



STRUCTURAL
CHEMISTRY

Volume 78 (2022)

Supporting information for article:

**Coordination chemistry of nitrile-functionalized mixed thia-aza
macrocycles [9]aneN₂S and [9]aneNS₂ towards silver(I)**

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Table S1. Short contacts in structure $[\text{Ag}(\text{L}^1)_2]\text{BF}_4$

D = donor atom, H = hydrogen atom, A = acceptor atom

D-H...A	D-H	H...A	D...A	D-H...A	Symm (A)
C2'-H2'B...N43	0.99	2.56	3.385 (2)	141	(1-x, 1-y, 1-z)
C2-H2B...N73'	0.99	2.62	3.321 (3)	128	
C5-H5A...F1	0.99	2.45	3.170 (2)	129	(1-x, 1-y, 2-z)
C6'-H6'B...N73	0.99	2.47	3.398 (3)	156	(x, y, -1+z)
C8-H8B...F4	0.99	2.37	3.197 (2)	140	
C41'-H41A...F2	0.99	2.36	3.274 (2)	154	(-x, 2-y, 1-z)
C41-H41D...F3	0.99	2.43	3.272 (2)	143	(1+x, -1+y, z)
C71'-H71B...F2	0.99	2.43	3.271 (2)	143	
C71-H71C...F3	0.99	2.38	3.329 (2)	161	(1-x, 2-y, 2-z)

Table S2. Short contacts in structure $[\text{Ag}(\text{L}^2)\text{SCN}]\text{BF}_4$

D = donor atom, H = hydrogen atom, A = acceptor atom

D-H...A	D-H	H...A	D...A	D-H...A	Symm (A)
C42-H42B...N74	0.99	2.34	3.276 (3)	157	(1-x, 1-y, -z)
C72-H72A...N	0.99	2.51	3.345 (3)	142	(1-x, 1-y, -z)

Table S3. Short contacts in structure $[\text{Ag}_2(\text{L}^3)_2(\mu\text{-SCN})]\text{BF}_4$

D = donor atom, H = hydrogen atom, A = acceptor atom

D-H...A	D-H	H...A	D...A	D-H...A	Symm (A)
C8A-H8AB...N	0.99	2.46	3.371 (8)	152	(-x, y, 1/2-z)
C5-H5A...F3	0.99	2.52	3.413 (6)	151	(1/2-x, 5/2-y, 1-z)
C6-H6A...N74A	0.99	2.56	3.542 (7)	170	(1/2-x, 5/2-y, 1-z)
C5A-H5AB...N74A	0.99	2.52	3.371 (7)	144	(x, -1+y, z)
C9A-H9AA...F1	0.99	2.41	3.356 (7)	159	(1/2-x, -1/2+y, 1/2-z)
C9A-H9AB...S4	0.99	2.79	3.766 (5)	171	(-x, y, 1/2-z)
C2A-H2AB...N	0.99	2.51	3.361 (7)	144	(-x, -1+y, 1/2-z)
C71-H71A...N74	0.99	2.58	3.454 (7)	147	(1/2-x, 5/2-y, 1-z)
C71A-H71C...N74	0.99	2.62	3.573 (7)	162	(1/2-x, 5/2-y, 1-z)

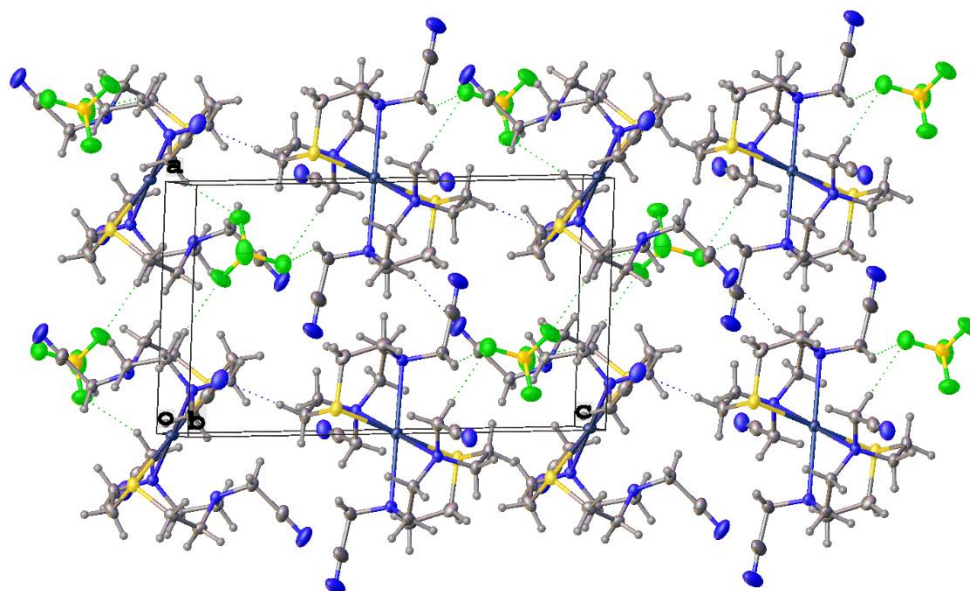


Figure S1. The extended structure of $[\text{Ag}(\text{L}^1)_2]\text{BF}_4$ viewed approximately along the b axis.

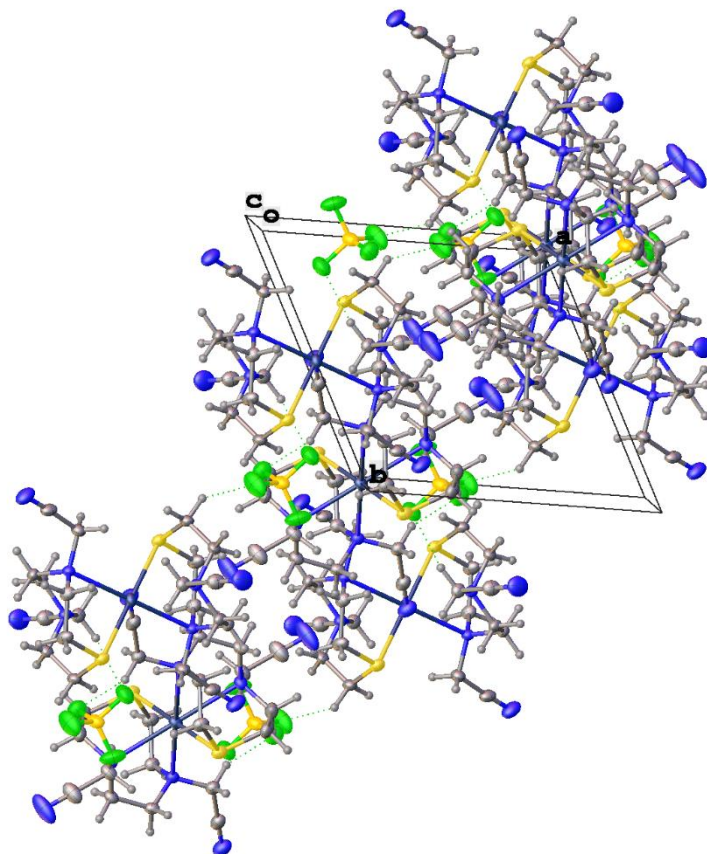
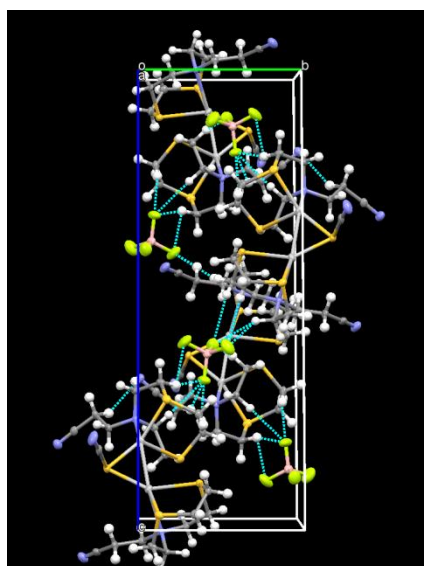


Figure S2. The extended structure of [Ag(L¹)₂]BF₄ viewed approximately along the *c* axis.



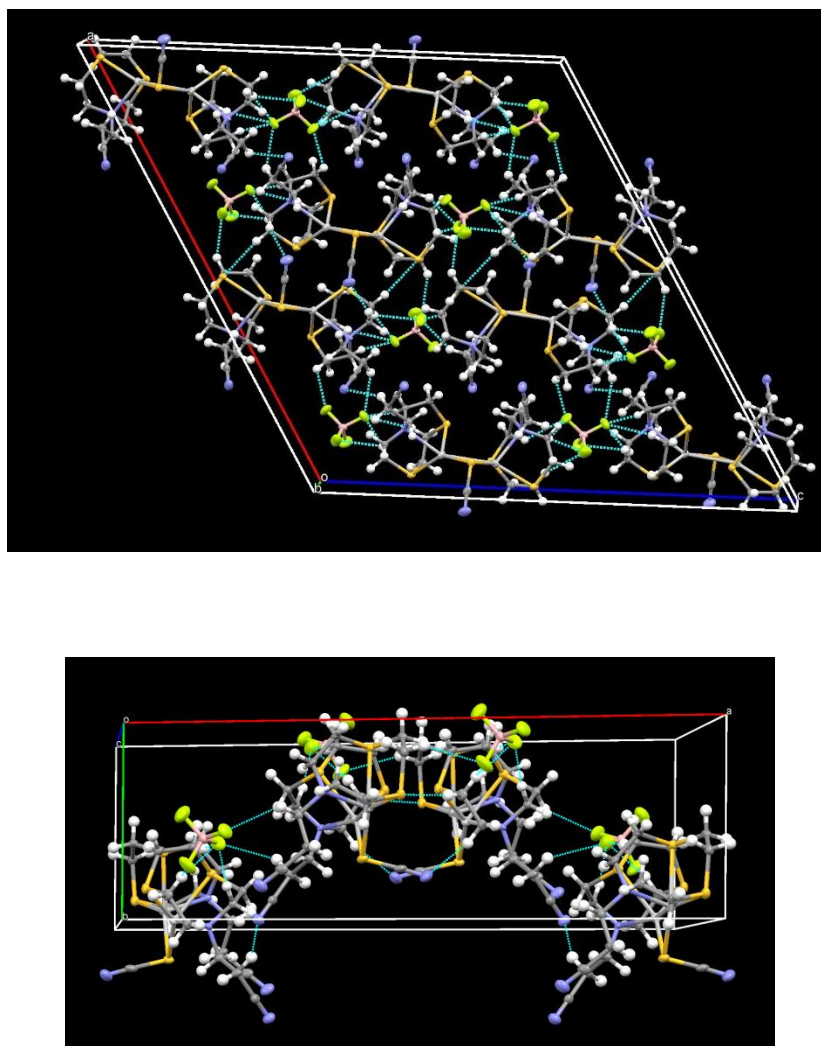


Figure S3. The extended structure of $[\text{Ag}_2(\text{L}^3)_2(\mu\text{-SCN})]\text{BF}_4$ viewed approximately along the a , b and c axes. The depth of the views along a and c have been restricted because of the length of these axes.