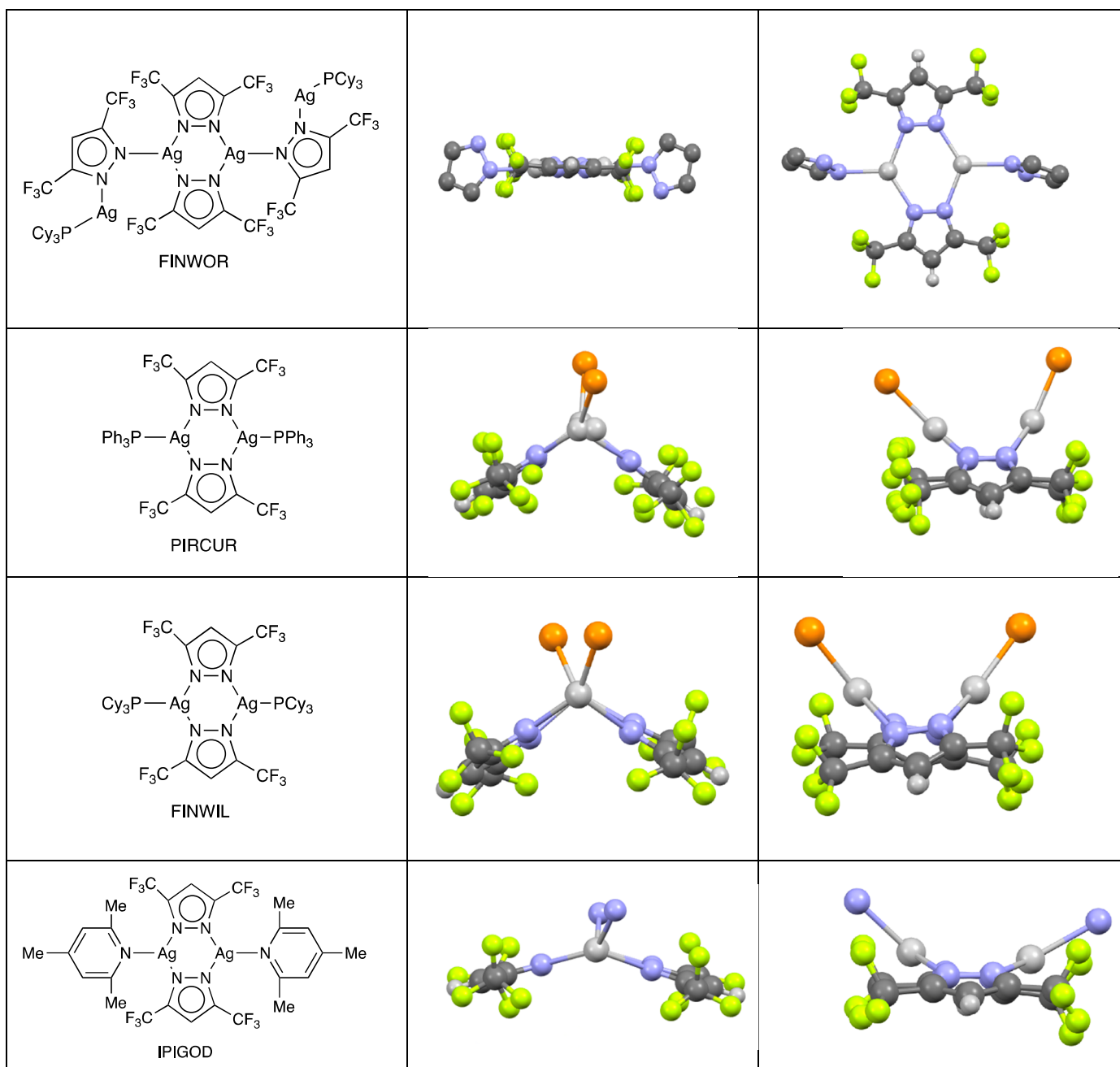


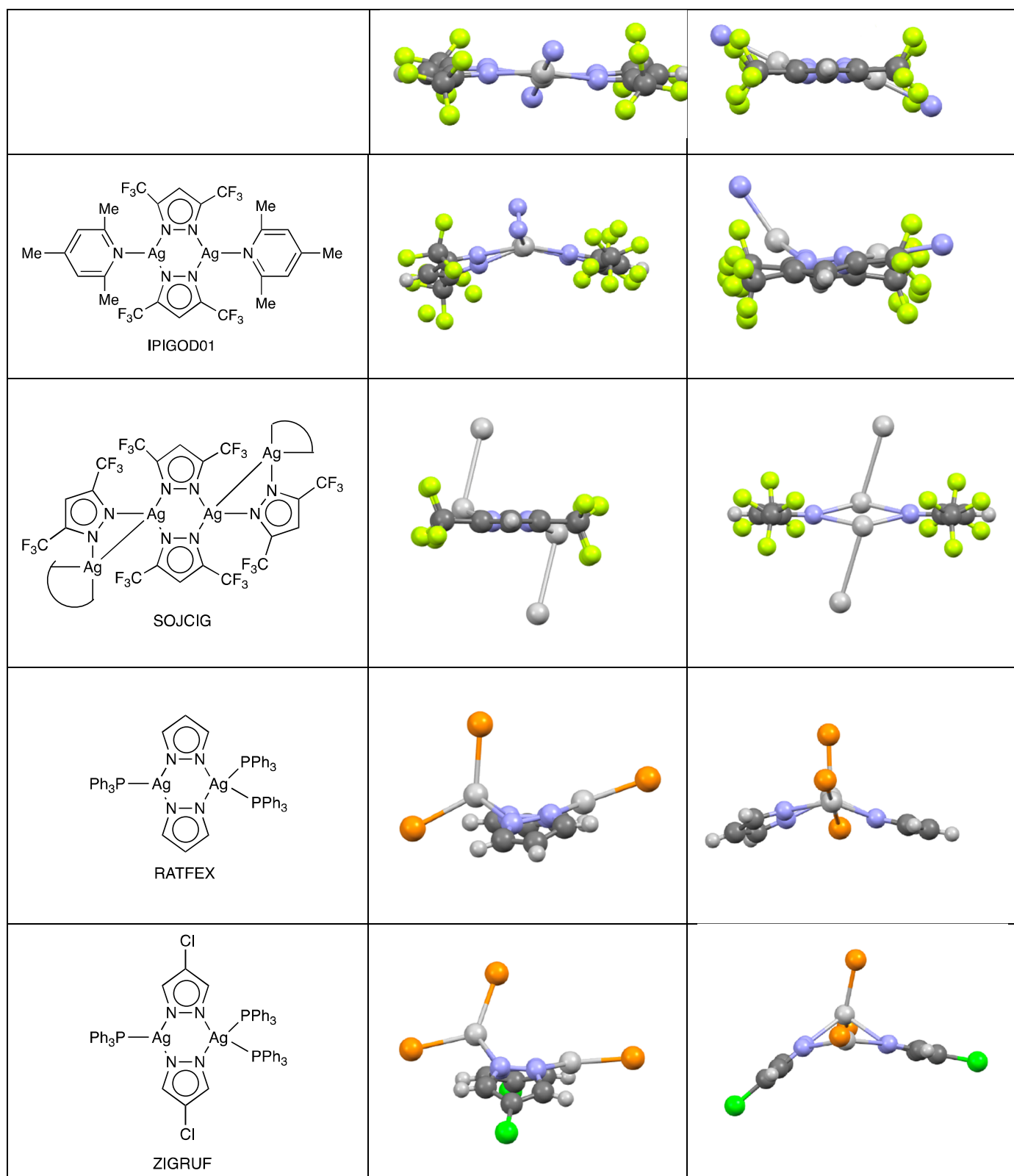
Supporting Information

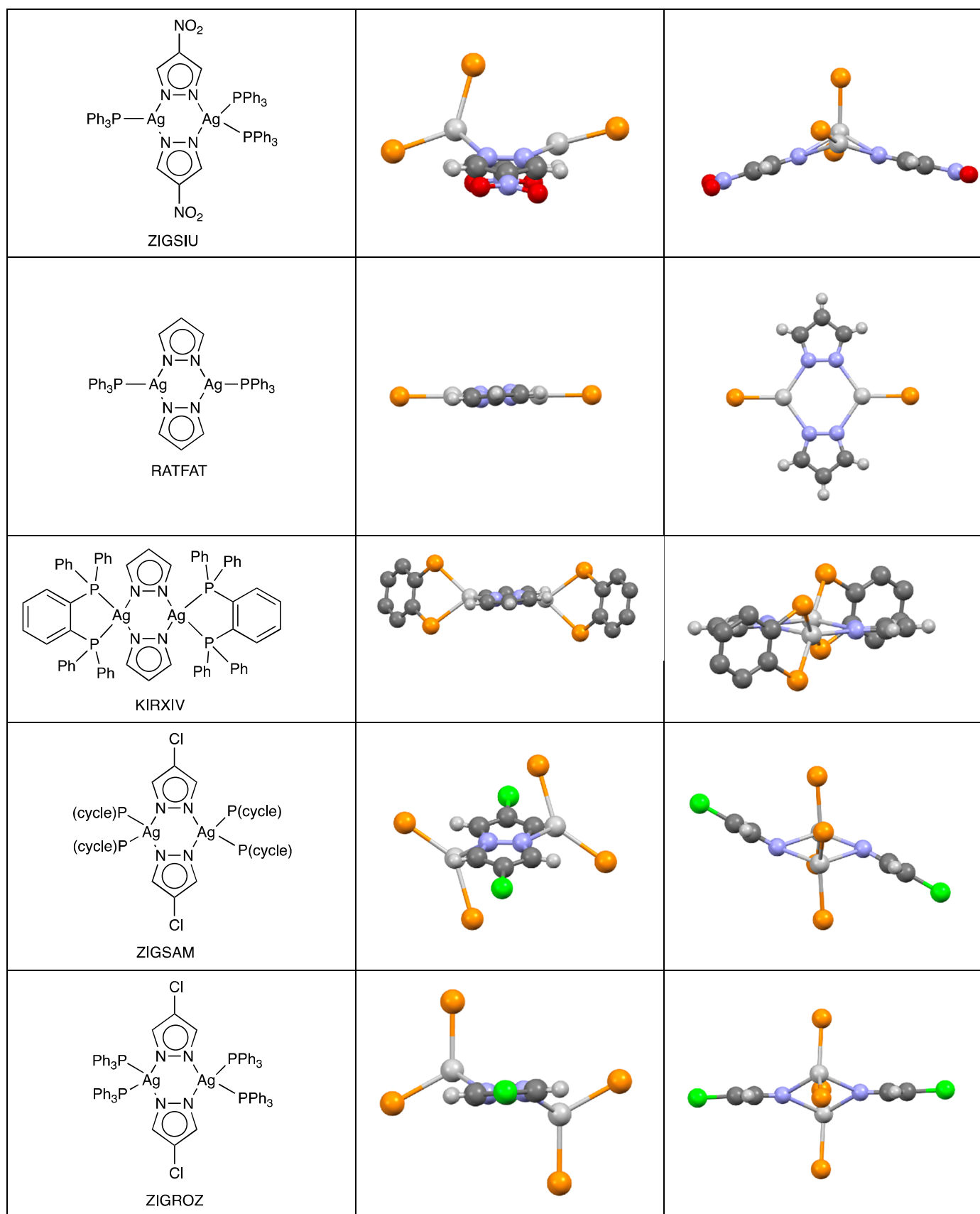
Regium Bonds between Silver(I) Pyrazolates Dinuclear Complexes and Lewis Bases (N_2 , OH_2 , NCH , SH_2 , NH_3 , PH_3 , CO and CNH)

Ibon Alkorta, José Elguero, Goar Sanchez-Sanz and Cristina Trujillo

Table S1. Two simplified views of the structures found in the CSD search.







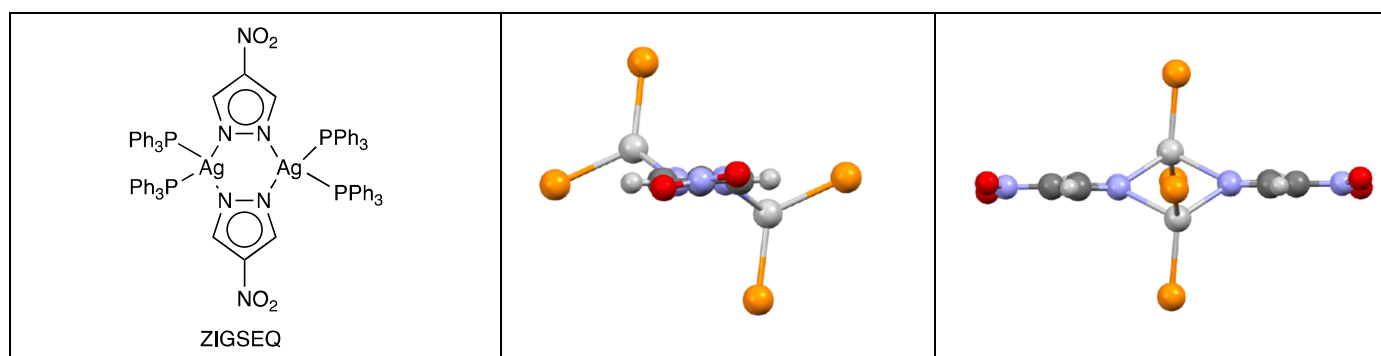
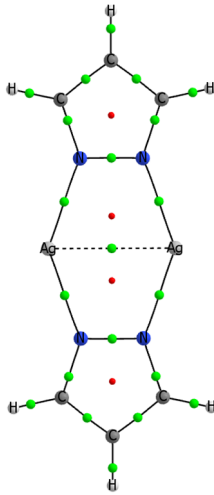
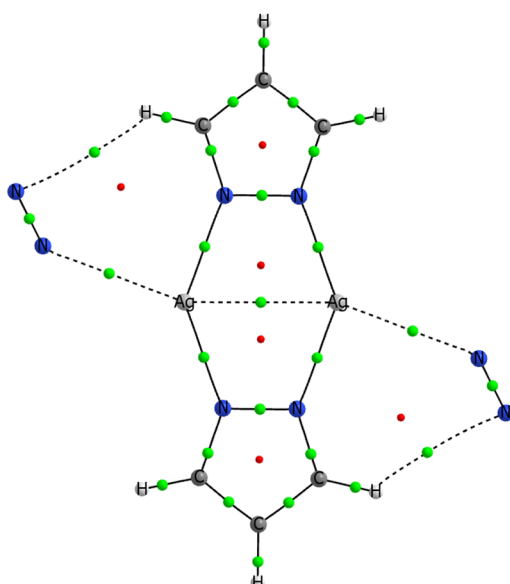


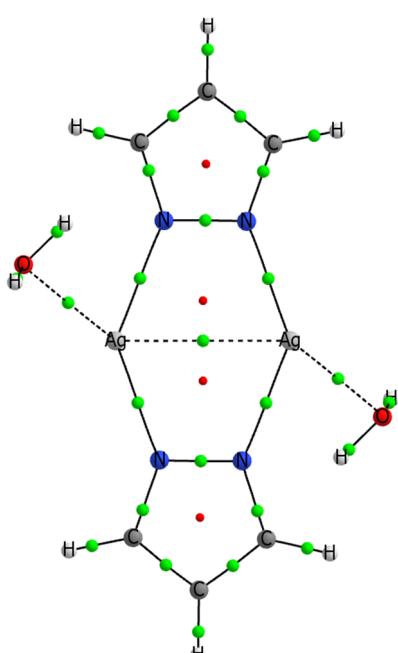
Table S2. Effect of the Ag(I)-Ag(I) distance (Å) on the relative energy (kJ·mol⁻¹) of the (PzAg)₂ system.

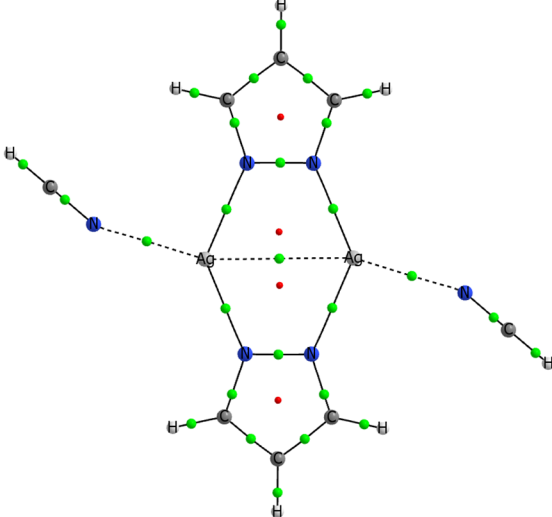
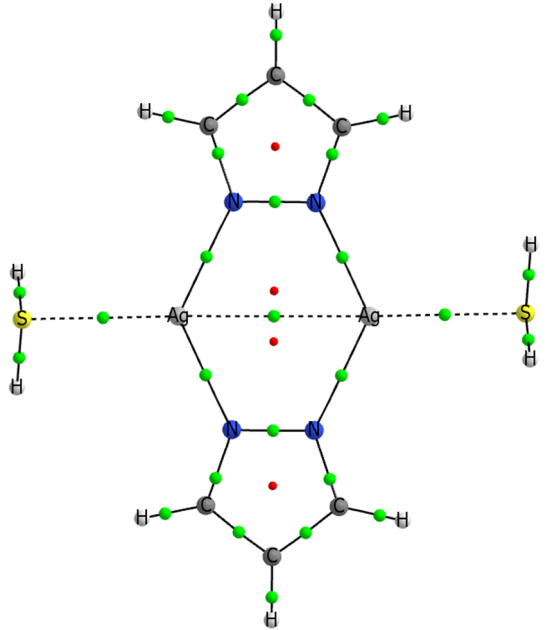
Ag-Ag dist.	E _{rel}
2.6	8.1
2.801	0.0
3.0	5.1
3.2	17.2
3.4	33.7
3.6	53.1
3.8	74.7
4.0	98.2

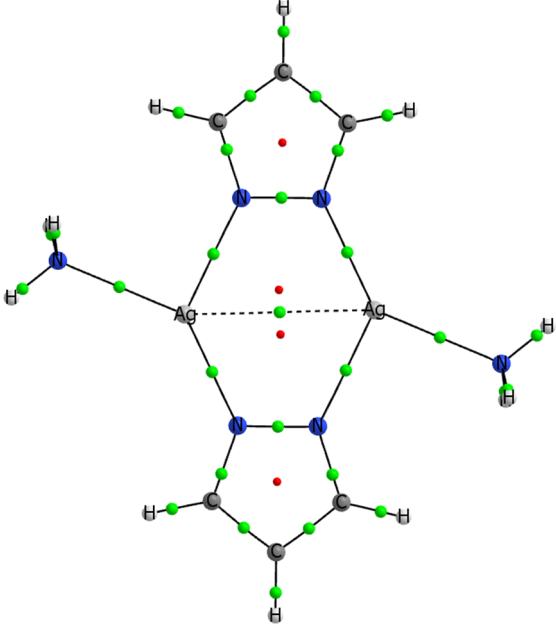
Table S3. Molecular graph and cartesian coordinates (Å) of the optimized systems at MP2/jul-cc-pVDZ/jul-cc-pVDZ-PP level.

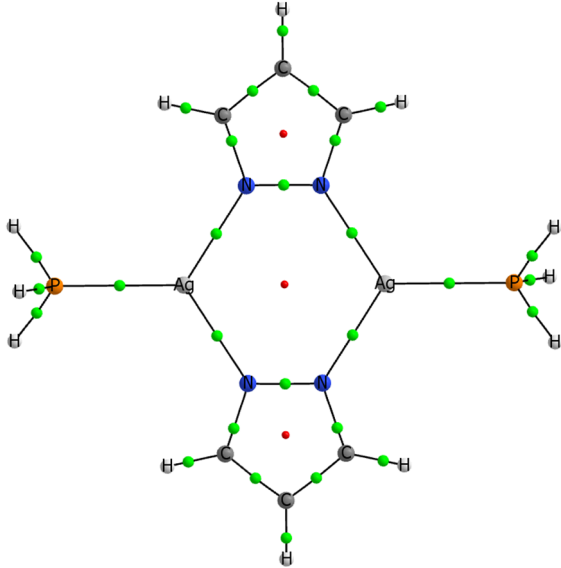
	(PzAg)₂	
	Ag	1.400583000
0.000000000		
Ag	-1.400583000	0.000000000
0.000000000		
N	-0.691776000	-1.983805000
0.000000000		
N	0.691776000	-1.983805000
0.000000000		
N	0.691776000	1.983805000
0.000000000		
N	-0.691776000	1.983805000
0.000000000		
C	-1.114431000	-3.281105000
0.000000000		
C	1.114431000	-3.281105000
0.000000000		
C	1.114431000	3.281105000
0.000000000		
C	-1.114431000	3.281105000
0.000000000		

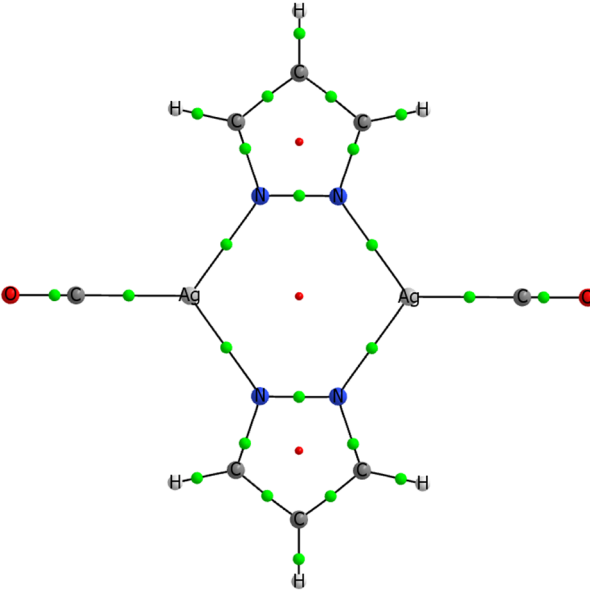
	C	0.000000000	-4.139000000
		0.000000000	
	C	0.000000000	4.139000000
		0.000000000	
	H	-2.179872000	-3.509934000
		0.000000000	
	H	2.179872000	-3.509934000
		0.000000000	
	H	2.179872000	3.509934000
		0.000000000	
	H	-2.179872000	3.509934000
		0.000000000	
	H	0.000000000	-5.227957000
		0.000000000	
	H	0.000000000	5.227957000
		0.000000000	
	(PzAg)₂(N₂)₂		
	Ag	0.,-0.1611193781,1.4163699803	
	Ag	0.,0.1611193781,-1.4163699803	
	N	0.,2.0450358941,-0.4696397968	
	N	0.,1.8984212204,0.905381866	
	N	0.,-2.0450358941,0.4696397968	
	N	0.,-1.8984212204,-0.905381866	
	C	0.,3.3796686318,-0.7543320252	
	C	0.,3.1447755441,1.4614592922	
	C	0.,-3.3796686318,0.7543320252	
	C	0.,-3.1447755441,-1.4614592922	
	C	0.,4.1159183689,0.4439640433	
	C	0.,-4.1159183689,-0.4439640433	
	H	0.,3.7189881129,-1.7900367255	
	H	0.,3.2664253685,2.5442731703	
	H	0.,-3.7189881129,1.7900367255	
	H	0.,-3.2664253685,-2.5442731703	
H	0.,5.1987498314,0.5592358352		
H	0.,-5.1987498314,-0.5592358352		
N	0.,0.5719801835,4.1567964283		
N	0.,-0.5719801835,-4.1567964283		
N	0.,1.5202282694,4.7759916665		
N	0.,-1.5202282694,-4.7759916665		

	<p>(PzAg)₂(OH)₂</p> <p>Ag,-0.0747810419,1.4452783447,-0.13908008 44</p> <p>Ag,0.0747810419,-1.4452783447,0.139080084 4</p> <p>N,-0.1556201465,-0.543031931,2.0409498475</p> <p>N,-0.1158386667,0.8322264997,1.9327942547</p> <p>N,0.1556201465,0.543031931,-2.0409498475</p> <p>N,0.1158386667,-0.8322264997,-1.932794254 7</p> <p>C,-0.259422122,-0.8648288678,3.3636183112</p> <p>C,-0.1985442381,1.3555181201,3.1943249859</p> <p>C,0.259422122,0.8648288678,-3.3636183112</p> <p>C,0.1985442381,-1.3555181201,-3.194324985 9</p> <p>C,-0.2925675616,0.3119854076,4.1343365578</p> <p>C,0.2925675616,-0.3119854076,-4.134336557 8</p> <p>H,-0.3034502589,-1.9093577404,3.672091211 1</p> <p>H,-0.1633302089,2.4358487009,3.3424004659</p> <p>H,0.3034502589,1.9093577404,-3.6720912111</p> <p>H,0.1633302089,-2.4358487009,-3.342400465 9</p> <p>H,-0.3682688734,0.3961276567,5.217663615</p> <p>H,0.3682688734,-0.3961276567,-5.217663615</p> <p>O,-1.9720229086,2.9931797046,0.8212859313</p> <p>O,1.9720229086,-2.9931797046,-0.821285931 3</p> <p>H,-2.0677251781,2.3632899941,1.5532572251</p> <p>H,-2.8546990605,3.0605477975,0.4325225512</p> <p>H,2.8546990605,-3.0605477975,-0.432522551 2</p> <p>H,2.0677251781,-2.3632899941,-1.553257225 1</p>
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	<p>(PzAg)₂(NCH)₂</p> <p>Ag,0.,-0.2061158801,1.5249267748 Ag,0.,0.2061158801,-1.5249267748 N,0.,2.038181774,-0.4538936708 N,0.,1.8681855476,0.9137734051 N,0.,-2.038181774,0.4538936708 N,0.,-1.8681855476,-0.9137734051 C,0.,3.3782726134,-0.7177602341 C,0.,3.1057888572,1.4900567987 C,0.,-3.3782726134,0.7177602341 C,0.,-3.1057888572,-1.4900567987 C,0.,4.0982006696,0.4915853694 C,0.,-4.0982006696,-0.4915853694 H,0.,3.7339221016,-1.7483658359 H,0.,3.204589072,2.5760143356 H,0.,-3.7339221016,1.7483658359 H,0.,-3.204589072,-2.5760143356 H,0.,5.179473828,0.6240703561 H,0.,-5.179473828,-0.6240703561 N,0.,0.2169442642,3.912432963 N,0.,-0.2169442642,-3.912432963 C,0.,0.8610789844,4.9023935731 C,0.,-0.8610789844,-4.9023935731 H,0.,1.4454822595,5.8093217777 H,0.,-1.4454822595,-5.8093217777</p>
	<p>(PzAg)₂(SH₂)₂</p> <p>Ag,-0.603654644,1.4793453249,0.0354414394 Ag,0.603654644,-1.4793453249,-0.0354414394 4 N,0.2438969147,-0.6897754458,1.9285194972 N,-0.2278821752,0.6028829598,1.9592972352 N,-0.2438969147,0.6897754458,-1.9285194972 2 N,0.2278821752,-0.6028829598,-1.9592972352 2 C,0.394873828,-1.1159259886,3.2179669471 C,-0.3680767066,0.9710947335,3.2676674414 C,-0.394873828,1.1159259886,-3.2179669471 C,0.3680767066,-0.9710947335,-3.2676674414 4 C,0.0169759901,-0.0916613289,4.1058410647</p>

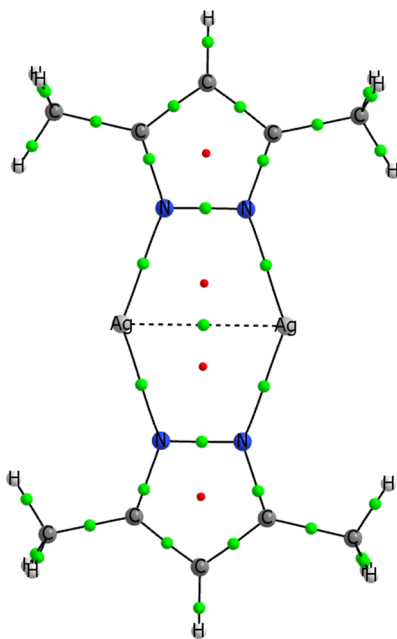
	<p>C,-0.0169759901,0.0916613289,-4.105841064 7</p> <p>H,0.756896311,-2.1236837799,3.4250844083</p> <p>H,-0.7281695024,1.9685545213,3.5225129286</p> <p>H,-0.756896311,2.1236837799,-3.4250844083</p> <p>H,0.7281695024,-1.9685545213,-3.522512928 6</p> <p>H,0.0215042134,-0.1159440748,5.1948567731</p> <p>H,-0.0215042134,0.1159440748,-5.194856773 1</p> <p>S,-1.84905466,3.7962110997,0.0944809692</p> <p>S,1.84905466,-3.7962110997,-0.0944809692</p> <p>H,-2.7423336701,3.5270359789,1.0723809142</p> <p>H,-2.751295645,3.5726863353,-0.8866839892</p> <p>H,2.751295645,-3.5726863353,0.8866839892</p> <p>H,2.7423336701,-3.5270359789,-1.072380914 2</p>
	<p>(PzAg)₂(NH₃)₂</p> <p>Ag, 0.0274153956,1.6135787098,-0.2111375282</p> <p>Ag,-0.0274153956,-1.6135787098,0.21113752 82</p> <p>N,-0.0282725571,-0.5063088859,2.012900411 9</p> <p>N,-0.0044846217,0.8617635907,1.8761663822</p> <p>N,0.0282725571,0.5063088859,-2.0129004119</p> <p>N,0.0044846217,-0.8617635907,-1.876166382 2</p> <p>C,-0.0466561618,-0.8071986255,3.346244220 6</p> <p>C,-0.0083856176,1.4028741244,3.1313010927</p> <p>C,0.0466561618,0.8071986255,-3.3462442206</p> <p>C,0.0083856176,-1.4028741244,-3.131301092 7</p> <p>C,-0.0349085465,0.3809530005,4.0997855041</p> <p>C,0.0349085465,-0.3809530005,-4.099785504 1</p> <p>H,-0.0670513723,-1.8468000942,3.674419546 5</p> <p>H,0.0080311304,2.4854829311,3.2672863236</p> <p>H,0.0670513723,1.8468000942,-3.6744195465</p>

	<p>H,-0.0080311304,-2.4854829311,-3.26728632 36</p> <p>H,-0.044099626,0.4853098951,5.1842517685</p> <p>H,0.044099626,-0.4853098951,-5.1842517685</p> <p>N,0.0545531187,3.8713251275,0.4701050867</p> <p>N,-0.0545531187,-3.8713251275,-0.47010508 67</p> <p>H,-0.7676912527,4.0505540098,1.0486657645</p> <p>H,0.8702300662,4.0261264666,1.0647854255</p> <p>H,0.0723113044,4.5927503747,-0.2513979334</p> <p>H,0.7676912527,-4.0505540098,-1.048665764 5</p> <p>H,-0.8702300662,-4.0261264666,-1.06478542 55</p> <p>H,-0.0723113044,-4.5927503747,0.251397933 4</p>
	<p>(PzAg)₂(PH₃)₂</p> <p>Ag,1.0483191436,1.5173572911,0.</p> <p>P,2.4335604114,3.4436300443,0.</p> <p>N,0.3821031759,0.5691704841,1.828359399</p> <p>N,-0.3821031759,-0.5691704841,1.828359399</p> <p>C,-0.6184358936,-0.9204801365,3.129020604 7</p> <p>H,-1.2126311382,-1.8061476966,3.357483515 9</p> <p>C,0.6184358936,0.9204801365,3.1290206047</p> <p>H,1.2126311382,1.8061476966,3.3574835159</p> <p>C,0.,0.,3.9946362558</p> <p>Ag,-1.0483191436,-1.5173572911,0.</p> <p>P,-2.4335604114,-3.4436300443,0.</p> <p>N,-0.3821031759,-0.5691704841,-1.82835939 9</p> <p>N,0.3821031759,0.5691704841,-1.828359399</p> <p>C,0.6184358936,0.9204801365,-3.1290206047</p> <p>H,1.2126311382,1.8061476966,-3.3574835159</p> <p>C,-0.6184358936,-0.9204801365,-3.12902060 47</p> <p>H,-1.2126311382,-1.8061476966,-3.35748351 59</p> <p>C,0.,0.,-3.9946362558</p> <p>H,0.,0.,5.0840192895</p>

	<p>H,0.,0.,-5.0840192895 H,2.3895012306,4.3841398886,1.0619031217 H,-2.3895012306,-4.3841398886,-1.0619031217 H,2.3895012306,4.3841398886,-1.0619031217 H,-2.3895012306,-4.3841398886,1.0619031217 H,3.8383532082,3.2477102048,0. H,-3.8383532082,-3.2477102048,0.</p>
	<p>(PzAg)₂(CO)₂ Ag,1.9213344677,0.,0. Ag,-1.9213344677,0.,0. N,-0.6844564829,-1.7592494843,0. N,0.6844564829,-1.7592494843,0. N,0.6844564829,1.7592494843,0. N,-0.6844564829,1.7592494843,0. C,-1.1082222493,-3.0607056699,0. C,1.1082222493,-3.0607056699,0. C,1.1082222493,3.0607056699,0. C,-1.1082222493,3.0607056699,0. C,0.,-3.9252867603,0. C,0.,3.9252867603,0. H,-2.1745984307,-3.2878817711,0. H,2.1745984307,-3.2878817711,0. H,2.1745984307,3.2878817711,0. H,-2.1745984307,3.2878817711,0. H,0.,-5.0143820835,0. H,0.,5.0143820835,0. C,3.9187330534,0.,0. C,-3.9187330534,0.,0. O,5.0708778876,0.,0. O,-5.0708778876,0.,0.</p>

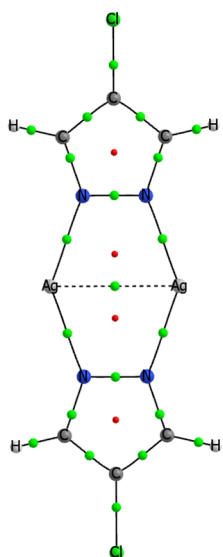
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		0.000000000	0.000000000
	Ag	-1.940154000	0.000000000
		0.000000000	0.000000000
	N	-0.684562000	-1.766790000
		0.000000000	0.000000000
	N	0.684562000	-1.766790000
		0.000000000	0.000000000
	N	0.684562000	1.766790000
		0.000000000	0.000000000
	N	-0.684562000	1.766790000
		0.000000000	0.000000000
	C	-1.108157000	-3.068009000
		0.000000000	0.000000000
	C	1.108157000	-3.068009000
		0.000000000	0.000000000
	C	1.108157000	3.068009000
		0.000000000	0.000000000
	C	-1.108157000	3.068009000
	0.000000000	0.000000000	
C	0.000000000	-3.934375000	
	0.000000000	0.000000000	
C	0.000000000	3.934375000	
	0.000000000	0.000000000	
H	-2.175101000	-3.293726000	
	0.000000000	0.000000000	
H	2.175101000	-3.293726000	
	0.000000000	0.000000000	
H	2.175101000	3.293726000	
	0.000000000	0.000000000	
H	-2.175101000	3.293726000	
	0.000000000	0.000000000	
H	0.000000000	-5.023757000	
	0.000000000	0.000000000	
H	0.000000000	5.023757000	
	0.000000000	0.000000000	
C	3.957788000	0.000000000	
	0.000000000	0.000000000	
C	-3.957788000	0.000000000	
	0.000000000	0.000000000	

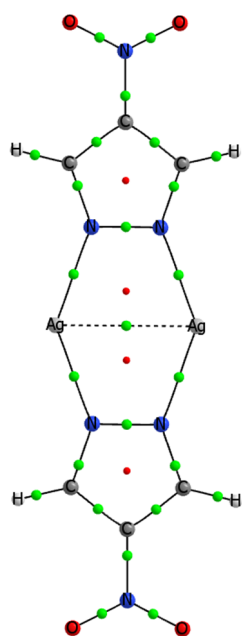
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		0.000000000	
	N	-5.145834000	0.000000000
		0.000000000	
	H	6.153545000	0.000000000
		0.000000000	
	H	-6.153545000	0.000000000
		0.000000000	
	(DMepzAg)₂		
	Ag	-0.111352000	1.824696000
		0.005233000	
	Ag	0.111352000	-1.824696000
		-0.005233000	
	P	-0.315932000	4.194458000
		-0.022085000	
	N	-0.000101000	0.683970000
		1.835448000	
	N	-0.000407000	-0.689412000
		1.831472000	
	C	0.000919000	-1.125934000
		3.128813000	
	C	-0.001849000	1.113763000
		3.134923000	
	C	-0.000448000	-0.008379000
		3.985794000	
	P	0.315932000	-4.194458000
		0.022085000	
	N	0.000101000	-0.683970000
		-1.835448000	
	N	0.000407000	0.689412000
		-1.831472000	
	C	-0.000919000	1.125934000
		-3.128813000	
	C	0.001849000	-1.113763000
		-3.134923000	
	C	0.000448000	0.008379000
		-3.985794000	
	H	-0.000774000	-0.011264000
		5.076693000	
	H	0.000774000	0.011264000
		-5.076693000	



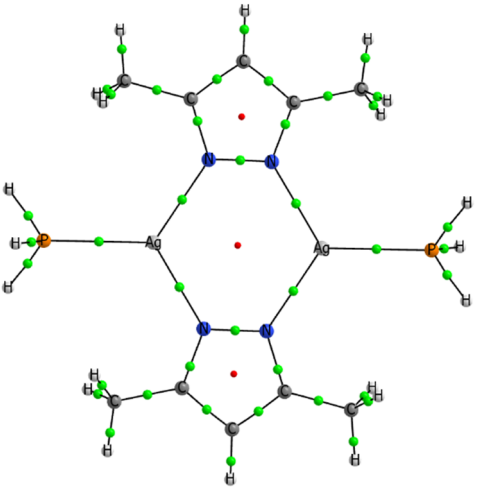
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1.073940000		
H	0.853527000	-4.919583000
-1.073940000		
H	-1.042706000	4.859534000
-1.044389000		
H	1.042706000	-4.859534000
1.044389000		
H	0.882188000	4.945162000
-0.150674000		
H	-0.882188000	-4.945162000
0.150674000		
C	-0.016654000	2.589504000
-3.468569000		
H	0.128488000	2.725397000
-4.551596000		
H	-0.976349000	3.061479000
-3.196529000		
H	0.791713000	3.130762000
-2.948105000		
C	0.016654000	-2.589504000
3.468569000		
H	0.976349000	-3.061479000
3.196529000		
H	-0.128488000	-2.725397000
4.551596000		
H	-0.791713000	-3.130762000
2.948105000		
C	-0.016885000	2.575717000
3.481830000		
H	-0.972075000	3.051644000
3.201235000		
H	0.117174000	2.705658000
4.566980000		
H	0.797904000	3.117246000
2.972013000		
C	0.016885000	-2.575717000
-3.481830000		
H	-0.117174000	-2.705658000
-4.566980000		

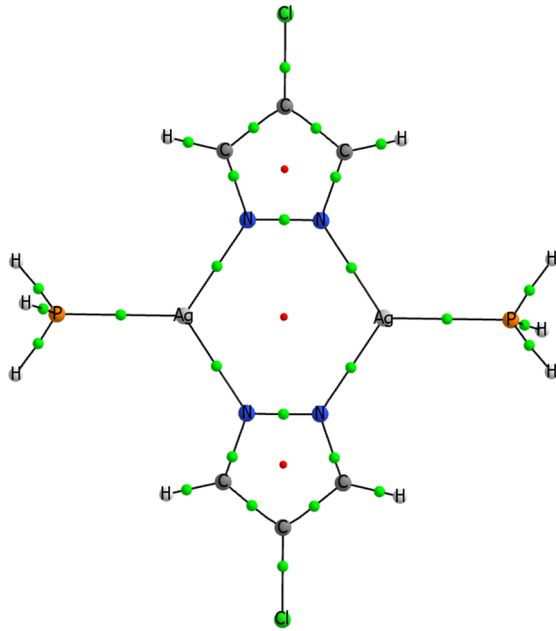
	H	0.972075000	-3.051644000
		-3.201235000	
	H	-0.797904000	-3.117246000
		-2.972013000	
	(4ClpzAg)₂		
	Ag	0.000000000	1.409496000
		0.000000000	
	Ag	0.000000000	-1.409496000
		0.000000000	
	N	0.000000000	0.691206000
		1.983935000	
	N	0.000000000	-0.691206000
		1.983935000	
	C	0.000000000	-1.122252000
		3.278585000	
	H	0.000000000	-2.183008000
		3.524003000	
	C	0.000000000	1.122252000
		3.278585000	
	H	0.000000000	2.183008000
		3.524003000	
	C	0.000000000	0.000000000
		4.121205000	
	N	0.000000000	-0.691206000
		-1.983935000	
	N	0.000000000	0.691206000
		-1.983935000	
	C	0.000000000	1.122252000
		-3.278585000	
	H	0.000000000	2.183008000
		-3.524003000	
	C	0.000000000	-1.122252000
		-3.278585000	
	H	0.000000000	-2.183008000
		-3.524003000	
	C	0.000000000	0.000000000
		-4.121205000	
	Cl	0.000000000	0.000000000
		-5.852896000	
	Cl	0.000000000	0.000000000
		5.852896000	

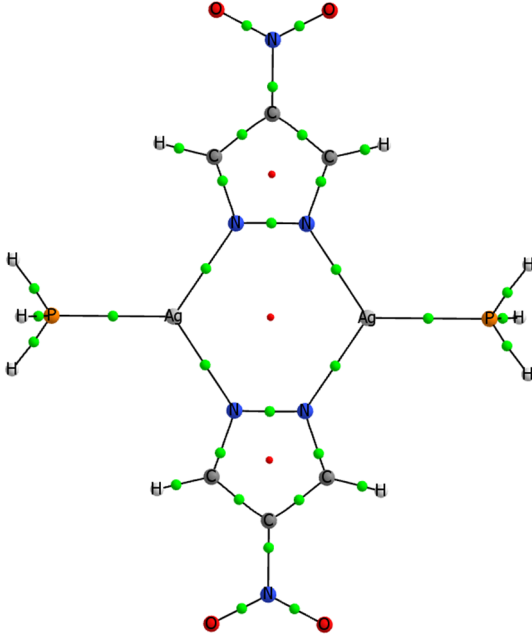


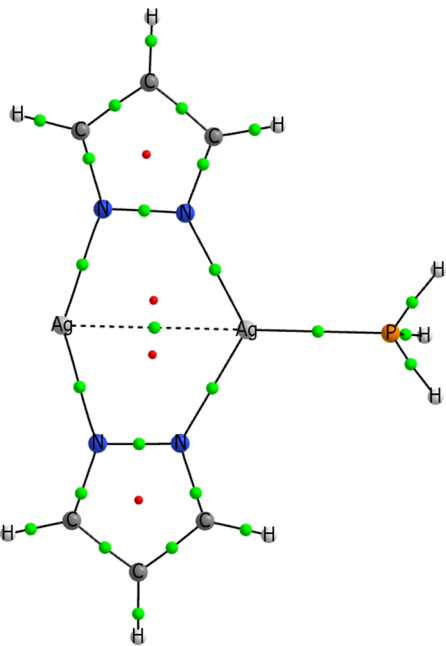
**(4NO₂pzAg)₂**

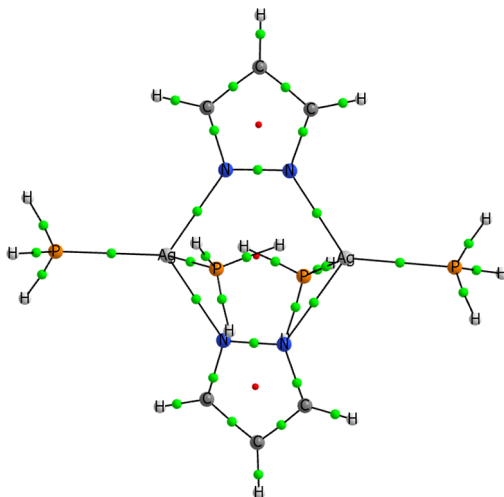
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0.000000000		
Ag	0.000000000	-1.420348000
0.000000000		
N	0.000000000	0.693388000
1.987084000		
N	0.000000000	-0.693388000
1.987084000		
C	0.000000000	-1.126784000
3.274415000		
H	0.000000000	-2.184930000
3.528103000		
C	0.000000000	1.126784000
3.274415000		
H	0.000000000	2.184930000
3.528103000		
C	0.000000000	0.000000000
4.110089000		
N	0.000000000	-0.693388000
-1.987084000		
N	0.000000000	0.693388000
-1.987084000		
C	0.000000000	1.126784000
-3.274415000		
H	0.000000000	2.184930000
-3.528103000		
C	0.000000000	-1.126784000
-3.274415000		
H	0.000000000	-2.184930000
-3.528103000		
C	0.000000000	0.000000000
-4.110089000		
N	0.000000000	0.000000000
5.550657000		
O	0.000000000	1.102008000
6.120597000		
O	0.000000000	-1.102008000
6.120597000		
N	0.000000000	0.000000000
-5.550657000		

	<p>O 0.000000000 -1.102008000 -6.120597000</p> <p>O 0.000000000 1.102008000 -6.120597000</p>
	<p>(DMepzAg)₂(PH₃)₂</p> <p>Ag,-0.1113520245,1.8246962613,0.005233473 8</p> <p>Ag,0.1113520245,-1.8246962613,-0.00523347 38</p> <p>P,-0.3159320509,4.194458478,-0.0220849664</p> <p>N,-0.0001009874,0.6839697055,1.8354481833</p> <p>N,-0.0004067572,-0.6894124902,1.83147178</p> <p>C,0.0009188074,-1.125934095,3.1288131816</p> <p>C,-0.001848743,1.1137632243,3.1349226836</p> <p>C,-0.0004475812,-0.0083794317,3.985793729 8</p> <p>P,0.3159320509,-4.194458478,0.0220849664</p> <p>N,0.0001009874,-0.6839697055,-1.835448183 3</p> <p>N,0.0004067572,0.6894124902,-1.83147178</p> <p>C,-0.0009188074,1.125934095,-3.1288131816</p> <p>C,0.001848743,-1.1137632243,-3.1349226836</p> <p>C,0.0004475812,0.0083794317,-3.9857937298</p> <p>H,-0.0007744601,-0.0112642348,5.076693288 1</p> <p>H,0.0007744601,0.0112642348,-5.0766932881</p> <p>H,-0.853527232,4.9195834464,1.0739397045</p> <p>H,0.853527232,-4.9195834464,-1.0739397045</p> <p>H,-1.0427058844,4.8595340849,-1.044388933 6</p> <p>H,1.0427058844,-4.8595340849,1.0443889336</p> <p>H,0.882188493,4.9451616518,-0.150674102</p> <p>H,-0.882188493,-4.9451616518,0.150674102</p> <p>C,-0.0166543242,2.5895036478,-3.468569416</p> <p>H,0.128488267,2.7253967554,-4.5515956174</p> <p>H,-0.9763490032,3.061479393,-3.1965287421</p> <p>H,0.7917128651,3.1307624683,-2.9481051355</p> <p>C,0.0166543242,-2.5895036478,3.468569416</p> <p>H,0.9763490032,-3.061479393,3.1965287421</p> <p>H,-0.128488267,-2.7253967554,4.5515956174</p>

	<p>H,-0.7917128651,-3.1307624683,2.948105135 5</p> <p>C,-0.0168850942,2.5757166286,3.4818297306</p> <p>H,-0.9720746763,3.051644145,3.201235434</p> <p>H,0.1171739449,2.70565753,4.5669801945</p> <p>H,0.7979037953,3.1172460315,2.9720131272</p> <p>C,0.0168850942,-2.5757166286,-3.481829730 6</p> <p>H,-0.1171739449,-2.70565753,-4.5669801945</p> <p>H,0.9720746763,-3.051644145,-3.201235434</p> <p>H,-0.7979037953,-3.1172460315,-2.97201312 72</p>
	<p>(4ClpzAg)₂(PH₃)₂</p> <p>Ag,-0.0085291906,1.8651144284,0.</p> <p>P,0.0183766361,4.2374143054,0.</p> <p>N,-0.0124631092,0.6850901575,1.8210222351</p> <p>N,0.0124631092,-0.6850901575,1.8210222351</p> <p>C,0.0198305777,-1.117181569,3.1186585603</p> <p>H,0.0394296395,-2.1783064593,3.3646618446</p> <p>C,-0.0198305777,1.117181569,3.1186585603</p> <p>H,-0.0394296395,2.1783064593,3.3646618446</p> <p>C,0.,0.,3.9671516371</p> <p>Ag,0.0085291906,-1.8651144284,0.</p> <p>P,-0.0183766361,-4.2374143054,0.</p> <p>N,0.0124631092,-0.6850901575,-1.821022235 1</p> <p>N,-0.0124631092,0.6850901575,-1.821022235 1</p> <p>C,-0.0198305777,1.117181569,-3.1186585603</p> <p>H,-0.0394296395,2.1783064593,-3.364661844 6</p> <p>C,0.0198305777,-1.117181569,-3.1186585603</p> <p>H,0.0394296395,-2.1783064593,-3.364661844 6</p> <p>C,0.,0.,-3.9671516371</p> <p>H,-0.5627071714,4.9743023826,1.0637226596</p> <p>H,0.5627071714,-4.9743023826,-1.063722659 6</p> <p>H,-0.5627071714,4.9743023826,-1.063722659 6</p> <p>H,0.5627071714,-4.9743023826,1.0637226596</p>

	<p>H,1.2796614926,4.8848095192,0. H,-1.2796614926,-4.8848095192,0. Cl,0.,0.,-5.7029839045 Cl,0.,0.,5.7029839045</p>
	<p>(4NO₂pzAg)₂(PH₃)₂ Ag,-0.003560636,1.8907561677,0. Ag,0.003560636,-1.8907561677,0. P,0.0215149758,4.2648744434,0. N,-0.0092784777,0.6875650606,1.8181091994 N,0.0092784777,-0.6875650606,1.8181091994 C,0.0147694182,-1.1215536185,3.1078188637 H,0.0293095759,-2.1799717125,3.3613637589 C,-0.0147694182,1.1215536185,3.1078188637 H,-0.0293095759,2.1799717125,3.3613637589 C,0.,0.,3.9515372891 P,-0.0215149758,-4.2648744434,0. N,0.0092784777,-0.6875650606,-1.8181091994 4 N,-0.0092784777,0.6875650606,-1.8181091994 4 C,-0.0147694182,1.1215536185,-3.1078188637 7 H,-0.0293095759,2.1799717125,-3.3613637589 9 C,0.0147694182,-1.1215536185,-3.1078188637 7 H,0.0293095759,-2.1799717125,-3.3613637589 9 C,0.,0.,-3.9515372891 H,-0.5650090283,4.9916046177,1.0664736702 H,0.5650090283,-4.9916046177,-1.0664736702 2 H,-0.5650090283,4.9916046177,-1.0664736702 2 H,0.5650090283,-4.9916046177,1.0664736702 H,1.2819687246,4.9120378213,0. H,-1.2819687246,-4.9120378213,0. N,0.,0.,5.3882531149 O,-0.0139164636,1.1010072615,5.9637256096 O,0.0139164636,-1.1010072615,5.9637256096 N,0.,0.,-5.3882531149</p>

	O,0.0139164636,-1.1010072615,-5.963725609 6 O,-0.0139164636,1.1010072615,-5.963725609 6
	(PzAg)₂(PH₃) Ag,-0.0198313786,1.784485932,-0.000000002 1 Ag,0.0056488108,-1.3021236041,0.000000001 6 N,-0.011224468,1.1449346135,1.9643602279 N,0.0067007551,-0.2333505314,1.9278202161 C,0.016828652,-0.6774248326,3.2209198636 H,0.0322427783,-1.7469943449,3.4326040131 C,-0.0119066564,1.5482215161,3.2671306033 H,-0.0245657325,2.6097089046,3.5138451805 C,0.0056710213,0.4175072322,4.1042894424 P,-0.0225370215,-3.711528228,0.0000000044 N,0.0067007551,-0.233350536,-1.9278202156 N,-0.011224468,1.1449346088,-1.9643602307 C,-0.0119066564,1.5482215083,-3.267130607 H,-0.0245657325,2.6097088962,-3.513845186 8 C,0.016828652,-0.6774248403,-3.220919862 H,0.0322427783,-1.7469943531,-3.432604009 C,0.0056710213,0.4175072224,-4.1042894434 H,0.009900249,0.3967308862,5.1932394342 H,0.009900249,0.3967308738,-5.1932394351 H,0.5592482489,-4.4481009364,-1.063675817 1 H,0.5592482489,-4.4481009338,1.0636758277 H,-1.2823962052,-4.3623826418,0.000000005 2

**(PzAg)₂(PH₃)₄**

Ag, -0.0808347102, 1.9314757844, 0.0391500405

Ag, -0.0491586997, -1.8657965759, 0.0709317071

P, 0.6142061725, 4.1905435367, 0.0454377393

P, -2.555077811, 1.2314296217, -0.1503900401

N, 0.2580366234, 0.6857738492, 1.8532309937

N, -0.1935852056, -0.6079477521, 1.8787187532

C, -0.2626512775, -1.0088913697, 3.1863204549

H, -0.5903609151, -2.0203617745, 3.4324081766

C, 0.4478736005, 1.0923450974, 3.1466703335

H, 0.7969876204, 2.1049444483, 3.3563319896

C, 0.1332422902, 0.0441795203, 4.0331529269

P, -0.9548528184, -4.051979479, -0.0431209313

P, 2.42878087, -1.3478431059, -0.4056283871

N, -0.398042305, -0.5606359367, -1.7655019255

N, 0.3052406814, 0.621656442, -1.7336670988

C, 0.7765399031, 0.8741467541, -2.9928161466

H, 1.3499923519, 1.7812770787, -3.1929962894

C, -0.3320595117, -1.0490460338, -3.0453508975

H, -0.8210153814, -1.9923607638, -3.2966328444

C, 0.4005853211, -0.1677819926, -3.8645362615

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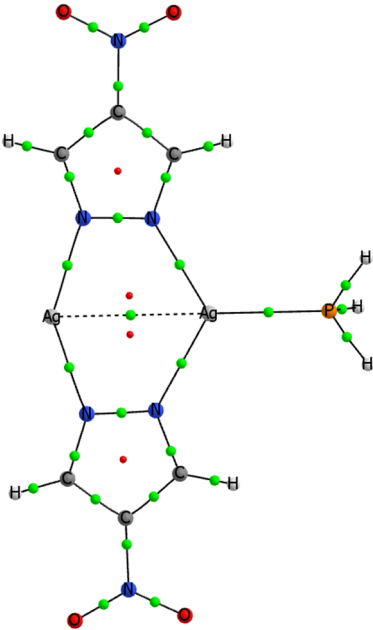
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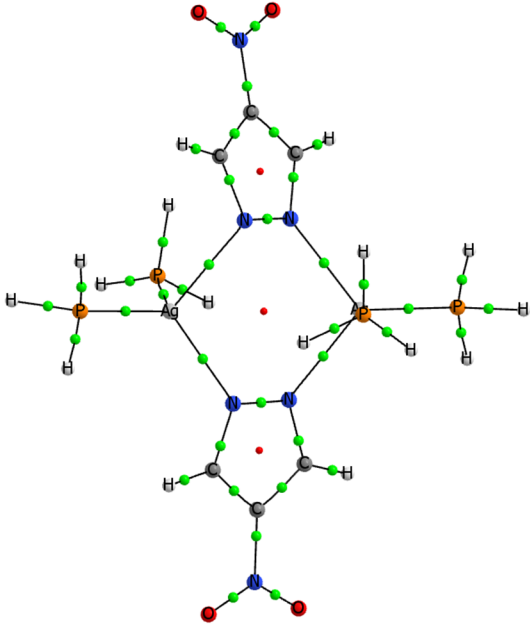
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H, 3.6288913596, -2.0764059433, -0.1572661317

H, -3.716364948, 1.8414294653, 0.408672068

	<p>H,2.6978376653,-1.0288275787,-1.764217532 5</p> <p>H,1.3693809523,4.7052406084,1.1324162582</p> <p>H,-0.1010896198,-5.1779972024,-0.17610179 76</p> <p>H,-0.3445376255,5.2362428356,0.0015221443</p> <p>H,-1.7514780614,-4.5728612857,1.010811924 9</p> <p>H,1.4510384494,4.691881241,-0.986619151</p> <p>H,-1.8404678448,-4.3886221658,-1.10076439 22</p>
	<p>(4NO₂pzAg)₂(PH₃)</p> <p>Ag,-0.0205183879,1.3972203155,0.</p> <p>Ag,-0.0000544396,-1.7543040267,0.</p> <p>N,-0.0133395592,0.7303098929,1.9650541199</p> <p>N,0.0015141153,-0.651365281,1.9240437996</p> <p>C,0.0101325617,-1.1099399986,3.2046540826</p> <p>H,0.022954397,-2.172834191,3.4381934646</p> <p>C,-0.0139448697,1.1404512422,3.2592783836</p> <p>H,-0.0242182952,2.1932893656,3.5339340188</p> <p>C,0.0006039213,-0.0051943344,4.0702389655</p> <p>P,-0.0207630491,-4.1630888328,0.</p> <p>N,0.0015141153,-0.651365281,-1.9240437996</p> <p>N,-0.0133395592,0.7303098929,-1.965054119 9</p> <p>C,-0.0139448697,1.1404512422,-3.259278383 6</p> <p>H,-0.0242182952,2.1932893656,-3.533934018 8</p> <p>C,0.0101325617,-1.1099399986,-3.204654082 6</p> <p>H,0.022954397,-2.172834191,-3.4381934646</p> <p>C,0.0006039213,-0.0051943344,-4.070238965 5</p> <p>H,0.5702293742,-4.8835577988,-1.067761359 8</p> <p>H,0.5702293742,-4.8835577988,1.0677613598</p> <p>H,-1.2790915708,-4.8140166881,0.</p> <p>N,0.0052808479,-0.0412217669,5.5085622888</p> <p>O,-0.0044802474,1.0446260624,6.1096888568</p> <p>O,0.0187485364,-1.1575299085,6.0524372941</p>

	<p>N,0.0052808479,-0.0412217669,-5.508562288 8</p> <p>O,0.0187485364,-1.1575299085,-6.052437294 1</p> <p>O,-0.0044802474,1.0446260624,-6.109688856 8</p>
	<p>(4NO₂pzAg)₂(PH₃)₄</p> <p>Ag,-0.1612245125,1.9736091666,0.027792054 7</p> <p>Ag,0.002330641,-1.8924163323,0.0456546796</p> <p>P,0.575891629,4.2279310539,0.0562281243</p> <p>P,-2.5986194813,1.2380040914,-0.1064420319</p> <p>N,0.2699974119,0.6915458285,1.8291465859</p> <p>N,-0.1807642191,-0.6082804091,1.856026317 5</p> <p>C,-0.2513070632,-1.0190536335,3.152689665 6</p> <p>H,-0.5734900086,-2.023254779,3.4243571764</p> <p>C,0.4645442788,1.1080419252,3.1108526639</p> <p>H,0.8115823259,2.1134908099,3.3448802735</p> <p>C,0.1475638828,0.0471907248,3.97642202</p> <p>P,-0.9594037474,-4.0653747526,-0.060886338 3</p> <p>P,2.4457962316,-1.3567784394,-0.4253860824</p> <p>N,-0.44260871,-0.5421755001,-1.7745853753</p> <p>N,0.2747239699,0.6376953309,-1.7373081319</p> <p>C,0.789194453,0.8791717153,-2.9735857929</p> <p>H,1.3816715701,1.7670574142,-3.1915039767</p> <p>C,-0.3548195803,-1.053400523,-3.036678796 6</p> <p>H,-0.8379736052,-1.9894108427,-3.31471539 87</p> <p>C,0.4146284701,-0.1782489741,-3.822113108 5</p> <p>H,-2.82306638,-0.0588811918,0.4217880256</p> <p>H,2.8992244432,-0.1417343447,0.1500098354</p> <p>H,-3.1755354387,1.0258023296,-1.385941646 6</p> <p>H,3.60518965,-2.1327649563,-0.1466184559</p> <p>H,-3.7253860779,1.8699214922,0.4910683077</p>

	H,2.7519213379,-1.0560727831,-1.779555052 3
	H,1.3439527863,4.7061372872,1.1491348226
	H,-0.1255952054,-5.2042879257,-0.19509970 82
	H,-0.3707701683,5.283273231,0.0295442315
	H,-1.7601752804,-4.5548682925,1.003090040 3
	H,1.4158869148,4.717372553,-0.9771107622
	H,-1.8565412725,-4.3740970674,-1.11557393 15
	N,0.2158911744,0.052009097,5.4101736621
	O,0.594260702,1.0973110729,5.9669269207
	O,-0.1076229798,-0.9891974498,6.007636051 5
	N,0.7467786308,-0.3289477779,-5.211361059 9
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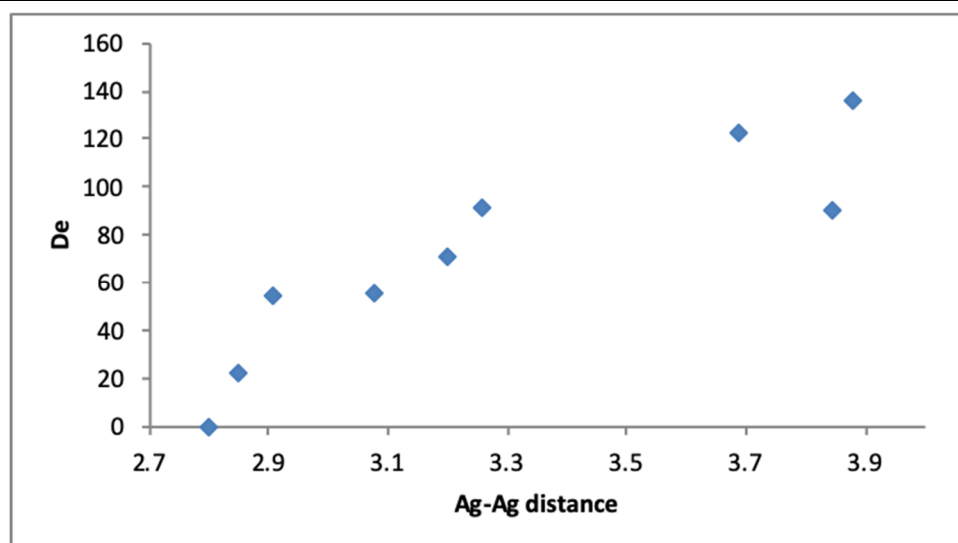


Figure S1. D_e ($\text{kJ}\cdot\text{mol}^{-1}$) vs. Ag-Ag dist. (\AA) in the $(\text{PzAg})_2\text{L}_2$ complexes.

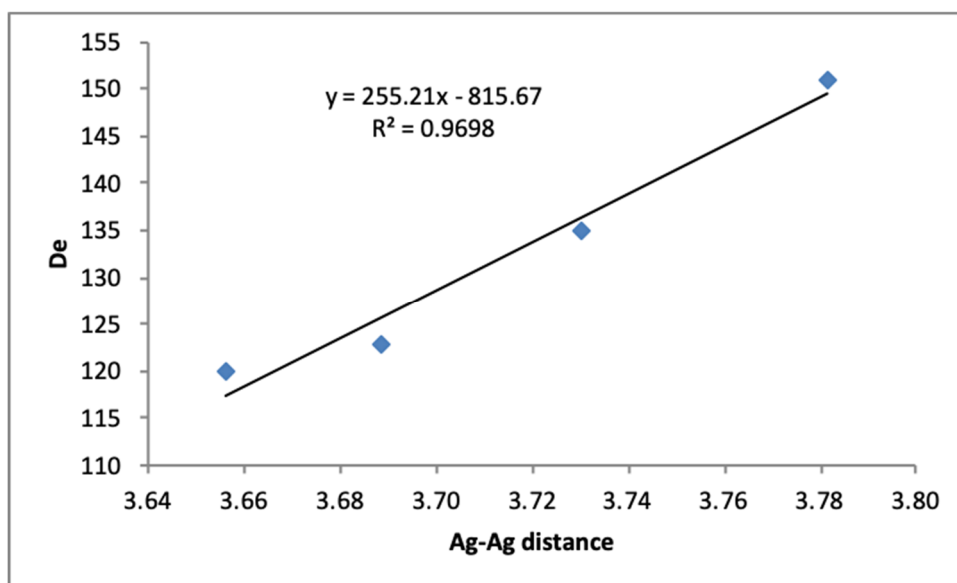


Figure S2. D_e ($\text{kJ}\cdot\text{mol}^{-1}$) vs. Ag-Ag dist. (\AA) in the $(R\text{-pzAg})_2(\text{PH}_3)_2$ complexes.

Table S4. Distance (\AA) and electron density properties (au) of the Ag-Ag BCPs.

System	Ag-Ag dist.	q_{BCP}	$\nabla^2 q_{\text{BCP}}$	H_{BCP}
(DMepzAg) ₂	2.793	0.032	0.098	-0.005
(PzAg) ₂	2.801	0.032	0.096	-0.005
(4ClpzAg) ₂	2.819	0.030	0.093	-0.004
(4NO ₂ pzAg) ₂	2.841	0.029	0.089	-0.004
(PzAg) ₂ (N ₂) ₂	2.851	0.029	0.087	-0.004
(PzAg) ₂ (OH ₂) ₂	2.908	0.026	0.077	-0.003
(PzAg) ₂ (PH ₃)	3.087	0.018	0.054	-0.001
(PzAg) ₂ (NCH) ₂	3.078	0.019	0.056	-0.001
(4NO ₂ pzAg) ₂ (PH ₃)	3.152	0.016	0.048	-0.0003
(PzAg) ₂ (SH ₂) ₂	3.196	0.015	0.045	-0.0002
(PzAg) ₂ (NH ₃) ₂	3.255	0.014	0.041	0.0002

Table S5. Distance (\AA) and electron density properties (au) of the Ag-L BCPs.

System	Interacting Atoms	Dist	q_{BCP}	$\nabla^2 q_{\text{BCP}}$	H_{BCP}
(PzAg) ₂ (N ₂) ₂	Ag-N*	2.837	0.017	0.062	0.001
(PzAg) ₂ (OH ₂) ₂	Ag-O*	2.630	0.026	0.099	-0.001
(PzAg) ₂ (NCH) ₂	Ag-N*	2.425	0.041	0.182	-0.001
(PzAg) ₂ (SH ₂) ₂	Ag-S*	2.631	0.048	0.142	-0.007
(PzAg) ₂ (NH ₃) ₂	Ag-N*	2.358	0.053	0.218	-0.004
(PzAg) ₂ (PH ₃) ₂	Ag-P*	2.373	0.082	0.153	-0.030
(PzAg) ₂ (CO) ₂	Ag-C*	1.998	0.119	0.397	-0.048
(PzAg) ₂ (CNH) ₂	Ag-C*	2.018	0.115	0.372	-0.046
(DMepzAg) ₂ (PH ₃) ₂	Ag-P*	2.379	0.081	0.153	-0.029
(4ClpzAg) ₂ (PH ₃) ₂	Ag-P*	2.372	0.082	0.152	-0.030
(4NO ₂ pzAg) ₂ (PH ₃) ₂	Ag-P*	2.374	0.082	0.150	-0.030
(PzAg) ₂ (PH ₃)	Ag-P	2.410	0.077	0.149	-0.026
(4NO ₂ pzAg) ₂ (PH ₃)	Ag-P	2.409	0.077	0.147	-0.026
(PzAg) ₂ (PH ₃) ₄	Ag-P	2.364	0.083	0.154	-0.031

	Ag-P	2.578	0.056	0.119	-0.014
	Ag-P	2.369	0.082	0.153	-0.030
	Ag-P	2.576	0.056	0.119	-0.014
(4NO₂pzAg)₂(PH₃)₄	Ag-P	2.379	0.081	0.150	-0.029
	Ag-P	2.545	0.060	0.125	-0.016
	Ag-P	2.372	0.082	0.152	-0.030
	Ag-P	2.550	0.059	0.125	-0.015

* Two contacts with identical values are found in these complexes.

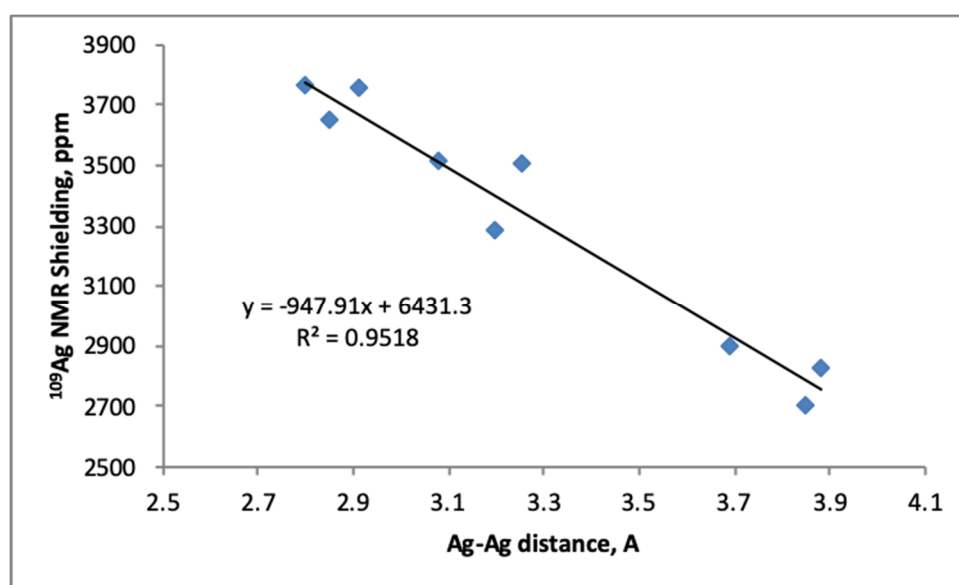


Figure 3. ¹⁰⁹Ag chemical shielding vs. Ag-Ag distance in the (PzAg)₂L₂ complexes.

Table S6. NICS values (ppm) from 0.0 to 2.0 Å of the center of the 6-membered ring in (PzAg)₂.

Distance to the Center	Ag-NICS Distance	NICS Value
0.00	1.40	-7.44
0.25	1.42	-6.81
0.50	1.49	-5.24
0.75	1.59	-3.40
1.00	1.72	-1.83
1.25	1.88	-0.78
1.50	2.05	-0.20
1.75	2.24	0.05
2.00	2.44	0.10