Supplementary Information

for

Modelling the Binding of Cytotoxic Dinuclear Nickel Complexes to two Neighboring Phosphate Esters of DNA Using Dicarboxylate Ligands

Thomas Riediger,[a] Maximilian Böhm,[a] Michael Kapiza,[a] Anja Stammler,[a] Jan Oldengott,[a], and Thorsten Glaser*[,a]

[a] *Lehrstuhl für Anorganische Chemie I, Fakultät für Chemie, Universität Bielefeld, Universitätsstr. 25, D-33615 Bielefeld, Germany*

* *To whom correspondence should be addressed. E-mail: thorsten.glaser@uni-bielefeld.de (T.G.)*

Table S1. Crystal data and refinement parameters.

	[(Htom$^{6\text{-Me}}$){Ni^{II}(μ-succ)Ni^{II}}]-(BPh$_4$)•2CH$_3$CN	[(Htom$^{6\text{-Me}}$){Ni^{II}(μ-glut)Ni^{II}}]-(BPh$_4$)•2CH$_3$CN
Empoirical formula	$C_{72}H_{71}BN_8Ni_2O_6$	$C_{73}H_{73}BN_8Ni_2O_6$
Formula weight	1272.59	1286.62
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a [Å]	18.6047(11)	18.6053(8)
b [Å]	24.1873(15)	24.5063(10)
c [Å]	14.9384(9)	14.9770(7)
α [°]	90	90
β [°]	113.012(2)	112.945(2)
γ [°]	90	90
V [Å^3]	6187.3(7)	6288.4(5)
Z	4	4
ρ [g cm^{-3}]	1.366	1.359
μ [mm^{-1}]	0.670	0.660
F(000)	2672.0	2704.0
Crystal size [mm^3]	0.37 × 0.19 × 0.03	0.42 × 0.28 × 0.23
Radiation	MoKα (λ = 0.71073 Å)	MoKα (λ = 0.71073 Å)
2Θ range [°]	2.91 to 60.39	3.32 to 66.69
	$-26 \le h \le 26$	$-28 \le h \le 28$
hkl ranges	$-34 \le k \le 34$	$-37 \le k \le 37$
	$-21 \le l \le 21$	$-23 \le l \le 23$
Collected refl.	231626	311779
Unique refl., R_{int}	18191, 0.0469	24173, 0.0427
Observed refl.($I > 2\sigma(I)$)	14261	19402
Completeness	0.990	0.992
Data/restraints/param.	18191/0/812	24173/0/821
Goodness-of-fit on F^2	1.008	1.052
R_1, wR_2 ($I > 2\sigma(I)$)	0.0335, 0.0794	0.0410, 0.0999
R_1, wR_2 (all data)	0.0508, 0.0876	0.0571, 0.1102
Largest peak/hole [e Å^{-3}]	0.48/-0.34	1.97/-0.71
CCDC numbers	2445426	2445427

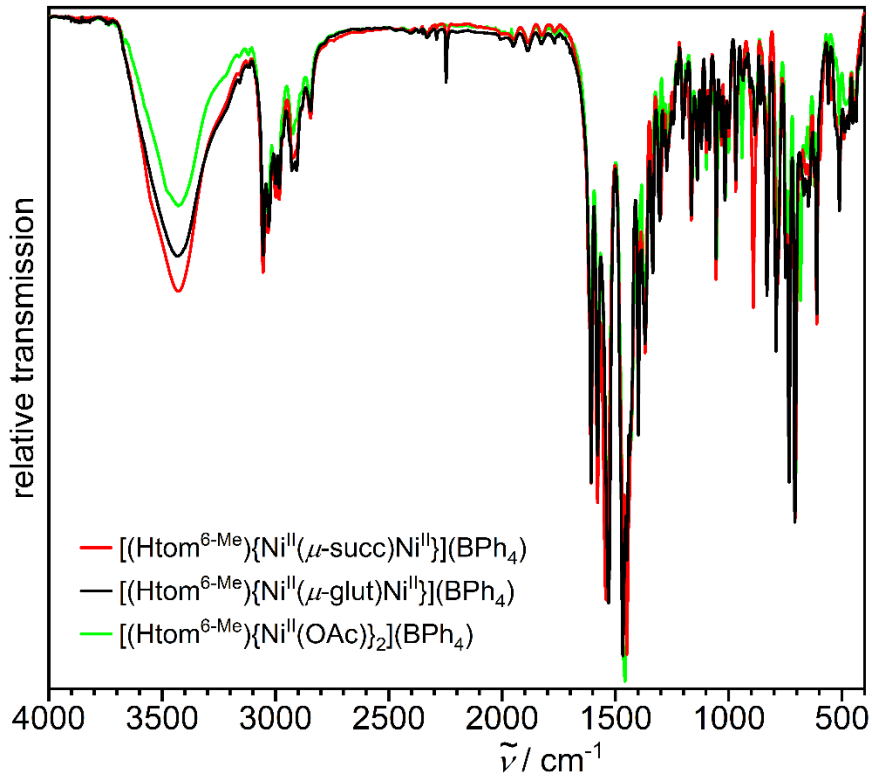

Figure S1. FTIR spectra of [(Htom$^{6\text{-Me}}$){Ni^{II}(μ-succ)Ni^{II}}](BPh$_4$), [(Htom$^{6\text{-Me}}$){Ni^{II}(μ-glut)Ni^{II}}](BPh$_4$), and [(Htom$^{6\text{-Me}}$){Ni^{II}(OAc)}$_2$](BPh$_4$) for comparison.

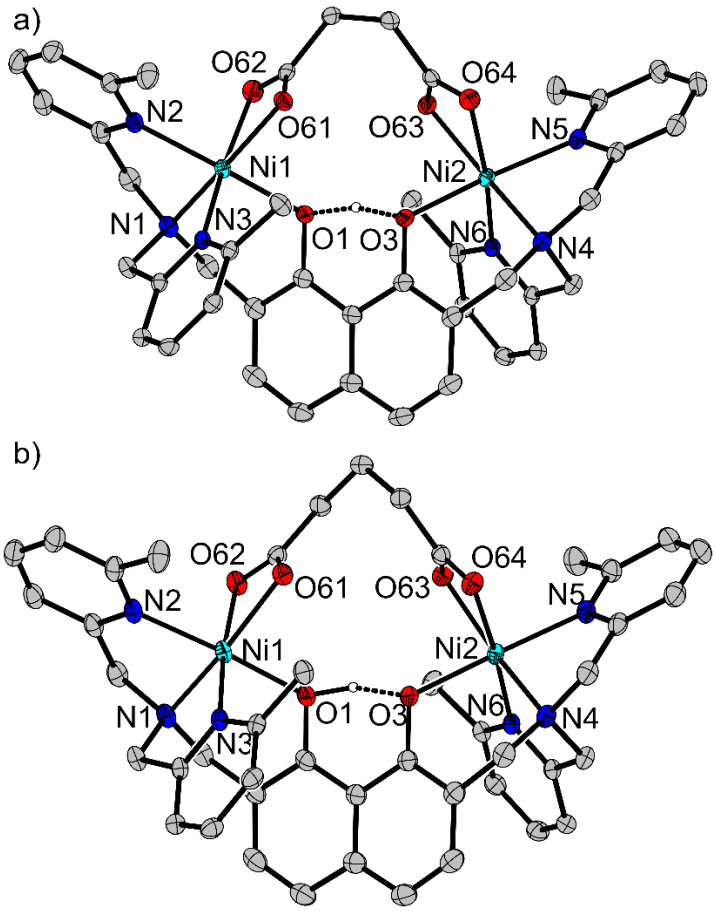

Figure S2. Theremal ellipsoid plots of a) $[(Htom^{6\text{-}Me})\{Ni^{II}(\mu\text{-succ})Ni^{II}\}]^{+}$ in single-crystals of $[(Htom^{6\text{-}Me})\{Ni^{II}(\mu\text{-succ})Ni^{II}\}](BPh_4)_2 \bullet 2CH_3CN$ and b) $[(Htom^{6\text{-}Me})\{Ni^{II}(\mu\text{-glut})Ni^{II}\}]^{+}$ in single-crystals of $[(Htom^{6\text{-}Me})\{Ni^{II}(\mu\text{-glut})Ni^{II}\}](BPh_4)_2 \bullet 2CH_3CN$ at the 50% probability level. Hydrogen atoms except those coordinated at oxygen atoms omitted for clarity.