**	**$d_{x^2-y^2}$**
d_z^2	0.52	-0.01
$d_{x^2-y^2}$	-0.01	0.66

Table S8- Previous literature on compounds containing O, S, Se, and Te ligands.

Species	**Condition**	**Result**	**Energy Barrier**	**Citation**
$Co(ClO_4)_2$ • 6MeCN + 2 [14]aneN4 + 2 NaSH= $C_{20}H_{48}N_2Ni_2S_2^{2+}$,2($Cl_1O_4^{1-}$),2($C_2H_3N_1$)	16-hour, Room Temp.	hydrogenation of a π bond (diazo benzene to di phenyl hydrazine product)	-	[10]
[{(η^5 -C_5H_4Me)Mo}$_2$(μ-SH)(μ-SCH_3)(S_2CH_2)]	20-60 ^{O}C	hydrogenation of unsaturated organic compounds	Found BDE(S-H) less than 90kcal/mol	[11]
[(triphos)Niμ-S_2)Ni(triphos)]ClO_4	22 ^{O}C	S = 1/2 spin system with g± = 2.0 and = 2.18	-	[6]
[{(triphos)M}$_2$(μ -η^2-Te_2)]$_2C_4H_8O$	60 ^{O}C for 3 h	Crystal structure formed	-	[9]
{[(Ni(Me_4[12]aneN$_4$)]$_2$(μ-η_2:η_2-Se_2)}(PF_6)$_2$	55 ^{O}C, overnight	DHA to anthracene	BDE(Se_H) bond= 80kcal/mol	[7]
[(PhTttBu)Ni]2(μ-η2 :η2 -S2)	-	Centrosymmetric, antiferromagnetically coupled, J=-487cm^{-1} Reactant with O2 and forms Ni2(μ-S) type complexes.	-	[4]
[Cp*2Co][Cp′2Ni2E2] E= S,Se,Te	100 K	Devision of Dichalcogenide, Subchalcogenide, chalcogenides. 1-3 complex falls in subchalcogenide category	-	[12]
LnNi2(η2 ,η2 -S2),[2] LnNi2(μ-1,2-S2),[3]	-	Three types of bonding modes of Sulphur ligand	-	[13]
butterfly like [NiII 2(μ-η2 :η2 -S2)] complex	-	Smaller activated S-S bond length.	-	[14]
[Ni$^{II}_2$(Me_nTPA)$_2$(μ-η^2:η^2-S_2)](ClO_4)$_2$	-	reactivity of these complexes is controlled by the steric effects as well as the electron donor ability of the supporting ligands		[15]
Facile Dissociation of [(LNiII)2E2] (E=Se,Te)	-	Dichalcogenides: Evidence for[LNiIIE2] Superselenides and Supertellurides in Solution	-	[8,8]
{(IPr)ClNi}2(μ2 -η2 ,η2 -S2)	-	Also, form Ni-Ni bonded bridging sulfide type species.	-	[16]
{[Ni(tmc)]2(μ-O2)}(OTf)2	-	DFT favored end on over side on type species	-	[17]

Table S9– Steric energies (in kJ/mol), **ΔE_{strain}** energy for lowest and first excited state of ***ts1*** for all complexes **1-4**.

First hydrogen atom transfer	**ΔE_{strain} (in kJ/mol)**	**ΔE_{steric}(in kJ/mol)**	**First hydrogen atom transfer**	**ΔE_{int} (in kJ/mol)**	**ΔE_{strain}(in kJ/mol)**
1-^{5}***ts1***$_{(t,t)}$	-67.0	70.5	**1**-^{1}***ts1***$_{(t,t)}$	10.2	75.4
2-^{1}***ts1***$_{(t,t)}$	-101.7	271.9	**2**-^{5}***ts1***$_{(t,t)}$	-3.14	306.9
3-^{5}***ts1***$_{(t,t)}$	-104.2	248.9	**3**-^{1}***ts1***$_{(t,t)}$	-220.0	250.5
4-^{5}***ts1***$_{(t,t)}$	-112.7	277.9	**4**-^{1}***ts1***$_{(t,t)}$	-120.9	225.3

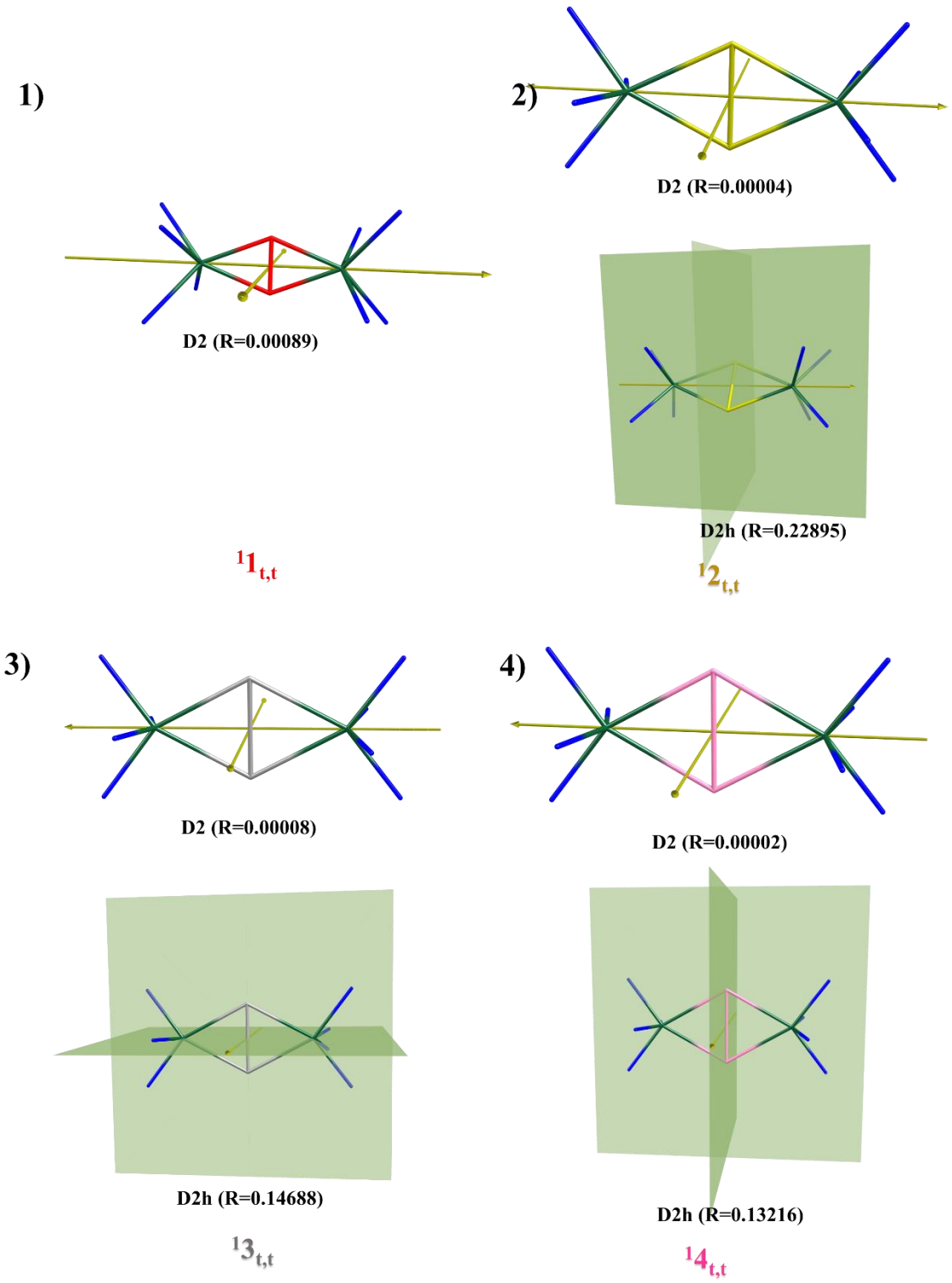


Figure S40. The symmetry measures of all four complexes (**1-4**) showed a minute deviations from D2h, ranging between 0.11-0.22 (plotted by Chemcraft software).

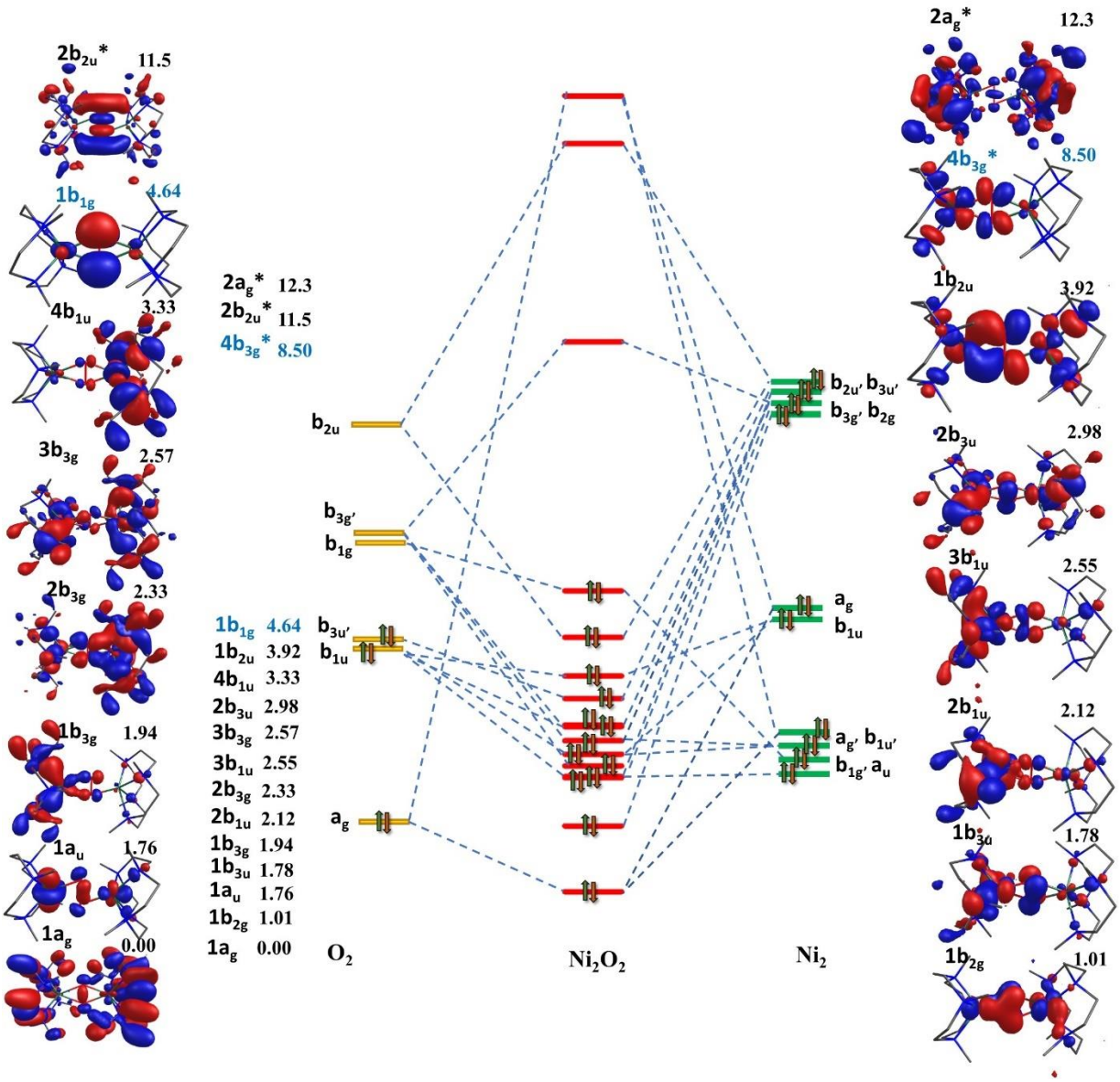


Figure S41. The qualitative molecular orbital diagram for complex $^{1}\mathbf{1}_{(t,t)}$. Here Homo-Lumo energy written in blue color code.

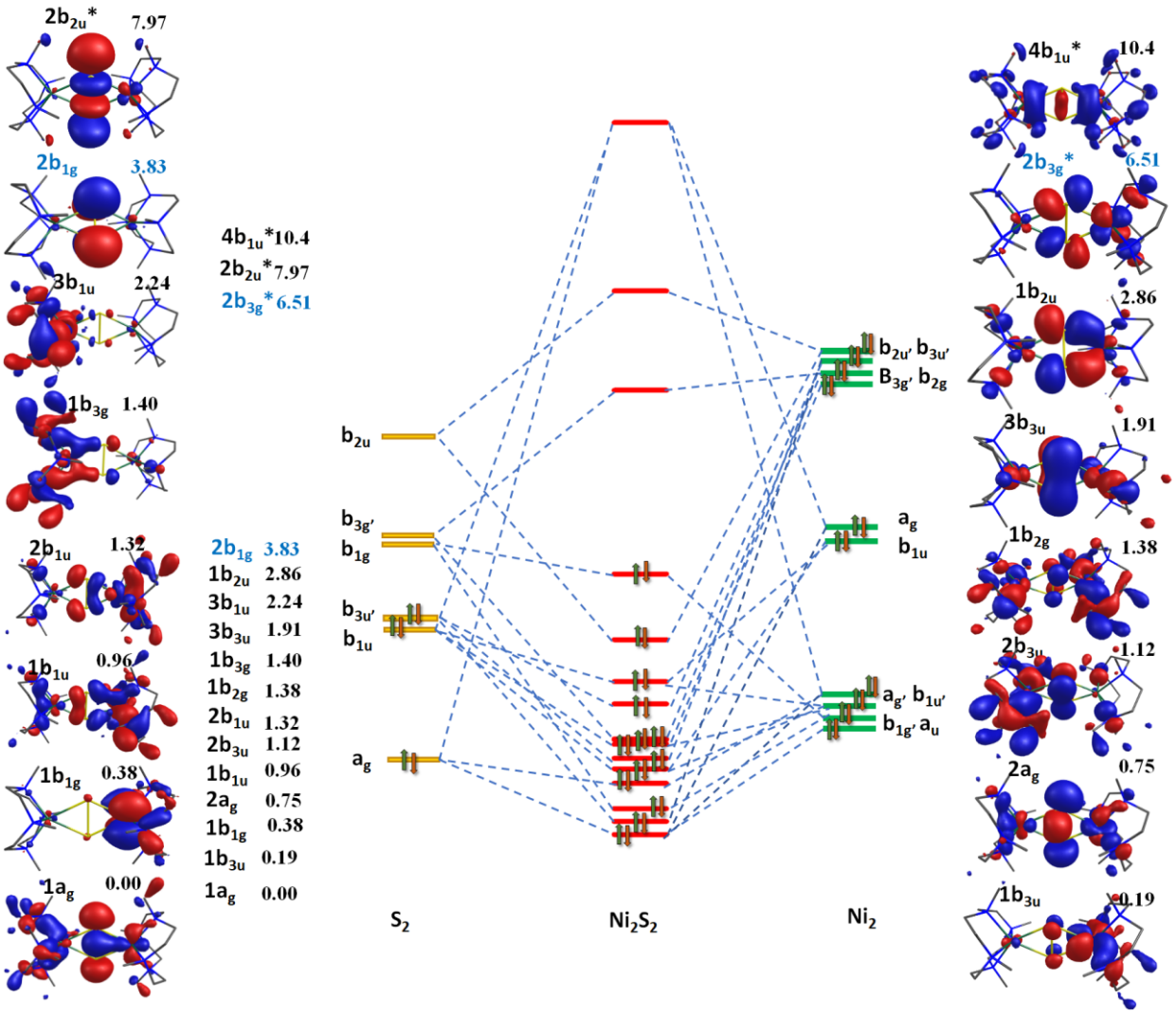


Figure S42. The qualitative molecular orbital diagram for complex $^{1}\mathbf{2}_{(t,t)}$. Here Homo-Lumo energy written in blue color code.

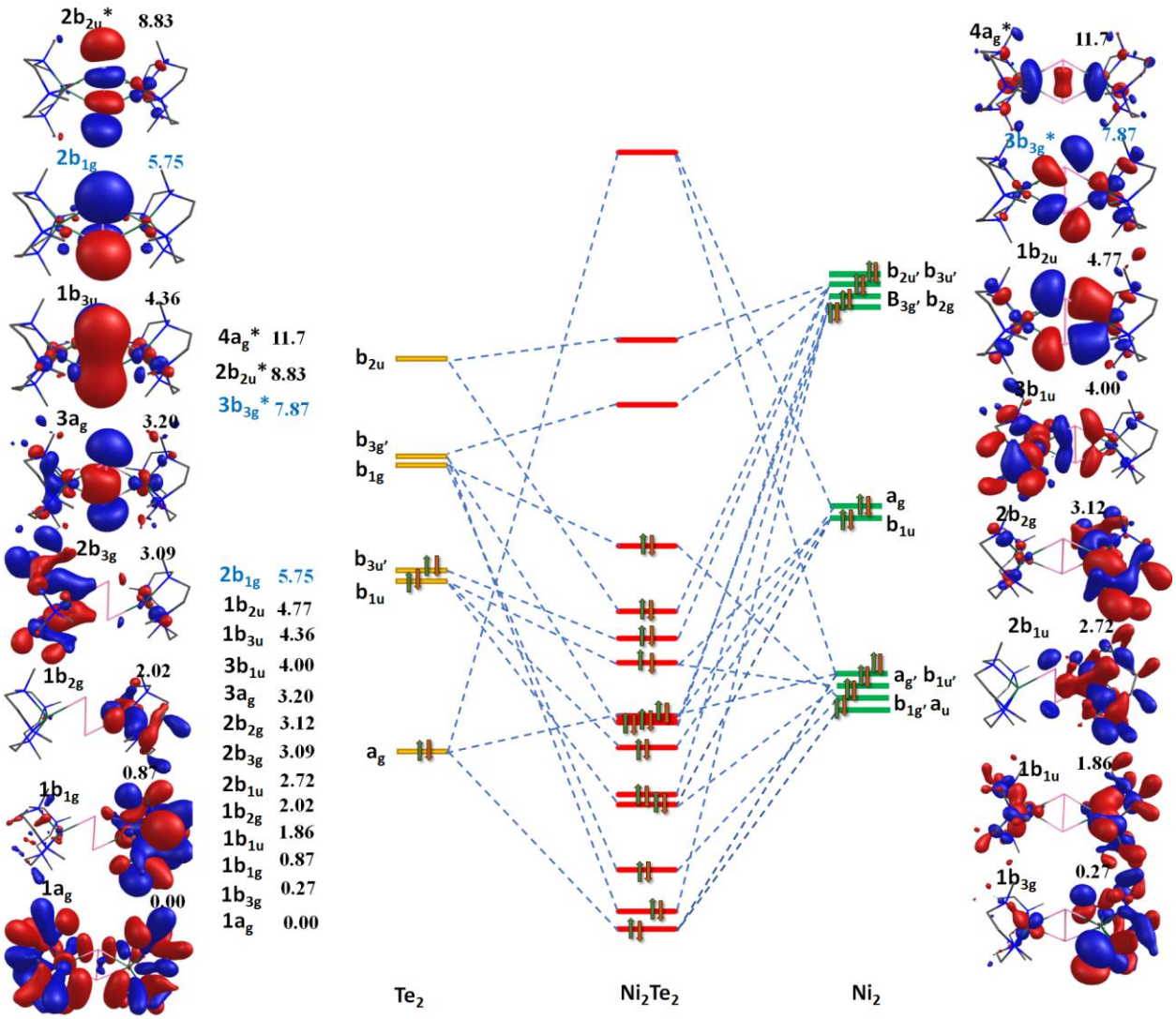


Figure S43. The qualitative molecular orbital diagram for complex $^{1}\mathbf{4}_{(t,t)}$. Here Homo-Lumo energy written in blue color code.

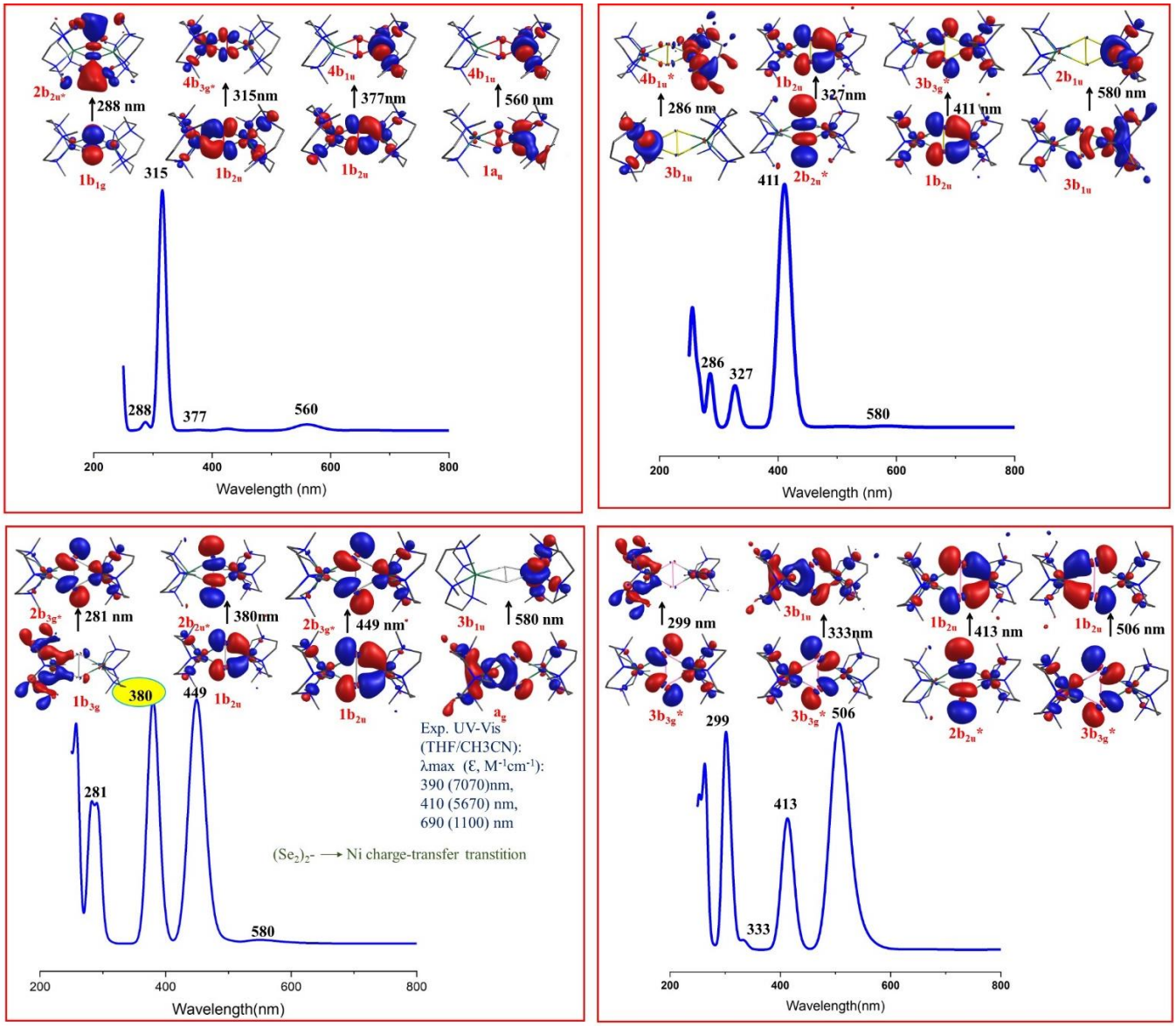


Figure S44. Electronic absorption spectra of ground state $^{1}\boldsymbol{R}_{(t,t)}$(A) Complex **1**, (B) Complex **2**, (C) Complex **3**, (D) Complex **4.**

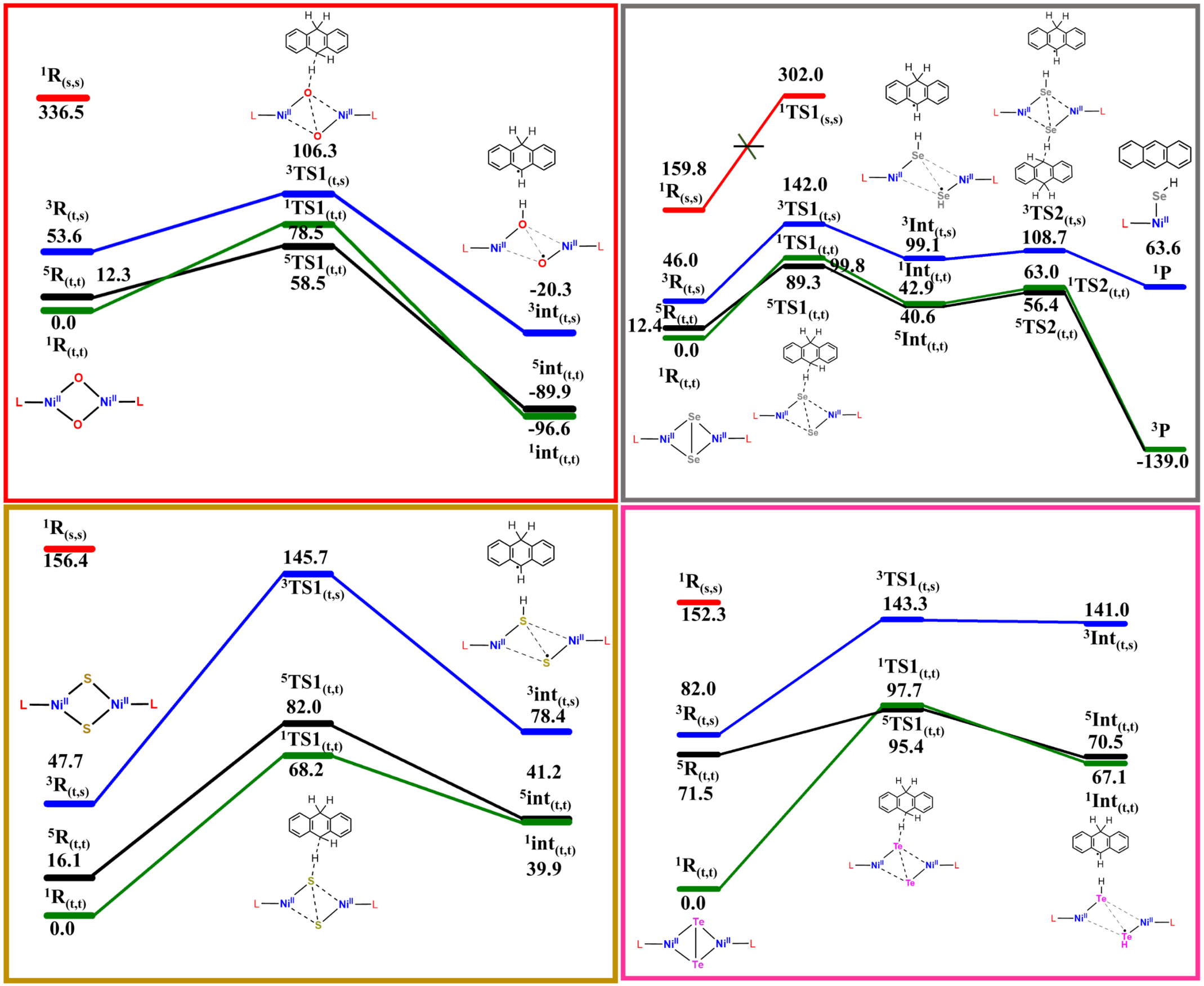


Figure S45. Computed potential energy surface for the C-H bond activation by complexes (a)**1**, (b) **2**, (c) **3** and (d) **4** (kJ/mol)

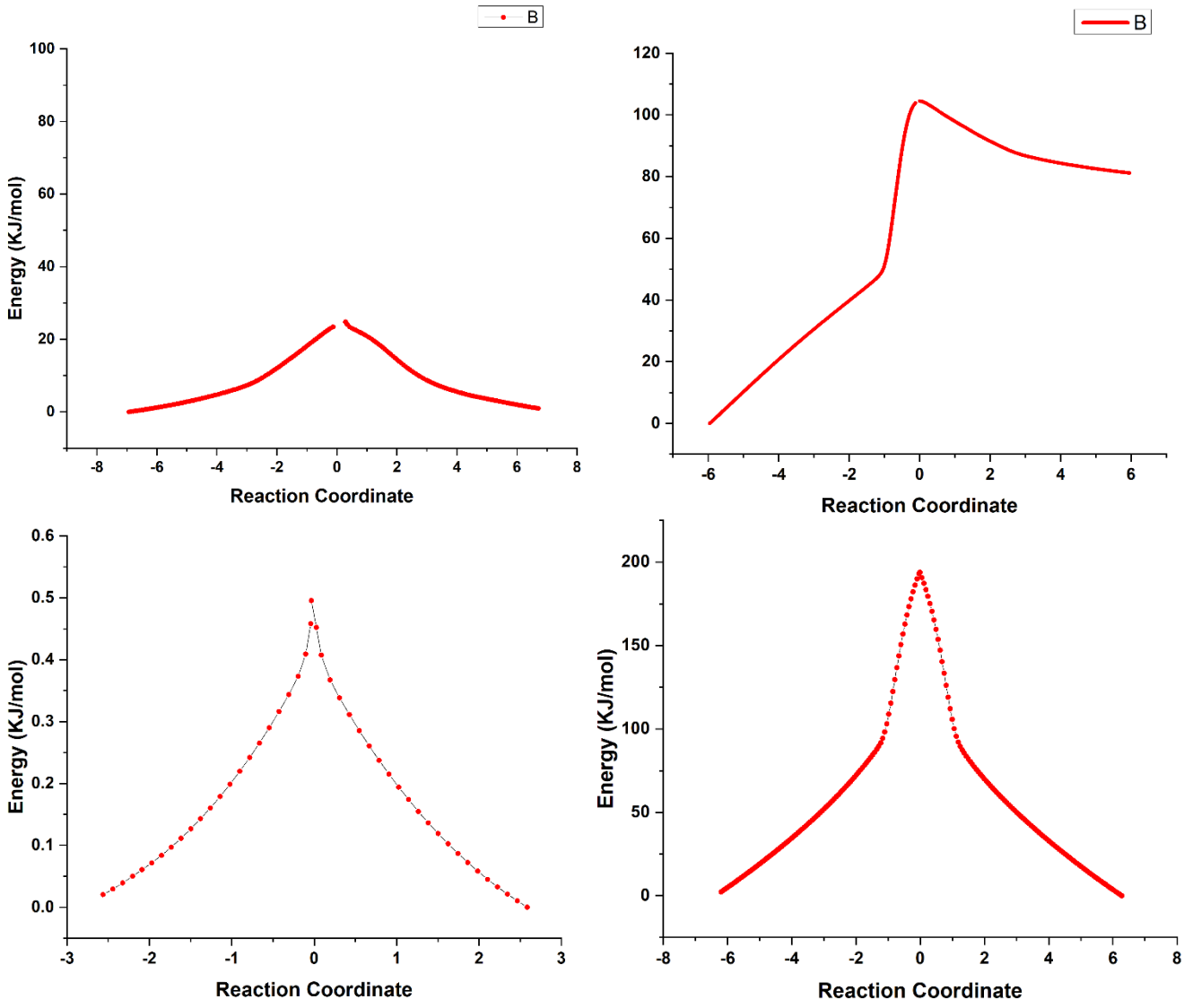


Figure S46. IRC plots for the first hydrogen abstraction transition state (***ts1***) for complex **3**.

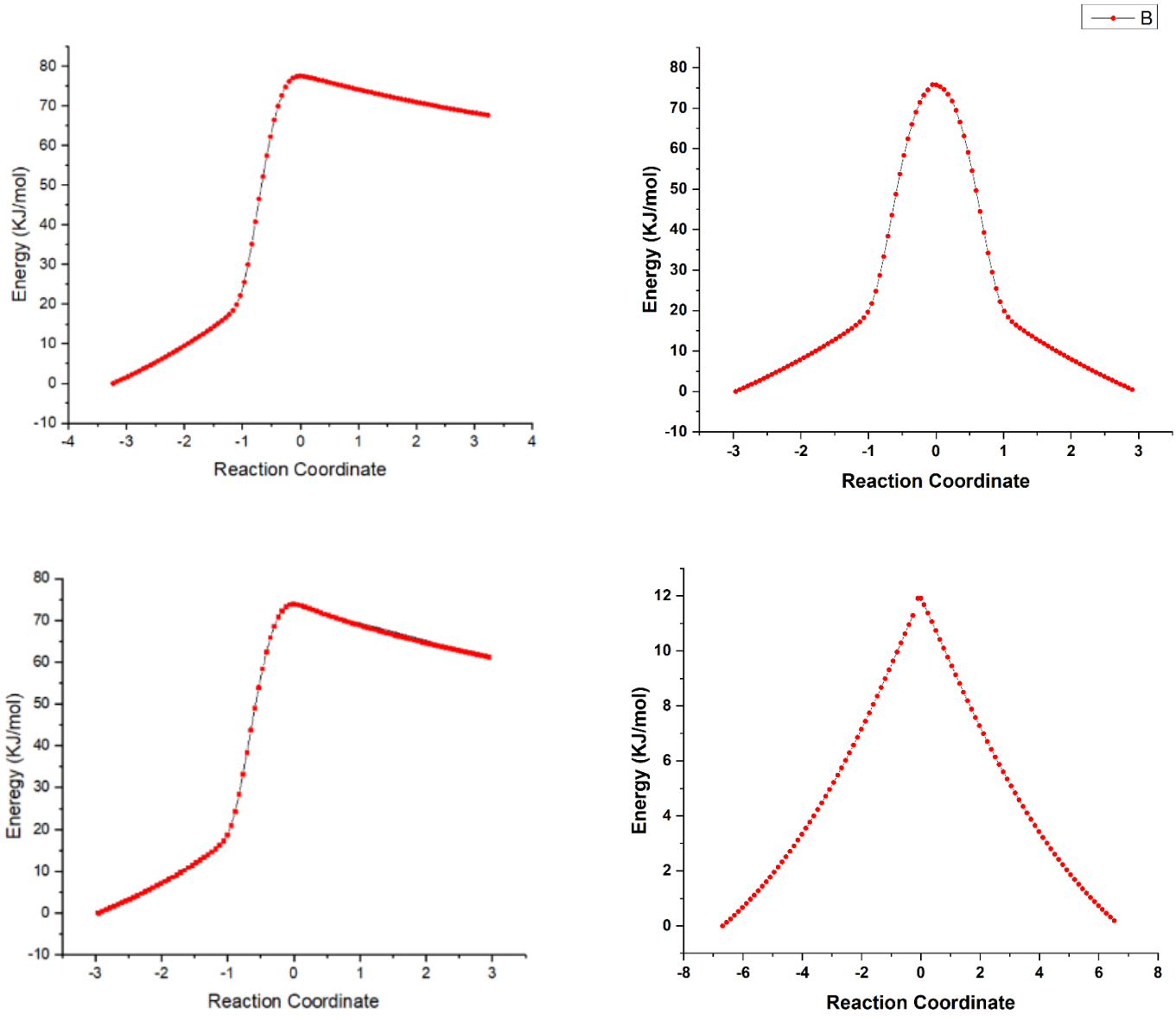


Figure S47. IRC plots for the second hydrogen abstraction transition state (***ts2***) for complex **3**.

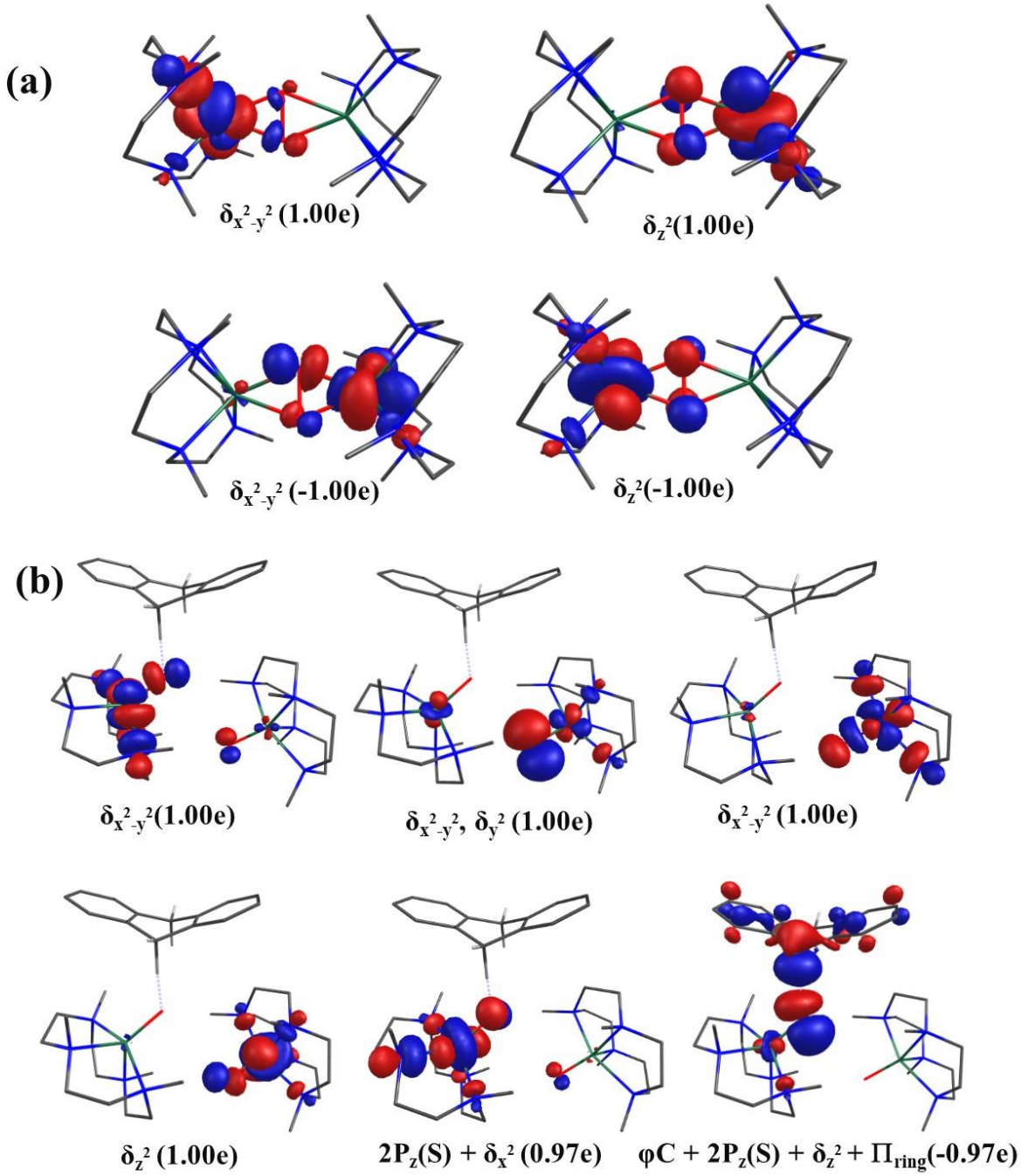


Figure S48. Spin natural orbitals and their occupations (noted in parenthesis) for complex **1** (a) $^{1}\boldsymbol{R}_{(t,t)}$ (top panel) and (b) $^{5}\boldsymbol{ts1}_{(t,t)}$ (bottom panel).

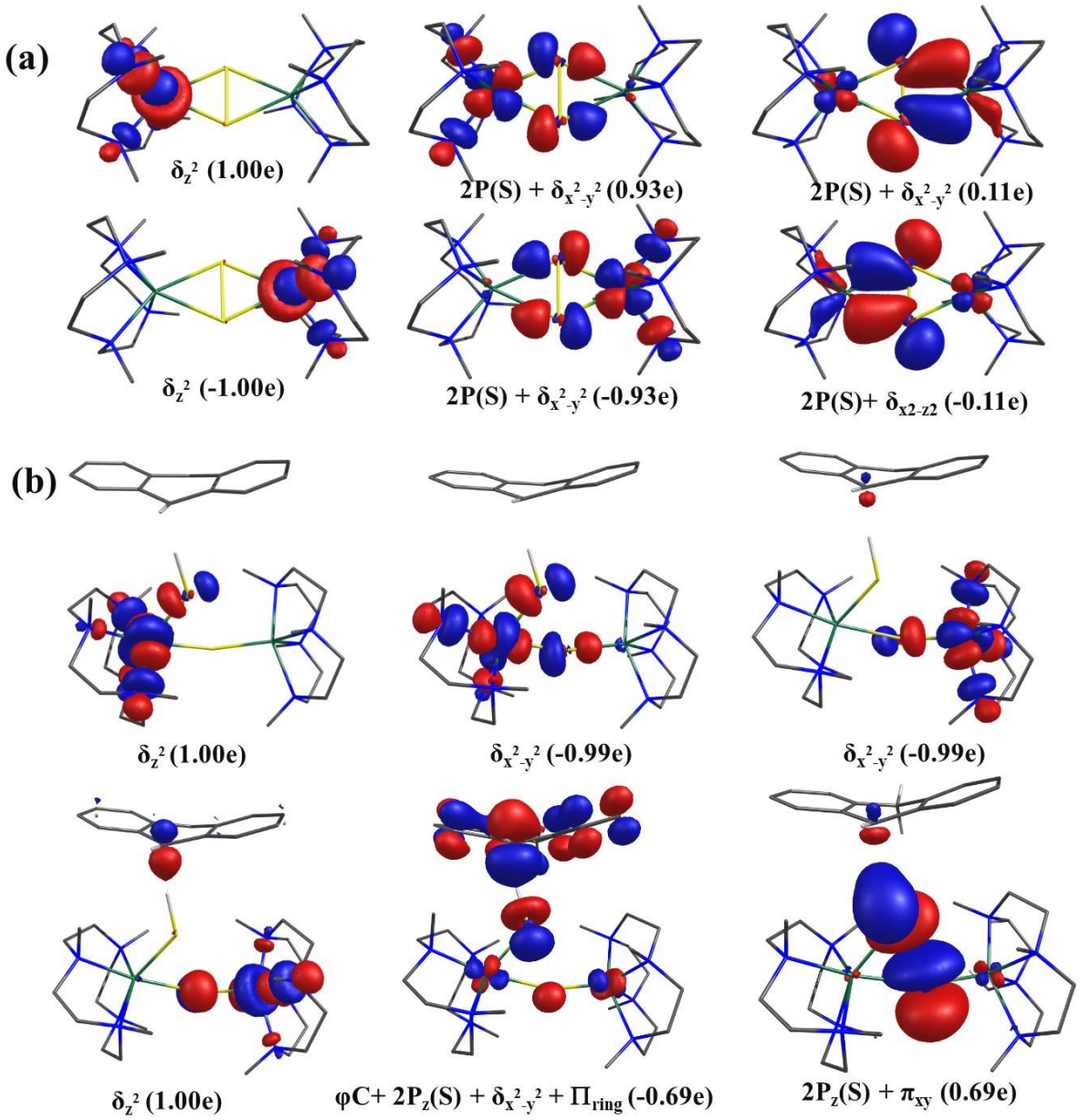


Figure S49. Spin natural orbitals and their occupations (noted in parenthesis) of Complex **2** (a) $^{1}\boldsymbol{R}_{(t,t)}$ (top panel) and (b) $^{1}\boldsymbol{ts1}_{(t,t)}$ (bottom panel).

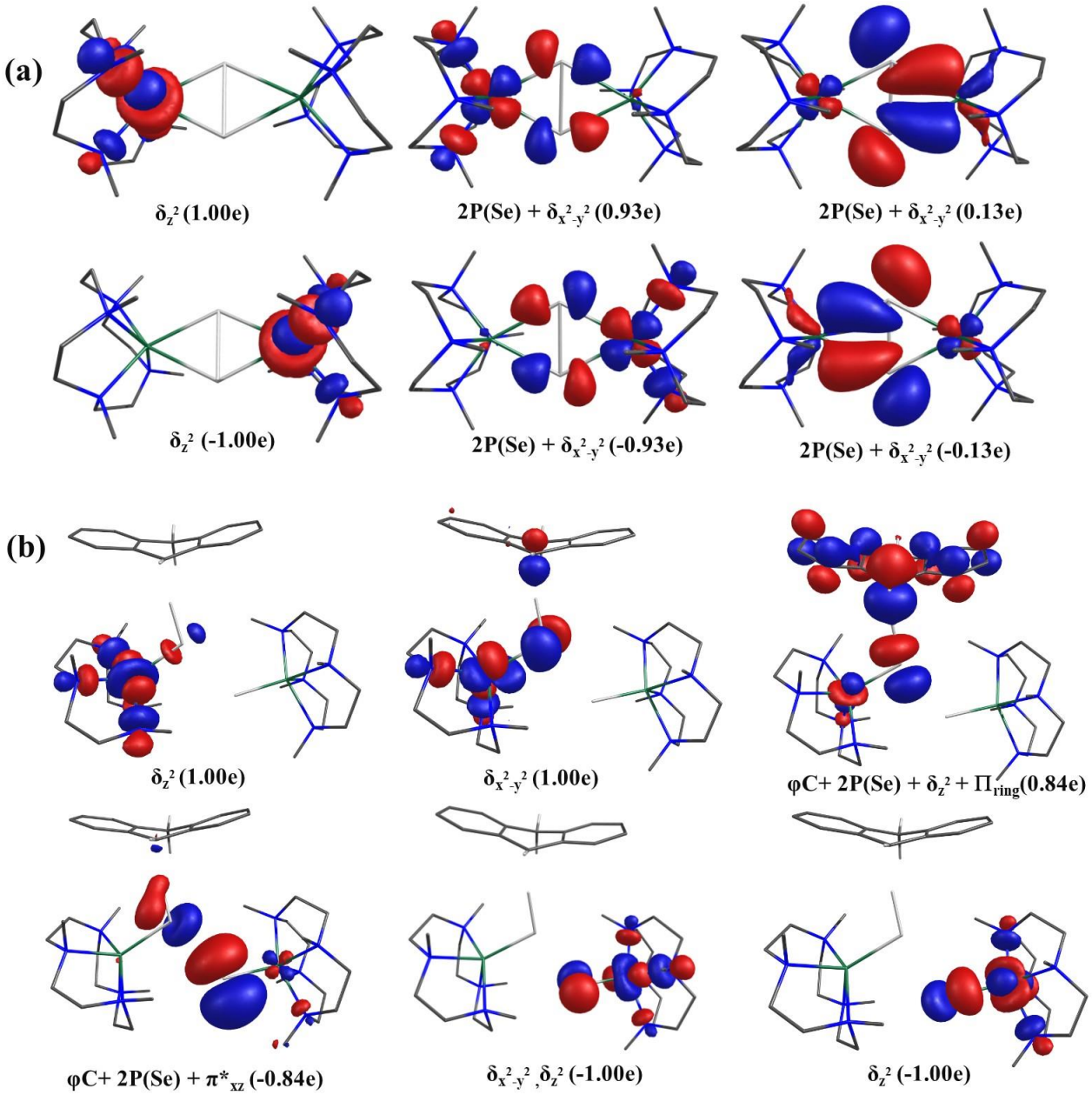


Figure S50. Spin natural orbitals and their occupations (noted in parenthesis) of Complex **3** (a) $^{1}\boldsymbol{R}_{(t,t)}$ (top panel) and (b) $^{5}\boldsymbol{ts1}_{(t,t)}$ (bottom panel).

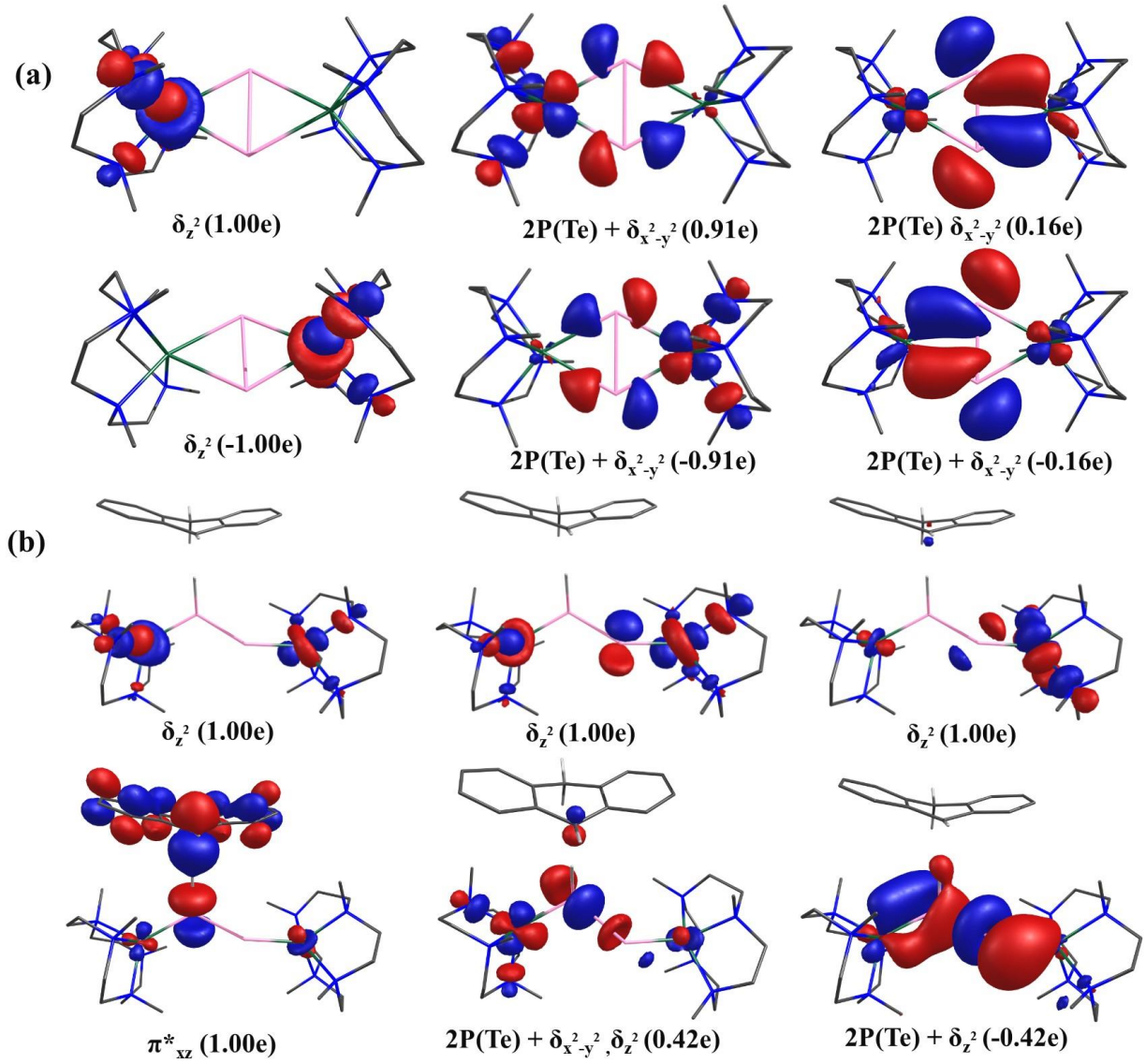


Figure S51. Spin natural orbitals and their occupations (noted in parenthesis) of Complex **4** (a) $^{1}\boldsymbol{R}_{(t,t)}$ (top panel) and (b) $^{5}\boldsymbol{ts1}_{(t,t)}$ (bottom panel).

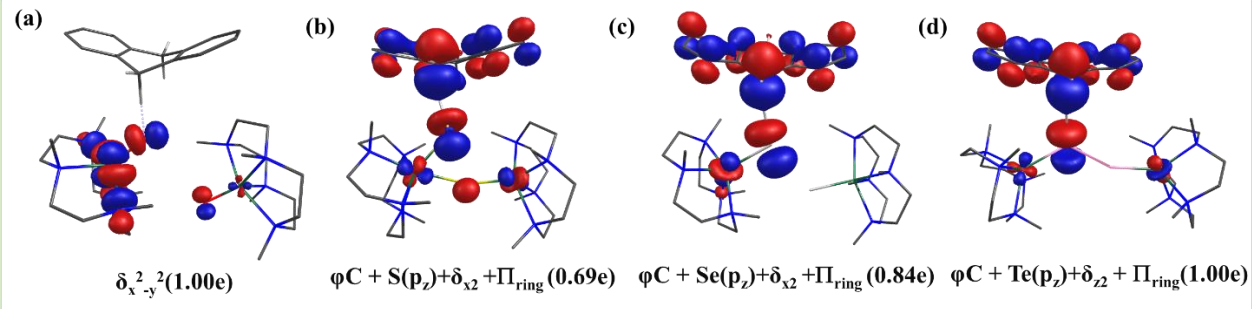


Figure S52- SNO plots for complexes **1-4**. (a) for complex **1**, (b) for complex **2**, (c) for complex **3**, (d) for complex **4**.

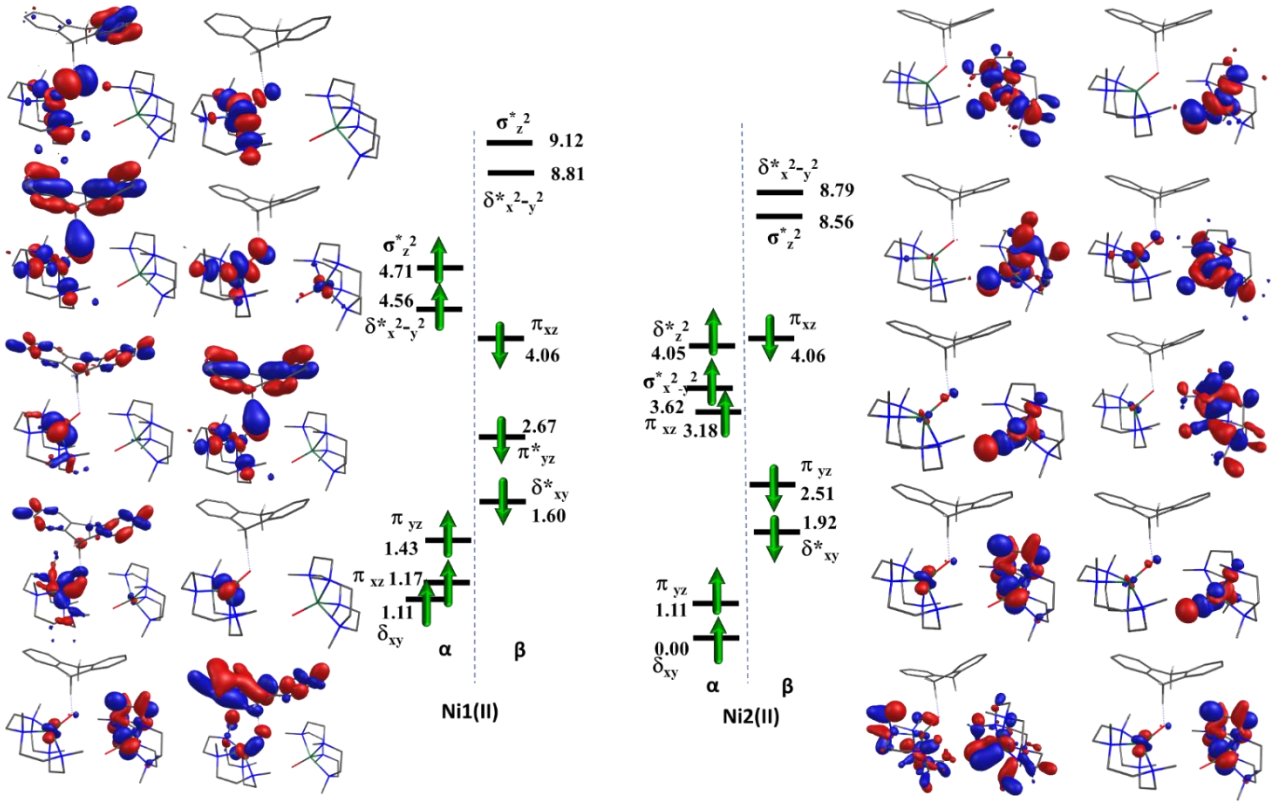


Figure S53- Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the ground state ^{5}**TS1**$_{(t,t)}$ of the complex **1** (energies are given in eV)

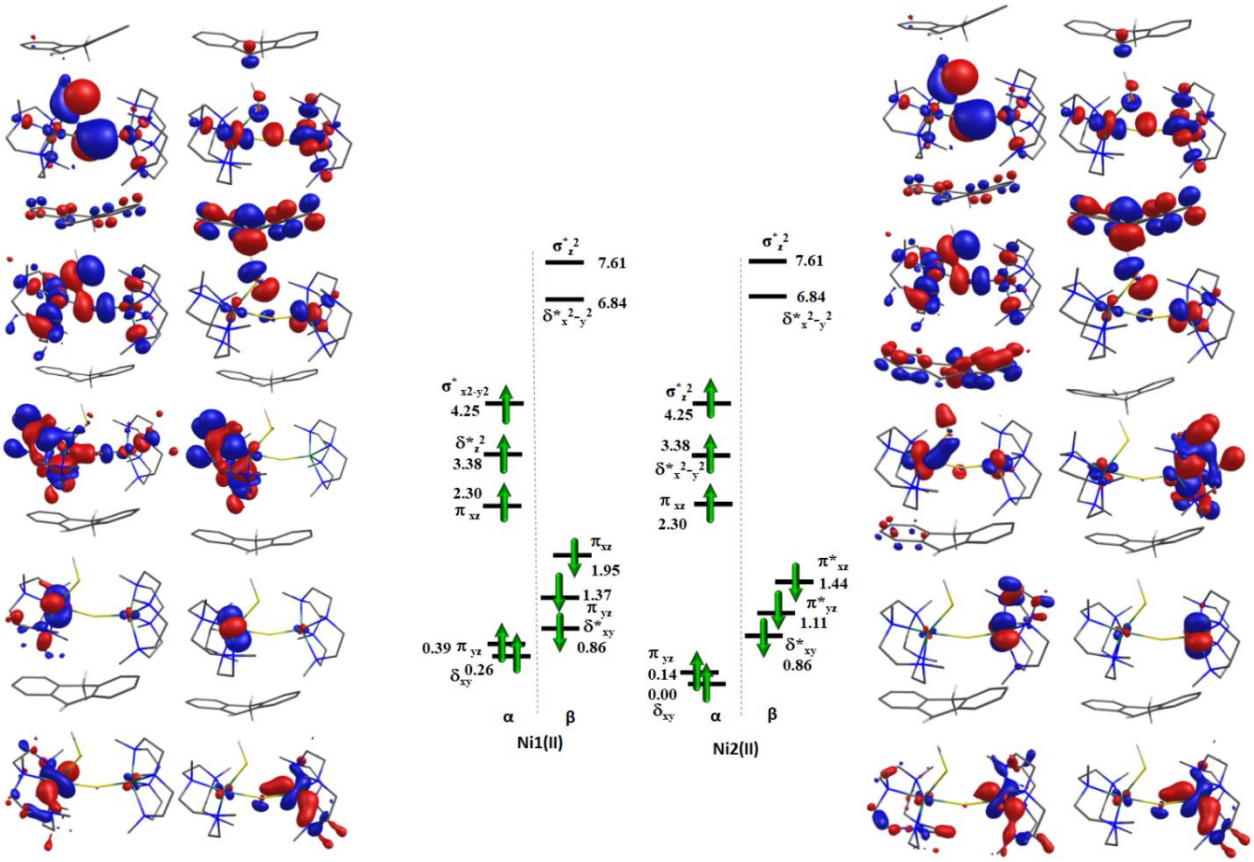


Figure S54- Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the state ^{5}**TS1**$_{(t,t)}$ of the complex **2** (energies are given in eV)

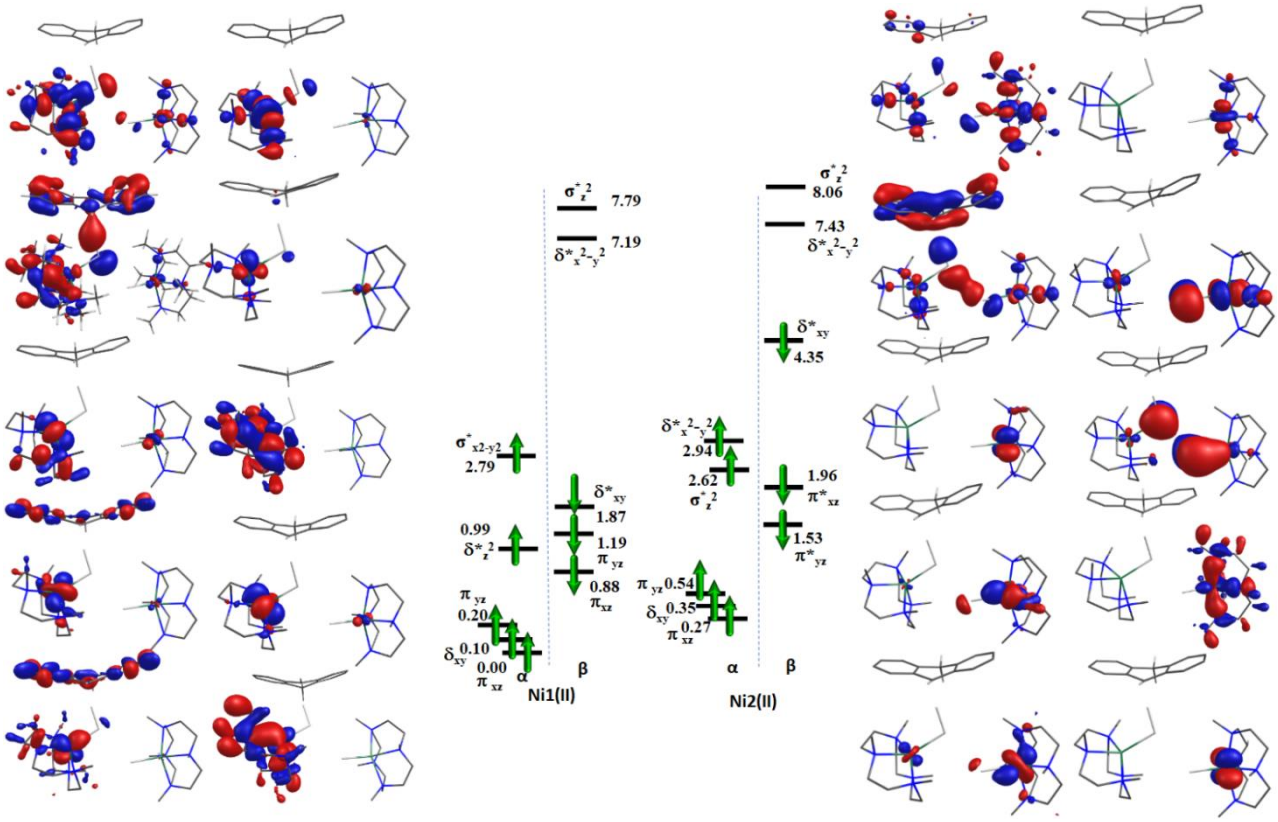


Figure S55- Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the ground state ^{5}**TS1**$_{(t,t)}$ of the complex **3** (energies are given in eV)

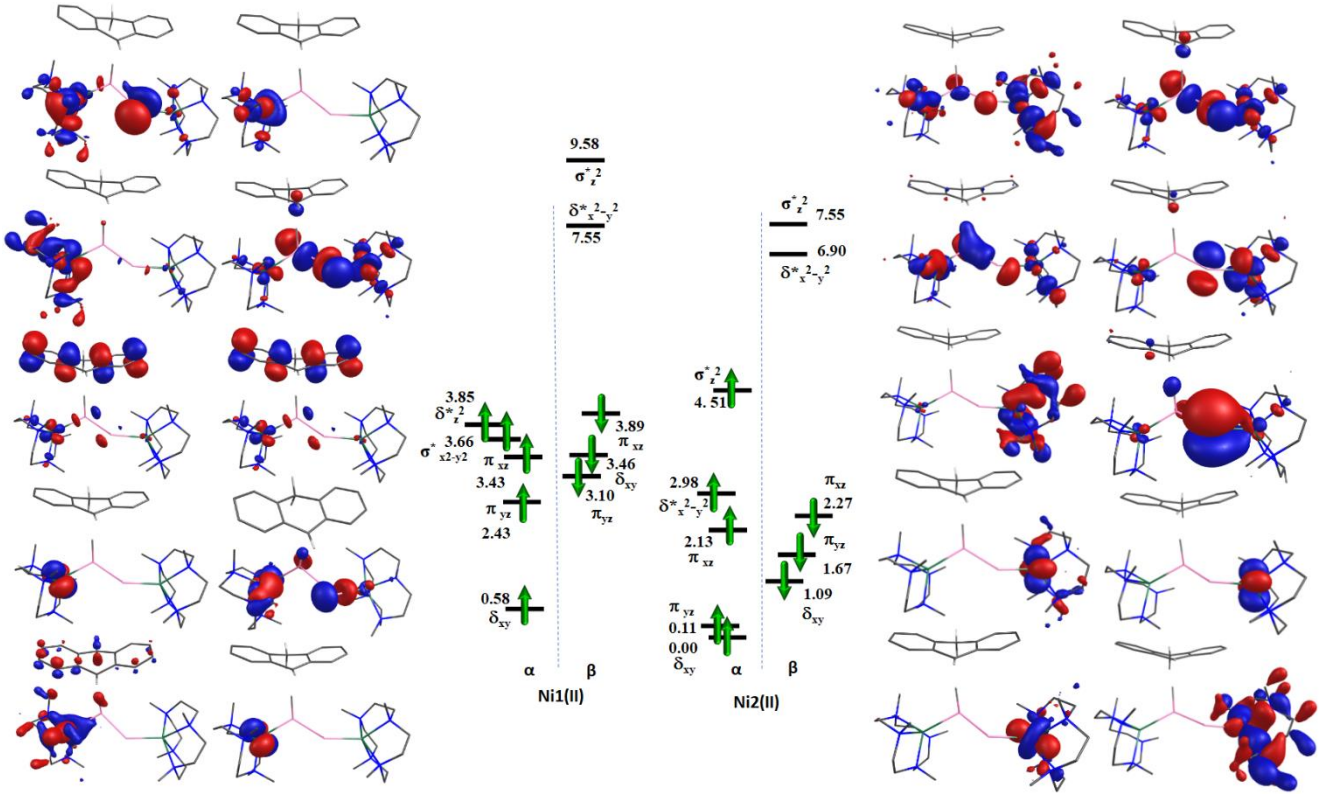


Figure S56- Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the ground state ^{5}**TS1**$_{(t,t)}$ of the complex **4** (energies are given in eV)

Table S10. Cartesian non-adiabatic coulpings parameters of the first hydrogen abstraction transition state TS1 of the complex **1**–**4**.

First hydrogen abstraction (TS1)	Norm of the NACs	RMS NACs	MAX NAC
^{5}**TS1**$_{(t,t)}$	2.66	0.14	1.33
^{1}**TS1**$_{(t,t)}$	1.97	0.10	1.21
^{5}**TS1**$_{(t,t)}$	0.56	0.03	0.34
^{5}**TS1**$_{(t,t)}$	0.52	0.03	0.29

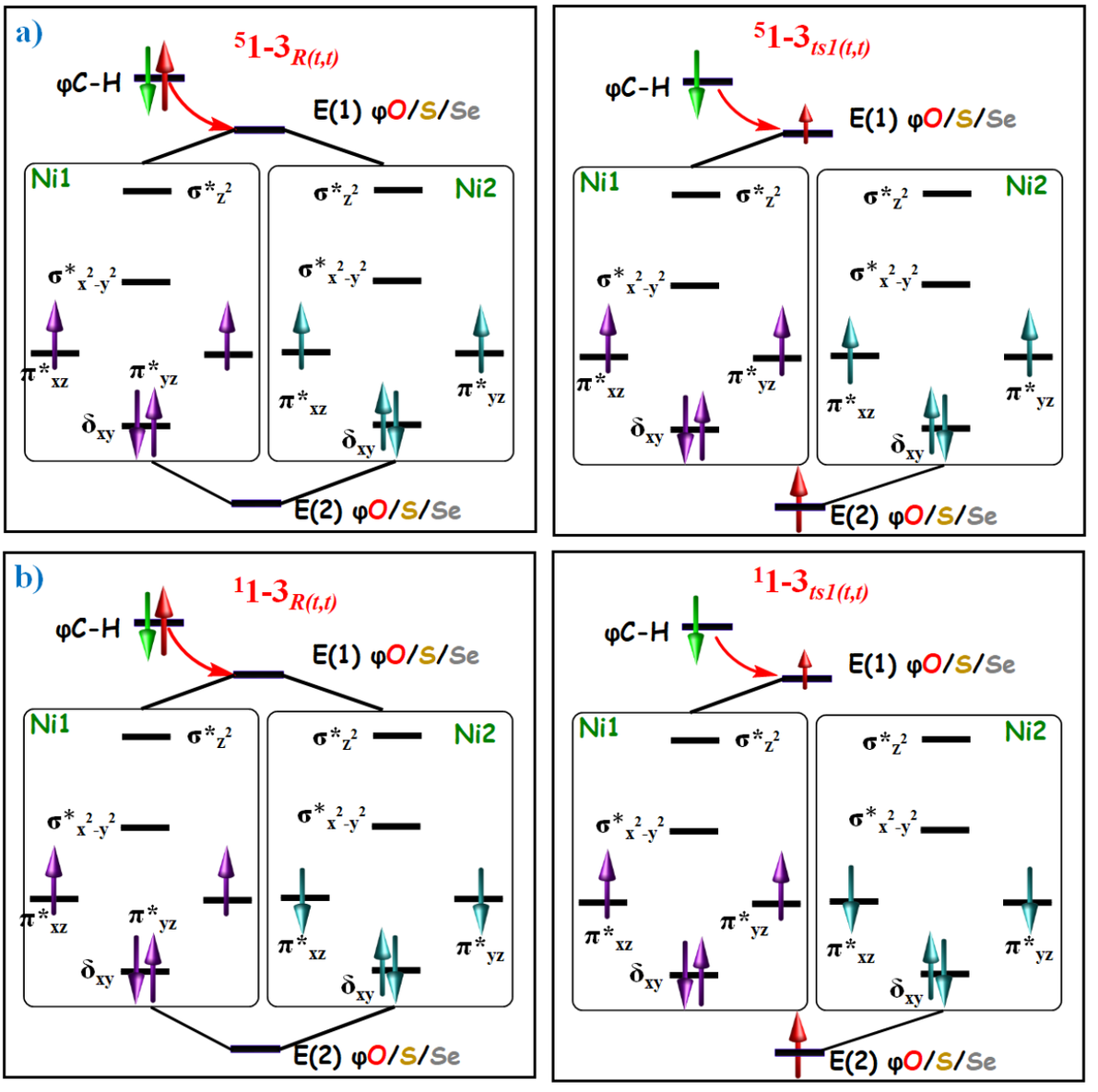


Figure S57. Electron shift diagrams for a) ferromagnetic reactant species (^{5}**1-3**$_{R(t,t)}$) and ground state ts1 (^{5}**1-3**$_{ts1(t,t)}$) b) for antiferromagntic reactant species (^{1}**1-3**$_{R(t,t)}$) and first excited transition state (^{1}**1-3**$_{ts1(t,t)}$), showed α-electron transfer from the substrate, triggers Ni–E bond cleavage, and the transferred electron is found to be located on the E(2) centre, resulting in the formation of Ni(II)-E• species.

Table S11. *J* values computed for single monomer core Ni(2)-E(2) core.

Half core of HAT ts1	***J* value**
1$_{ts1}$	366.6
2$_{ts1}$	147.0
3$_{ts1}$	163.4
4$_{ts1}$	129.5

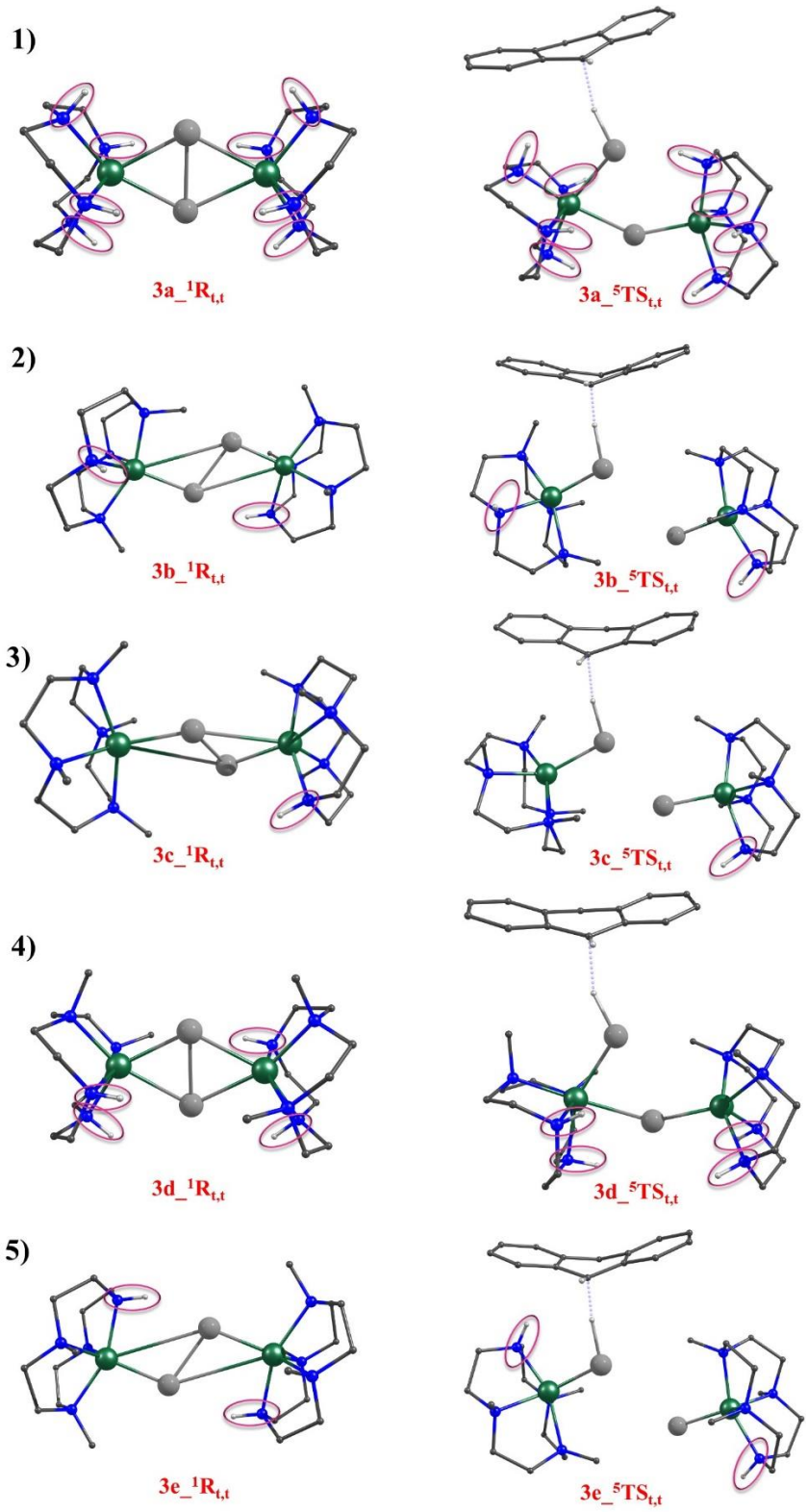


Figure S58- Optimized geometries of substituted reactant ($^{1}\mathbf{R_{t,t}}$) and first hydrogen abstraction transition state ($^{5}\mathbf{TS_{t,t}}$) species of complex **3 (3a-3e)**. Pink circle shows the substituted area.

Table S12- The correlation of J value with barrier height of first hydrogen abstraction transition state (TS1) by substituted geometries of complex **3**.

Substituted Geometries	J value (cm^{-1})	Barrier height (kJ/mol)
1	300.2	60.1
2	302.5	96.2
3	333.3	97.8
4	334.6	113.1
5	338.5	121.3

Table S13: Computed spin densities and Mulliken charges of complex **1** for all possible spin states of reactants (***R***) along with bond lengths and bond angle obtained from optimized geometries in Gaussian 09.

Spin Density of Reactant (Complex 1)				
Spin Density	$^{5}R_{(t,t)}$	$^{1}R_{(t,t)}$	$^{3}R_{(s,t)}$	$^{1}R_{(s,s)}$
Ni1	1.64	1.58	1.57	0.00
Ni2	1.64	-1.58	0.17	0.00
O1	0.14	0.00	-0.01	0.00
O2	0.14	0.00	-0.01	0.00
N_{1a}	0.06	0.05	0.05	0.00
N_{1b}	0.05	0.05	0.05	0.00
N_{1c}	0.06	0.05	0.05	0.00
N_{1d}	0.05	0.05	0.05	0.00
N_{2a}	0.06	-0.05	-0.02	0.00
N_{2b}	0.05	-0.05	0.05	0.00
N_{2c}	0.06	-0.05	-0.02	0.00
N_{2d}	0.05	-0.05	0.05	0.00
Mulliken Atomic Charges of Reactant (Complex 1)				
Spin Density	$^{5}R_{(t,t)}$	$^{1}R_{(t,t)}$	$^{3}R_{(s,t)}$	$^{1}R_{(s,s)}$
Ni_A	0.86	0.84	0.83	0.72
Ni_B	0.86	0.84	0.81	0.72
O_A	-0.51	-0.47	-0.45	-0.37
O_B	-0.51	-0.47	-0.45	-0.37
N_{1a}	-0.29	-0.29	-0.29	-0.27
N_{1b}	-0.23	-0.23	-0.24	-0.22
N_{1c}	-0.29	-0.29	-0.29	-0.28
N_{1d}	-0.23	-0.23	-0.24	-0.21
N_{2a}	-0.29	-0.29	-0.29	-0.27
N_{2b}	-0.23	-0.23	-0.23	-0.22
N_{2c}	-0.29	-0.29	-0.29	-0.28
N_{2d}	-0.23	-0.23	-0.23	-0.21

Bond parameter of the Reactant (Complex 1)				
Bond Parameter	$^{5}R_{(t,t)}$	$^{1}R_{(t,t)}$	$^{3}R_{(s,t)}$	$^{1}R_{(s,s)}$
Ni_1-Ni_2	3.850	3.810	3.844	3.821
Ni_1-O_1	2.069	2.047	2.062	2.044
Ni_1-O_2	2.070	2.048	2.061	2.050
Ni_1-N_1	2.180	2.183	2.183	2.183
Ni_1-N_2	2.288	2.288	2.284	2.281
Ni_1-N_3	2.180	2.183	2.182	2.185
Ni_1-N_4	2.286	2.287	2.285	2.280
O_1-O_2	1.519	1.500	1.488	1.470
Ni_2-O_1	2.070	2.048	2.060	2.050
Ni_2-O_2	2.069	2.047	2.060	2.044
Ni_2-N_1	2.180	2.183	2.188	2.183
Ni_2-N_2	2.287	2.288	2.287	2.282
Ni_2-N_3	2.180	2.183	2.188	2.185
Ni_2-N_4	2.286	2.288	2.286	2.281
The bond angle of the Reactant (Complex 1)				
Bond Angle	$^{5}R_{(t,t)}$	$^{1}R_{(t,t)}$	$^{3}R_{(s,t)}$	$^{1}R_{(s,s)}$
∠Ni_1-O_1-O_2	68.5	68.5	68.8	69.2
∠Ni_1-O_2-O_1	68.4	68.5	68.8	68.7
∠Ni_2-O_1-O_2	68.4	68.5	68.9	68.7
∠Ni_2-O_2-O_1	68.5	68.5	68.8	69.2
∠Ni_1-O_1-Ni_2	136.9	137.0	137.7	137.9
∠Ni_1-O_2-Ni_2	136.9	137.0	137.7	137.9
∠N_1-Ni_1-N_2	81.4	81.3	81.7	81.4
∠N2-Ni_1-N3	81.3	81.5	80.7	81.9
∠N_3-Ni_1-N_4	81.4	81.3	81.7	81.4
∠N_4-Ni_1-N_1	81.4	81.5	80.7	81.9
∠N_1-Ni_2-N_2	81.4	81.3	81.7	81.4
∠N2-Ni_2-N3	81.3	81.5	80.7	81.9

∠N_3-Ni_2-N_4	81.4	81.3	81.6	81.4
∠N_4-Ni_2-N_1	81.4	81.5	80.7	81.8

Table S14- Computed spin densities and Mulliken charges of complex **1** for all possible spin states of the first hydrogen abstraction transition state (***ts1***) along with bond lengths and bond angle obtained from optimized geometries in Gaussian 09.

Mulliken spin density and charges values of the transition state (TS1)							
Spin Density	$^5ts1_{(t,t)}$	$^1ts1_{(t,t)}$	$^3ts1_{(s,t)}$	**Mulliken Charges**	$^5ts1_{(t,t)}$	$^1ts1_{(t,t)}$	$^3ts1_{(s,t)}$
Ni1	1.59	1.60	1.65	**Ni1**	0.80	0.81	0.80
Ni2	1.61	-1.59	-0.04	**Ni2**	0.68	0.70	0.69
O1	-0.58	-0.58	0.80	**O1**	-0.61	-0.61	-0.59
O2	1.08	0.85	-1.02	**O2**	-0.49	-0.50	-0.49
N_{1a}	0.07	0.07	0.08	**N_{1a}**	-0.28	-0.28	-0.28
N_{1b}	0.05	0.06	0.08	**N_{1b}**	-0.22	-0.22	-0.21
N_{1c}	0.05	0.06	0.05	**N_{1c}**	-0.29	-0.28	-0.29
N_{1d}	0.05	0.05	0.07	**N_{1d}**	-0.24	-0.24	-0.23
N_{2a}	0.07	-0.08	0.03	**N_{2a}**	-0.28	-0.28	-0.28
N_{2b}	0.09	-0.06	0.05	**N_{2b}**	-0.21	-0.21	-0.21
N_{2c}	0.06	-0.06	-0.06	**N_{2c}**	-0.29	-0.29	-0.28
N_{2d}	0.08	-0.06	0.05	**N_{2d}**	-0.22	-0.23	-0.22
C_{DHA}	-0.19	-0.19	0.19	**C_{DHA}**	-0.20	-0.20	-0.21
Bond parameters and Bond angles of the transition state (TS1)							
Bond Parameter	$^5ts1_{(t,t)}$	$^1ts1_{(t,t)}$	$^3ts1_{(s,t)}$	**Bond Angle**	$^5ts1_{(t,t)}$	$^1ts1_{(t,t)}$	$^3ts1_{(s,t)}$
Ni_1-Ni_2	5.789	5.789	5.727	**∠Ni_1-O_1-O_2**	91.3	91.0	83.1
Ni_1-O_1	1.860	1.862	1.830	**∠Ni_1-O_2-O_1**	24.7	25.1	24.9
Ni_1-O_2	4.452	4.383	4.320	**∠Ni_2-O_1-O_2**	20.9	21.5	20.6
Ni_1-N_1	2.149	2.150	2.225	**∠Ni_2-O_2-O_1**	106.4	107.3	107.7
Ni_1-N_2	2.233	2.231	2.171	**∠Ni_1-O_1-Ni_2**	112.0	112.2	103.3
Ni_1-N_3	2.175	2.174	2.143	**∠Ni_1-O_2-Ni_2**	130.8	132.0	131.9
Ni_1-N_4	2.278	2.280	2.223	**∠N_1-Ni_1-N_2**	83.0	82.9	83.5
O_1-O_2	4.003	2.938	4.139	**∠N2-Ni_1-N3**	82.1	82.2	83.4
Ni_2-O_1	4.828	4.824	5.022	**∠N_3-Ni_1-N_4**	80.8	80.8	82.0
Ni_2-O_2	1.797	1.854	1.854	**∠N_4-Ni_1-N_1**	82.5	82.4	82.7
Ni_2-N_1	2.145	2.130	2.137	**∠N_1-Ni_2-N_2**	83.1	83.5	83.3

Ni_2-N_2	2.217	2.211	2.209	**∠N2-Ni_2-N3**	82.9	83.3	83.5
Ni_2-N_3	2.158	2.146	2.142	**∠N_3-Ni_2-N_4**	82.6	82.6	82.8
Ni_2-N_4	2.222	2.223	2.221	**∠N_4-Ni_2-N_1**	83.3	83.6	83.5
C-$H_{abs(DHA)}$	1.203	1.205	1.221	**∠O_1-H-C_{DHA}**	165.8	165.7	167.1
O-$H_{abs(DHA)}$	1.459	1.456	1.410	**∠ H-O_1-Ni**	124.7	124.5	132.0

Table S15- Computed spin densities and Mulliken charges of complex **1** for all possible spin states of intermediates (**Int1**), along with bond lengths and angles obtained from optimized geometries in Gaussian 09.

Mulliken spin density and charges values of intermediate (Int1)							
Spin Density	$^5Int1_{(t,t)}$	$^1Int1_{(t,t)}$	$^3Int1_{(s,t)}$	**Mulliken Charges**	$^5Int1_{(t,t)}$	$^1Int1_{(t,t)}$	$^3Int1_{(s,t)}$
Ni1	1.65	1.62	1.65	**Ni1**	0.80	0.67	0.79
Ni2	1.61	-1.64	-0.09	**Ni2**	0.68	0.77	0.62
O1	0.11	-0.11	0.12	**O1**	-0.74	-0.74	-0.74
O2	1.09	1.06	-0.82	**O2**	-0.49	-0.51	-0.49
N_{1a}	0.07	0.05	0.07	**N_{1a}**	-0.28	-0.29	-0.28
N_{1b}	0.06	0.09	0.06	**N_{1b}**	-0.23	-0.22	-0.23
N_{1c}	0.05	0.09	0.05	**N_{1c}**	-0.29	-0.26	-0.29
N_{1d}	0.05	0.08	0.05	**N_{1d}**	-0.22	-0.21	-0.22
N_{2a}	0.07	-0.05	0.00	**N_{2a}**	-0.28	-0.30	-0.25
N_{2b}	0.09	-0.06	-0.08	**N_{2b}**	-0.21	-0.22	-0.20
N_{2c}	0.06	-0.07	0.02	**N_{2c}**	-0.28	-0.28	-0.28
N_{2d}	0.08	-0.05	-0.06	**N_{2d}**	-0.22	-0.21	-0.20
C_{DHA}	-0.70	-0.71	0.70	**C_{DHA}**	-0.27	-0.29	-0.27
Bond parameters and Bond angles of Intermediate (Int1)							
Bond Parameter	$^5Int1_{(t,t)}$	$^1Int1_{(t,t)}$	$^3Int1_{(s,t)}$	**Bond Angle**	$^5Int1_{(t,t)}$	$^1Int1_{(t,t)}$	$^3Int1_{(s,t)}$
Ni_1-Ni_2	5.640	5.603	5.823	**∠Ni_1-O_1-O_2**	93.8	123.9	97.2
Ni_1-O_1	1.880	1.806	1.876	**∠Ni_1-O_2-O_1**	25.0	21.5	24.9
Ni_1-O_2	4.439	3.910	4.415	**∠Ni_2-O_1-O_2**	23.0	25.8	20.9
Ni_1-N_1	2.142	2.171	2.144	**∠Ni_2-O_2-O_1**	98.9	109.8	111.3

Ni_1-N_2	2.226	2.211	2.224	**∠Ni_1-O_1-Ni_2**	116.7	131.1	116.7
Ni_1-N_3	2.156	2.136	2.160	**∠Ni_1-O_2-Ni_2**	123.8	149.4	134.6
Ni_1-N_4	2.250	2.204	2.250	**∠N_1-Ni_1-N_2**	83.0	81.9	83.0
O_1-O_2	3.900	2.910	3.769	**∠N2-Ni_1-N3**	82.6	84.4	82.7
Ni_2-O_1	4.538	4.249	4.732	**∠N_3-Ni_1-N_4**	82.6	83.5	82.3
Ni_2-O_2	1.797	1.872	1.802	**∠N_4-Ni_1-N_1**	83.2	82.5	82.8
Ni_2-N_1	2.154	2.165	2.242	**∠N_1-Ni_2-N_2**	83.5	82.0	83.2
Ni_2-N_2	2.217	2.240	2.169	**∠N2-Ni_2-N3**	82.9	83.4	83.8
Ni_2-N_3	2.165	2.121	2.112	**∠N_3-Ni_2-N_4**	82.4	83.6	83.9
Ni_2-N_4	2.221	2.242	2.152	**∠N_4-Ni_2-N_1**	83.7	81.9	84.1
C-$H_{abs(DHA)}$	3.401	5.939	4.179	**∠O_1-H-C_{DHA}**	141.2	-	136.7
O-$H_{abs(DHA)}$	0.970	0.977	0.969	**∠ H-O_1-Ni**	114.3	-	114.5

Table S16- Computed spin densities and Mulliken charges of complex **2** for all possible spin states of reactants (**R**) along with bond lengths and bond angle obtained from optimized geometries in Gaussian 09 (Ni1, Ni48 or Ni2, S1 or S47, S2 or S48).

Spin Density of Reactant (Complex 2)				
Spin Density	$^5R_{(t,t)}$	$^1R_{(t,t)}$	$^3R_{(s,t)}$	$^1R_{(s,s)}$
Ni1	1.61	1.53	1.52	0.00
Ni2	1.61	-1.53	0.18	0.00
S1	0.12	0.00	-0.02	0.00
S2	0.12	0.00	-0.02	0.00
N_{1a}	0.07	0.07	0.07	0.00

N_{1b}	0.06	0.05	0.05	0.00
N_{1c}	0.07	0.07	0.07	0.00
N_{1d}	0.06	0.05	0.05	0.00
N_{2a}	0.07	-0.07	-0.02	0.00
N_{2b}	0.06	-0.05	0.06	0.00
N_{2c}	0.07	-0.07	-0.02	0.00
N_{2d}	0.06	-0.05	0.06	0.00
Mulliken Atomic Charges of Reactant (Complex 2)				
Spin Density	**$^{5}R_{(t,t)}$**	**$^{1}R_{(t,t)}$**	**$^{3}R_{(s,t)}$**	**$^{1}R_{(s,s)}$**
Ni1	0.89	0.86	0.86	0.41
Ni2	0.89	0.86	0.87	0.44
S1	-0.56	-0.52	-0.50	-0.37
S2	-0.56	-0.52	-0.50	-0.36
N_{1a}	-0.30	-0.30	-0.29	-0.25
N_{1b}	-0.23	-0.23	-0.23	-0.18
N_{1c}	-0.30	-0.30	-0.29	-0.22
N_{1d}	-0.23	-0.23	-0.23	-0.18
N_{2a}	-0.30	-0.30	-0.29	-0.25
N_{2b}	-0.23	-0.23	-0.23	-0.20
N_{2c}	-0.30	-0.30	-0.29	-0.22
N_{2d}	-0.23	-0.23	-0.23	-0.21
Bond parameter of reactant (Complex 2)				
Bond Parameter	**$^{5}R_{(t,t)}$**	**$^{1}R_{(t,t)}$**	**$^{3}R_{(s,t)}$**	**$^{1}R_{(s,s)}$**
Ni_1-Ni_2	4.713	4.635	4.623	5.526
Ni_1-S_1	2.634	2.595	2.580	2.325
Ni_1-S_2	2.632	2.595	2.581	3.583
Ni_1-N_1	2.193	2.198	2.200	2.022
Ni_1-N_2	2.235	2.244	2.246	2.045
Ni_1-N_3	2.193	2.198	2.200	2.564
Ni_1-N_4	2.235	2.244	2.246	2.045

S_1-S_2	2.348	2.335	2.326	2.329
Ni_2-S_1	2.632	2.595	2.595	3.512
Ni_2-S_2	2.634	2.595	2.594	2.324
Ni_2-N_1	2.193	2.198	2.200	2.022
Ni_2-N_2	2.235	2.244	2.246	2.051
Ni_2-N_3	2.193	2.198	2.200	2.549
Ni_2-N_4	2.235	2.244	2.246	2.051
The bond angle of the Reactant (Complex 2)				
Bond Angle	$^5R_{(t,t)}$	$^1R_{(t,t)}$	$^3R_{(s,t)}$	$^1R_{(s,s)}$
∠Ni_1-S_1-S_2	63.6	63.3	63.2	100.6
∠Ni_1-S_2-S_1	63.5	63.3	63.2	39.6
∠Ni_2-S_1-S_2	63.5	63.3	63.4	100.6
∠Ni_2-S_2-S_1	63.6	63.3	63.4	39.6
∠Se_1-Ni_1-Se_2	53.0	53.5	53.6	37.8
∠Se_1-Ni_2-Se_2	52.9	53.3	53.2	37.8
∠Ni_1-S_1-Ni_2	127.0	126.5	126.6	141.6
∠Ni_1-S_2-Ni_2	127.0	126.5	126.6	137.6
∠N_1-Ni_1-N_2	82.3	82.1	82.1	86.1
∠N2-Ni_1-N3	81.7	81.6	81.7	83.9
∠N_3-Ni_1-N_4	82.3	82.1	82.1	83.9
∠N_4-Ni_1-N_1	81.7	81.6	81.7	86.1
∠N_1-Ni_2-N_2	82.3	82.1	82.1	86.0
∠N2-Ni_2-N3	81.7	81.6	81.6	83.8
∠N_3-Ni_2-N_4	82.3	82.1	82.1	83.8
∠N_4-Ni_2-N_1	81.7	81.6	81.6	86.0

Table S17- Computed spin densities and Mulliken charges of complex **2** for all possible spin states of the first hydrogen abstraction transition state along with bond lengths and bond angle obtained from optimized geometries in Gaussian 09.

	Mulliken spin density and charges values of the transition state (TS1)								
Spin Density	$^{5}ts1_{(t,t)}$	$^{1}ts1_{(t,t)}$	$^{3}ts1_{(s,t)}$	$^{1}ts1_{(s,s)}$	**Mulliken Charges**	$^{5}ts1_{(t,t)}$	$^{1}ts1_{(t,t)}$	$^{3}ts1_{(s,t)}$	$^{1}ts1_{(s,s)}$
Ni1	1.60	1.57	1.60	0.00	**Ni1**	0.82	0.70	0.77	0.58
Ni2	1.61	-1.60	0.11	0.00	**Ni2**	0.70	0.68	0.74	0.40
S1	0.15	0.19	0.04	0.00	**S1**	-0.47	-0.41	-0.27	-0.43
S2	0.78	0.53	-0.67	0.00	**S2**	-0.56	-0.41	-0.53	-0.56
N_{1a}	0.06	0.07	0.09	0.00	**N_{1a}**	-0.27	-0.29	-0.29	-0.20
N_{1b}	0.05	0.07	0.06	0.00	**N_{1b}**	-0.23	-0.23	-0.23	-0.19
N_{1c}	0.05	0.07	0.05	0.00	**N_{1c}**	-0.26	-0.29	-0.30	-0.26
N_{1d}	0.05	0.06	0.07	0.00	**N_{1d}**	-0.23	-0.23	-0.20	-0.23
N_{2a}	0.08	-0.08	-0.03	0.00	**N_{2a}**	-0.27	-0.28	-0.26	-0.19
N_{2b}	0.07	-0.07	0.06	0.00	**N_{2b}**	-0.23	-0.21	-0.23	-0.20
N_{2c}	0.06	-0.06	0.00	0.00	**N_{2c}**	-0.29	-0.29	-0.28	-0.25
N_{2d}	0.05	-0.06	0.06	0.00	**N_{2d}**	-0.23	-0.23	-0.20	-0.20
C_{DHA}	-0.46	-0.46	0.43	0.00	**C_{DHA}**	-0.36	-0.30	-0.29	-0.40
	Bond parameters and Bond angles of the transition state (TS1)								
Bond Parameter	$^{5}ts1_{(t,t)}$	$^{1}ts1_{(t,t)}$	$^{3}ts1_{(s,t)}$	$^{1}ts1_{(s,s)}$	**Bond Angle**	$^{5}ts1_{(t,t)}$	$^{1}ts1_{(t,t)}$	$^{3}ts1_{(s,t)}$	$^{1}ts1_{(s,s)}$
Ni_1-Ni_2	4.746	4.865	4.817	5.547	**∠Ni_1-S_1-S_2**	54.4	96.8	42.9	78.4
Ni_1-S_1	2.522	2.507	2.495	2.309	**∠Ni_1-S_2-S_1**	54.0	25.6	83.8	42.3
Ni_1-S_2	2.534	2.595	2.568	3.363	**∠Ni_2-S_1-S_2**	32.1	26.9	57.5	23.7
Ni_1-N_1	2.289	2.248	2.255	2.605	**∠Ni_2-S_2-S_1**	104.7	90.8	53.5	124.2
Ni_1-N_2	2.248	2.242	2.247	2.065	**∠Ni_1-S_1-Ni_2**	86.4	123.7	100.3	101.5
Ni_1-N_3	2.231	2.272	2.285	2.045	**∠Ni_1-S_2-Ni_2**	158.1	116.4	137.3	163.5
Ni_1-N_4	2.244	2.225	2.230	2.061	**∠N_1-Ni_1-N_2**	79.7	83.4	83.3	81.8
S_1-S_2	2.960	2.817	2.826	2.956	**∠N2-Ni_1-N3**	80.7	82.9	81.7	86.2
Ni_2-S_1	4.183	4.151	4.106	4.604	**∠N_3-Ni_1-N_4**	79.6	83.1	80.8	85.1
Ni_2-S_2	2.229	2.330	2.322	2.240	**∠N_4-Ni_1-N_1**	80.6	82.7	83.1	82.1
Ni_2-N_1	2.147	2.131	2.170	2.580	**∠N_1-Ni_2-N_2**	83.9	83.8	80.5	83.2
Ni_2-N_2	2.229	2.227	2.199	2.059	**∠N2-Ni_2-N3**	105.3	83.0	81.1	85.6
Ni_2-N_3	2.180	2.168	2.152	2.056	**∠N_3-Ni_2-N_4**	81.0	82.7	81.5	85.5
Ni_2-N_4	2.310	2.278	2.278	2.067	**∠N_4-Ni_2-N_1**	81.2	83.1	78.9	83.2
C-$H_{abs(DHA)}$	1.882	1.744	1.697	1.791	**∠S_1-H-C_{DHA}**	148.2	126.6	151.9	158.9
S-$H_{abs(DHA)}$	1.456	1.485	1.500	1.462	**∠ H-S_1-Ni**	121.3	103.5	98.6	112.9

Table S18- Computed spin densities and Mulliken charges of complex **2** for all possible spin states of intermediates (**Int1**), along with bond lengths and angles obtained from optimized geometries in Gaussian 09.

Mulliken spin density and charges values of intermediate (Int1)							
Spin Density	$^{5}Int1_{(t,t)}$	$^{1}Int1_{(t,t)}$	$^{3}Int1_{(s,t)}$	**Mulliken Charges**	$^{5}Int1_{(t,t)}$	$^{1}Int1_{(t,t)}$	$^{3}Int1_{(s,t)}$
Ni1	1.61	1.62	1.61	**Ni1**	0.80	0.70	0.77
Ni2	1.61	-1.64	0.13	**Ni2**	0.83	0.68	0.74
S1	-0.15	0.10	0.27	**S1**	-0.32	-0.41	-0.27
S2	-0.52	0.90	0.63	**S2**	-0.53	-0.41	-0.53
N_{1a}	0.05	0.07	0.05	**N_{1a}**	-0.28	-0.29	-0.29
N_{1b}	0.05	0.07	0.06	**N_{1b}**	-0.23	-0.23	-0.23
N_{1c}	0.06	0.07	0.06	**N_{1c}**	-0.28	-0.29	-0.30
N_{1d}	0.05	0.06	0.09	**N_{1d}**	-0.20	-0.21	-0.20
N_{2a}	0.05	-0.07	-0.03	**N_{2a}**	-0.29	-0.28	-0.26
N_{2b}	0.05	-0.07	0.06	**N_{2b}**	-0.23	-0.23	-0.23
N_{2c}	0.06	-0.07	0.00	**N_{2c}**	-0.28	-0.29	-0.27
N_{2d}	0.05	-0.06	0.06	**N_{2d}**	-0.21	-0.21	-0.20
C_{DHA}	0.70	-0.69	-0.70	**C_{DHA}**	-0.28	-0.30	-0.29
Bond parameters and Bond angles of Intermediate (Int1)							
Bond Parameter	$^{5}Int1_{(t,t)}$	$^{1}Int1_{(t,t)}$	$^{3}Int1_{(s,t)}$	**Bond Angle**	$^{5}Int1_{(t,t)}$	$^{1}Int1_{(t,t)}$	$^{3}Int1_{(s,t)}$
Ni_1-Ni_2	4.332	6.711	4.662	**∠Ni_1-S_1-S_2**	54.7	96.8	57.5
Ni_1-S_1	2.657	2.329	3.543	**∠Ni_1-S_2-S_1**	59.6	25.6	53.5
Ni_1-S_2	2.514	5.346	2.424	**∠Ni_2-S_1-S_2**	54.5	26.9	42.9
Ni_1-N_1	2.238	2.131	2.153	**∠Ni_2-S_2-S_1**	59.7	90.8	83.8
Ni_1-N_2	2.278	2.239	2.243	**∠Ni_1-S_1-Ni_2**	109.1	123.7	100.3
Ni_1-N_3	2.254	2.140	2.186	**∠Ni_1-S_2-Ni_2**	119.3	116.4	137.2
Ni_1-N_4	2.301	2.252	2.272	**∠N_1-Ni_1-N_2**	80.4	83.4	83.3
S_1-S_2	2.810	4.546	2.859	**∠N2-Ni_1-N3**	80.4	82.9	81.7
Ni_2-S_1	2.659	5.134	2.463	**∠N_3-Ni_1-N_4**	148.8	82.5	80.7
Ni_2-S_2	2.506	2.324	2.582	**∠N_4-Ni_1-N_1**	80.9	83.1	83.1
Ni_2-N_1	2.274	2.141	2.311	**∠N_1-Ni_2-N_2**	80.0	83.8	80.5
Ni_2-N_2	2.278	2.221	2.249	**∠N2-Ni_2-N3**	80.4	83.0	81.1
Ni_2-N_3	2.250	2.145	2.238	**∠N_3-Ni_2-N_4**	81.1	82.7	81.5
Ni_2-N_4	2.284	2.238	2.265	**∠N_4-Ni_2-N_1**	79.9	83.1	78.9

C-H$_{abs(DHA)}$	1.087	1.087	1.088	**∠S$_1$-H-C$_{DHA}$**	149.4	126.6	151.9
S-H$_{abs(DHA)}$	1.374	1.371	1.374	**∠ H-S$_1$-Ni**	97.2	103.5	98.6

Table S19- Computed spin densities and Mulliken charges of complex **3** for all possible spin states of reactants (**R**) along with bond lengths and bond angle obtained from optimized geometries in Gaussian 09.

Spin Density of reactant (Complex 3)				
Spin Density	$^5R_{(t,t)}$	$^1R_{(t,t)}$	$^3R_{(s,t)}$	$^1R_{(s,s)}$
Ni1	1.59	1.48	1.47	0.00
Ni2	1.59	-1.48	0.26	0.00
Se1	0.14	0.00	-0.03	0.00
Se2	0.14	0.00	-0.03	0.00
N$_{1a}$	0.07	0.07	0.07	0.00
N$_{1b}$	0.06	0.05	0.06	0.00
N$_{1c}$	0.07	0.07	0.07	0.00
N$_{1d}$	0.06	0.05	0.06	0.00
N$_{2a}$	0.07	-0.07	-0.02	0.00
N$_{2b}$	0.06	-0.05	0.06	0.00
N$_{2c}$	0.07	-0.07	-0.02	0.00
N$_{2d}$	0.06	-0.05	0.06	0.00
Mulliken Atomic Charges of Reactant (Complex 3)				
Mulliken Charges	$^5R_{(t,t)}$	$^1R_{(t,t)}$	$^3R_{(s,t)}$	$^1R_{(s,s)}$
Ni1	0.68	0.66	0.66	0.41
Ni2	0.68	0.66	0.63	0.41
Se1	-0.48	-0.42	-0.39	-0.40
Se2	-0.48	-0.42	-0.39	-0.40
N$_{1a}$	-0.28	-0.28	-0.28	-0.22
N$_{1b}$	-0.22	-0.21	-0.21	-0.19
N$_{1c}$	-0.28	-0.28	-0.28	-0.25
N$_{1d}$	-0.22	-0.21	-0.21	-0.21
N$_{2a}$	-0.28	-0.28	-0.27	-0.22

N_{2b}	-0.22	-0.21	-0.21	-0.19
N_{2c}	-0.28	-0.28	-0.27	-0.25
N_{2d}	-0.22	-0.21	-0.21	-0.19
Bond parameter of reactant (Complex 3)				
Bond Parameter	$^{5}R_{(t,t)}$	$^{1}R_{(t,t)}$	$^{3}R_{(s,t)}$	$^{1}R_{(s,s)}$
Ni_1-Ni_2	4.884	4.781	4.763	5.753
Ni_1-Se_1	2.749	2.699	2.696	3.703
Ni_1-Se_2	2.749	2.699	2.696	2.448
Ni_1-N_1	2.204	2.210	2.207	2.541
Ni_1-N_2	2.232	2.241	2.244	2.054
Ni_1-N_3	2.204	2.210	2.207	2.028
Ni_1-N_4	2.231	2.241	2.244	2.054
Se_1-Se_2	2.525	2.503	2.492	2.514
Ni_2-Se_1	2.749	2.699	2.679	2.448
Ni_2-Se_2	2.750	2.699	2.679	3.703
Ni_2-N_1	2.204	2.210	2.215	2.541
Ni_2-N_2	2.232	2.241	2.244	2.054
Ni_2-N_3	2.204	2.210	2.215	2.028
Ni_2-N_4	2.231	2.241	2.244	2.054
The bond angle of Reactant (Complex 3)				
Bond Angle	$^{5}R_{(t,t)}$	$^{1}R_{(t,t)}$	$^{3}R_{(s,t)}$	$^{1}R_{(s,s)}$
∠Ni_1-Se_1-Se_2	62.7	62.4	62.5	41.1
∠Ni_1-Se_2-Se_1	62.7	62.4	62.5	96.5
∠Ni_2-Se_1-Se_2	62.7	62.4	62.3	96.5
∠Ni_2-Se_2-Se_1	62.7	62.4	62.3	41.1
∠Ni_1-Se_1-Ni_2	125.3	124.7	124.8	137.6
∠Ni_1-Se_2-Ni_2	125.3	124.7	124.8	137.6
∠N_1-Ni_1-N_2	82.4	82.3	82.3	84.1
∠N2-Ni_1-N3	81.9	81.7	81.8	86.0
∠N_3-Ni_1-N_4	82.4	82.3	82.3	86.0

∠N_4-Ni_1-N_1	81.9	81.7	81.8	84.1
∠N_1-Ni_2-N_2	82.4	82.3	82.3	84.1
∠N2-Ni_2-N3	81.9	81.7	81.7	86.0
∠N_3-Ni_2-N_4	82.4	82.3	82.3	86.0
∠N_4-Ni_2-N_1	81.9	81.7	81.7	84.1

Table S20- Computed spin densities and Mulliken charges of complex **3** for all possible spin states of the first hydrogen abstraction transition state (**TS1**) along with bond lengths and bond angle as obtained from optimized geometries in Gaussian 09.

Mulliken spin density values of Transition State (TS1)				
Spin Density	$^5ts1_{(t,t)}$	$^1ts1_{(t,t)}$	$^3ts1_{(s,t)}$	$^1ts1_{(s,s)}$
Ni1	1.64	1.64	1.62	0.00
Ni2	1.56	-1.63	-0.03	0.00
Se1	-0.06	-0.06	0.16	0.00
Se2	0.97	0.67	-0.76	0.00
N_{1a}	0.06	0.08	0.08	0.00
N_{1b}	0.06	0.06	0.06	0.00
N_{1c}	0.08	0.07	0.06	0.00
N_{1d}	0.06	0.06	0.06	0.00
N_{2a}	0.07	-0.07	-0.09	0.00
N_{2b}	0.07	-0.07	0.05	0.00
N_{2c}	0.07	-0.06	0.05	0.00
N_{2d}	0.06	-0.06	0.06	0.00
C_{DHA}	-0.48	-0.48	0.48	0.00
Mulliken Atomic Charges of for Transition State (TS1)				
Spin Density	$^5ts1_{(t,t)}$	$^1ts1_{(t,t)}$	$^3ts1_{(s,t)}$	$^1ts1_{(s,s)}$
Ni1	0.76	0.76	0.76	0.57
Ni2	0.66	0.66	0.66	0.44
Se1	-0.47	-0.47	-0.39	-0.36
Se2	-0.56	-0.59	-0.63	-0.73
N_{1a}	-0.30	-0.30	-0.29	-0.23
N_{1b}	-0.23	-0.22	-0.23	-0.17

N_{1c}	-0.28	-0.28	-0.30	-0.27
N_{1d}	-0.22	-0.23	-0.21	-0.20
N_{2a}	-0.29	-0.29	-0.27	-0.19
N_{2b}	-0.21	-0.21	-0.21	-0.19
N_{2c}	-0.29	-0.29	-0.30	-0.26
N_{2d}	-0.20	-0.21	-0.21	-0.18
C_{DHA}	-0.14	-0.14	-0.15	-0.26
Bond parameter of TS1 in Å				
Bond Parameter	$^{5}ts1_{(t,t)}$	$^{1}ts1_{(t,t)}$	$^{3}ts1_{(s,t)}$	$^{1}ts1_{(s,s)}$
Ni_1-Ni_2	6.847	6.847	6.580	6.201
Ni_1-Se_1	2.489	2.489	2.487	2.469
Ni_1-Se_2	4.577	4.577	4.296	3.894
Ni_1-N_1	2.166	2.166	2.142	2.443
Ni_1-N_2	2.251	2.251	2.265	2.057
Ni_1-N_3	2.141	2.141	2.154	2.058
Ni_1-N_4	2.260	2.260	2.251	2.067
Se_1-Se_2	3.370	3.370	3.211	3.345
Ni_2-Se_1	5.153	5.153	4.946	5.054
Ni_2-Se_2	2.400	2.400	2.414	2.393
Ni_2-N_1	2.165	2.165	2.187	2.187
Ni_2-N_2	2.230	2.230	2.220	2.553
Ni_2-N_3	2.166	2.166	2.166	2.064
Ni_2-N_4	2.289	2.289	2.225	2.058
C-$H_{abs(DHA)}$	1.692	1.692	1.691	2.070
Se-$H_{abs(DHA)}$	1.628	1.628	1.633	1.572
The bond angle of TS1				
Bond Angle	$^{5}ts1_{(t,t)}$	$^{1}ts1_{(t,t)}$	$^{3}ts1_{(s,t)}$	$^{1}ts1_{(s,s)}$
∠Ni_1-Se_1-Se_2	101.7	101.7	97.0	82.6
∠Ni_1-Se_2-Se_1	32.2	32.2	35.1	39.0
∠Ni_2-Se_1-Se_2	22.2	22.2	24.3	23.5
∠Ni_2-Se_2-Se_1	125.7	125.7	122.5	122.6
∠Ni_1-Se_1-Ni_2	123.4	123.4	120.9	105.8
∠Ni_1-Se_2-Ni_2	156.7	156.6	156.4	160.5
∠N_1-Ni_1-N_2	81.3	81.3	81.9	83.3

∠N2-Ni_1-N3	83.6	83.5	82.7	86.2
∠N_3-Ni_1-N_4	82.2	82.2	82.3	85.0
∠N_4-Ni_1-N_1	81.9	81.9	82.9	83.3
∠N_1-Ni_2-N_2	83.0	83.0	83.5	82.5
∠N2-Ni_2-N3	82.7	82.7	82.6	85.8
∠N_3-Ni_2-N_4	82.2	82.2	82.4	85.6
∠N_4-Ni_2-N_1	81.6	81.6	83.8	83.4
∠Se_1-H-C_{DHA}	163.8	163.8	159.2	154.6
∠ Ni_1-Se_1-H	104.5	104.5	108.7	107.3

Table S21- Computed spin densities and Mulliken charges of complex **3** for all possible spin states of Intermediate (**Int1**) along with respective bond lengths and bond angles as obtained from optimized geometries in Gaussian 09.

Mulliken spin density and charges values of Intermediate (Int1)							
Spin Density	$^5Int1_{(t,t)}$	$^1Int1_{(t,t)}$	$^3Int1_{(s,t)}$	**Mulliken Charges**	$^5Int1_{(t,t)}$	$^1Int1_{(t,t)}$	$^3Int1_{(s,t)}$
Ni1	1.62	1.59	1.62	**Ni1**	0.71	0.75	0.65
Ni2	1.56	-1.55	0.00	**Ni2**	0.70	0.63	0.63
Se1	0.12	0.27	0.12	**Se1**	-0.56	-0.30	-0.46
Se2	1.13	0.65	0.92	**Se2**	-0.50	-0.59	-0.48
N_{1a}	0.07	0.09	0.07	**N_{1a}**	-0.28	-0.27	-0.29
N_{1b}	0.07	0.06	0.07	**N_{1b}**	-0.23	-0.22	-0.21
N_{1c}	0.07	0.05	0.07	**N_{1c}**	-0.29	-0.30	-0.29
N_{1d}	0.06	0.06	0.06	**N_{1d}**	-0.22	-0.20	-0.20
N_{2a}	0.07	-0.06	0.06	**N_{2a}**	-0.27	-0.25	-0.27
N_{2b}	0.07	-0.05	0.03	**N_{2b}**	-0.22	-0.21	-0.20
N_{2c}	0.07	-0.05	-0.07	**N_{2c}**	-0.29	-0.26	-0.29
N_{2d}	0.07	-0.05	0.03	**N_{2d}**	-0.23	-0.20	-0.20
C_{DHA}	-0.68	-0.70	-0.68	**C_{DHA}**	-0.22	-0.27	-0.20
Bond parameters and Bond angles of Intermediate (Int1)							
Bond Parameter	$^5Int1_{(t,t)}$	$^1Int1_{(t,t)}$	$^3Int1_{(s,t)}$	**Bond Angle**	$^5Int1_{(t,t)}$	$^1Int1_{(t,t)}$	$^3Int1_{(s,t)}$
Ni_1-Ni_2	6.981	4.845	7.083	**∠Ni_1-Se_1-Se_2**	95.8	44.7	96.7

Ni_1-Se_1	2.437	3.581	2.436	**∠Ni_1-Se_2-Se_1**	26.6	79.6	26.4
Ni_1-Se_2	5.424	2.546	5.446	**∠Ni_2-Se_1-Se_2**	22.2	57.0	25.8
Ni_1-N_1	2.141	2.164	2.141	**∠Ni_2-Se_2-Se_1**	95.0	54.4	98.0
Ni_1-N_2	2.247	2.247	2.248	**∠Ni_1-Se_1-Ni_2**	122.1	101.3	122.5
Ni_1-N_3	2.144	2.207	2.143	**∠Ni_1-Se_2-Ni_2**	121.5	133.9	124.3
Ni_1-N_4	2.263	2.253	2.263	**∠N_1-Ni_1-N_2**	82.8	83.4	82.8
Se_1-Se_2	4.608	3.017	4.594	**∠N2-Ni_1-N3**	82.9	81.4	83.0
Ni_2-Se_1	5.373	2.634	5.471	**∠N_3-Ni_1-N_4**	82.6	81.0	82.6
Ni_2-Se_2	2.395	2.719	2.401	**∠N_4-Ni_1-N_1**	82.8	83.4	82.8
Ni_2-N_1	2.148	2.280	2.188	**∠N_1-Ni_2-N_2**	83.3	81.1	83.6
Ni_2-N_2	2.243	2.245	2.209	**∠N2-Ni_2-N3**	82.2	80.9	83.0
Ni_2-N_3	2.163	2.269	2.152	**∠N_3-Ni_2-N_4**	82.6	81.4	83.2
Ni_2-N_4	2.246	2.259	2.215	**∠N_4-Ni_2-N_1**	82.9	80.0	83.3
C-$H_{abs(DHA)}$	3.925	3.860	3.966	**∠Se_1-H-C_{DHA}**	106.8	142.9	105.3
Se-$H_{abs(DHA)}$	1.488	1.493	1.488	**∠ H-Se_1-Ni**	100.2	97.4	100.3

Table S22- Computed spin densities and Mulliken charges of complex **3** for all possible spin states of second hydrogen abstraction transition state from other DHA molecule (**TS2**) along with respective bond lengths and bond angles obtained from optimized geometries in Gaussian 09.

Mulliken spin density values of Transition State (TS2)				
Spin Density	$^5ts2_{(t,t)}$	$^1ts2_{(t,t)}$	$^3ts2_{(s,t)}$	$^1ts2_{(s,s)}$
Ni1	1.57	1.56	1.56	0.00
Ni2	1.57	-1.57	-0.15	0.00
Se1	-0.05	-0.06	0.13	0.00
Se2	0.13	-0.27	-0.02	0.00
N_{1a}	0.06	0.06	0.06	0.00
N_{1b}	0.05	0.05	0.05	0.00
N_{1c}	0.05	0.06	0.05	0.00
N_{1d}	0.05	0.05	0.05	0.00
N_{2a}	0.06	-0.06	0.02	0.00
N_{2b}	0.05	-0.05	-0.06	0.00
N_{2c}	0.06	-0.06	0.02	0.00
N_{2d}	0.05	-0.05	-0.06	0.00

C_{DHA1}	0.69	0.69	0.69	0.00
C_{DHA2}	-0.46	-0.44	-0.47	0.00
Mulliken Atomic Charges of for Transition State (TS2)				
Spin Density	$^{5}ts2_{(t,t)}$	$^{1}ts2_{(t,t)}$	$^{3}ts2_{(s,t)}$	$^{1}ts2_{(s,s)}$
Ni1	0.75	0.74	0.74	0.67
Ni2	0.78	0.79	0.76	0.71
Se1	-0.32	-0.33	-0.52	-0.45
Se2	-0.53	-0.51	-0.30	-0.19
N_{1a}	-0.26	-0.26	-0.26	-0.25
N_{1b}	-0.22	-0.22	-0.22	-0.20
N_{1c}	-0.25	-0.25	-0.25	-0.23
N_{1d}	-0.22	-0.22	-0.21	-0.19
N_{2a}	-0.25	-0.25	-0.22	-0.23
N_{2b}	-0.23	-0.23	-0.26	-0.21
N_{2c}	-0.26	-0.26	-0.21	-0.25
N_{2d}	-0.21	-0.21	-0.24	-0.19
C_{DHA1}	-0.19	-0.19	-0.19	-0.44
C_{DHA2}	-0.34	-0.30	-0.37	-0.35
Bond parameter of TS2 in Å				
Bond Parameter	$^{5}ts2_{(t,t)}$	$^{1}ts2_{(t,t)}$	$^{3}ts2_{(s,t)}$	$^{1}ts2_{(s,s)}$
Ni_1-Ni_2	4.468	4.502	4.500	4.523
Ni_1-Se_1	2.696	2.683	2.707	2.688
Ni_1-Se_2	2.756	2.782	2.743	2.758
Ni_1-N_1	2.267	2.263	2.268	2.271
Ni_1-N_2	2.261	2.257	2.261	2.262
Ni_1-N_3	2.323	2.309	2.321	2.347
Ni_1-N_4	2.274	2.263	2.275	2.276
Se_1-Se_2	3.134	3.131	3.104	3.080
Ni_2-Se_1	2.680	2.720	2.650	2.648
Ni_2-Se_2	2.793	2.790	2.843	2.262
Ni_2-N_1	2.317	2.304	2.350	2.346
Ni_2-N_2	2.278	2.275	2.275	2.273
Ni_2-N_3	2.271	2.256	2.262	2.258
Ni_2-N_4	2.266	2.264	2.265	2.262

C-$H_{abs(DHA1)}$	4.029	3.935	4.176	4.193
Se-$H_{abs(DHA1)}$	1.494	1.495	1.493	1.492
C-$H_{abs(DHA2)}$	1.651	1.599	1.690	1.735
Se-$H_{abs(DHA2)}$	1.661	1.688	1.644	1.631
The bond angle of TS2				
Bond Angle	$^{5}ts2_{(t,t)}$	$^{1}ts2_{(t,t)}$	$^{3}ts2_{(s,t)}$	$^{1}ts2_{(s,s)}$
∠Ni_1-Se_1-Se_2	55.8	56.6	55.8	56.6
∠Ni_1-Se_2-Se_1	54.0	53.6	54.7	54.5
∠Ni_2-Se_1-Se_2	56.8	56.4	58.6	59.4
∠Ni_2-Se_2-Se_1	53.4	54.3	52.7	52.8
∠Ni_1-Se_1-Ni_2	112.5	112.8	114.3	115.9
∠Ni_1-Se_2-Ni_2	107.3	107.8	107.3	107.2
∠N_1-Ni_1-N_2	80.8	80.9	80.7	80.9
∠N2-Ni_1-N3	79.7	79.9	80.0	80.0
∠N_3-Ni_1-N_4	79.7	80.2	80.0	80.0
∠N_4-Ni_1-N_1	79.9	80.0	80.0	80.2
∠N_1-Ni_2-N_2	80.0	80.1	79.9	80.1
∠N2-Ni_2-N3	80.0	80.0	80.2	80.3
∠N_3-Ni_2-N_4	80.7	80.8	81.0	81.1
∠N_4-Ni_2-N_1	79.5	80.0	79.4	79.6
∠Se_1-H-C_{DHA1}	151.9	160.2	147.7	149.0
∠H-Se_1-C_{DHA1}	103.5	104.9	103.1	102.0
∠Se_2-H-C_{DHA2}	174.3	175.4	173.1	172.1
∠H-Se_2-C_{DHA2}	122.0	125.7	121.5	129.1

Table S23- Computed spin densities and Mulliken charges of complex **3** for all possible spin states of Product (**P**) along with respective bond lengths and angles obtained from optimized geometries in Gaussian 09.

Mulliken spin density values of Product (P)					
Spin Density	^{3}P	^{1}P	**Charge Density**	^{3}P	^{1}P
Ni	1.61	0.00	**Ni**	0.64	0.43
Se	0.13	0.00	**Se**	-0.44	-0.36
N_{1a}	0.06	0.00	**N_{1a}**	-0.21	-0.19
N_{1b}	0.07	0.00	**N_{1b}**	-0.29	-0.21

N_{1c}	0.07	0.00	**N_{1c}**	-0.22	-0.20
N_{1d}	0.07	0.00	**N_{1d}**	-0.29	-0.25
	Bond parameter of P in Å				
Bond Parameter	**^3P**	**^1P**	**Bond Angle**	**^3P**	**^1P**
Ni-Se	2.410	2.405	**∠Ni-Se-H**	100.8	100.7
Ni_1-N_1	2.265	2.070	**$\angle N_1$-Ni-N_2**	82.6	83.2
Ni_1-N_2	2.152	2.551	**∠N2-Ni-N3**	82.8	84.5
Ni_1-N_3	2.255	2.040	**$\angle N_3$-Ni-N_4**	82.8	86.4
Ni_1-N_4	2.153	2.039	**$\angle N_4$-Ni-N_1**	82.6	86.0

Table S24- Computed spin densities and Mulliken charges of complex **4** for all possible spin states of Reactant (R) along with respective bond lengths and bond angles obtained from optimized geometries in Gaussian 09.

Spin Density of reactant (Complex 4)				
Spin Density	**$^5R_{(t,t)}$**	**$^1R_{(t,t)}$**	**$^3R_{(s,t)}$**	**$^1R_{(s,s)}$**
Ni1	1.71	1.43	1.59	0.00
Ni2	1.64	-1.43	-0.12	0.00
Te1	0.10	0.00	0.17	0.00
Te2	0.14	0.00	0.17	0.00
N_{1a}	-0.01	0.07	0.06	0.00
N_{1b}	0.04	0.05	0.06	0.00
N_{1c}	0.06	0.07	0.06	0.00
N_{1d}	0.04	0.05	0.06	0.00
N_{2a}	0.09	-0.07	0.02	0.00
N_{2b}	0.06	-0.05	-0.06	0.00
N_{2c}	0.05	-0.07	0.02	0.00
N_{2d}	0.06	-0.05	-0.06	0.00
Mulliken Atomic Charges of reactant (Complex 4)				
Spin Density	**$^5R_{(t,t)}$**	**$^1R_{(t,t)}$**	**$^3R_{(s,t)}$**	**$^1R_{(s,s)}$**
Ni1	0.63	0.52	0.55	0.37

Ni2	0.61	0.52	0.53	0.37
Te1	-0.48	-0.15	-0.37	-0.38
Te2	-0.46	-0.15	-0.37	-0.38
N_{1a}	-0.29	-0.26	-0.26	-0.21
N_{1b}	-0.23	-0.23	-0.20	-0.18
N_{1c}	-0.30	-0.26	-0.26	-0.26
N_{1d}	-0.22	-0.23	-0.20	-0.19
N_{2a}	-0.26	-0.26	-0.26	-0.22
N_{2b}	-0.21	-0.23	-0.19	-0.18
N_{2c}	-0.31	-0.26	-0.26	-0.26
N_{2d}	-0.21	-0.23	-0.19	-0.18
Bond parameter of reactant (Complex 4)				
Bond Parameter	$^5R_{(t,t)}$	$^1R_{(t,t)}$	$^3R_{(s,t)}$	$^1R_{(s,s)}$
Ni_1-Ni_2	6.083	5.033	4.988	6.219
Ni_1-Te_1	3.912	2.885	2.875	4.049
Ni_1-Te_2	2.719	2.885	2.875	2.665
Ni_1-N_1	2.136	2.228	2.226	2.476
Ni_1-N_2	2.246	2.239	2.242	2.066
Ni_1-N_3	2.185	2.228	2.226	2.053
Ni_1-N_4	2.241	2.239	2.242	2.071
Te_1-Te_2	2.882	2.823	2.808	2.859
Ni_2-Te_1	2.719	2.885	2.849	2.653
Ni_2-Te_2	3.910	2.885	2.849	4.047
Ni_2-N_1	2.135	2.228	2.238	2.479
Ni_2-N_2	2.246	2.239	2.245	2.069
Ni_2-N_3	2.185	2.228	2.238	2.052
Ni_2-N_4	2.241	2.239	2.245	2.069
The bond angle of the reactant (Complex 4)				
Bond Angle	$^5R_{(t,t)}$	$^1R_{(t,t)}$	$^3R_{(s,t)}$	$^1R_{(s,s)}$
∠Ni_1-Te_1-Te_2	44.0	60.7	60.8	40.8

∠Ni_1-Te_2-Te_1	88.5	60.7	60.8	94.4
∠Ni_2-Te_1-Te_2	88.5	60.7	60.5	94.4
∠Ni_2-Te_2-Te_1	44.0	60.7	60.5	40.8
∠Te_1-Ni_1-Te_2	47.4	58.6	58.5	44.8
∠Te_1-Ni_2-Te_2	47.5	58.6	59.0	44.8
∠Ni_1-Te_1-Ni_2	132.3	121.4	121.3	135.2
∠Ni_1-Te_2-Ni_2	132.3	121.4	121.3	135.2
∠N_1-Ni_1-N_2	84.5	82.3	82.3	84.3
∠N2-Ni_1-N3	81.2	81.9	81.9	85.5
∠N_3-Ni_1-N_4	81.8	82.3	82.3	85.5
∠N_4-Ni_1-N_1	84.3	81.9	81.9	81.8
∠N_1-Ni_2-N_2	84.6	82.3	82.3	84.4
∠N2-Ni_2-N3	81.2	81.9	81.9	85.5
∠N_3-Ni_2-N_4	81.8	82.3	82.3	85.5
∠N_4-Ni_2-N_1	84.3	81.9	81.9	84.2

Table S25- Computed spin densities and Mulliken charges of complex **4** for all possible spin states of the first hydrogen abstraction transition state (**TS1**) along with respective bond lengths and bond angle as obtained from optimized geometries in Gaussian 09.

Mulliken spin density and charges values of the transition state (TS1)							
Spin Density	$^5ts1_{(t,t)}$	$^1ts1_{(t,t)}$	$^3ts1_{(s,t)}$	**Mulliken Charges**	$^5ts1_{(t,t)}$	$^1ts1_{(t,t)}$	$^3ts1_{(s,t)}$
Ni1	1.32	1.63	1.63	**Ni1**	0.70	0.70	0.69
Ni2	1.60	-1.63	-0.09	**Ni2**	0.73	0.65	0.63
Te1	0.06	0.01	0.10	**Te1**	-0.15	-0.37	0.04
Te2	-0.03	0.64	0.98	**Te2**	-0.57	-0.56	-0.52
N_{1a}	0.05	0.07	0.05	**N_{1a}**	-0.28	-0.27	-0.30
N_{1b}	0.04	0.06	0.06	**N_{1b}**	-0.20	-0.22	-0.21
N_{1c}	0.04	0.07	0.08	**N_{1c}**	-0.28	-0.27	-0.28
N_{1d}	0.04	0.06	0.06	**N_{1d}**	-0.22	-0.24	-0.21
N_{2a}	0.07	-0.07	-0.04	**N_{2a}**	-0.29	-0.27	-0.28
N_{2b}	0.06	-0.06	-0.04	**N_{2b}**	-0.21	-0.23	-0.20
N_{2c}	0.07	-0.07	0.06	**N_{2c}**	-0.30	-0.28	-0.29

N_{2d}	0.06	-0.05	-0.03	**N_{2d}**	-0.21	-0.22	-0.20
C_{DHA}	0.44	-0.48	-0.62	**C_{DHA}**	-0.16	-0.36	-0.28
Bond parameters and Bond angles of the transition state (TS1)							
Bond Parameter	**$^{5}ts1_{(t,t)}$**	**$^{1}ts1_{(t,t)}$**	**$^{3}ts1_{(s,t)}$**	**Bond Angle**	**$^{5}ts1_{(t,t)}$**	**$^{1}ts1_{(t,t)}$**	**$^{3}ts1_{(s,t)}$**
Ni_1-Ni_2	6.861	7.248	7.216	**∠Ni_1-Te_1-Te_2**	110.1	98.9	95.7
Ni_1-Te_1	2.630	2.656	2.667	**∠Ni_1-Te_2-Te_1**	32.5	33.3	34.0
Ni_1-Te_2	4.591	4.781	2.746	**∠Ni_2-Te_1-Te_2**	28.5	23.2	21.4
Ni_1-N_1	2.185	2.147	2.163	**∠Ni_2-Te_2-Te_1**	118.9	118.6	127.0
Ni_1-N_2	2.249	2.278	2.259	**∠Ni_1-Te_1-Ni_2**	131.6	122.1	117.1
Ni_1-N_3	2.211	2.157	2.144	**∠Ni_1-Te_2-Ni_2**	141.9	157.3	160.9
Ni_1-N_4	2.290	2.257	2.284	**∠N_1-Ni_1-N_2**	83.4	82.0	81.5
Te_1-Te_2	2.967	3.585	3.669	**∠N2-Ni_1-N3**	82.5	82.5	83.2
Ni_2-Te_1	4.828	5.480	5.599	**∠N_3-Ni_1-N_4**	82.1	81.7	82.0
Ni_2-Te_2	2.635	2.599	2.562	**∠N_4-Ni_1-N_1**	82.5	82.8	81.7
Ni_2-N_1	2.149	2.159	2.198	**∠N_1-Ni_2-N_2**	82.7	83.0	82.1
Ni_2-N_2	2.253	2.254	2.275	**∠N2-Ni_2-N3**	82.5	82.0	82.0
Ni_2-N_3	2.160	2.177	2.191	**∠N_3-Ni_2-N_4**	82.2	81.6	81.5
Ni_2-N_4	2.303	2.295	2.294	**∠N_4-Ni_2-N_1**	81.9	82.1	82.1
C-$H_{abs(DHA)}$	1.792	1.819	2.155	**∠Te_1-H-C_{DHA}**	172.3	159.4	149.4
Te-$H_{abs(DHA)}$	1.782	1.787	1.736	**∠ H-Te_1-Ni**	109.9	98.1	96.7

Table S26- Computed spin densities and Mulliken charges of complex **4** for all possible spin states of Intermediate (**Int1**) along with respective bond lengths and bond angles as obtained from optimized geometries in Gaussian 09.

Mulliken spin density and charges values of intermediate (Int1)							
Spin Density	**$^{5}Int1_{(t,t)}$**	**$^{1}Int1_{(t,t)}$**	**$^{3}Int1_{(s,t)}$**	**Mulliken Charges**	**$^{5}Int1_{(t,t)}$**	**$^{1}Int1_{(t,t)}$**	**$^{3}Int1_{(s,t)}$**
Ni1	1.47	1.54	1.66	**Ni1**	0.70	0.68	0.69
Ni2	1.61	-1.57	0.04	**Ni2**	0.66	0.64	0.62
Te1	-0.10	-0.09	0.30	**Te1**	-0.18	-0.22	-0.24
Te2	-0.45	-0.88	0.67	**Te2**	-0.69	-0.64	-0.65
N_{1a}	0.07	0.07	0.07	**N_{1a}**	-0.28	-0.29	-0.29
N_{1b}	0.05	0.06	0.06	**N_{1b}**	-0.20	-0.20	-0.20

N_{1c}	0.05	0.06	0.07	**N_{1c}**	-0.29	-0.29	-0.29
N_{1d}	0.05	0.06	0.06	**N_{1d}**	-0.16	-0.21	-0.21
N_{2a}	0.06	-0.07	-0.07	**N_{2a}**	-0.29	-0.29	-0.29
N_{2b}	0.06	-0.06	0.03	**N_{2b}**	-0.20	-0.20	-0.19
N_{2c}	0.06	-0.06	0.06	**N_{2c}**	-0.29	-0.28	-0.28
N_{2d}	0.06	-0.05	0.01	**N_{2d}**	-0.20	-0.20	-0.19
C_{DHA}	0.69	0.68	-0.68	**C_{DHA}**	-0.16	-0.18	-0.18
Bond parameters and Bond angles of intermediate (Int1)							
Bond Parameter	$^{5}Int1_{(t,t)}$	$^{1}Int1_{(t,t)}$	$^{3}Int1_{(s,t)}$	**Bond Angle**	$^{5}Int1_{(t,t)}$	$^{1}Int1_{(t,t)}$	$^{3}Int1_{(s,t)}$
Ni_1-Ni_2	7.199	7.352	7.360	**∠Ni_1-Te_1-Te_2**	108.6	110.1	108.8
Ni_1-Te_1	2.623	2.617	2.618	**∠Ni_1-Te_2-Te_1**	31.4	32.5	30.0
Ni_1-Te_2	4.774	4.972	4.957	**∠Ni_2-Te_1-Te_2**	26.1	28.5	24.6
Ni_1-N_1	2.149	2.143	2.142	**∠Ni_2-Te_2-Te_1**	121.1	118.9	122.0
Ni_1-N_2	2.266	2.262	2.262	**∠Ni_1-Te_1-Ni_2**	134.3	131.5	133.3
Ni_1-N_3	2.175	2.155	2.156	**∠Ni_1-Te_2-Ni_2**	151.9	141.9	151.4
Ni_1-N_4	2.271	2.271	2.270	**∠N_1-Ni_1-N_2**	83.3	83.4	83.2
Te_1-Te_2	3.240	3.484	3.449	**∠N2-Ni_1-N3**	82.5	82.5	82.5
Ni_2-Te_1	5.118	5.308	5.314	**∠N_3-Ni_1-N_4**	82.2	82.0	82.5
Ni_2-Te_2	2.628	2.603	2.608	**∠N_4-Ni_1-N_1**	83.2	82.5	83.0
Ni_2-N_1	2.155	2.164	2.164	**∠N_1-Ni_2-N_2**	82.2	82.7	82.7
Ni_2-N_2	2.258	2.245	2.226	**∠N2-Ni_2-N3**	82.5	82.5	83.1
Ni_2-N_3	2.160	2.169	2.197	**∠N_3-Ni_2-N_4**	82.2	82.1	82.5
Ni_2-N_4	2.289	2.302	2.266	**∠N_4-Ni_2-N_1**	82.2	81.9	82.3
C-$H_{abs(DHA)}$	3.322	3.583	3.516	**∠Te_1-H-C_{DHA}**	157.4	173.6	157.4
Te-$H_{abs(DHA)}$	1.661	1.660	1.660	**∠ H-Te_1-Ni**	98.7	110.0	99.2

Table S27- Optimized geometries of ground state reactant, transition sate, intermediate, and product complex of complexes **1**-**4**.

1-$^{1}R_{(t,t)}$

Ni	1.904918000	0.000148000	-0.000128000
N	3.237094000	0.778927000	-1.543735000
N	2.464893000	-1.978066000	-1.003106000
N	3.235775000	-0.778872000	1.544635000
C	4.124221000	-0.323749000	-1.985766000
H	4.921116000	-0.432841000	-1.248344000
H	4.613448000	-0.077965000	-2.940426000
C	3.349600000	-1.631229000	-2.154831000
H	2.711471000	-1.552114000	-3.038253000
H	4.058831000	-2.446527000	-2.358364000
C	3.161696000	-2.769667000	0.045580000
H	3.793485000	-3.550931000	-0.403096000
H	2.391535000	-3.285965000	0.624989000
C	4.013456000	-1.914823000	0.982627000
H	4.412131000	-2.550839000	1.786310000
H	4.876195000	-1.509372000	0.452111000
C	2.396057000	1.247867000	-2.672976000
H	1.751459000	2.062756000	-2.342403000
H	3.022147000	1.600177000	-3.505095000
C	1.322577000	-2.758365000	-1.528477000
H	1.659662000	-3.653432000	-2.071215000
H	0.731895000	-2.122519000	-2.188085000
H	0.686486000	-3.068702000	-0.700481000
C	2.393867000	-1.247660000	2.673257000
N	2.464309000	1.978243000	1.003165000
C	4.014537000	1.914794000	-0.981201000
H	4.876848000	1.509258000	-0.450042000
H	4.413874000	2.550722000	-1.784623000
C	3.162209000	2.769807000	-0.044806000
H	2.392706000	3.286412000	-0.624819000

H	3.793856000	3.550824000	0.404497000
C	3.347926000	1.631222000	2.155700000
H	4.056961000	2.446509000	2.359951000
H	2.708955000	1.552022000	3.038507000
C	4.122662000	0.323753000	1.987201000
H	4.611276000	0.078016000	2.942189000
H	4.919997000	0.432803000	1.250250000
H	1.751256000	0.440315000	-3.021009000
C	1.321537000	2.758519000	1.527592000
H	1.658122000	3.652981000	2.071625000
H	0.686818000	3.069904000	0.698932000
H	0.729657000	2.122221000	2.185713000
H	3.019325000	-1.600161000	3.505770000
H	1.749017000	-0.439971000	3.020862000
H	1.749257000	-2.062310000	2.342169000
O	0.000561000	-0.001424000	0.749977000
O	-0.000512000	-0.001192000	-0.750011000
Ni	-1.904876000	0.000149000	0.000122000
N	-3.237069000	0.778800000	1.543804000
N	-2.464925000	-1.978154000	1.002975000
N	-3.235765000	-0.778726000	-1.544699000
C	-4.124330000	-0.323871000	1.985576000
H	-4.921136000	-0.432803000	1.248034000
H	-4.613666000	-0.078173000	2.940203000
C	-3.349841000	-1.631438000	2.154577000
H	-2.711891000	-1.552518000	3.038145000
H	-4.059178000	-2.446712000	2.357840000
C	-3.161506000	-2.769696000	-0.045896000
H	-3.793188000	-3.551156000	0.402593000
H	-2.391199000	-3.285743000	-0.625336000
C	-4.013341000	-1.914838000	-0.982854000
H	-4.411918000	-2.550793000	-1.786632000
H	-4.876142000	-1.509559000	-0.452310000

C	-2.396066000	1.247465000	2.673185000
H	-1.751467000	2.062443000	2.342826000
H	-1.751272000	0.439835000	3.021046000
C	-1.322674000	-2.758466000	1.528464000
H	-1.659826000	-3.653632000	2.071000000
H	-0.732162000	-2.122704000	2.188304000
H	-0.686389000	-3.068642000	0.700558000
C	-2.393910000	-1.247259000	-2.673470000
H	-3.019410000	-1.599536000	-3.506047000
H	-1.749324000	-2.062020000	-2.342605000
H	-1.749043000	-0.439508000	-3.020899000
N	-2.464301000	1.978343000	-1.003024000
C	-4.014386000	1.914844000	0.981438000
H	-4.876768000	1.509497000	0.450251000
H	-4.413613000	2.550716000	1.784956000
C	-3.161970000	2.769858000	0.045132000
H	-2.392315000	3.286201000	0.625177000
H	-3.793497000	3.551079000	-0.403986000
C	-3.348131000	1.631454000	-2.155437000
H	-4.057253000	2.446731000	-2.359425000
H	-2.709336000	1.552431000	-3.038387000
C	-4.122764000	0.323914000	-1.987001000
H	-4.611494000	0.078278000	-2.941957000
H	-4.920007000	0.432822000	-1.249929000
H	-3.022182000	1.599579000	3.505369000
C	-1.321588000	2.758621000	-1.527572000
H	-1.658237000	3.653182000	-2.071406000
H	-0.686673000	3.069845000	-0.699004000
H	-0.729882000	2.122399000	-2.185922000

2-$^{1}R_{(t,t)}$

Ni	-2.316288000	-0.000004000	0.000091000
N	-3.636493000	-0.176341000	-1.745223000

N	-2.846677000	2.173846000	-0.206955000
N	-3.636345000	0.176329000	1.745523000
C	-4.357277000	1.112897000	-1.914419000
H	-5.244359000	1.107722000	-1.278511000
H	-4.716662000	1.226264000	-2.946739000
C	-3.449288000	2.285778000	-1.564177000
H	-2.621389000	2.331319000	-2.276780000
H	-4.009914000	3.227272000	-1.662038000
C	-3.815771000	2.504624000	0.882541000
H	-4.544927000	3.251200000	0.538427000
H	-3.250433000	2.977340000	1.688536000
C	-4.562990000	1.292981000	1.441538000
H	-5.116041000	1.602322000	2.341271000
H	-5.304695000	0.928406000	0.729620000
C	-2.854345000	-0.474964000	-2.972841000
H	-2.225884000	-1.351643000	-2.817663000
H	-3.528218000	-0.652103000	-3.822932000
C	-1.707204000	3.114961000	-0.133089000
H	-2.034243000	4.154017000	-0.283204000
H	-0.981235000	2.841659000	-0.897891000
H	-1.231409000	3.022215000	0.843330000
C	-2.854079000	0.474962000	2.973064000
N	-2.846638000	-2.173843000	0.207201000
C	-4.563100000	-1.292999000	-1.441148000
H	-5.304741000	-0.928428000	-0.729163000
H	-5.116232000	-1.602348000	-2.340829000
C	-3.815818000	-2.504633000	-0.882216000
H	-3.250542000	-2.977341000	-1.688258000
H	-4.544937000	-3.251217000	-0.538042000
C	-3.449135000	-2.285787000	1.564473000
H	-4.009748000	-3.227286000	1.662375000
H	-2.621179000	-2.331327000	2.277008000
C	-4.357104000	-1.112912000	1.914791000

H	-4.716395000	-1.226278000	2.947143000
H	-5.244242000	-1.107749000	1.278963000
H	-2.196665000	0.363240000	-3.204266000
C	-1.707153000	-3.114937000	0.133233000
H	-2.034159000	-4.154000000	0.283372000
H	-1.231443000	-3.022174000	-0.843224000
H	-0.981124000	-2.841625000	0.897975000
H	-3.527870000	0.652113000	3.823218000
H	-2.196379000	-0.363242000	3.204435000
H	-2.225628000	1.351635000	2.817816000
S	0.000090000	0.000018000	1.072142000
S	-0.000091000	0.000031000	-1.072145000
Ni	2.316288000	-0.000004000	-0.000091000
N	3.636492000	-0.176360000	1.745222000
N	2.846678000	2.173843000	0.206980000
N	3.636346000	0.176348000	-1.745521000
C	4.357279000	1.112875000	1.914431000
H	5.244360000	1.107706000	1.278523000
H	4.716663000	1.226232000	2.946752000
C	3.449290000	2.285761000	1.564202000
H	2.621393000	2.331298000	2.276806000
H	4.009919000	3.227254000	1.662071000
C	3.815769000	2.504634000	-0.882515000
H	4.544925000	3.251207000	-0.538395000
H	3.250431000	2.977356000	-1.688505000
C	4.562990000	1.292998000	-1.441524000
H	5.116040000	1.602348000	-2.341255000
H	5.304695000	0.928416000	-0.729610000
C	2.854343000	-0.474995000	2.972836000
H	2.225882000	-1.351672000	2.817649000
H	2.196664000	0.363208000	3.204269000
C	1.707204000	3.114959000	0.133124000
H	2.034242000	4.154013000	0.283250000

H	0.981236000	2.841648000	0.897924000
H	1.231407000	3.022222000	-0.843295000
C	2.854080000	0.474992000	-2.973059000
H	3.527871000	0.652151000	-3.823212000
H	2.225629000	1.351664000	-2.817803000
H	2.196380000	-0.363209000	-3.204439000
N	2.846638000	-2.173841000	-0.207225000
C	4.563098000	-1.293016000	1.441136000
H	5.304741000	-0.928439000	0.729156000
H	5.116229000	-1.602375000	2.340815000
C	3.815816000	-2.504643000	0.882191000
H	3.250538000	-2.977358000	1.688227000
H	4.544934000	-3.251225000	0.538010000
C	3.449137000	-2.285771000	-1.564496000
H	4.009752000	-3.227267000	-1.662407000
H	2.621182000	-2.331305000	-2.277034000
C	4.357106000	-1.112891000	-1.914802000
H	4.716398000	-1.226246000	-2.947155000
H	5.244244000	-1.107734000	-1.278973000
H	3.528216000	-0.652142000	3.822926000
C	1.707152000	-3.114934000	-0.133269000
H	2.034157000	-4.153996000	-0.283418000
H	1.231440000	-3.022182000	0.843189000
H	0.981123000	-2.841613000	-0.898009000

3-$^{1}R_{(t,t)}$

Ni	2.390718000	-0.000005000	-0.000096000
N	3.720378000	-0.126203000	1.760754000
N	2.910096000	2.175727000	0.143005000
N	3.720242000	0.126116000	-1.761053000
C	4.433178000	1.174259000	1.878051000
H	5.315531000	1.155632000	1.236347000
H	4.799324000	1.325872000	2.902924000

C	3.509814000	2.326312000	1.498207000
H	2.678868000	2.375532000	2.206919000
H	4.057460000	3.277490000	1.574261000
C	3.885617000	2.473807000	-0.951163000
H	4.608665000	3.234720000	-0.625940000
H	3.323150000	2.917225000	-1.775573000
C	4.643165000	1.248909000	-1.467361000
H	5.210590000	1.537801000	-2.364986000
H	5.373589000	0.901818000	-0.735967000
C	2.981755000	-0.394361000	3.022770000
H	2.358198000	-1.282199000	2.920278000
H	3.688580000	-0.539185000	3.852059000
C	1.774875000	3.122791000	0.037330000
H	2.114097000	4.163257000	0.143051000
H	1.050663000	2.891678000	0.818377000
H	1.289891000	2.994540000	-0.930935000
C	2.981533000	0.394347000	-3.023002000
N	2.909897000	-2.175717000	-0.143243000
C	4.643178000	-1.249079000	1.466989000
H	5.373572000	-0.902051000	0.735535000
H	5.210654000	-1.538020000	2.364566000
C	3.885474000	-2.473909000	0.950846000
H	3.323035000	-2.917279000	1.775299000
H	4.608421000	-3.234888000	0.625557000
C	3.509489000	-2.326385000	-1.498491000
H	4.057043000	-3.277614000	-1.574573000
H	2.678481000	-2.375549000	-2.207134000
C	4.432922000	-1.174409000	-1.878422000
H	4.798956000	-1.326049000	-2.903330000
H	5.315337000	-1.155860000	-1.236803000
H	2.327149000	0.445858000	3.255845000
C	1.774531000	-3.122619000	-0.037481000
H	2.113598000	-4.163135000	-0.143183000

H	1.289597000	-2.994261000	0.930800000
H	1.050311000	-2.891428000	-0.818508000
H	3.688296000	0.539087000	-3.852358000
H	2.326810000	-0.445801000	-3.256009000
H	2.358086000	1.282255000	-2.920453000
Se	-0.000038000	0.000091000	-1.251701000
Se	0.000038000	0.000102000	1.251703000
Ni	-2.390719000	-0.000006000	0.000094000
N	-3.720378000	-0.126221000	-1.760754000
N	-2.910098000	2.175724000	-0.143028000
N	-3.720241000	0.126135000	1.761054000
C	-4.433179000	1.174239000	-1.878066000
H	-5.315533000	1.155617000	-1.236364000
H	-4.799322000	1.325840000	-2.902941000
C	-3.509816000	2.326296000	-1.498232000
H	-2.678870000	2.375511000	-2.206945000
H	-4.057463000	3.277473000	-1.574296000
C	-3.885619000	2.473816000	0.951136000
H	-4.608668000	3.234724000	0.625905000
H	-3.323152000	2.917244000	1.775541000
C	-4.643165000	1.248923000	1.467350000
H	-5.210588000	1.537825000	2.364972000
H	-5.373590000	0.901823000	0.735961000
C	-2.981753000	-0.394391000	-3.022766000
H	-2.358195000	-1.282227000	-2.920264000
H	-2.327147000	0.445827000	-3.255847000
C	-1.774877000	3.122789000	-0.037364000
H	-2.114098000	4.163254000	-0.143095000
H	-1.050664000	2.891667000	-0.818408000
H	-1.289893000	2.994547000	0.930903000
C	-2.981530000	0.394382000	3.022998000
H	-3.688292000	0.539130000	3.852354000
H	-2.358087000	1.282291000	2.920437000

H	-2.326804000	-0.445761000	3.256014000
N	-2.909898000	-2.175715000	0.143266000
C	-4.643178000	-1.249095000	-1.466980000
H	-5.373575000	-0.902059000	-0.735533000
H	-5.210651000	-1.538047000	-2.364556000
C	-3.885476000	-2.473920000	-0.950819000
H	-3.323038000	-2.917301000	-1.775266000
H	-4.608424000	-3.234894000	-0.625521000
C	-3.509487000	-2.326370000	1.498517000
H	-4.057041000	-3.277598000	1.574609000
H	-2.678477000	-2.375528000	2.207157000
C	-4.432918000	-1.174390000	1.878440000
H	-4.798947000	-1.326019000	2.903352000
H	-5.315337000	-1.155849000	1.236827000
H	-3.688575000	-0.539224000	-3.852055000
C	-1.774531000	-3.122617000	0.037511000
H	-2.113597000	-4.163133000	0.143224000
H	-1.289601000	-2.994269000	-0.930773000
H	-1.050309000	-2.891417000	0.818532000

4-$^{1}R_{(t,t)}$

Ni	2.516278000	0.000004000	0.000126000
N	3.856570000	0.112946000	-1.776493000
N	3.027196000	-2.176200000	-0.129130000
N	3.856414000	-0.112925000	1.776868000
C	4.567483000	-1.191686000	-1.864584000
H	5.444014000	-1.165763000	-1.215761000
H	4.943529000	-1.360645000	-2.883036000
C	3.636948000	-2.337083000	-1.479425000
H	2.811239000	-2.389920000	-2.193877000
H	4.182563000	-3.290352000	-1.543562000
C	3.999626000	-2.463564000	0.971477000
H	4.714599000	-3.237530000	0.659092000

H	3.431557000	-2.887156000	1.802463000
C	4.770770000	-1.239614000	1.470152000
H	5.351252000	-1.529305000	2.359160000
H	5.491306000	-0.897990000	0.727118000
C	3.163592000	0.372059000	-3.066113000
H	2.541067000	1.263682000	-2.995281000
H	3.900935000	0.507122000	-3.870182000
C	1.898458000	-3.134675000	-0.019748000
H	2.252388000	-4.172169000	-0.101421000
H	1.178990000	-2.931577000	-0.814140000
H	1.398994000	-2.993614000	0.939685000
C	3.163325000	-0.372009000	3.066434000
N	3.027171000	2.176204000	0.129426000
C	4.770899000	1.239629000	-1.469682000
H	5.491358000	0.898010000	-0.726570000
H	5.351471000	1.529320000	-2.358632000
C	3.999695000	2.463575000	-0.971095000
H	3.431697000	2.887151000	-1.802139000
H	4.714630000	3.237552000	-0.658651000
C	3.636808000	2.337096000	1.479771000
H	4.182412000	3.290369000	1.543949000
H	2.811043000	2.389928000	2.194159000
C	4.567322000	1.191706000	1.864998000
H	4.943295000	1.360673000	2.883476000
H	5.443899000	1.165782000	1.216235000
H	2.516579000	-0.468740000	-3.317853000
C	1.898427000	3.134662000	0.019943000
H	2.252334000	4.172162000	0.101642000
H	1.399051000	2.993589000	-0.939534000
H	1.178891000	2.931557000	0.814273000
H	3.900599000	-0.507068000	3.870568000
H	2.516306000	0.468807000	3.318107000
H	2.540792000	-1.263624000	2.995568000

Te	-0.000057000	-0.000012000	1.411301000
Te	0.000057000	-0.000031000	-1.411309000
Ni	-2.516278000	0.000004000	-0.000124000
N	-3.856567000	0.112965000	1.776495000
N	-3.027197000	-2.176198000	0.129155000
N	-3.856417000	-0.112944000	-1.776864000
C	-4.567481000	-1.191666000	1.864601000
H	-5.444013000	-1.165749000	1.215779000
H	-4.943526000	-1.360614000	2.883056000
C	-3.636947000	-2.337067000	1.479453000
H	-2.811238000	-2.389899000	2.193905000
H	-4.182563000	-3.290335000	1.543600000
C	-3.999628000	-2.463574000	-0.971447000
H	-4.714600000	-3.237537000	-0.659053000
H	-3.431559000	-2.887175000	-1.802429000
C	-4.770772000	-1.239630000	-1.470134000
H	-5.351256000	-1.529330000	-2.359139000
H	-5.491308000	-0.897997000	-0.727103000
C	-3.163587000	0.372091000	3.066111000
H	-2.541060000	1.263712000	2.995269000
H	-2.516575000	-0.468707000	3.317859000
C	-1.898458000	-3.134673000	0.019782000
H	-2.252387000	-4.172167000	0.101468000
H	-1.178989000	-2.931567000	0.814171000
H	-1.398996000	-2.993623000	-0.939653000
C	-3.163330000	-0.372042000	-3.066428000
H	-3.900604000	-0.507111000	-3.870559000
H	-2.540796000	-1.263656000	-2.995553000
H	-2.516312000	0.468771000	-3.318111000
N	-3.027171000	2.176203000	-0.129447000
C	-4.770896000	1.239646000	1.469675000
H	-5.491357000	0.898018000	0.726568000
H	-5.351466000	1.529346000	2.358623000

C	-3.999693000	2.463585000	0.971073000
H	-3.431693000	2.887171000	1.802110000
H	-4.714628000	3.237559000	0.658622000
C	-3.636811000	2.337080000	-1.479793000
H	-4.182415000	3.290352000	-1.543980000
H	-2.811047000	2.389906000	-2.194183000
C	-4.567324000	1.191685000	-1.865007000
H	-4.943299000	1.360642000	-2.883486000
H	-5.443901000	1.165769000	-1.216243000
H	-3.900928000	0.507163000	3.870181000
C	-1.898426000	3.134661000	-0.019977000
H	-2.252333000	4.172161000	-0.101690000
H	-1.399050000	2.993600000	0.939501000
H	-1.178891000	2.931545000	-0.814305000

1-^{5}TS1$_{(t,t)}$

Ni	2.183090000	-1.573734000	-0.093622000
N	3.889561000	-2.273870000	-1.196406000
N	1.065188000	-2.844464000	-1.550481000
N	1.675202000	-3.201052000	1.256774000
C	3.486755000	-3.522175000	-1.886326000
H	3.522307000	-4.335621000	-1.159361000
H	4.197941000	-3.780114000	-2.685457000
C	2.085802000	-3.386037000	-2.493769000
H	2.132214000	-2.704922000	-3.346821000
H	1.769248000	-4.361023000	-2.891367000
C	0.392085000	-3.903594000	-0.747899000
H	0.155671000	-4.775560000	-1.376499000
H	-0.555872000	-3.484896000	-0.401662000
C	1.217308000	-4.362681000	0.456287000
H	0.610436000	-5.046768000	1.067811000
H	2.096583000	-4.926150000	0.138245000
C	4.219909000	-1.217225000	-2.185615000

H	4.521122000	-0.307707000	-1.666811000
H	5.037928000	-1.544596000	-2.843292000
C	0.040751000	-2.088097000	-2.310532000
H	-0.431588000	-2.725582000	-3.074005000
H	0.511176000	-1.228313000	-2.789393000
H	-0.715646000	-1.728942000	-1.612068000
C	0.562731000	-2.686607000	2.095617000
N	3.750232000	-1.212099000	1.519262000
C	5.027202000	-2.467717000	-0.261661000
H	4.934762000	-3.456313000	0.192293000
H	5.984695000	-2.459984000	-0.802531000
C	5.049812000	-1.374232000	0.810462000
H	5.284670000	-0.411581000	0.349398000
H	5.859529000	-1.588127000	1.524149000
C	3.544134000	-2.238051000	2.581432000
H	4.498458000	-2.502003000	3.059144000
H	2.928529000	-1.780553000	3.359356000
C	2.856443000	-3.516443000	2.090089000
H	2.575815000	-4.125802000	2.962957000
H	3.537460000	-4.123551000	1.491069000
H	3.344858000	-0.976825000	-2.790105000
C	3.699448000	0.137573000	2.132925000
H	4.485629000	0.265256000	2.891100000
H	3.823535000	0.894119000	1.359874000
H	2.725057000	0.283396000	2.604650000
H	0.281592000	-3.429342000	2.857155000
H	0.871035000	-1.766176000	2.594651000
H	-0.307964000	-2.459892000	1.476567000
Ni	-3.482746000	-0.444508000	0.274403000
N	-3.538099000	1.073848000	-1.239733000
N	-2.489616000	1.147569000	1.455714000
N	-5.121547000	-0.052433000	1.621836000
C	-3.377625000	2.386184000	-0.567774000

H	-4.347494000	2.678614000	-0.159461000
H	-3.080406000	3.165593000	-1.282908000
C	-2.310999000	2.305078000	0.528059000
H	-1.327692000	2.204314000	0.066563000
H	-2.294250000	3.249847000	1.087466000
C	-3.408405000	1.456604000	2.589325000
H	-3.244963000	2.481725000	2.950884000
H	-3.141659000	0.790326000	3.413418000
C	-4.891005000	1.270902000	2.248988000
H	-5.487331000	1.385554000	3.166159000
H	-5.231487000	2.041128000	1.554180000
C	-2.385066000	0.809335000	-2.140094000
H	-2.507358000	-0.162249000	-2.620336000
H	-1.451819000	0.783897000	-1.575496000
C	-1.162536000	0.743496000	1.990411000
H	-0.725283000	1.547481000	2.601430000
H	-0.480868000	0.506718000	1.167866000
H	-1.289659000	-0.144588000	2.613511000
C	-5.083553000	-1.127413000	2.646536000
H	-5.899757000	-1.003518000	3.372263000
H	-4.130175000	-1.109943000	3.175732000
H	-5.174128000	-2.105008000	2.171817000
N	-5.091295000	-1.360384000	-0.954732000
C	-4.818085000	0.941358000	-1.975441000
H	-5.597245000	1.445810000	-1.400059000
H	-4.770726000	1.445933000	-2.951718000
C	-5.170180000	-0.534009000	-2.195937000
H	-4.473433000	-0.968146000	-2.916654000
H	-6.170186000	-0.606539000	-2.646170000
C	-6.343864000	-1.298054000	-0.143087000
H	-7.226962000	-1.251910000	-0.795255000
H	-6.417662000	-2.236085000	0.411753000
C	-6.379503000	-0.123343000	0.842270000

H	-7.252563000	-0.238676000	1.501831000
H	-6.505804000	0.825228000	0.316451000
H	-2.317643000	1.586455000	-2.913784000
C	-4.803510000	-2.772591000	-1.317737000
H	-5.599350000	-3.199363000	-1.943858000
H	-3.855914000	-2.818101000	-1.857259000
H	-4.704947000	-3.367817000	-0.407975000
C	4.862192000	2.446497000	-0.859335000
C	5.984497000	2.872798000	-0.148231000
C	5.820797000	3.626739000	1.017193000
C	4.536928000	3.963270000	1.452755000
H	4.989449000	1.906619000	-1.795189000
H	6.981099000	2.643561000	-0.514690000
H	6.688784000	3.974898000	1.569168000
H	4.413346000	4.577973000	2.341128000
C	3.408120000	3.537779000	0.747414000
C	3.566874000	2.758574000	-0.416195000
C	2.347198000	2.312905000	-1.158610000
C	2.004619000	3.904453000	1.185934000
H	1.908068000	1.299800000	-0.680414000
H	2.024771000	4.785332000	1.836464000
C	1.247789000	3.329669000	-1.141654000
C	1.085520000	4.135848000	0.003459000
C	0.111478000	5.137981000	0.008648000
C	-0.706210000	5.345527000	-1.106015000
C	-0.552537000	4.542101000	-2.240321000
C	0.417518000	3.538655000	-2.252861000
H	0.011806000	5.782833000	0.878839000
H	-1.435522000	6.150868000	-1.100562000
H	-1.158715000	4.723217000	-3.124086000
H	0.563933000	2.936423000	-3.146745000
H	2.583418000	1.993301000	-2.179143000
H	1.595975000	3.082905000	1.800588000

O	1.270801000	0.008989000	-0.441121000
O	-2.248654000	-1.751016000	0.291803000

Imaginary frequency *i*640.9

2-^{1}TS1$_{(t,t)}$

Ni	1.339928000	-1.969502000	-0.062390000
N	3.436542000	-2.211162000	-0.823083000
N	0.962859000	-3.278904000	-1.871529000
N	0.982782000	-3.957066000	0.996355000
C	3.467962000	-3.500492000	-1.546306000
H	3.474694000	-4.304980000	-0.811332000
H	4.394734000	-3.603720000	-2.132061000
C	2.272733000	-3.623974000	-2.497505000
H	2.421171000	-2.948103000	-3.342037000
H	2.248150000	-4.640157000	-2.916318000
C	0.274419000	-4.474238000	-1.319965000
H	0.227596000	-5.275891000	-2.073620000
H	-0.752241000	-4.172216000	-1.097133000
C	0.928921000	-5.012268000	-0.048144000
H	0.360387000	-5.883431000	0.306910000
H	1.938191000	-5.372410000	-0.252696000
C	3.784583000	-1.115778000	-1.756740000
H	3.874270000	-0.184155000	-1.204090000
H	4.742732000	-1.330480000	-2.253740000
C	0.084186000	-2.641581000	-2.880040000
H	-0.128783000	-3.325300000	-3.715227000
H	0.563907000	-1.737554000	-3.258611000
H	-0.842841000	-2.345014000	-2.387732000
C	-0.278817000	-3.987737000	1.774429000
N	2.424294000	-1.568062000	1.841639000
C	4.353155000	-2.171714000	0.345143000
H	4.477437000	-3.181598000	0.739687000
H	5.354737000	-1.833101000	0.045345000

C	3.808895000	-1.228713000	1.417089000
H	3.783369000	-0.209157000	1.024112000
H	4.488679000	-1.226047000	2.282927000
C	2.376824000	-2.795606000	2.692100000
H	3.301726000	-2.894014000	3.277943000
H	1.568998000	-2.661182000	3.414863000
C	2.134168000	-4.093949000	1.913581000
H	1.975449000	-4.909039000	2.637187000
H	3.009425000	-4.368391000	1.324874000
H	3.001621000	-0.983070000	-2.502211000
C	1.858798000	-0.425779000	2.596630000
H	2.414993000	-0.244756000	3.528269000
H	1.896039000	0.464913000	1.968549000
H	0.812011000	-0.634217000	2.825249000
H	-0.334979000	-4.913035000	2.367384000
H	-0.345606000	-3.122841000	2.433121000
H	-1.130159000	-3.937396000	1.096970000
Ni	-2.978941000	0.087443000	0.265952000
N	-3.506908000	1.348871000	-1.369026000
N	-2.376748000	1.991798000	1.244175000
N	-4.608145000	0.234322000	1.686351000
C	-3.438772000	2.759136000	-0.901713000
H	-4.399793000	3.024680000	-0.455966000
H	-3.285360000	3.441494000	-1.749241000
C	-2.302376000	2.943512000	0.101336000
H	-1.344622000	2.769875000	-0.394182000
H	-2.296661000	3.982676000	0.460931000
C	-3.424982000	2.354421000	2.244208000
H	-3.572633000	3.442973000	2.275626000
H	-3.049969000	2.067761000	3.229169000
C	-4.775702000	1.672222000	2.004324000
H	-5.408924000	1.810007000	2.893990000
H	-5.302549000	2.134588000	1.167613000

C	-2.507611000	1.117535000	-2.446336000
H	-2.489899000	0.061717000	-2.716422000
H	-1.506790000	1.369982000	-2.094306000
C	-1.055146000	1.952461000	1.915362000
H	-0.802006000	2.935697000	2.339197000
H	-0.300114000	1.646522000	1.190408000
H	-1.079978000	1.211344000	2.716552000
C	-4.184512000	-0.528707000	2.888619000
H	-4.926798000	-0.431800000	3.693860000
H	-3.218512000	-0.168438000	3.244512000
H	-4.067209000	-1.583529000	2.635615000
N	-4.492288000	-1.318095000	-0.771758000
C	-4.865814000	0.967281000	-1.821489000
H	-5.583693000	1.375573000	-1.107616000
H	-5.096705000	1.421795000	-2.796796000
C	-5.016438000	-0.553827000	-1.942416000
H	-4.471107000	-0.895052000	-2.824699000
H	-6.074280000	-0.793521000	-2.122645000
C	-5.529716000	-1.577530000	0.259257000
H	-6.458335000	-1.948189000	-0.201146000
H	-5.152962000	-2.381098000	0.898079000
C	-5.847059000	-0.354124000	1.115620000
H	-6.546434000	-0.641022000	1.913944000
H	-6.351632000	0.410729000	0.522006000
H	-2.758504000	1.718665000	-3.332162000
C	-3.958946000	-2.618634000	-1.238746000
H	-4.746245000	-3.232603000	-1.700571000
H	-3.162354000	-2.445098000	-1.963038000
H	-3.529706000	-3.157048000	-0.392140000
C	5.186429000	2.056904000	-0.704415000
C	6.266767000	2.114504000	0.167075000
C	6.138981000	2.791505000	1.386885000
C	4.935957000	3.421505000	1.714655000

H	5.294820000	1.574378000	-1.672337000
H	7.214136000	1.660324000	-0.107907000
H	6.983385000	2.852592000	2.066916000
H	4.856597000	3.975085000	2.647079000
C	3.842219000	3.375728000	0.849144000
C	3.956006000	2.670423000	-0.375773000
C	2.833608000	2.646426000	-1.293925000
C	2.544397000	4.072333000	1.192904000
H	1.937793000	1.317699000	-0.772060000
H	2.748759000	4.967840000	1.791300000
C	1.821104000	3.680588000	-1.202263000
C	1.695688000	4.430461000	-0.006953000
C	0.780909000	5.484233000	0.042782000
C	-0.013762000	5.796707000	-1.063254000
C	0.090905000	5.042072000	-2.239848000
C	0.996407000	3.990195000	-2.305326000
H	0.705897000	6.084589000	0.946388000
H	-0.696460000	6.640467000	-1.016444000
H	-0.510722000	5.297440000	-3.107462000
H	1.102160000	3.414633000	-3.221334000
H	3.015493000	2.231649000	-2.282979000
H	1.953398000	3.412953000	1.853236000
S	0.854591000	0.313610000	-0.867022000
S	-1.085075000	-1.226690000	0.229956000

Imaginary frequency *i*855.7

3-^{5}TS1$_{(t,t)}$

Ni	2.639291000	-1.718983000	-0.099216000
N	4.498540000	-2.362275000	-1.005094000
N	1.797231000	-3.134138000	-1.633414000
N	2.087762000	-3.264507000	1.276085000
C	4.272469000	-3.712154000	-1.569065000
H	4.283567000	-4.421840000	-0.739992000

H	5.090615000	-4.000885000	-2.246700000
C	2.947193000	-3.780789000	-2.335338000
H	3.066285000	-3.276606000	-3.297059000
H	2.719733000	-4.831079000	-2.565845000
C	1.012479000	-4.091047000	-0.805876000
H	0.786323000	-5.003776000	-1.378432000
H	0.060057000	-3.604497000	-0.578569000
C	1.718175000	-4.475488000	0.494066000
H	1.060703000	-5.129712000	1.083808000
H	2.625358000	-5.048634000	0.290335000
C	4.782353000	-1.378895000	-2.079977000
H	4.984682000	-0.402085000	-1.639550000
H	5.652857000	-1.691017000	-2.675314000
C	0.897133000	-2.531046000	-2.651854000
H	0.549401000	-3.294728000	-3.363061000
H	1.434960000	-1.749751000	-3.191977000
H	0.040672000	-2.070976000	-2.159577000
C	0.920223000	-2.790640000	2.065518000
N	4.030795000	-1.141571000	1.585710000
C	5.582319000	-2.343711000	0.010861000
H	5.578936000	-3.300649000	0.536449000
H	6.567331000	-2.256136000	-0.469985000
C	5.393506000	-1.185334000	0.989505000
H	5.549316000	-0.233959000	0.474446000
H	6.161046000	-1.248222000	1.775803000
C	3.839894000	-2.165046000	2.656625000
H	4.787919000	-2.362469000	3.176549000
H	3.164552000	-1.736315000	3.399862000
C	3.255519000	-3.491094000	2.158524000
H	2.978961000	-4.105416000	3.028975000
H	3.997256000	-4.059330000	1.595091000
H	3.916758000	-1.273787000	-2.736221000
C	3.801549000	0.207082000	2.161372000

H	4.492171000	0.403856000	2.994151000
H	3.949842000	0.961539000	1.389559000
H	2.770515000	0.279247000	2.510645000
H	0.668379000	-3.525792000	2.843963000
H	1.143994000	-1.829285000	2.528153000
H	0.060106000	-2.636265000	1.412907000
Se	1.106454000	0.227597000	-0.339794000
Se	-1.914261000	-1.256014000	-0.159472000
Ni	-4.017432000	-0.125747000	0.082770000
N	-5.414878000	0.380751000	-1.490989000
N	-3.548626000	2.052114000	-0.007265000
N	-4.964994000	0.436969000	1.947843000
C	-5.591978000	1.853327000	-1.483397000
H	-6.331190000	2.104268000	-0.720055000
H	-5.997662000	2.207090000	-2.442950000
C	-4.265483000	2.563577000	-1.209036000
H	-3.596888000	2.421958000	-2.061336000
H	-4.444017000	3.645891000	-1.124747000
C	-4.050424000	2.646827000	1.264666000
H	-4.330660000	3.700179000	1.118962000
H	-3.216935000	2.643030000	1.970611000
C	-5.233099000	1.893435000	1.881174000
H	-5.434288000	2.304777000	2.882085000
H	-6.140674000	2.042930000	1.293241000
C	-4.807936000	-0.064529000	-2.771611000
H	-4.589367000	-1.131820000	-2.731330000
H	-3.860849000	0.449356000	-2.936901000
C	-2.100878000	2.360737000	-0.147398000
H	-1.929025000	3.444252000	-0.205837000
H	-1.710991000	1.881193000	-1.045320000
H	-1.554353000	1.948416000	0.701182000
C	-4.010416000	0.131963000	3.043281000
H	-4.432229000	0.425176000	4.015981000

H	-3.070815000	0.660110000	2.880193000
H	-3.781450000	-0.933808000	3.053473000
N	-5.412054000	-1.930301000	0.280991000
C	-6.683417000	-0.341464000	-1.237895000
H	-7.237163000	0.205640000	-0.472590000
H	-7.318287000	-0.352829000	-2.137108000
C	-6.427275000	-1.787425000	-0.802409000
H	-6.063518000	-2.356786000	-1.660730000
H	-7.381184000	-2.248041000	-0.506136000
C	-5.997010000	-1.806483000	1.645021000
H	-6.953952000	-2.345778000	1.709124000
H	-5.310667000	-2.305919000	2.333153000
C	-6.205000000	-0.362119000	2.102856000
H	-6.543339000	-0.365990000	3.149838000
H	-6.994092000	0.117730000	1.521816000
H	-5.485962000	0.140142000	-3.613081000
C	-4.773902000	-3.265624000	0.160332000
H	-5.510560000	-4.073595000	0.280606000
H	-4.299407000	-3.355295000	-0.818472000
H	-3.999177000	-3.368107000	0.922107000
C	5.289621000	2.424198000	-0.931911000
C	6.494488000	2.568642000	-0.252755000
C	6.530885000	3.283172000	0.952347000
C	5.363170000	3.859323000	1.459122000
H	5.260531000	1.915931000	-1.893184000
H	7.409617000	2.157361000	-0.669555000
H	7.470867000	3.412989000	1.480393000
H	5.404854000	4.435207000	2.380414000
C	4.146738000	3.728204000	0.786947000
C	4.100110000	2.993234000	-0.424459000
C	2.849275000	2.894695000	-1.149895000
C	2.874335000	4.342589000	1.327493000
H	2.096322000	1.503273000	-0.548938000

H	3.106720000	5.238792000	1.913815000
C	1.827229000	3.896667000	-0.930393000
C	1.848817000	4.662380000	0.262560000
C	0.916076000	5.684774000	0.433171000
C	-0.035281000	5.958224000	-0.554033000
C	-0.067600000	5.196370000	-1.729563000
C	0.850586000	4.169443000	-1.912040000
H	0.943883000	6.289417000	1.336403000
H	-0.735027000	6.777549000	-0.415686000
H	-0.791568000	5.423477000	-2.506996000
H	0.848314000	3.588756000	-2.831044000
H	2.891514000	2.451589000	-2.143269000
H	2.420673000	3.633564000	2.042694000

Imaginary frequency *i*606.6

4-^{5}TS1$_{(t,t)}$

Ni	3.026668000	-1.438966000	0.185940000
N	5.114611000	-0.816822000	0.351606000
N	3.452268000	-1.368166000	-2.021713000
N	2.976336000	-3.617683000	-0.187514000
C	5.740558000	-1.134085000	-0.954808000
H	5.990364000	-2.196487000	-0.965650000
H	6.689470000	-0.589557000	-1.080850000
C	4.819167000	-0.785979000	-2.125774000
H	4.702101000	0.299751000	-2.172391000
H	5.303710000	-1.093512000	-3.065456000
C	3.370962000	-2.776298000	-2.501698000
H	4.011411000	-2.925033000	-3.384474000
H	2.342848000	-2.941069000	-2.833612000
C	3.724296000	-3.828418000	-1.447760000
H	3.521620000	-4.826212000	-1.869129000
H	4.791103000	-3.800501000	-1.218792000
C	5.228040000	0.632677000	0.639536000

H	4.713616000	0.870659000	1.571983000
H	6.283798000	0.933132000	0.728402000
C	2.528237000	-0.546579000	-2.839711000
H	2.804602000	-0.569147000	-3.905078000
H	2.557265000	0.484959000	-2.487759000
H	1.507259000	-0.917585000	-2.727643000
C	1.580060000	-4.087797000	-0.324176000
N	3.375688000	-2.138407000	2.338678000
C	5.701756000	-1.612185000	1.454141000
H	5.930546000	-2.608722000	1.072775000
H	6.658131000	-1.180297000	1.789704000
C	4.762872000	-1.696433000	2.659823000
H	4.685158000	-0.705329000	3.114116000
H	5.214457000	-2.353037000	3.419326000
C	3.227255000	-3.619771000	2.294952000
H	3.794786000	-4.092309000	3.111761000
H	2.172879000	-3.838881000	2.483408000
C	3.636264000	-4.264948000	0.968582000
H	3.395932000	-5.339206000	1.016162000
H	4.716068000	-4.197074000	0.827537000
H	4.759853000	1.215498000	-0.154060000
C	2.470753000	-1.616657000	3.391202000
H	2.730514000	-2.014828000	4.383778000
H	2.529634000	-0.526980000	3.420794000
H	1.440031000	-1.893824000	3.158730000
H	1.545097000	-5.163472000	-0.561110000
H	1.034768000	-3.913417000	0.605079000
H	1.066683000	-3.528775000	-1.107981000
Te	0.978051000	0.157756000	0.595597000
Te	-1.336390000	-0.713542000	-1.044066000
Ni	-3.763359000	-0.493099000	-0.041090000
N	-5.231366000	0.947345000	-0.664970000
N	-3.712514000	0.787186000	1.812938000

N	-4.787160000	-1.865438000	1.275533000
C	-5.698098000	1.688961000	0.534201000
H	-6.467220000	1.090736000	1.025727000
H	-6.175388000	2.636939000	0.245671000
C	-4.541219000	1.983334000	1.487502000
H	-3.873345000	2.719609000	1.034516000
H	-4.937497000	2.441024000	2.405983000
C	-4.298463000	-0.046900000	2.903147000
H	-4.767633000	0.588473000	3.668171000
H	-3.468275000	-0.559289000	3.394657000
C	-5.314461000	-1.085435000	2.422646000
H	-5.570002000	-1.747539000	3.263515000
H	-6.244508000	-0.608558000	2.108619000
C	-4.564391000	1.874812000	-1.616982000
H	-4.156313000	1.319218000	-2.461495000
H	-3.729866000	2.375304000	-1.126029000
C	-2.371598000	1.256422000	2.248254000
H	-2.445143000	1.867676000	3.159465000
H	-1.912985000	1.849177000	1.456485000
H	-1.728455000	0.397896000	2.441577000
C	-3.784522000	-2.859009000	1.739029000
H	-4.247880000	-3.584429000	2.423312000
H	-2.964504000	-2.353912000	2.250529000
H	-3.356760000	-3.386215000	0.885910000
N	-4.800762000	-1.764453000	-1.656678000
C	-6.343065000	0.227223000	-1.333333000
H	-6.986621000	-0.193029000	-0.558672000
H	-6.965685000	0.922994000	-1.915246000
C	-5.822295000	-0.863909000	-2.268996000
H	-5.355266000	-0.395023000	-3.137751000
H	-6.673153000	-1.447079000	-2.650599000
C	-5.407127000	-2.898844000	-0.902980000
H	-6.256701000	-3.322706000	-1.458867000

H	-4.649424000	-3.684212000	-0.846190000
C	-5.865813000	-2.539503000	0.510545000
H	-6.193203000	-3.457392000	1.020870000
H	-6.729791000	-1.873919000	0.481734000
H	-5.278269000	2.625956000	-1.984875000
C	-3.973660000	-2.333186000	-2.754640000
H	-4.590647000	-2.921282000	-3.449222000
H	-3.490880000	-1.524737000	-3.306630000
H	-3.195240000	-2.973353000	-2.336432000
C	3.547006000	3.254634000	-2.067213000
C	4.883459000	3.615687000	-1.938914000
C	5.318740000	4.274746000	-0.781047000
C	4.407309000	4.571784000	0.236416000
H	3.194493000	2.786995000	-2.983649000
H	5.581995000	3.414861000	-2.746489000
H	6.357302000	4.576482000	-0.682559000
H	4.746659000	5.103217000	1.122451000
C	3.061599000	4.220242000	0.122709000
C	2.614391000	3.550696000	-1.046059000
C	1.212065000	3.235386000	-1.189858000
C	2.072096000	4.528843000	1.227167000
H	1.152604000	1.637304000	-0.381671000
H	2.372494000	5.439726000	1.758072000
C	0.231745000	3.962848000	-0.416332000
C	0.637894000	4.648748000	0.757360000
C	-0.295126000	5.407978000	1.464341000
C	-1.620301000	5.505151000	1.031831000
C	-2.027228000	4.829189000	-0.126632000
C	-1.113629000	4.058137000	-0.837529000
H	0.020826000	5.949059000	2.353013000
H	-2.323684000	6.125930000	1.579137000
H	-3.044798000	4.943749000	-0.492330000
H	-1.410796000	3.557935000	-1.756299000

H	0.884249000	2.814427000	-2.139231000
H	2.123704000	3.723616000	1.981071000

Imaginary frequency *i*514.3

1-$^{1}Int_{(t,t)}$

Ni	2.005377000	-2.159163000	-0.457252000
N	3.486081000	-3.699275000	-0.845445000
N	1.014934000	-3.821324000	0.612459000
N	2.366487000	-1.390336000	1.502830000
C	3.374201000	-4.698516000	0.240288000
H	3.874346000	-4.289636000	1.120570000
H	3.896742000	-5.632291000	-0.017569000
C	1.903029000	-5.021953000	0.542590000
H	1.511473000	-5.672184000	-0.242948000
H	1.846116000	-5.598294000	1.475969000
C	0.858463000	-3.288550000	1.996748000
H	0.667448000	-4.108282000	2.705264000
H	-0.025076000	-2.645148000	1.982838000
C	2.073322000	-2.484135000	2.463182000
H	1.878080000	-2.081940000	3.467552000
H	2.957039000	-3.120819000	2.546909000
C	3.122047000	-4.298031000	-2.154898000
H	3.182105000	-3.545065000	-2.942363000
H	3.794597000	-5.130479000	-2.406065000
C	-0.328581000	-4.156837000	0.071679000
H	-0.785349000	-4.981360000	0.639342000
H	-0.231354000	-4.459999000	-0.973527000
H	-0.962392000	-3.268689000	0.131334000
C	1.445722000	-0.244856000	1.736178000
N	3.668634000	-0.824668000	-1.016048000
C	4.821850000	-3.059341000	-0.922797000
H	5.211296000	-2.951516000	0.091596000
H	5.535902000	-3.691158000	-1.470572000

C	4.719479000	-1.696758000	-1.611660000
H	4.464148000	-1.838715000	-2.665020000
H	5.698585000	-1.197682000	-1.587895000
C	4.123040000	-0.158285000	0.246276000
H	5.204168000	0.026692000	0.216270000
H	3.654661000	0.825932000	0.289918000
C	3.779055000	-0.941302000	1.520798000
H	3.982949000	-0.296854000	2.388455000
H	4.411648000	-1.825933000	1.624618000
H	2.095116000	-4.665366000	-2.131420000
C	3.260021000	0.203350000	-2.007689000
H	4.095552000	0.868571000	-2.264771000
H	2.896714000	-0.290386000	-2.911210000
H	2.444939000	0.797851000	-1.591526000
H	1.595354000	0.154272000	2.749779000
H	1.647401000	0.549333000	1.017227000
H	0.406099000	-0.552570000	1.606384000
Ni	-3.231781000	-0.245343000	0.093971000
N	-4.352163000	1.488561000	0.746187000
N	-4.528587000	-1.265582000	1.608228000
N	-4.466005000	-1.293904000	-1.306273000
C	-5.572176000	1.026938000	1.451138000
H	-6.329793000	0.791081000	0.700892000
H	-5.991700000	1.825414000	2.081094000
C	-5.273116000	-0.194407000	2.326166000
H	-4.659009000	0.112440000	3.176597000
H	-6.214620000	-0.579668000	2.743707000
C	-5.421926000	-2.165015000	0.822613000
H	-6.373994000	-2.326014000	1.348406000
H	-4.931303000	-3.139634000	0.767526000
C	-5.715260000	-1.667123000	-0.599405000
H	-6.260373000	-2.452188000	-1.144410000
H	-6.365843000	-0.790744000	-0.577973000

C	-3.456001000	2.216480000	1.679097000
H	-2.541801000	2.521857000	1.167652000
H	-3.172159000	1.567085000	2.509203000
C	-3.741206000	-2.065546000	2.577016000
H	-4.391286000	-2.599628000	3.284696000
H	-3.072859000	-1.403383000	3.130391000
H	-3.122131000	-2.776063000	2.029295000
C	-3.725104000	-2.508318000	-1.732293000
H	-4.310156000	-3.076328000	-2.469645000
H	-3.518891000	-3.141316000	-0.869539000
H	-2.764180000	-2.229818000	-2.165877000
N	-2.803881000	1.083272000	-1.659913000
C	-4.656635000	2.317978000	-0.442726000
H	-5.518721000	1.875500000	-0.945313000
H	-4.950366000	3.337895000	-0.151563000
C	-3.451796000	2.400516000	-1.387480000
H	-2.693230000	3.054769000	-0.951899000
H	-3.766797000	2.877948000	-2.326384000
C	-3.412894000	0.371437000	-2.818872000
H	-3.627259000	1.073162000	-3.638227000
H	-2.663084000	-0.328837000	-3.194594000
C	-4.691253000	-0.396027000	-2.466686000
H	-5.020840000	-0.965696000	-3.347927000
H	-5.503370000	0.289867000	-2.217161000
H	-3.954010000	3.111110000	2.080257000
C	-1.356517000	1.294514000	-1.922632000
H	-1.200946000	1.912510000	-2.818666000
H	-0.907954000	1.803323000	-1.066515000
H	-0.859739000	0.330274000	-2.048564000
C	4.289714000	3.167768000	2.107926000
C	5.609603000	2.949750000	1.738875000
C	6.013689000	3.188858000	0.416558000
C	5.083143000	3.646847000	-0.520991000

H	3.977834000	3.013399000	3.138487000
H	6.333566000	2.619189000	2.478612000
H	7.050031000	3.043161000	0.126001000
H	5.407806000	3.853717000	-1.539001000
C	3.751746000	3.878848000	-0.170689000
C	3.333636000	3.639530000	1.169906000
C	1.985989000	3.901948000	1.555682000
C	2.775089000	4.409157000	-1.201446000
H	1.699093000	3.740742000	2.592106000
H	2.716479000	3.702172000	-2.045275000
C	1.021324000	4.440579000	0.655034000
C	1.375062000	4.701099000	-0.699773000
C	0.426382000	5.256766000	-1.558849000
C	-0.860685000	5.573276000	-1.115112000
C	-1.215514000	5.325687000	0.220161000
C	-0.291374000	4.761520000	1.089069000
H	0.704427000	5.471415000	-2.588688000
H	-1.569875000	6.037243000	-1.794528000
H	-2.200111000	5.609224000	0.583668000
H	-0.549646000	4.598004000	2.133083000
H	-0.919506000	-0.995249000	-0.132745000
H	3.190800000	5.326528000	-1.644196000
O	-1.626131000	-1.102874000	0.533409000
O	0.586707000	-1.453485000	-1.323699000

2-$^{1}\mathrm{Int}_{(t,t)}$

Ni	2.581116000	-1.837042000	0.019332000
N	4.277143000	-2.252226000	-1.207707000
N	1.599029000	-3.396470000	-1.264205000
N	2.474742000	-3.380548000	1.499172000
C	4.058450000	-3.570362000	-1.854693000
H	4.327356000	-4.348838000	-1.138106000
H	4.722784000	-3.696489000	-2.722153000

C	2.606376000	-3.725586000	-2.314408000
H	2.423354000	-3.052796000	-3.155222000
H	2.454417000	-4.747105000	-2.691980000
C	1.302766000	-4.544746000	-0.358262000
H	1.279148000	-5.488427000	-0.922264000
H	0.295815000	-4.390533000	0.035841000
C	2.288845000	-4.678336000	0.804049000
H	1.920443000	-5.446944000	1.499270000
H	3.265806000	-5.015566000	0.452331000
C	4.342119000	-1.173096000	-2.229027000
H	4.450753000	-0.201737000	-1.745479000
H	5.189826000	-1.339800000	-2.908780000
C	0.338239000	-2.969200000	-1.924711000
H	-0.067466000	-3.774471000	-2.554643000
H	0.537466000	-2.092745000	-2.544082000
H	-0.402251000	-2.700698000	-1.167510000
C	1.289357000	-3.068350000	2.342584000
N	4.151021000	-1.010167000	1.421250000
C	5.488661000	-2.231570000	-0.351272000
H	5.561247000	-3.195531000	0.155676000
H	6.398617000	-2.125985000	-0.960226000
C	5.433380000	-1.083185000	0.660049000
H	5.550426000	-0.131290000	0.137055000
H	6.287461000	-1.169403000	1.347550000
C	4.133844000	-1.904787000	2.615043000
H	5.115325000	-1.909050000	3.110577000
H	3.428161000	-1.473986000	3.329299000
C	3.717557000	-3.345277000	2.307325000
H	3.587096000	-3.888356000	3.255096000
H	4.498714000	-3.868915000	1.752353000
H	3.415173000	-1.144256000	-2.801698000
C	3.947751000	0.388958000	1.876623000
H	4.737278000	0.699220000	2.575365000

H	3.959447000	1.063249000	1.019468000
H	2.978758000	0.469390000	2.373537000
H	1.172980000	-3.820641000	3.135577000
H	1.404568000	-2.083027000	2.795890000
H	0.383546000	-3.043232000	1.734867000
H	1.791315000	0.939831000	0.139065000
Ni	-4.000326000	-0.585602000	0.236840000
N	-3.690646000	0.737913000	-1.417276000
N	-3.005345000	1.043723000	1.394951000
N	-5.743841000	0.110454000	1.286714000
C	-3.394454000	2.087379000	-0.873040000
H	-4.342668000	2.574643000	-0.635853000
H	-2.893606000	2.715305000	-1.623491000
C	-2.496658000	1.992967000	0.362279000
H	-1.507264000	1.639853000	0.062605000
H	-2.357505000	2.997919000	0.786069000
C	-4.053037000	1.641789000	2.273764000
H	-3.841864000	2.704231000	2.461043000
H	-3.989552000	1.138876000	3.241240000
C	-5.478235000	1.500099000	1.728845000
H	-6.189818000	1.809832000	2.508982000
H	-5.639839000	2.162747000	0.876061000
C	-2.523376000	0.221263000	-2.179203000
H	-2.699367000	-0.814194000	-2.472262000
H	-1.625762000	0.238036000	-1.560281000
C	-1.866998000	0.590901000	2.235417000
H	-1.427067000	1.432781000	2.790322000
H	-1.102880000	0.142508000	1.597505000
H	-2.218111000	-0.162312000	2.943829000
C	-5.917779000	-0.789229000	2.458056000
H	-6.777382000	-0.471301000	3.064918000
H	-5.018769000	-0.785506000	3.074573000
H	-6.072903000	-1.815401000	2.123983000

N	-5.543058000	-1.480275000	-1.130033000
C	-4.914220000	0.704846000	-2.252960000
H	-5.664381000	1.342739000	-1.781623000
H	-4.722664000	1.126457000	-3.251116000
C	-5.433467000	-0.728673000	-2.415027000
H	-4.747865000	-1.285795000	-3.057385000
H	-6.400675000	-0.706226000	-2.937018000
C	-6.853368000	-1.273447000	-0.450358000
H	-7.675553000	-1.273414000	-1.180531000
H	-7.016728000	-2.134120000	0.202487000
C	-6.913918000	0.010731000	0.379794000
H	-7.855706000	0.027005000	0.947546000
H	-6.921730000	0.891639000	-0.265219000
H	-2.356022000	0.831885000	-3.078350000
C	-5.356723000	-2.931028000	-1.391393000
H	-6.138022000	-3.323286000	-2.057756000
H	-4.378662000	-3.093301000	-1.848188000
H	-5.383403000	-3.475632000	-0.445748000
C	4.666966000	2.990888000	-1.554808000
C	5.885110000	2.833559000	-0.908172000
C	6.055566000	3.335178000	0.391897000
C	4.998503000	3.994432000	1.025941000
H	4.536265000	2.632937000	-2.573533000
H	6.715356000	2.353615000	-1.419873000
H	7.012361000	3.235249000	0.896123000
H	5.143809000	4.399155000	2.025472000
C	3.767570000	4.171029000	0.391666000
C	3.584838000	3.662058000	-0.926062000
C	2.342155000	3.847680000	-1.596664000
C	2.657193000	4.935904000	1.081997000
H	3.020179000	5.951653000	1.304451000
C	1.239841000	4.522526000	-1.000018000
C	1.353717000	5.047417000	0.318767000

C	0.261377000	5.701687000	0.888632000
C	-0.934894000	5.865337000	0.184448000
C	-1.049800000	5.363750000	-1.121883000
C	0.018844000	4.697105000	-1.702333000
H	0.352148000	6.112456000	1.892033000
H	-1.760499000	6.406505000	0.637924000
H	-1.964329000	5.522850000	-1.687628000
H	-0.055349000	4.320595000	-2.719861000
H	2.235277000	3.469617000	-2.610205000
H	2.465651000	4.491803000	2.070946000
S	1.125990000	-0.107690000	-0.389184000
S	-2.679158000	-2.371732000	0.724868000

3-^{5}Int$_{(t,t)}$

Ni	2.946651000	-1.662188000	0.020857000
N	4.726585000	-1.894503000	-1.145453000
N	2.084678000	-3.033861000	-1.536658000
N	2.773172000	-3.398924000	1.266110000
C	4.592744000	-3.154498000	-1.916396000
H	4.823677000	-3.985395000	-1.247042000
H	5.327444000	-3.195253000	-2.734552000
C	3.187685000	-3.297444000	-2.508688000
H	3.071682000	-2.584256000	-3.327663000
H	3.083389000	-4.298347000	-2.951120000
C	1.663946000	-4.251120000	-0.786008000
H	1.606433000	-5.120367000	-1.457554000
H	0.650805000	-4.066745000	-0.420056000
C	2.579021000	-4.584693000	0.391992000
H	2.144957000	-5.420918000	0.958845000
H	3.559026000	-4.917133000	0.044238000
C	4.803164000	-0.724859000	-2.061704000
H	4.872082000	0.201495000	-1.490169000
H	5.678973000	-0.812432000	-2.720599000

C	0.908912000	-2.508244000	-2.279053000
H	0.560299000	-3.234565000	-3.027823000
H	1.182495000	-1.578015000	-2.780107000
H	0.096026000	-2.303790000	-1.579161000
C	1.581801000	-3.200013000	2.134416000
N	4.417023000	-1.025237000	1.618914000
C	5.895364000	-1.910728000	-0.230206000
H	6.009677000	-2.922326000	0.163573000
H	6.822139000	-1.679551000	-0.775278000
C	5.719735000	-0.900271000	0.903855000
H	5.764855000	0.113465000	0.498145000
H	6.559834000	-0.997217000	1.607519000
C	4.414261000	-2.123232000	2.633312000
H	5.399083000	-2.206111000	3.114859000
H	3.711625000	-1.833451000	3.417825000
C	4.007885000	-3.492609000	2.081524000
H	3.871938000	-4.186870000	2.924233000
H	4.795521000	-3.912732000	1.453124000
H	3.898748000	-0.661576000	-2.666877000
C	4.136141000	0.255361000	2.316901000
H	4.881701000	0.449410000	3.101453000
H	4.155312000	1.080352000	1.603345000
H	3.143849000	0.209846000	2.769857000
H	1.469573000	-4.044742000	2.828995000
H	1.683036000	-2.275370000	2.703611000
H	0.680094000	-3.111933000	1.526705000
Se	1.334778000	0.152911000	-0.191416000
H	2.029846000	1.214531000	0.585036000
Se	-2.404948000	-2.487384000	0.330291000
Ni	-3.963629000	-0.678889000	0.137296000
N	-3.743368000	0.960492000	-1.232640000
N	-3.147229000	0.794100000	1.618715000
N	-5.787068000	-0.341408000	1.251468000

C	-3.538882000	2.201019000	-0.439354000
H	-4.516684000	2.584085000	-0.138914000
H	-3.063346000	2.984491000	-1.045756000
C	-2.658516000	1.925422000	0.779385000
H	-1.651135000	1.663720000	0.446162000
H	-2.566274000	2.845766000	1.374509000
C	-4.277554000	1.178317000	2.515799000
H	-4.171209000	2.221269000	2.846488000
H	-4.203066000	0.561566000	3.414260000
C	-5.665110000	0.987557000	1.893945000
H	-6.425815000	1.121230000	2.678224000
H	-5.859873000	1.745408000	1.132951000
C	-2.551997000	0.701222000	-2.083331000
H	-2.655878000	-0.256710000	-2.593429000
H	-1.651916000	0.650069000	-1.469571000
C	-2.020382000	0.298059000	2.449854000
H	-1.685751000	1.067460000	3.161586000
H	-1.185772000	0.024011000	1.802082000
H	-2.339088000	-0.587960000	3.002917000
C	-5.885340000	-1.413687000	2.275942000
H	-6.767769000	-1.258853000	2.913375000
H	-4.988633000	-1.427123000	2.895776000
H	-5.957387000	-2.388682000	1.793383000
N	-5.396842000	-1.426118000	-1.421437000
C	-4.975054000	0.999728000	-2.055748000
H	-5.763841000	1.464328000	-1.460651000
H	-4.836471000	1.632573000	-2.945519000
C	-5.385972000	-0.405081000	-2.512858000
H	-4.682012000	-0.752579000	-3.272140000
H	-6.368586000	-0.350863000	-3.002728000
C	-6.712652000	-1.517880000	-0.727935000
H	-7.537519000	-1.501845000	-1.455477000
H	-6.747027000	-2.492904000	-0.235859000

C	-6.932456000	-0.418376000	0.310907000
H	-7.871295000	-0.615323000	0.848756000
H	-7.047499000	0.554058000	-0.171658000
H	-2.436772000	1.500057000	-2.830365000
C	-5.071443000	-2.756825000	-1.997893000
H	-5.816322000	-3.060926000	-2.747093000
H	-4.086061000	-2.719054000	-2.465815000
H	-5.041581000	-3.501219000	-1.200175000
C	4.286682000	3.657618000	-1.663621000
C	5.481078000	3.373956000	-1.017451000
C	5.596062000	3.590524000	0.365163000
C	4.508182000	4.099827000	1.082279000
H	4.194582000	3.507309000	-2.736496000
H	6.335014000	3.015008000	-1.586064000
H	6.536998000	3.397588000	0.873077000
H	4.612502000	4.293139000	2.148124000
C	3.302158000	4.404027000	0.449787000
C	3.174198000	4.175265000	-0.950413000
C	1.946911000	4.467423000	-1.609831000
C	2.168120000	5.037461000	1.228090000
H	2.494958000	6.038038000	1.556423000
C	0.796544000	4.942267000	-0.918865000
C	0.859298000	5.191033000	0.482366000
C	-0.282735000	5.638058000	1.147173000
C	-1.479853000	5.863867000	0.460903000
C	-1.544823000	5.638004000	-0.923406000
C	-0.425516000	5.178331000	-1.601314000
H	-0.231037000	5.840338000	2.215050000
H	-2.346303000	6.244836000	0.994316000
H	-2.461707000	5.849260000	-1.467650000
H	-0.463322000	5.014181000	-2.675553000
H	1.880227000	4.303820000	-2.682409000
H	2.001392000	4.482180000	2.162238000

4-^{1}Int$_{(t,t)}$

Ni	-3.326904000	-1.431810000	-0.062660000
N	-5.355574000	-0.854360000	-0.438424000
N	-3.741554000	-0.557545000	1.982179000
N	-3.374749000	-3.288592000	1.030741000
C	-6.017059000	-0.645651000	0.875111000
H	-6.318480000	-1.620045000	1.262761000
H	-6.937406000	-0.054622000	0.758962000
C	-5.089904000	0.069936000	1.858399000
H	-4.937394000	1.100838000	1.529685000
H	-5.582433000	0.122716000	2.840774000
C	-3.724321000	-1.716180000	2.924976000
H	-4.376609000	-1.520017000	3.788323000
H	-2.707331000	-1.794717000	3.315959000
C	-4.117646000	-3.051857000	2.291500000
H	-3.926975000	-3.856536000	3.017668000
H	-5.185541000	-3.081047000	2.067690000
C	-5.362310000	0.409790000	-1.222904000
H	-4.798163000	0.281912000	-2.147032000
H	-6.394298000	0.702338000	-1.464665000
C	-2.793299000	0.464266000	2.496676000
H	-3.074696000	0.786408000	3.509875000
H	-2.792439000	1.335758000	1.840746000
H	-1.785703000	0.044896000	2.523347000
C	-1.967178000	-3.670297000	1.318704000
N	-3.685406000	-2.810696000	-1.830575000
C	-5.990925000	-1.948445000	-1.215382000
H	-6.264231000	-2.744217000	-0.520288000
H	-6.925412000	-1.604449000	-1.683215000
C	-5.058271000	-2.472091000	-2.309106000
H	-4.948650000	-1.706162000	-3.080391000
H	-5.524608000	-3.341197000	-2.795503000

C	-3.583869000	-4.192626000	-1.277840000
H	-4.160862000	-4.899521000	-1.892133000
H	-2.536341000	-4.492411000	-1.358897000
C	-4.029136000	-4.312822000	0.180027000
H	-3.799307000	-5.327063000	0.539046000
H	-5.109946000	-4.188493000	0.267120000
H	-4.888957000	1.213007000	-0.658011000
C	-2.748557000	-2.698156000	-2.978208000
H	-3.012618000	-3.401980000	-3.780428000
H	-2.775103000	-1.682000000	-3.375975000
H	-1.731577000	-2.914050000	-2.643650000
H	-1.932257000	-4.602740000	1.900787000
H	-1.410855000	-3.805679000	0.390774000
H	-1.463687000	-2.878325000	1.873463000
Te	-1.216888000	-0.180796000	-0.975908000
Te	1.606396000	-1.547312000	0.541356000
Ni	3.979977000	-0.618970000	0.013343000
N	5.024533000	1.006279000	0.988939000
N	3.793281000	0.894718000	-1.634071000
N	5.410979000	-1.517294000	-1.346775000
C	5.511268000	1.920848000	-0.071180000
H	6.415472000	1.485328000	-0.500576000
H	5.801199000	2.895084000	0.351099000
C	4.446130000	2.147525000	-1.147512000
H	3.659128000	2.790293000	-0.746875000
H	4.896808000	2.698682000	-1.985613000
C	4.502064000	0.284508000	-2.792405000
H	4.788246000	1.056164000	-3.522599000
H	3.786952000	-0.372817000	-3.293549000
C	5.739130000	-0.518797000	-2.395725000
H	6.152574000	-1.009482000	-3.289033000
H	6.520396000	0.139520000	-2.012225000
C	4.048323000	1.700320000	1.868879000

H	3.641063000	1.000538000	2.599096000
H	3.212923000	2.083763000	1.282763000
C	2.403464000	1.213346000	-2.047229000
H	2.391542000	1.939845000	-2.872659000
H	1.859028000	1.629724000	-1.199292000
H	1.896932000	0.299635000	-2.358997000
C	4.770285000	-2.709765000	-1.960049000
H	5.471428000	-3.216337000	-2.639130000
H	3.880525000	-2.410330000	-2.514308000
H	4.446993000	-3.405719000	-1.186118000
N	5.163075000	-1.870769000	1.541075000
C	6.136396000	0.448357000	1.798793000
H	6.997769000	0.295860000	1.146012000
H	6.454151000	1.164104000	2.571264000
C	5.729065000	-0.859049000	2.475178000
H	4.959682000	-0.652921000	3.223492000
H	6.595075000	-1.270313000	3.015681000
C	6.208854000	-2.592080000	0.757918000
H	7.113079000	-2.744004000	1.365486000
H	5.816024000	-3.587090000	0.538171000
C	6.601957000	-1.913632000	-0.557922000
H	7.240783000	-2.604103000	-1.129606000
H	7.197339000	-1.017328000	-0.375752000
H	4.532990000	2.536442000	2.394093000
C	4.411424000	-2.868955000	2.345834000
H	5.076706000	-3.398126000	3.043656000
H	3.626718000	-2.365546000	2.913172000
H	3.938931000	-3.595104000	1.682041000
C	-3.885126000	4.133790000	1.633788000
C	-5.131579000	4.132894000	1.021866000
C	-5.225855000	4.271521000	-0.371526000
C	-4.061952000	4.407645000	-1.135324000
H	-3.808112000	4.065660000	2.716618000

H	-6.033017000	4.061658000	1.624964000
H	-6.198532000	4.304078000	-0.854092000
H	-4.140808000	4.534184000	-2.213173000
C	-2.799785000	4.409733000	-0.540903000
C	-2.694958000	4.276122000	0.873043000
C	-1.416075000	4.331445000	1.501966000
C	-1.552806000	4.534725000	-1.392010000
H	-1.122522000	1.018731000	0.167281000
H	-1.697192000	5.326149000	-2.140174000
C	-0.222088000	4.628283000	0.781092000
C	-0.264610000	4.782430000	-0.634187000
C	0.895599000	5.148627000	-1.315898000
C	2.100733000	5.359924000	-0.637820000
C	2.154238000	5.193935000	0.754710000
C	1.011107000	4.829812000	1.452459000
H	0.854430000	5.293218000	-2.393597000
H	2.981177000	5.684335000	-1.185821000
H	3.079188000	5.386629000	1.292263000
H	1.038682000	4.732332000	2.535153000
H	-1.361944000	4.241435000	2.584285000
H	-1.438844000	3.608237000	-1.981007000

3-^{5}TS2$_{(t,t)}$

Ni	0.012461000	-1.716109000	-0.696894000
N	1.233484000	-3.403731000	0.197873000
N	1.191422000	-2.321726000	-2.529423000
N	-1.608143000	-2.905633000	-1.861516000
C	1.949313000	-4.090817000	-0.907945000
H	1.313942000	-4.879222000	-1.313363000
H	2.855259000	-4.588529000	-0.534392000
C	2.344503000	-3.093775000	-1.991606000
H	3.050118000	-2.368053000	-1.580010000
H	2.861919000	-3.623828000	-2.805875000

C	0.317620000	-3.148110000	-3.415407000
H	0.916517000	-3.897138000	-3.953690000
H	-0.095751000	-2.481633000	-4.175968000
C	-0.837266000	-3.850307000	-2.697999000
H	-1.479912000	-4.322754000	-3.457807000
H	-0.473536000	-4.655336000	-2.060093000
C	2.227578000	-2.911228000	1.181060000
H	1.763361000	-2.244246000	1.905755000
H	2.688711000	-3.761164000	1.705468000
C	1.732631000	-1.190474000	-3.315987000
H	2.342874000	-1.546552000	-4.159268000
H	2.340425000	-0.566421000	-2.660460000
H	0.904473000	-0.594673000	-3.703095000
C	-2.475649000	-2.075238000	-2.732931000
N	-1.349498000	-2.330530000	1.017957000
C	0.264897000	-4.285643000	0.883291000
H	-0.260916000	-4.870917000	0.129883000
H	0.781653000	-5.007164000	1.535566000
C	-0.709250000	-3.472636000	1.735867000
H	-0.167523000	-3.058886000	2.589333000
H	-1.477004000	-4.142285000	2.149411000
C	-2.637494000	-2.724720000	0.382675000
H	-3.281879000	-3.246315000	1.105049000
H	-3.157712000	-1.804145000	0.107219000
C	-2.465785000	-3.591588000	-0.858403000
H	-3.460952000	-3.805057000	-1.271030000
H	-2.025199000	-4.556616000	-0.605394000
H	3.002194000	-2.346149000	0.668039000
C	-1.626835000	-1.265343000	2.006776000
H	-2.250000000	-1.639383000	2.832654000
H	-0.682174000	-0.888423000	2.401142000
H	-2.151952000	-0.446369000	1.516350000
H	-3.129901000	-2.720867000	-3.336995000

H	-3.098232000	-1.418565000	-2.125428000
H	-1.880118000	-1.444952000	-3.392532000
Se	-1.017912000	0.672848000	-1.404930000
Se	1.622433000	0.312911000	0.245144000
Ni	0.365561000	2.727385000	-0.382711000
N	-1.247864000	4.295852000	-0.936896000
N	1.171622000	3.432752000	-2.393224000
N	2.055924000	4.074959000	0.311965000
C	-0.753778000	5.034690000	-2.127784000
H	-0.132131000	5.870436000	-1.803944000
H	-1.591100000	5.476755000	-2.686258000
C	0.021037000	4.105248000	-3.055275000
H	-0.644040000	3.314766000	-3.412467000
H	0.362985000	4.669452000	-3.936740000
C	2.304724000	4.372007000	-2.141320000
H	2.351265000	5.138530000	-2.928238000
H	3.228708000	3.794893000	-2.221203000
C	2.266375000	5.057225000	-0.773530000
H	3.209465000	5.607934000	-0.632138000
H	1.466264000	5.794913000	-0.723280000
C	-2.571777000	3.710370000	-1.257101000
H	-2.937745000	3.099760000	-0.432299000
H	-2.497069000	3.072928000	-2.137800000
C	1.647599000	2.351717000	-3.285870000
H	2.042593000	2.756200000	-4.229578000
H	0.816558000	1.681717000	-3.507678000
H	2.426580000	1.782813000	-2.776658000
C	3.306723000	3.317029000	0.541195000
H	4.134473000	4.005975000	0.766915000
H	3.555361000	2.720269000	-0.335640000
H	3.169539000	2.630224000	1.374778000
N	-0.413433000	3.262617000	1.677100000
C	-1.368436000	5.154226000	0.262171000

H	-0.510488000	5.825992000	0.289604000
H	-2.261814000	5.795710000	0.202264000
C	-1.462712000	4.318391000	1.542402000
H	-2.433270000	3.817479000	1.566567000
H	-1.441637000	4.991934000	2.411613000
C	0.787415000	3.749997000	2.407283000
H	0.490867000	4.234194000	3.350471000
H	1.377683000	2.866361000	2.665751000
C	1.641363000	4.710581000	1.588877000
H	2.519785000	5.006399000	2.179921000
H	1.096413000	5.630387000	1.374089000
H	-3.301031000	4.510671000	-1.452348000
C	-0.974484000	2.127721000	2.445286000
H	-1.257020000	2.435843000	3.463026000
H	-1.861261000	1.750597000	1.935036000
H	-0.227784000	1.334872000	2.493336000
C	-6.441310000	-2.722595000	-1.092921000
C	-6.504859000	-4.070125000	-0.766403000
C	-6.432614000	-4.467473000	0.577281000
C	-6.310487000	-3.501476000	1.581250000
H	-6.513401000	-2.407595000	-2.131481000
H	-6.630415000	-4.814008000	-1.548385000
H	-6.495460000	-5.519191000	0.840783000
H	-6.284019000	-3.813490000	2.623517000
C	-6.253477000	-2.140974000	1.275679000
C	-6.308728000	-1.730054000	-0.086945000
C	-6.220028000	-0.345489000	-0.418269000
C	-6.206683000	-1.107941000	2.382721000
H	-6.309201000	-0.050076000	-1.461082000
H	-5.484241000	-1.413420000	3.153182000
C	-5.998947000	0.664672000	0.563821000
C	-5.926092000	0.314396000	1.943205000
C	-5.674256000	1.308378000	2.888685000

C	-5.519291000	2.646886000	2.513680000
C	-5.617400000	3.004342000	1.160392000
C	-5.846061000	2.027801000	0.200040000
H	-5.629716000	1.039383000	3.942114000
H	-5.360503000	3.407768000	3.272599000
H	-5.545457000	4.048409000	0.865967000
H	-5.942406000	2.301978000	-0.848250000
H	-2.340558000	0.699903000	-0.711499000
H	-7.180708000	-1.117483000	2.900044000
C	6.519246000	-2.282018000	-2.143470000
C	6.074392000	-0.970885000	-2.366339000
C	5.521684000	-0.246580000	-1.319929000
C	6.414084000	-2.842636000	-0.871096000
H	6.966220000	-2.852317000	-2.952414000
H	6.179782000	-0.519260000	-3.348616000
H	5.191589000	0.777131000	-1.481999000
H	6.790846000	-3.847846000	-0.694937000
C	5.397324000	-0.805475000	-0.026938000
C	5.861709000	-2.124654000	0.196117000
C	5.818875000	-2.745457000	1.575019000
C	4.809702000	-0.038767000	1.057975000
H	6.830539000	-3.088723000	1.836553000
H	3.209288000	0.055419000	0.663719000
C	4.850663000	-0.540912000	2.418977000
C	5.307223000	-1.854526000	2.685427000
C	5.325295000	-2.315583000	4.006023000
C	4.905239000	-1.505803000	5.059968000
C	4.466870000	-0.198707000	4.804090000
C	4.444044000	0.273597000	3.500604000
H	5.691910000	-3.318462000	4.213426000
H	4.934994000	-1.882089000	6.078132000
H	4.160709000	0.443864000	5.624345000
H	4.121149000	1.292267000	3.297940000

H	4.839240000	1.043366000	0.945574000
H	5.219490000	-3.668963000	1.541789000

Imaginary frequency *i*865.2

3-$^{3}P_{(t,t)}$

Ni	0.024057000	0.235007000	-0.000383000
Se	0.754346000	2.531188000	-0.001609000
H	-0.553758000	3.240463000	-0.003022000
N	-2.241254000	0.245588000	-0.000351000
N	-0.259555000	-1.014781000	-1.729851000
N	2.068188000	-0.716066000	0.000437000
C	-2.890172000	1.582481000	-0.000565000
H	-3.986118000	1.494380000	-0.000411000
H	-2.577406000	2.141056000	0.883230000
C	-2.639261000	-0.475430000	-1.243762000
H	-2.734802000	0.275219000	-2.031559000
H	-3.632570000	-0.933121000	-1.126435000
C	-1.642548000	-1.547674000	-1.691519000
H	-1.658423000	-2.402754000	-1.012894000
H	-1.948078000	-1.924030000	-2.679399000
C	-0.063028000	-0.156271000	-2.927640000
H	-0.172892000	-0.748467000	-3.847580000
H	0.925533000	0.302371000	-2.904515000
H	-0.790113000	0.655949000	-2.931789000
C	0.763964000	-2.086861000	-1.685104000
H	0.878006000	-2.563734000	-2.670241000
H	0.412511000	-2.861682000	-1.000945000
C	2.123203000	-1.539869000	-1.241142000
H	2.827432000	-2.376298000	-1.122092000
H	2.527712000	-0.902663000	-2.030762000
C	3.215071000	0.230816000	-0.001555000
H	4.174316000	-0.306083000	-0.001388000
N	-0.259561000	-1.011600000	1.731494000

H	-2.577667000	2.140676000	-0.884696000
C	-2.639541000	-0.475204000	1.243158000
H	-2.736888000	0.275771000	2.030421000
H	-3.632142000	-0.934231000	1.125121000
C	-1.641957000	-1.545929000	1.692658000
H	-1.656371000	-2.401657000	1.014822000
H	-1.947861000	-1.921661000	2.680671000
C	-0.065183000	-0.150524000	2.927774000
H	-0.176748000	-0.740748000	3.848776000
H	0.923464000	0.307971000	2.905475000
H	-0.792177000	0.661792000	2.928798000
C	0.765097000	-2.082763000	1.690006000
H	0.879447000	-2.556648000	2.676545000
H	0.414692000	-2.860027000	1.008071000
C	2.123819000	-1.535572000	1.244782000
H	2.829140000	-2.371513000	1.128819000
H	2.527162000	-0.895122000	2.032371000
H	3.160273000	0.868329000	-0.885315000
H	3.161446000	0.870703000	0.880704000

References-

1. S. Hikichi, M. Yoshizawa, Y. Sasakura, M. Akita and Y. Moro-oka, *J. Am. Chem. Soc.*, 1998, **120**, 10567-10568.
2. R. Schenker, B. S. Mandimutsira, C. G. Riordan and T. C. Brunold, *J. Am. Chem. Soc.*, 2002, **124**, 13842-13855.
3. M. T. Kieber-Emmons and C. G. Riordan, *Acc. Chem. Res.*, 2007, **40**, 618-625.
4. J. Cho, K. M. Van Heuvelen, G. P. Yap, T. C. Brunold and C. G. Riordan, *Inorg. Chem.*, 2008, **47**, 3931-3933.
5. S. A. Yao, V. Martin-Diaconescu, I. Infante, K. M. Lancaster, A. W. Götz, S. DeBeer and J. F. Berry, *J. Am. Chem. Soc.*, 2015, **137**, 4993-5011.
6. C. Mealli and S. Midollini, *Inorg. Chem.*, 1983, **22**, 2785-2786.
7. J. Wallick, C. G. Riordan and G. P. Yap, *J. Am. Chem. Soc.*, 2013, **135**, 14972-14974.
8. S. Yao, Y. Xiong, X. Zhang, M. Schlangen, H. Schwarz, C. Milsmann and M. Driess, *Angew. Chem.*, 2009, **121**, 4621-4624.
9. M. Di Vaira, M. Peruzzini and P. Stoppioni, *J. Chem. Soc., Chem. Commun.*, 1986, 374-375.
10. R. J. Pleus, H. Waden, W. Saak, D. Haase and S. Pohl, *J. Chem. Soc., Dalton Trans.*, 1999, 2601-2610.
11. C. Casewit, D. Coons, L. Wright, W. Miller and M. R. DuBois, *Organometallics*, 1986, **5**, 951-955.
12. L. Fohlmeister, K. R. Vignesh, F. Winter, B. Moubaraki, G. Rajaraman, R. Pöttgen, K. S. Murray and C. Jones, *Dalton Trans.*, 2015, **44**, 1700-1708.
13. V. M. Iluc, C. A. Laskowski, C. K. Brozek, N. D. Harrold and G. L. Hillhouse, *Inorg. Chem.*, 2010, **49**, 6817-6819.
14. S. Yao, C. Milsmann, E. Bill, K. Wieghardt and M. Driess, *J. Am. Chem. Soc.*, 2008, **130**, 13536-13537.
15. M. Inosako, A. Kunishita, M. Kubo, T. Ogura, H. Sugimoto and S. Itoh, *Dalton Trans.*, 2009, 9410-9417.
16. F. Olechnowicz, G. L. Hillhouse and R. F. Jordan, *Inorg. Chem.*, 2015, **54**, 2705-2712.
17. M. T. Kieber-Emmons, J. Annaraj, M. S. Seo, K. M. Van Heuvelen, T. Tosha, T. Kitagawa, T. C. Brunold, W. Nam and C. G. Riordan, *J. Am. Chem. Soc.*, 2006, **128**, 14230-14231.