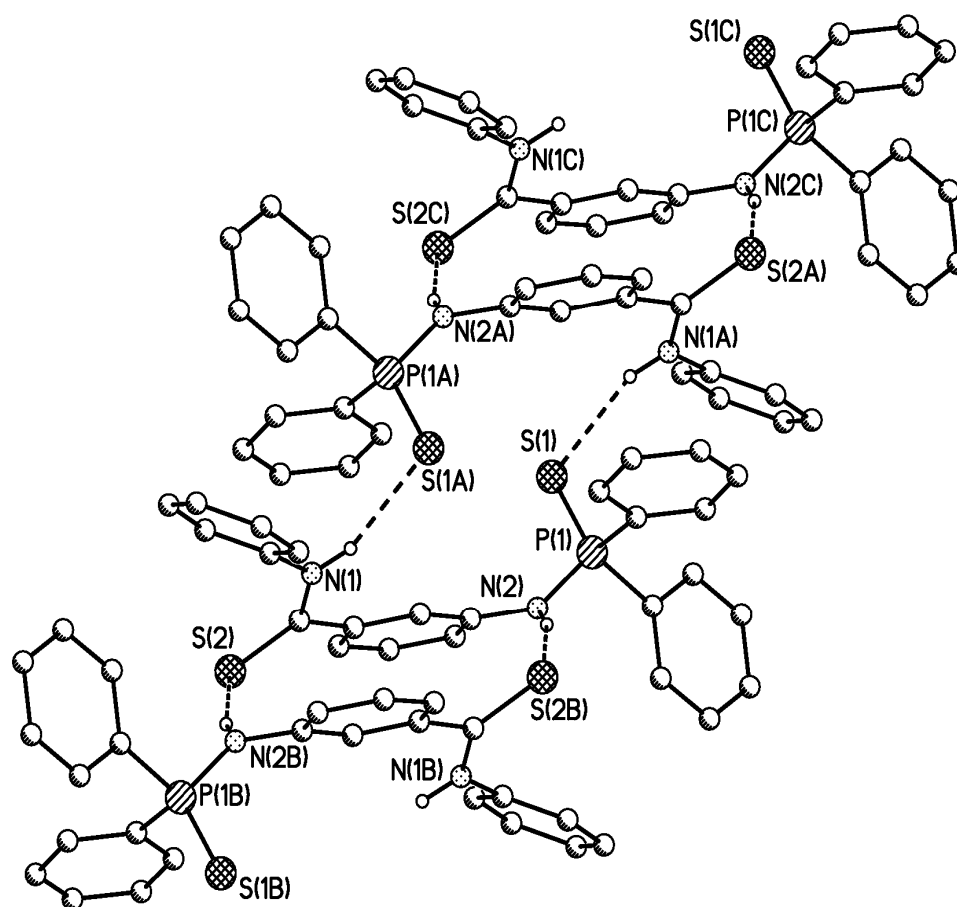
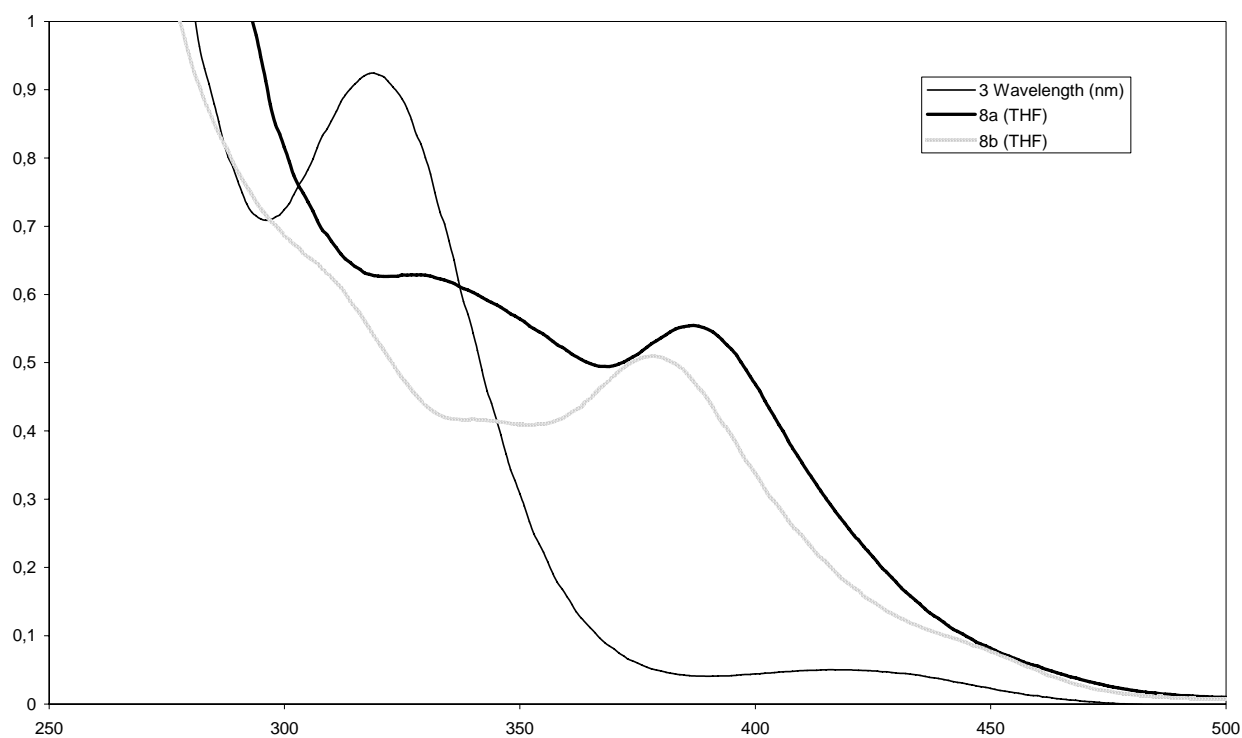


**Supplementary data for**  
**Synthesis, catalytic activity, and photophysical properties of 5,6-membered**  
**palladium and platinum SCS'-pincer complexes based on thiophosphorylated 3-**  
**amino(hydroxy)-benzoic acid thioanilides**

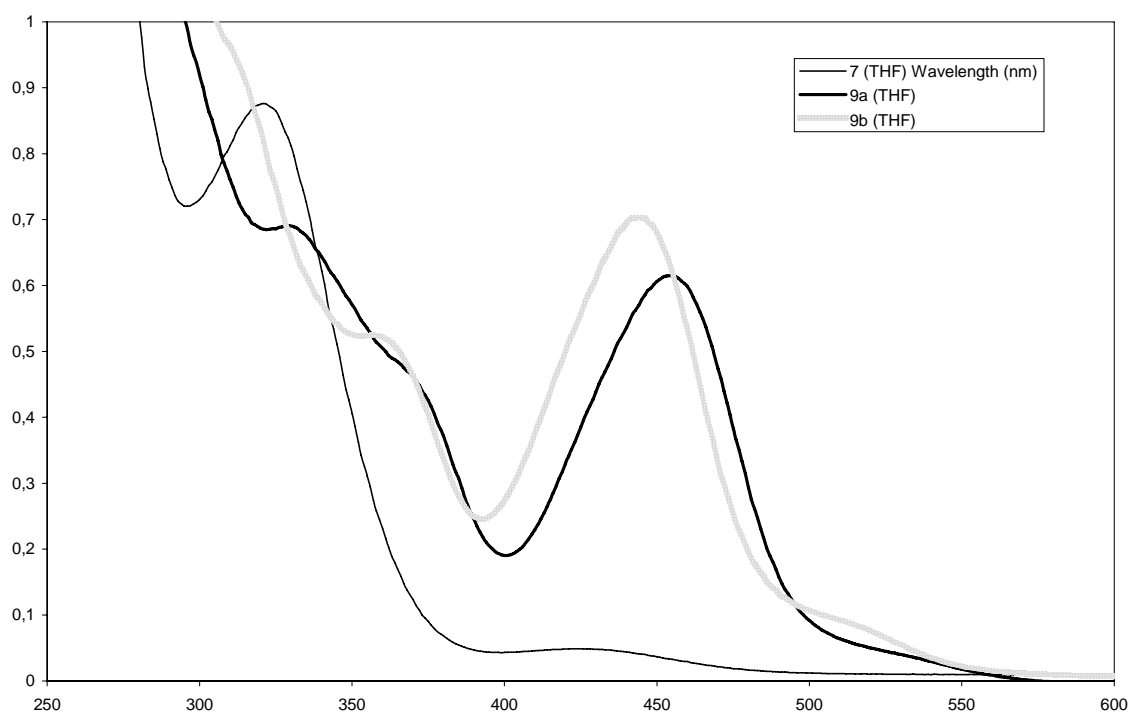
*Diana V. Aleksanyan, Vladimir A. Kozlov, Yulia V. Nelyubina, Konstantin A. Lyssenko,  
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Irina L. Odinet*



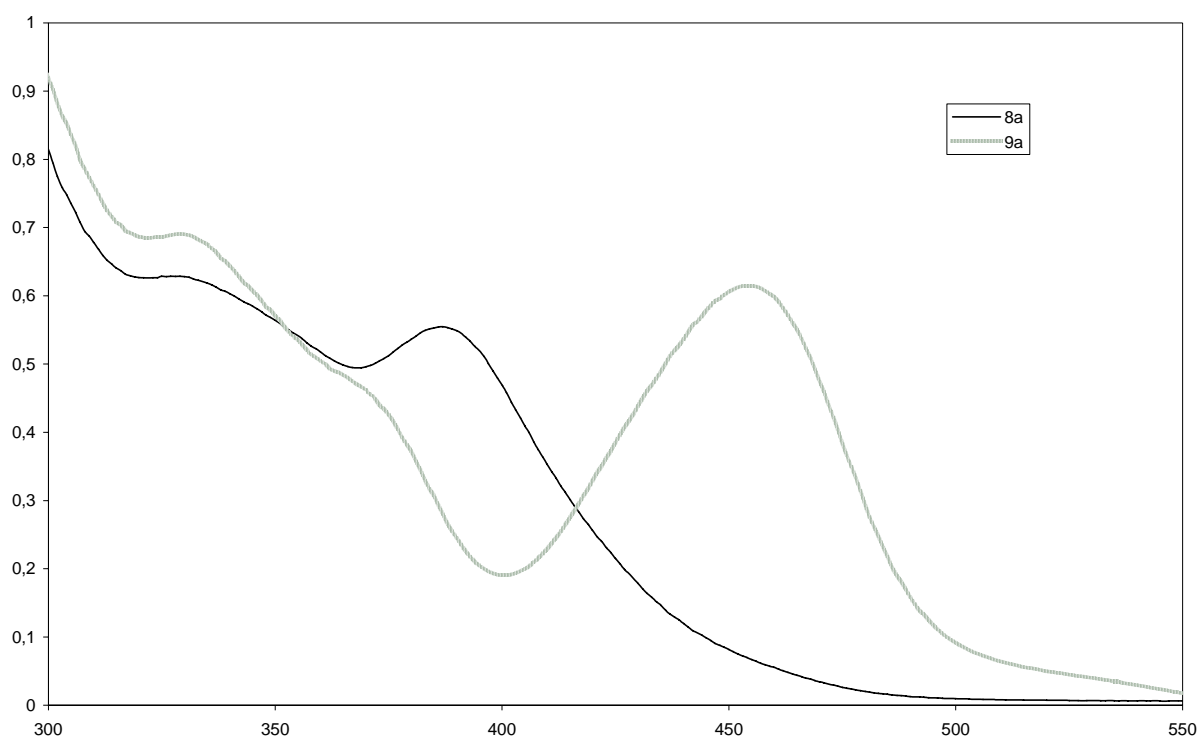
**Fig.S1.** Fragment of the infinite N-H...S-bonded tape in the crystal of **3**.



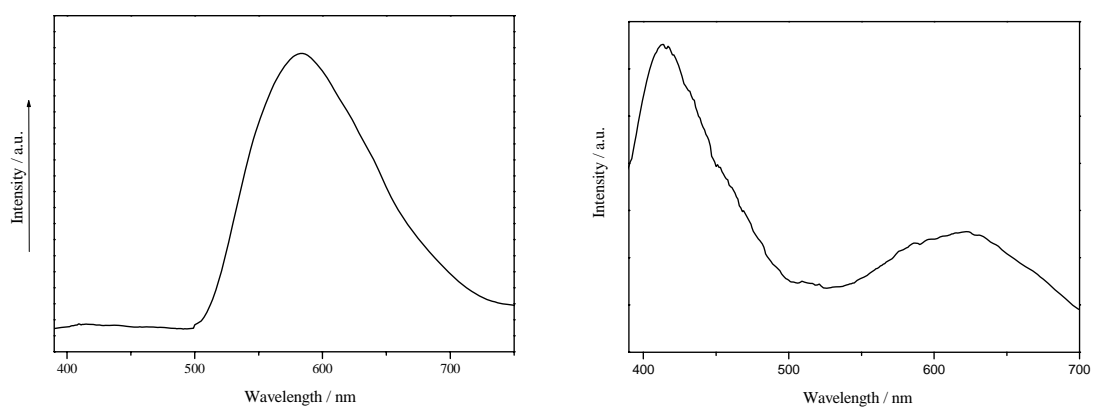
**Fig.S2.** The absorption spectra of the NH-bridged ligand **3** and its palladium and platinum pincer complexes **8a,8b** in THF at 293 K



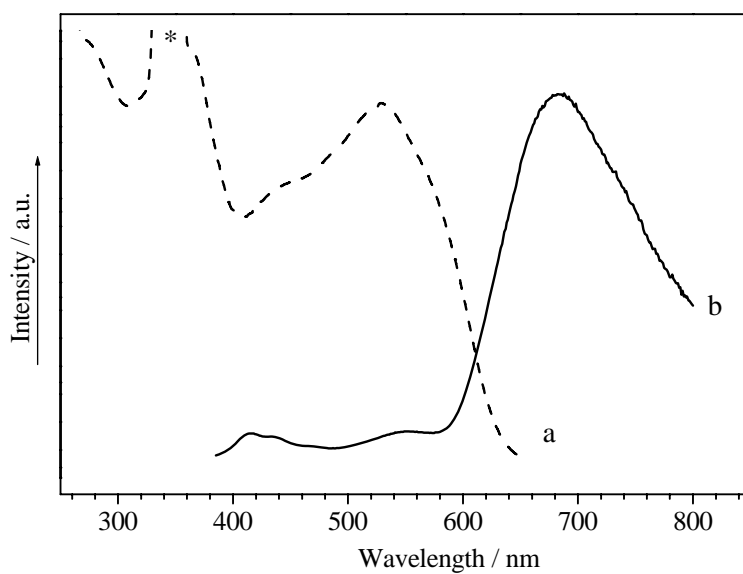
**Fig.S3.** The absorption spectra of the O-bridged ligand **7** and its palladium and platinum pincer complexes **9a,9b** in THF at 293 K



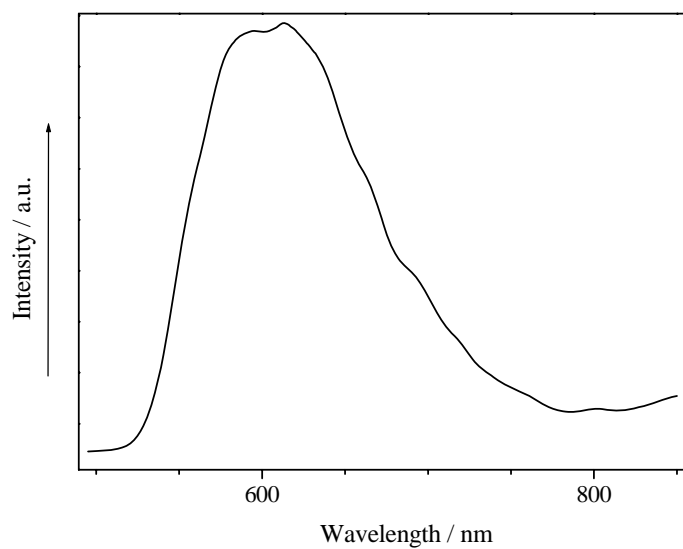
**Fig.S4.** The absorption spectra of the palladium pincer complexes **8a** and **9a** in THF at 293 K



**Fig. S5.** Emission spectra of **3** (left) and **7** (right) at 77K.



**Fig. S6.** Excitation (dash line) and luminescence (solid line) spectra of platinum complex **9b** at 77K.



**Fig. S6.** Luminescence spectra of palladium complex **9a** at 77 K

## Results of DFT calculations

The DFT calculations were carried out at the B3LYP level using a 6-311G\*\* basis set. As convergence criteria, the extremely tight threshold limits of  $2 \cdot 10^{-6}$  and  $6 \cdot 10^{-6}$  au were applied for the maximum force and displacement, respectively. To enhance the accuracy in the DFT calculation the pruned (99,590) grid (keyword Grid=Ultrafine) has been used.

All data (geometry, frequency analysis and etc) are summarized below in the archive

```
1\1\GINC-PLANEWAVE\Freq\RB3LYP\6-311G(d,p)\C25H21N2P1S2\KOSTYA\15-Jul-2010\0\#\#P B3LYP/6-311G** geom=allcheck #freq SCF=tight\odin_lada B3LYP\0,1\P,0.3073884837,0.4609839716,0.2519113065\S,-0.4572282539,1.7096520729,1.5627606932\S,-1.0594035397,-6.6470677656,3.3293522141\N,0.5255323405,-4.7256018452,4.4073610344\H,0.6486505763,-3.7223050896,4.4493020611\N,0.4880069803,-1.1825925965,0.7204103176\H,1.4362341748,-1.3896294213,1.0062524327\C,-0.9433624721,-3.9710134561,2.7063421189\C,-0.0365322994,-3.0715892756,2.1345769385\H,1.030631214,-3.2288974558,2.2594751643\C,-0.4768478787,-2.0035216105,1.3428110308\C,-1.8516708992,-1.8193925862,1.159527297\H,-2.2209283064,-0.9900302515,0.5720795868\C,-2.7505628417,-2.7122845179,1.7365720392\H,-3.8130277275,-2.5565751826,1.5891281987\C,-2.3136783345,-3.7937804234,2.4906425843\H,-3.0146741282,-4.4953480957,2.9221787036\C,-0.6366535147,0.3705064246,-1.3187970488\C,-1.3054878277,1.5117495774,-1.7751757403\H,-1.2987797754,2.4123880862,-1.1731769503\C,-1.9897376442,1.4807042627,-2.9866784486\H,-2.5053318315,2.3684773321,-3.3345087751\C,-2.021540013,0.3112080914,-3.7440578738\H,-2.5615978177,0.2876043164,-4.6838355928\C,-1.3674334537,-0.8309407124,-3.2875394326\H,-1.4022798137,-1.7468918689,-3.8663022982\C,-0.6735723365,-0.803954556,-2.0801361109\H,-0.1826305177,-1.6984294431,-1.7173029717\C,2.0537033514,0.8134153035,-0.2067077291\C,2.7099873276,0.0571372881,-1.1874430674\H,2.1906386416,-0.739911954,-1.7055925966\C,4.0338404429,0.3369340704,-1.5128314809\H,4.5361647808,-0.2502260253,-2.2731288013\C,4.7078828757,1.3740148482,-0.8693081239\H,5.7379574126,1.5925571637,-1.1273754431\C,4.0554005764,2.1319582194,0.0996385118\H,4.5753056235,2.9417972901,0.5985287941\C,2.7309182701,1.855573646,0.4312671196\H,2.2144645512,2.4425871514,1.1814406877\C,-0.4440748265,-5.113462326,3.534781182\C,1.3468419142,-5.4105476428,5.3301668466\C,1.445187024,-6.8026406489,5.4370168754\H,0.8431903166,-7.432622543,4.8027627343\C,2.3158799064,-7.3564887818,6.3733943153\H,2.3834972628,-8.4360759122,6.446492208\C,3.0875068074,-6.5541730623,7.2078659478\H,3.7574220247,-7.0002895196,7.9333928371\C,2.9870603637,-5.1673596354,7.1012519863\H,3.5781628318,-4.5242444089,7.7430612281\C,2.1267348295,-4.6006791328,6.1723993212\H,2.0525851487,-3.5197213691,6.0964541682\Version=EM64L-G09RevA.01\State=1-A\HF=-2212.9224285\RMSD=4.535e-09\RMSF=1.707e-06\ZeroPoint=0.3977594\Thermal=0.424233\Dipole=1.6937477,0.7638983,-1.2076255\DipoleDeriv=1.7694555,-0.1659262,-0.0912654,0.1446384,2.2428576,-0.2070823,-0.2185441,-0.1610323,2.1258621,-0.597898,0.1508219,0.1426101,0.0638199,-0.822917,-0.1676766,0.1418555,-0.251441,-0.8099758,-0.4164448,-0.1389616,-0.1623242,-0.4269316,-0.9037439,-0.1650551,-0.1036154,0.1042698,-0.417916,-1.0045812,-0.0146645,-0.8951655,-0.1276679,-0.4960154,0.0213537,-0.8006936,0.1821144,-1.1025351,0.1762177,-0.0691834,-0.0045241,-0.0010523,0.1442555,-0.0039968,-0.0446227,-0.1157354,0.2409647,-0.886129,-0.6583798,0.4837015,-0.4134203,-1.7288944,0.7383514,0.4243248,0.7603259,-1.0106282,0.1561565,-0.0041664,-0.0067292,0.0576404,0.1039769,0.0516433,-0.110746,-0.0250249,0.1635369,0.1224265,-0.0408347,-0.0265663,0.092425,-0.1602118,0.0897406,-0.0895778,0.0241917,-0.0734064,-0.0882985,0.0451831,-0.0765852,-0.2617371,-0.2346843,0.0353892,0.0831011,0.2109531,-0.2694784,-0.0838787,0.0068909,-0.0104469,-0.0010965,0.0825862,0.015432,-0.0064017,-0.026173,0.1177673,0.4720654,1.1978941,-0.8136123,0.4082579,0.7966394,-0.495214,-0.3227263,-0.588888,0.4874608,-0.1730879,-0.4409685,0.3396464,0.0296042,-0.1177645,0.0146244,-0.0287781,0.0772761,-0.1664371,0.0816011,0.0592368,-0.0554333,0.0192399,-0.0065894,0.0710544,-0.0102778,0.0476025,0.0743044,0.2122714,0.0776648,-0.0562097,-0.0911652,0.1192063,-0.1645535,0.0685184,-0.1170046,0.0025258,-0.0883788,0.0202321,-0.0246046,0.0290509,0.0645995,0.0344
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