

## **SUPPORTING INFORMATION**

### **Indium-catalyzed cycloisomerization of 1,6-cyclohexenylalkynes**

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## Experimental section

All reactions were carried out under argon atmosphere in flame-dried glassware unless otherwise noted. Syringes, which were used to transfer anhydrous solvents or reagents, were purged with nitrogen prior to use. Commercially available starting materials, reagents and anhydrous solvents were used without further purification unless otherwise stated. All reactions were monitored by thin layer chromatography (T.L.C.) or HPLC-MS. Thin-layer chromatography (T.L.C.) were carried out on ready-for-use silica plates silica gel 60 F254 art. 5554 (Merck). Products were eluted with mixture of solvents (volume/volume) and were visualized with U.V. light (254 nm). Products were purified by flash chromatography using packed silica gel columns. Reaction monitoring was conducted with HPLC-MS Agilent instrument, fitted with Quadrupole 6120 detectors (ESI source in positive mode).

The 1,6-enynes **1a-1p** were prepared according to described procedures.<sup>1</sup> Compounds **2** to **4** are known derivatives from our previous report<sup>1</sup> and the spectral data were found to be consistent with authentic samples.

*Typical procedure for indium-catalyzed cyclization.* To a screw-cap vial, equipped with an argon inlet was added the alkynyl arylcyclohexene functional derivative in anhydrous toluene ( $c = 0.12 - 0.15\text{M}$ ). After stirring for 5 min under argon, was added indium trichloride catalyst (5 or 7 mol %). The reaction mixture was stirred at 40°C, 80°C or 110°C under Ar. After cooling the mixture was filtrated through a short pad of celite and concentrated in vacuum. The crude was purified by flash chromatography.

*Ethyl 4-(4-methoxyphenyl)-6-methylene-bicyclo[3.2.1]oct-3-ene-1-carboxylate (2a).* According to the described typical procedure for indium-catalyzed cyclization, 0.10 g (90%) of **2a** (colorless oil) was obtained from ethyl 4-(4-methoxyphenyl)-1-prop-2-ynyl-cyclohex-3-ene-1-carboxylate **1a** (0.368 mmol, 0.110 g) in toluene (2.45 mL,  $c=0.15\text{ M}$ ), in the presence of indium trichloride (0.05 eq., 0.00184 mmol, 4.10 mg) at 40°C for 2 h. The compound was purified by column chromatography on silica gel (98/2 to 90/10 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 6-methylene-4-phenyl-bicyclo[3.2.1]oct-3-ene-1-carboxylate (2b).* According to the described typical procedure for indium-catalyzed cyclization, 0.312 g (78%) of **2b** (colorless oil) was obtained from ethyl 4-phenyl-1-prop-2-ynyl-cyclohex-3-ene-1-carboxylate **1b** (1.49 mmol, 0.400 g) in toluene (10 mL,  $c=0.15\text{M}$ ), in the presence of indium trichloride (0.05 eq., 0.0745 mmol, 16.5 mg). Reaction at 40°C, 15 h. The compound was purified by column chromatography on silica gel (98/2 to 93/7 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 6-methylene-4-(4-propylphenyl)bicyclo[3.2.1]oct-3-ene-1-carboxylate (2c).* According to the described typical procedure for indium-catalyzed cyclization, 0.150 g (75%) of **2c** (colorless oil) was obtained from ethyl 4-(4-propylphenyl)-1-prop-2-ynyl-cyclohex-3-ene-1-carboxylate **1c** (0.644 mmol, 0.200 g) in toluene (4.30 mL,  $c = 0.15\text{ M}$ ), in the presence of indium trichloride (0.05 eq., 0.0745 mmol, 7.2 mg). Reaction at 40°C, 2 h. The compound was purified by column

<sup>1</sup> Davenel, V.; Nisole, C.; Fontaine-Vive, F.; Fourquez, J.-M.; Chollet, A.-M.; Michelet, V *J. Org. Chem.* **2020**, *85*, 12657–12669.

chromatography on silica gel (98/2 to 95/5 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(4-chlorophenyl)-6-methylenebicyclo[3.2.1]oct-3-ene-1-carboxylate (2d).* According to the described typical procedure for indium-catalyzed cyclization, 0.078 g (39%) of **2d** (colorless oil) was obtained from ethyl 4-(4-chlorophenyl)-1-prop-2-ynyl-cyclohex-3-ene-1-carboxylate **1d** (0.726 mmol, 0.200 g) in toluene (4.40 mL, *c* = 0.15 M), in the presence of indium trichloride (0.05eq., 0.0073 mmol, 7.0 mg) Reaction at 40°C, 15 h The crude contains the homologue with the isomerized double bond (65 : 35). The compound was purified by column chromatography on silica gel (98/2 to 90/10 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(4-methoxyphenyl)-6-methylbicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4e).* According to the described typical procedure for indium-catalyzed cyclization, 0.130 g (87%) of **4e** (thick colorless oil) was obtained from ethyl 1-but-2-ynyl-4-(4-methoxyphenyl)cyclohex-3-ene-1-carboxylate **1e** (0.48 mmol, 0.150 g) in toluene 4.0 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.0336 mmol, 7.4 mg) Reaction at 110°C, 5h. The compound was purified by column chromatography on silica gel (98/2 to 85/15 heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(4-methoxyphenyl)-6-phenylbicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4f).* According to the described typical procedure for indium-catalyzed cyclization, 0.131 g (87%) of **4f** (off white solid) was obtained from ethyl 4-(4-methoxyphenyl)-1-(3-phenylprop-2-ynyl)cyclohex-3-ene-1-carboxylate **1f** (0.40 mmol, 0.150 g) in toluene (3.35 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.028 mmol, 6.2 mg) Reaction at 110°C, 5 h. The crude contains the homologue *exo* product (12 : 88)The compound was purified by column chromatography on silica gel (98/2 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4,6-bis(4-methoxyphenyl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4g).* According to the described typical procedure for indium-catalyzed cyclization, 0.10 g (66%) of **4g** (off white solid) was obtained from ethyl 4-(4-methoxyphenyl)-1-[3-(4-methoxyphenyl)prop-2-ynyl]cyclohex-3-ene-1-carboxylate **1g** (0.371 mmol, 0.150 g) in toluene (3.10 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.026 mmol, 5.8 mg) Reaction at 110°C, 5 h The crude contains the homologue *exo* product (5 : 95). The compound was purified by column chromatography on silica gel (95/2 to 95/5 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(4-chlorophenyl)-6-(4-methoxyphenyl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4h).* According to the described typical procedure for indium-catalyzed cyclization, 0.082 g (54%) of **4h** (off-white solid) was obtained from ethyl 1-[3-(4-chlorophenyl)prop-2-ynyl]-4-(4-methoxyphenyl)cyclohex-3-ene-1-carboxylate **1h** (0.49 mmol, 0.150 g) in toluene (3.15 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.026 mmol, 5.8 mg). Reaction at 110°C, 5 h. The crude contains the homologue *exo* product (45 : 55). The compound was

purified by column chromatography on silica gel (95/5 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(4-fluorophenyl)-6-(4-methoxyphenyl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4i).* According to the described typical procedure for indium-catalyzed cyclization, 0.10 g (65%) of **4i** (white solid) was obtained from ethyl 1-[3-(4-fluorophenyl)prop-2-ynyl]-4-(4-methoxyphenyl)cyclohex-3-ene-1-carboxylate **1i** (0.393 mmol, 0.154 g) in toluene (3.20 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.028 mmol, 6.1 mg). Reaction at 110°C, 5 h. The crude contains the homologue *exo* product (10 : 90). The compound was purified by column chromatography on silica gel (95/5 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(3-fluorophenyl)-6-(4-methoxyphenyl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4j).* According to the described typical procedure for indium-catalyzed cyclization, 0.0752 g (57%) of **4j** (thick oil) was obtained from ethyl 1-[3-(3-fluorophenyl)prop-2-ynyl]-4-(4-methoxyphenyl)cyclohex-3-ene-1-carboxylate **1j** (0.339 mmol, 0.133 g) in toluene (2.80 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.024 mmol, 5.3 mg). Reaction at 110°C, 5 h. The crude contains the homologue *exo* product (35 : 65). The compound was purified by column chromatography on silica gel (95/5 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(2-fluorophenyl)-6-(4-methoxyphenyl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4k).* According to the described typical procedure for indium-catalyzed cyclization, 0.104 g (69%) of **4k** (thick oil) was obtained from ethyl 1-[3-(2-fluorophenyl)prop-2-ynyl]-4-(4-methoxyphenyl)cyclohex-3-ene-1-carboxylate **1k** (0.382 mmol, 0.150 g) in toluene (3.20 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.0268 mmol, 5.9 mg). Reaction at 110°C, 5 h. The crude contains the homologue *exo* product (25 : 75). The compound was purified by column chromatography on silica gel (95/5 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(4-(methoxycarbonyl)phenyl)-6-(4-methoxyphenyl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4l).* According to the described typical procedure for indium-catalyzed cyclization, 0.073 g (49%) of **4l** (white solid) was obtained from ethyl methyl 4-[3-[1-ethoxycarbonyl-4-(4-methoxyphenyl)-cyclohex-3-en-1-yl]prop-1-ynyl]benzoate **1l** (0.347 mmol, 0.150 g) in toluene (2.95 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.0243 mmol, 5.4 mg). Reaction at 110°C, 5 h. The crude contains the homologue *exo* product (51 : 49). The compound was purified by column chromatography on silica gel (95/5 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(4-methoxyphenyl)-6-(4-(trifluoromethyl)phenyl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4m).* in the presence of to the described typical procedure for indium-catalyzed cyclization, 0.0614 g (41%) of **4m** (yellow solid) was obtained from ethyl 4-(4-methoxyphenyl)-1-[3-[4-(trifluoromethyl)phenyl]prop-2-ynyl]cyclohex-3-ene-1-carboxylate **1m** (0.339 mmol, 0.150 g) in toluene (7.50 mL, *c* = 0.12 M), catalyst indium trichloride (0.07eq., 0.0237 mmol, 5.2 mg). Reaction at 110°C, 5 h. The crude contains the homologue *exo* product (55 : 45).

The compound was purified by column chromatography on silica gel (95/5 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl 4-(4-methoxyphenyl)-6-(3-nitrophenyl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4n).* According to the described typical procedure for indium-catalyzed cyclization, 0.0720 g (48%) of **4n** (thick yellow oil) was obtained from ethyl 4-(4-methoxyphenyl)-1-[3-(3-nitrophenyl)prop-2-ynyl]cyclohex-3-ene-1-carboxylate **1n** (0.357 mmol, 0.150 g) in toluene (3.0 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.025 mmol, 5.5 mg). Reaction at 110°C, 5 h. The crude contains the homologue *exo* product (46 : 54). The compound was purified by column chromatography on silica gel (95/5 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

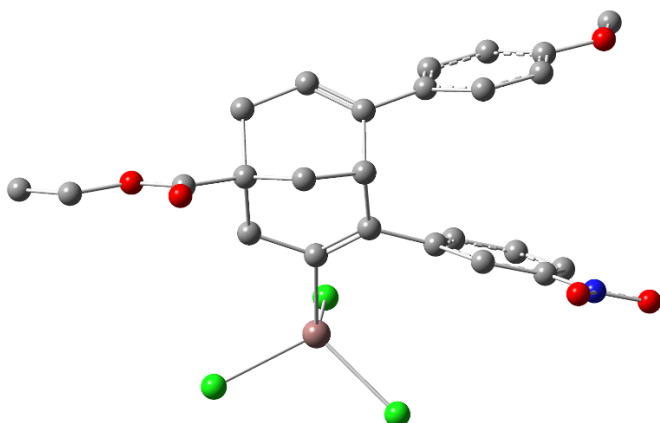
*Ethyl-4-(furan-2-yl)-6-(4-methoxyphenyl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4o).* According to the described typical procedure for indium-catalyzed cyclization, 0.008 g (5%) of **4o** (off-white solid) was obtained from ethyl 1-[3-(2-furyl)prop-2-ynyl]-4-(4-methoxyphenyl)cyclohex-3-ene-1-carboxylate **1o** (0.604 mmol, 0.220 g) in toluene 3.40 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.0288 mmol, 5.5 mg). Reaction at 110°C, 5 h. The compound was purified by column chromatography on silica gel (95/5 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

*Ethyl-4-(4-methoxyphenyl)-6-(thiophen-2-yl)bicyclo[3.3.1]nona-3,6-diene-1-carboxylate (4p).* According to the described typical procedure for indium-catalyzed cyclization, 0.066 g (44%) of **4p** (pale yellow solid) was obtained from ethyl 1-[3-(2-furyl)prop-2-ynyl]-4-(4-methoxyphenyl)cyclohex-3-ene-1-carboxylate **1p** (0.394 mmol, 0.150 g) in toluene 3.30 mL, *c* = 0.12 M), in the presence of indium trichloride (0.07eq., 0.0276 mmol, 6.1 mg). Reaction at 110°C, 5 h. The compound was purified by column chromatography on silica gel (95/5 to 85/15 Heptane / EtOAc). The spectral analyses are in full agreement with published spectra.<sup>1</sup>

**DFT calculations.** We performed DFT calculations with the Gaussian 16 suite of programs (Revision A.03). Gold and indium intermediates were optimized with the dispersion corrected B3LYP-D3 exchange-correlation functional. The effective-core potential of Hay and Wadt with a double- $\xi$  valence basis set (LANL2DZ) was used to describe Au and In and the other atoms were described by the 6-31g(d,p) basis set. The PCM implicit solvation model was used to modelize the solvation effects of toluene. The reported Gibbs free energies were obtained by computing vibrational frequencies and summing electronic and thermal free energies. Only positive frequencies were obtained and the cartesian coordinates of gold and indium intermediates are presented below and hydrogen atoms were hidden for clarity.

***InCl<sub>3</sub> endo***

43% (absolute Gibbs free energy= -2780.372304 Hartree, number of imaginary frequencies= 0)

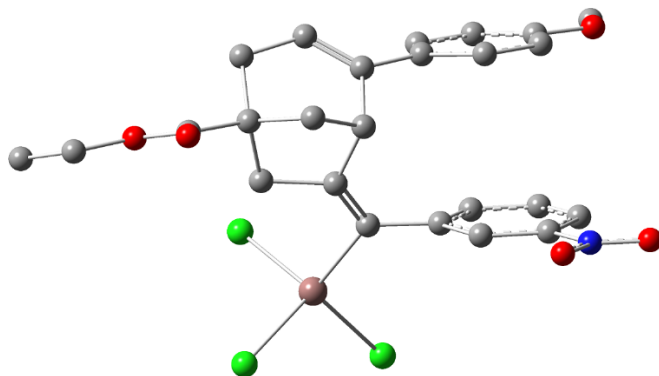


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C	-0.01726600	1.68832700	1.21264200
C	1.78969900	2.58781700	-0.38894300
C	2.85053900	2.60769800	0.53729000
C	4.17294400	2.51156000	0.12804400
C	4.48390700	2.38934000	-1.23447700
C	3.44901500	2.37704600	-2.17668900
C	2.12415700	2.46950400	-1.74574200
O	5.81271400	2.28065100	-1.53323200
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H	4.98624200	2.51874000	0.84660600
H	3.65477300	2.26574400	-3.23451300
H	1.32752300	2.40048500	-2.48002800
H	7.26649000	2.01705300	-2.90705400
H	5.74240400	1.18139800	-3.31084000
H	5.87385400	2.95214300	-3.51435900
C	-1.36671300	2.08772700	1.81404700
C	-1.20477600	-0.24143300	0.15293700
H	-1.63471600	1.40663400	2.62688900
H	-1.31752100	3.09819700	2.23356800
H	0.74911900	1.75081500	1.99170100
C	-0.59429800	3.21266700	-0.65546400
H	-0.32055200	3.84661300	-1.49715100
C	-2.06726000	3.09918700	-0.36479800
H	-2.43747400	4.08041000	-0.02742300
H	-2.61723700	2.88707400	-1.28910000
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H	-8.00954300	2.63148400	-0.28946500
H	-6.66219300	3.20419800	-1.29531000
H	-6.86551500	1.46786100	-0.99135100
C	-2.48706500	0.57485400	0.13184100
H	-2.87994700	0.61636800	-0.89136200
H	-3.24709900	0.00926600	0.68816000
C	1.24179000	-0.45787700	0.62804000
C	1.78694700	-0.89937300	-0.58991700
C	1.99204600	-0.63905600	1.79632000
C	3.03752100	-1.51786600	-0.64291900
H	1.23007400	-0.73472000	-1.50599600
C	3.23939600	-1.25206300	1.72179000
H	1.61789500	-0.31379200	2.75888500
C	3.78392800	-1.69875700	0.51658800
H	3.43314900	-1.84913700	-1.59729700
N	4.01778800	-1.41942100	2.95399500
O	3.53586700	-1.00134000	4.00986600
O	5.12265900	-1.96301700	2.87430100
H	4.76042500	-2.16471700	0.50599500
In	-1.40379300	-2.23895800	-0.62171400
Cl	-3.73843200	-2.80958700	-0.54598500
Cl	-0.76188100	-2.37149800	-2.94423200
Cl	-0.21104200	-3.95953000	0.53049500

### ***InCl<sub>3</sub> exo***

57% (absolute Gibbs free energy= -2780.372589 Hartree, number of imaginary frequencies= 0)

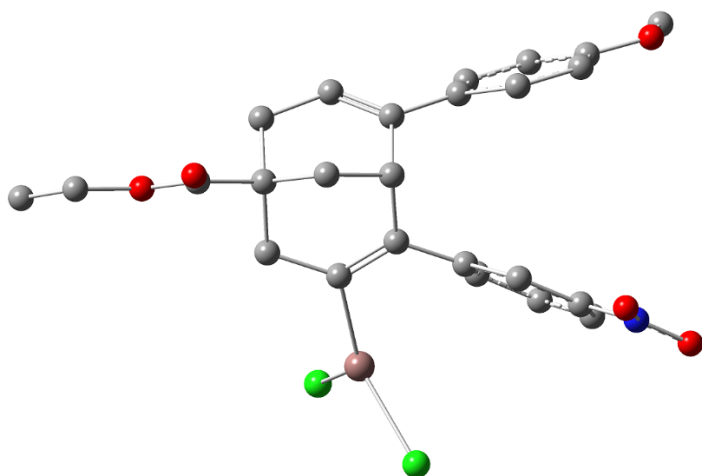


C	0.76914900	-0.49122800	0.55381500
C	2.53918100	-2.19252900	0.48148000
C	-0.14293400	-2.51114100	-0.42402600
C	0.23619100	-1.88234100	0.91931300
C	-1.54082600	-2.36194800	-0.88814900
C	-2.63489900	-2.59322700	-0.03213400
C	-3.93931900	-2.39099300	-0.45707800
C	-4.19420700	-1.93339400	-1.75864800
C	-3.12488600	-1.70395300	-2.63099900
C	-1.81735900	-1.91528900	-2.18733000
O	-5.51021700	-1.72702900	-2.06662000
C	-5.82095600	-1.20404700	-3.35075400

H	-2.46131500	-2.93463200	0.98395400
H	-4.78054100	-2.55711100	0.20780100
H	-3.28941800	-1.33502500	-3.63625300
H	-0.99000500	-1.68637300	-2.85171800
H	-5.50450100	-1.88259000	-4.15383300
H	-6.90653900	-1.09683300	-3.37965700
H	-5.35648600	-0.22218700	-3.51090700
C	1.46572500	-2.58342000	1.51147100
C	2.25981300	-0.67373600	0.26530200
H	2.84687000	-0.07353800	0.97088800
C	0.07072100	0.64852600	0.40325300
H	1.34087100	-3.66649700	1.60239700
H	1.71513800	-2.18004900	2.49746100
H	-0.61578200	-1.85529200	1.59704800
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C	2.29031500	-3.00269800	-0.81757500
H	2.87935200	-2.56470000	-1.63283600
H	2.66586300	-4.03020900	-0.69295500
H	2.54061900	-0.34546000	-0.74019400
C	3.95396100	-2.41950400	0.97139300
O	4.26839500	-2.90780400	2.03976600
O	4.85097000	-1.99473900	0.05720000
C	6.24582200	-2.10525800	0.42163100
C	7.05212200	-1.52159300	-0.72256000
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H	6.40977500	-1.56428700	1.35915300
H	6.86462500	-2.07192200	-1.64929100
H	6.78659700	-0.47327300	-0.88458100
H	8.12086900	-1.57955900	-0.49378500
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C	-1.87046200	0.44694500	1.98919200
C	-2.31223000	1.04407400	-0.30009900
C	-3.24447300	0.48099900	2.22656200
H	-1.19181100	0.21386800	2.79944600
C	-3.68175600	1.07606800	-0.04226400
H	-1.95127300	1.25849000	-1.30056900
C	-4.16990100	0.79010900	1.23011200
H	-4.37579200	1.31340200	-0.84192800
N	-3.73573600	0.16742400	3.57187400
O	-4.95292800	0.21770700	3.77466100
O	-2.91238700	-0.14004100	4.43796300
H	-5.22771800	0.80058200	1.45686000
In	1.05192900	2.38603700	-0.39506700
Cl	2.91851700	3.09134400	0.93479500
Cl	1.94071900	1.93119900	-2.58927400
Cl	-0.44511600	4.23582400	-0.63697600

***InCl<sub>2</sub> endo***

96% (absolute Gibbs free energy= -2319.971691 Hartree, number of imaginary frequencies= 0)

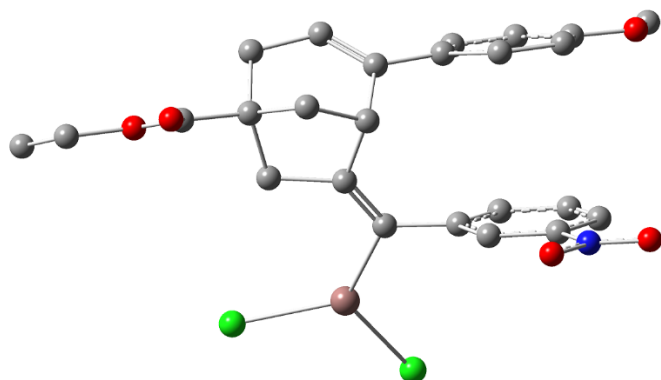


C	0.28919600	-0.09225700	0.60230800
C	2.79781400	-1.59139900	0.69787300
C	0.04072800	-2.47257600	0.12898700
C	0.37198400	-1.47603800	1.24059400
C	-1.38563100	-2.70083300	-0.20167400
C	-2.36948600	-2.83299100	0.79796900
C	-3.70872400	-3.00318200	0.47791700
C	-4.11657700	-3.04173700	-0.86464900
C	-3.15751000	-2.91076400	-1.87730700
C	-1.81504800	-2.73869000	-1.53667300
O	-5.45364900	-3.19922500	-1.07326000
C	-5.92554400	-3.24915100	-2.41483400
H	-2.08418400	-2.81802400	1.84547200
H	-4.46252500	-3.11013900	1.25104800
H	-3.44184700	-2.92261900	-2.92257400
H	-1.08607400	-2.60057500	-2.32965300
H	-7.00585100	-3.38452300	-2.34925500
H	-5.71039400	-2.31723700	-2.95334700
H	-5.48806900	-4.09163900	-2.96542700
C	1.76629000	-1.72245800	1.82477200
C	1.38810400	0.50052000	0.09523600
H	1.98052300	-1.00114400	2.61895800
H	1.81848600	-2.72143900	2.26651900
H	-0.37297800	-1.54537200	2.03914400
C	1.05037200	-2.99067900	-0.58857900
H	0.83036600	-3.70542000	-1.37910700
C	2.50884500	-2.67928100	-0.37789600
H	3.01749700	-3.61088100	-0.08773800
H	2.97257700	-2.38830600	-1.32804900
C	4.20399400	-1.83276900	1.23719800
O	4.48228200	-2.10709600	2.38696700
O	5.12179800	-1.70114600	0.25844300
C	6.50508400	-1.90770200	0.64152200
C	7.34836600	-1.70027000	-0.60089600
H	6.75851000	-1.20057100	1.43765000

H	6.60902800	-2.91805100	1.04960100
H	8.40566700	-1.84663400	-0.36070700
H	7.06912200	-2.41222600	-1.38285600
H	7.21957000	-0.68721900	-0.99274000
C	2.75979800	-0.13403700	0.13658900
H	3.21453000	-0.11799000	-0.86010400
H	3.40735500	0.49992000	0.75897500
C	-1.04811100	0.53448400	0.45238500
C	-1.50833100	0.92425800	-0.82441700
C	-1.85715300	0.79959200	1.56597300
C	-2.72005800	1.61085700	-0.98011400
H	-0.95982800	0.59906100	-1.70554100
C	-3.05584600	1.47582200	1.38244600
H	-1.55286200	0.51050300	2.56385400
C	-3.50366300	1.90240300	0.13017400
H	-3.05526400	1.89686600	-1.97122400
N	-3.89146400	1.75857900	2.56714400
O	-3.49197400	1.35590300	3.65878500
O	-4.94101500	2.37471700	2.39116400
H	-4.44564500	2.42814200	0.04603100
In	1.00403500	2.41381200	-0.72774900
Cl	0.31728900	4.29095900	0.47240900
Cl	1.41870800	2.94826000	-2.96920000

### ***InCl<sub>2</sub> exo***

4% (absolute Gibbs free energy= -2319.968668 Hartree, number of imaginary frequencies= 0)

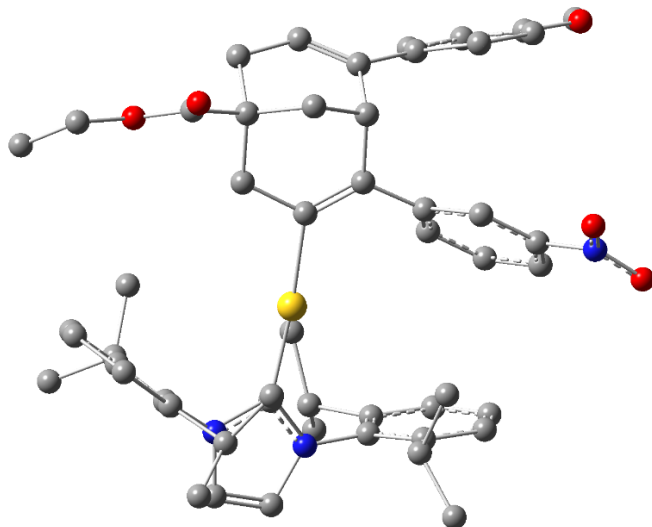


C	0.90400700	-0.29517700	0.48491900
C	2.71856500	-1.94069800	0.50768200
C	0.03645000	-2.38314900	-0.37103400
C	0.40842600	-1.67030900	0.93565300
C	-1.37581700	-2.33805700	-0.81089000
C	-2.43762200	-2.54804400	0.09101400
C	-3.75907000	-2.45873200	-0.31726600
C	-4.06799100	-2.14174900	-1.64963100
C	-3.03053700	-1.93834500	-2.56744300
C	-1.70479200	-2.03510900	-2.13950300
O	-5.39574700	-2.03976600	-1.93941500
C	-5.77115700	-1.71259900	-3.27240400
H	-2.22691000	-2.79082600	1.12805300

H	-4.57525200	-2.61457800	0.38016500
H	-3.23751700	-1.68606600	-3.60042600
H	-0.90657900	-1.83892900	-2.84925200
H	-5.42362000	-2.46900700	-3.98737400
H	-6.86146200	-1.68429800	-3.28028900
H	-5.38187800	-0.73062300	-3.57143500
C	1.65799400	-2.30659500	1.55865000
C	2.40213200	-0.43998700	0.22979400
H	2.95491000	0.19502500	0.93247800
C	0.14152800	0.79889000	0.28225000
H	1.55669400	-3.38542900	1.70051300
H	1.89958900	-1.85290100	2.52427200
H	-0.44071400	-1.61768200	1.61446200
C	1.02611500	-2.90464800	-1.11866600
H	0.78494100	-3.42241600	-2.04451200
C	2.48577500	-2.80945000	-0.75479800
H	3.05940900	-2.39243300	-1.59216700
H	2.89253800	-3.81787900	-0.58922300
H	2.70497400	-0.13247900	-0.77503900
C	4.14158000	-2.10969500	1.00589800
O	4.45872800	-2.52227900	2.10327700
O	5.02524400	-1.72614700	0.06436200
C	6.42813000	-1.81404600	0.42210600
C	7.22321200	-1.30053300	-0.76184800
H	6.66420100	-2.85582800	0.66151200
H	6.59758500	-1.21876500	1.32478600
H	7.03049900	-1.90696500	-1.65155600
H	6.95823400	-0.26317100	-0.98502800
H	8.29317500	-1.34486800	-0.53767200
C	-1.31837100	0.82715800	0.57218500
C	-1.78481300	0.68559900	1.88499800
C	-2.26101600	0.99196700	-0.45861300
C	-3.15743400	0.67822200	2.12533800
H	-1.09485500	0.57422100	2.71166000
C	-3.62976200	0.98696800	-0.19526000
H	-1.91538900	1.09311700	-1.48241600
C	-4.09686100	0.82628800	1.10726500
H	-4.33743900	1.09033300	-1.01058700
N	-3.62907400	0.50045700	3.50690300
O	-4.84470500	0.49882000	3.70550600
O	-2.78331100	0.35753300	4.39184300
H	-5.15350100	0.81049300	1.33983700
In	0.97369800	2.56700400	-0.49477400
Cl	-0.34994000	4.38142900	-1.10732200
Cl	3.23799800	2.94452700	-0.89339100

***IPrAu endo***

99 % (absolute Gibbs free energy= -2692.764728 Hartree, number of imaginary frequencies= 0)



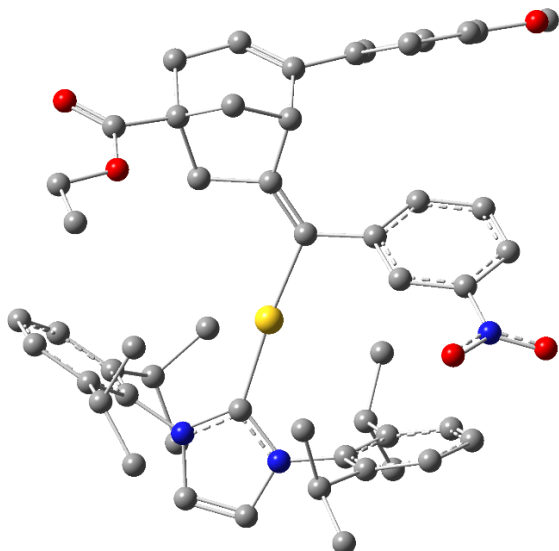
C	-1.53584100	1.49320800	-0.68291200
C	-0.19163000	4.10580000	-0.39595400
C	-2.89430300	3.27157900	0.33458800
C	-2.23868900	2.82494300	-0.96999100
C	-4.16221700	2.61265300	0.73285400
C	-5.19413900	2.36333500	-0.19300100
C	-6.35806500	1.70477500	0.17729000
C	-6.53049200	1.26153000	1.49712400
C	-5.51996300	1.49559600	2.43722800
C	-4.35514900	2.15919400	2.04575200
O	-7.70353600	0.61166800	1.75698900
C	-7.92370800	0.12799400	3.07479900
H	-5.08959000	2.69536300	-1.22119100
H	-7.15020600	1.51649400	-0.54020200
H	-5.61653000	1.15278300	3.46052700
H	-3.56104900	2.30063800	2.77271800
H	-8.90411300	-0.35072500	3.06166900
H	-7.16557800	-0.61059700	3.36689900
H	-7.93025000	0.94304200	3.81035700
C	-1.24358700	3.87156700	-1.48407800
C	-0.25317200	1.46622300	-0.26241400
H	-0.76544200	3.51711100	-2.40215000
H	-1.75775500	4.80932800	-1.72059900
H	-3.01026500	2.67362600	-1.73172800
C	-2.24709800	4.13087500	1.13918000
H	-2.71276800	4.44539600	2.07166700
C	-0.89342200	4.72212100	0.84448300
H	-1.01031000	5.80665400	0.69007600
H	-0.24005200	4.62476000	1.71986200
C	0.87834800	5.07538000	-0.87142500
O	0.93327100	5.60960400	-1.96189500
O	1.81878100	5.25281800	0.08582000

C	2.97009700	6.04754400	-0.27148400
C	3.99891300	5.85087300	0.82620800
H	3.34169500	5.71714100	-1.24651500
H	2.66551700	7.09522600	-0.37057200
H	4.90275700	6.42639800	0.60353600
H	3.60650500	6.18144100	1.79229800
H	4.26689100	4.79316100	0.90674200
C	0.53535800	2.75452800	-0.09261700
H	0.95276400	2.79440200	0.92047200
H	1.41829000	2.67988100	-0.74338700
C	-2.35399400	0.25971400	-0.79540900
C	-2.42953200	-0.65669000	0.27185500
C	-3.07060200	-0.03467200	-1.96229900
C	-3.16260200	-1.83830400	0.17083300
H	-1.90644200	-0.42149000	1.19170700
C	-3.79142500	-1.22452000	-2.04802700
H	-3.05184000	0.63315800	-2.81430800
C	-3.85013300	-2.14387100	-1.00026700
H	-3.18823200	-2.52959900	1.00571700
Au	0.87955600	-0.21745200	0.04008300
C	3.21371600	-3.79993400	0.44750100
C	4.19131700	-2.86315800	0.33209700
H	3.25949100	-4.87135100	0.55583200
H	5.26559400	-2.94966500	0.31640200
C	2.19587800	-1.78115000	0.26233900
N	2.00107400	-3.11619400	0.40812500
N	3.54792500	-1.63687900	0.21896700
C	0.70329300	-3.73753500	0.49471600
C	0.19140200	-4.03430900	1.77233700
C	0.00729400	-4.01226600	-0.69410900
C	-1.05037700	-4.67657300	1.83261000
C	-1.22847300	-4.66183200	-0.57786800
C	-1.74561800	-5.00194700	0.66830800
H	-1.48074100	-4.92325100	2.79726400
H	-1.79578400	-4.88902100	-1.47462000
H	-2.70568700	-5.50576500	0.73566100
C	4.17427600	-0.35129800	0.03278200
C	4.42282700	0.44319000	1.16509500
C	4.41817300	0.08568200	-1.28152900
C	4.96614700	1.71583700	0.94994400
C	4.95762100	1.36747500	-1.44199600
C	5.23198400	2.17349000	-0.33884500
H	5.16863200	2.35952900	1.80048600
H	5.15094500	1.74272500	-2.44204600
H	5.64751700	3.16637200	-0.48505100
C	0.91521400	-3.59489100	3.04005200
C	0.37964100	-2.22084200	3.49420200
C	0.82988600	-4.62425500	4.17810000
H	-0.68371800	-2.29061800	3.74986000
H	0.92193000	-1.86985900	4.37916700
H	0.48896500	-1.47215800	2.70430100
H	1.46083000	-4.30751400	5.01468500

H	-0.19042300	-4.72346100	4.56279400
H	1.16548300	-5.61325300	3.85041400
C	0.52693300	-3.60448500	-2.06616100
C	-0.42453700	-2.58605500	-2.72222700
C	0.75870900	-4.82691000	-2.97190200
H	-1.40391000	-3.02983100	-2.92886800
H	-0.58002600	-1.72175900	-2.07104500
H	-0.00630700	-2.23324200	-3.67086300
H	1.16889700	-4.51119100	-3.93691400
H	1.46055800	-5.53286200	-2.51560000
H	-0.17669500	-5.36179500	-3.16751200
C	4.08060600	-0.01894000	2.57546000
C	2.96766600	0.85600000	3.18292500
C	5.32619000	-0.05244800	3.47914000
H	3.29624100	1.89524200	3.29153700
H	2.07585900	0.84594100	2.54902000
H	2.69035200	0.48372100	4.17508600
H	5.06540000	-0.43477500	4.47164900
H	6.10505000	-0.69627600	3.05766800
H	5.75269600	0.94766200	3.61033000
C	4.06813700	-0.75997900	-2.49965000
C	2.91115300	-0.12331400	-3.29364400
C	5.29598200	-1.00495100	-3.39492600
H	3.19747600	0.85684000	-3.68993400
H	2.63468500	-0.76193300	-4.13966000
H	2.02911600	0.01136400	-2.66034200
H	5.03038100	-1.66102600	-4.23036900
H	5.67804200	-0.06970900	-3.81738100
H	6.10939800	-1.47649800	-2.83383600
H	1.97579400	-3.46825900	2.80031800
H	3.69217000	-1.03976300	2.51589700
H	1.49078000	-3.10532300	-1.93534500
H	3.72161800	-1.73707100	-2.15101000
N	-4.49651500	-1.53349400	-3.29639200
O	-4.51294100	-0.67817300	-4.18473000
O	-5.03729800	-2.63852200	-3.39910300
H	-4.42108400	-3.05608900	-1.11208500

**IPrAu exo**

1% (absolute Gibbs free energy= -2692.752605 Hartree, number of imaginary frequencies= 0)



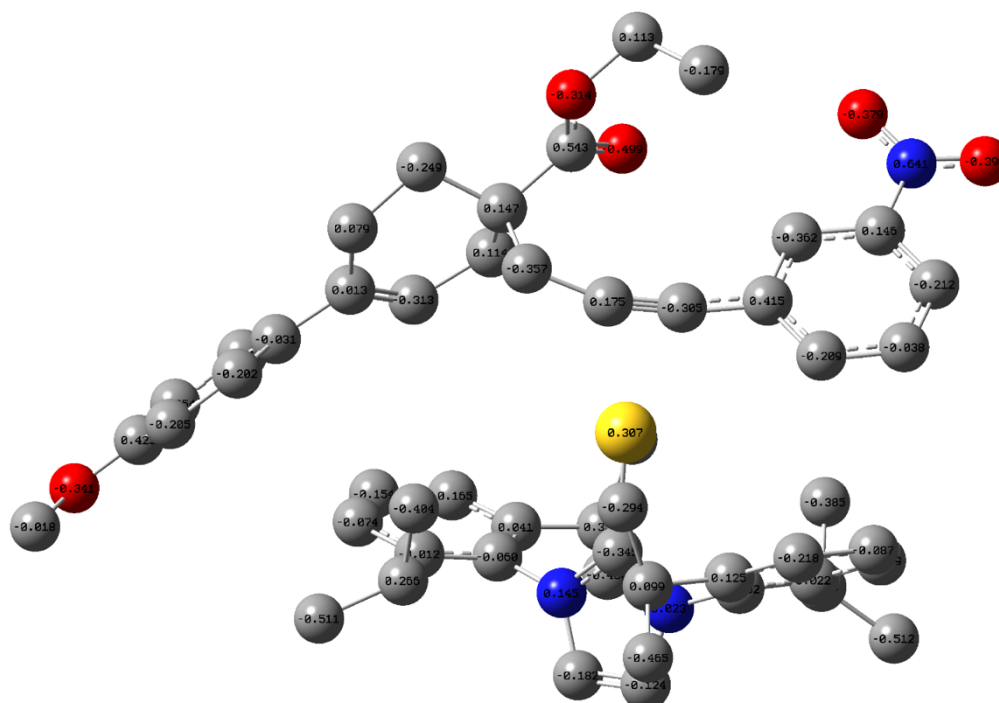
C	1.69194100	1.60462700	0.46798500
C	1.72315900	4.05756100	0.68026600
C	3.96820300	2.47831700	-0.05897400
C	3.00826100	2.09390800	1.07129600
C	4.98669100	1.49154100	-0.48522500
C	5.76397500	0.78271100	0.45123900
C	6.67286700	-0.18647600	0.05180600
C	6.82963200	-0.49067400	-1.30918600
C	6.07626400	0.20734000	-2.26113600
C	5.16977700	1.18434900	-1.84081000
O	7.72547400	-1.48082600	-1.59579400
C	7.91933700	-1.83549800	-2.95893300
H	5.65373000	0.99328200	1.51063100
H	7.26785800	-0.73319900	0.77615700
H	6.16999100	-0.00947900	-3.31849200
H	4.56203500	1.69523100	-2.58157700
H	8.66469100	-2.63221100	-2.96088600
H	6.99271100	-2.20673600	-3.41588800
H	8.29451300	-0.98879400	-3.54822900
C	2.54060400	3.36553200	1.80284900
C	0.91850100	2.86129100	0.06963500
H	0.83088100	2.96595900	-1.01744600
C	1.19871800	0.35732800	0.40174100
H	1.89658200	3.11013500	2.64810400
H	3.36687500	3.99012600	2.15846000
H	3.45485200	1.35091700	1.73511500
C	3.80428500	3.65673500	-0.68724800
H	4.48717500	3.93799600	-1.48677400
C	2.71382000	4.64020800	-0.34600000
H	2.16972200	4.93345000	-1.25335000
H	3.14880600	5.57115400	0.04308500
H	-0.09663300	2.81902800	0.47199100

C	0.77652300	5.13610300	1.16980000
O	0.66051000	6.24561100	0.68435100
O	0.03111600	4.71002600	2.21515600
C	-0.94300100	5.64210900	2.73650800
C	-1.45338000	5.07387300	4.04669000
H	-1.74524200	5.75829600	1.99848500
H	-0.46931000	6.61945200	2.86688900
H	-2.20541200	5.74339400	4.47562400
H	-1.90811800	4.09173200	3.89416400
H	-0.63463700	4.96702200	4.76397500
Au	-0.71536500	-0.10037600	-0.20513700
C	-4.80146300	-0.89853300	-1.26765600
C	-4.40224500	-2.12549700	-0.84603300
H	-5.75044200	-0.54734700	-1.63685100
H	-4.93192900	-3.06090000	-0.76819700
C	-2.62176900	-0.73006800	-0.67313800
N	-3.06469100	-2.00257000	-0.48311400
N	-3.69648500	-0.05812400	-1.16424000
C	-2.20849400	-3.06083300	0.00612700
C	-1.32210700	-3.67618500	-0.89742200
C	-2.23848100	-3.37473100	1.37770800
C	-0.45088300	-4.64546400	-0.38623400
C	-1.33869500	-4.34349400	1.83783900
C	-0.45249400	-4.97291300	0.96660000
H	0.24920300	-5.13578000	-1.05528800
H	-1.30020100	-4.58025900	2.89484600
H	0.25511800	-5.69939100	1.35352700
C	-3.67738500	1.34547400	-1.51306100
C	-3.37336100	1.70597700	-2.84689400
C	-3.94439000	2.30662800	-0.51425600
C	-3.35993600	3.07217200	-3.15787900
C	-3.91289400	3.65709500	-0.89667000
C	-3.62546400	4.04332300	-2.19843800
H	-3.12626600	3.37390300	-4.17493000
H	-4.11330800	4.41477900	-0.14383800
H	-3.60863800	5.09565700	-2.46597800
C	-2.96506100	0.76112300	-3.98355700
C	-1.47441100	0.38102400	-3.88273800
C	-3.83437200	-0.48487700	-4.22321800
H	-1.16715500	-0.17883100	-4.77325200
H	-1.27994700	-0.23992600	-3.00668200
H	-0.84465800	1.27174400	-3.79984300
H	-3.64286200	-1.27756600	-3.49881300
H	-4.90244400	-0.24705500	-4.19377300
H	-3.60853700	-0.89076900	-5.21492200
H	-3.06930100	1.37011900	-4.88967900
C	-4.19083900	2.06846800	0.98146800
C	-2.87260000	2.23596400	1.76648300
C	-4.91348700	0.78542800	1.41431600
H	-3.06409100	2.17779000	2.84366600
H	-2.15897300	1.44966300	1.50538700
H	-2.39700600	3.19696000	1.55100000

H	-4.27122800	-0.09213700	1.34163700
H	-5.81858900	0.60470000	0.82837900
H	-5.20751200	0.88345100	2.46448800
H	-4.84485200	2.89673300	1.28365300
C	-1.27313700	-3.31953200	-2.37671500
C	0.13110000	-2.85129700	-2.79951800
C	-1.76003800	-4.49377400	-3.24539700
H	0.11908800	-2.51902100	-3.84290300
H	0.86578000	-3.65852600	-2.71319300
H	0.46902200	-2.01819200	-2.17605600
H	-1.75768000	-4.21256500	-4.30404200
H	-1.11122700	-5.36839100	-3.12771000
H	-2.77765500	-4.79225700	-2.97268000
C	-3.14736200	-2.64444600	2.35793000
C	-2.35206000	-1.55876400	3.10957000
C	-3.84711600	-3.59756700	3.34170000
H	-3.00606400	-1.00854000	3.79499500
H	-1.54056400	-2.01009600	3.68887300
H	-1.90930600	-0.84312100	2.41072100
H	-4.56340200	-3.04046200	3.95446300
H	-3.13473500	-4.07231000	4.02356600
H	-4.38927300	-4.38905900	2.81424400
H	-1.95395800	-2.48371100	-2.54995500
H	-3.93463600	-2.14494800	1.78628200
C	1.96698600	-0.84406700	0.81514100
C	1.48455400	-1.65307600	1.85939800
C	3.11432500	-1.28373500	0.12850700
C	2.12626600	-2.84821900	2.16647300
H	0.58752800	-1.37247500	2.39557100
C	3.75474300	-2.48171700	0.46272900
H	3.49816600	-0.68383400	-0.68746400
C	3.26103700	-3.29151500	1.48039000
H	4.64483500	-2.78058400	-0.08232600
N	1.56499500	-3.69195100	3.22121400
O	1.95665200	-4.86072000	3.30245500
O	0.71293900	-3.20805400	3.97266600
H	3.72237000	-4.23378900	1.74599600

We calculated partial charges using the MKUFF method for Au and In alkyne complexes. The Merz-Kollman-Singh approximate charges with electronic embedding but using UFF radii. Atomic charges are fitted to reproduce the molecular electrostatic potential.

#### Au -alkyne complex:

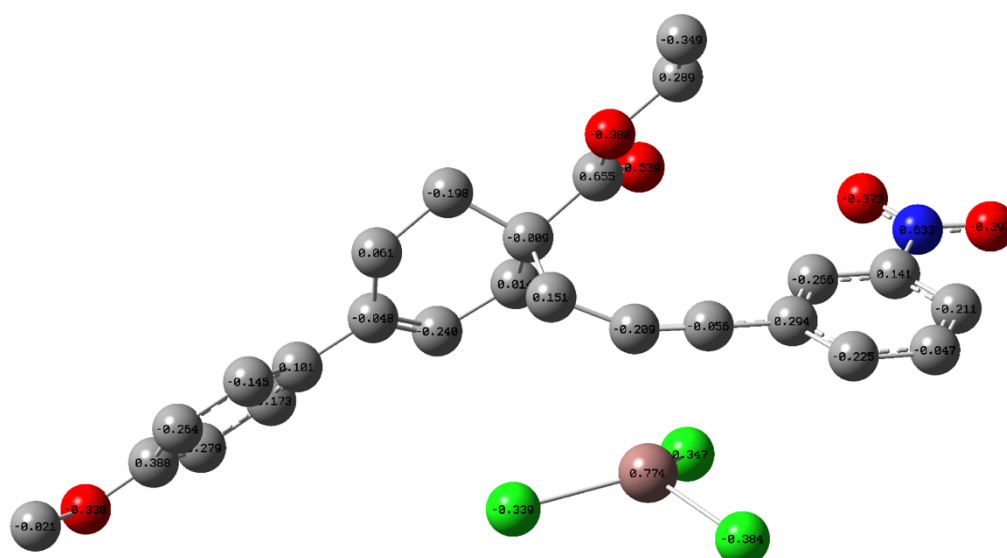


C	-1.24364100	2.96446000	-0.90014500
C	-0.79961900	3.58136400	0.43872900
C	-1.95929900	4.42215000	1.01833500
C	-3.21562700	3.57697100	1.26916600
C	-3.53836200	2.64661000	0.11589500
C	-2.63070100	2.38273600	-0.84126900
C	-4.88671800	2.02802500	0.08193700
C	-0.41862300	2.46324300	1.46819500
C	0.46580200	4.41885500	0.22767800
O	1.19002100	4.32245900	-0.74558600
O	0.71259900	5.21287600	1.28086100
C	1.94371500	5.99115500	1.27094800
C	3.04457400	5.23314300	1.99351200
C	0.79511000	1.74094100	1.05433500
C	1.95859600	1.47417300	0.73535100
C	-5.61591000	1.94098700	-1.11934500
C	-6.84701800	1.30296900	-1.17601700
C	-7.39970900	0.72811700	-0.01946900
C	-6.70860500	0.83352400	1.19535700
C	-5.47510200	1.48970500	1.23425600
O	-8.60205500	0.11141700	-0.18040500
C	-9.20975900	-0.49020700	0.95820300
H	-0.52902600	2.19661600	-1.21848500
H	-1.19046000	3.73635000	-1.67883000
H	-2.19262800	5.20866600	0.29149500
H	-1.64295400	4.92043700	1.93777100

H	-3.10463800	2.99762400	2.19747700
H	-4.06783500	4.24192300	1.44921600
H	-2.88885900	1.69274200	-1.63963700
H	-1.25535500	1.76904100	1.56889000
H	-0.22917300	2.91653000	2.44776700
H	2.21531300	6.21194300	0.23707700
H	1.68522800	6.91744900	1.78749700
H	3.94843000	5.84809400	2.03982500
H	2.74026300	4.98595100	3.01463300
H	3.29000900	4.30808800	1.46582000
H	-5.20446400	2.38693900	-2.01945300
H	-7.40793300	1.24092600	-2.10286500
H	-7.11666600	0.41831000	2.10878700
H	-4.95775100	1.55585600	2.18681500
H	-10.14428800	-0.92716800	0.60482900
H	-8.57652200	-1.28127500	1.38034500
H	-9.42853900	0.25106300	1.73687600
C	3.34718600	1.39375100	0.37844400
C	4.14990900	0.32700800	0.82319600
C	3.88979000	2.40725100	-0.42792000
C	5.49675700	0.27884300	0.47192400
H	3.71346300	-0.46112700	1.42780700
C	5.23968200	2.32774800	-0.74937800
H	3.27763100	3.22714300	-0.78569900
C	6.05614400	1.28211800	-0.31937000
H	6.11010200	-0.54697200	0.81352100
H	7.10050800	1.26759500	-0.60430500
Au	0.67845300	-0.40050200	0.28144100
C	-0.82799000	-4.19169300	-0.83857900
C	0.33234300	-4.55730800	-0.23121400
H	-1.60710800	-4.77371900	-1.30299400
H	0.77562400	-5.52398400	-0.05617400
N	0.95300200	-3.38383100	0.17421500
N	-0.89190000	-2.80479000	-0.78141500
C	0.20114100	-2.30836100	-0.16214200
C	2.23519800	-3.28831400	0.83107000
C	2.25912000	-3.16420800	2.23136300
C	3.39098100	-3.28125400	0.02869100
C	3.51675400	-3.05389600	2.83910700
C	4.62097700	-3.17544000	0.68908400
C	4.68425100	-3.06820100	2.07788600
H	3.58076500	-2.96403100	3.91873600
H	5.53792000	-3.16766300	0.10990200
H	5.64939400	-2.98989600	2.56955200
C	-1.93370900	-2.00736100	-1.38641000
C	-1.69968700	-1.48793800	-2.67112500
C	-3.13035900	-1.81050700	-0.67022000
C	-2.74786500	-0.77351900	-3.26673100
C	-4.14068900	-1.08871400	-1.31222900
C	-3.95642700	-0.59129100	-2.60181700
H	-2.61287400	-0.36019800	-4.26111800
H	-5.07643500	-0.89373500	-0.80312000

H	-4.75947200	-0.03698600	-3.07598300
C	0.98998800	-3.14954000	3.07419700
H	0.12881800	-3.19891600	2.40163400
C	0.92652600	-4.38128500	3.99633300
H	1.75453300	-4.38375800	4.71266800
H	-0.00881300	-4.38265200	4.56491200
H	0.97840700	-5.30992300	3.41949300
C	0.86140900	-1.84232800	3.87830900
H	1.67111100	-1.73839700	4.60765000
H	0.88560100	-0.96787900	3.21967000
H	-0.08582200	-1.83023000	4.42688900
C	3.32243000	-3.31713500	-1.49399700
H	2.32102700	-3.64857600	-1.78512000
C	4.32154000	-4.31131300	-2.10931700
H	4.16350500	-4.37642800	-3.19015000
H	5.35812900	-3.99810500	-1.95047900
H	4.20164600	-5.31223000	-1.68391600
C	3.52118500	-1.90057700	-2.07018600
H	3.44918700	-1.92016100	-3.16240400
H	2.76329400	-1.20788200	-1.69245300
H	4.50396500	-1.50212800	-1.79833100
C	-3.29781400	-2.29477400	0.76636200
H	-2.65322100	-3.16871400	0.91265200
C	-4.73692800	-2.72626300	1.09444500
H	-4.76724400	-3.19146200	2.08459300
H	-5.41897900	-1.87025500	1.11441900
H	-5.11579900	-3.44800600	0.36455600
C	-2.82901400	-1.20052700	1.74955900
H	-1.77341800	-0.95419200	1.60249700
H	-3.41437000	-0.28802300	1.60323300
H	-2.95773300	-1.53440200	2.78484900
C	-0.37466300	-1.65601700	-3.40499000
H	0.28682600	-2.27838600	-2.79559400
C	-0.55575400	-2.37428500	-4.75426400
H	-1.17413500	-1.78838500	-5.44155500
H	0.41657900	-2.52936300	-5.23279200
H	-1.03280000	-3.35042000	-4.62204900
C	0.32309300	-0.29407000	-3.58489100
H	0.49178000	0.19332100	-2.61874900
H	1.29342200	-0.42456800	-4.07423900
H	-0.27866900	0.38154200	-4.20126600
N	5.82728100	3.39739200	-1.57976900
O	7.00203200	3.27162800	-1.92065500
O	5.10708200	4.34877200	-1.87505700

### In -alkyne complex



C	0.80399200	-1.35520600	-1.16651800
C	0.44026700	-2.06953100	0.14556700
C	1.55364500	-3.09090300	0.47667100
C	2.91684400	-2.41118900	0.65904700
C	3.21644400	-1.36828600	-0.40306800
C	2.23784000	-0.89988600	-1.19924200
C	4.61089400	-0.87166700	-0.49946200
C	0.30885100	-1.04868800	1.32528100
C	-0.90794000	-2.77894200	-0.00604900
O	-1.61003300	-2.74714100	-0.99751800
O	-1.25275300	-3.41836400	1.12584500
C	-2.54752000	-4.07639800	1.12458400
C	-2.74321800	-4.67853300	2.50111500
C	-0.90156900	-0.22208200	1.14292400
C	-2.09526900	0.01588500	0.97304100
C	5.14923400	-0.41427600	-1.72025900
C	6.44566600	0.06908300	-1.80717200
C	7.26606100	0.10657500	-0.66858400
C	6.76307300	-0.35758500	0.55165400
C	5.45454300	-0.84257000	0.62072200
O	8.52472700	0.59706500	-0.85969100
C	9.39835500	0.65880500	0.26062500
H	0.13209100	-0.50663100	-1.33862400
H	0.59878600	-2.03511500	-2.00291300
H	1.60866200	-3.80022500	-0.35752600
H	1.28718400	-3.66293500	1.36999500
H	2.96994700	-1.94691400	1.65423900
H	3.70251000	-3.17553800	0.65643700
H	2.46424700	-0.12033600	-1.92124400
H	1.20646800	-0.43060300	1.37443400
H	0.20407000	-1.58328700	2.27469400
H	-3.31497700	-3.33428200	0.88271600
H	-2.55467000	-4.83163400	0.33312000
H	-3.71058100	-5.18717400	2.54824900

H	-1.95817600	-5.40726100	2.72164900
H	-2.72255900	-3.90192200	3.27120100
H	4.54566200	-0.45995000	-2.62131100
H	6.85495700	0.41323600	-2.75152000
H	7.37032500	-0.34523700	1.44875300
H	5.08997600	-1.18630300	1.58343700
H	10.33426400	1.08029600	-0.10901400
H	8.99739300	1.30704900	1.05043800
H	9.59137100	-0.33785500	0.67846900
C	-3.45765500	0.26093900	0.63943500
C	-4.29126000	1.04136100	1.46433500
C	-3.95153300	-0.30757900	-0.54983200
C	-5.61703500	1.25858100	1.09828400
H	-3.88610000	1.48210000	2.36726800
C	-5.28165900	-0.07768700	-0.87244400
H	-3.31852400	-0.91722000	-1.18344500
C	-6.12320500	0.69930700	-0.07495400
H	-6.25899600	1.86647000	1.72583600
H	-7.15061300	0.85355300	-0.37985700
N	-5.82277200	-0.67698600	-2.10754600
O	-6.99940300	-0.44542000	-2.38290700
O	-5.06739400	-1.37295600	-2.78148700
In	-0.57673300	2.14033000	0.32063400
Cl	1.71548400	2.19909800	0.68936900
Cl	-1.28679000	2.02334400	-1.89099300
Cl	-1.82349400	3.52390100	1.72151600