Electronic Supporting Information

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Synthesis, structures, electrochemical and quantum chemical investigations of Ni(II) and Cu(II) complexes with a tetradentate Schiff base derived from 1-(2-thienyl)-1,3-butanedione

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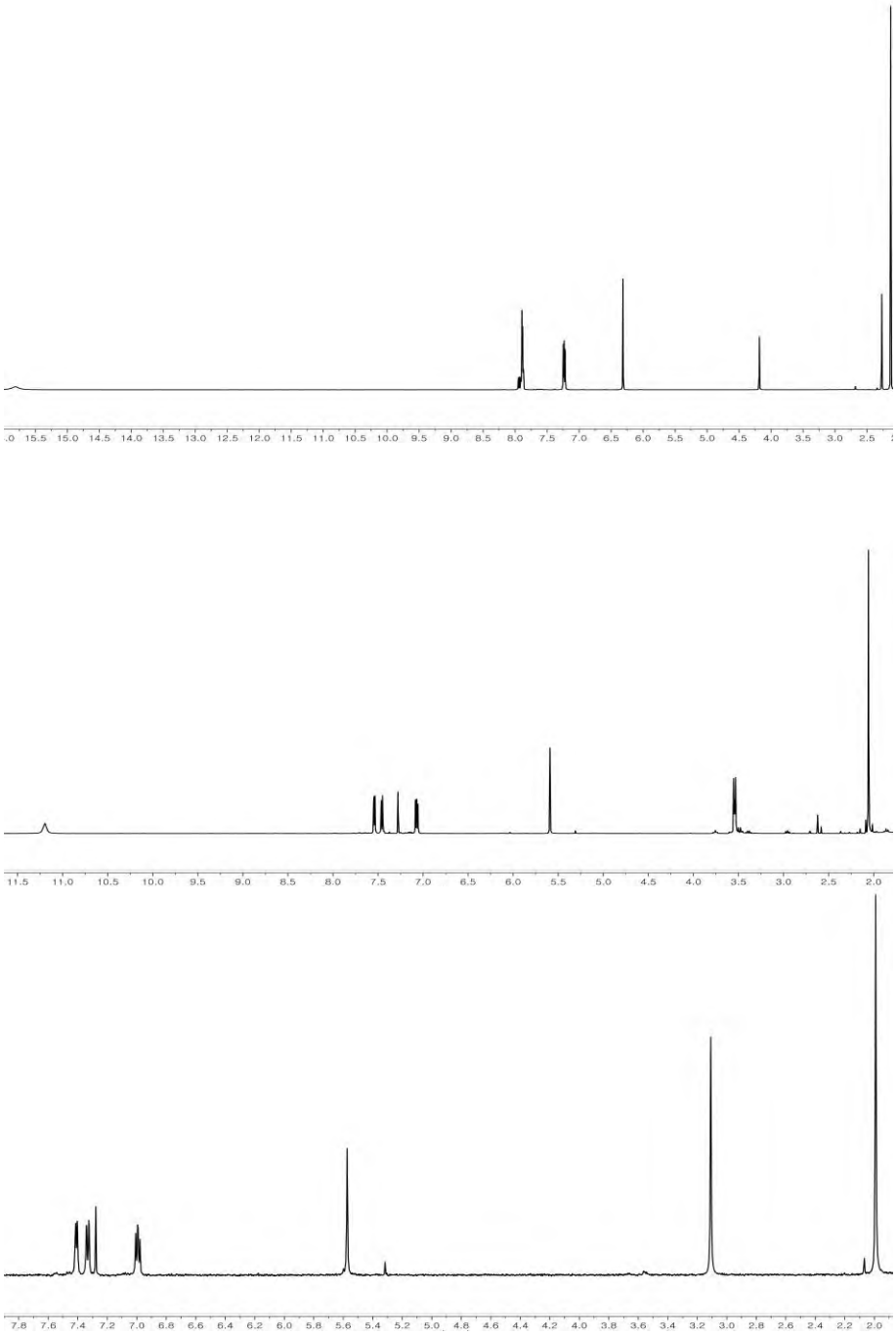


Fig. S1 ^{1}H NMR spectra recorded at 298 K of the β-diketone **1** (top, in $(CD_3)_2CO$), the free Schiff base **2** (middle, in $CDCl_3$), and of the Ni(II) complex **3** (bottom, in $CDCl_3$).

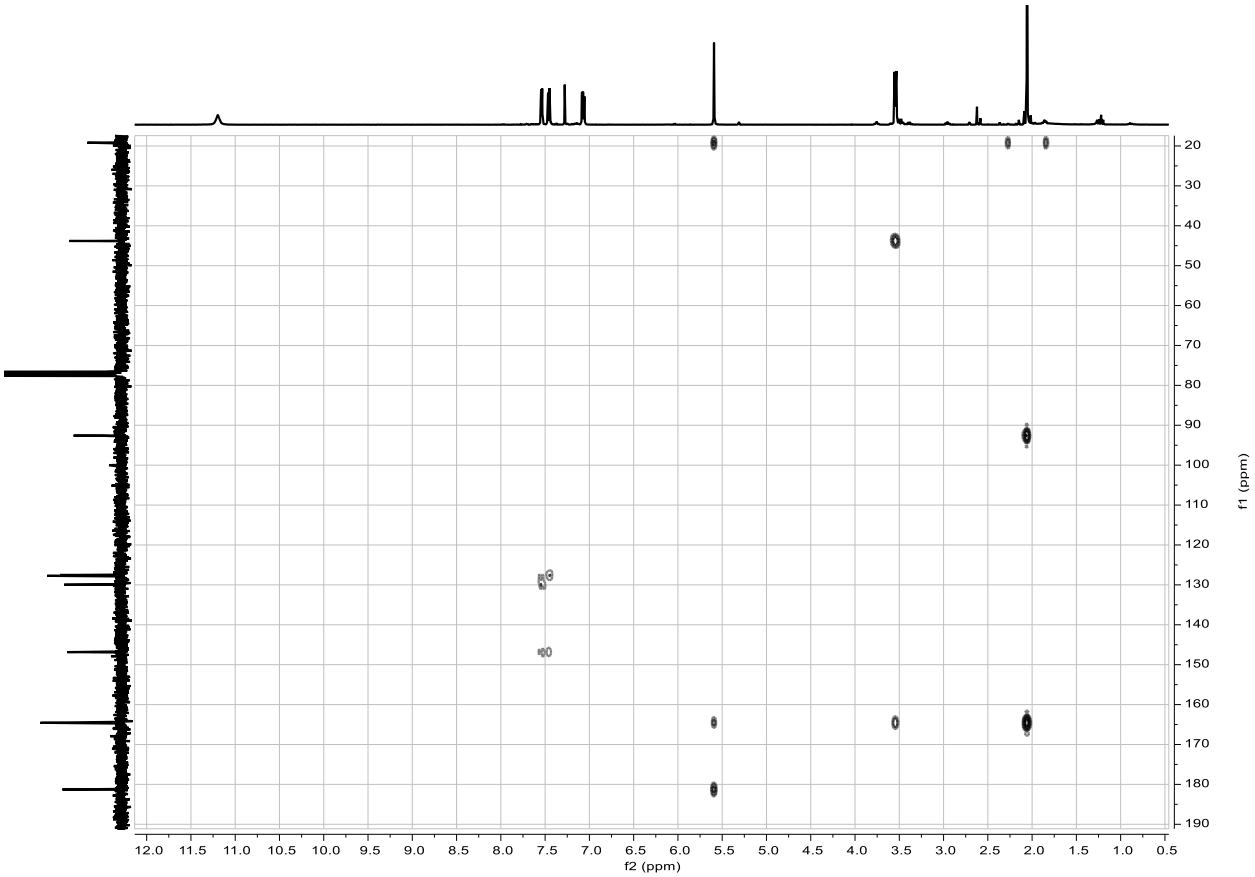
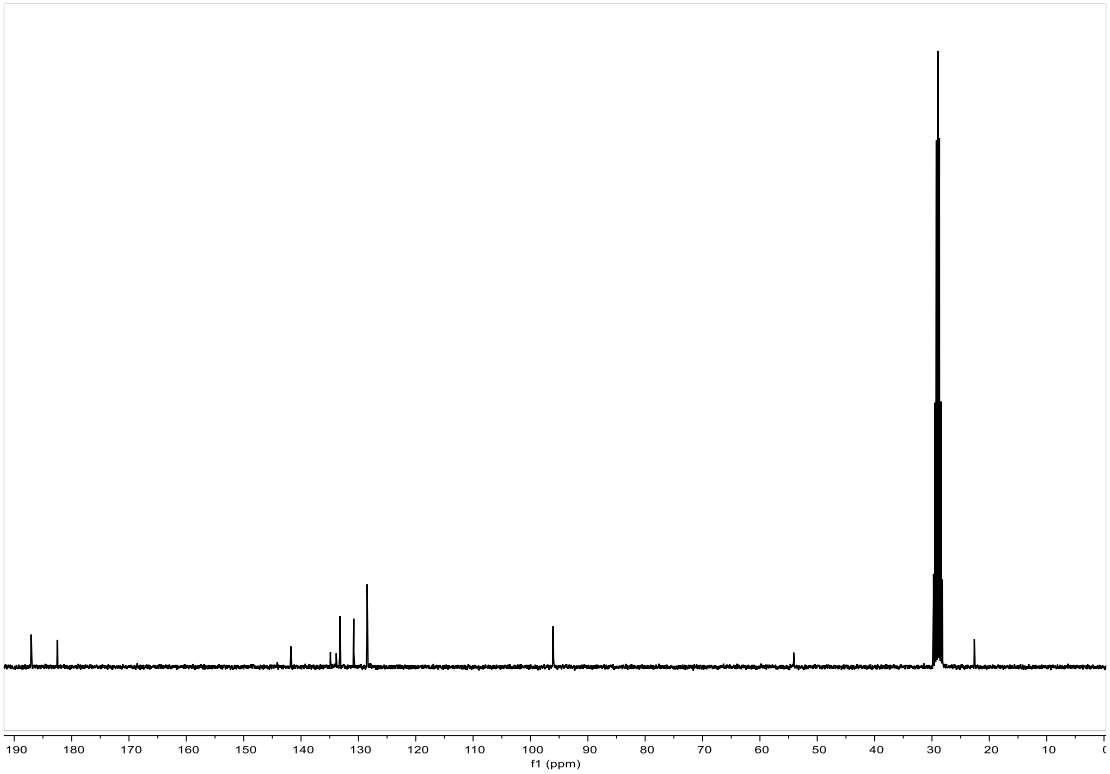


Fig. S2 HMBC ^{1}H-^{13}C spectra of the free Schiff base **2**.



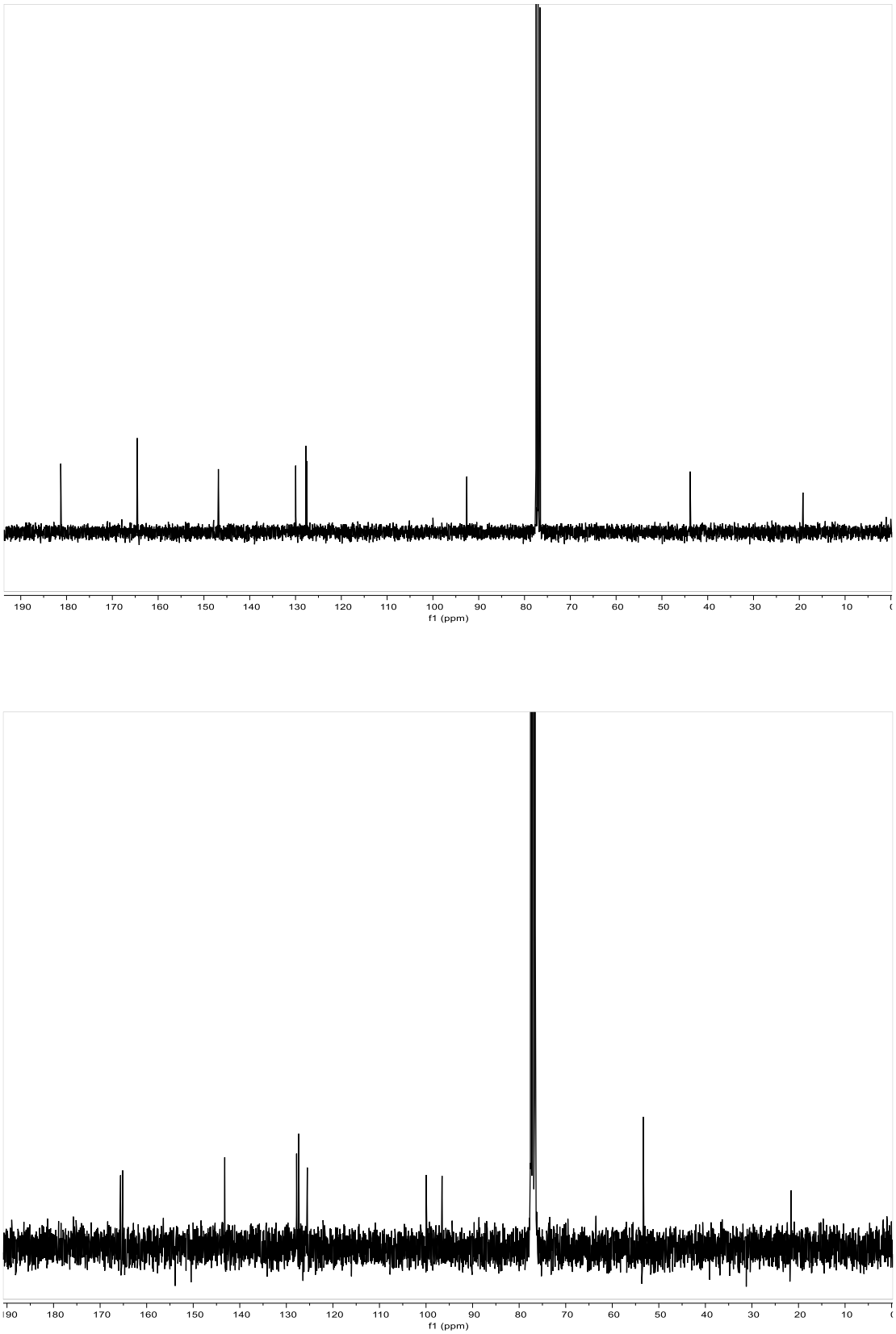


Fig. S3 $^{13}C\{^{1}H\}$ NMR spectra recorded at 298 K of the β-diketone **1** (top, in $(CD_3)_2CO$), the free Schiff base **2** (middle, in $CDCl_3$), and of the Ni(II) complex **3** (bottom, in $CDCl_3$).

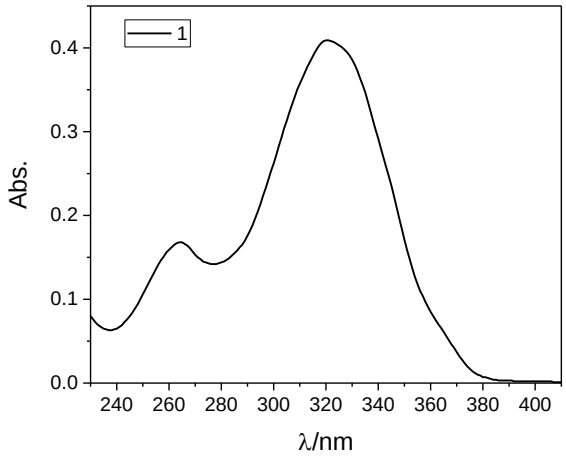


Fig. S4 UV spectrum of 2-thenoylacetone **1** measured in CH_2Cl_2 (10^{-6} M) solution at 20 °C.

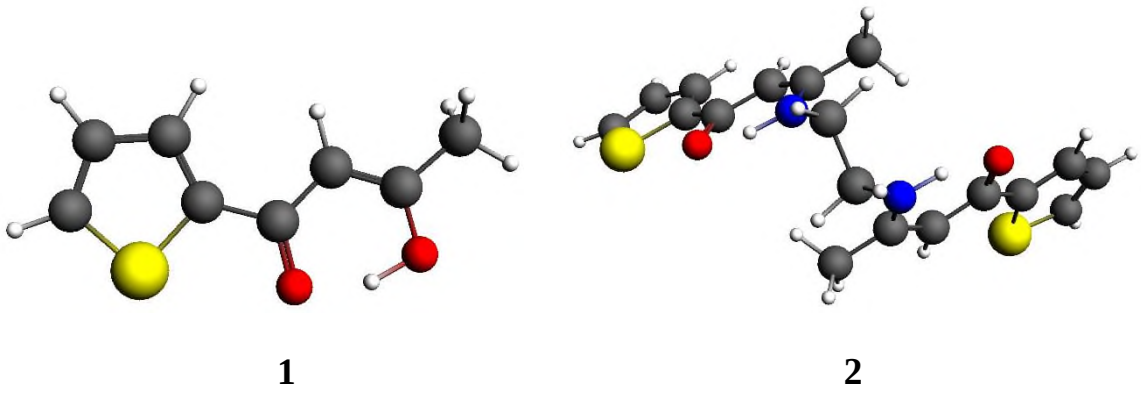


Fig. S5 Optimized geometries of the 1-(2-thienyl)-1,3-butanedione **1** (left) and of the free Schiff base **2** (right).

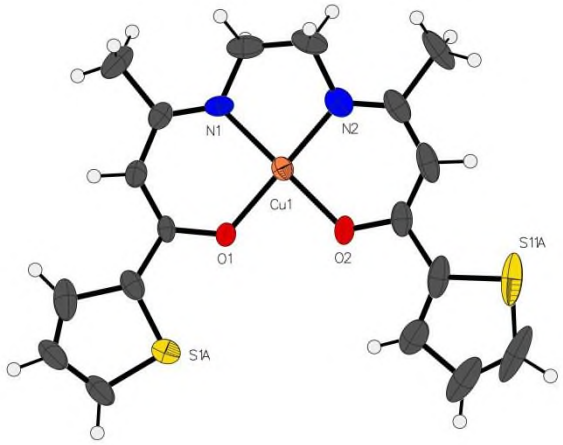


Fig. S6 Molecular structures of the Cu(II) complex **4** with a selected atom numbering scheme. Thermal ellipsoids are drawn at the 50% probability level.

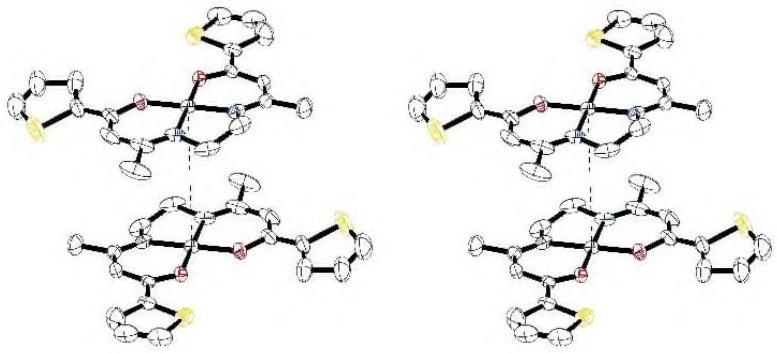


Fig. S7 Arrangement of molecules of **3** (left) and **4** (right) in the packing.

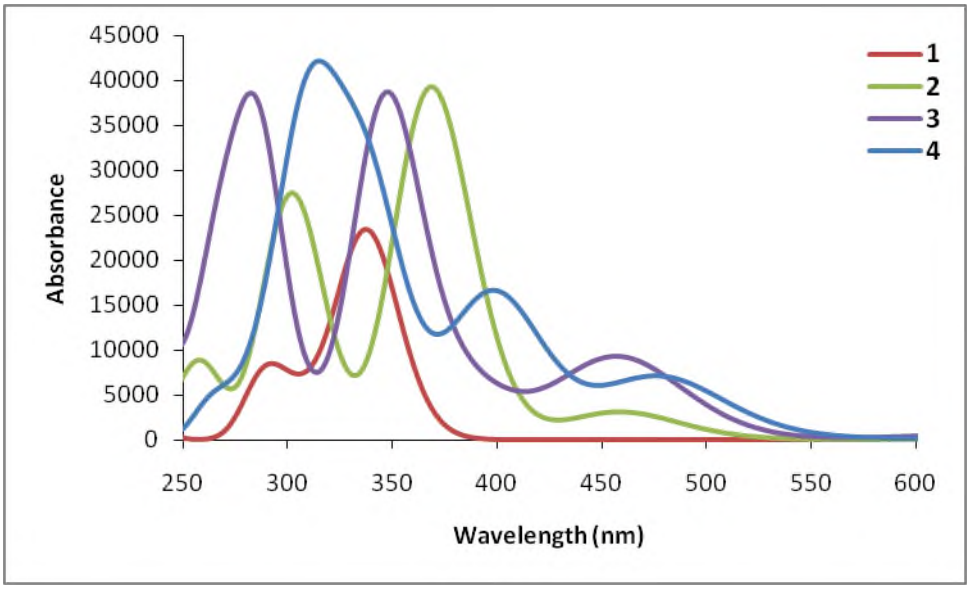


Fig. S8 TD-DFT simulated spectra of compounds **1**-**4** with Gaussian half-height bandwidths of 3000 cm^{-1}.

Table S1. Selected X-ray and corresponding DFT-optimized (in square brackets) bond distances (Å) and angles (°) *for the Schiff base ligands in* compound **3** and **4**.[a]
[A] M = Ni, **3**; Cu, **4**.

	3	**4**
Bond distances		
O(1)-C(6)	1.288(4) [1.291]	1.311(9) [1.288]
N(1)-C(8)	1.306(6) [1.326]	1.309(12) [1.321]
N(1)-C(10)	1.469(6) [1.461]	1.436(13) [1.455]
C(6)-C(7)	1.368(6) [1.397]	1.377(12) [1.402]
C(7)-C(8)	1.396(7) [1.406]	1.381(13) [1.411]
O(2)-C(16)	1.292(5) [1.288]	1.286(11) [1.285]
N(2)-C(18)	1.308(7) [1.326]	1.285(14) [1.321]
N(2)-C(20)	1.464(7) [1.461]	1.479(14) [1.455]
C(16)-C(17)	1.369(8) [1.398]	1.360(16) [1.403]
C(17)-C(18)	1.417(9) [1.406]	1.405(18) [1.411]
C(10)-C(20)	1.480(9) [1.516]	1.504(16) [1.529]
Bond angles		
M(1)-O(1)-C(6)	126.20(3) [126]	125.40(5) [125]
M(1)-O(2)-C(16)	126.60(3) [126]	124.30(7) [125]
M(1)-N(1)-C(8)	126.80(3) [127]	125.90(7) [126]
M(1)-N(2)-C(18)	126.10(4) [126]	126.60(9) [126]
M(1)-N(1)-C(10)	112.40(4) [112]	110.70(7) [111]
M(1)-N(2)-C(20)	113.20(4) [112]	113.70(7) [111]
O(1)-C(6)-C(7)	124.70(4) [125]	123.00(8) [126]
N(1)-C(8)-C(7)	122.20(4) [123]	122.00(9) [123]
O(2)-C(16)-C(17)	124.20(5) [125]	125.80(11) [126]
N(2)-C(18)-C(17)	123.10(4) [123]	122.50(11) [123]
C(6)-C(7)-C(8)	124.90(4) [125]	128.40(9) [126]
C(16)-C(17)-C(18)	124.60(5) [124]	126.40(11)[126]