SUPPORTING INFORMATION

Key Mechanistic Features of a Silver(I)-Mediated Deconstructive Fluorination of Cyclic Amines: Multi-State Reactivity versus Single Electron Transfer

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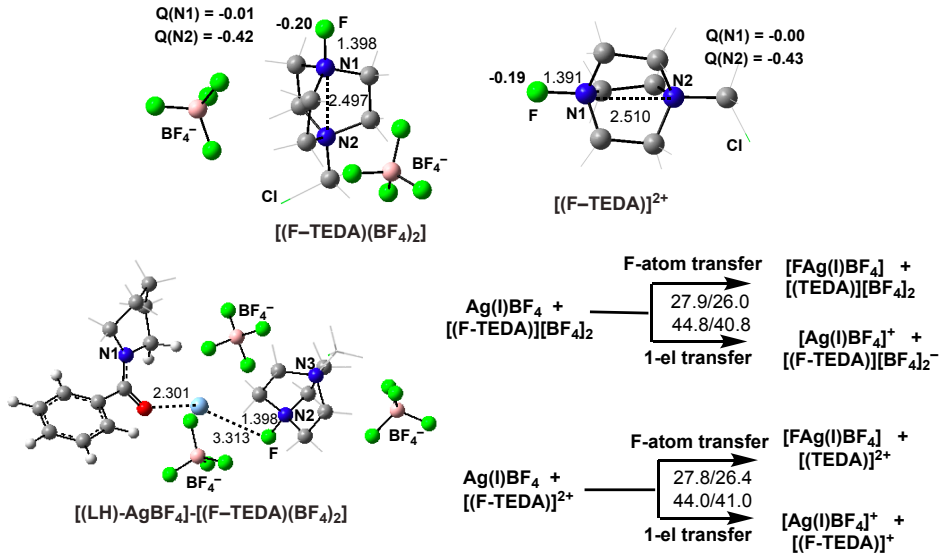


Figure S1. Validation of the used $[F–TEDA]^{2+}$ as a model of the Selectfluor®. See also the cartesian coordinates of the $[F–TEDA]^{2+}$ and $[F–TEDA][BF_4]_2$ species, below.

Table 1S. Energies (in kcal/mol) of several important steps of the Ag(I)-mediated deconstructive C–H bond fluorination of *N*-protected cyclic amines (**LH**) with Selectfluor®**,** calculated at the [B3LYP-D3(BJ)+PCM]/[6-31G(d,p) + Lanl2dz(Ag)], [B3LYP-D3(BJ)+PCM]/[cc-pVTZ + Lanl2dz(f)(Ag)], and [wB97XD+PCM]/[cc-pVTZ + Lanl2dz(f)(Ag)] levels of theory

B3LYP – D3(BJ)				wB97XD	
[6-31G(d,p) + Lanl2dz(Ag)]		[cc-pVTZ + Lanl2dz(f)(Ag)]		[cc-pVTZ + Lanl2dz(f)(Ag)]	
ΔH	ΔG	ΔH	ΔG	ΔH	ΔG
Reaction Energy: **LH** + $AgBF_4$ → [(**LH**)-$AgBF_4$]					
-20.5	-8.9	-16.6	-7.0	-13.7	-3.6
		(**5c-s**) - (**5c-t**), (S-T) splitting			
13.4	13.5	**3.5**	**4.4**	14.8	13.8
		(**11c-s**) - (**11c-t**), (S-T) splitting			
12.7	11.0	9.2	10.2	22.1	17.0

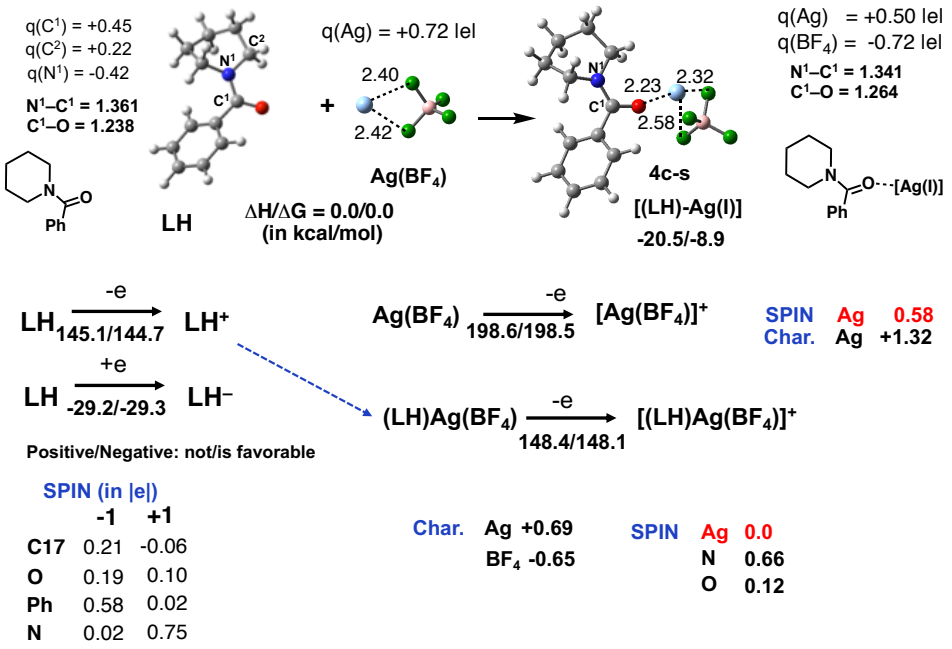


Figure S2. Selected structural and electronic parameters (distances are in Å and Mulliken charges, **Q**, are in |e|), as well as relative energy (ΔH/ΔG in kcal/mol) for **LH** (or **1**), $AgBF_4$, and singlet state adduct (**LH**)[$AgBF_4$], **4c-s**. Comparison of the calculated ionization potential, electron affinity, and relevant properties of **LH** and $AgBF_4$.

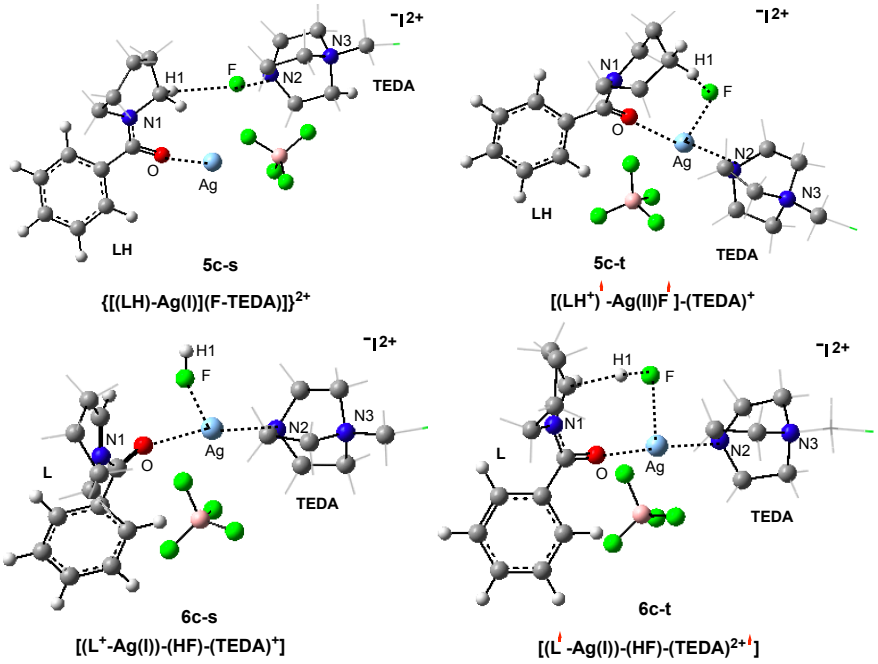


Figure S3. Selected structural and electronic parameters (distances are in Å and Mulliken charges, **Q**, are in |e|) for complexes **5c-s**, **5c-t**, **6c-s**, and **6c-t**. See also the cartesian coordinates for these species, below.

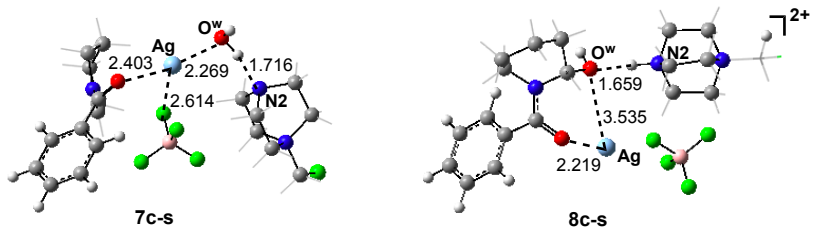


Figure S4. Selected structural and electronic parameters (distances are in Å and Mulliken charges, **Q**, are in |e|) for complexes **7c-s** and **8c-s**. See also the cartesian coordinates for these species, below.

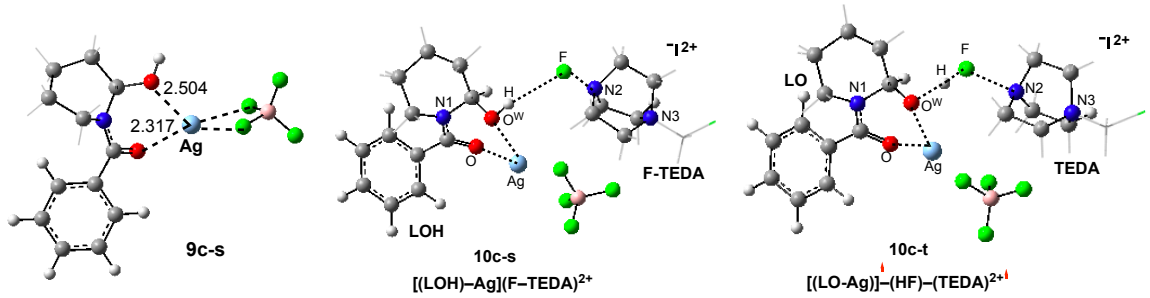


Figure S5. Selected structural and electronic parameters for complexes **9c-s**, **10c-s** and **10c-t.** See also the cartesian coordinates for these species, below.

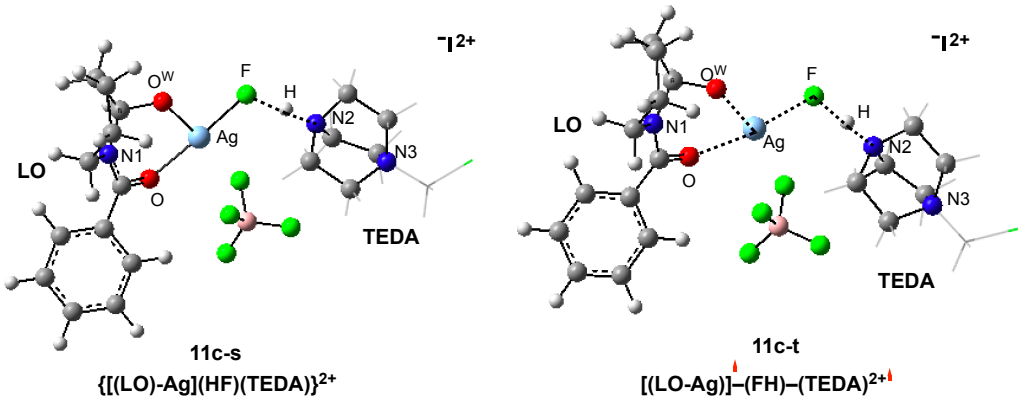


Figure S6. Selected structural and electronic parameters for complexes **11c-s** and **11c-t.** See also the cartesian coordinates for these species, below.

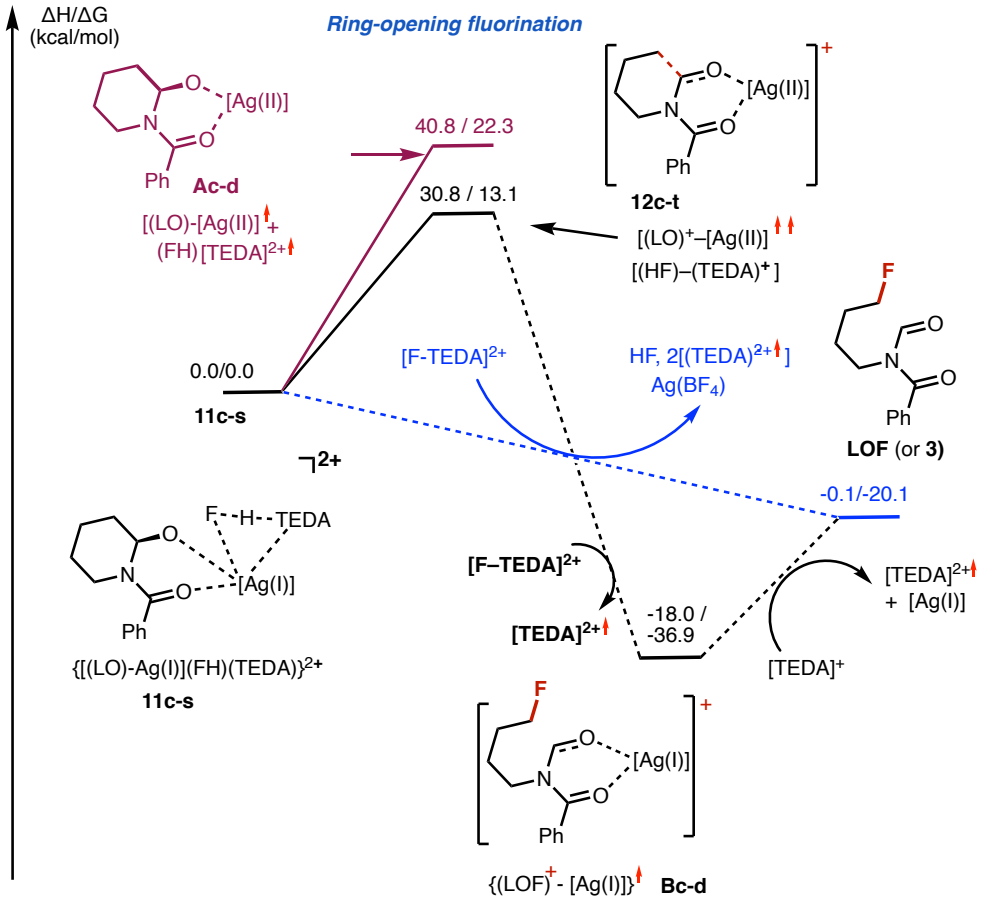


Figure S7. Energy profile of the reaction **11c-s** + $[F\text{-}TEDA]^{2+}$ → **LOF** (or **3**) + HF + Ag(I) + $2[TEDA]^{2+}$. (equation (1) of main text).

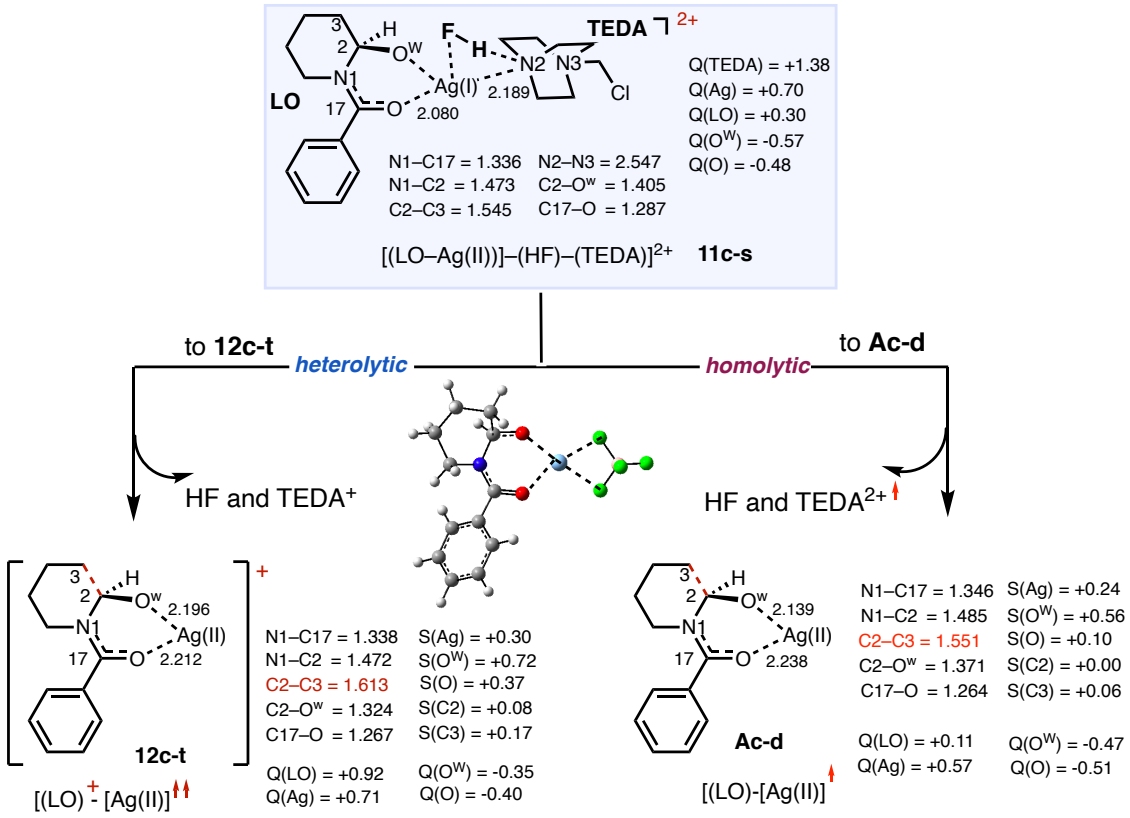


Figure S8. Schematic presentation of the calculated intermediates **11c-s**, **Ac-d**, and **12c-t**, along with their important geometry (distances are in Å) and electronic (the Mulliken charges, **Q**, and spin densities, **S**, are in |e|) parameters.

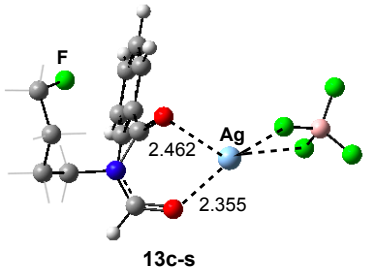


Figure S9. Schematic presentation of the calculated intermediate **13c-s**, along with its important geometry (distances are in Å) parameters.

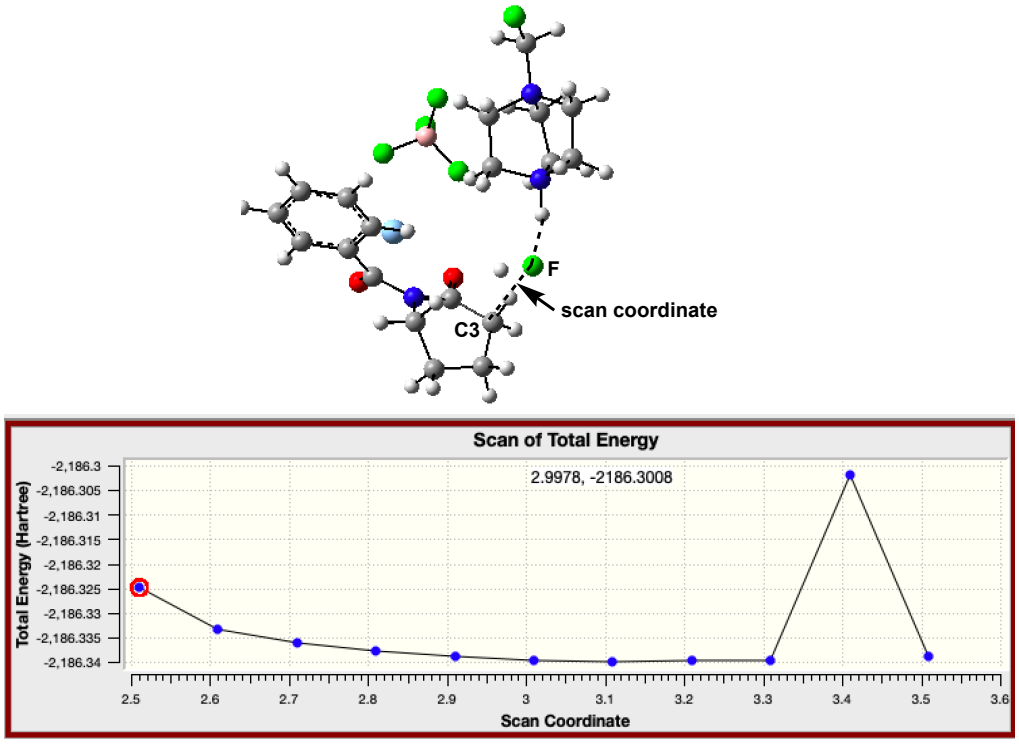


Figure S10. Schematic presentation of potential energy surface scanning by the F–C3 bond formation in **11c-s** via the "internal geometrical rearrangement" pathway (path-2).

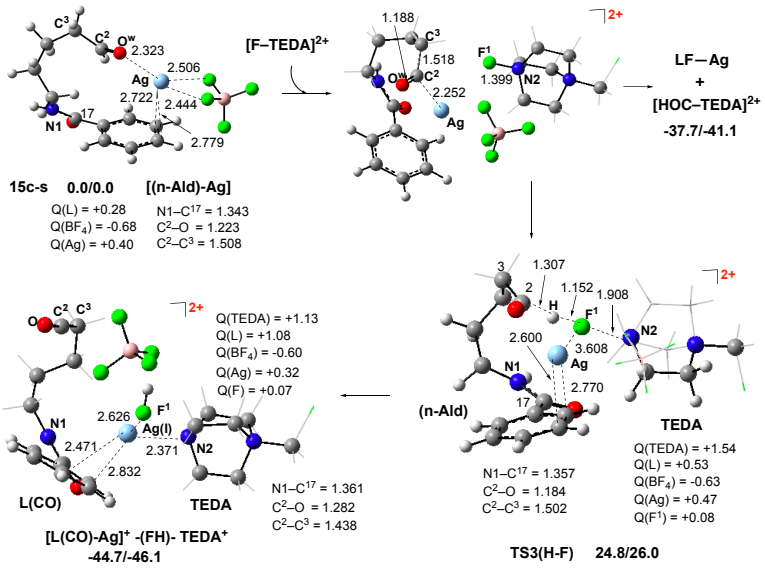


Figure S11. Schematic presentation of intermediates and transition states of the "deformylative fluorination" pathway, along with their important geometry and electronic structure parameters (distances are in Å, and Mulliken charges, **Q**, are in |e|), as well as relative energies (presented as ΔH/ΔG, in kcal/mol).

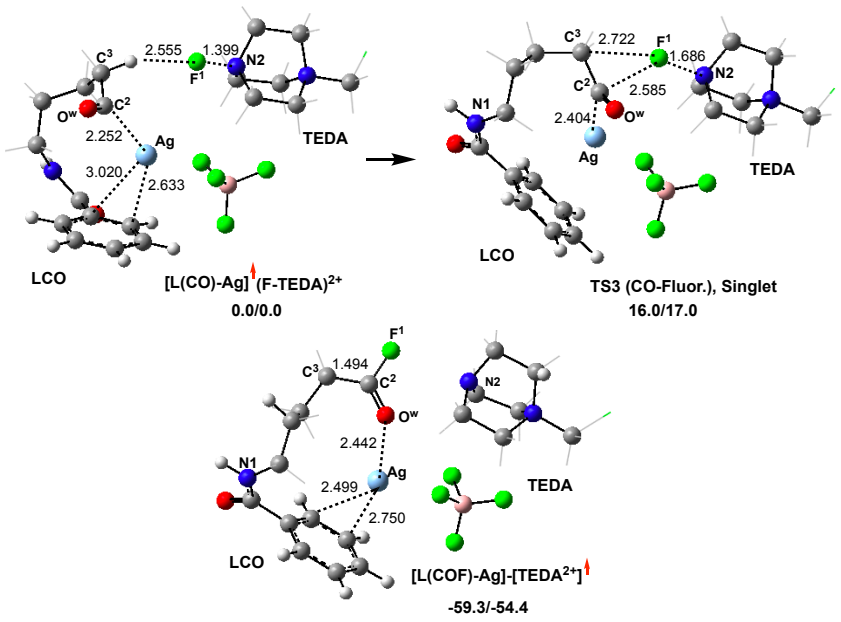


Figure S11 (Continued). Schematic presentation of intermediates and transition states of the "deformylative fluorination" pathway, along with their important geometry and electronic structure parameters (distances are in Å, and Mulliken charges, **Q**, are in |e|), as well as relative energies (presented as ΔH/ΔG, in kcal/mol)

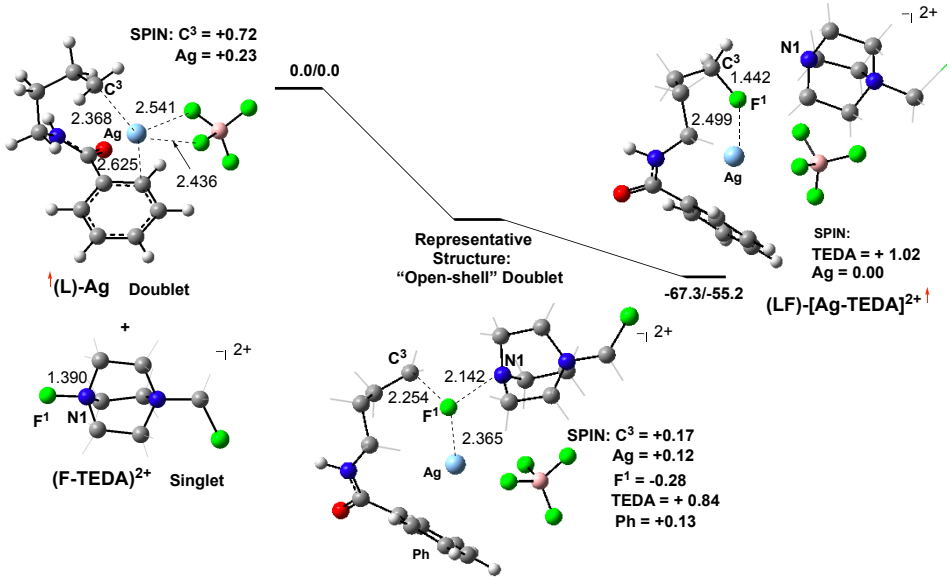
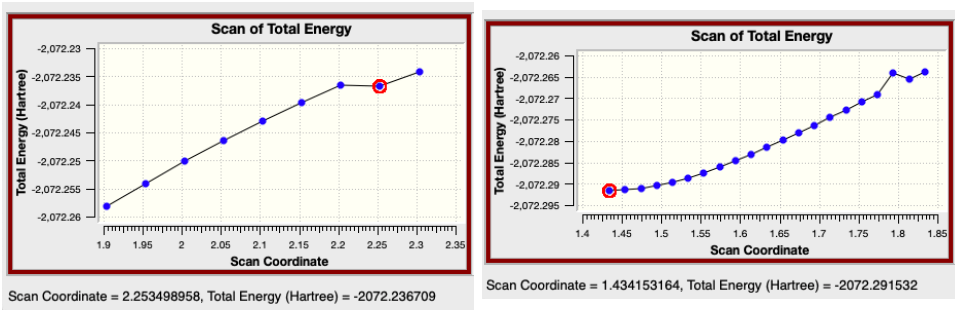


Figure S12. Schematic presentation of the calculated intermediates, along with their important geometry (distances are in Å) parameters and spin densities (in |e|), of the reaction [(L)–Ag], (**18c-d**) + $[F–TEDA]^{2+}$ → (LF)–Ag–$[TEDA]^{2+}$.



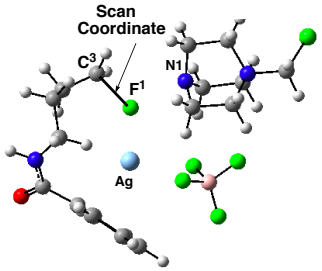


Figure S13. Scanning of the potential energy surface of the reaction [(L)–Ag], (**18c-d**) + $[F–TEDA]^{2+}$ → (LF)–Ag–$[TEDA]^{2+}$.

Table S1. Cartesian coordinates of all reported structures (in Å)

Substrate, LH

N -1.52938600 1.09288300 0.51336700
C -0.57932800 1.30378100 -0.58974400
C -0.49029000 2.79737500 -0.94166200
C -1.86621800 3.45736300 -0.79792900
C -2.32570700 3.42651800 0.67733600
C -1.69688600 2.23262800 1.41753100
H 0.40606300 0.89690000 -0.32665200
H 0.23115700 3.30370000 -0.28960800
H -1.84686700 4.48541900 -1.17164500
H -2.02846900 4.34601300 1.19318300
H -2.28855800 1.93174600 2.27939500
H -3.41820900 3.37116500 0.72902800
H -0.70398900 2.50842200 1.79524000
H -2.58413600 2.90830200 -1.41872800
H -0.10901900 2.89345600 -1.96269800
H -0.94427800 0.72888600 -1.44449400
C -1.97735800 -0.17468000 0.72670500
O -1.53774100 -1.13354000 0.07780800
C -3.05843500 -0.39590600 1.74624400
C -4.22277400 0.38297200 1.78211500
C -2.93607100 -1.48874600 2.61348600
C -5.24088100 0.08379100 2.68786300
H -4.34024000 1.20974100 1.08909300
C -3.94540500 -1.77628900 3.53046300
H -2.04501400 -2.10531100 2.55900200
C -5.10022600 -0.99008300 3.56931400
H -6.14362200 0.68662500 2.70240200
H -3.83563100 -2.61612700 4.20964600
H -5.88999300 -1.21827000 4.27847800

Substrate, 1plus, LH^+

N -1.44819700 1.15318000 0.62901000
C -0.88767100 1.28691100 -0.70794700
C -0.70637400 2.74594900 -1.10252600
C -1.96677400 3.54555000 -0.73886600
C -2.23222000 3.50568900 0.77889500
C -1.50611000 2.32176200 1.47756800
H 0.05251800 0.71646200 -0.71549800
H 0.17278500 3.16869100 -0.60412200
H -1.86470000 4.57923800 -1.07513000
H -1.87003800 4.41033800 1.27189900
H -1.94712300 2.05513700 2.43579600
H -3.30168700 3.42390200 0.98737600
H -0.45629500 2.60920600 1.64982700
H -2.81872900 3.11434600 -1.27530600
H -0.51148800 2.77999800 -2.17659500
H -1.56805400 0.75118000 -1.38470300

C -1.64787700 -0.20707000 1.17138500
O -0.74440400 -0.98454600 0.95707200
C -2.88679500 -0.45047200 1.90520900
C -4.02119400 0.36342900 1.73903900
C -2.93648300 -1.57535000 2.74807800
C -5.19227500 0.05795000 2.42374400
H -4.00338700 1.20637400 1.05727500
C -4.10625100 -1.86375500 3.43900100
H -2.05456000 -2.19646900 2.85526800
C -5.23169900 -1.04760000 3.27831400
H -6.07215200 0.67735300 2.29074300
H -4.14586000 -2.72144600 4.10137200
H -6.14441700 -1.27720400 3.81836000

$AgBF_4$
B -0.87978300 0.45528800 -0.04354200
F 0.52517900 0.60309200 0.22575900
F -1.38894000 1.79728000 -0.15032000
F -1.49183400 -0.18864000 1.01499100
Ag 0.63609100 3.02212700 0.24803000
F -1.05748300 -0.20336000 -1.24490100

$[AgBF_4]^+$
B -0.65380300 0.41576600 0.00873800
F 0.74140200 0.76348000 0.28044300
F -1.20235900 1.85801400 -0.08080200
F -1.22498200 -0.17767300 1.06548200
Ag 0.55771400 2.96873600 0.18676200
F -0.79387800 -0.14787300 -1.19929300

$[F\text{-}TEDA]^{2+}$
C -1.64552900 0.56271700 0.38460400
C -0.12890000 0.42896200 0.13609000
H -1.86895200 1.33226400 1.12199300
H -2.21501800 0.74288500 -0.52528400
N -2.11231600 -0.74720000 0.94797900
N 0.25701700 -1.04140300 0.17348900
H 0.13707600 0.82622400 -0.84108600
H 0.45674800 0.93481600 0.90203000
C -1.28896600 -1.14833200 2.13530400
C 0.10644600 -1.54238900 1.60354600
H -1.79172300 -1.98951500 2.60912500
H -1.26487200 -0.29763500 2.81404300
H 0.88819400 -1.08767100 2.21002000
H 0.24256300 -2.62208200 1.58952600
C -2.10117700 -1.81762200 -0.10226700
C -0.68627300 -1.83320800 -0.71942400
H -2.86127600 -1.55705900 -0.83627900
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F -3.42586900 -0.58712900 1.37449700
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H 1.94301700 -2.29442500 -0.10719800
Cl 1.98925700 -0.78755900 -1.92545200
H 2.32091200 -0.61594000 0.40727400

$TEDA^{2+}$, radical
C -1.66602600 0.55142400 0.41081400
C -0.12503600 0.43099500 0.11753100
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H -2.23448400 0.76088200 -0.49299900
N -2.02302800 -0.75814500 0.91894200
N 0.26092200 -1.04185100 0.17380100
H 0.10555300 0.81133500 -0.87531200
H 0.46751400 0.95438300 0.86577000
C -1.32158100 -1.15656100 2.12297800
C 0.12040100 -1.52904900 1.61337700
H -1.80211600 -2.02757800 2.56852000
H -1.29693600 -0.32749700 2.82761600
H 0.87695300 -1.03524800 2.22144800
H 0.27756800 -2.60578100 1.62044800
C -2.12285300 -1.79076700 -0.09265100
C -0.67818900 -1.84776600 -0.71544700
H -2.85181700 -1.50749700 -0.85135100
H -2.39936000 -2.73540500 0.37154900
H -0.31739000 -2.87443700 -0.75682200
H -0.65827400 -1.40502200 -1.70822400
C 1.71306900 -1.24414500 -0.24067800
H 1.94536900 -2.29899200 -0.11149000
Cl 1.99287600 -0.78908800 -1.92778500
H 2.32919800 -0.62289200 0.40533400

$[H\text{-}TEDA]^{2+}$
C -1.64697900 0.55283400 0.36192700
C -0.12861500 0.42973600 0.16053200
H -1.88621600 1.36100000 1.05113000
H -2.18386800 0.70894600 -0.57300600
N -2.13898800 -0.74349600 0.95748400
N 0.25376600 -1.04116200 0.17262200
H 0.17517900 0.85238900 -0.79482300
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H -2.86792400 -1.62994700 -0.82338100
H -2.31441800 -2.77369700 0.41443600

H -0.30454300 -2.82441400 -0.84326900
H -0.69394900 -1.32261700 -1.70010900
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H 1.94096800 -2.29021200 -0.10615900
Cl 1.99241800 -0.77806600 -1.92036400
H 2.31234000 -0.61310300 0.41501700
H -3.10612500 -0.62358600 1.27397700

TEDA^{+}, singlet
C -1.68235500 0.50093500 0.46413900
C -0.17788200 0.41482800 0.08454500
H -1.82062600 1.25693400 1.23951600
H -2.27299800 0.79436300 -0.40566800
N -2.17922800 -0.78727600 0.95340000
N 0.24915200 -1.04285600 0.16687400
H 0.02126600 0.75053100 -0.93155600
H 0.46518300 0.96343700 0.77388500
C -1.35025300 -1.23446600 2.07327900
C 0.11069500 -1.50586800 1.61381300
H -1.77429100 -2.14879700 2.49261400
H -1.36230400 -0.46538100 2.84787800
H 0.84589300 -0.95251300 2.19868700
H 0.36523700 -2.56570700 1.62784400
C -2.11430600 -1.77624000 -0.12552900
C -0.67369600 -1.88661500 -0.69972900
H -2.80247300 -1.48382500 -0.92084900
H -2.43714300 -2.74254900 0.26671100
H -0.28405500 -2.90494700 -0.67955800
H -0.59418300 -1.49695600 -1.71278300
C 1.69086200 -1.22210800 -0.21690700
H 1.94497200 -2.27193100 -0.08609200
Cl 2.02159100 -0.77107000 -1.90797200
H 2.29223100 -0.58965300 0.43255000

LOF, alkylfluoride
C -0.16300600 1.35098600 -0.39455900
C -0.66204500 0.51002800 0.78325000
H -0.30454000 0.93373100 1.72904200
H 0.93296600 1.33934500 -0.42827700
H -0.52021000 0.92437700 -1.33947500
C -0.18586000 -0.93943000 0.68044800
H -1.75805600 0.52420200 0.81675200
H 0.90297700 -0.98909300 0.69877100
H -0.55265000 -1.40546400 -0.23417200
N -0.67482800 -1.74636800 1.80968600
C -0.63377500 2.79024000 -0.29957800
H -0.26269300 3.27002100 0.61385400
H -1.72856400 2.85084300 -0.30619700
F -0.15382700 3.51687300 -1.39528300
C -1.93246700 -2.36402300 1.68653700
O -2.47083300 -2.45250900 0.59110800
C -2.60538100 -2.86281900 2.92177500
C -3.32078700 -4.06540500 2.83794600
C -2.63839900 -2.11447800 4.10766000
C -4.02726100 -4.53538100 3.94169600
H -3.30954600 -4.62191300 1.90717000
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LF
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C -0.69005500 0.55305300 0.69963300
H -0.51761800 1.08600900 1.64288000
H 1.09169200 1.30051200 -0.28673900
H -0.16365300 0.74316200 -1.39409600
C -0.20325700 -0.89295000 0.84347900
H -1.77319200 0.53548000 0.53390500
H 0.87251000 -0.91701100 1.03889700
H -0.39041600 -1.43837600 -0.08614800
N -0.87134900 -1.60482400 1.92337900
C -0.48930700 2.70466600 -0.60744300
H -0.30110600 3.29187800 0.29931800
H -1.56432800 2.72872700 -0.82203800
F 0.17735900 3.32686700 -1.67018700
H -0.40058300 -1.69149900 2.81024400
C -2.09028700 -2.17986000 1.75196100
O -2.66794200 -2.17848800 0.65898600
C -2.69591500 -2.83713300 2.95770100
C -3.65149600 -3.83788400 2.73896100
C -2.37068100 -2.47439000 4.27211100
C -4.25253500 -4.48657500 3.81502900
H -3.90757300 -4.09292000 1.71662600
C -2.97948300 -3.11803900 5.34959700
H -1.66928100 -1.66855600 4.46534000
C -3.91586300 -4.12896100 5.12347700
H -4.98427400 -5.26818500 3.63565100
H -2.72817700 -2.82461500 6.36399000
H -4.38676400 -4.63074100 5.96319200

LH_AgBF$_4$, 4c-s
N -1.49161500 1.23146800 0.28670100
C -0.65902100 1.54677200 -0.88744800
C -0.64278100 3.06093900 -1.14467900
C -2.02295000 3.66003700 -0.84813800
C -2.36499700 3.51523500 0.65210800

C -1.62872900 2.31484100 1.26847400
H 0.35727000 1.15563900 -0.73511200
H 0.11709300 3.54855600 -0.52373800
H -2.06184800 4.71061000 -1.14905600
H -2.06936500 4.41275000 1.20486700
H -2.13049900 1.93734600 2.15610700
H -3.44558900 3.40033000 0.78267700
H -0.61496700 2.60399500 1.56778400
H -2.77086200 3.13051400 -1.45007300
H -0.35205000 3.22881600 -2.18551300
H -1.08752000 1.01425700 -1.73879700
C -1.91932800 -0.02885100 0.44975100
O -1.55861900 -0.94279500 -0.34455000
C -2.86319800 -0.36576300 1.55580900
C -4.07417700 0.32253200 1.71111800
C -2.55895900 -1.44621300 2.39649700
C -4.97254800 -0.06159000 2.70582000
H -4.31931600 1.14158400 1.04261600
C -3.45400600 -1.81284100 3.40045300
H -1.62375300 -1.98329700 2.27640400
C -4.66047700 -1.12523100 3.55518900
H -5.91395300 0.46723500 2.81542100
H -3.21075600 -2.63902100 4.06109100
H -5.35719000 -1.41962500 4.33387300
Ag 0.49678700 -1.78788800 -0.14942000
B 1.71675600 -3.43444600 2.08030200
F 2.03879800 -4.77793700 2.05433400
F 2.18128900 -2.79430900 3.21435300
F 2.29341900 -2.79298800 0.91191400
F 0.30752000 -3.26358100 1.95924200

LH_AgBF$_4$, 4c-t

N -1.55955900 1.41359600 0.17363600
C -0.71956600 1.76833400 -0.97886200
C -0.80383100 3.27372400 -1.26603200
C -2.23011900 3.77881300 -1.02217300
C -2.60125300 3.63598700 0.47069700
C -1.80633300 2.49675900 1.12834900
H 0.31713100 1.45291700 -0.79178800
H -0.10152900 3.82565100 -0.63062300
H -2.33541600 4.81878400 -1.34380600
H -2.38249100 4.56069800 1.01443100
H -2.31100200 2.10383600 2.01028000
H -3.67556400 3.45171800 0.57405700
H -0.82914400 2.86105700 1.47289500
H -2.92110900 3.18620400 -1.63312900
H -0.49169100 3.44567000 -2.30005500
H -1.07621500 1.19064300 -1.83573100
C -1.69945000 0.08609900 0.46438000
O -1.02773900 -0.77228400 -0.21176300
C -2.66262100 -0.37610700 1.42727600
C -3.87246200 0.39437900 1.82024500
C -2.46452700 -1.69183200 2.06771200
C -4.54801600 0.06121500 2.94885700
H -4.21210900 1.19868400 1.17859200
C -3.14808300 -1.98595900 3.19862400
H -1.71548500 -2.36800100 1.67629800
C -4.16794900 -1.09205400 3.71818300
H -5.41691900 0.63662100 3.25325600
H -2.95266600 -2.91542900 3.72426900
H -4.70332500 -1.34699300 4.62465800
Ag 0.83613000 -1.59153700 0.61187600
B 1.38957000 -3.98939400 2.37332800
F 1.99931900 -5.17790200 2.01778900
F 1.19801700 -3.87428300 3.73808700
F 2.22466000 -2.88646700 1.92615400
F 0.15120400 -3.84606900 1.68641400

LH_AgBF$_4$_[F-TEDA]$^{2+}$, 5c-s: Singlet

C 0.80009500 0.17196100 0.89335600
C -0.17635900 0.23974800 -0.29995400
H 1.46058800 1.03529900 0.88147400
H 0.26718800 0.10640200 1.83841000
N 1.67362000 -1.06422500 0.76926600
N 0.13720000 -0.91395000 -1.20273400
H -1.21567400 0.12564300 0.00142700
H -0.03912200 1.15808600 -0.86830500
C 2.48906100 -0.96588700 -0.51223500
C 1.53907200 -0.86547500 -1.72581200
H 3.11859800 -1.85170800 -0.57294500
H 3.09568300 -0.06597200 -0.44550200
H 1.66575100 0.07583700 -2.25778500
H 1.64778000 -1.70657500 -2.40700300
C 0.80078900 -2.30276300 0.70713000
C -0.13683600 -2.21877700 -0.52011100
H 0.23177100 -2.35205900 1.63215600
H 1.46009900 -3.16654000 0.63980600
H 0.05585100 -3.00757700 -1.24425100
H -1.18780900 -2.21909600 -0.23789400
F -0.72313700 -0.83098900 -2.30096100
Ag -0.32624300 2.21718000 -3.85463100
O -1.78912000 1.45430600 -5.33334600
C -1.51723300 1.10272100 -6.51674100
N -0.57273600 0.18265900 -6.77427300
C 0.07346400 -0.49054500 -5.63425700
C 0.02122900 -0.05083400 -8.10902600
C 0.83569900 -1.72550300 -6.10540700
H 0.76549200 0.20780000 -5.13607200
C 1.54101400 -0.15495500 -7.97661300
H -0.39068100 -0.96831200 -8.54351100
C 1.95493300 -1.35654000 -7.09808000
H 1.24339900 -2.24046100 -5.23069800

H 1.97554400 -0.23224300 -8.97704500
H 2.18209800 -2.22530600 -7.72313600
C -2.30736800 1.70666300 -7.62525900
C -2.56473100 3.08424100 -7.57793600
C -2.86633200 0.92920300 -8.64908000
C -3.34350300 3.68283600 -8.56507900
H -2.14508200 3.67507000 -6.77075500
C -3.66243100 1.52900200 -9.62366600
H -2.69884300 -0.14222500 -8.67074400
C -3.89408000 2.90576100 -9.58804400
H -3.52592200 4.75215300 -8.53491900
H -4.10297900 0.92181100 -10.40766500
H -4.50716500 3.37193300 -10.35281300
H -0.70150500 -0.75047200 -4.91198200
H 0.12379100 -2.41612600 -6.57030100
H 2.87194100 -1.10969900 -6.55373300
H 1.90951600 0.78126100 -7.54295700
H -0.25495100 0.77831200 -8.75753300
B 1.98597200 2.72773500 -1.91834400
F 2.41856800 1.97962600 -0.80746900
F 0.57229000 2.96717100 -1.75864500
F 2.66861200 3.90033500 -2.05789200
F 2.09716500 1.90761500 -3.08271900
C 2.66168800 -1.14297500 1.92140100
Cl 1.85783400 -1.29472800 3.49103900
H 3.28786700 -2.01642000 1.75586100
H 3.24857800 -0.22723700 1.90637200

LH_AgBF$_4$_[F-TEDA]$^{2+}$, 5c-t: Triplet
C 0.98197100 0.37565700 0.75641600
C 0.09096900 0.63331700 -0.48139800
H 1.41763800 1.29941900 1.13591000
H 0.44250300 -0.12125100 1.55982700
N 2.12002100 -0.54796300 0.35064500
N 0.39130700 -0.39725100 -1.50737000
H -0.96029300 0.56522800 -0.20210300
H 0.27999200 1.60917300 -0.92445500
C 2.75237200 0.00206500 -0.91969400
C 1.73973000 -0.14774500 -2.07758200
H 3.66758400 -0.55747700 -1.11144900
H 3.00083700 1.04462600 -0.72438300
H 1.71473100 0.77137600 -2.65997300
H 1.99069300 -0.98665700 -2.72598900
C 1.55257700 -1.92356100 0.04076500
C 0.34386400 -1.75259900 -0.90380000
H 1.26380400 -2.38721800 0.98202800
H 2.35956800 -2.49998300 -0.41110300
H 0.35862900 -2.48380800 -1.71082700
H -0.59953500 -1.84620400 -0.36569400
F -0.70307000 -2.25666600 -3.59412400
Ag -1.09276200 -0.29507500 -3.19410400
O -2.33509900 0.00768600 -5.11327200
C -1.80102400 0.35025900 -6.17096100
N -0.76269900 -0.51552600 -6.69297700
C -0.90254600 -1.94990700 -6.52882700
C 0.49973600 0.00578700 -7.16468400
C 0.38911200 -2.68319000 -6.83625400
H -1.18611800 -2.12517300 -5.47196800
C 1.67577600 -0.55875800 -6.30404300
H 0.63006600 -0.35522500 -8.19425800
C 1.51285500 -2.05846600 -5.98937600
H 0.24146500 -3.73520900 -6.58231100
H 2.57722500 -0.36031100 -6.88818800
H 2.45125500 -2.58970000 -6.16030600
C -2.15714400 1.53704900 -6.92146700
C -2.80862700 2.57218200 -6.21764200
C -1.92175500 1.65367900 -8.30773800
C -3.19714300 3.71817400 -6.89383300
H -2.96179000 2.47056500 -5.15093000
C -2.33329200 2.79817900 -8.97588400
H -1.45693800 0.84608000 -8.86102000
C -2.96303900 3.83016200 -8.27000700
H -3.67625100 4.52801400 -6.35544500
H -2.16854700 2.88947200 -10.04333500
H -3.27267800 4.72738200 -8.79573600
H -1.76227400 -2.27225100 -7.13742700
H 0.63013800 -2.64174500 -7.90446100
H 1.22780600 -2.18969400 -4.94153700
H 1.71456000 0.04447400 -5.39738200
H 0.47805000 1.09116800 -7.14969700
B -0.21500500 2.58461300 -3.68376000
F 0.80283800 2.81586400 -2.76526200
F -1.31601700 1.93545100 -2.96074300
F -0.68512800 3.71621500 -4.28563500
F 0.21673400 1.61940600 -4.63437700
C 3.19867200 -0.61581800 1.40350400
Cl 2.57333100 -1.12464400 2.98563000
H 3.94021700 -1.33896400 1.07120700
H 3.63440100 0.37655300 1.49886300

TS1 (H-F form)-t, triplet
C 0.98221800 0.48018600 0.79291300
C 0.08107900 0.73370000 -0.44016000
H 1.48592700 1.39166400 1.11285700
H 0.42931400 0.06364000 1.63203900
N 2.05025400 -0.53475500 0.41611000
N 0.31621600 -0.35101100 -1.42416900
H -0.96759300 0.72602200 -0.14275000
H 0.31107600 1.67994200 -0.92498600
C 2.70225700 -0.08590600 -0.88423200
C 1.66672900 -0.20998300 -2.02478200
H 3.57251800 -0.71692500 -1.06318300

H 3.02501800 0.94408000 -0.73642500
H 1.68927700 0.69002200 -2.63668900
H 1.83652900 -1.08458300 -2.65148700
C 1.39022800 -1.88175100 0.17901500
C 0.18972100 -1.67867900 -0.77339600
H 1.07427800 -2.27520400 1.14320000
H 2.15186600 -2.53544700 -0.24558600
H 0.17890200 -2.43993000 -1.55220200
H -0.75780000 -1.70115000 -0.23545200
F -0.34041200 -2.12996700 -3.65227900
Ag -1.12160200 -0.24897400 -3.13937200
O -2.34105200 -0.02867000 -5.04207800
C -1.77499500 0.29927100 -6.09786900
N -0.73481100 -0.54196400 -6.58683500
C -0.77026100 -1.92731200 -6.28803900
C 0.50018200 0.01176300 -7.15381400
C 0.33592400 -2.70099300 -6.97452300
C 1.70755000 -0.62048100 -6.43907000
H 0.52373800 -0.23989200 -8.22192700
C 1.72135900 -2.15961300 -6.56168300
H 0.23133200 -3.75701900 -6.71946300
H 2.60554900 -0.17440300 -6.87248500
H 2.46338800 -2.48533400 -7.29371400
C -2.14757200 1.48070000 -6.85713800
C -2.74938000 2.54358500 -6.15211300
C -1.97506600 1.55890000 -8.25414200
C -3.14634000 3.68152500 -6.83870200
H -2.85762300 2.47093700 -5.07758700
C -2.39436400 2.69497400 -8.93228600
H -1.55311900 0.72643400 -8.80470700
C -2.97184900 3.75672800 -8.22548200
H -3.58644600 4.51277300 -6.29948700
H -2.27705600 2.75633700 -10.00825600
H -3.28795000 4.64690700 -8.75936600
H -1.78839000 -2.31729900 -6.39577400
H 0.20660200 -2.61842600 -8.06152400
H 2.00023800 -2.59424000 -5.59788000
H 1.65798400 -0.30563600 -5.39453100
H 0.48139400 1.09192900 -7.03925900
B -0.14637500 2.57735200 -3.66930200
F 0.86341500 2.79658100 -2.73775200
F -1.29197300 2.00609200 -2.94651700
F -0.55031700 3.70572000 -4.32168400
F 0.26448400 1.55877300 -4.57324300
C 3.13590800 -0.62371300 1.46199500
Cl 2.49823800 -1.02214900 3.07010100
H 3.82759300 -1.40535200 1.15607900
H 3.63214000 0.34344500 1.50751700
H -0.59067600 -2.04347800 -5.13029600

[(L-Ag)-HF_(TEDA)]$^{2+}$, 6c-s: Singlet

C 0.96629200 0.83001000 0.75707300
C 0.12922200 0.79494300 -0.54405400
H 1.59557200 1.71795200 0.81899100
H 0.35190100 0.76816200 1.65299800
N 1.88716100 -0.37877900 0.77302900
N 0.26490400 -0.52138300 -1.21379100
H -0.92202600 0.96464500 -0.31064700
H 0.46100600 1.55945800 -1.24414800
C 2.65684900 -0.41267200 -0.54110800
C 1.65907300 -0.66769400 -1.69499100
H 3.40677300 -1.19944800 -0.46087600
H 3.15715600 0.55139000 -0.63327500
H 1.82630500 0.05370200 -2.49190300
H 1.76887000 -1.67188000 -2.10385500
C 1.04805600 -1.63956700 0.86937900
C -0.02847300 -1.59685500 -0.24176400
H 0.61188500 -1.66895600 1.86610600
H 1.73473300 -2.47864100 0.75546400
H -0.05186400 -2.55248900 -0.76595600
H -1.01657900 -1.41192800 0.18113700
F 0.37792700 -2.67232900 -3.93536900
Ag -1.15746400 -0.60477800 -3.07899700
O -2.23269900 -0.20642300 -5.21032800
C -1.75286600 0.27897900 -6.21880900
N -0.59962900 -0.41689800 -6.83270500
C -0.53084400 -1.70364800 -6.69984400
C 0.50689100 0.39666100 -7.43446700
C 0.61212100 -2.52741600 -7.13213800
C 1.82818700 -0.34655200 -7.30345400
H 0.25030700 0.57542400 -8.47976000
C 1.70822400 -1.76023300 -7.87608900
H 0.97681200 -2.96451400 -6.18897200
H 2.59015900 0.22911200 -7.83452300
H 1.46220400 -1.70899900 -8.94158800
C -2.21821400 1.49771300 -6.86997500
C -2.69774200 2.53182600 -6.04522800
C -2.25772900 1.62271100 -8.27021200
C -3.19324600 3.69271200 -6.62529000
H -2.61936700 2.42695300 -4.97032600
C -2.78127100 2.77877500 -8.83802000
H -1.92796500 0.80977300 -8.90748700
C -3.23930600 3.81456300 -8.01789200
H -3.54068900 4.50484300 -5.99608200
H -2.83381100 2.87312800 -9.91692900
H -3.63316300 4.72070200 -8.46657000
H -1.37254600 -2.17386400 -6.19885200
H 0.21555500 -3.37980700 -7.69757100
H 2.65271600 -2.30090400 -7.78738500
H 2.10681400 -0.37566500 -6.24577000
H 0.51535500 1.34392100 -6.89885600
B 0.42155600 1.94361700 -4.07526500

F 1.39927000 2.31213500 -3.15246400
F -0.85461700 1.96047700 -3.44731500
F 0.41467600 2.76004200 -5.19772000
F 0.66735300 0.59089100 -4.48707000
C 2.89974000 -0.29942300 1.88323000
Cl 2.14983600 -0.15982000 3.49019800
H 3.49684600 -1.20840800 1.85698700
H 3.51571500 0.58012700 1.70907900
H -0.08991900 -3.44371400 -3.70063800

[(L-Ag)-HF-(TEDA)]$^{2+}$, 6c-t: TRIPLET
C 0.75993200 0.61117700 0.82102300
C 0.03727200 0.79170000 -0.53440100
H 1.24374800 1.53237300 1.14363400
H 0.09221400 0.26422600 1.60646200
N 1.83739800 -0.44728500 0.65566400
N 0.34596700 -0.36844600 -1.40929000
H -1.03983500 0.84367700 -0.37585100
H 0.36470400 1.69108900 -1.05070100
C 2.65664100 -0.10500200 -0.58116400
C 1.77028700 -0.30183300 -1.83162600
H 3.52709800 -0.75951800 -0.59978100
H 2.98369400 0.92832600 -0.46699800
H 1.89975000 0.54261600 -2.50494200
H 2.00924800 -1.22384700 -2.35890700
C 1.17257300 -1.79317400 0.43455100
C 0.10638800 -1.63466800 -0.67453900
H 0.72725800 -2.10624300 1.37679400
H 1.96107500 -2.49295200 0.15880300
H 0.17080500 -2.46832800 -1.37386400
H -0.90009600 -1.60044100 -0.25738500
F 0.45241400 -2.27020400 -3.85107600
Ag -0.93444100 -0.32468000 -3.25935600
O -2.18827400 -0.14851700 -5.03708800
C -1.64571100 0.21287300 -6.13171900
N -0.72770000 -0.59121100 -6.74158000
C -0.62318400 -1.93095900 -6.40224800
C 0.32068200 -0.04497400 -7.64408200
C 0.36260500 -2.73990700 -7.18139900
C 1.68391900 -0.55096000 -7.16827500
H 0.10753000 -0.36889500 -8.66666500
C 1.77001500 -2.09348200 -7.18920200
H 0.39042700 -3.76024900 -6.79302800
H 2.45182500 -0.10679700 -7.80637900
H 2.30742500 -2.44138700 -8.07431100
C -2.11541100 1.45346500 -6.75141700
C -2.49384500 2.52367400 -5.90322500
C -2.29096000 1.56020200 -8.14675300
C -2.98272200 3.69881400 -6.45489500
H -2.36468900 2.42192800 -4.83454600
C -2.78922600 2.73554600 -8.68508400
H -2.05453500 0.72296700 -8.79257600
C -3.13080700 3.80918600 -7.84073400
H -3.24938700 4.52888800 -5.81058300
H -2.92207300 2.82702100 -9.75718200
H -3.52053300 4.72525000 -8.27201400
H -1.51892900 -2.36161500 -5.96452800
H -0.00431000 -2.81946800 -8.21781600
H 2.33254600 -2.43792100 -6.31687000
H 1.83763600 -0.16419900 -6.15756600
H 0.26908000 1.04059200 -7.60161900
B 0.32327800 2.39984300 -3.82865400
F 1.30585900 2.63726800 -2.86997600
F -0.91612700 2.10614500 -3.14039800
F 0.14964000 3.44115800 -4.69891900
F 0.64666300 1.19286500 -4.53489000
C 2.78228600 -0.48197000 1.83141800
Cl 1.94187000 -0.75864900 3.37119000
H 3.48791600 -1.29322400 1.66561700
H 3.29103600 0.47853400 1.87538800
H 0.19949800 -2.24065700 -4.77829500

[(L-Ag)-(TEDA)]$^{2+}$, Singlet
C 0.85828000 0.81054000 0.78126800
C 0.11342400 0.74199000 -0.57153100
H 1.45193700 1.71963700 0.87821800
H 0.18743100 0.73249700 1.63437400
N 1.81448400 -0.36701300 0.86342200
N 0.28936400 -0.59589100 -1.19372000
H -0.95007700 0.92156700 -0.41386100
H 0.49312400 1.48464300 -1.27045400
C 2.64218600 -0.39337300 -0.41528000
C 1.70962700 -0.74248600 -1.59839400
H 3.43346700 -1.13090900 -0.28240100
H 3.08706600 0.59640400 -0.51868000
H 1.90818800 -0.06978400 -2.42996400
H 1.86346200 -1.77072800 -1.92793600
C 1.01132200 -1.65303000 0.93945700
C -0.03836000 -1.64033900 -0.19616900
H 0.55213400 -1.69895300 1.92517000
H 1.72640200 -2.46992800 0.83989300
H -0.05730100 -2.61312000 -0.68800800
H -1.03518800 -1.43316600 0.19514500
Ag -1.06182100 -0.70894300 -3.08663500
O -2.18002300 -0.22218300 -5.14283800
C -1.74212400 0.26256300 -6.17090300
N -0.64427000 -0.45689300 -6.85580200
C -0.61379300 -1.74771900 -6.75525800
C 0.45680000 0.33445500 -7.49598900
C 0.46773700 -2.60005700 -7.28234400
C 1.75429700 -0.45943200 -7.45840900
H 0.15069500 0.55206300 -8.52037800

C 1.54920700 -1.84902000 -8.06439200
H 0.87648000 -3.10613900 -6.39220100
H 2.50791000 0.10399200 -8.01383500
H 1.24418500 -1.75432300 -9.11141700
C -2.20859000 1.49977500 -6.78315200
C -2.62052300 2.53520600 -5.92379600
C -2.31594700 1.64216400 -8.17844300
C -3.11679400 3.71391900 -6.46582700
H -2.48990200 2.41546000 -4.85560200
C -2.83997000 2.81643800 -8.70649600
H -2.03939000 0.82882600 -8.83993800
C -3.23100900 3.85280700 -7.85298200
H -3.41255800 4.52654800 -5.81141500
H -2.94533000 2.92450800 -9.78020800
H -3.62603500 4.77278800 -8.27140300
H -1.44126600 -2.20181400 -6.21579200
H -0.00253800 -3.40767700 -7.85811100
H 2.47575400 -2.42620600 -8.04769100
H 2.08846400 -0.53106700 -6.41872000
H 0.52914900 1.26475800 -6.93584800
B 0.59778700 1.78933500 -4.10582600
F 1.59985300 2.10670700 -3.18934500
F -0.66873900 1.86178500 -3.46444800
F 0.61603900 2.61536800 -5.22144400
F 0.77734600 0.42975900 -4.52946900
C 2.76888500 -0.23880100 2.01932500
Cl 1.93604200 -0.08991600 3.58394400
H 3.39016400 -1.13141500 2.04007700
H 3.36835400 0.65442400 1.85797900

[(L-Ag)-H_2O-(TEDA)$^{2+}$, 7c-s, singlet
C 0.94810400 -1.04876000 -0.35405700
C 1.69840200 -1.33228700 -1.67759200
H 0.01140500 -0.52262600 -0.53170200
H 0.76586100 -1.94966800 0.22815800
N 1.80720300 -0.13053400 0.49855500
N 2.97719500 -0.59688000 -1.73098800
H 1.91940400 -2.39678200 -1.76914500
H 1.07517400 -1.03299900 -2.51753600
C 2.01652000 1.17146500 -0.26528800
C 2.74573800 0.85304000 -1.59288300
H 2.59025900 1.83282000 0.38350900
H 1.02816000 1.58945300 -0.44854400
H 2.14359900 1.20657800 -2.42701300
H 3.71424900 1.35472900 -1.62449200
C 3.15900300 -0.77832300 0.74365800
C 3.83740700 -1.05050800 -0.62556100
H 2.97700700 -1.69202400 1.30600800
H 3.72892200 -0.08665100 1.36432300
H 4.79070900 -0.52333600 -0.68453800
H 4.02676800 -2.11791200 -0.74608300
O 3.79150600 -0.94181800 -4.29673800
Ag 2.07330000 0.05263400 -5.39572200
O 0.67911800 1.11228500 -7.04151700
C -0.53803700 1.04426900 -7.08392100
N -1.12800800 -0.30790100 -7.01809200
C -2.02529400 -0.54998200 -6.11290800
C -0.48081200 -1.38215500 -7.83081600
C -2.52789600 -1.90018300 -5.79345300
C -0.55572800 -2.71898500 -7.10793300
H -1.00813700 -1.40213100 -8.78865300
C -1.99999500 -3.01693300 -6.69822100
H -2.23101600 -2.04258600 -4.74271200
H -0.16949200 -3.49121400 -7.77732300
H -2.62623000 -3.09204500 -7.59296900
C -1.45186200 2.17030600 -7.17147100
C -0.98543200 3.41811600 -6.71441500
C -2.74452400 2.04618100 -7.71483100
C -1.81365700 4.52802800 -6.79289200
H 0.00084400 3.47999400 -6.27042800
C -3.55906700 3.16948400 -7.80311900
H -3.09474700 1.09276000 -8.09369700
C -3.09714800 4.40460100 -7.33929600
H -1.46918300 5.48824900 -6.42524100
H -4.55040400 3.08464900 -8.23381600
H -3.74046200 5.27617900 -7.40185200
H -2.36860300 0.29780000 -5.52761400
H -3.62337200 -1.84753600 -5.76786400
H -2.06836600 -3.97223400 -6.17404400
H 0.09581700 -2.68811100 -6.22664200
H 0.54512200 -1.06171700 -8.00396400
B -0.39763800 1.09113900 -3.60255900
F -0.40396200 1.03787000 -2.20814700
F -0.24387600 -0.23902200 -4.12167600
F -1.57619800 1.63384200 -4.10422700
F 0.71808300 1.84039500 -4.05355500
C 1.12237100 0.22715500 1.78827400
Cl 0.78714800 -1.18901000 2.81374200
H 1.77481600 0.90259800 2.33723300
H 0.17857600 0.70781300 1.54059100
H 4.60008000 -0.43426700 -4.45119000
H 3.58675500 -0.84378400 -3.31620100

[(LOH-Ag)-(H-TEDA)$^{2+}$, 8c-s, singlet
C 0.31217300 0.08064800 0.41608400
C -0.27227000 0.03225700 -1.00501200
H 0.87324000 0.99863700 0.57906000
H -0.46216600 -0.03149500 1.17166100
N 1.29543900 -1.06453600 0.58711600
N 0.53987700 -0.92422800 -1.82922100
H -1.30207900 -0.32133700 -1.02004500
H -0.21706500 1.01960700 -1.45841400

C 2.49313800 -0.82107700 -0.32068000
C 1.99749400 -0.57665000 -1.75689300
H 3.13181300 -1.69984700 -0.24508900
H 3.01263700 0.06022400 0.04868900
H 2.11801000 0.46494100 -2.04574400
H 2.52887100 -1.20925600 -2.46647100
C 0.63052600 -2.36519800 0.17752500
C 0.33114800 -2.32441800 -1.33430300
H -0.27546100 -2.46290700 0.77108800
H 1.30949900 -3.17925100 0.42813600
H 0.99381400 -2.97754600 -1.90079700
H -0.70160100 -2.60563800 -1.53638000
H 0.21265600 -0.86567000 -2.83264700
Ag 0.66430800 2.59275100 -3.94024800
O -0.95163400 2.02594900 -5.35164200
C -1.12868800 1.31843200 -6.36762100
N -0.47912800 0.13956700 -6.56408400
C 0.37257000 -0.37999500 -5.49567200
C -0.39923600 -0.54698700 -7.87306600
C 1.23195300 -1.53595300 -5.98775000
H 1.01543100 0.42462700 -5.12560300
C 1.05420800 -0.61434800 -8.35272100
H -0.83183100 -1.54651400 -7.77549500
C 2.00855400 -1.13317500 -7.24679800
H 1.91229100 -1.81771900 -5.18051200
H 1.08381500 -1.26194100 -9.23361900
H 2.58881700 -1.98876800 -7.59991000
C -2.13691900 1.78193700 -7.36311000
C -2.10298900 3.12434100 -7.76360900
C -3.16388700 0.94197100 -7.81645000
C -3.06768100 3.61221200 -8.64194300
H -1.31631800 3.77188400 -7.39138100
C -4.13975400 1.44137100 -8.67730100
H -3.20936600 -0.08962100 -7.48255100
C -4.08713300 2.77231600 -9.09788700
H -3.02841600 4.64702100 -8.96596900
H -4.94020600 0.79283600 -9.01776500
H -4.84267400 3.15610600 -9.77590600
O -0.42603100 -0.74417100 -4.35887000
H 0.59444900 -2.40561100 -6.18621200
H 2.73050400 -0.35416100 -6.98013600
H 1.35971400 0.38398300 -8.67896600
H -1.00610500 0.00155700 -8.58681400
B 2.03770800 3.07139100 -1.26475500
F 2.41484600 2.17802400 -0.24986000
F 0.61992900 3.03959000 -1.40726100
F 2.49271300 4.34082400 -1.03834900
F 2.55440700 2.56233700 -2.51550200
C 1.81997000 -1.12230700 2.00421900
Cl 0.54914500 -1.49531500 3.18464600
H 2.57887500 -1.90067600 2.04367200
H 2.24347600 -0.14735000 2.23599100
H -1.00908800 -1.47873400 -4.60693800

LOH-Ag, 9c-s
N -1.50502500 0.91704200 0.68400800
C -0.52016000 0.94385300 -0.38497600
C -0.36404200 2.36717000 -0.93581300
C -1.70408300 3.11001600 -0.88469400
C -2.14249800 3.31131200 0.58036300
C -1.62191500 2.16103300 1.46141600
H 0.38321700 2.89574500 -0.33292000
H -1.62779900 4.07101600 -1.39960000
H -1.74099000 4.25030600 0.97448800
H -2.25484900 1.98307900 2.32747400
H -3.23262000 3.37918600 0.64248600
H -0.61939400 2.39099000 1.83586100
H -2.45708800 2.52205200 -1.42194400
H 0.02460400 2.30686600 -1.95626000
H -0.87628800 0.26177800 -1.16209800
C -2.14091500 -0.25024100 0.96220000
O -1.77009000 -1.33759100 0.46601400
C -3.33819700 -0.24118700 1.85042900
C -4.38466600 0.67400100 1.67222800
C -3.44873700 -1.24563000 2.82150600
C -5.52393000 0.59374800 2.47137200
H -4.31948900 1.42711900 0.89472100
C -4.58000200 -1.31004200 3.63158900
H -2.64243000 -1.96206300 2.93697600
C -5.61855200 -0.39118500 3.45708200
H -6.33699900 1.29675900 2.32208400
H -4.65519600 -2.07866700 4.39399300
H -6.50298400 -0.44720900 4.08387700
Ag 0.44648400 -2.00906300 0.52505200
B 3.02743900 -3.40841100 1.21192800
F 4.25965500 -2.84031700 0.93738300
F 2.28290600 -2.55499700 2.08584400
F 2.25778700 -3.48685600 -0.00318500
F 3.13779800 -4.67098700 1.76789400
O 0.72100900 0.45170700 0.15267300
H 1.40883400 0.56163900 -0.52070200

[(LOH-Ag)(F-TEDA)]$^{2+}$, 10c-s, Singlet
N -2.06234500 1.29873300 0.83190400
C -1.16723400 1.76657600 -0.21061600
C -1.31746500 3.27849200 -0.41431200
C -2.77365900 3.70181700 -0.19009600
C -3.17085200 3.47120500 1.28258200
C -2.38652900 2.28639600 1.87465800
H -0.66171600 3.79600000 0.29544500
H -2.91261100 4.74954400 -0.46759300
H -2.94874800 4.35941700 1.88227300

H -2.92621300 1.79236400 2.67885600
H -4.24764500 3.29544300 1.35950700
H -1.43272900 2.62856300 2.28881600
H -3.42058700 3.11114200 -0.84866100
H -0.97327400 3.53222700 -1.42112900
H -1.42418500 1.21983100 -1.12180800
C -2.43218000 -0.00903300 0.83670000
O -1.86937300 -0.84920700 0.09769800
C -3.55071200 -0.45561300 1.71236300
C -4.76798600 0.23703600 1.77264800
C -3.39665800 -1.65731300 2.41743300
C -5.81473300 -0.26148300 2.54620700
H -4.90487700 1.14500600 1.19583600
C -4.43814200 -2.14132800 3.20521000
H -2.45795300 -2.19663000 2.34823600
C -5.64783200 -1.44442000 3.26989800
H -6.75954200 0.27094900 2.58103900
H -4.30985700 -3.06285000 3.76366200
H -6.46142000 -1.82634600 3.87835200
Ag 0.45326700 -1.01332000 0.07784900
B 3.42551800 -1.90148600 0.01760700
F 4.28985600 -2.12780200 -1.07584400
F 3.06256400 -0.50645800 -0.00367600
F 2.22154400 -2.62470600 -0.18114900
F 4.01758500 -2.22370600 1.20916100
O 0.18175400 1.42729500 0.17928600
H 0.78980100 1.87787400 -0.42385000
C 4.19999300 2.28361000 -3.90529100
C 5.50513900 1.48997800 -4.13241200
H 4.39493500 3.33516900 -3.70346300
H 3.49328100 2.18635100 -4.72710000
N 3.54308400 1.70585600 -2.68749300
N 5.44711800 0.20932100 -3.32201700
H 5.61353700 1.22760000 -5.18270800
H 6.38326500 2.04432800 -3.80343400
C 4.49008300 1.66326700 -1.52656900
C 5.52236700 0.56245900 -1.84170700
H 3.91163300 1.39093500 -0.64611600
H 4.92607700 2.65508800 -1.42711300
H 6.53103400 0.90983100 -1.62619200
H 5.30329200 -0.35256200 -1.29520000
C 2.98552300 0.34246800 -2.96813700
C 4.12308000 -0.49087300 -3.58823600
H 2.14859600 0.46669900 -3.65208300
H 2.66379000 -0.06027600 -2.01087200
H 4.16081200 -1.46559000 -3.10627500
H 4.02115100 -0.59849700 -4.66491500
F 2.47799800 2.54197800 -2.34340000
C 6.61696200 -0.70942700 -3.61736800
H 6.52849800 -1.55771000 -2.94139700
Cl 6.61067400 -1.28495800 -5.29121200
H 7.53097600 -0.14874800 -3.43442200

[(LOH-Ag)(F-TEDA)]$^{2+}$, 10c-t, Triplet

N -2.20712200 1.30501600 1.06908700
C -1.25450300 1.71664200 0.03257400
C -1.13555000 3.25965800 -0.00200900
C -2.52360800 3.88024300 0.19201100
C -3.07572600 3.56761000 1.59865500
C -2.46212800 2.27308100 2.15309100
H -0.44635800 3.58090300 0.78496600
H -2.46236000 4.95994700 0.03234200
H -2.83510800 4.37485600 2.29656700
H -3.09138300 1.80488400 2.90594900
H -4.16574000 3.48750800 1.56473000
H -1.49364600 2.47597600 2.62025600
H -3.19833100 3.48291900 -0.57389800
H -0.68902000 3.52531100 -0.96192300
H -1.65086800 1.37112600 -0.92945500
C -2.67153500 0.04425600 1.03437600
O -2.13855000 -0.83947800 0.29508600
C -3.85460300 -0.36709400 1.82287600
C -5.00926000 0.42890300 1.88036400
C -3.82834000 -1.62141200 2.45261200
C -6.11953100 -0.01904700 2.58996500
H -5.04467600 1.37583400 1.35368700
C -4.93631600 -2.05403200 3.17508100
H -2.93702000 -2.23475000 2.38232000
C -6.08073600 -1.25462500 3.24354500
H -7.01506300 0.59159100 2.63014200
H -4.91102700 -3.01409600 3.67930300
H -6.94685600 -1.59746400 3.80022500
Ag 0.03748700 -0.96775200 0.07333200
B 2.41806400 -2.80816100 -0.14448600
F 3.58752400 -2.65168400 -0.90012900
F 2.26342300 -1.63796900 0.69026500
F 1.29269600 -2.76183500 -1.03145100
F 2.42004000 -3.94510500 0.60761200
O 0.02451500 1.19339900 0.24973800
H 0.73576600 1.47220100 -0.97655800
C 3.66200700 1.67726700 -3.22556700
C 5.05010400 1.07963900 -3.63902700
H 3.78148800 2.61460300 -2.68527700
H 3.01799900 1.81995800 -4.09113200
N 3.07908400 0.67929600 -2.34990300
N 5.18883100 -0.30609800 -3.02218100
H 5.13013700 0.97341500 -4.71809500
H 5.87385300 1.68559000 -3.26556000
C 3.78935400 0.49945500 -1.09867200
C 5.14027600 -0.18148800 -1.50057300
H 3.22489800 -0.15183400 -0.43378100
H 3.95627700 1.47213500 -0.63962000

H 5.99531800 0.41476900 -1.18761700
H 5.18901300 -1.18631000 -1.08879600
C 2.68874800 -0.54041600 -3.02890000
C 4.03719600 -1.19510400 -3.47965900
H 2.06412600 -0.28734900 -3.88342600
H 2.15756400 -1.20224600 -2.34928400
H 4.16318900 -2.16216400 -2.99866000
H 4.09884600 -1.28502200 -4.56112800
F 1.07401200 1.63884800 -1.89967400
C 6.52615000 -0.92823300 -3.37101400
H 6.57654500 -1.89591100 -2.87649600
Cl 6.73045400 -1.15976600 -5.11736100
H 7.30526900 -0.26031800 -3.01053600

[(LO)-Ag](HF)(TEDA)$^{2+}$, 11c-s, Singlet
C 1.36065100 1.37396600 1.40046800
C 0.27286700 2.11326400 0.59026700
H 2.07837300 2.05829500 1.85262400
H 0.91874600 0.74967800 2.17453200
N 2.14127000 0.47623000 0.45798900
N 0.62013400 2.03859700 -0.85816800
H -0.71467400 1.66889300 0.70658400
H 0.23963200 3.16125200 0.88756300
C 2.95912100 1.35384700 -0.47463000
C 2.03975200 2.45327000 -1.05250600
H 3.36683000 0.70387100 -1.24758200
H 3.77652700 1.79248800 0.09685600
H 2.19339100 3.40492500 -0.55066200
H 2.23719900 2.58552300 -2.11493600
C 1.16331500 -0.31898000 -0.38608000
C 0.43865900 0.64765900 -1.35068900
H 0.47219000 -0.80740500 0.29721900
H 1.72364200 -1.07728200 -0.93173000
H 0.83379300 0.59148900 -2.36379200
H -0.61990600 0.40778100 -1.35700600
Ag -0.64397700 3.47087300 -1.92664300
O -1.72224400 4.87632000 -3.01660900
C -1.83771800 4.65061900 -4.27842000
N -2.13080400 3.42697300 -4.72665000
C -2.65234300 2.46336600 -3.74288000
C -1.81928000 2.95034100 -6.09626500
C -3.19221300 1.21824000 -4.48081300
O -1.66021200 2.00120200 -2.86188100
C -1.16668200 1.57454100 -5.98905700
H -2.73946200 2.91007200 -6.68632600
C -2.12793800 0.54321400 -5.35698800
H -3.60374800 0.53671100 -3.73449300
H -0.85541200 1.25867400 -6.98765100
H -2.64612900 -0.01846900 -6.13944700
C -1.67907600 5.81834000 -5.14967200
C -0.72912100 6.79784500 -4.78969600
C -2.50896800 5.99943100 -6.27328100
C -0.57852700 7.92291200 -5.59038600
H -0.11713800 6.66032500 -3.90793600
C -2.35526100 7.13522100 -7.05541400
H -3.27180000 5.26858800 -6.51406600
C -1.38790400 8.09344200 -6.71778200
H 0.16268300 8.67143400 -5.33343600
H -2.98673600 7.28242200 -7.92437300
H -1.27519700 8.97997200 -7.33315300
H -4.03252500 1.58691400 -5.08008700
H -1.55720000 -0.17719400 -4.76710100
H -0.26147100 1.67146500 -5.38113400
H -1.14988700 3.67601400 -6.55679800
B 1.39293800 5.68444500 -1.69337700
F 2.58462400 5.57920500 -1.02305200
F 0.35443600 5.02449800 -0.81618300
F 0.97816000 6.96466900 -1.93255200
F 1.37382100 4.89437800 -2.85992000
C 3.10011600 -0.41669100 1.21057900
Cl 2.25972400 -1.59152000 2.24085400
H 3.69878800 -0.95205400 0.47662500
H 3.72141900 0.22075500 1.83550600
H -3.45547400 2.95954600 -3.19007000
F -2.50569900 1.13570400 -0.61076200
H -2.34957600 1.41581900 -1.50995300

[(LO)-Ag](HF)(TEDA)$^{2+}$, 11c-t, Triplet
C 0.01062700 -0.99825200 1.34408100
C -0.13017100 -1.47147200 -0.11182800
H -0.81165100 -0.34241200 1.62735900
H 0.07071300 -1.82270100 2.05132800
N 1.29778300 -0.20051900 1.47256400
N 1.18520400 -1.30682100 -0.80930300
H -0.39779900 -2.52600400 -0.15745900
H -0.86912200 -0.89085900 -0.65574200
C 1.30991000 0.85040000 0.36806000
C 1.52101000 0.14282500 -0.97773900
H 2.11129000 1.55679700 0.58112800
H 0.34623700 1.35664900 0.39570000
H 0.87418900 0.58149500 -1.73418600
H 2.55472400 0.19889600 -1.31694100
C 2.48525900 -1.12941200 1.27225600
C 2.25639400 -1.96409200 -0.00340000
H 2.56865300 -1.76136200 2.15382000
H 3.36892300 -0.49565700 1.20100600
H 3.16550900 -2.01238400 -0.60169300
H 1.93024200 -2.97820500 0.22443500
Ag -0.53257900 -1.10826700 -4.19622700
O -1.70732600 0.05895200 -5.63742900
C -1.18170100 0.72777800 -6.55430200
N -0.07761400 0.21469000 -7.23763000

C 0.17901600 -1.23757300 -7.13455100
C 0.94554800 1.05666500 -7.88498500
C 1.11817300 -1.70634800 -8.23912900
O 0.80689300 -1.25971400 -5.88631300
C 2.34042200 0.46844400 -7.65832500
H 0.72665600 1.07803900 -8.95965600
C 2.46495000 -0.95433200 -8.23723200
H 1.25756200 -2.78262100 -8.11484400
H 3.06260200 1.14451200 -8.12168600
H 2.83387300 -0.91032700 -9.26514500
C -1.75508200 2.01823600 -6.93551300
C -2.39541600 2.75789400 -5.91964100
C -1.75593100 2.48443500 -8.26475200
C -2.98599700 3.97543200 -6.23282200
H -2.40508700 2.38093300 -4.90399600
C -2.37057400 3.69276300 -8.56620500
H -1.32083000 1.89167200 -9.05981200
C -2.97505500 4.44278200 -7.55118200
H -3.45894200 4.56046200 -5.45169600
H -2.38550000 4.04853900 -9.59028100
H -3.44586900 5.39044700 -7.79139500
H 0.57610300 -1.56230800 -9.18005200
H 3.20267800 -1.51136900 -7.65543900
H 2.53034600 0.46589300 -6.58121300
H 0.85985700 2.06664600 -7.48869700
B -1.73702700 1.05059900 -2.34338800
F -1.45358200 1.23466500 -0.98891800
F -1.98248200 -0.37355600 -2.54757600
F -2.82929100 1.77131600 -2.76144400
F -0.59125600 1.35159900 -3.11937300
C 1.37578600 0.52682700 2.79287500
Cl 1.25816400 -0.57167000 4.18269200
H 2.33310500 1.04154800 2.83292900
H 0.54838200 1.23247100 2.82937900
H -0.77304900 -1.77244300 -7.14346000
F 0.56188800 -2.37106000 -2.95187300
H 1.04661700 -1.77961500 -1.79422900

[(LO)-Ag]$^{+}$, triplet, 12c-t

N -1.90816700 0.90490400 0.38352000
C -1.00807300 0.98703600 -0.77771100
C 0.13806700 2.07579300 -0.45967200
C -0.50841200 3.45423800 -0.24787600
C -2.00337900 3.37084700 0.09942100
C -2.31453100 2.19700300 1.01571900
H 0.64263900 1.69450800 0.43054100
H 0.03232000 3.93892800 0.57155000
H -2.32846500 4.28323800 0.60412100
H -3.37913100 2.15745800 1.23553300
H -2.60382800 3.29139100 -0.81326900
H -1.77237900 2.28056600 1.96291800
H -0.37854400 4.06450300 -1.14373900
H 0.82691300 2.04993100 -1.30212900
H -1.58823000 1.40954700 -1.62087300
C -2.28277600 -0.26479500 0.91463200
O -1.78557800 -1.39334500 0.62563500
C -3.38888200 -0.36680800 1.89954900
C -4.68723000 0.06587900 1.57385200
C -3.12351300 -1.01332500 3.12218000
C -5.70236100 -0.09178100 2.50694900
H -4.89078900 0.50965500 0.60527400
C -4.14558300 -1.14644400 4.05443700
H -2.12441900 -1.37671000 3.33344800
C -5.43131900 -0.69024700 3.74761800
H -6.70582900 0.24665800 2.27445500
H -3.94603200 -1.61464400 5.01163300
H -6.23188100 -0.81053300 4.46975800
Ag 0.37370100 -1.63737100 0.21459700
B 2.70130500 -3.10681100 1.13110100
F 3.44498500 -2.68949400 2.20325700
F 1.31272700 -3.27432000 1.53175900
F 2.63028700 -2.04307000 0.13977000
F 3.15558700 -4.25749900 0.54348500
O -0.40724100 -0.12455400 -1.17199400

[(LO)-Ag], neutral, doublet, Ac-d

N -1.50322600 1.00316000 0.74834400
C -0.45458900 0.98698000 -0.30305000
C -0.29658200 2.41346300 -0.89189500
C -1.67145100 3.08060900 -1.00890800
C -2.28805100 3.32443200 0.38439600
C -1.75847900 2.29867600 1.39731400
H 0.36727800 2.99297000 -0.24253300
H -1.57838400 4.02095100 -1.55922300
H -2.03241700 4.32363100 0.75037800
H -2.43760900 2.15495600 2.23454100
H -3.37945300 3.27454700 0.32613200
H -0.80187200 2.63297000 1.81260300
H -2.32777700 2.43129500 -1.59904500
H 0.19547500 2.31347300 -1.86101500
H -0.82883600 0.32740200 -1.09870000
C -1.99599600 -0.17985700 1.15908300
O -1.45667500 -1.27663800 0.83888900
C -3.23576400 -0.23911400 1.97778100
C -4.35997100 0.53969500 1.66813700
C -3.29182100 -1.16278800 3.03088900
C -5.52391300 0.40820200 2.42239200
H -4.33028200 1.22343800 0.82688200
C -4.45171900 -1.27731700 3.79300800
H -2.42251400 -1.77429200 3.24642600
C -5.56772000 -0.49275800 3.48948300
H -6.39615800 1.00435000 2.17529000

H -4.48822900 -1.98043900 4.61864400
H -6.47358800 -0.58846900 4.07968300
Ag 0.76641800 -1.49269100 0.70672600
B 2.80847100 -3.59290500 1.08497900
F 3.51219600 -3.75512700 2.25841800
F 1.39132900 -3.66929900 1.35287500
F 3.00615700 -2.25562000 0.57901300
F 3.14822800 -4.51163600 0.11596200
O 0.76948700 0.57408000 0.15555300

[(LO)-AgF], singlet
Ag -0.59576200 -1.00125100 -4.28757400
O -1.76381300 0.03911600 -5.64070700
C -1.18655200 0.69399700 -6.58209800
N -0.13203900 0.17846200 -7.22054700
C 0.15416700 -1.25773500 -6.97895900
C 0.87508200 0.98151200 -7.95161200
C 1.21511400 -1.73685500 -7.99212900
O 0.67640200 -1.49373200 -5.71490400
C 2.26940300 0.53070500 -7.51978200
H 0.73535900 0.84929000 -9.02933100
C 2.52746000 -0.94333600 -7.89701200
H 1.36842600 -2.80444700 -7.82788700
H 3.00832500 1.18920200 -7.98370200
H 3.03281400 -1.00455700 -8.86538500
C -1.76265500 2.00421500 -6.92580600
C -2.27153500 2.79828000 -5.88344700
C -1.85257800 2.43569100 -8.26015000
C -2.82794500 4.03873100 -6.18129600
H -2.21481000 2.44577100 -4.86139200
C -2.42554600 3.67040300 -8.54549900
H -1.50010000 1.80052000 -9.06473800
C -2.90471100 4.47514500 -7.50655200
H -3.20600700 4.66391300 -5.37934100
H -2.50236300 4.00434400 -9.57463200
H -3.34518100 5.44095200 -7.73298800
H 0.75290400 -1.62016900 -8.97842700
H 3.19060100 -1.39936800 -7.15869400
H 2.34764000 0.66113800 -6.43610400
H 0.70732400 2.03065300 -7.71405600
B -1.79975900 1.05112000 -2.42557300
F -1.55738200 1.16204100 -1.08010900
F -1.95925300 -0.40454200 -2.73434200
F -2.95626200 1.68408900 -2.83070300
F -0.69887900 1.45931900 -3.19766200
H -0.78207800 -1.80380500 -7.13822500
F 0.47894400 -1.99264400 -3.02799300

[(LO)-AgF], triplet
Ag -0.62914000 -1.09371200 -4.08375600
O -1.79112800 0.00135800 -5.64583900
C -1.20895100 0.67974400 -6.51535600
N -0.07120500 0.18928400 -7.13844600
C 0.19806600 -1.25822000 -7.03399500
C 0.95569900 1.04200500 -7.77109000
C 1.15629800 -1.71335300 -8.12342400
O 0.79609500 -1.29038700 -5.76741400
C 2.34919600 0.46937100 -7.51116600
H 0.76181500 1.07250700 -8.84935700
C 2.49902500 -0.95319200 -8.08753400
H 1.30373700 -2.79009300 -8.00911000
H 3.08020700 1.14914600 -7.95603300
H 2.89579300 -0.90644200 -9.10536700
C -1.75714800 1.98789300 -6.91344000
C -2.36882800 2.75914000 -5.90872600
C -1.75786300 2.42841100 -8.24783300
C -2.94095700 3.98272400 -6.24219100
H -2.37693200 2.40124200 -4.88619200
C -2.35395800 3.64287200 -8.57104100
H -1.33306400 1.81208500 -9.03136800
C -2.93572200 4.42441800 -7.56826400
H -3.39674400 4.59045100 -5.46761500
H -2.37002600 3.97737400 -9.60270100
H -3.39214600 5.37554900 -7.82333800
H 0.63684400 -1.56462900 -9.07656200
H 3.22483600 -1.50621400 -7.48692300
H 2.51428900 0.46527900 -6.43023300
H 0.85413700 2.04941100 -7.37119300
B -1.83018300 1.11628200 -2.38752900
F -1.50773900 1.41846300 -1.08210000
F -2.09638800 -0.31378600 -2.49131000
F -2.95014300 1.80505200 -2.83242900
F -0.73084200 1.36501800 -3.24974900
H -0.75413000 -1.79377700 -7.05787900
F 0.42195700 -2.19510700 -2.80285600

[(LOF)-Ag], 13c-s
Ag -0.86729000 -2.52111800 -4.28084900
O -0.82883300 -1.16121100 -6.33314000
C -0.21890900 -0.09822900 -6.31089400
N 1.20137900 -0.08359800 -6.16334900
C 1.83862000 -0.89788000 -5.26863900
C 2.04500500 0.74045100 -7.06910400
C 0.91459500 -0.30215000 -9.86440600
O 1.33420300 -1.71278300 -4.49939400
C 2.77778600 -0.12816600 -8.10045100
H 1.38570200 1.44797300 -7.56345300
C 1.87839800 -1.03443500 -8.95222300
H 0.36706600 -1.00047400 -10.50429000
H 3.34724600 0.54895500 -8.74853500
H 2.51442700 -1.66244000 -9.58658900
C -0.90056400 1.21014800 -6.37165800

C -0.35747400 2.35183700 -5.76297900
C -2.15658600 1.27612600 -6.99433400
C -1.06634100 3.55076100 -5.78281100
H 0.59974700 2.29470000 -5.25633300
C -2.85311600 2.47894400 -7.02351800
H -2.55985400 0.38417800 -7.45958400
C -2.30870600 3.61653900 -6.41800100
H -0.65196100 4.43058400 -5.30205100
H -3.81817600 2.53395000 -7.51618800
H -2.85549200 4.55392400 -6.43921000
H 1.43060000 0.43232200 -10.49233400
H 1.30881900 -1.71799100 -8.31208200
H 3.51630100 -0.75238300 -7.58480300
H 2.75984000 1.30696000 -6.46709300
B -3.08308000 -4.11018300 -3.02141600
F -2.89582100 -5.05095800 -2.02425400
F -2.29945400 -4.46488600 -4.17222700
F -4.41138500 -3.97980500 -3.38542400
F -2.57381800 -2.83951400 -2.58813800
H 2.92461800 -0.72780800 -5.25716700
F -0.04140600 0.40076100 -9.10071100

[(LOF)-Ag]$^{+}$, Bc-d
Ag -3.09124900 -0.11596900 -5.16655600
O -1.10400500 -0.96109600 -5.80120400
C -0.27893300 -0.08060500 -6.14717600
N 1.05301200 -0.30973100 -6.17528200
C 1.55441000 -1.44632700 -5.49021700
C 2.00204000 0.58947900 -6.88015100
C 0.90866700 -0.19831600 -9.75211100
O 2.73530400 -1.68541100 -5.43177300
C 2.78883200 -0.11699400 -7.99484200
H 1.41230700 1.40554900 -7.29160600
C 1.96450800 -0.95682400 -8.97796600
H 0.44154500 -0.82436700 -10.51624900
H 3.31522300 0.67581700 -8.53853800
H 2.65066400 -1.39791500 -9.70989000
C -0.87366700 1.26382600 -6.38782900
C -0.48133700 2.37245400 -5.64347200
C -2.04194200 1.32618600 -7.23779600
C -1.22394000 3.54653800 -5.75274400
H 0.37474600 2.32209200 -4.98155300
C -2.76147200 2.51415000 -7.34482200
H -2.28976900 0.46677000 -7.85053600
C -2.36943200 3.61602300 -6.59461800
H -0.92933000 4.42285900 -5.18688600
H -3.62482600 2.56574600 -7.99627600
H -2.93123100 4.53967800 -6.64514900
H 1.30804600 0.70855100 -10.21624900
H 1.48626200 -1.79937900 -8.46529000
H 3.55080000 -0.75259400 -7.54145000
H 2.68859800 0.99844300 -6.13653800
B -4.43085800 2.30981700 -4.06589300
F -5.06519600 2.47420500 -2.86115400
F -4.93741400 1.09717700 -4.71202400
F -4.61490400 3.37219300 -4.93326900
F -3.03979500 2.06062600 -3.88342900
H 0.76556300 -2.04330800 -5.01641800
F -0.12752000 0.21233900 -8.87253200

[(l-Ald)-Ag], 14c-s
C -0.30129500 0.68479400 -0.82337300
C -0.89995100 0.16490900 0.48529200
H -0.71742000 0.87489400 1.30056600
H 0.77251300 0.86488200 -0.70227900
H -0.40061500 -0.07692200 -1.60594400
C -0.33841500 -1.20772800 0.87355600
H -1.99148800 0.09139600 0.38868600
H 0.72277400 -1.13107500 1.12237400
H -0.42155500 -1.90941700 0.03903800
N -1.01724100 -1.79240600 2.02669800
C -0.99240500 1.95659700 -1.30638800
H -0.92863700 2.76142800 -0.55793600
H -2.06153500 1.77979300 -1.47021000
C -0.42893600 2.50321500 -2.58981300
H -0.99587500 3.35465800 -3.02185400
O 0.57769600 2.09179500 -3.13415000
H -0.60124600 -1.65365100 2.93551100
C -2.13102200 -2.53900700 1.95532300
O -2.68496200 -2.84868400 0.87332500
C -2.70089900 -3.04486800 3.23838400
C -3.48109700 -4.20856000 3.19758300
C -2.50194900 -2.38726600 4.46120200
C -4.03227600 -4.72343000 4.36813000
H -3.63898000 -4.69999100 2.24444200
C -3.06352600 -2.90002900 5.62935000
H -1.94323400 -1.45769800 4.50764400
C -3.82311900 -4.07107800 5.58598100
H -4.62564100 -5.63132600 4.33142000
H -2.91442400 -2.38067900 6.57033000
H -4.25693600 -4.46982500 6.49755600
Ag -3.03669700 -1.83751000 -1.08627300
B -3.18345700 -0.07155600 -3.50633500
F -2.39153600 -1.25613200 -3.31447200
F -3.75994500 0.20822300 -2.21972400
F -2.36393600 0.97866300 -3.88917400
F -4.18488500 -0.31953500 -4.42353400

[(n-Ald)-Ag], isomer-1, 15c-s
N -4.40687200 1.32754600 -0.35108500
C -0.76194600 1.47455500 -0.94991100
C -1.01081200 2.68005800 -1.79585000

C -2.49556600 2.93229200 -2.12616400
C -3.32678600 3.46610200 -0.95216800
C -3.62274400 2.45065100 0.15810200
H -0.53930400 3.54939600 -1.32811500
H -2.53046400 3.66217800 -2.93970100
H -2.81971700 4.32526300 -0.49783900
H -4.15970900 2.95646800 0.96976800
H -4.28111400 3.84390200 -1.33910800
H -2.69889000 2.06409200 0.59158500
H -2.94581900 2.01313300 -2.51938200
H -0.47979900 2.47880300 -2.73882400
H -1.29069600 0.54877800 -1.23887700
C -4.20878700 -0.01390000 -0.21047000
O -4.79171900 -0.82438400 -0.93637500
C -3.27649100 -0.49224000 0.86426200
C -3.24760300 0.07331300 2.14689100
C -2.47867800 -1.61014600 0.58380000
C -2.41357000 -0.45618400 3.13223800
H -3.89114700 0.91293600 2.38490700
C -1.63221600 -2.13659500 1.56422500
H -2.53283900 -2.06191500 -0.40056800
C -1.59783300 -1.55698400 2.84575400
H -2.40496100 -0.01891700 4.12518000
H -1.00792700 -2.99799100 1.35564200
H -0.94453800 -1.98329100 3.59780800
Ag 0.42964100 -0.37090400 1.36133700
B 1.83297200 -2.71277000 2.62711200
F 3.10224100 -3.20047900 2.86564800
F 1.70426200 -1.39307500 3.17841800
F 1.60965000 -2.57698100 1.22185600
F 0.84008200 -3.52673000 3.17078100
O 0.00426400 1.46970800 0.00943900
H -5.09781900 1.54623800 -1.05964200

[(n-Ald)-Ag], isomer-2, 16c-s

N -2.76995000 1.10108400 -0.42054200
C 0.20414500 1.39569200 -0.35147000
C 0.01153800 2.85316300 -0.03972700
C -1.07002400 3.51573000 -0.91817900
C -2.48724200 3.56864300 -0.31763100
C -2.99060100 2.30505700 0.38734600
H -0.15494700 2.98384000 1.03345400
H -0.77062600 4.54236600 -1.14442400
H -2.53970900 4.37338700 0.42349500
H -4.05291700 2.43027400 0.61988900
H -3.18654200 3.84124600 -1.11622300
H -2.47001700 2.16365000 1.33736800
H -1.09242600 3.00185400 -1.88761600
H 0.98315200 3.31521200 -0.26918500
H 0.13083500 1.13174200 -1.42456100
C -2.53140500 -0.14170000 0.05095300
O -2.06281800 -1.02585700 -0.69893300
C -2.89218000 -0.42834600 1.47386700
C -4.20616100 -0.19156800 1.90512600
C -1.97575600 -1.02519800 2.34904900
C -4.59837500 -0.55959400 3.19096800
H -4.92498200 0.25411500 1.22519300
C -2.37021700 -1.38970900 3.63516600
H -0.94438300 -1.18345400 2.05826900
C -3.68097000 -1.15923200 4.05724300
H -5.62023700 -0.38513800 3.51244800
H -1.64922100 -1.87135900 4.28513100
H -3.98867000 -1.44855500 5.05732800
Ag 0.06601100 -1.89781800 -0.10392600
B 0.82541200 -3.51723600 2.37660800
F 1.94865000 -4.29428300 2.59840100
F 1.21159300 -2.16426600 2.11909600
F 0.15237700 -3.96954500 1.19247800
F -0.05475600 -3.54734500 3.45218200
O 0.46497200 0.53171300 0.47297800
H -2.64753000 1.20681400 -1.42062300

[(LCO)-Ag], 17c-d

N -3.44601400 0.88563700 -0.65403500
C -0.43984100 2.07738200 1.80308500
C 0.06967400 2.76956000 0.55025100
C -0.69654700 2.39407100 -0.73435900
C -2.11756300 2.96741100 -0.81497400
C -3.17971900 2.18101700 -0.03650400
H 0.03365100 3.84921300 0.73498500
H -0.10229900 2.78897200 -1.56322900
H -2.12050100 4.00230600 -0.45329000
H -4.10425200 2.76892500 0.00704300
H -2.42285500 3.01296900 -1.86698400
H -2.86455200 2.01656200 0.99253700
H -0.71669600 1.30536100 -0.85880600
H 1.11463900 2.45851100 0.45139800
C -3.37914500 -0.37600900 -0.14366800
O -3.42162600 -1.36244800 -0.88458100
C -3.24940300 -0.55330300 1.34186600
C -3.95905500 0.20744600 2.27904500
C -2.41878200 -1.59810000 1.79053300
C -3.80685100 -0.04110400 3.64492200
H -4.64579500 0.97892300 1.94894600
C -2.25135000 -1.82939700 3.16141300
H -1.92008300 -2.23128800 1.06590600
C -2.94190800 -1.04284500 4.08909700
H -4.36638400 0.55075000 4.36207900
H -1.58710500 -2.62451300 3.47866000
H -2.81787200 -1.22250300 5.15207300
Ag -0.15523500 -0.13164300 1.83427400
B 0.92011300 -2.93241800 1.66197100

F 2.12869100 -3.54295400 1.40460700
F 1.05912000 -2.00724200 2.75464100
F 0.51505000 -2.13905200 0.53873300
F -0.08794100 -3.84035600 1.96718400
O -0.91823000 2.55643300 2.78114600
H -3.56814500 0.88736400 -1.66040700

[L-Ag], radical, 18c-d
N -2.25911800 0.29862100 -1.11184500
C -1.19324000 3.23786100 1.25553800
C -0.86652100 2.89109600 -0.16292500
C -2.07178300 2.76928800 -1.10241300
C -2.96403200 1.55012200 -0.84569800
H -2.16256800 3.68160500 1.48081200
H -0.19814800 3.68227800 -0.54321800
H -2.69366800 3.66815900 -1.01825400
H -3.85767000 1.61341500 -1.47750600
H -1.71490000 2.73670100 -2.13869600
H -3.30670100 1.54498200 0.18947400
H -0.25259900 1.97980100 -0.20566400
H -0.37187900 3.54671000 1.90155100
C -1.99117500 -0.74924600 -0.28391000
O -1.15756800 -1.60826800 -0.58173900
C -2.75097100 -0.84678900 1.00967200
C -4.13962300 -0.66800300 1.08829700
C -2.03711300 -1.22535700 2.16490000
C -4.80076200 -0.84050800 2.30485900
H -4.70421700 -0.41396700 0.19766800
C -2.70206900 -1.36455000 3.39096900
H -0.97314000 -1.42486900 2.09651500
C -4.08443600 -1.17123000 3.45787100
H -5.87727400 -0.71157800 2.35280100
H -2.12324000 -1.62086600 4.26989500
H -4.60251700 -1.28793800 4.40426500
Ag -1.44139900 1.29569700 2.58730600
B 0.54578300 -0.08193500 4.43404000
F 1.65939000 0.27900200 5.16648700
F -0.56475000 0.75714400 4.79581300
F 0.77664200 0.14163800 3.04127900
F 0.18793100 -1.41337100 4.63208500
H -1.72811700 0.25812900 -1.97453600

(LF)-[Ag-TEDA]$^{2+}$, 19c-d
N -3.30638000 1.46250600 0.08444600
C 0.80018500 2.02067300 0.39645300
C -0.40767600 2.32010200 -0.45651500
C -1.50127500 3.13532200 0.25364900
C -2.52736500 2.28129200 1.01210200
H 1.27703900 2.93151500 0.76790400
H -0.02783900 2.87545800 -1.32211200
H -1.04935800 3.84363000 0.95850500
H -3.19547900 2.93514800 1.58435500
H -2.03682700 3.74311700 -0.48412100
H -2.02325900 1.62376500 1.71860400
H -0.82314900 1.38609800 -0.85174100
H 1.53396700 1.39338100 -0.11198800
C -3.41905600 0.10749100 0.01429500
O -3.79329700 -0.45931900 -1.01511300
C -3.12412900 -0.69967700 1.24633700
C -3.57194800 -0.33127900 2.51823100
C -2.48380000 -1.94765800 1.07239700
C -3.36910000 -1.17940900 3.61134800
H -4.09843400 0.60713400 2.65391700
C -2.26283900 -2.78645300 2.18086300
H -2.24624400 -2.27955000 0.06622200
C -2.70437900 -2.39306900 3.45248200
H -3.72819100 -0.88389400 4.59133900
H -1.78766100 -3.75155600 2.03852900
H -2.52357500 -3.03461100 4.30656900
Ag -0.19224600 -1.12979000 1.67718100
B 0.68839500 -1.10628600 4.53282800
F 1.33641500 -0.72446400 5.72482200
F -0.38455700 -0.20995400 4.28542500
F 1.60271500 -0.93699900 3.43868300
F 0.24626300 -2.40745700 4.57892800
H -3.59716000 1.91776600 -0.77384400
F 0.40866900 1.29359400 1.57846500
N 1.67814900 3.12956800 3.75434100
C 2.60774500 2.03191200 3.59678700
C 0.38542800 2.74929300 4.27875200
C 2.24365300 4.33427100 4.33003800
C 3.01970800 1.66559300 5.06936300
H 3.47588800 2.35574900 3.02422000
H 2.10899400 1.18894300 3.12397300
C 0.69600900 2.27793100 5.74719800
H -0.01560600 1.91522300 3.70821800
H -0.28612500 3.60566800 4.26968500
C 2.50113800 3.96523900 5.84106500
H 1.53152200 5.15500200 4.25155600
H 3.17407400 4.58121300 3.82217600
H 2.80546500 0.61721700 5.26509200
H 4.06341000 1.90043000 5.26059100
N 2.17860400 2.49522300 6.03029900
H 0.13094500 2.86381700 6.46912000
H 0.49103600 1.21562800 5.85043600
H 3.54462400 4.12524700 6.10301800
H 1.85390600 4.53538400 6.50512100
C 2.40878500 2.03600000 7.46072400
Cl 4.09620700 2.22655100 7.96459500
H 1.77423200 2.63852500 8.10669800
H 2.13456100 0.98332400 7.49519500

[Ag-TEDA]$^{2+}$,
C -6.06930800 -3.45605900 -8.99628900
C -5.94778000 -2.14505700 -9.81789700
H -5.58558000 -3.37917900 -8.02365300
H -7.11320700 -3.73313600 -8.86201300
N -5.37386800 -4.57219600 -9.75387900
N -4.88323900 -2.35310300 -10.83284600
H -6.87387200 -1.89960000 -10.33502600
H -5.67579400 -1.31567000 -9.16451200
C -3.87693800 -4.30547500 -9.75016400
C -3.63413300 -2.83891700 -10.20097400
H -3.42092000 -5.02355200 -10.42938700
H -3.49868900 -4.46611300 -8.74162600
H -3.39545700 -2.19068900 -9.35828200
H -2.82160300 -2.80327300 -10.92876400
C -5.85527100 -4.57618800 -11.19291300
C -5.33676000 -3.28840900 -11.88981600
H -6.94165400 -4.62138800 -11.17572000
H -5.46211300 -5.46710300 -11.68112800
H -4.49568100 -3.49659500 -12.55009300
H -6.14413100 -2.83115500 -12.46251900
Ag -4.50879200 -0.37543600 -11.77136300
B -6.03699800 2.03704800 -11.42370600
F -7.11273100 2.34297800 -12.19954100
F -4.86483400 1.80368700 -12.26132500
F -5.74199700 2.93879100 -10.44722000
F -6.24516400 0.71034700 -10.80837300
C -5.60005800 -5.91657100 -9.08555600
Cl -7.29919800 -6.41338100 -9.13702000
H -4.99664900 -6.64932000 -9.61711300
H -5.28669300 -5.82217900 -8.04834500

(FH)-(TEDA)$^{2+}$, doublet
C -1.54562600 0.60745500 0.39588800
C -0.01224600 0.43958700 0.10413800
H -1.70846100 1.36801600 1.15965400
H -2.10579500 0.84772300 -0.50546300
N -1.95230700 -0.69517800 0.88690300
N 0.32651300 -1.04544700 0.14868600
H 0.23590500 0.82076100 -0.88409100
H 0.59727400 0.93368900 0.85870800
C -1.26646300 -1.13228900 2.08734200
C 0.16360500 -1.53680800 1.58584700
H -1.78404600 -1.98812200 2.51713500
H -1.22591800 -0.31433600 2.80384500
H 0.93327600 -1.06785100 2.19679000
H 0.29600200 -2.61672700 1.58357500
C -2.07647400 -1.71332800 -0.13776900
C -0.63623000 -1.81530000 -0.75048400
H -2.79451000 -1.39722400 -0.89322500
H -2.39316300 -2.64938000 0.31678300
H -0.30513300 -2.85185400 -0.79587800
H -0.59030900 -1.36806300 -1.74059500
C 1.77106500 -1.28890200 -0.25828900
H 1.97085400 -2.35124100 -0.13750100
Cl 2.07800700 -0.82896500 -1.94030500
H 2.40314600 -0.69279200 0.39610200
H -4.70830500 -0.40086500 1.75298100
F -4.16255400 -1.15559000 1.76064200

(FH)–(TEDA)$^{+}$
F 0.98511700 0.73658900 -0.43345500
C 2.86626400 1.11140000 -3.62413000
C 4.20504800 0.66001500 -4.26160700
H 2.85799300 2.19551100 -3.50463000
H 2.02284100 0.82898000 -4.25545300
N 2.69151300 0.48044200 -2.30708400
N 4.77212700 -0.48270000 -3.43305400
H 4.07986600 0.29381400 -5.27880700
H 4.96036900 1.44626700 -4.25599000
C 3.87062600 0.75077000 -1.46611600
C 5.12159800 0.05005900 -2.04718400
H 3.66381900 0.39127400 -0.45760100
H 4.01895000 1.83055000 -1.42099300
H 5.96345600 0.73195900 -2.16444100
H 5.43655200 -0.80853100 -1.45425700
C 2.53187000 -0.97580300 -2.47190000
C 3.71547000 -1.56570500 -3.27586800
H 1.59384600 -1.16881300 -2.99411600
H 2.46694900 -1.42285300 -1.47925200
H 4.19051600 -2.40656300 -2.77008500
H 3.42660400 -1.87266200 -4.27908400
H 1.49159400 0.80416300 -1.25107600
C 6.04228000 -1.02124100 -4.03242600
H 6.43371300 -1.77902100 -3.35732700
Cl 5.79350000 -1.76033500 -5.63175400
H 6.73846300 -0.19202800 -4.13862700

Selectfluor: F–TEDA](BF$_4$)$_2$
C -1.20689500 1.02741900 0.26097800
C 0.10361100 0.39601100 -0.26159100
H -1.05106000 2.03107400 0.65170400
H -1.98839200 1.01086100 -0.49594700
N -1.69047000 0.18462800 1.40299500
N 0.29706100 -0.94915600 0.40243200
H 0.02030300 0.25313100 -1.33693600
H 0.97426900 1.00557600 -0.02429200
C -0.66078900 0.07131800 2.47840500
C 0.52027300 -0.72562800 1.89019700
H -1.11203600 -0.47678400 3.30198800
H -0.38941400 1.08363100 2.77113300
H 1.45220600 -0.17332900 1.99915000

H 0.59317100 -1.70760900 2.35076000
C -2.13627000 -1.16657300 0.93433900
C -0.95036400 -1.78972400 0.17449100
H -2.97633700 -1.00149500 0.26284700
H -2.40036100 -1.74506400 1.81626500
H -0.75652200 -2.79035800 0.54879700
H -1.13972500 -1.80015000 -0.89820700
F -2.80014500 0.82984600 1.95651900
C 1.52010100 -1.68433600 -0.09946500
H 1.56006800 -2.61832400 0.45821300
Cl 1.43661400 -2.02667800 -1.83605800
H 2.38821500 -1.05875500 0.09588500
B -2.43253100 -0.23431900 -2.82407200
F -1.76927200 -1.47774500 -2.77188300
F -1.46598700 0.79627000 -2.76206200
F -3.19718200 -0.12487800 -3.97083300
F -3.26124800 -0.12196000 -1.66788200
B -0.81450700 -3.90522900 2.85307300
F -0.73125800 -4.92292300 3.78097900
F -1.78340300 -4.16700200 1.87155200
F -1.14468300 -2.67452300 3.48620200
F 0.44472100 -3.72751700 2.19800800

[(LH)-AgBF$_4$][F–TEDA](BF$_4$)$_2$
C -0.33312000 -1.10046000 -1.40255000
C 0.94843400 -0.54100100 -0.76000800
H -1.14487100 -0.38607300 -1.29571000
H -0.17634100 -1.33008300 -2.45378600
N -0.68734200 -2.38995600 -0.68691000
N 1.64833200 -1.70288600 -0.12568700
H 1.60812700 -0.11505500 -1.51054200
H 0.73368500 0.17901600 0.02510900
C -0.53272300 -2.14679300 0.81310000
C 0.96486800 -2.09034900 1.14851800
H -0.99091800 -2.96841600 1.35657700
H -1.03405700 -1.20142800 1.01974500
H 1.17941500 -1.31573500 1.88258600
H 1.35462600 -3.05646400 1.46126500
C 0.29497600 -3.44809100 -1.15333500
C 1.71974200 -2.86802100 -1.06692700
H 0.04772000 -3.69245100 -2.18466800
H 0.16900200 -4.31540800 -0.51211600
H 2.40325600 -3.59469700 -0.63161000
H 2.08932000 -2.47833300 -2.01463500
F 2.95559500 -1.31607000 0.17687600
Ag -0.05221000 2.22583700 -3.24219900
O -1.80107800 1.94614000 -4.73084700
C -2.67092600 1.07084500 -4.46797400
N -3.75481000 1.39458000 -3.74093200
C -3.89337200 2.81517400 -3.35587600
C -4.69482800 0.43770300 -3.13105200
C -5.18311500 3.04198200 -2.57542900
H -3.03511200 3.09153300 -2.73560100
C -4.86226200 0.70012200 -1.62932600
H -5.66136400 0.50643800 -3.64337800
C -5.20201500 2.17890900 -1.30735400
H -5.24546100 4.10395200 -2.31848000
H -5.64425800 0.02581300 -1.26630100
H -6.17851200 2.25767300 -0.81996800
C -2.48598000 -0.31155500 -5.01030600
C -1.18163200 -0.82471300 -5.05117700
C -3.53557500 -1.07176700 -5.54497900
C -0.93790600 -2.09831300 -5.55703400
H -0.35305800 -0.22530600 -4.70368300
C -3.28763100 -2.34253900 -6.06581500
H -4.54201200 -0.66958200 -5.57384100
C -1.99211500 -2.86552800 -6.05908100
H 0.07627700 -2.48491600 -5.55189100
H -4.10675900 -2.92132300 -6.48049400
H -1.80570500 -3.85962200 -6.45333600
H -3.85473000 3.42081200 -4.26537000
H -6.04973700 2.82187500 -3.20969500
H -4.45677500 2.57321600 -0.61028800
H -3.93190300 0.42329800 -1.13200900
H -4.31252200 -0.56885000 -3.28175000
B 2.33095700 0.34285800 -4.01119500
F 1.82312700 -0.93090600 -3.65154800
F 2.25602700 1.18917000 -2.85191300
F 3.62893600 0.25366400 -4.45595400
F 1.48361000 0.91921700 -4.98169600
C -2.11355200 -2.83876100 -0.89214100
Cl -2.53155800 -2.98980900 -2.60720300
H -2.20250400 -3.80525200 -0.39969500
H -2.75759200 -2.09080300 -0.43565100
B -0.03397700 -5.36125400 1.87431800
F -0.07426700 -6.61943700 2.43853400
F -0.15675500 -4.34917300 2.84289000
F 1.18929200 -5.16114500 1.17418800
F -1.09713400 -5.20243500 0.93405700
B -1.28031400 2.08877900 -0.30525900
F -0.00461300 2.55014900 -0.73672500
F -2.06886800 3.13404000 0.12845200
F -1.88188900 1.45581100 -1.43530500
F -1.10080500 1.11739300 0.69772100

(*p*-NO$_2$)-5c-s
C 0.87956000 0.21578700 0.88366700
C -0.10363400 0.24953800 -0.30543700
H 1.51740900 1.09587200 0.86457200
H 0.35195200 0.14196800 1.83112600
N 1.78408000 -0.99818700 0.76302100
N 0.24958800 -0.88958000 -1.21247000

H -1.13700300 0.09595300 -0.00099800
H -0.00281500 1.17415300 -0.87128200
C 2.59927900 -0.88254900 -0.51748000
C 1.65010300 -0.79307200 -1.73234000
H 3.24304600 -1.75805500 -0.57906900
H 3.19124200 0.02683500 -0.44757500
H 1.74904100 0.15868900 -2.25129000
H 1.78548500 -1.62143900 -2.42431600
C 0.93939600 -2.25660500 0.70383200
C 0.01660200 -2.20579100 -0.53659800
H 0.36015000 -2.30665400 1.62246100
H 1.61642400 -3.10768100 0.65467100
H 0.24865000 -2.98459500 -1.25992500
H -1.03720400 -2.24697500 -0.26835900
F -0.61015500 -0.83003000 -2.31269100
Ag -0.32728000 2.20991300 -3.86817500
O -1.82670500 1.45890200 -5.33333100
C -1.57605500 1.07624800 -6.50872200
N -0.70007100 0.09610800 -6.76651600
C -0.08446600 -0.60134500 -5.62242400
C -0.14603100 -0.19800800 -8.10703300
C 0.60706500 -1.87933500 -6.08640200
H 0.64501100 0.06698100 -5.13851600
C 1.36808600 -0.38219700 -7.99776500
H -0.61804800 -1.09996400 -8.51104800
C 1.73352100 -1.58168000 -7.09450400
H 0.99566000 -2.40397100 -5.20890500
H 1.77793100 -0.50847800 -9.00347400
H 1.91733500 -2.47345100 -7.70087200
C -2.33222500 1.72519900 -7.62296200
C -2.45133900 3.12204000 -7.61110500
C -2.99153200 0.97065000 -8.60284400
C -3.19564900 3.76894900 -8.59005700
H -1.95487900 3.69498700 -6.83658600
C -3.75468000 1.60533000 -9.57732300
H -2.92494400 -0.11110400 -8.59636700
C -3.83567700 2.99538000 -9.55660800
H -3.29016500 4.84639500 -8.61173200
H -4.28029600 1.04482200 -10.33871400
H -0.86936400 -0.81048000 -4.89442700
H -0.14439100 -2.53763900 -6.53547400
H 2.66433800 -1.36372200 -6.56150900
H 1.79401400 0.54380400 -7.59624800
H -0.38545900 0.63142800 -8.76972700
B 1.94975300 2.81619800 -1.92217000
F 2.42644000 2.05908000 -0.83581000
F 0.53049300 2.99354600 -1.74504300
F 2.58440000 4.01752900 -2.04143200
F 2.07976300 2.02789500 -3.10806900
C 2.77304900 -1.04945800 1.91589400
Cl 1.97251200 -1.22369600 3.48474600
H 3.42421300 -1.90461100 1.75068200
H 3.33381300 -0.11750100 1.90113200
N -4.63157700 3.67162100 -10.58966800
O -4.69210900 4.90054400 -10.55562800
O -5.19360300 2.97200800 -11.43216000

(*p*-NO_2)-5c-t

C 1.08228800 0.42392900 0.75453900
C 0.17155300 0.68610000 -0.46806200
H 1.54758400 1.34248700 1.11068000
H 0.54796500 -0.04817500 1.57608600
N 2.18970700 -0.53139600 0.33852700
N 0.42861900 -0.36572700 -1.48448500
H -0.87488400 0.64610300 -0.16580100
H 0.37363700 1.65072000 -0.92965100
C 2.80818300 -0.01154400 -0.95101600
C 1.76924600 -0.15470400 -2.08685000
H 3.70675800 -0.59320900 -1.15499200
H 3.08316900 1.02782600 -0.77457300
H 1.75220300 0.75703700 -2.68117700
H 1.98829700 -1.00816300 -2.72758300
C 1.58514800 -1.89764200 0.05901000
C 0.36054200 -1.71193000 -0.86289900
H 1.30511500 -2.34164400 1.01231200
H 2.36873700 -2.49883800 -0.40203000
H 0.34278900 -2.45401800 -1.65988100
H -0.57362100 -1.77578500 -0.30486300
F -0.75221000 -2.22010400 -3.53750200
Ag -1.09289400 -0.25248300 -3.14055800
O -2.38543800 0.06303800 -5.08409300
C -1.85890300 0.35805100 -6.15223300
N -0.85849300 -0.54431300 -6.67742600
C -1.02551200 -1.96874100 -6.46791500
C 0.40396900 -0.06348400 -7.18914800
C 0.23898200 -2.73969900 -6.79025500
H -1.28138700 -2.10735500 -5.39682800
C 1.58424600 -0.63242900 -6.33573300
H 0.50570100 -0.45497700 -8.21095200
C 1.40027300 -2.12207400 -5.98859000
H 0.07330300 -3.78146000 -6.50725100
H 2.47874200 -0.46028100 -6.93841100
H 2.32128500 -2.67658400 -6.17830000
C -2.19001200 1.55478500 -6.92342500
C -2.73374400 2.64221800 -6.21535100
C -2.02112900 1.61410100 -8.31864600
C -3.08752600 3.79680600 -6.89750200
H -2.84076300 2.58206800 -5.14066300
C -2.39053000 2.76195500 -9.00649600
H -1.63459900 0.76602300 -8.87081700
C -2.90967400 3.83044500 -8.27902800
H -3.48851900 4.65868300 -6.38176200

H -2.28468300 2.83752500 -10.08000400
H -1.91249900 -2.28968400 -7.03735900
H 0.45316600 -2.72934000 -7.86500600
H 1.14406200 -2.22807900 -4.93066400
H 1.64570900 -0.01085400 -5.44264700
H 0.40845100 1.02230100 -7.20387000
B -0.18053400 2.59272600 -3.70857500
F 0.87405300 2.79357000 -2.82710300
F -1.27676400 1.97617700 -2.94604900
F -0.64032800 3.73627400 -4.29525400
F 0.18516200 1.61324500 -4.67262300
C 3.28667600 -0.60942700 1.37240100
Cl 2.67894800 -1.08128100 2.97238900
H 4.00550300 -1.35381600 1.03739300
H 3.74580900 0.37424000 1.44452600
N -3.28851400 5.05752700 -9.00792000
O -3.76039500 5.98359200 -8.35333900
O -3.10779600 5.07475800 -10.22301200

(*p*-NO_2)-6c-s
C 0.97015400 0.83136300 0.76388700
C 0.12646200 0.78680700 -0.53266400
H 1.59831900 1.72062800 0.81712500
H 0.36025800 0.77430200 1.66319300
N 1.89260600 -0.37618100 0.78275500
N 0.25815300 -0.53462200 -1.19304800
H -0.92349500 0.95885400 -0.29516300
H 0.45497800 1.54595100 -1.24008400
C 2.65393600 -0.41871600 -0.53591200
C 1.64928300 -0.68498200 -1.68141400
H 3.40629000 -1.20303100 -0.45453100
H 3.15124500 0.54578000 -0.63905500
H 1.81237500 0.02921600 -2.48557400
H 1.75753100 -1.69278200 -2.08185700
C 1.05545300 -1.63707100 0.89312400
C -0.02908600 -1.60219100 -0.21030400
H 0.62647200 -1.66073100 1.89312300
H 1.74204700 -2.47620200 0.77942100
H -0.05744500 -2.56205100 -0.72664600
H -1.01388300 -1.41276200 0.21825900
F 0.35535900 -2.67633200 -3.93666800
Ag -1.18452000 -0.63940700 -3.04732600
O -2.24711500 -0.19899000 -5.22736600
C -1.75116800 0.27798200 -6.22670200
N -0.60138100 -0.41100400 -6.83752700
C -0.51853900 -1.69683800 -6.68991000
C 0.48861300 0.40844100 -7.46302000
C 0.62750800 -2.51146500 -7.12612900
C 1.81873600 -0.32101200 -7.34392800
H 0.21416400 0.57586000 -8.50581300
C 1.70410300 -1.74310300 -7.89637800
H 1.00821600 -2.93053000 -6.18054300
H 2.56604500 0.25552800 -7.89429600
H 1.44141900 -1.70906700 -8.95852600
C -2.21657800 1.50953200 -6.88059700
C -2.62242000 2.56833600 -6.05206700
C -2.32039400 1.60249100 -8.27756500
C -3.11597700 3.73345500 -6.62356600
H -2.49970600 2.48284600 -4.98008200
C -2.83567600 2.75845700 -8.85114100
H -2.04027800 0.77155900 -8.91446700
C -3.21505800 3.80244900 -8.01131200
H -3.41814000 4.57686700 -6.01755200
H -2.94486400 2.85788200 -9.92246600
H -1.34984600 -2.17009600 -6.17479200
H 0.23342200 -3.37812600 -7.67149800
H 2.65524700 -2.27285600 -7.81454700
H 2.11426300 -0.33409100 -6.29048400
H 0.49753600 1.35949100 -6.93371800
B 0.39867300 1.89755300 -4.08263800
F 1.37717800 2.27346200 -3.16710400
F -0.87794700 1.91417900 -3.45144300
F 0.38022000 2.71009300 -5.20921200
F 0.64189400 0.54456600 -4.49172300
C 2.91195900 -0.28805300 1.88631900
Cl 2.17148000 -0.13680400 3.49649400
H 3.50911500 -1.19709900 1.86331400
H 3.52657700 0.59035500 1.70179200
H -0.08555200 -3.46142500 -3.69493100
N -3.74520200 5.03627400 -8.61988400
O -4.08061700 5.94585800 -7.86432900
O -3.81979300 5.08086200 -9.84611000

(*p*-NO_2)-6c-t
C 0.79374900 0.61651200 0.80412100
C 0.05530400 0.80332700 -0.54329800
H 1.27865800 1.53923600 1.12011700
H 0.13357100 0.26906000 1.59560700
N 1.86941500 -0.44074600 0.62247800
N 0.35526700 -0.36379900 -1.41263800
H -1.01982800 0.85664100 -0.37286400
H 0.38262700 1.69936000 -1.06449700
C 2.67073400 -0.09767900 -0.62559100
C 1.77054200 -0.30715200 -1.86508800
H 3.54529800 -0.74586400 -0.65699500
H 2.99053900 0.93889100 -0.52289500
H 1.89296100 0.53065100 -2.54833800
H 1.99549400 -1.23720500 -2.38480300
C 1.20190900 -1.78668900 0.41251100
C 0.11177300 -1.62807000 -0.67422800
H 0.77126700 -2.10195200 1.36080400
H 1.98302100 -2.48741400 0.11971900

H 0.15608400 -2.46525700 -1.37037000
H -0.88565200 -1.58050100 -0.23817400
F 0.24604200 -2.33051900 -3.77428900
Ag -0.92977400 -0.31913500 -3.23702000
O -2.18854300 -0.12801300 -5.00624100
C -1.65922200 0.22249200 -6.10838500
N -0.74358600 -0.58592400 -6.71717200
C -0.65080700 -1.92622500 -6.37422000
C 0.30703600 -0.05408400 -7.62702100
C 0.33448200 -2.74412700 -7.14336500
C 1.66819200 -0.56309700 -7.14779000
H 0.09065300 -0.38950500 -8.64510900
C 1.74523000 -2.10603800 -7.15077100
H 0.35404000 -3.76304800 -6.75076900
H 2.43586700 -0.13078600 -7.79420700
H 2.28455200 -2.46717900 -8.02929100
C -2.12185500 1.46642300 -6.74278900
C -2.49918600 2.53465300 -5.90676100
C -2.27858100 1.56760900 -8.13800800
C -2.98098700 3.71219400 -6.46162200
H -2.38363300 2.44291400 -4.83600200
C -2.77014800 2.73797600 -8.69710200
H -2.04078200 0.72933300 -8.78114300
C -3.10471400 3.79218700 -7.84621900
H -3.25628900 4.55658400 -5.84438200
H -2.90310600 2.84266800 -9.76530600
H -1.55726600 -2.34949400 -5.95037000
H -0.03064900 -2.82655300 -8.18038300
H 2.30113200 -2.44456300 -6.27190700
H 1.82770700 -0.16460500 -6.14269700
H 0.26294300 1.03174900 -7.59621800
B 0.31246100 2.39573400 -3.81520400
F 1.28629100 2.63760600 -2.85074700
F -0.92421800 2.05344600 -3.12351100
F 0.10233700 3.44748400 -4.65931100
F 0.65575700 1.20758600 -4.53631300
C 2.83182900 -0.47512400 1.78718600
Cl 2.01042400 -0.75126200 3.33557300
H 3.53481100 -1.28637700 1.61052800
H 3.34090000 0.48558900 1.82268600
H 0.08899000 -2.27403500 -4.72436300
N -3.61760100 5.03871200 -8.43874400
O -3.90888000 5.95661500 -7.67424400
O -3.72295500 5.08753400 -9.66307900

(*p*-NO_2)-10c-s

N -2.07395200 1.29726000 0.83264500
C -1.17371500 1.76904400 -0.20736400
C -1.31601700 3.28268200 -0.39594600
C -2.77541100 3.70643200 -0.19302500
C -3.20226500 3.46102700 1.26953700
C -2.41759300 2.28280400 1.87224000
H -0.67023900 3.79062700 0.32949600
H -2.90652600 4.75742400 -0.46115900
H -3.00467700 4.34693100 1.88075100
H -2.96305400 1.78608300 2.67123700
H -4.27818700 3.27123000 1.32158300
H -1.47111500 2.62908700 2.29868800
H -3.41119400 3.12525600 -0.87051500
H -0.95483000 3.54533200 -1.39439000
H -1.43657300 1.23300600 -1.12336300
C -2.44003100 -0.00675300 0.83092900
O -1.89395200 -0.85125200 0.08911500
C -3.55770400 -0.45650400 1.71681400
C -4.79613300 0.19944700 1.72524500
C -3.37121600 -1.62216400 2.47185800
C -5.84193900 -0.29406900 2.49791600
H -4.95122200 1.08138600 1.11499000
C -4.40279900 -2.11463600 3.26230400
H -2.41592200 -2.13330300 2.44113500
C -5.62154000 -1.43892700 3.25962300
H -6.80964700 0.18899900 2.51543600
H -4.27975500 -3.00338600 3.86667000
Ag 0.44401200 -1.02616400 0.05724900
B 3.41668000 -1.90793100 0.00445000
F 4.28627700 -2.13233600 -1.08464800
F 3.05399900 -0.51270600 -0.01530100
F 2.21286000 -2.63032100 -0.20274700
F 4.00116200 -2.23334300 1.19867400
O 0.16922800 1.41388800 0.18141300
H 0.78303400 1.86369300 -0.41662900
C 4.21191900 2.28890200 -3.90280600
C 5.51604300 1.49343700 -4.12925000
H 4.40841400 3.33957000 -3.69797500
H 3.50669000 2.19508300 -4.72633500
N 3.55161900 1.70922700 -2.68776200
N 5.45415400 0.21074600 -3.32223800
H 5.62611500 1.23355100 -5.18000500
H 6.39448100 2.04528200 -3.79700100
C 4.49605300 1.66163800 -1.52494100
C 5.52715700 0.55987200 -1.84088700
H 3.91481700 1.38848900 -0.64651600
H 4.93371800 2.65234600 -1.42171600
H 6.53599000 0.90505400 -1.62256300
H 5.30566700 -0.35619500 -1.29709600
C 2.99213000 0.34762700 -2.97294400
C 4.12945800 -0.48651400 -3.59252600
H 2.15695300 0.47510000 -3.65842900
H 2.66783100 -0.05663400 -2.01716000
H 4.16460500 -1.46214000 -3.11225400
H 4.02941800 -0.59195200 -4.66958700
F 2.48740800 2.54611500 -2.34313200

C 6.62306400 -0.70921200 -3.61796300
H 6.53221300 -1.55899900 -2.94421700
Cl 6.61857900 -1.28070100 -5.29312900
H 7.53764000 -0.15039400 -3.43221600
N -6.71883500 -1.95772300 4.08760100
O -6.50577300 -2.96926100 4.75558300
O -7.78991200 -1.35151200 4.06773200

(*p*-NO_2)-10c-t
N -1.78070300 1.85776800 0.06804700
C -1.44060200 2.65322200 -1.16075900
C -1.43358400 4.14003900 -0.81855800
C -2.49112200 4.44855500 0.24742000
C -2.13599600 3.75899100 1.57903100
C -1.36192300 2.43079500 1.33195100
H -0.43390500 4.40914500 -0.46286500
H -2.57481900 5.52676600 0.39531700
H -1.48748500 4.39002000 2.19110700
H -1.47352900 1.70400400 2.13175500
H -3.03483600 3.54109300 2.16052000
H -0.29429800 2.65387400 1.21643300
H -3.46980400 4.10005200 -0.10252500
H -1.61301800 4.69942100 -1.73906200
H -2.18256300 2.39432700 -1.91633400
C -2.35718800 0.57618600 -0.08362900
O -2.44566300 0.11877100 -1.22058700
C -2.86962300 -0.12047400 1.12351400
C -3.84538300 0.49542200 1.92200500
C -2.43239900 -1.42499100 1.39666200
C -4.39233400 -0.19341200 2.99822800
H -4.20155300 1.49265200 1.69074300
C -2.96490600 -2.10911500 2.48464600
H -1.66016300 -1.89115700 0.79711100
C -3.93614300 -1.48237300 3.25972200
H -5.15589200 0.24970500 3.62311200
H -2.63957700 -3.11074500 2.73224400
Ag -1.10155700 -1.56124600 -2.33595900
B 0.93464600 -3.49013100 -0.94842500
F 2.28720800 -3.11367500 -0.87151000
F 0.15561100 -2.49018100 -0.27166600
F 0.53055700 -3.42894200 -2.32208900
F 0.70492700 -4.72980100 -0.41987900
O -0.16856100 2.17237100 -1.46393500
H -0.18508900 1.38754600 -2.12529300
C 2.83756400 1.35318300 -2.74362300
C 4.30753300 1.14652600 -2.25443900
H 2.37522200 2.21003100 -2.25565100
H 2.79330600 1.47431600 -3.82422000
N 2.12634000 0.14213800 -2.36432100
N 4.43732900 -0.24680000 -1.65079600
H 5.01618500 1.21545700 -3.07655200
H 4.57858400 1.85905200 -1.47666000
C 2.05427500 -0.03066500 -0.91917000
C 3.49955300 -0.36560100 -0.45190300
H 1.38203100 -0.84664400 -0.66754600
H 1.69195000 0.89764200 -0.48176500
H 3.84799000 0.32478500 0.31426300
H 3.55612500 -1.39380300 -0.10072100
C 2.56423300 -1.02580200 -3.11601900
C 4.03152200 -1.29979200 -2.67491100
H 2.50371300 -0.79486900 -4.17786800
H 1.93693500 -1.88168300 -2.88395800
H 4.10776900 -2.26790500 -2.18347400
H 4.72841600 -1.23667700 -3.50689400
F 0.09181900 0.29723900 -3.00495200
C 5.83895700 -0.49445600 -1.14048900
H 5.85323600 -1.48545700 -0.69276700
Cl 7.05701400 -0.42715700 -2.42972800
H 6.06510300 0.27353100 -0.40429700
N -4.50544700 -2.21233400 4.40567000
O -4.09381300 -3.35094400 4.61810500
O -5.35782200 -1.63857600 5.08067400

(*p*-NO_2)-11c-s
C 1.38818100 1.36289900 1.37907800
C 0.28023500 2.10697200 0.60001400
H 2.11468400 2.04564300 1.81927500
H 0.96379900 0.73397800 2.15917600
N 2.14775500 0.47163800 0.41344300
N 0.59659800 2.03907000 -0.85654300
H -0.70413000 1.66133200 0.73547500
H 0.25389400 3.15311500 0.90423900
C 2.94425900 1.35436900 -0.53204900
C 2.01181500 2.45660400 -1.08338800
H 3.33524600 0.71001400 -1.31814100
H 3.77372900 1.79220200 0.02239100
H 2.17674700 3.40575500 -0.58081800
H 2.18338300 2.59275500 -2.14973100
C 1.15325300 -0.31978400 -0.41394100
C 0.40115900 0.65135000 -1.35383200
H 0.48010400 -0.81776700 0.28007000
H 1.70351900 -1.07032500 -0.98023400
H 0.76783300 0.60149300 -2.37768500
H -0.65709300 0.41122000 -1.33097900
Ag -0.67016800 3.47561800 -1.89110600
O -1.73534600 4.89096600 -2.98767200
C -1.83911300 4.66434200 -4.24695000
N -2.12093200 3.43999000 -4.69813200
C -2.66141500 2.48311100 -3.71589400
C -1.79507500 2.95432700 -6.06250500
C -3.19652800 1.23478300 -4.45757700
O -1.68674600 2.01427100 -2.82127500

C -1.15005700 1.57640000 -5.93916600
H -2.71018500 2.91374400 -6.66035700
C -2.12457200 0.55190800 -5.31686600
H -3.62156600 0.55981300 -3.71319200
H -0.82673400 1.25548900 -6.93214500
H -2.63649100 -0.00831600 -6.10447200
C -1.67026200 5.82982200 -5.13376600
C -0.71966900 6.80365400 -4.77939600
C -2.49083100 5.99642300 -6.26280100
C -0.55834500 7.92467800 -5.58435200
H -0.11183500 6.67877800 -3.89343400
C -2.33858800 7.12152500 -7.06119800
H -3.25409100 5.26688600 -6.50331000
C -1.36892600 8.05914300 -6.70794700
H 0.17323200 8.68627500 -5.35033800
H -2.95388000 7.28202400 -7.93602500
H -4.02672300 1.60821600 -5.06794800
H -1.56584600 -0.17055300 -4.71829300
H -0.25268800 1.67218100 -5.31962500
H -1.11731900 3.67335300 -6.52038800
B 1.36066100 5.68922900 -1.70384000
F 2.57070000 5.57846300 -1.07223400
F 0.34866700 5.01457000 -0.79809900
F 0.93206100 6.96835200 -1.91649700
F 1.30209000 4.90849500 -2.87572200
C 3.12316200 -0.42668900 1.13980900
Cl 2.30413800 -1.60651600 2.18067200
H 3.70456600 -0.95784700 0.38915800
H 3.75876000 0.20683600 1.75425800
H -3.46926000 2.98598700 -3.17678700
F -2.52309300 1.13962600 -0.54978500
H -2.39719100 1.42029900 -1.45023600
N -1.20354500 9.25302800 -7.55871900
O -0.35450100 10.07616900 -7.22521800
O -1.92494400 9.34999500 -8.54903600

(*p*-NO_2)-11c-t

C 1.84418100 1.65770700 1.30736800
C 0.74077300 2.47621400 0.60033000
H 2.79759000 2.18467200 1.33586100
H 1.55387900 1.38351300 2.31959100
N 2.07480200 0.37785500 0.52344400
N 0.54923700 1.94865200 -0.77691400
H -0.21364000 2.40302000 1.12166400
H 1.03091800 3.52336900 0.53500800
C 2.70248800 0.74299700 -0.81426200
C 1.86600900 1.87095600 -1.46286900
H 2.71646700 -0.16477100 -1.41638200
H 3.72573800 1.06747900 -0.62724000
H 2.35564500 2.83870900 -1.36983900
H 1.71063500 1.65345800 -2.51916700
C 0.73587700 -0.28790900 0.25815200
C -0.07116500 0.60061000 -0.71699400
H 0.23884800 -0.40174600 1.21915400
H 0.93140100 -1.27373800 -0.16235400
H -0.07492600 0.18398600 -1.72399500
H -1.09783700 0.70729700 -0.37114600
Ag -0.77831800 3.35736900 -1.88639700
O -2.03722700 4.72365900 -3.04475200
C -2.04449400 4.58033100 -4.29945500
N -2.24735700 3.38045000 -4.88846100
C -2.82908400 2.26710200 -4.12479500
C -1.93733800 3.09702300 -6.30470900
C -2.46833100 0.87033400 -4.82662800
O -2.46289400 2.17004900 -2.84295600
C -0.83222400 2.02843300 -6.38506000
H -2.85559200 2.76171200 -6.79243900
C -1.02878700 0.92753700 -5.32479300
H -2.63004600 0.09495500 -4.07848300
H -0.86103400 1.61147000 -7.39508000
H -0.78301500 -0.05568400 -5.73925300
C -1.86196300 5.81295400 -5.10745600
C -0.81482000 6.67886400 -4.75536200
C -2.76809000 6.14782800 -6.12585300
C -0.64819700 7.86768000 -5.45661200
H -0.12851400 6.41954100 -3.95950800
C -2.61508500 7.34456400 -6.81443300
H -3.59517200 5.48987500 -6.36652800
C -1.55160300 8.17641300 -6.46979400
H 0.15884400 8.54934600 -5.22385800
H -3.29861200 7.63627300 -7.60022500
H -3.19482300 0.73129300 -5.63016200
H -0.36112800 1.08942500 -4.47418100
H 0.14066600 2.50777400 -6.25373100
H -1.62077700 4.01730100 -6.78590000
B 1.40926600 5.40335200 -1.82217300
F 2.59807200 5.00684200 -1.23525300
F 0.33027300 5.14325700 -0.87694600
F 1.38176900 6.71938100 -2.20603800
F 1.11981600 4.55331800 -2.93876800
C 3.03052800 -0.54775500 1.23798200
Cl 2.37516900 -1.14358300 2.77624400
H 3.22018100 -1.39587100 0.58361200
H 3.94417500 0.00808100 1.43637200
H -3.93116800 2.35865100 -4.18955800
F -2.71960800 2.20331100 -0.25050900
H -3.09209100 1.99486900 -1.08730900
N -1.38122700 9.44097500 -7.20705000
O -0.44089500 10.16530700 -6.88776900
O -2.18962400 9.69504200 -8.09796600

(*p*-NH_2)-5c-s

C 0.89544500 0.22975500 0.85330300
C -0.09479500 0.25206000 -0.33015200
H 1.53131700 1.11100100 0.82360300
H 0.37370200 0.16199000 1.80445700
N 1.80201300 -0.98309400 0.73660900
N 0.25664800 -0.89221600 -1.23120800
H -1.12587600 0.09756100 -0.01848300
H 0.00005600 1.17282500 -0.90324600
C 2.60982100 -0.87561900 -0.54925500
C 1.65399500 -0.79479400 -1.75936300
H 3.25394300 -1.75103100 -0.60813900
H 3.20131800 0.03474400 -0.48881200
H 1.74816300 0.15468300 -2.28352500
H 1.78748800 -1.62620200 -2.44821200
C 0.95966500 -2.24369700 0.69150500
C 0.03151200 -2.20444100 -0.54526700
H 0.38462400 -2.28723900 1.61304300
H 1.63799000 -3.09393800 0.64619500
H 0.26308500 -2.98727000 -1.26438800
H -1.02100200 -2.24744000 -0.27224700
F -0.60928700 -0.84317300 -2.32671200
Ag -0.34908300 2.18983800 -3.89600800
O -1.84852600 1.46285800 -5.34495600
C -1.59733300 1.08798200 -6.53112900
N -0.71908300 0.08934200 -6.76000500
C -0.17027500 -0.63052700 -5.59972100
C -0.07525000 -0.17113900 -8.06485500
C 0.49345100 -1.93064100 -6.04349400
H 0.56750000 0.00462200 -5.08335300
C 1.42091400 -0.41140200 -7.85754400
H -0.53659000 -1.04123000 -8.54579300
C 1.68050400 -1.66226900 -6.98951600
H 0.81622200 -2.48178000 -5.15526000
H 1.90057000 -0.50674700 -8.83569500
H 1.84236400 -2.53895800 -7.62399000
C -2.31831800 1.73796600 -7.64253700
C -2.62461500 3.10631600 -7.52850000
C -2.80332200 1.03882900 -8.76200000
C -3.34603700 3.76344000 -8.50963500
H -2.27938300 3.65084100 -6.65611600
C -3.54493700 1.68195700 -9.73997300
H -2.63038300 -0.02772400 -8.85348600
C -3.82076100 3.06277500 -9.64075000
H -3.55513300 4.82483500 -8.41443500
H -3.92440600 1.12180900 -10.58921000
H -0.98644000 -0.81453000 -4.89989400
H -0.25935800 -2.55209700 -6.54062200
H 2.59771000 -1.51790100 -6.40950100
H 1.84667600 0.47928700 -7.38207400
H -0.24287400 0.69196100 -8.70696600
B 1.95012100 2.81180900 -1.97099600
F 2.43415500 2.06460000 -0.88039300
F 0.52935600 2.98078900 -1.79001500
F 2.57503200 4.01801600 -2.09616700
F 2.08316900 2.01940000 -3.15142600
C 2.79778100 -1.02277500 1.88377100
Cl 2.00711500 -1.18770800 3.45877600
H 3.45078100 -1.87704100 1.72118200
H 3.35537900 -0.08913500 1.85879500
N -4.49733200 3.71917300 -10.64078300
H -4.91255500 4.61121500 -10.41407600
H -5.04778200 3.15995500 -11.27622400

(*p*-NH_2)-5c-t

C 1.09065600 0.65307500 0.73320200
C 0.33817900 0.92590800 -0.59134000
H 1.80877600 1.44041000 0.96079500
H 0.41565900 0.53171200 1.57756400
N 1.86254100 -0.65022400 0.59626200
N 0.30054600 -0.32295100 -1.38997900
H -0.68224000 1.24426900 -0.37950000
H 0.83112400 1.69056200 -1.18626600
C 2.65713200 -0.59947700 -0.70169400
C 1.66515600 -0.63696100 -1.88410100
H 3.33709000 -1.45068800 -0.71526500
H 3.23507300 0.32419800 -0.68057100
H 1.95059800 0.11316000 -2.62064600
H 1.61768700 -1.61600300 -2.36026700
C 0.87356400 -1.79966400 0.50511300
C -0.19362700 -1.44245900 -0.54974000
H 0.43664400 -1.94166600 1.49174000
H 1.44920400 -2.68585400 0.23716300
H -0.39726900 -2.28420200 -1.21046600
H -1.12397900 -1.12121700 -0.08063500
F -0.73079800 -2.25306500 -3.25759600
Ag -0.93927000 -0.21009800 -3.26655200
O -2.14595800 -0.13175800 -5.12918400
C -1.62236700 0.14705600 -6.24856600
N -0.76595200 -0.64559300 -6.88720600
C -0.45829200 -1.99749500 -6.36267500
C 0.07658600 -0.21787000 -8.01615000
C 0.99121800 -2.39347900 -6.67162500
H -0.62865900 -2.01184900 -5.28680100
C 1.54288300 -0.09111700 -7.55422600
H -0.02700400 -0.97125100 -8.80146400
C 1.90730200 -1.17606000 -6.51816000
H 1.27294300 -3.19222000 -5.97966400
H 2.17140100 -0.17106400 -8.44656800
H 2.95626100 -1.46581100 -6.62315100
C -2.10927300 1.41029800 -6.88501300
C -2.17608200 2.58044800 -6.08840800
C -2.63369300 1.41085600 -8.20248000

C -2.68703900 3.74102700 -6.60832800
H -1.81663800 2.55399200 -5.06986500
C -3.16809000 2.55557000 -8.73710700
H -2.62544400 0.49800100 -8.78644700
C -3.19420300 3.75525000 -7.94946500
H -2.71730600 4.65105100 -6.01988500
H -3.57468800 2.56641500 -9.74206700
H -1.17206700 -2.69205500 -6.82194500
H 1.07838500 -2.80579200 -7.68284700
H 1.78295300 -0.76285200 -5.51236100
H 1.69602500 0.89970900 -7.12228500
H -0.27943500 0.73037200 -8.41055300
B 0.57212900 2.37839000 -3.96734700
F 1.63046100 2.38097000 -3.06269000
F -0.65852000 2.09199100 -3.21797000
F 0.41281800 3.57472900 -4.61857200
F 0.70977400 1.30077500 -4.86746000
C 2.84317900 -0.85243000 1.72216400
Cl 2.06859200 -0.79327100 3.32064700
H 3.29970200 -1.83140300 1.59233900
H 3.58748500 -0.06112700 1.66411300
N -3.69767500 4.87580300 -8.45804500
H -3.73091000 5.73263500 -7.91637500
H -4.06824800 4.91316400 -9.40126200

(*p*-NH$_2$)-10c-s
N -2.04615400 1.30118600 0.83662600
C -1.16055700 1.74487200 -0.21980400
C -1.34392200 3.24446800 -0.48940200
C -2.80028200 3.65581500 -0.24647300
C -3.15259200 3.48485800 1.24479700
C -2.35475000 2.31696000 1.85534300
H -0.68152700 3.80509400 0.18062900
H -2.96377600 4.68805300 -0.56610700
H -2.90629300 4.39452800 1.80167400
H -2.87588200 1.84464500 2.68442200
H -4.22815800 3.32279300 1.36095000
H -1.39480400 2.67615100 2.24100000
H -3.45499200 3.02606900 -0.85953500
H -1.02837700 3.45901100 -1.51462500
H -1.39768700 1.15346400 -1.10786500
C -2.40059600 -0.01693100 0.88788200
O -1.79536900 -0.86803400 0.18805300
C -3.51945100 -0.45199200 1.74399800
C -4.70973700 0.28191900 1.89070600
C -3.43340600 -1.71309100 2.36121200
C -5.76410800 -0.21006800 2.64224800
H -4.82948800 1.22913400 1.37737200
C -4.47149500 -2.20469100 3.13267000
H -2.52983900 -2.29957700 2.23288000
C -5.66157100 -1.45974100 3.29179100
H -6.68196100 0.36328500 2.72944800
H -4.37879200 -3.17072400 3.61992100
Ag 0.51157600 -0.97927900 0.17790100
B 3.48313300 -1.86230900 0.09286300
F 4.32252600 -2.10638400 -1.01662900
F 3.09968200 -0.47267900 0.04139500
F 2.28611200 -2.60626300 -0.05206800
F 4.11266600 -2.13999100 1.27666900
O 0.19924800 1.45975700 0.18563900
H 0.79485600 1.91519900 -0.42595200
C 4.15699100 2.26977900 -3.91181900
C 5.46686000 1.48262300 -4.13569600
H 4.34513700 3.32525500 -3.72383200
H 3.44709800 2.15688700 -4.72864700
N 3.50972900 1.70242400 -2.68394200
N 5.42441100 0.21417200 -3.30574700
H 5.57081600 1.20495100 -5.18245300
H 6.34273200 2.04896900 -3.82157300
C 4.46274700 1.68524100 -1.52728100
C 5.50289900 0.58936500 -1.83123400
H 3.89257100 1.42001900 -0.63957500
H 4.89001700 2.68236000 -1.44513600
H 6.50957200 0.94739000 -1.62421500
H 5.29342500 -0.31963400 -1.27143800
C 2.96213400 0.33120200 -2.94630800
C 4.10576700 -0.50216200 -3.55560700
H 2.12452500 0.44080700 -3.63195300
H 2.64140700 -0.06246700 -1.98505100
H 4.15435700 -1.46841200 -3.05760900
H 4.00113500 -0.62854100 -4.63013600
F 2.43864300 2.53421000 -2.34696700
C 6.60141500 -0.69831000 -3.59144000
H 6.52204700 -1.53751800 -2.90298800
Cl 6.59569300 -1.29764900 -5.25685500
H 7.51096000 -0.12698800 -3.41906100
N -6.67737700 -1.92156400 4.09236200
H -6.69223500 -2.90804900 4.30698500
H -7.59227900 -1.51194900 3.97169200

(*p*-NH$_2$)-10c-t
N -1.66395100 1.78825000 0.09917000
C -1.30068900 2.60428200 -1.09623100
C -1.28205300 4.08090000 -0.68939400
C -2.35706000 4.38309000 0.35912400
C -2.04938400 3.64566200 1.68044500
C -1.27698600 2.34439700 1.40199700
H -0.28577200 4.31489900 -0.29672800
H -2.43094600 5.45956400 0.53258200
H -1.43767400 4.27061900 2.33835400
H -1.43122800 1.59579700 2.17931100
H -2.97715900 3.42728700 2.21801800

H -0.20052300 2.53353800 1.35321000
H -3.33070600 4.05986100 -0.02743600
H -1.41742500 4.68212100 -1.59181300
H -2.09405500 2.41142600 -1.82399300
C -2.31362500 0.63396500 -0.06050200
O -2.56947000 0.11922100 -1.17221400
C -2.85829700 -0.08354100 1.14108600
C -3.98979800 0.44960000 1.80759100
C -2.33162500 -1.34527700 1.51439500
C -4.57577000 -0.23779600 2.84037100
H -4.39353100 1.40643400 1.49698400
C -2.89668000 -2.04426400 2.55093000
H -1.47054800 -1.75009900 0.99571400
C -4.03608700 -1.50687500 3.23568200
H -5.43778400 0.16249200 3.36230700
H -2.49531200 -3.00212300 2.86293000
Ag -1.16403300 -1.48899400 -2.22635900
B 0.89638200 -3.43113200 -0.80287400
F 2.25786200 -3.08087900 -0.77726300
F 0.16054600 -2.40792400 -0.11894300
F 0.44446300 -3.39929900 -2.16007600
F 0.66485300 -4.65800300 -0.23679100
O -0.04964300 2.25316100 -1.60840900
H -0.12834400 1.47950000 -2.22034700
C 2.78020300 1.29395200 -2.89300700
C 4.24981600 1.14814000 -2.39180400
H 2.29541400 2.16843400 -2.46064500
H 2.73696800 1.34920300 -3.97942400
N 2.07966000 0.09848100 -2.44769400
N 4.40356800 -0.19934900 -1.69440000
H 4.96204200 1.17219000 -3.21349800
H 4.50991300 1.91500000 -1.66318200
C 2.01301200 0.01827100 -0.99256900
C 3.45822200 -0.25540000 -0.49555000
H 1.35719300 -0.79252200 -0.68833200
H 1.61877700 0.96410200 -0.62524600
H 3.79288600 0.48979900 0.22450100
H 3.53701800 -1.25645000 -0.07555300
C 2.55700000 -1.10681200 -3.11245000
C 4.02307100 -1.32637900 -2.64768000
H 2.50141900 -0.94852300 -4.18784300
H 1.93797900 -1.95354700 -2.83077400
H 4.11685800 -2.25753400 -2.09185500
H 4.72740700 -1.30710700 -3.47590800
F 0.14060300 0.20250600 -3.16592900
C 5.80253300 -0.38253700 -1.15982300
H 5.83586700 -1.34029400 -0.64537900
Cl 7.03376100 -0.37661300 -2.44100700
H 6.00836600 0.43783800 -0.47592200
N -4.59319600 -2.18666600 4.23466500
H -4.23060100 -3.08743600 4.52699000
H -5.40294600 -1.83269000 4.73160000

(*p*-NH$_2$)-11c-s

N -1.93096600 1.89099600 0.05406000
C -1.74717100 2.48991600 -1.39795000
C -1.96540900 3.99540700 -1.24813500
C -3.01610700 4.33008300 -0.18516400
C -2.51609100 3.96189300 1.22926600
C -1.54985300 2.76583500 1.18322900
H -0.99994700 4.45111700 -1.00345100
H -3.26939200 5.39165800 -0.22632400
H -1.97839500 4.80069800 1.67991400
H -1.54829200 2.18257500 2.10426700
H -3.36183800 3.72678600 1.88056100
H -0.52464300 3.07843300 0.97443200
H -3.93827900 3.78039100 -0.40688700
H -2.25595100 4.37397400 -2.23156500
H -2.55749700 2.01184200 -1.96116700
C -2.40753500 0.72827500 0.22674000
O -2.84263800 -0.24879500 -0.51172000
C -2.79072000 -0.37233500 1.09478400
C -4.12830800 -0.39798200 1.70053500
C -1.76171300 -1.30835100 1.56055300
C -4.36888900 -1.21164200 2.74293600
H -4.89097800 0.25935800 1.30024000
C -2.02291500 -2.13252600 2.58936000
H -0.79056200 -1.29651300 1.08087300
C -3.32586100 -2.10314700 3.22981700
H -5.34024100 -1.23098300 3.22391000
H -1.26852600 -2.82960200 2.93425500
Ag -0.61195500 -1.49316100 -2.08612300
B 0.85653800 -3.08556300 0.09578800
F 2.08610400 -3.62833000 -0.24182000
F 0.95104900 -1.64913900 0.03949300
F -0.12247200 -3.44107900 -0.88654200
F 0.42698900 -3.46436400 1.35436400
O -0.51292300 2.18655600 -1.85992600
H -0.55143800 1.35910300 -2.48157200
C 4.59236600 1.50797800 -2.77602300
C 5.18132900 0.20473600 -2.16638600
H 4.97332300 2.37883900 -2.23835500
H 4.89979000 1.59197200 -3.82027300
N 3.12943200 1.51487000 -2.70378400
N 4.04656100 -0.56923500 -1.52099200
H 5.62116200 -0.44905000 -2.91731900
H 5.91895900 0.39536200 -1.38605300
C 2.71609200 1.52985900 -1.29839200
C 3.34622500 0.34301300 -0.51734500
H 1.62723400 1.48497200 -1.25276000
H 3.03421400 2.47119800 -0.84435700
H 4.11064100 0.66153500 0.19223700

H 2.60017500 -0.26596900 -0.01013200
C 2.60434800 0.30838400 -3.35472600
C 3.03687200 -0.96962800 -2.58511000
H 2.99220200 0.27527400 -4.37534900
H 1.51369600 0.36082200 -3.40279400
H 2.22107600 -1.44664100 -2.04412600
H 3.51863700 -1.70691000 -3.22503400
F -0.60687400 0.25489400 -3.31822600
C 4.53488700 -1.76342900 -0.75331400
H 3.66828200 -2.28701900 -0.35513600
Cl 5.44379800 -2.91508000 -1.77082600
H 5.19767100 -1.40779900 0.03242500
N -3.57104500 -2.89480700 4.23805800
H -2.86773400 -3.53720700 4.58962000
H -4.47284400 -2.90393500 4.70419900

(*p*-NH$_2$)-11c-t
N -1.44667800 1.51187300 -0.33304400
C -1.23422600 2.17450500 -1.65184700
C -0.92137800 3.65556000 -1.42216400
C -1.84906100 4.24509700 -0.35421000
C -1.60036600 3.58371400 1.02141100
C -0.92658100 2.21524600 0.85005100
H 0.12932400 3.76836500 -1.13367400
H -1.71389100 5.32718200 -0.28837500
H -0.94376400 4.20223900 1.64055300
H -1.04809400 1.58158100 1.72819500
H -2.54198500 3.47314400 1.56677200
H 0.14859100 2.34816400 0.70600400
H -2.88719300 4.07736300 -0.66284200
H -1.04022600 4.16561100 -2.38093100
H -2.19520100 2.07942500 -2.18142700
C -2.19856500 0.40352400 -0.27611200
O -2.66244600 -0.17045100 -1.28128900
C -2.56157600 -0.18756900 1.05629200
C -3.51479300 0.46358500 1.87772900
C -2.04959200 -1.45866800 1.41880000
C -3.91876100 -0.10588700 3.05879700
H -3.92496200 1.41905100 1.57211700
C -2.43330600 -2.04194000 2.60004800
H -1.34588800 -1.96876800 0.77198600
C -3.37314400 -1.37327400 3.45262000
H -4.64041400 0.38861500 3.69922100
H -2.03662600 -3.00582100 2.89975400
Ag -1.54801000 -1.96094700 -2.40948400
B 0.94694600 -3.56565300 -1.45376200
F 2.25485400 -3.26822500 -1.03555200
F 0.02835500 -2.88913700 -0.57805800
F 0.73957500 -3.00732900 -2.74689400
F 0.70051800 -4.91607000 -1.45184800
O -0.29375800 1.54743800 -2.45847700
H -0.64829100 0.49103500 -3.26090000
C 2.53162100 1.91342000 -1.42253100
C 3.98619500 1.36729700 -1.36235700
H 2.26587500 2.41188300 -0.49024000
H 2.42102800 2.61908600 -2.24505900
N 1.62587500 0.78439600 -1.63393400
N 3.92159300 -0.14637200 -1.23623400
H 4.54760300 1.58866600 -2.26751500
H 4.53146900 1.74794600 -0.49942200
C 1.55805200 -0.06958600 -0.44881500
C 3.00119900 -0.49844700 -0.07225600
H 0.94566400 -0.94191700 -0.66186300
H 1.11397100 0.48188200 0.37722600
H 3.38269600 0.02971500 0.80064900
H 3.05323700 -1.57514600 0.07504800
C 2.01751700 0.02259900 -2.82500400
C 3.32817400 -0.73457200 -2.50936400
H 2.14399900 0.72605000 -3.64741000
H 1.23633000 -0.68620000 -3.08796700
H 3.14428100 -1.78761200 -2.30277700
H 4.06612800 -0.62441700 -3.30128600
F -0.82721500 -0.27879100 -3.90474100
C 5.26650900 -0.74943600 -0.93171100
H 5.14381300 -1.83010300 -0.90854000
Cl 6.49339300 -0.33907400 -2.15158700
H 5.59412700 -0.36875100 0.03347800
N -3.73965500 -1.92791800 4.60508800
H -3.36605100 -2.82180600 4.90490800
H -4.40316600 -1.47698700 5.22550700

[(*p*-NH$_2$)-TS1(H-F form)-t]
C 1.18672900 0.80762900 0.56845600
C 0.06674300 0.80876800 -0.50027100
H 1.92182700 1.59465700 0.39855400
H 0.79373100 0.89602500 1.57952800
N 1.94208000 -0.50964300 0.48456700
N 0.27671500 -0.31290100 -1.43806700
H -0.91458200 0.69001700 -0.03958500
H 0.08899400 1.73933100 -1.06332100
C 2.67171300 -0.56263600 -0.85276100
C 1.65537600 -0.25859000 -1.97741000
H 3.10339800 -1.56017200 -0.93334400
H 3.47454500 0.17396900 -0.81802200
H 1.80907700 0.73660000 -2.39156800
H 1.72349600 -1.00272400 -2.77193800
C 0.95094300 -1.66045600 0.53019600
C 0.07422700 -1.60077400 -0.74294000
H 0.36722000 -1.53882600 1.44038900
H 1.52583400 -2.58376900 0.59738700
H 0.32282700 -2.39124600 -1.45178300
H -0.97781100 -1.69251400 -0.47011000

F 0.17208900 -2.13474800 -3.77624300
Ag -1.09401600 -0.32899200 -3.30573500
O -2.34478800 -0.25638400 -5.20065800
C -1.71224500 0.16498000 -6.19922200
N -0.70275300 -0.59325500 -6.73757300
C -0.56834400 -1.95316200 -6.31181300
C 0.43258200 0.00115600 -7.47062400
C 0.49610700 -2.69716100 -7.09676100
H -0.22672400 -1.98459900 -5.18853700
C 1.74256300 -0.49501000 -6.84269800
H 0.36889200 -0.30276900 -8.52145200
C 1.87654600 -2.03063400 -6.92238600
H 0.51393100 -3.73451200 -6.75613800
H 2.56672600 0.00549200 -7.35710800
H 2.52437000 -2.32203000 -7.75290400
C -2.11066800 1.43966000 -6.82136800
C -2.65776200 2.44503900 -5.98142100
C -2.08311700 1.62550000 -8.22833200
C -3.11406900 3.62005700 -6.51453700
H -2.66799200 2.28718600 -4.91174700
C -2.55240100 2.78706800 -8.78415000
H -1.71666800 0.83769000 -8.87433100
C -3.07190900 3.81919500 -7.93292100
H -3.49919300 4.40952200 -5.87921400
H -2.54634800 2.93474700 -9.85805600
H -1.55357500 -2.42719300 -6.28022500
H 0.21435500 -2.71444900 -8.15743100
H 2.34100200 -2.39703100 -6.00285600
H 1.74815100 -0.15313600 -5.80519500
H 0.36014300 1.08396400 -7.40502900
B -0.03643000 2.53521600 -3.85735000
F 0.95828200 2.74596000 -2.90243600
F -1.23942800 2.11232600 -3.17539700
F -0.30208000 3.66104000 -4.60263900
F 0.33876600 1.44938600 -4.70092600
C 2.98100800 -0.62196100 1.56753200
Cl 2.27159200 -0.68450000 3.19766000
H 3.54249300 -1.53810500 1.39674800
H 3.62570400 0.25172600 1.50401400
N -3.51541300 4.95543300 -8.46203500
H -3.88989900 5.69725100 -7.88150300
H -3.49418800 5.11868100 -9.46215800

[(*p*-NH$_2$)-TS2(H-F form)-t]
N -1.64670000 1.77166900 0.08067000
C -1.22837100 2.55738700 -1.14169700
C -1.21492800 4.04361200 -0.75353300
C -2.31251100 4.37381400 0.26244000
C -2.03436700 3.66839600 1.60737500
C -1.27091000 2.35256400 1.37386300
H -0.22613700 4.27859500 -0.34212500
H -2.39322100 5.45403900 0.40993900
H -1.42723500 4.30441700 2.25924600
H -1.44088100 1.62678700 2.16989300
H -2.97284100 3.47206500 2.13524800
H -0.19239500 2.53156900 1.33214900
H -3.27731900 4.03852500 -0.13676300
H -1.32452200 4.63006200 -1.66970400
H -2.03176500 2.36659100 -1.86381700
C -2.31526300 0.63281000 -0.05737800
O -2.59966000 0.10289600 -1.15992500
C -2.85244100 -0.07577500 1.15255100
C -3.98892000 0.45010600 1.81615700
C -2.31162200 -1.32858500 1.53737400
C -4.56375600 -0.23293900 2.85804200
H -4.40367000 1.39950600 1.49710200
C -2.86639200 -2.02371200 2.58177900
H -1.44922800 -1.73013000 1.01793400
C -4.00985600 -1.49229000 3.26414200
H -5.42795800 0.16343700 3.37949100
H -2.45388500 -2.97415800 2.90184200
Ag -1.24347600 -1.50938800 -2.20601000
B 0.88379300 -3.44413300 -0.86401100
F 2.24795500 -3.10065100 -0.83649200
F 0.15687000 -2.43812100 -0.14746500
F 0.42780200 -3.36841500 -2.21885200
F 0.65051500 -4.68604800 -0.33481400
O 0.00427200 2.16431500 -1.60817600
H -0.08833900 1.16925400 -2.43176600
C 2.75922200 1.32767400 -2.82686500
C 4.21993000 1.17894300 -2.29180500
H 2.24908400 2.18443900 -2.38692800
H 2.74017300 1.39468600 -3.91298100
N 2.07702800 0.11460900 -2.40842500
N 4.37703800 -0.19960900 -1.65821400
H 4.95002100 1.25783500 -3.09425700
H 4.44467100 1.91197000 -1.51840700
C 1.98261000 0.00064800 -0.95935400
C 3.42455000 -0.31323300 -0.46947800
H 1.31540300 -0.81151200 -0.68361600
H 1.59467800 0.94512200 -0.58097900
H 3.75524200 0.39094300 0.29219000
H 3.48826300 -1.33639900 -0.10468300
C 2.53261000 -1.07342900 -3.11041200
C 4.01013700 -1.28504000 -2.66505100
H 2.46430600 -0.89268900 -4.18144500
H 1.92095200 -1.92669500 -2.83212900
H 4.12453000 -2.24233100 -2.15949800
H 4.70434400 -1.20756000 -3.49799400
F 0.04934500 0.25894200 -3.13894200
C 5.77559400 -0.39968100 -1.12421700
H 5.80701000 -1.37524400 -0.64458500

Cl 7.00889100 -0.34608400 -2.40078900
H 5.97639900 0.39634300 -0.41081900
N -4.55801500 -2.16902600 4.27060900
H -4.18554000 -3.06315600 4.57014500
H -5.37066200 -1.81907000 4.76528100