Supporting Information

Density functional theory study on silver and bis-silver complexes with lighter tetrylene – Are silver and bis-silver carbenes candidates for SARS-CoV-2 inhibition? An insight from molecular docking simulation

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Table S1. Cartesian coordinates of the optimized ligands NHC_{Ph} to $NHGe_{Ph}$ (**NHC** – **NHGe**) at the BP86/def2-SVP level of theory.

$[NHC_{Ph}]$ (**NHC**)

C	-0.70886000	1.22998500	-0.09997800
C	0.70886100	1.22998100	-0.09997500
C	1.43613400	2.42014000	-0.27766500
C	0.70655900	3.61025600	-0.43915500
C	-0.70652700	3.61026100	-0.43916200
C	-1.43611600	2.42015400	-0.27767900
C	-0.00000500	-0.97779300	0.06392400
H	2.53468400	2.42019800	-0.31097900
H	1.24886000	4.55812800	-0.58077500
H	-1.24881800	4.55813800	-0.58079000
H	-2.53466600	2.42022900	-0.31100600
N	1.08431600	-0.12580000	0.01265900
N	-1.08432500	-0.12579200	0.01265400
C	2.42842100	-0.61369900	0.07005500
C	3.40111200	0.04576600	0.84849600
C	2.76713500	-1.78325800	-0.63983600
C	4.71341100	-0.45535400	0.89603200
H	3.12479500	0.93105700	1.44018600
C	4.07738600	-2.28084100	-0.57665500
H	1.98418700	-2.29120000	-1.22124200
C	5.05750400	-1.61676800	0.18376500
H	5.46819500	0.06188200	1.50941700
H	4.33624900	-3.19581100	-1.13286700
H	6.08618900	-2.00778200	0.22559600
C	-2.42842800	-0.61369100	0.07005300
C	-3.40113700	0.04580600	0.84844400
C	-2.76712500	-1.78328800	-0.63978500
C	-4.71343500	-0.45531900	0.89598300
H	-3.12483800	0.93112400	1.44010200
C	-4.07737400	-2.28087600	-0.57660200
H	-1.98416300	-2.29125500	-1.22115000
C	-5.05751000	-1.61677000	0.18376700
H	-5.46823100	0.06194400	1.50933000
H	-4.33622200	-3.19587500	-1.13277300
H	-6.08619400	-2.00778700	0.22559900

$[NHSi_{Ph}]$ (**NHSi**)

C	-0.71491200	1.03104800	-0.16157800
C	0.71490600	1.03106200	-0.16160600
C	1.42131800	2.24011700	-0.33331000
C	0.70522800	3.43702200	-0.48992200
C	-0.70533000	3.43700500	-0.48987900
C	-1.42137400	2.24007700	-0.33323300
H	2.52090300	2.23702700	-0.35607200

H	1.25455600	4.38195600	-0.62459500
H	-1.25469100	4.38192500	-0.62451100
H	-2.52096100	2.23694500	-0.35592700
N	1.24153100	-0.26418200	-0.04170400
N	-1.24150100	-0.26421400	-0.04165500
C	2.64508600	-0.51596300	0.04844700
C	3.42838300	0.07604000	1.06598000
C	3.25386400	-1.41110000	-0.85796200
C	4.79702100	-0.21883700	1.16314300
H	2.95005000	0.75516400	1.78832400
C	4.62135300	-1.71446100	-0.74389100
H	2.64395300	-1.85846500	-1.65835600
C	5.39915700	-1.11606800	0.26147100
H	5.39664800	0.24692000	1.96150500
H	5.08239500	-2.41753600	-1.45569200
H	6.47235200	-1.34860800	0.34500900
C	-2.64506600	-0.51599900	0.04848300
C	-3.42831100	0.07580500	1.06616900
C	-3.25389000	-1.41091400	-0.85811000
C	-4.79695600	-0.21904700	1.16330400
H	-2.94993100	0.75476400	1.78863800
C	-4.62138800	-1.71425700	-0.74406600
H	-2.64401300	-1.85812400	-1.65861500
C	-5.39914200	-1.11606300	0.26145000
H	-5.39654900	0.24655000	1.96178500
H	-5.08247300	-2.41715800	-1.45601200
H	-6.47234200	-1.34858700	0.34496700
Si	0.00001500	-1.57048600	0.08240900

[$NHGe_{Ph}$] (**NHGe**)

C	-0.71746100	1.18661200	-0.17415200
C	0.71745900	1.18661700	-0.17417500
C	1.41779600	2.40439900	-0.33633900
C	0.70556200	3.60282000	-0.48173300
C	-0.70560600	3.60281300	-0.48170300
C	-1.41782100	2.40438500	-0.33627900
H	2.51730400	2.40196700	-0.36199000
H	1.25635000	4.54795800	-0.60911200
H	-1.25640900	4.54794700	-0.60905300
H	-2.51732900	2.40193600	-0.36188100
N	1.27472800	-0.09002400	-0.07098300
N	-1.27471800	-0.09003500	-0.07094300
C	2.67681700	-0.31740200	0.03263200
C	3.44487000	0.28204600	1.05931900
C	3.30897200	-1.20512500	-0.86713000
C	4.81503800	0.00130300	1.17214100
H	2.95166600	0.95534000	1.77709000
C	4.67809800	-1.49399700	-0.73751600
H	2.71445700	-1.65542300	-1.67772300

C	5.43812800	-0.88874600	0.27736600
H	5.40002900	0.47281400	1.97805900
H	5.15502700	-2.19041700	-1.44549200
H	6.51272200	-1.10965500	0.37325600
C	-2.67681400	-0.31740500	0.03264900
C	-3.44482800	0.28187300	1.05946300
C	-3.30899900	-1.20496900	-0.86724500
C	-4.81499700	0.00113100	1.17227300
H	-2.95158800	0.95503100	1.77733800
C	-4.67813200	-1.49382700	-0.73766000
H	-2.71450400	-1.65514900	-1.67791900
C	-5.43812500	-0.88874100	0.27734700
H	-5.39996200	0.47250600	1.97828900
H	-5.15509000	-2.19011600	-1.44574400
H	-6.51272000	-1.10964900	0.37322600
Ge	0.00000700	-1.51398200	0.04967500

Table S2. Cartesian coordinates of the optimized silver- tetrylene complexes AgCl-NHC_{Ph} to AgCl-$NHGe_{Ph}$ (**Ag-NHC** – **Ag-NHGe**) at the BP86/def2-SVP level of theory.

[AgCl-NHC_{Ph}] (**Ag-NHC**)

C	-0.70929300	2.31930600	-0.09334500
C	0.70620900	2.32003100	-0.09340300
C	1.43844000	3.51554100	-0.19118200
C	0.70489700	4.70965600	-0.27566300
C	-0.71043700	4.70892600	-0.27565900
C	-1.44274900	3.51405400	-0.19112500
C	-0.00043900	0.13849600	-0.00370600
H	2.53754300	3.51208500	-0.20999000
H	1.24407100	5.66642500	-0.35219800
H	-1.25059200	5.66514100	-0.35218300
H	-2.54184400	3.50945900	-0.20992000
Ag	0.00135200	-1.91693300	0.08390600
Cl	0.00364600	-4.21974700	0.14116200
N	1.09536800	0.97077400	-0.03762600
N	-1.09705500	0.96963200	-0.03754900
C	2.45620800	0.51078700	-0.01175300
C	3.33819600	0.99999700	0.97112700
C	2.89229600	-0.43406400	-0.95993500
C	4.66635800	0.54332600	0.99641100
H	2.97739200	1.71545200	1.72572800
C	4.21871200	-0.89316300	-0.91660700
H	2.19006900	-0.80566600	-1.72089800
C	5.10808000	-0.40397800	0.05608800
H	5.35478200	0.91943800	1.76926300
H	4.55632600	-1.63967200	-1.65192700
H	6.14727700	-0.76679000	0.08540500
C	-2.45735800	0.50808300	-0.01158900
C	-3.34026200	0.99731800	0.97046600
C	-2.89195800	-0.43842800	-0.95879900
C	-4.66785100	0.53899400	0.99587000
H	-2.98058400	1.71403900	1.72440100
C	-4.21780500	-0.89915800	-0.91533600
H	-2.18900200	-0.80996200	-1.71912800
C	-5.10808800	-0.40996600	0.05651800
H	-5.35699200	0.91511400	1.76808000
H	-4.55426600	-1.64691700	-1.64991100
H	-6.14684800	-0.77402000	0.08591600

[AgCl-$NHSi_{Ph}$] (**Ag-NHSi**)

C	-0.90871900	2.29256300	-0.15892200
C	0.51667000	2.40200600	-0.16196300
C	1.12946600	3.65934900	-0.33539800
C	0.32178600	4.79588300	-0.49187100
C	-1.08471000	4.68783000	-0.48757900

C	-1.70786800	3.44106800	-0.32764300
H	2.22588400	3.73943300	-0.35960600
H	0.79607800	5.77989300	-0.62947200
H	-1.70460000	5.58780400	-0.62138400
H	-2.80362600	3.35162200	-0.34541100
Ag	0.21015400	-2.48322700	0.07306600
Cl	0.46242100	-4.76715700	-0.11444700
N	1.15119500	1.15141800	-0.03819000
N	-1.34538600	0.95970700	-0.03380800
C	2.57458300	0.99697600	0.03984000
C	3.31426400	1.64260100	1.05505300
C	3.23398800	0.15046600	-0.87577900
C	4.70154400	1.44743200	1.14040300
H	2.79292300	2.28181700	1.78394700
C	4.62057400	-0.05346600	-0.77111100
H	2.65445300	-0.34142000	-1.67256200
C	5.35848500	0.59792300	0.23117700
H	5.27207000	1.95191400	1.93616200
H	5.12493000	-0.72291400	-1.48523300
H	6.44563900	0.44107300	0.30801400
C	-2.73007800	0.59404200	0.04352600
C	-3.55275100	1.10402000	1.07184300
C	-3.26137100	-0.32166500	-0.88834100
C	-4.89611900	0.70585700	1.15412000
H	-3.12855600	1.79908100	1.81266200
C	-4.60307100	-0.72773600	-0.78790600
H	-2.61842500	-0.70763700	-1.69475300
C	-5.42500100	-0.21187300	0.22784400
H	-5.53143400	1.10555600	1.96025100
H	-5.00667000	-1.44874200	-1.51581000
H	-6.47732300	-0.52736300	0.30177100
Si	-0.00217700	-0.18102400	0.08379800

[AgCl-NHGe$_{Ph}$] (**Ag-NHGe**)

C	-0.96998800	2.31819400	-0.19402700
C	0.45703500	2.46377300	-0.20015800
C	1.03140700	3.73825100	-0.40511800
C	0.19916500	4.85038700	-0.58787100
C	-1.20492100	4.70725100	-0.57893000
C	-1.79284300	3.44988400	-0.38911600
H	2.12522900	3.84570000	-0.43501900
H	0.65003700	5.84153800	-0.75073300
H	-1.84851700	5.58697200	-0.73397700
H	-2.88603100	3.33310200	-0.40552400
Ag	0.28456000	-2.60240400	0.05529400
Cl	0.57980800	-4.87011500	-0.20278700
N	1.14848300	1.25542500	-0.05200500
N	-1.40287500	0.99521100	-0.04333600
C	2.57129700	1.15931400	0.04463300
C	3.28258800	1.87481400	1.03474300

C	3.26990100	0.29295700	-0.82414000
C	4.67430000	1.72883700	1.14068900
H	2.73520900	2.52941900	1.73010900
C	4.66101700	0.13925000	-0.69842100
H	2.71549500	-0.25188400	-1.60445600
C	5.36822100	0.85997800	0.27836900
H	5.21984400	2.28817800	1.91716500
H	5.19352000	-0.54491700	-1.37739100
H	6.45907300	0.74281700	0.37146000
C	-2.77924600	0.61886800	0.05116700
C	-3.60595400	1.14362400	1.07025600
C	-3.30475200	-0.32897300	-0.85314500
C	-4.94284300	0.72862600	1.17042300
H	-3.18796500	1.86366300	1.79044700
C	-4.64007100	-0.75060300	-0.73522700
H	-2.66113300	-0.72497400	-1.65434400
C	-5.46413900	-0.22018700	0.27136500
H	-5.57938400	1.14014900	1.96969000
H	-5.03758200	-1.49500300	-1.44273000
H	-6.51161200	-0.54798500	0.35922000
Ge	0.00945200	-0.21568000	0.13153400

Table S3. Cartesian coordinates of the optimized bis-silver-tetrylene complexes (NHC_{Ph}-$AgCl)_2$ to ($NHGe_{Ph}$-$AgCl)_2$ (**Ag-NHC-bis** – **Ag-NHGe-bis**) at the BP86/def2-SVP level of theory.

[(NHC_{Ph}-$AgCl)_2$] (**Ag-NHC-bis**)

C	5.37519200	0.70768400	-0.26940400
C	5.37520000	-0.70767400	-0.26930300
C	6.48803400	-1.44069000	-0.71458600
C	7.60478200	-0.70772200	-1.14731100
C	7.60477200	0.70763800	-1.14741400
C	6.48801200	1.44065300	-0.71480000
C	3.32303900	0.00004300	0.46773700
H	6.47776100	-2.53990600	-0.73137300
H	8.49627200	-1.24730100	-1.50263500
H	8.49625700	1.24717800	-1.50281200
H	6.47772500	2.53986600	-0.73172900
Ag	1.37515900	0.00038600	1.16117300
Cl	0.76229800	0.00026500	-2.16050400
N	4.10451600	-1.09494200	0.18732700
N	4.10452100	1.09499600	0.18723000
C	3.65071200	-2.45539500	0.28073500
C	4.35235800	-3.37038000	1.08915600
C	2.51390300	-2.85287100	-0.44890600
C	3.91319000	-4.70276500	1.16181900
H	5.22466100	-3.03303300	1.66982600
C	2.08246500	-4.18738500	-0.35963200
H	1.98301900	-2.11865100	-1.08045000
C	2.77883600	-5.11265400	0.43849600
H	4.45522800	-5.42055000	1.79741400
H	1.19443500	-4.50227200	-0.92954900
H	2.43705000	-6.15808300	0.49903000
C	3.65073400	2.45546400	0.28062900
C	4.35247700	3.37047400	1.08894000
C	2.51381400	2.85290200	-0.44885600
C	3.91328500	4.70284700	1.16165700
H	5.22486500	3.03315100	1.66949700
C	2.08234700	4.18740500	-0.35951300
H	1.98284200	2.11867800	-1.08032900
C	2.77880600	5.11269800	0.43850500
H	4.45539700	5.42065200	1.79716800
H	1.19420600	4.50225500	-0.92927900
H	2.43698700	6.15811200	0.49909500
C	-5.37533200	0.70703800	0.26937000
C	-5.37496800	-0.70831900	0.26954600
C	-6.48758700	-1.44153700	0.71503300
C	-7.60451100	-0.70877500	1.14765300
C	-7.60487900	0.70658500	1.14746100
C	-6.48833000	1.43980600	0.71465100
C	-3.32302500	-0.00019400	-0.46772400
H	-6.47703000	-2.54074700	0.73203500
H	-8.49584500	-1.24851800	1.50312300

H	-8.49649400	1.24596200	1.50278200
H	-6.47832800	2.53902500	0.73135600
Ag	-1.37516100	0.00015000	-1.16122200
Cl	-0.76237000	0.00136000	2.16030100
N	-4.10421000	-1.09533400	-0.18710600
N	-4.10477900	1.09460300	-0.18737000
C	-3.65009600	-2.45569200	-0.28044000
C	-4.35169600	-3.37093200	-1.08861600
C	-2.51302400	-2.85282100	0.44898000
C	-3.91222700	-4.70321800	-1.16124500
H	-5.22420200	-3.03385000	-1.66913500
C	-2.08129100	-4.18724500	0.35974400
H	-1.98215700	-2.11842800	1.08033100
C	-2.77761500	-5.11276400	-0.43813000
H	-4.45423200	-5.42119500	-1.79665300
H	-1.19305200	-4.50185800	0.92948800
H	-2.43559000	-6.15811600	-0.49863300
C	-3.65133700	2.45517500	-0.28089900
C	-4.35314100	3.36986600	-1.08951500
C	-2.51471700	2.85303800	0.44882200
C	-3.91430400	4.70235200	-1.16231400
H	-5.22529900	3.03221300	-1.67022600
C	-2.08360000	4.18764700	0.35939200
H	-1.98371300	2.11903300	1.08052800
C	-2.78011900	5.11262500	-0.43894000
H	-4.45645800	5.41991700	-1.79805900
H	-1.19569700	4.50283500	0.92934300
H	-2.43858000	6.15812700	-0.49960200

[$(NHC_{Ph}\text{-}AgCl)_2$] (**Ag-NHSi-bis**)

C	5.16591100	0.71479300	-0.25691800
C	5.16610000	-0.71434500	-0.25684200
C	6.34319800	-1.41815200	-0.57078100
C	7.51864700	-0.70287900	-0.86285000
C	7.51846000	0.70388600	-0.86292800
C	6.34282200	1.41887900	-0.57093700
H	6.33602500	-2.51766000	-0.59483100
H	8.44032900	-1.25492300	-1.10428700
H	8.43999500	1.25614800	-1.10442700
H	6.33535700	2.51838200	-0.59510900
Ag	0.63848600	-0.00023400	1.34770100
Cl	1.69162100	-0.00034200	-2.17355700
N	3.89285900	-1.26240600	0.02113500
N	3.89252700	1.26254700	0.02100400
C	3.65991200	-2.65366900	0.22602100
C	4.41878800	-3.38463400	1.16979500
C	2.62744900	-3.30620800	-0.48395500
C	4.15013900	-4.74448000	1.38787000
H	5.20972700	-2.87406100	1.74013000

C	2.35403000	-4.66438300	-0.24543000
H	2.05794500	-2.74312000	-1.23950500
C	3.11574200	-5.39071300	0.68525300
H	4.74766200	-5.30220500	2.12668700
H	1.54589400	-5.15874300	-0.80762600
H	2.90668500	-6.45713600	0.86358500
C	3.65921800	2.65376500	0.22577500
C	4.41793100	3.38501400	1.16946100
C	2.62655500	3.30596700	-0.48421900
C	4.14892400	4.74480600	1.38743000
H	5.20902700	2.87470200	1.73981100
C	2.35277300	4.66408700	-0.24579400
H	2.05718200	2.74266400	-1.23970700
C	3.11432400	5.39070000	0.68480000
H	4.74632400	5.30275500	2.12617800
H	1.54447600	5.15817700	-0.80799700
H	2.90498600	6.45708100	0.86305100
C	-5.16581600	0.71480200	0.25732700
C	-5.16600800	-0.71433500	0.25725300
C	-6.34302200	-1.41814800	0.57148600
C	-7.51839000	-0.70286700	0.86385900
C	-7.51820000	0.70390100	0.86393800
C	-6.34264100	1.41889700	0.57164100
H	-6.33584200	-2.51765700	0.59551000
H	-8.44001400	-1.25490500	1.10553100
H	-8.43967500	1.25615900	1.10567300
H	-6.33516600	2.51840200	0.59578700
Ag	-0.63837400	-0.00024300	-1.34762700
Cl	-1.69148800	-0.00033200	2.17348300
N	-3.89284200	-1.26238200	-0.02108500
N	-3.89250500	1.26253800	-0.02095900
C	-3.65998800	-2.65363400	-0.22618400
C	-4.41915400	-3.38448100	-1.16981100
C	-2.62737100	-3.30627000	0.48347300
C	-4.15060200	-4.74431700	-1.38808000
H	-5.21024800	-2.87383600	-1.73986700
C	-2.35404400	-4.66442600	0.24474200
H	-2.05767300	-2.74324800	1.23892400
C	-3.11602400	-5.39064000	-0.68581200
H	-4.74834400	-5.30196000	-2.12678200
H	-1.54577200	-5.15886400	0.80667500
H	-2.90704500	-6.45705100	-0.86430500
C	-3.65928000	2.65374400	-0.22594100
C	-4.41826200	3.38487600	-1.16949700
C	-2.62646600	3.30603700	0.48374500
C	-4.14934000	4.74465500	-1.38766100
H	-5.20950400	2.87449500	-1.73958200
C	-2.35276700	4.66413600	0.24511700
H	-2.05691200	2.74279800	1.23914200
C	-3.11456800	5.39063600	-0.68536300
H	-4.74694100	5.30252400	-2.12630600
H	-1.54434000	5.15830100	0.80706600

H	-2.90529900	6.45700300	-0.86377400
Si	2.65330100	-0.00008900	0.11282300
Si	-2.65333900	-0.00008400	-0.11299700

[$(NHC_{Ph}$-AgCl$)_2$] (**Ag-NHGe-bis**)

C	5.36085500	0.71612500	-0.22777400
C	5.36048700	-0.71703400	-0.22800100
C	6.53350100	-1.41700100	-0.57909500
C	7.69915000	-0.70501500	-0.90405100
C	7.69951500	0.70315200	-0.90379600
C	6.53422600	1.41561900	-0.57860700
H	6.52472900	-2.51632500	-0.60535200
H	8.61289100	-1.25789700	-1.17223300
H	8.61353900	1.25566000	-1.17178200
H	6.52600300	2.51495800	-0.60448700
Ag	0.62208300	0.00048400	1.39300000
Cl	1.62955800	0.00069600	-2.24553600
N	4.11446200	-1.28895800	0.08104400
N	4.11511500	1.28858700	0.08139900
C	3.88880900	-2.68867100	0.21449000
C	4.64645500	-3.46247800	1.12484800
C	2.86199600	-3.30763100	-0.53330200
C	4.38169400	-4.83259700	1.27288600
H	5.43193600	-2.97744000	1.72434100
C	2.59311500	-4.67695900	-0.36440900
H	2.29488500	-2.70589300	-1.26131600
C	3.35313700	-5.44579700	0.53326500
H	4.97726100	-5.42484600	1.98594800
H	1.79017000	-5.14661100	-0.95454100
H	3.14666300	-6.52037800	0.65739900
C	3.89017700	2.68838000	0.21521200
C	4.64820300	3.46154500	1.12579300
C	2.86374700	3.30808700	-0.53248700
C	4.38415900	4.83176500	1.27418400
H	5.43342200	2.97593900	1.72517300
C	2.59556800	4.67750700	-0.36322900
H	2.29635500	2.70684000	-1.26069000
C	3.35594800	5.44570200	0.53469400
H	4.98001400	5.42350900	1.98742400
H	1.79289500	5.14774000	-0.95326900
H	3.15003100	6.52035700	0.65911000
C	-5.36090000	0.71613100	0.22708800
C	-5.36053000	-0.71703800	0.22730100
C	-6.53377500	-1.41699800	0.57763100
C	-7.69965800	-0.70503000	0.90179700
C	-7.70002500	0.70313300	0.90156700
C	-6.53450800	1.41560000	0.57718300
H	-6.52502200	-2.51632300	0.60389900

H	-8.61357600	-1.25792800	1.16934500
H	-8.61423100	1.25564300	1.16893200
H	-6.52631300	2.51493800	0.60310000
Ag	-0.62245100	0.00046900	-1.39370300
Cl	-1.62979100	0.00069100	2.24604900
N	-4.11430100	-1.28898100	-0.08089500
N	-4.11496100	1.28862600	-0.08125100
C	-3.88860300	-2.68869100	-0.21413100
C	-4.64583100	-3.46249100	-1.12486000
C	-2.86220200	-3.30772800	0.53417100
C	-4.38108400	-4.83262200	-1.27275600
H	-5.43098500	-2.97741300	-1.72474800
C	-2.59331500	-4.67707600	0.36541300
H	-2.29536200	-2.70608100	1.26247400
C	-3.35292800	-5.44588500	-0.53262500
H	-4.97633200	-5.42483800	-1.98611300
H	-1.79068400	-5.14675700	0.95595000
H	-3.14646100	-6.52048000	-0.65664900
C	-3.88998500	2.68841900	-0.21484900
C	-4.64752000	3.46156000	-1.12588100
C	-2.86401200	3.30821400	0.53341000
C	-4.38348100	4.83178900	-1.27413400
H	-5.43235400	2.97589800	-1.72571700
C	-2.59582900	4.67765600	0.36429400
H	-2.29693400	2.70707000	1.26194300
C	-3.35573800	5.44580700	-0.53405600
H	-4.97896100	5.42348700	-1.98772800
H	-1.79351400	5.14793000	0.95479100
H	-3.14982100	6.52047500	-0.65836300
Ge	2.77461300	0.00013200	0.26212700
Ge	-2.77417900	0.00014300	-0.26080600

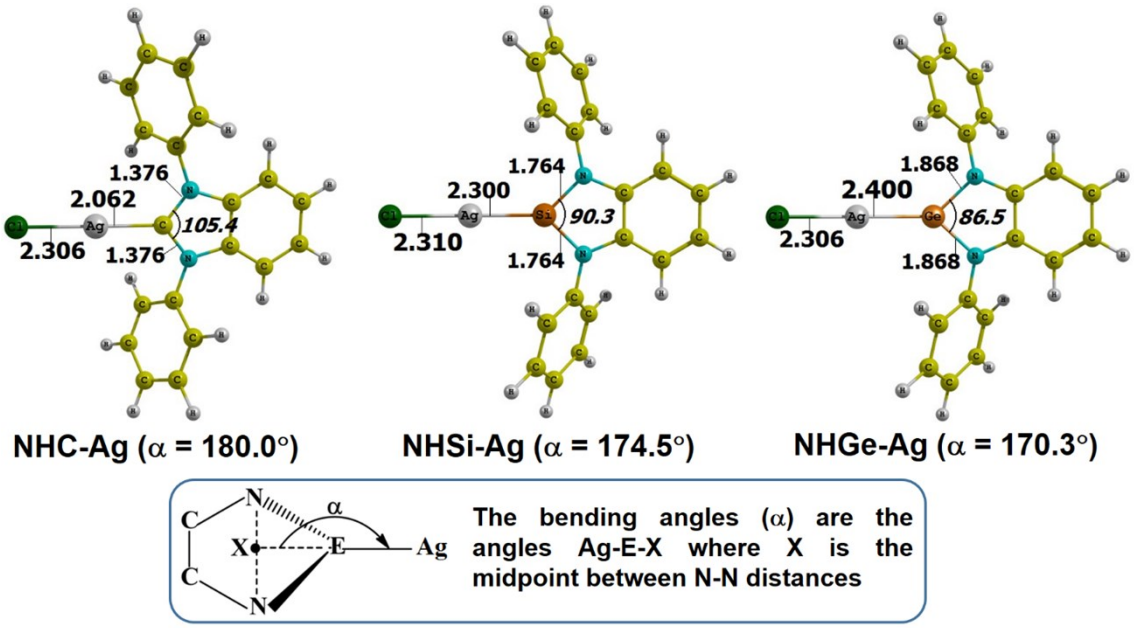

Figure S1. Optimized geometries of silver-complexes **NHE-Ag** (E = C, Si, Ge) at the BP86/def2-SVP level with dispersive effect. Bond lengths are given in Å; angles in degrees.

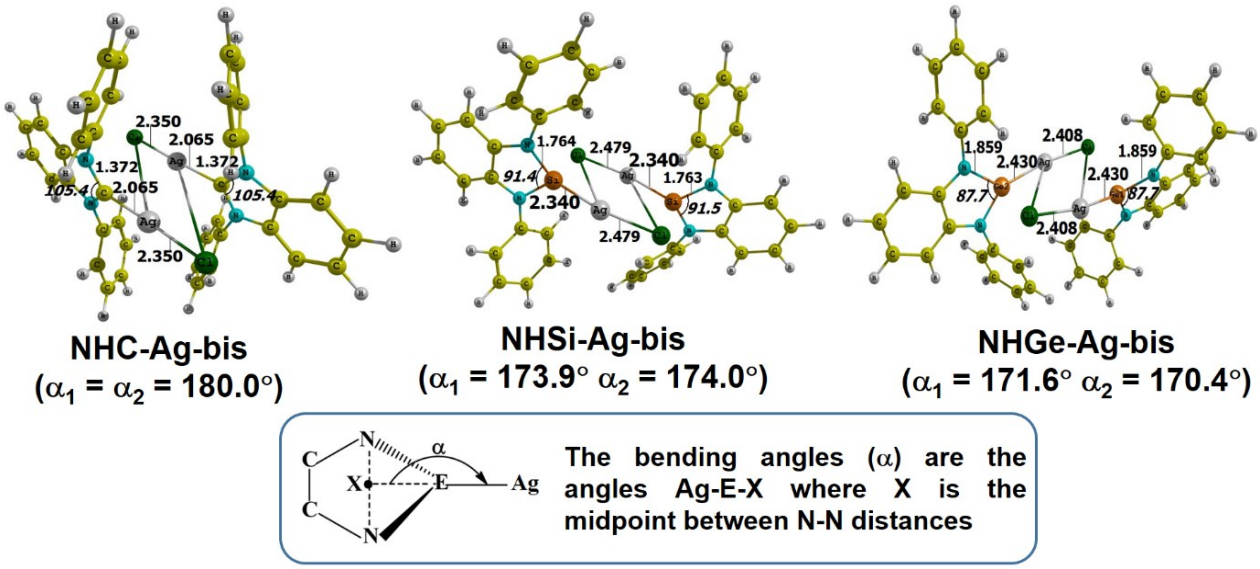

Figure S2. Optimized geometries of silver-complexes **NHE-Ag-bis** (E = C, Si, Ge) at the BP86/def2-SVP level with dispersive effect. Bond lengths are given in Å; angles in degrees