

Electronic Supplementary Material for CrystEngComm
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Moderation of metal... π supramolecular synthons by introducing pyridine-nitrogen into aromatic rings†

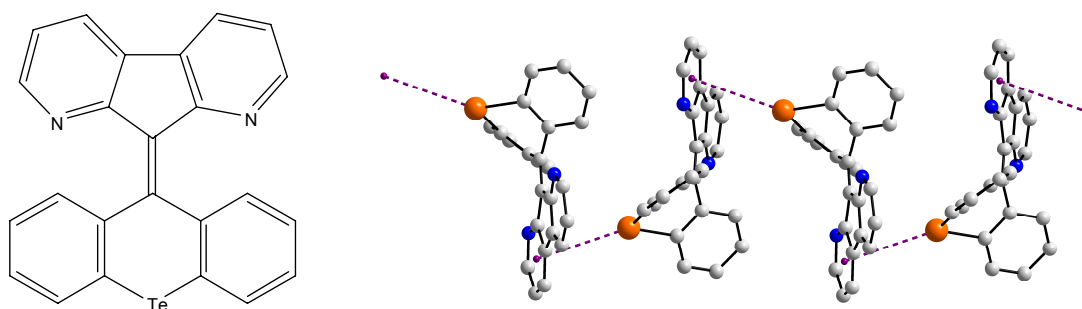
Edward R.T. Tiekink* and Julio Zukerman-Schpector*

Universidade Federal de São Carlos, Laboratório de Cristalografia, Estereodinâmica e Modelagem Molecular, Departamento de Química, C.P. 676, São Carlos, São Paulo, 13565-905, Brazil. Fax 55 16 3351 8350; Tel: 55 16 3351 8208; E-mail: Edward.Tiekink@gmail.com and julio@power.ufscar.br

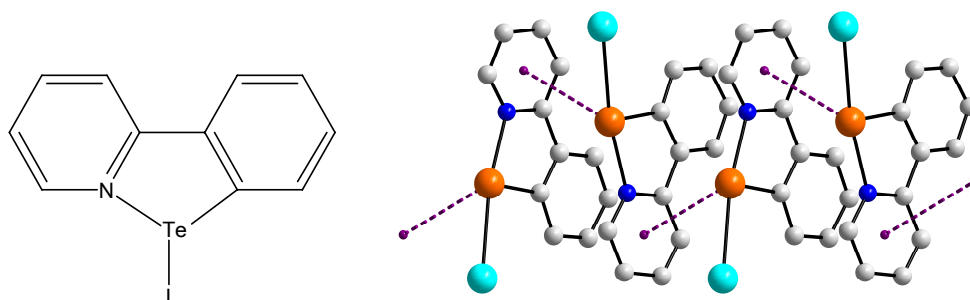
Table S(1) Chemical structures and other descriptors describing intermolecular Te... π interactions, (1) – (3).

Compound number; Te...C(g), d (Å); Te...C(g)...plane, α^a (°); [reference] and REFCODE

(1), 3.81, 17.2 [A. Levy, S. Cohen and I. Agranat, *Org. Biomol. Chem.* **1** (2003) 2755] EKALEH



(2), 3.94, 19.5 [T. A. Hamor, H. Chen, W. R. McWhinnie, S. L. W. McWhinnie and Z. Majeed, *J. Organomet. Chem.* **523** (1996) 53] REWPUE



(3), 3.98, 15.4 [K. K. Bhasin, N. Singh, S. Doomra, E. Arora, G. Ram, S. Singh, Y. Nagpal, S. K. Mehta and T. M. Klapötke, *Bioinorg. Chem. Appl.* (2007) 69263; doi:10.1155/2007/69263]

DIHHAE

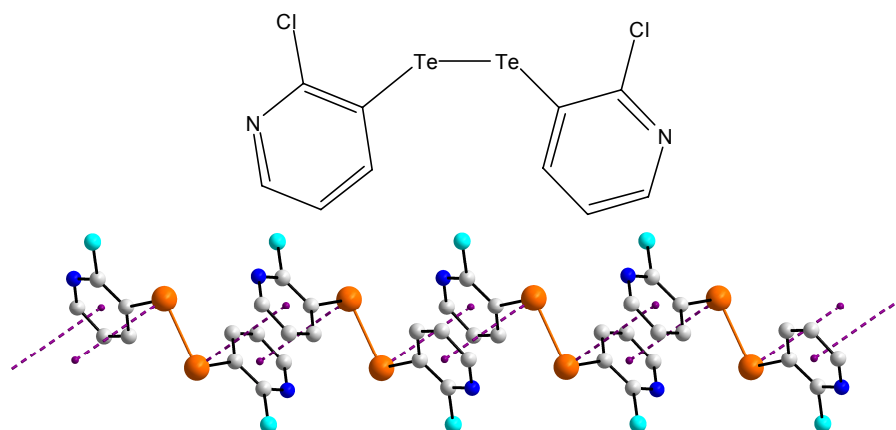
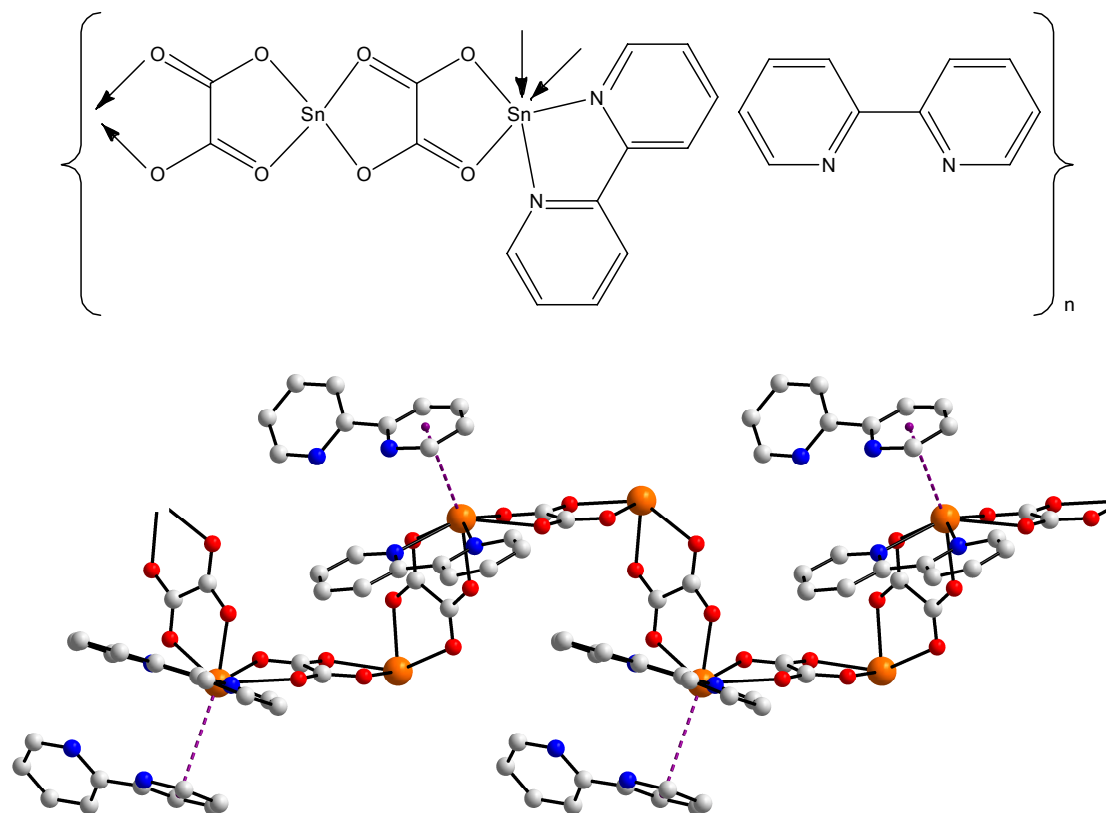


Table S(2) Chemical structures and other descriptors describing intermolecular Sn... π interactions, (4) – (6).

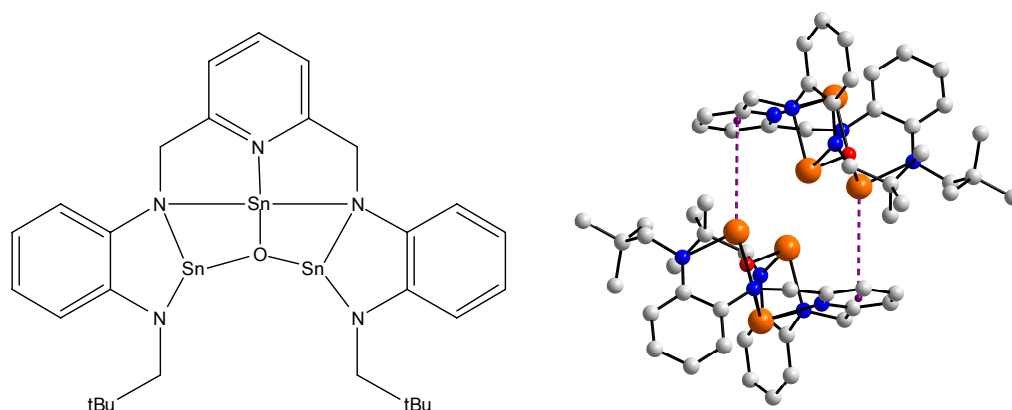
Compound number; Sn...C(g), d (Å); Sn...C(g)...plane, α^a (°); [ref.] and REFCODE

(4), 3.72, 10.1 [P. Ramaswamy, A. Datta and S. Natarajan, *Eur. J. Inorg. Chem.* (2008) 1376]

CIXSUY

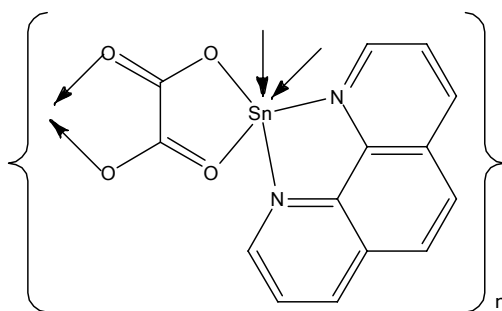


(5), 3.87, 3.5 [A. V. Zabula, T. Pape, A. Hepp, F. M. Schappacher, U. Ch. Rodewald, R. Pöttgen and F. E. Hahn, *J. Am. Chem. Soc.* **130** (2008) 5648] HOCWIG



(6), 3.87, 16.7 [P. Ramaswamy, A. Datta and S. Natarajan, *Eur. J. Inorg. Chem.* (2008) 1376]

CIXTAF



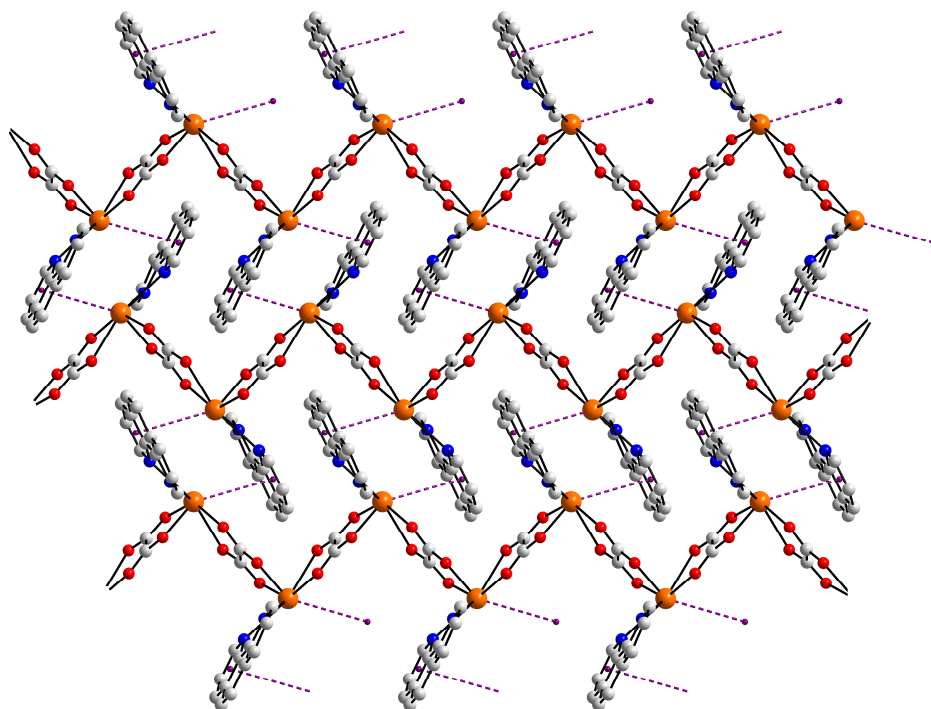


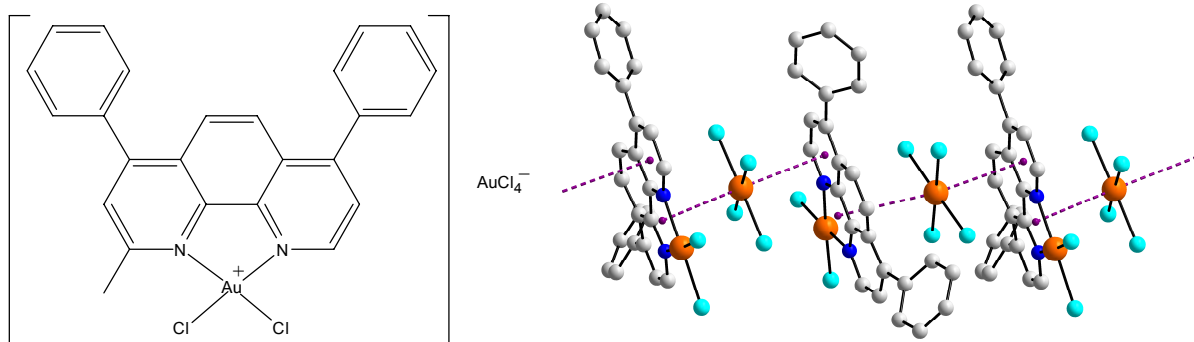
Table S(3) Chemical structures and other descriptors describing intermolecular Au... π interactions, (7) – (28). Species not engaged in Au... π interactions are shown in blue.

Compound number; Au...C(g), d (Å); Au...C(g)...plane, α^a (°); [ref.] and REFCODE

Pyridine derivatives

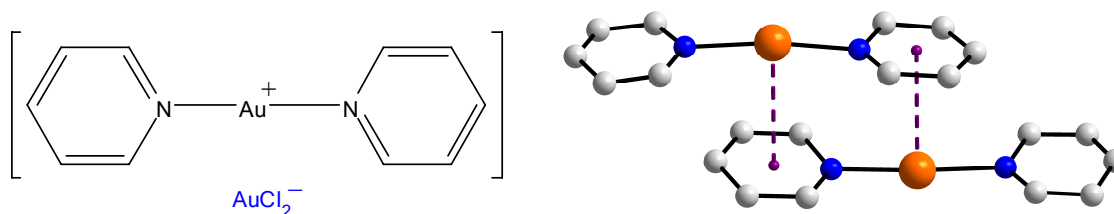
(7), 3.44, 4.7 [R. Ahmadi, V. Amani and H. R. Khavasi, *Acta Crystallogr., Sect. E: Struct. Rep.*

Online. **64** (2008) m1156] BOFSEV

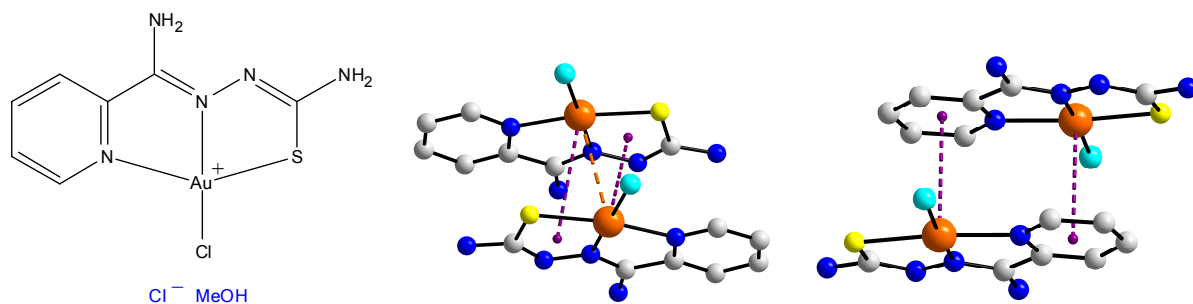


(8), 3.46, 8.0 [H.-N. Adams, W. Hiller and J. Strahle, *Z. Anorg. Allg. Chem.* **485** (1982) 81]

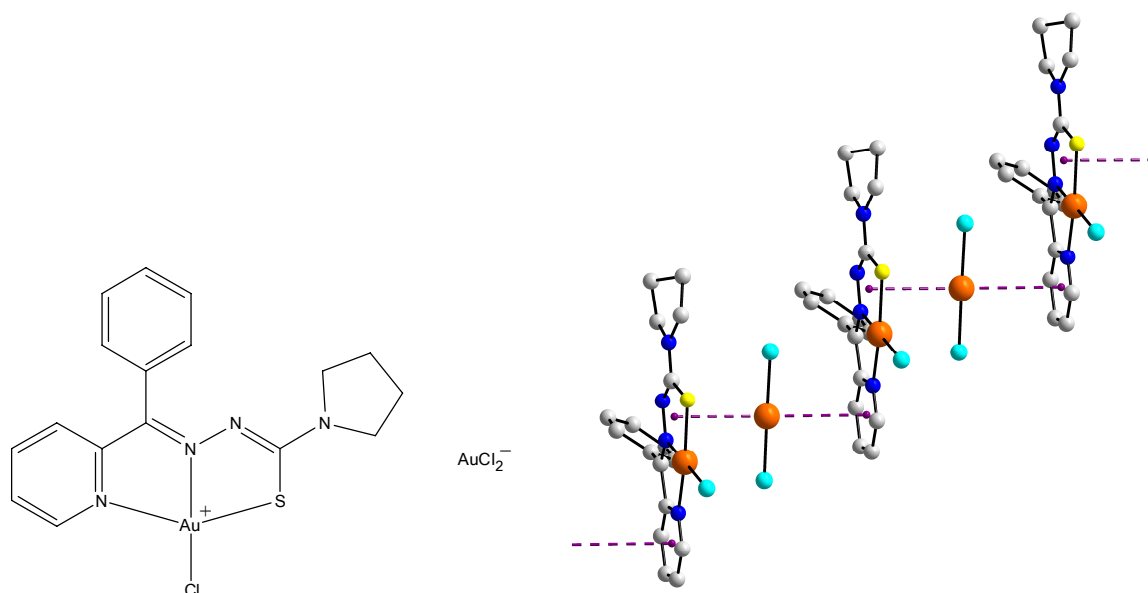
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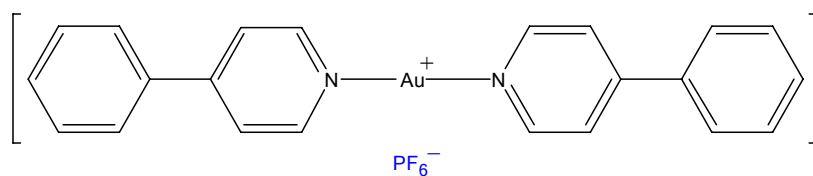
(9) Two independent molecules: 3.46, 17.9 (left-hand molecule) & 3.48, 6.6 (right-hand molecule) [I. Garcia Santos, A. Hagenbach and U. Abram, *Dalton Trans.* (2004) 677] ATOPII

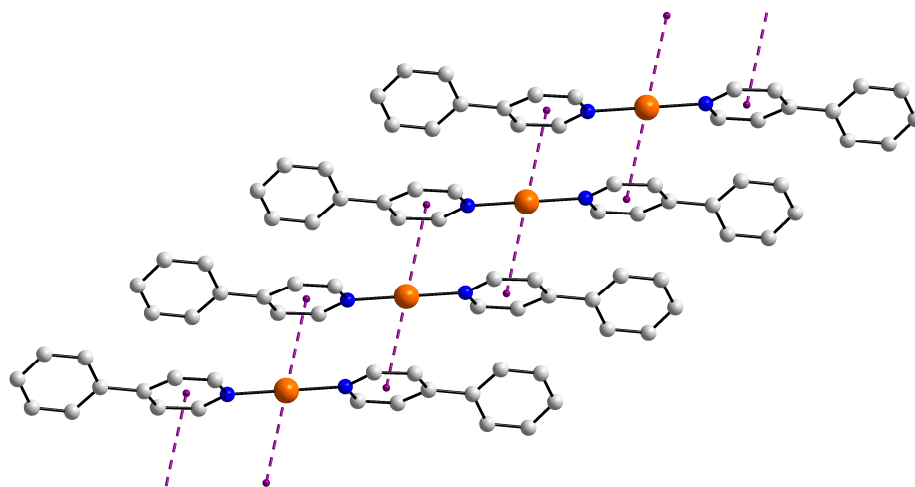


(10), 3.48, 7.3 & 3.41, 3.7 for Au... π {AuSCN₂} ring [A. Srekanth, H.-K. Fun and M. R. P. Kurup, *Inorg. Chem. Commun.* **7** (2004) 1250] QALDAJ

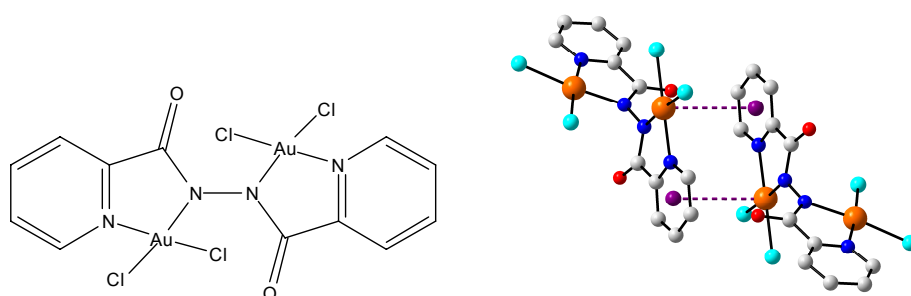


(11), 3.49, 19.1 [J. C. Y. Lin, S. S. Tang, C. S. Vasam, W. C. You, T. W. Ho, C. H. Huang, B. J. Sun, C. Y. Huang, C. S. Lee, W. S. Hwang, A. H. H. Chang and I. J. B. Lin, *Inorg. Chem.* **47** (2008) 2543] PIZKOZ

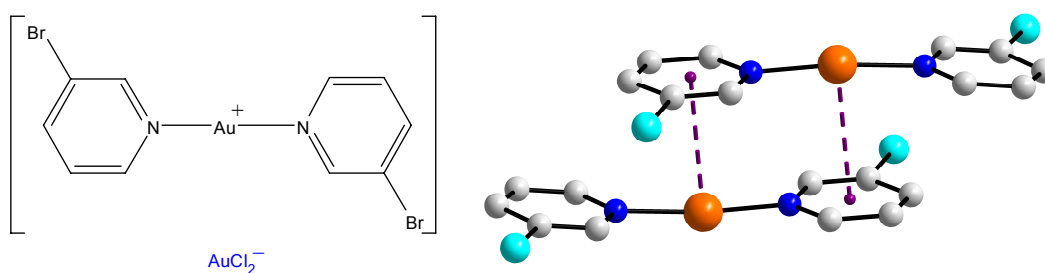




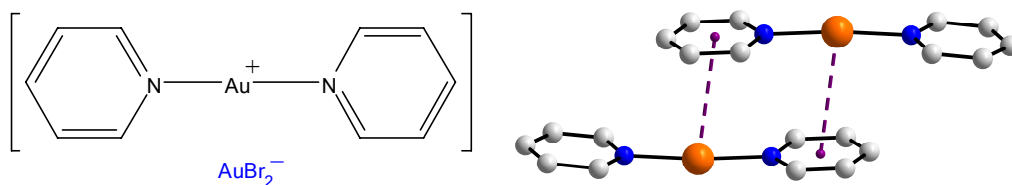
(12), 3.51, 17.3 [A. Dogan, B. Schwederski, T. Schleid, F. Lissner, J. Fiedler and W. Kaim, *Inorg. Chem. Commun.* **7** (2004) 220] ESOKOM



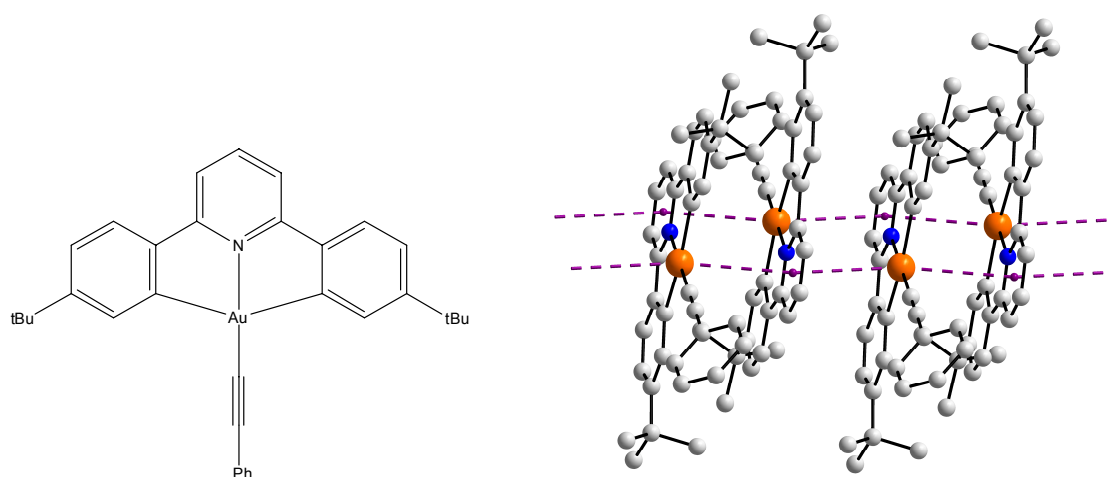
(13), 3.53, 9.3 [M. Freytag and P. G. Jones, *Chem. Commun.*, (2000) 277] KANJIS



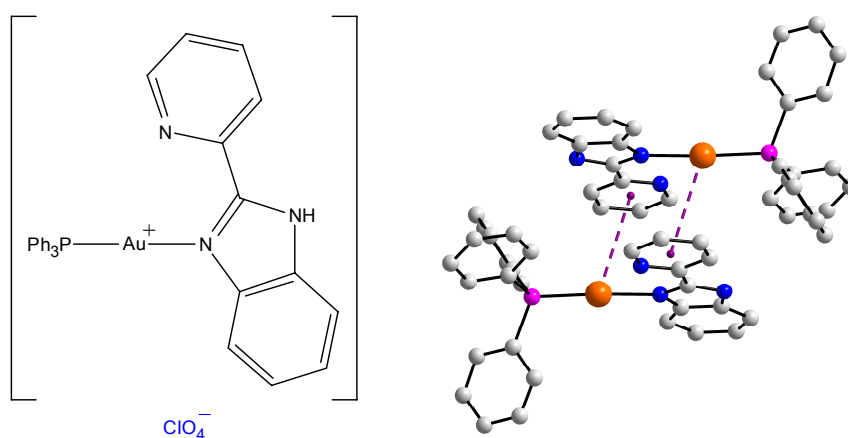
(14), 3.55, 11.9 [W. Conzelmann, W. Hiller, J. Strahle and G. M. Sheldrick, *Z. Anorg. Allg. Chem.*, **512** (1984) 169] COCVUL



(15), 3.62, 10.2 [K. M.-C. Wong, L.-L. Hung, W. H. Lam, N. Zhu and V.W.-W. Yam, *J. Am. Chem. Soc.* **129** (2007) 4350] SICRUS



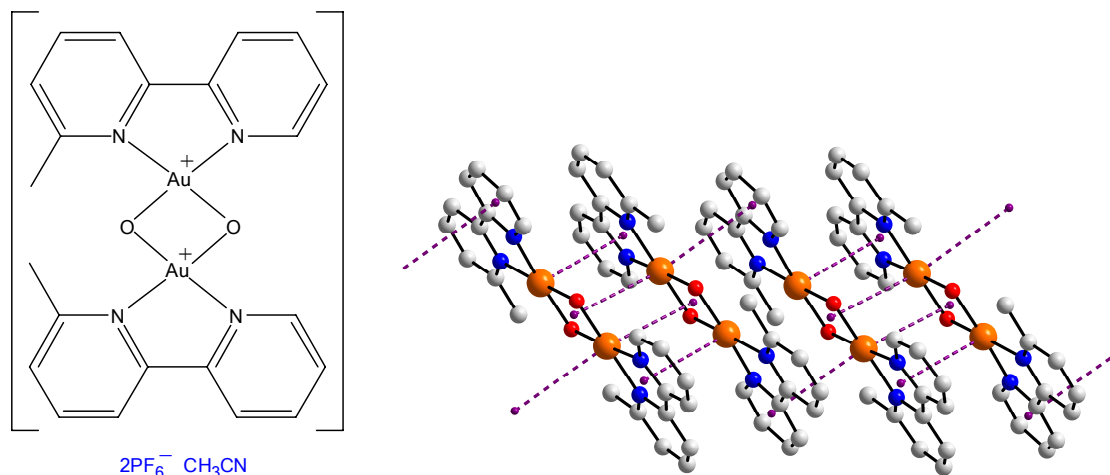
(16), 3.63, 19.1 [M. Munakata, S.-G. Yan, M. Maekawa, M. Akiyama and S. Kitagawa, *J. Chem. Soc., Dalton Trans.*, (1997) 4257] PABSEQ



(17), 3.64, 16.0; 3.65, 17.6 between Au... π {AuNC₂N}; 3.56, 18.5 between Au... π {Au₂O₂}

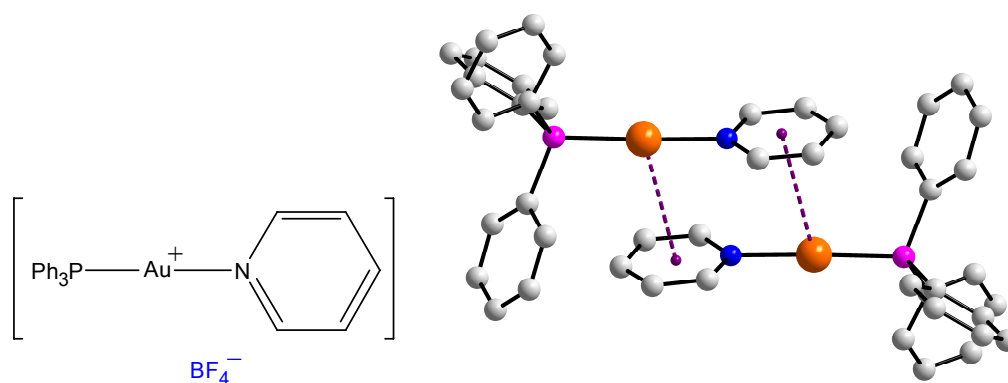
linked into a chain via 3.64, 16.0 [C. Gabbiani, A. Casini, L. Messori, A. Guerri, M. A. Cinellu, G. Minghetti, M. Corsini, C. Rosani, P. Zanello and M. Arca, *Inorg. Chem.*, **47** (2008) 2368]

QIYZAA



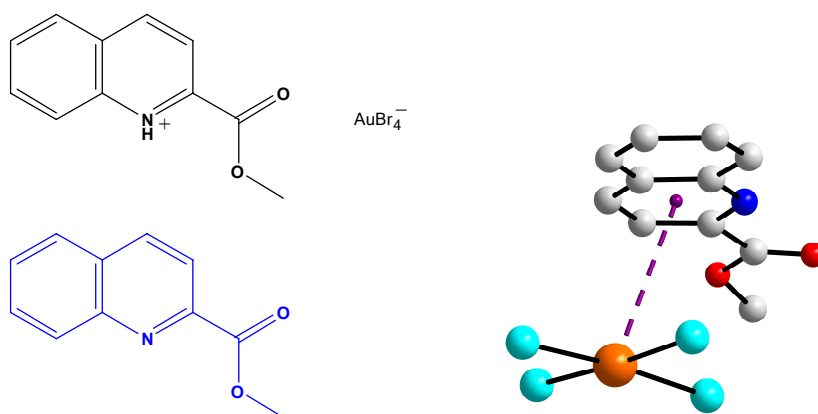
(18), 3.66, 8.5 [S. E. Thwaite, A. Schier and H. Schmidbaur, *Inorg. Chim. Acta*, **357** (2004)

1549] IWABEN

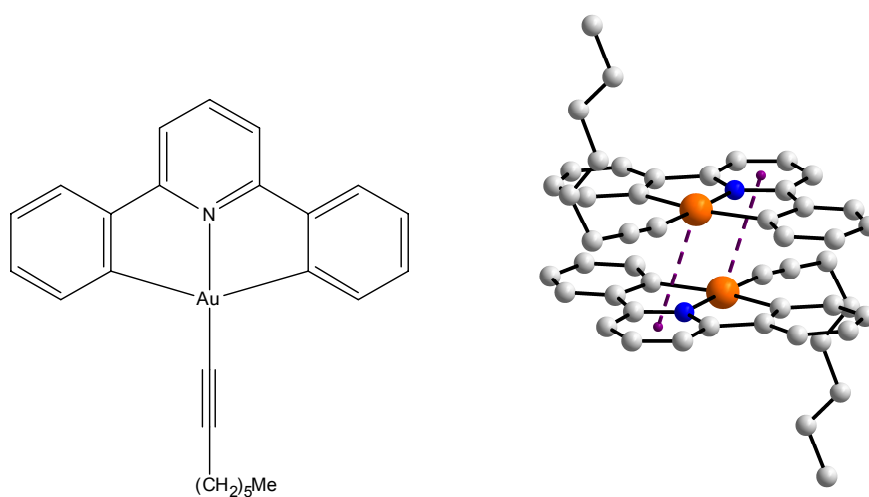


(19), 3.69, 19.3 [M. A. S. Goher, A. K. Hafez, W.-H. Yip and T. C. W. Mak, *J. Crystallogr.*

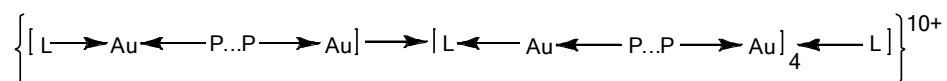
Spectrosc. Res., **22** (1992) 317] VUGDUW



(**20**), 3.70, 18.8 [K. M.-C. Wong, L.-L. Hung, W. H. Lam, N. Zhu and V.W.-W. Yam, *J. Am. Chem. Soc.* **129** (2007) 4350] SICSAZ

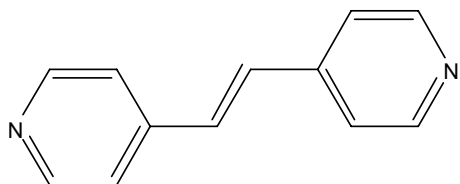


(**21**), 3.73, 10.3; 3.90, 15.2; 3.90, 16.8; 3.98, 11.0 [C. A. Wheaton, M. C. Jennings and R. J. Puddephatt, *J. Am. Chem. Soc.*, **128** (2006) 15370] DEVRUS

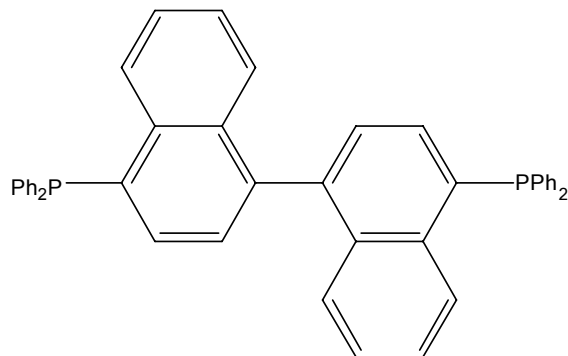


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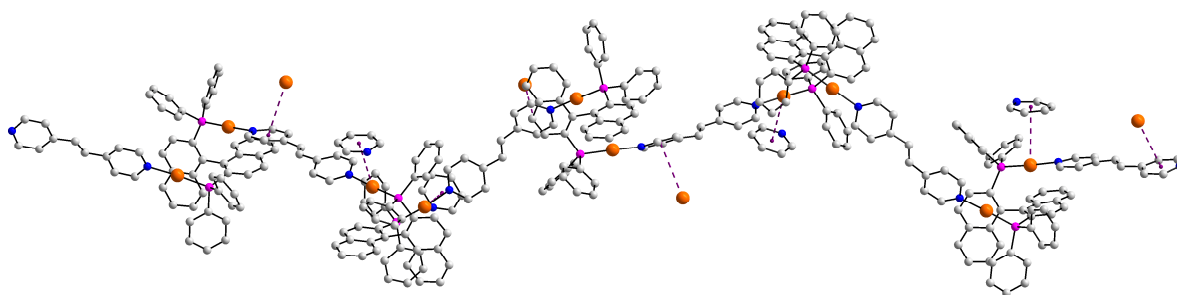
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P...P =

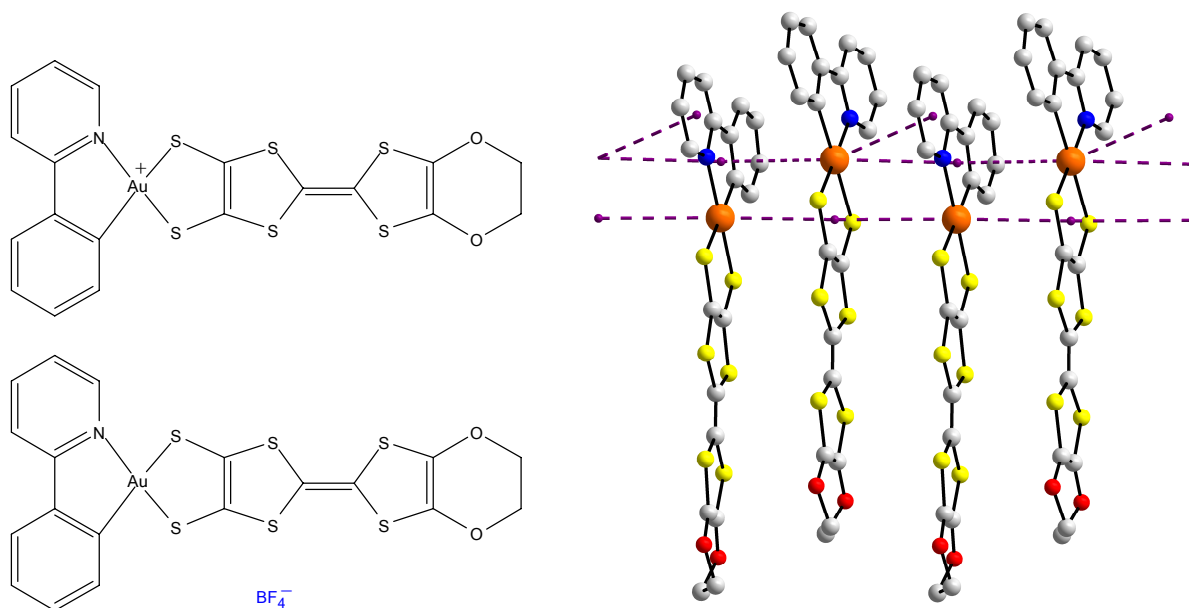


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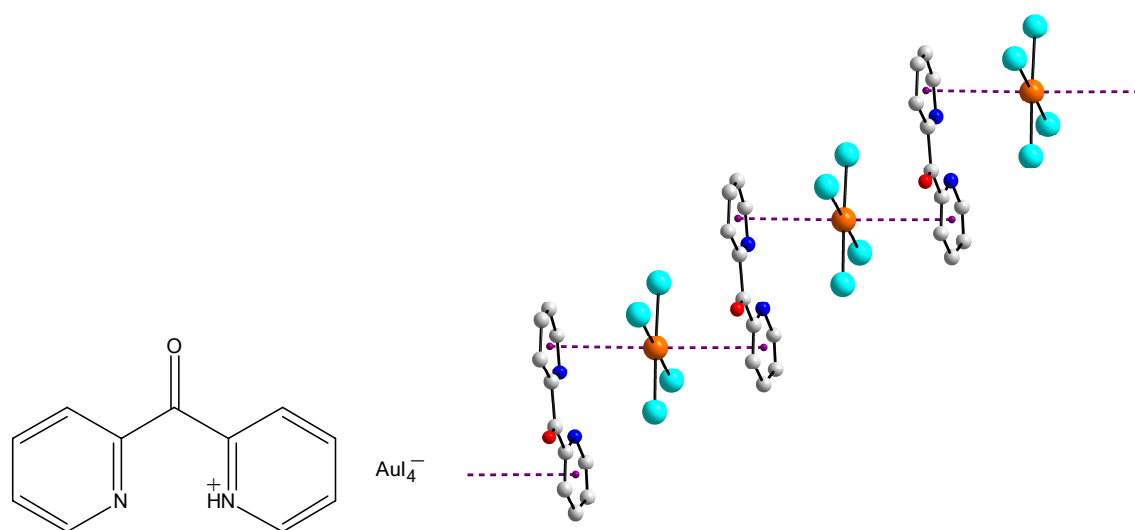


(22), 3.73, 16.6 [K. Kubo, A. Nakao, Y. Ishii, R. Kato and G. Matsubayashi, *Synth. Met.*, **153**

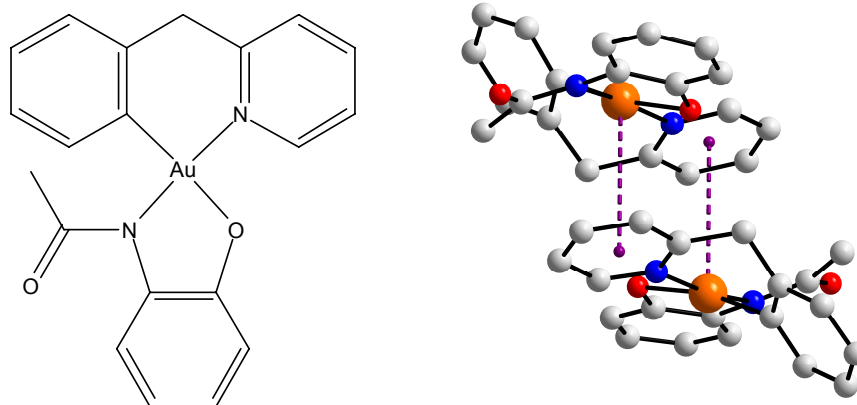
(2005) 425] YEDPON



(23), 3.80, 11.8; 3.88, 16.2 [T. C. W. Mak, *Private Communication to CCDC*] IPUNAI



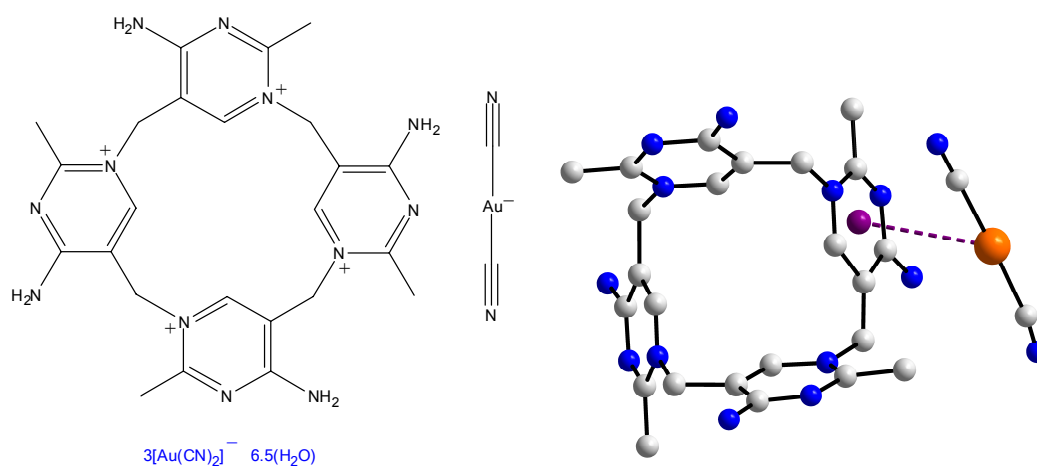
(24), 4.00, 5.5 & 3.99, 10.6 between two independent molecules [C. H. A. Goss, W. Henderson, A. L. Wilkins and C. Evans, *J. Organomet. Chem.*, **679** (2003) 194] BAZSEB



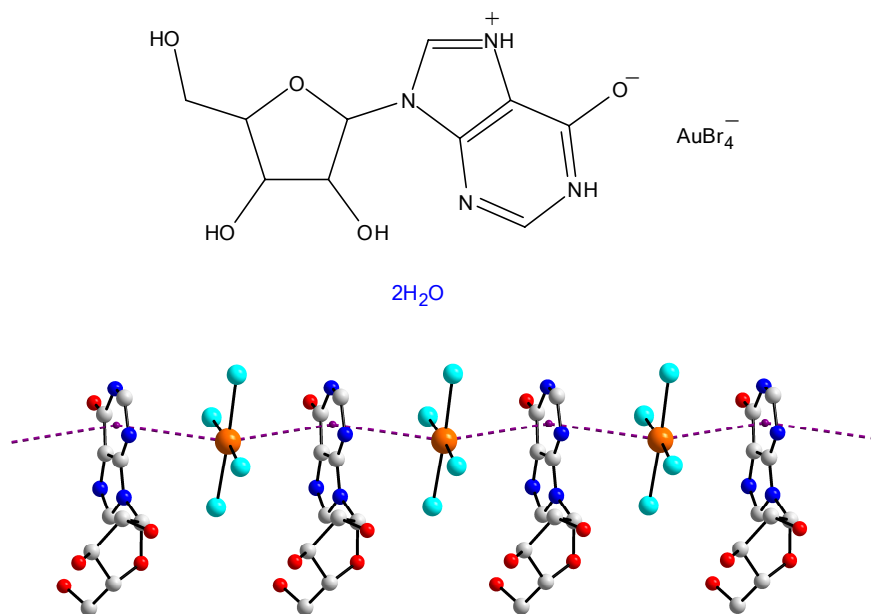
Pyrimidine derivatives

(25), 3.66, 16.8 [R. E. Cramer, D. W. Smith and W. VanDorne, *Inorg. Chem.* **37** (1998) 5895]

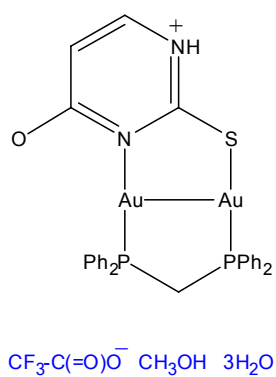
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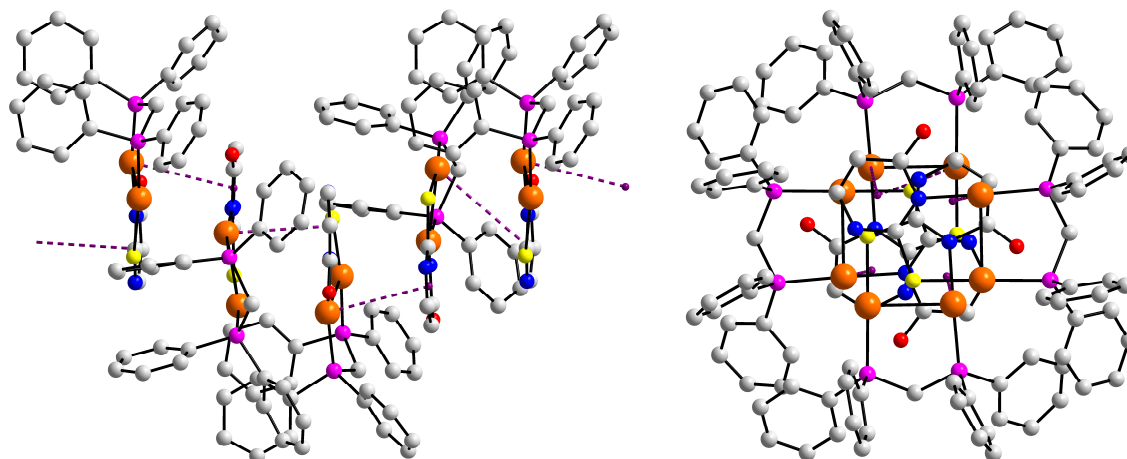


(26), 3.67, 13.9 and 3.86, 15.9 [J. M. Salas, M. Quiros, M. P. Sanchez and A. L. Beauchamp, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **45** (1989) 1874] VAYZEA



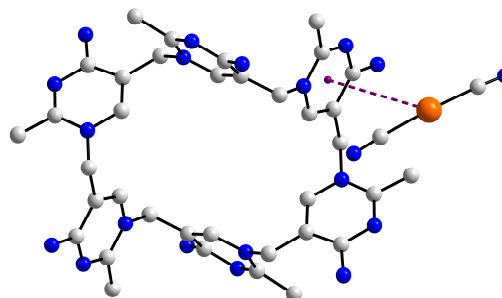
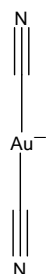
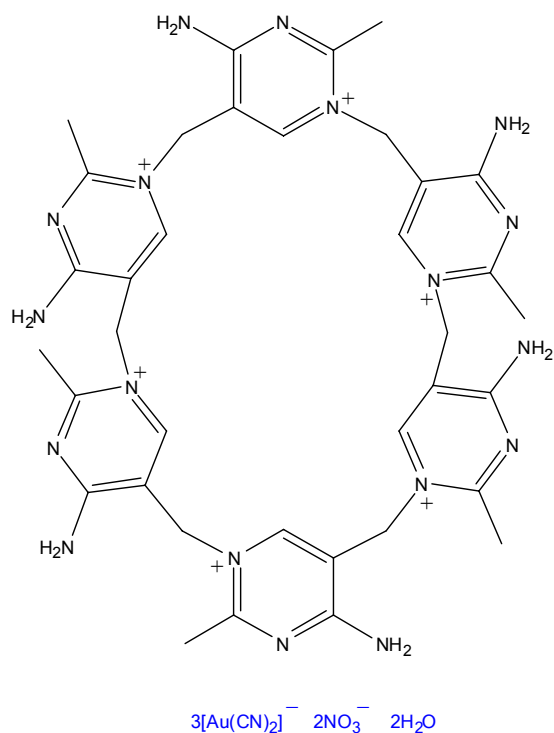
(27), 3.73, 12.3 [Y. Lee and R. Eisenberg, *J. Am. Chem. Soc.* **125** (2003) 7778] EJOHEQ





(28), 3.77, 18.4 [R. E. Cramer, D. W. Smith and W. VanDorpe, *Inorg. Chem.* **37** (1998) 5895]

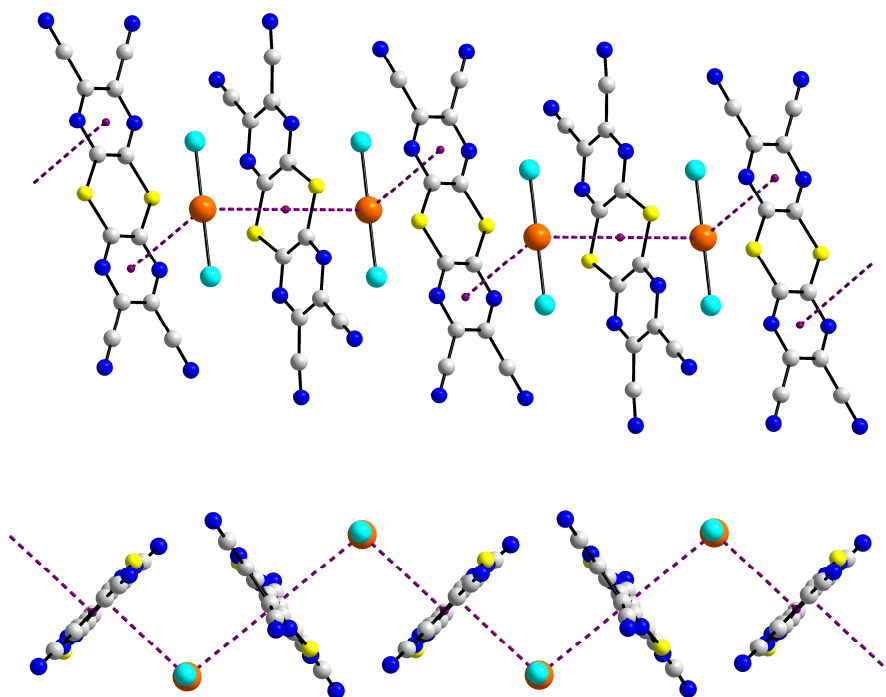
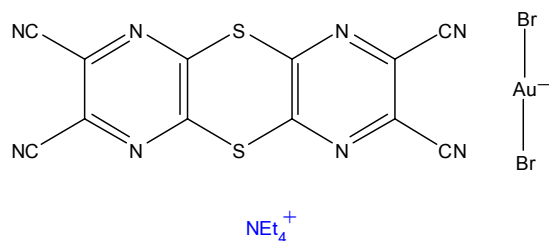
SOCVEL



Pyrazine and 1,4-dithiine derivative

(29), 3.66, 18.8 (pyrazine) & 3.48, 4.9 [D. Belo, I. C. Santos and M. Almeida, *Polyhedron*, **23**

(2004) 1351] AXUHOQ



Thiopyran derivative

(30), 3.65, 10.3 [S. Wang and J. P. Fackler Jr, *Chem. Commun.*, 1988, 22] FOZJIN

