# SUPPLEMENTARY MATERIALS

belonging to the paper **KD5008**

## Synchrotron powder diffraction in a systematic study of *N*-(4´-benzo-15-crown-5)-2-(amino-*N*-tosyl)phenylaldimine complexes

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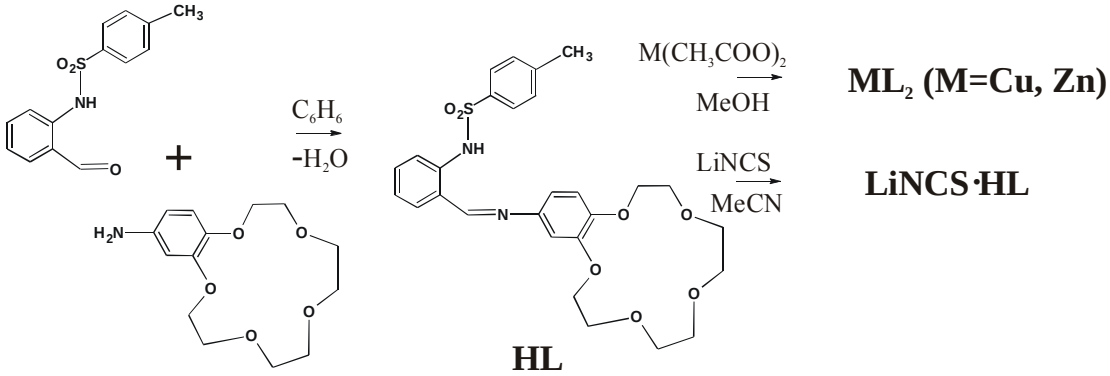
CONTENT

1. *Syntheses*.

*Reagents and techniques*. Commercial grade chemicals were used without further purification unless otherwise stated. Acetonitrile and benzene were dried by refluxing over potassium carbonate and sodium respectively. Elemental (CHN) analysis was performed with Carlo Erba Strumentazione-1106 analyzer. IR spectra were recorded on a FTIR NEXUS (Nicolet) spectrometer (suspensions in liquid paraffin, KBr plates). *N*-(4′-benzo-15-crown-5)-2-(amino-*N*-tosyl)-phenylaldimine (Minacheva *et al*., 2004a) and its complexes were prepared as depicted in Scheme.




HL (Minacheva *et al*., 2004a):

A solution of 4'-aminobenzo-15-crown-5 (0.283 g) in benzene (5 ml) was added to a solution of 2-tosylaminobenzaldehyde (0.275) in benzene (10 ml). The mixture was refluxed for 2 h with the use of a Dean–Stark apparatus for 2 h until water was completely separated. After removal of two-thirds of the solvent, the resulting precipitate was separated and recrystallized from methanol. Beige crystals were obtained, m.p. 140–141 C°. Analysis calcd. for $C_{28}H_{32}N_2O_7S$: C 62.2, H 6.0, N 5.2, S 5.9 %; found C 62.2, H 6.0, N 5.1, S 6.1 %.

$CuL_2$ and $ZnL_2$ (Minacheva *et al*., 2006):

Copper(II) acetate (0.00002 mol) was added to a solution of *N*-(4′-benzo-15-crown-5)-2-(amino-*N*-tosyl)-phenylaldimine (0.00001 mol) in methanol (10 ml). The mixture was refluxed for 2 h and then allowed to cool to ambient temperature. The black ($CuL_2$) or yellow ($ZnL_2$) substances formed were recrystallized from methanol. Analysis calcd. for $C_{56}H_{62}CuN_4O_{14}S_2$: C 58.9, H 5.5, N 4.9, S 5.6 %; found C 59.4, H 4.8, N 4.9, S 5.8 %. Calcd. for $C_{56}H_{62}N_4O_{14}S_2Zn$: C 58.8, H 5.5, N 4.9, S 5.6 %; found C 58.5, H 4.8, N 4.7, S 5.9 %.

LiNCS·HL (Ivanova *et al*., 2005):

The equimolar quantities of crown ether HL and LiNCS were dissolved in acetonitrile. The solutions were mixed together and allowed to stay in air for 5–7 days. After the precipitate was formed, the raw product was recrystallized from acetonitrile and dried over $CaCl_2$. Analysis calcd. for $C_{29}H_{32}LiN_3O_7S_2$: C 58.9, H 5.5, N 4.9, S 5.6 %; found C 59.4, H 4.8, N 4.9, S 5.8 %.

2. *Membranes and ISEs preparation.*

The neutral carrier (HL, $ZnL_2$ or $CuL_2$), plasticizer (o-nitrophenyloctyl ether, Fluka) and high molecular weight polyvinylchloride (PVC) (Aldrich) were dissolved in the appropriate volume of cyclohexanone and mechanically stirred. All membrane cocktails were cast in glass rings placed on glass plates. Solvent from PVC membrane was allowed to evaporate for a week at room temperature. The thickness of the resulting membranes was about 0.2 - 0.3 mm. Small disks were punched from the cast membranes and mounted in the electrode bodies (Fig. 1).

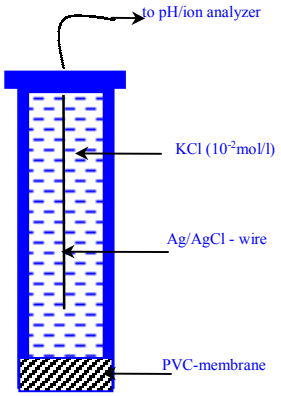
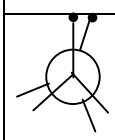
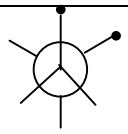
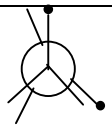
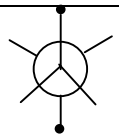
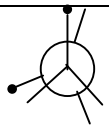
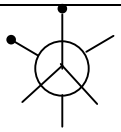



Fig.1. Scheme of the electrode designed for the investigation of membrane' potentiometric properties.

Macrocycle conformation is determined by the sequence of the ethylene glycol units O-CH2-CH2-O conformations. The conformation of the single unit is completely defined by the value of three torsion angles which can be described by different ways (table 1).

Table 1. The most wide-spread ways of conformation descriptions.

| Newman formula | Angle | Indication | |
|---|---|---|---|
| | | (used in this article) | Klyne and Prelog system (Klyne W., Prelog V., 1960) |
|  | $\varphi^o$ ($0\pm30^o$) | cis (C) | ± synperiplanar (±sp) |

| | | | |
|---|---|---|---|
|  | $\varphi^1$ (60±30°) | gauche (G) | +synclinal (+sc) |
|  | $\varphi^2$ (120±30°) | skew (S) | +anticlinal (+ac) |
|  | $\varphi^3$ (180±30°) | trans (T) | ±antiperiplanar (±ap) |
|  | $\varphi^4$ (-120±30°) | see $\varphi^2$ | -anticlinal (-ac) |
|  | $\varphi^5$ (-60±30°) | see $\varphi^1$ | -synclinal (-sc) |

**References.**


Ivanova, I.S., Dorokhov, A.V., Pyatova, E.N., Bicherov, A.V., Burlov, A.S., Garnovskii, A.D., Tsivadze, A. Yu. (2005). *Russ. J. Coord. Chem.* **31**, 483–488.

Klyne, W. & Prelog, V. (1960). *Experientia*, **16**, 521-523.

Minacheva, L.Kh., Ivanova, I.S., Dorokhov, A.V., Bicherov, A.V., Burlov, A.S., Garnovskii, A.D., Sergienko, V. S., Tsivadze, A. Yu (2004a). *Doklady Chemistry,* **398,** 179–183.

Minacheva, L.Kh., Ivanova, I.S., Dorokhov, A.V., Burlov, A.S., Garnovskii, A.D., Sergienko, V.S., Tsivadze, A.Yu. (2006). *Russ. J. Coord. Chem.* **32**, 166 – 172.

## DFT optimized (*in vacuo*) Cartesian coordinates

**HL:**

Atomic Coordinates (Angstroms)

| | | | |
|---|---|---|---|
| 6 | 3.20111483 | 21.96898492 | 4.77429523 |
| 1 | 2.32533992 | 21.44803027 | 5.15261755 |
| 6 | 4.28520302 | 22.23585863 | 5.61746371 |
| 6 | 5.40866854 | 22.93098751 | 5.15398895 |
| 1 | 6.22989697 | 23.15084139 | 5.82995594 |
| 6 | 5.44058882 | 23.35828762 | 3.82326476 |
| 1 | 6.31134752 | 23.90507921 | 3.46328513 |
| 6 | 4.36785656 | 23.10088294 | 2.94871338 |
| 6 | 3.25131693 | 22.40384697 | 3.44588327 |
| 1 | 2.40531482 | 22.20316484 | 2.79038156 |
| 6 | 4.41696433 | 23.57705672 | 1.50836301 |
| 1 | 3.52660162 | 23.26499682 | 0.95173295 |
| 1 | 5.29884265 | 23.17865120 | 0.98904341 |
| 1 | 4.47996187 | 24.67263693 | 1.45710709 |
| 16 | 4.22513537 | 21.66189299 | 7.35257860 |
| 7 | 4.61793603 | 19.97218913 | 7.32616987 |
| 1 | 3.79551718 | 19.41283377 | 7.01665064 |
| 6 | 5.82658489 | 19.42511038 | 6.84361408 |
| 6 | 7.07915971 | 20.00440962 | 7.12895493 |
| 1 | 7.11517999 | 20.91288258 | 7.72162841 |
| 6 | 8.25941406 | 19.40915729 | 6.68091698 |
| 1 | 9.21218526 | 19.87933957 | 6.91756401 |
| 6 | 8.22903291 | 18.20831692 | 5.95519541 |
| 1 | 9.15200359 | 17.74143819 | 5.61939025 |
| 6 | 7.00043240 | 17.61541644 | 5.68120076 |
| 1 | 6.96107953 | 16.67905499 | 5.12532933 |
| 6 | 5.78050218 | 18.19778536 | 6.09955728 |
| 6 | 4.54641864 | 17.49916409 | 5.74402025 |
| 1 | 4.68956074 | 16.57513964 | 5.16171227 |
| 7 | 3.35881872 | 17.89406444 | 6.08611670 |
| 6 | 2.19126191 | 17.21686186 | 5.65989835 |
| 6 | 1.06533632 | 17.30410685 | 6.50928395 |
| 1 | 1.16653559 | 17.87458628 | 7.42726330 |
| 6 | -0.13984474 | 16.67838794 | 6.17262855 |
| 6 | -0.22755883 | 15.93786959 | 4.95980588 |
| 6 | 0.87874104 | 15.89191539 | 4.10730778 |
| 1 | 0.77262839 | 15.35812582 | 3.16496478 |
| 6 | 2.08205785 | 16.52473229 | 4.43876716 |
| 1 | 2.91276788 | 16.50262148 | 3.73808215 |
| 8 | 5.28332243 | 22.37464396 | 8.10336004 |
| 8 | 2.81437349 | 21.67398220 | 7.79957645 |
| 8 | -1.29307584 | 16.74278191 | 6.91865648 |
| 8 | -1.41773276 | 15.34708674 | 4.56418123 |
| 6 | -1.81765766 | 14.16355535 | 5.32806375 |
| 1 | -1.26403929 | 13.29209063 | 4.94876525 |
| 1 | -1.59808734 | 14.29990083 | 6.39182256 |
| 6 | -3.31964431 | 13.97096537 | 5.12120843 |
| 1 | -3.56347274 | 14.01979364 | 4.04693612 |
| 1 | -3.87274279 | 14.75420071 | 5.65121168 |
| 8 | -3.64646573 | 12.65903068 | 5.64120881 |
| 6 | -4.99828195 | 12.50193215 | 6.10928572 |
| 1 | -5.28103564 | 11.46078632 | 5.89842695 |
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   1    -3.36555709  17.84178249   8.03076176
   6    -1.26185282  17.39810333   8.20896433
   1    -0.92333196  18.43964057   8.10316510
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Energy:     -2120.46867836
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**LiNCS.HL:**

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Atomic Coordinates (Angstroms)
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   1     7.59635241   5.12401638  -1.42623312
   6     8.84570223   6.29170758  -0.09145557
   1     9.76968990   5.83938406  -0.44833038
   6     8.89256028   7.26268519   0.92248447
   6     7.67859476   7.82368919   1.36975761
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   6    10.21119034   7.69631707   1.53565040
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   1    10.25138322   7.44202329   2.60374443
   1    10.34668075   8.78330063   1.45751971
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   6     5.81762985   7.16876973  -3.79758907
   1     5.84554803   6.08550760  -3.72717972
   6     6.53025239   7.82758644  -4.80066843
   1     7.12816596   7.24305207  -5.49740354
   6     6.46535174   9.22377156  -4.92924916
   1     7.01429341   9.73189928  -5.71854198
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   1     5.61400143  11.03358952  -4.13382007
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   6     4.16549735  10.17580939  -2.11431014
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   6     1.01988298  12.03712435   1.46706553
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   1    -1.94440160  13.87929623   5.82432905
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   6    -0.22290955  13.32458075   7.01065299
   1     0.82958273  13.62388158   7.15122620
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   8    -0.29317729  11.96703204   6.53558807
   6     0.18215865  10.95626305   7.44089206
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   6    -0.07837566   9.61639948   6.76259061
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   6    -3.20847162  11.65967458   4.31854064
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Energy:     -2619.18710937
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**$CuL_2$:**

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Atomic Coordinates (Angstroms)
   ------------------------------

  29    -0.08150700   3.33187772   5.63648443
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   6     3.92264421   1.65962104   5.87946275
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   1     2.14089524   0.42079417   5.84969539
   6     3.94069974  -0.72635695   6.20070305
   1     3.39782983  -1.66806176   6.26971250
   6     5.33935905  -0.71636507   6.34905448
   6     6.01243087   0.51644421   6.25598707
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| | | | |
|---|---|---|---|
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| 1 | 6.65644996 | -1.95118320 | 7.55696512 |
| 1 | 6.85539349 | -2.17768700 | 5.81633061 |
| 16 | 3.01909897 | 3.21427701 | 5.50357801 |
| 7 | 1.69443862 | 3.24221659 | 6.60863861 |
| 6 | 1.91644122 | 3.34529678 | 7.96749925 |
| 6 | 3.19120187 | 3.62746456 | 8.55119979 |
| 1 | 4.02080803 | 3.87784778 | 7.90168478 |
| 6 | 3.39113976 | 3.62949240 | 9.92356713 |
| 1 | 4.38512293 | 3.85202491 | 10.30869083 |
| 6 | 2.33468622 | 3.36361970 | 10.81543523 |
| 1 | 2.49734597 | 3.36239676 | 11.89042552 |
| 6 | 1.07669333 | 3.12373961 | 10.28933131 |
| 1 | 0.23939212 | 2.93504391 | 10.96057421 |
| 6 | 0.81684592 | 3.12120868 | 8.88988931 |
| 6 | -0.56990739 | 2.91830447 | 8.54304407 |
| 1 | -1.21143644 | 2.68733895 | 9.40273462 |
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| 6 | -4.77060549 | 3.41818692 | 6.53604443 |
| 6 | -5.33353474 | 2.26880424 | 7.17277139 |
| 6 | -4.48398736 | 1.35434463 | 7.80499528 |
| 1 | -4.88115863 | 0.43628450 | 8.22712980 |
| 6 | -3.10480813 | 1.59216629 | 7.87911870 |
| 1 | -2.45266280 | 0.84631697 | 8.32475173 |
| 8 | 2.36165553 | 3.05113668 | 4.17568321 |
| 8 | 3.97728296 | 4.34419696 | 5.66747244 |
| 8 | -5.67192442 | 4.18704869 | 5.83534891 |
| 8 | -6.70099331 | 2.18322898 | 7.10302609 |
| 6 | -7.39287340 | 1.06675064 | 7.70269034 |
| 1 | -6.93531273 | 0.78926993 | 8.66389185 |
| 1 | -7.35804709 | 0.20375727 | 7.02244949 |
| 6 | -8.82841032 | 1.50117171 | 7.97271805 |
| 1 | -9.33411208 | 0.70649304 | 8.55368050 |
| 1 | -8.80381034 | 2.41206834 | 8.59239872 |
| 8 | -9.51969405 | 1.72763112 | 6.73752843 |
| 6 | -10.71646247 | 2.51831230 | 6.88308949 |
| 1 | -11.25770159 | 2.22879953 | 7.80119119 |
| 1 | -11.34788927 | 2.27161859 | 6.02145929 |
| 6 | -10.47218876 | 4.03183555 | 6.90299440 |
| 1 | -11.37724821 | 4.53422524 | 7.29749567 |
| 1 | -9.63483930 | 4.27369151 | 7.57849422 |
| 8 | -10.21272361 | 4.48301476 | 5.56494487 |
| 6 | -9.87991456 | 5.87955699 | 5.46307574 |
| 1 | -10.45465153 | 6.46894074 | 6.19992522 |
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| 6 | -8.38734612 | 6.18926106 | 5.63159287 |
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| 8 | -7.69307009 | 5.66202874 | 4.49261301 |
| 6 | -6.30916763 | 6.00683991 | 4.37817468 |
| 1 | -6.18349934 | 7.10114414 | 4.25917653 |
| 1 | -5.98447134 | 5.52044356 | 3.45203473 |
| 6 | -5.38981157 | 5.56629818 | 5.53078745 |
| 1 | -4.35504950 | 5.71813827 | 5.19287762 |
| 1 | -5.54461063 | 6.16754676 | 6.44055801 |

| | | | |
|---|---|---|---|
| 6 | -0.98191039 | -1.11358116 | 2.28579630 |
| 1 | -1.94061551 | -1.47572618 | 2.64709147 |
| 6 | -0.34297697 | -0.05596465 | 2.93720242 |
| 6 | 0.89426918 | 0.43154234 | 2.49427302 |
| 1 | 1.38530830 | 1.25778772 | 3.00424034 |
| 6 | 1.48809106 | -0.16090686 | 1.37745179 |
| 1 | 2.44805982 | 0.21846636 | 1.02849323 |
| 6 | 0.87295458 | -1.23260735 | 0.69950956 |
| 6 | -0.36519228 | -1.69862671 | 1.17207681 |
| 1 | -0.85975969 | -2.52631230 | 0.66509780 |
| 6 | 1.53719889 | -1.85821215 | -0.51389067 |
| 1 | 0.95031760 | -2.69639119 | -0.90590894 |
| 1 | 2.54020436 | -2.23232877 | -0.26799294 |
| 1 | 1.65783331 | -1.12329100 | -1.32162393 |
| 16 | -1.11903123 | 0.65948391 | 4.43929637 |
| 7 | -1.09233011 | 2.36280470 | 4.17011563 |
| 6 | -1.84350471 | 2.92380888 | 3.15591874 |
| 6 | -2.82096605 | 2.21070354 | 2.39386470 |
| 1 | -3.07163146 | 1.19704470 | 2.68121922 |
| 6 | -3.48235672 | 2.78607288 | 1.31901374 |
| 1 | -4.21735052 | 2.19342163 | 0.77636370 |
| 6 | -3.22771745 | 4.11586525 | 0.93244470 |
| 1 | -3.74617122 | 4.56094656 | 0.08673766 |
| 6 | -2.31200480 | 4.84964120 | 1.66756862 |
| 1 | -2.11045696 | 5.88571396 | 1.39679521 |
| 6 | -1.61568875 | 4.30930451 | 2.78527272 |
| 6 | -0.74540510 | 5.24625114 | 3.45540190 |
| 1 | -0.65024646 | 6.20982611 | 2.93867882 |
| 7 | -0.11863634 | 5.12560428 | 4.59866336 |
| 6 | 0.70734620 | 6.21765798 | 5.01303900 |
| 6 | 0.59186908 | 6.69547383 | 6.33731649 |
| 1 | -0.11200151 | 6.21299829 | 7.00911986 |
| 6 | 1.35467087 | 7.77982471 | 6.77242027 |
| 6 | 2.28110779 | 8.39691253 | 5.87666815 |
| 6 | 2.40842030 | 7.89588941 | 4.57613426 |
| 1 | 3.13831927 | 8.32413783 | 3.89576507 |
| 6 | 1.62841195 | 6.81598279 | 4.14246631 |
| 1 | 1.78277583 | 6.40412341 | 3.14905418 |
| 8 | -0.17772854 | 0.47164643 | 5.58003856 |
| 8 | -2.48440987 | 0.07552345 | 4.56661811 |
| 8 | 1.28311674 | 8.33679703 | 8.02578396 |
| 8 | 2.99218897 | 9.45008349 | 6.39259989 |
| 6 | 4.14888471 | 9.93543573 | 5.67366287 |
| 1 | 3.83944153 | 10.43833718 | 4.74335765 |
| 1 | 4.81737622 | 9.09824582 | 5.42744574 |
| 6 | 4.86694546 | 10.93423804 | 6.57266368 |
| 1 | 5.62246541 | 11.47153367 | 5.96810735 |
| 1 | 4.14200604 | 11.67169072 | 6.95578709 |
| 8 | 5.48047530 | 10.22467865 | 7.65381224 |
| 6 | 5.98490910 | 11.05934827 | 8.71035604 |
| 1 | 5.33923893 | 11.94179130 | 8.84877712 |
| 1 | 7.00562132 | 11.40889584 | 8.47036249 |
| 6 | 6.00786744 | 10.25391318 | 10.00567497 |
| 1 | 6.41943018 | 9.25055742 | 9.80524853 |
| 1 | 6.66303938 | 10.75823979 | 10.74106457 |
| 8 | 4.66550853 | 10.15954500 | 10.50278058 |
| 6 | 4.47776761 | 9.18306339 | 11.53725658 |
| 1 | 4.92093442 | 9.53227095 | 12.48916854 |
| 1 | 4.95645083 | 8.22880935 | 11.26121828 |

| | | | |
|---|---|---|---|
| 6 | 2.98054626 | 8.96243948 | 11.72618772 |
| 1 | 2.79709972 | 8.46228838 | 12.69523336 |
| 1 | 2.47274941 | 9.94117857 | 11.74100041 |
| 8 | 2.49111148 | 8.15633136 | 10.64329061 |
| 6 | 1.08288844 | 8.26341470 | 10.41382132 |
| 1 | 0.78332220 | 9.32318969 | 10.34449759 |
| 1 | 0.50728942 | 7.79589585 | 11.23540820 |
| 6 | 0.73820978 | 7.55100792 | 9.11189011 |
| 1 | 1.17416107 | 6.54331146 | 9.09958825 |
| 1 | -0.35743003 | 7.47442967 | 9.02078088 |

Energy: -5880.43999841

**$ZnL_2$:**

Atomic Coordinates (Angstroms)

| | | | |
|---|---|---|---|
| 30 | 5.89039200 | 8.99935816 | 9.37240294 |
| 16 | 7.75945234 | 7.07103668 | 10.87660555 |
| 8 | 2.45252383 | 11.53913376 | 5.40270491 |
| 8 | 1.26660536 | 11.03388959 | 2.79007727 |
| 8 | 0.39991340 | 14.37686519 | 1.49109775 |
| 8 | 2.33893356 | 15.96795241 | 3.49522731 |
| 8 | 2.95385900 | 14.09000120 | 5.68638809 |
| 8 | 6.30704153 | 6.98865556 | 11.22532961 |
| 8 | 8.71224869 | 7.39405240 | 11.98010177 |
| 7 | 7.77246953 | 8.22055673 | 9.63057994 |
| 7 | 6.52664367 | 10.31760569 | 7.87282188 |
| 6 | 3.87326642 | 13.23428081 | 6.25077372 |
| 6 | 5.02260956 | 13.62858457 | 6.94200425 |
| 6 | 5.90626055 | 12.67298319 | 7.47037413 |
| 6 | 5.63603803 | 11.30781452 | 7.32019434 |
| 6 | 4.47056647 | 10.89679410 | 6.64038041 |
| 6 | 3.59552591 | 11.84250367 | 6.09635114 |
| 6 | 2.30851186 | 10.20009410 | 4.84945562 |
| 6 | 1.07684224 | 10.20248202 | 3.95153968 |
| 6 | 0.46140526 | 12.23160578 | 2.73519457 |
| 6 | 1.24008171 | 13.26957963 | 1.90892858 |
| 6 | 0.11764383 | 15.38718181 | 2.47809236 |
| 6 | 1.24289365 | 16.41964379 | 2.66420106 |
| 6 | 2.13590392 | 16.20267634 | 4.89767966 |
| 6 | 3.23515362 | 15.50626560 | 5.68710946 |
| 6 | 7.78562921 | 10.40093304 | 7.53180899 |
| 6 | 8.93084313 | 9.64170759 | 7.99128440 |
| 6 | 10.14878129 | 10.00105884 | 7.34636657 |
| 6 | 11.36418861 | 9.41579326 | 7.65805617 |
| 6 | 11.38887308 | 8.43748262 | 8.66606249 |
| 6 | 10.22643204 | 8.05542841 | 9.32455948 |
| 6 | 8.95515604 | 8.61720235 | 9.01320724 |
| 6 | 8.27815334 | 5.45356403 | 10.17977673 |
| 6 | 9.11004400 | 4.63279216 | 10.95135788 |
| 6 | 9.47379866 | 3.37750264 | 10.45589861 |
| 6 | 9.02641316 | 2.93416998 | 9.19647333 |
| 6 | 8.19456189 | 3.78446327 | 8.44699826 |
| 6 | 7.81126502 | 5.04221006 | 8.92804527 |
| 6 | 9.44833554 | 1.57739621 | 8.66208912 |

| | | | |
|---|---|---|---|
| 16 | 4.02272586 | 7.07285358 | 7.86401331 |
| 8 | 9.33861675 | 11.53988025 | 13.32523651 |
| 8 | 10.55705134 | 11.03796819 | 15.92504146 |
| 8 | 11.44840391 | 14.37386214 | 17.22262250 |
| 8 | 9.45695066 | 15.95570340 | 15.25537639 |
| 8 | 8.82278395 | 14.09000534 | 13.06056867 |
| 8 | 5.47510193 | 6.99285564 | 7.51458588 |
| 8 | 3.06942234 | 7.39761491 | 6.76146202 |
| 7 | 4.00908731 | 8.21948225 | 9.11261686 |
| 7 | 5.25331398 | 10.31340298 | 10.87588960 |
| 6 | 7.90338511 | 13.23318309 | 12.49791840 |
| 6 | 6.74723223 | 13.62597778 | 11.81716435 |
| 6 | 5.86485537 | 12.66927025 | 11.28891045 |
| 6 | 6.14241566 | 11.30439407 | 11.42917022 |
| 6 | 7.31429051 | 10.89518274 | 12.09900649 |
| 6 | 8.18871963 | 11.84192199 | 12.64218893 |
| 6 | 9.48866798 | 10.20120099 | 13.87813141 |
| 6 | 10.72978660 | 10.20336248 | 14.76307298 |
| 6 | 11.35201172 | 12.24376130 | 15.95289809 |
| 6 | 10.60027179 | 13.26631243 | 16.82207083 |
| 6 | 11.69982176 | 15.39195625 | 16.23530496 |
| 6 | 10.55995450 | 16.41268532 | 16.07426821 |
| 6 | 9.63838770 | 16.20270059 | 13.85209733 |
| 6 | 8.53341098 | 15.50457553 | 13.07229349 |
| 6 | 3.99464800 | 10.39247048 | 11.21929336 |
| 6 | 2.85025701 | 9.63294763 | 10.75824943 |
| 6 | 1.63236638 | 9.98791821 | 11.40574841 |
| 6 | 0.41742675 | 9.40253511 | 11.09245511 |
| 6 | 0.39306503 | 8.42878971 | 10.08002614 |
| 6 | 1.55547893 | 8.05094430 | 9.41905240 |
| 6 | 2.82635175 | 8.61263160 | 9.73217275 |
| 6 | 3.50576720 | 5.45320885 | 8.55721180 |
| 6 | 2.67641147 | 4.63233518 | 7.78298808 |
| 6 | 2.31432568 | 3.37544631 | 8.27558867 |
| 6 | 2.76085266 | 2.93052613 | 9.53475985 |
| 6 | 3.59013452 | 3.78091299 | 10.28694112 |
| 6 | 3.97173197 | 5.04028729 | 9.80877094 |
| 6 | 2.34095337 | 1.57181981 | 10.06586191 |
| 1 | 5.24682022 | 14.68244680 | 7.07727163 |
| 1 | 6.77888234 | 12.99796166 | 8.03096144 |
| 1 | 4.26890470 | 9.83765371 | 6.51850664 |
| 1 | 2.19080063 | 9.45731873 | 5.64994212 |
| 1 | 3.20507387 | 9.95313770 | 4.26412603 |
| 1 | 0.90356133 | 9.17116762 | 3.60884809 |
| 1 | 0.19386403 | 10.52383567 | 4.52309380 |
| 1 | 0.26647202 | 12.60342705 | 3.75069647 |
| 1 | -0.50399295 | 12.02082167 | 2.24420222 |
| 1 | 2.12133570 | 13.61953847 | 2.45972241 |
| 1 | 1.57332917 | 12.79944134 | 0.97665896 |
| 1 | -0.15917773 | 14.94130503 | 3.44682980 |
| 1 | -0.76691844 | 15.91356206 | 2.09187101 |
| 1 | 1.68185590 | 16.64677439 | 1.68491755 |
| 1 | 0.81859202 | 17.35257490 | 3.07769421 |
| 1 | 1.15688565 | 15.82683301 | 5.23635399 |
| 1 | 2.17879021 | 17.28749492 | 5.10800125 |
| 1 | 4.21252380 | 15.70283864 | 5.22239492 |
| 1 | 3.24242647 | 15.89165616 | 6.71950269 |
| 1 | 8.03792392 | 11.15657558 | 6.77775306 |
| 1 | 10.10621253 | 10.77211348 | 6.57813480 |

```
   1    12.27391202   9.71331867   7.14269580
   1    12.33012882   7.96772957   8.94804608
   1    10.30442826   7.31965683  10.11529167
   1     9.46593868   4.97492105  11.91931743
   1    10.11769595   2.73624430  11.05718949
   1     7.83579123   3.46442153   7.46981678
   1     7.16057370   5.68008196   8.33434434
   1     9.26169574   0.78402502   9.39774115
   1    10.52362675   1.56016504   8.43517559
   1     8.90913008   1.32340153   7.74285094
   1     6.51680861  14.67951774  11.68999259
   1     4.98717933  12.99346884  10.73580970
   1     7.52175499   9.83639636  12.21395258
   1     9.59838930   9.45763636  13.07725283
   1     8.59806067   9.95495242  14.47278798
   1    10.90277059   9.17275349  15.10765565
   1    11.60809246  10.51929071  14.18130892
   1    11.49687958  12.62490181  14.93264441
   1    12.34057179  12.03932433  16.39857851
   1     9.69605367  13.61752913  16.31055218
   1    10.30667395  12.78203308  17.76038451
   1    11.96421010  14.95385240  15.25954848
   1    12.58516052  15.92642410  16.60826738
   1    10.13287789  16.62690535  17.06170666
   1    10.96753470  17.35371030  15.66237775
   1    10.61528035  15.83675023  13.49685591
   1     9.58460243  17.28877638  13.65083049
   1     7.56058983  15.69227026  13.55009328
   1     8.51131891  15.89664520  12.04263801
   1     3.74179184  11.14478097  11.97647421
   1     1.67454384  10.75575859  12.17721036
   1    -0.49225230   9.69672547  11.60980805
   1    -0.54790906   7.95943022   9.79645129
   1     1.47775109   7.31875584   8.62498123
   1     2.32104380   4.97560975   6.81524196
   1     1.67242683   2.73413327   7.67221797
   1     3.94829512   3.45963740  11.26394119
   1     4.62061251   5.67814073  10.40445374
   1     2.53253843   0.77994739   9.32984619
   1     1.26491964   1.55114274  10.28889171
   1     2.87764070   1.31816622  10.98666210

Energy:     -6019.33530796
```

### HL ligand from LiNCS.HL:

```
Atomic Coordinates (Angstroms)
   ------------------------------

   6     6.05297739   7.33735017   0.92710725
   1     5.07747562   7.70230117   1.23810108
   6     6.16736413   6.45964886  -0.15936520
   6     7.41099226   5.96289949  -0.55720902
   1     7.47843855   5.26768345  -1.38892986
   6     8.55696203   6.35631503   0.14636651
   1     9.52619443   5.96531731  -0.15958676
   6     8.47508063   7.23770919   1.23707964
   6     7.20525464   7.71961418   1.61571181
   1     7.11637103   8.39757772   2.46378209
```

| | | | |
|---|---|---|---|
| 6 | 9.71646031 | 7.66116057 | 2.00063473 |
| 1 | 10.62153296 | 7.21448245 | 1.57480098 |
| 1 | 9.65406497 | 7.35830119 | 3.05471187 |
| 1 | 9.83777890 | 8.75269362 | 1.98543994 |
| 16 | 4.65706927 | 5.95469105 | -1.06229049 |
| 7 | 4.17179670 | 7.31577315 | -2.01757008 |
| 1 | 3.62033411 | 7.98763345 | -1.44147913 |
| 6 | 5.01837980 | 7.99186084 | -2.92465080 |
| 6 | 5.84766728 | 7.29914405 | -3.82787982 |
| 1 | 5.83830827 | 6.21341389 | -3.82238652 |
| 6 | 6.65098339 | 7.99213983 | -4.73545438 |
| 1 | 7.27913622 | 7.43068347 | -5.42463878 |
| 6 | 6.63803831 | 9.39451553 | -4.77809530 |
| 1 | 7.25772246 | 9.93148208 | -5.49260640 |
| 6 | 5.81223101 | 10.09166418 | -3.90076428 |
| 1 | 5.78742494 | 11.18074715 | -3.92891673 |
| 6 | 4.99190764 | 9.42682187 | -2.95886456 |
| 6 | 4.16824061 | 10.25425870 | -2.07785340 |
| 1 | 4.33130283 | 11.33818061 | -2.18543667 |
| 7 | 3.31487064 | 9.77928541 | -1.22286500 |
| 6 | 2.49781459 | 10.59759114 | -0.40970323 |
| 6 | 1.91324218 | 9.97172447 | 0.71824128 |
| 1 | 2.12474032 | 8.91934825 | 0.88278263 |
| 6 | 1.08874451 | 10.67848535 | 1.59409855 |
| 6 | 0.81184347 | 12.05516309 | 1.33839097 |
| 6 | 1.36541806 | 12.66231243 | 0.20265535 |
| 1 | 1.13609645 | 13.70076567 | -0.02020087 |
| 6 | 2.20119522 | 11.94812088 | -0.66539006 |
| 1 | 2.58370159 | 12.44553723 | -1.55273610 |
| 8 | 5.02999366 | 4.84963517 | -1.97403791 |
| 8 | 3.55285983 | 5.81261706 | -0.08517411 |
| 8 | 0.48974415 | 10.15209175 | 2.70998466 |
| 8 | -0.01563116 | 12.67329369 | 2.24034969 |
| 6 | -0.08364588 | 14.11685268 | 2.25960235 |
| 1 | -0.65546078 | 14.48656525 | 1.39335676 |
| 1 | 0.92952466 | 14.54313468 | 2.23158761 |
| 6 | -0.78899310 | 14.52887205 | 3.54592550 |
| 1 | -1.03184246 | 15.60691279 | 3.48419221 |
| 1 | -1.73239962 | 13.96660238 | 3.64455061 |
| 8 | 0.07719717 | 14.25522430 | 4.65226465 |
| 6 | -0.54677368 | 14.35662574 | 5.94418517 |
| 1 | -1.59860167 | 14.03207974 | 5.89224150 |
| 1 | -0.52206978 | 15.40220915 | 6.30105589 |
| 6 | 0.19997879 | 13.46091445 | 6.92742818 |
| 1 | 1.28679521 | 13.60301501 | 6.80134206 |
| 1 | -0.06998777 | 13.74823765 | 7.96147221 |
| 8 | -0.16574230 | 12.09896894 | 6.66767412 |
| 6 | 0.63415785 | 11.12698584 | 7.35622182 |
| 1 | 0.40691296 | 11.13139414 | 8.43914050 |
| 1 | 1.70781540 | 11.34505482 | 7.22663261 |
| 6 | 0.32282393 | 9.74967336 | 6.77923703 |
| 1 | 0.68497292 | 8.96713945 | 7.47068048 |
| 1 | -0.76932422 | 9.64304311 | 6.67656184 |
| 8 | 0.96559922 | 9.62493943 | 5.49995720 |
| 6 | 0.34503039 | 8.69365058 | 4.60500547 |
| 1 | -0.74301934 | 8.86691489 | 4.56140926 |
| 1 | 0.51843228 | 7.65059873 | 4.92999834 |
| 6 | 0.94585171 | 8.87632681 | 3.21747439 |
| 1 | 2.04349373 | 8.86505026 | 3.27637750 |

```
   1     0.61315018   8.05897798   2.55927116

Energy:     -2120.46836294
```

**HL ligand from $ZnL_2$:**

```
Atomic Coordinates (Angstroms)
   ----------------------------

   6     7.68704746  -5.47531786  10.52869759
   1     8.19187720  -5.43151373  11.48936202
   6     6.94225168  -6.60481982  10.18018857
   6     6.26265035  -6.67379845   8.95667026
   1     5.67221482  -7.55096118   8.70466926
   6     6.33803275  -5.59380758   8.07577263
   1     5.80590037  -5.64477892   7.12663155
   6     7.08237498  -4.44044292   8.39779639
   6     7.75055650  -4.40005412   9.63290152
   1     8.32665717  -3.51716794   9.90577461
   6     7.14146811  -3.26989742   7.43377797
   1     7.84719205  -2.50439841   7.77446975
   1     7.44919096  -3.59551887   6.43144709
   1     6.15552936  -2.79573400   7.33048187
  16     6.84074458  -8.01740002  11.33926851
   7     7.83077078  -9.27477945  10.67523418
   1     7.30171764  -9.82197636   9.96371127
   6     9.18446713  -9.11714644  10.30750376
   6    10.10258942  -8.42266568  11.11926197
   1     9.75690572  -7.99354396  12.05476885
   6    11.44254372  -8.30831841  10.74483563
   1    12.13022082  -7.76884378  11.39355010
   6    11.90875491  -8.89636671   9.55912780
   1    12.95526929  -8.81331194   9.27516353
   6    11.01567716  -9.59802988   8.75463365
   1    11.36627538 -10.06624435   7.83523632
   6     9.64776980  -9.72687948   9.09291469
   6     8.79337171 -10.47741751   8.17385593
   1     9.29436240 -10.81301322   7.25202314
   7     7.53925043 -10.73292163   8.38977721
   6     6.75209878 -11.50371729   7.50403101
   6     5.35040464 -11.32146584   7.58732252
   1     4.97324574 -10.61000257   8.31533593
   6     4.47755540 -12.03098992   6.76245081
   6     5.00459261 -12.98136768   5.83749358
   6     6.38975919 -13.18171076   5.78005376
   1     6.80288432 -13.92143225   5.10036477
   6     7.26069158 -12.45263594   6.60087965
   1     8.32620687 -12.66147779   6.55398076
   8     5.47558604  -8.58729094  11.26684554
   8     7.43146032  -7.58490666  12.62576159
   8     3.10936367 -11.90236156   6.76609825
   8     4.07460801 -13.65420833   5.08128584
   6     4.52876408 -14.48437505   3.98820354
   1     5.17073029 -13.90136019   3.31190915
   1     5.09589164 -15.34707148   4.37237071
   6     3.29821652 -14.98503117   3.24404169
   1     2.59350923 -15.42049629   3.97010836
   1     3.60678088 -15.78298288   2.54332815
   8     2.71230452 -13.89129469   2.52249369
```

```
   6     1.41409071 -14.17506630   1.95482936
   1     1.28574829 -13.44674032   1.14491311
   1     1.40274419 -15.18922485   1.51337625
   6     0.23793550 -14.04249723   2.93720570
   1     0.40547510 -14.66165535   3.83561943
   1    -0.66246802 -14.42111021   2.43210733
   8    -0.07779428 -12.69526779   3.31825034
   6     0.79608564 -12.11049183   4.31705712
   1     1.09579906 -12.87275817   5.05108218
   1     1.70716067 -11.70734356   3.85652830
   6     0.00483587 -10.97949993   4.99383334
   1    -0.88149322 -11.38516473   5.50703243
   1    -0.33800149 -10.26785087   4.23368511
   8     0.82306300 -10.21331504   5.90432491
   6     1.02203103 -10.78921090   7.21070776
   1     0.52246323 -10.15053587   7.95783377
   1     0.58521204 -11.79606116   7.27555593
   6     2.50607465 -10.84983478   7.55772508
   1     2.63023216 -11.06357245   8.63100609
   1     2.98051686  -9.88554932   7.32745955

Energy:     -2120.46601714
```

### HL ligand A from $CuL_2$:

```
Atomic Coordinates (Angstroms)
   ------------------------------

6     4.15996221   1.85339635   6.38239293
   1     4.84668338   2.62805841   6.71100478
   6     2.88023927   2.19613932   5.92976256
   6     1.99006873   1.21962237   5.47016625
   1     1.00798822   1.50159543   5.09923914
   6     2.39222706  -0.11998027   5.47147978
   1     1.70352252  -0.88018362   5.10608857
   6     3.66936352  -0.49743117   5.92552409
   6     4.54392434   0.50912548   6.37693282
   1     5.54190374   0.24197447   6.72264265
   6     4.10407378  -1.95170441   5.92408540
   1     3.31574484  -2.60596414   5.53613218
   1     4.35643116  -2.29026917   6.93815351
   1     4.99896886  -2.09610208   5.30379454
  16     2.35461966   3.94786453   5.93473494
   7     1.34900620   4.15681438   7.33148069
   1     0.39452361   3.77770608   7.15421839
   6     1.75234053   3.93656789   8.66671750
   6     3.00759045   4.35542236   9.15097622
   1     3.69687570   4.84450031   8.47010301
   6     3.35408014   4.17062041  10.49045288
   1     4.33068448   4.50507826  10.83573296
   6     2.45218487   3.58424310  11.39159611
   1     2.72103536   3.45393544  12.43729256
   6     1.20208877   3.18200809  10.93129848
   1     0.48860108   2.73218828  11.62124380
   6     0.82035084   3.33226922   9.57697531
   6    -0.51148506   2.86300248   9.19799924
   1    -1.09565859   2.42188777  10.02116744
   7    -1.00754168   2.95969368   8.00231930
   6    -2.27746604   2.43781370   7.66497532
```

| | | | |
|---|---|---|---|
| 6 | -2.93683054 | 3.03738699 | 6.56574078 |
| 1 | -2.43725053 | 3.85890934 | 6.06135883 |
| 6 | -4.19478916 | 2.60033110 | 6.14937011 |
| 6 | -4.82850448 | 1.52736704 | 6.84301389 |
| 6 | -4.15135991 | 0.90513339 | 7.90122969 |
| 1 | -4.60420429 | 0.05449295 | 8.40372453 |
| 6 | -2.89007064 | 1.35179603 | 8.31524844 |
| 1 | -2.37815911 | 0.82525490 | 9.11681585 |
| 8 | 1.41770674 | 4.15678923 | 4.80831931 |
| 8 | 3.56508876 | 4.78359780 | 6.10193022 |
| 8 | -4.89662845 | 3.12104390 | 5.08719944 |
| 8 | -6.07339401 | 1.17043917 | 6.39004106 |
| 6 | -6.97938316 | 0.49054807 | 7.29201045 |
| 1 | -6.80545458 | 0.82332598 | 8.32430048 |
| 1 | -6.82576306 | -0.59831698 | 7.23105313 |
| 6 | -8.40517470 | 0.83415211 | 6.87890794 |
| 1 | -8.54670222 | 0.63998326 | 5.80302212 |
| 1 | -9.09579678 | 0.18156206 | 7.44585197 |
| 8 | -8.63843903 | 2.21655241 | 7.17491900 |
| 6 | -9.96075911 | 2.68740523 | 6.84979408 |
| 1 | -10.62843195 | 2.55079832 | 7.71891457 |
| 1 | -10.37802895 | 2.12828835 | 5.99798945 |
| 6 | -9.88545748 | 4.16537398 | 6.47763380 |
| 1 | -10.87380039 | 4.63810834 | 6.62649391 |
| 1 | -9.16056482 | 4.66292811 | 7.14135334 |
| 8 | -9.49826698 | 4.27055249 | 5.09555696 |
| 6 | -8.95612362 | 5.54585159 | 4.70433619 |
| 1 | -9.36767944 | 6.35651827 | 5.32882946 |
| 1 | -9.27786287 | 5.71085723 | 3.66799482 |
| 6 | -7.42555639 | 5.59540454 | 4.75853494 |
| 1 | -7.09876678 | 6.63682761 | 4.56971986 |
| 1 | -7.06987072 | 5.29666689 | 5.75790995 |
| 8 | -6.91640486 | 4.71713355 | 3.74287323 |
| 6 | -5.51362890 | 4.81450534 | 3.47554991 |
| 1 | -5.24650078 | 5.83752697 | 3.14658638 |
| 1 | -5.34343526 | 4.12862507 | 2.63760914 |
| 6 | -4.56751986 | 4.44949629 | 4.62648279 |
| 1 | -3.53877165 | 4.49443378 | 4.23497346 |
| 1 | -4.64539199 | 5.15545633 | 5.46712318 |

Energy: -2120.46282555

### HL ligand B from $CuL_2$:

Atomic Coordinates (Angstroms)

| | | | |
|---|---|---|---|
| 6 | -0.54388240 | 0.17208991 | 3.21058455 |
| 1 | -1.52703206 | -0.28865467 | 3.17865518 |
| 6 | -0.25469004 | 1.14301928 | 4.17320737 |
| 6 | 1.01684227 | 1.72698215 | 4.25385101 |
| 1 | 1.23407504 | 2.46436239 | 5.02240092 |
| 6 | 2.00385738 | 1.32946833 | 3.35033448 |
| 1 | 2.99501201 | 1.77651826 | 3.41757731 |
| 6 | 1.74217238 | 0.35635270 | 2.36427537 |
| 6 | 0.45922116 | -0.21387027 | 2.31212819 |
| 1 | 0.23711326 | -0.97504858 | 1.56568524 |
| 6 | 2.82910102 | -0.06403822 | 1.39197693 |
| 1 | 2.47158693 | -0.83250616 | 0.69788548 |

| | | | |
|---|---|---|---|
| 1 | 3.70090549 | -0.46807556 | 1.92421032 |
| 1 | 3.18144361 | 0.79061276 | 0.79852474 |
| 16 | -1.55083616 | 1.66739124 | 5.35209744 |
| 7 | -2.16715259 | 3.17786907 | 4.76614587 |
| 1 | -1.51281351 | 3.95475994 | 5.00002017 |
| 6 | -2.77332576 | 3.37477167 | 3.50562745 |
| 6 | -3.69888782 | 2.45913647 | 2.96671516 |
| 1 | -3.93855831 | 1.56215038 | 3.52872197 |
| 6 | -4.32074471 | 2.70945912 | 1.74229265 |
| 1 | -5.03220228 | 1.98413583 | 1.35165252 |
| 6 | -4.05580290 | 3.88913121 | 1.03007137 |
| 1 | -4.55217677 | 4.08669466 | 0.08277094 |
| 6 | -3.15697987 | 4.81067349 | 1.55880127 |
| 1 | -2.94731256 | 5.73466128 | 1.02055106 |
| 6 | -2.49027047 | 4.58481751 | 2.78628087 |
| 6 | -1.55548098 | 5.61247032 | 3.24268140 |
| 1 | -1.45160704 | 6.47499464 | 2.56532344 |
| 7 | -0.89750694 | 5.55804108 | 4.36010173 |
| 6 | 0.04401619 | 6.54642814 | 4.72980001 |
| 6 | 0.25691396 | 6.73348495 | 6.11657052 |
| 1 | -0.31575131 | 6.12124130 | 6.80670761 |
| 6 | 1.16365327 | 7.68350648 | 6.58697729 |
| 6 | 1.90928567 | 8.46553919 | 5.65296313 |
| 6 | 1.71767949 | 8.25480853 | 4.28132884 |
| 1 | 2.30068830 | 8.82046845 | 3.55995891 |
| 6 | 0.79487308 | 7.30667614 | 3.81718406 |
| 1 | 0.69934450 | 7.14083999 | 2.74710238 |
| 8 | -0.89817084 | 2.03797934 | 6.62757280 |
| 8 | -2.64084634 | 0.66684984 | 5.30090764 |
| 8 | 1.41651063 | 7.94134835 | 7.91038726 |
| 8 | 2.78439763 | 9.36869976 | 6.20107905 |
| 6 | 3.79567543 | 9.96963452 | 5.36251301 |
| 1 | 3.34068407 | 10.70173267 | 4.67594656 |
| 1 | 4.30943288 | 9.19517840 | 4.77466750 |
| 6 | 4.79080221 | 10.67797076 | 6.27362869 |
| 1 | 5.44837931 | 11.31331010 | 5.65003936 |
| 1 | 4.24643264 | 11.32941137 | 6.97736262 |
| 8 | 5.54621232 | 9.69076263 | 6.98319520 |
| 6 | 6.34819848 | 10.20568252 | 8.06031320 |
| 1 | 5.84269974 | 11.05517152 | 8.54742179 |
| 1 | 7.32515546 | 10.55396523 | 7.67868588 |
| 6 | 6.56285568 | 9.10034893 | 9.08940150 |
| 1 | 6.82619819 | 8.16271142 | 8.57125008 |
| 1 | 7.40312740 | 9.37699468 | 9.75435878 |
| 8 | 5.35235588 | 8.94086336 | 9.84121334 |
| 6 | 5.31316118 | 7.76679742 | 10.66540228 |
| 1 | 5.99547627 | 7.87397847 | 11.52984887 |
| 1 | 5.62026907 | 6.87750538 | 10.08959549 |
| 6 | 3.88556844 | 7.57766698 | 11.16808695 |
| 1 | 3.88262705 | 6.87532757 | 12.02162167 |
| 1 | 3.49643330 | 8.54839753 | 11.51661971 |
| 8 | 3.07923687 | 7.06580422 | 10.09470991 |
| 6 | 1.67882761 | 7.34023632 | 10.21630190 |
| 1 | 1.51247277 | 8.40781207 | 10.43775718 |
| 1 | 1.22330465 | 6.74193647 | 11.02784075 |
| 6 | 0.99428265 | 6.97811516 | 8.90472803 |
| 1 | 1.28295233 | 5.96425885 | 8.59402097 |
| 1 | -0.09848352 | 7.01618475 | 9.03677688 |

Energy:  -2120.46892128

Table 2. The differences in energies of B3LYP optimized HL ligands, when starting from different structural geometries.

| Initial structural geometry of HL taken from | ΔE, kJ $mol^{-1}$ |
|---|---|
| HL | 0.6 |
| LiNCS·HL | 1.5 |
| $ZnL_2$ | 7.6 |
| $CuL_2$, ligand A | 16.0 |
| $CuL_2$, ligand B | 0 |