Supporting Information for

Room-temperature phosphorescence and dual-emission behavior of simple biphenyl derivatives unlocked by intermolecular interaction with cyclic silver pyrazolate

Arina P. Olbrykh,[a,b] Alisia V. Tsorieva,[c] Vladislav M. Korshunov,[c] Alexander F. Smol'yakov,[a] Ivan A. Godovikov,[a] Alexander A. Korlykov,[a] Ilya V. Taydakov,[c] Aleksei A. Titov,*[a] Oleg A. Filippov,*[a] Elena S. Shubina[a]

a A.N. Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences (INEOS RAS), 119991 Moscow, Vavilov St. 28, bld. 1, Russia.

E-mail: tit@ineos.ac.ru (AAT); *h-bond@ineos.ac.ru (OAF)*

b Higher Chemical College, Mendeleev University of Chemical Technology of Russia, Miusskaya Sq. 9, 125047 Moscow, Russia

c P.N. Lebedev Physical Institute of the Russian Academy of Sciences, 53 Leninskiy Prospekt, 119991 Moscow, Russia

1. Physical measurement and instrumentation

^{1}H, ^{19}F, and ^{13}C NMR measurements were carried out on Bruker Avance-III-500 spectrometer with CryoProbe Prodigy operating at 500.13 MHz.

The diffuse reflectance spectra of investigated compounds were recorded with a JASCO V-770 spectrophotometer operating within 200–2500 nm (HPLC SuperGradient, Panreac, Spain).

The photoluminescence spectra were obtained using a Horiba Fluorolog QM spectrofluorimeter with a 75 W xenon arc lamp as excitation source and a R13456 (/Hamamatsu, Japan) photomultiplier tube sensitive in the 200-980 nm emission range as a detector.

The photoluminescence quantum yields were measured for solid samples by an absolute method using the same experimental setup equipped with a G8 (GMP, Switzerland) integration sphere.

Single-crystal X-ray diffraction study

Single crystals of compounds **1Ag**, **2Ag** and **7Ag** were selected for the data collection under an optical microscope. For the diffraction experiments the crystals were coated with an oil-based cryoprotectant and mounted on cryoloops. Studies were conducted using a Rigaku SuperNova XtaLAB (**2Ag**) and Rigaku XtaLAB Synergy-S (**1Ag** and **7Ag**) X-ray diffractometers, where the former is operated with monochromatic micro-focus CuKα tube (λ = 1.54184 Å) at 50 kV and 1.0 mA and equipped with a CCD HyPix 3000 hybrid photon counting detector, and the latter is

operated with monochromatic micro-focus CuKα tube PhotoJet-S (λ[CuKα] for **7Ag**, λ[MoKα] for **1Ag**) at 50 kV and 1.0 mA and equipped with a CCD HyPix 6000HE hybrid photon counting detector. All data collection strategies were designed to collect more than half of the Ewald sphere. Frame widths were 0.5 s. CrysAlisPro software was used for the integration and correction of diffraction data for polarization, for background and Lorentz effects, for a numerical absorption correction based on Gaussian integration over a multifaceted crystal model, and for an empirical absorption correction based on spherical harmonics implemented in the SCALE3 ABSPACK algorithm.[S1] The unit cell parameters were refined using a least-squares technique. The structure was solved by a dual-space algorithm and refined using SHELX programs, which were incorporated in the *OLEX*2 program package.[S2-S4] The carbon-bound H atoms were placed in calculated positions and were included in the refinement in the 'riding' model approximation, with C–H bond lengths of 0.95 Å. The U_{iso}(H) parameters were fixed at 1.2U_{eq}(C) for the C–H bonds.

Table S1. Crystallographic data, data collection and refinement parameters of crystal structures of samples **1Ag**, **2Ag**, **7Ag**.

Compound	**7Ag**	**2Ag**	**1Ag**
Formula	$C_{15}H_3Ag_3F_{18}N_6$, $C_{12}H_8I_2$	$C_{15}H_3Ag_3F_{18}N_6$, $C_{12}H_8F_2$	$C_{15}H_3Ag_3F_{18}N_6$, $C_{12}H_{10}$
Space group	$P2_1/c$	$P2_1/n$	$C2/c$
a [Å]	13.3886(3)	12.9970(1)	27.1546(3)
b [Å]	18.1861(4)	21.2672(3)	12.88400(15)
c [Å]	15.3291(3)	35.6158(4)	28.4468(4)
α [°]	90	90	90
β [°]	109.789(2)	92.443(1)	97.3645(11)
γ [°]	90	90	90
V [Å^3]	3512.01(14)	9835.61(19)	9870.3(2)
Z	4	12	12
Calculated density [g/cm^3]	2.53	2.27	2.19
μ [mm^{-1}]	28.3	15.62	1.90
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Mo $K\alpha$
Angle range 2ϑ [°]	7.02 – 139.99	4.84 – 138.55	3.72 – 76.07
Index range	-16 ≤ h ≤ 13, -22 ≤ k ≤ 21, -18 ≤ l ≤ 18	-15 ≤ h ≤ 15, -25 ≤ k ≤ 23, -42 ≤ l ≤ 43	-44 ≤ h ≤ 46, -20 ≤ k ≤ 21, -48 ≤ l ≤ 49
Total reflections, unique reflections and reflections with $F^2 > 2\sigma(F^2)$	24362, 6598, 5480	111104, 18286, 15516	220298, 25668, 19871
R_{int}, R_σ	0.0551, 0.0504	0.0940, 0.0556	0.0687, 0.0321
R_1 [$F^2 > 2\sigma(F^2)$], wR_2 [$F^2 > 2\sigma(F^2)$]	0.0322, 0.0771	0.0469, 0.1237	0.0441, 0.0947
R_1 and wR_2 (all data)	0.0419, 0.0811	0.0553, 0.1295	0.0643, 0.1043
S	1.049	1.024	1.078
ρ_{max}, ρ_{min} [e$^-$ Å^{-3}]	1.07, -0.90	1.13, -1.04	1.74, -1.56

Single-crystal X-ray diffraction experiments of complexes **3Ag, 4Ag, 3/4Ag**, **5Ag** were carried out with a Bruker APEX-II diffractometer. The APEX II software[S5] was used for collecting frames of data, indexing reflections, determination of lattice constants, integration of intensities of reflections, scaling, and absorption correction. The structures were solved by dual-space algorithm and refined in anisotropic approximation for non-hydrogen atoms against F 2 (*hkl*). Hydrogen atoms of aromatic fragments were calculated according to those idealized geometry and refined with constraints applied to C-H bond lengths and equivalent displacement parameters (U eq (H) = 1.2U eq (X), X - cental atom of XH_2 group; U eq (H) = 1.5U eq (Y), Y - central atom of YH_3 group). All structures were solved with the ShelXT[S2] program and refined with the ShelXL[S3] program. Molecular graphics was drawn using OLEX2[S4] program.

Table S2. Crystallographic data, data collection and refinement parameters of crystal structures of **3Ag, 4Ag, 3/4Ag**, **5Ag** samples.

Compound	**3Ag**	**4Ag**	**3/4Ag,**	**5Ag**
Empirical formula	$C_{27}H_{11}Ag_3Cl_2F_{18}N_6$	$C_{27}H_{11}Ag_3Br_2F_{18}N_6$	$C_{27}H_{11}Ag_3BrClF_{18}N_6$	$C_{27}H_{11}Ag_3ClF_{19}N_6$
Formula weight	1155.93	1244.85	1200.39	1139.51
Temperature/K	120	296.15	120.00	120.00
Crystal system	triclinic	triclinic	triclinic	triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1
a/Å	12.3392(6)	12.2479(8)	12.2937(5)	12.6900(11
b/Å	12.6908(7)	12.6464(8)	12.6654(5)	13.0350(11)
c/Å	12.8767(7)	12.8813(9)	12.8884(5)	22.228(2)
α/°	78.070(2)	80.986(3)	79.543(2)	89.400(3)
β/°	64.247(2)	65.501(3)	65.004(2)	83.802(4)
γ/°	73.652(2)	76.007(3)	74.907(2)	69.652(3)
Volume/Å^3	1734.38(16)	1758.1(2)	1750.22(12)	3425.8(5)
Z	2	2	2	4
ρ_{calc}g/cm^3	2.213	2.352	2.278	2.209
μ/mm^{-1}	1.960	4.055	3.008	1.912
F(000)	1104.0	1176.0	1140.0	2176.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.36 to 56.638	3.326 to 61.07	3.342 to 52	3.334 to 56.622
Index ranges	-16 ≤ h ≤ 16, -16 ≤ k ≤ 16, -17 ≤ l ≤ 17	-17 ≤ h ≤ 13, -15 ≤ k ≤ 18, -18 ≤ l ≤ 18	-15 ≤ h ≤ 15, -15 ≤ k ≤ 15, -15 ≤ l ≤ 15	-16 ≤ h ≤ 16, -17 ≤ k ≤ 17, -29 ≤ l ≤ 29
Reflections collected	28076	21252	25252	51396
Independent reflections	8584 [R_{int} = 0.0459, R_{sigma} = 0.0519]	9909 [R_{int} = 0.0264, R_{sigma} = 0.0431]	6850 [R_{int} = 0.0377, R_{sigma} = 0.0398]	16829 [R_{int} = 0.0290, R_{sigma} = 0.0402]
Data/restraints/parameters	8584/0/521	9909/0/506	6850/0/447	16829/66/871
Goodness-of-fit on F^2	1.158	1.080	1.094	1.136
Final R indexes [I>=2σ (I)]	R_1 = 0.0365, wR_2 = 0.0936	R_1 = 0.0314, wR_2 = 0.0675	R_1 = 0.0383, wR_2 = 0.0930	R_1 = 0.0340, wR_2 = 0.0817
Final R indexes [all data]	R_1 = 0.0489, wR_2 = 0.0966	R_1 = 0.0478, wR_2 = 0.0705	R_1 = 0.0499, wR_2 = 0.0969	R_1 = 0.0498, wR_2 = 0.0848
Largest diff. peak/hole / e Å^{-3}	1.64/-1.05	1.13/-0.89	1.76/-1.91	1.27/-1.21

The low quality crystals of **6Ag** do not allowed the complete refinement of the XRD structure. Needles crystals splicing due to growthing leading to the twinning/ Moreover, the presence of two different halogens leads to a superposition of their locations, similar to that observed for **5Ag**. The positions of silver atoms do not raise any doubts, and the typical structure of {biphenyl - $[AgL]_3\}_\infty$ can be observed in complex **6Ag**. Furthermore, the distances between Ag3-Ag3 centroids and planes fall within the range observed for other complexes (6.3-6.4 Å and 6.15-6.25 Å correspondingly). The ball-and-stick diagram of unspecified structure is given below:

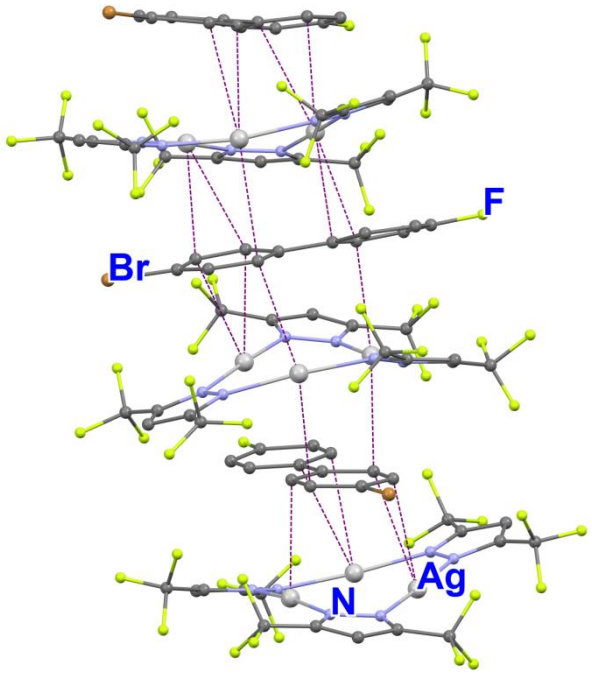


Figure S1. Ball-and-stick diagram demonstrating main structural motive of 6Ag.

X-ray powder diffraction study

Prior to the powder XRD study, all samples were ground to a fine powder and placed on a Si(911) zero-background flat holder. All measurements were carried out with a D8 Advance (Bruker AXS) diffractometer in the Bragg-Brentano focusing geometry using CuKα radiation, the scan rate was 0.5 deg·min^{-1} and the angular step was 0.02°. Several scans for each sample were measured and patterns were processed with DIFFRACplus EVA.[S6] The phase analysis of all samples was carried out with DIFFRAC TOPAS 5.0[S7] software using single-crystal X-ray data and Rietveld refinement procedure. To verify the phase composition of studied compounds the Rietveld refinement of collected powder X-ray data was carried out starting from single-crystal X-ray data. Atomic coordinates were fixed, while cell and March-Dollase preferred orientation parameters were refined. As a result, powder samples of 3Ag, 4Ag, 3-4Ag and 7Ag are almost identical to corresponding single-crystal data. At the same time, 1Ag, 2Ag and 5Ag, some low-intensive X-ray maxima near 10° cannot be satisfactorily described by X-ray data. These maxima are probably the results of sample decomposition due to the grinding process.

2. Experimental section

General Information

All manipulations were performed under a dry argon atmosphere by standard Schlenk techniques. Commercially available argon (99.9%) was additionally purified from traces of oxygen and moisture by sequential passage through a Ni/Cr catalyst column and 4 Å molecular

sieves. HPLC-grade toluene were additionally purified by standard dehydration over Na and freshly distilled under argon before use. Dichloromethane, CCl_4 were dried over CaH_2 and freshly distilled under argon. Biphenyls 1-4, 7 were purchased from commercial producers.

General procedure for synthesis of biphenyls 5-6.[S8]

4-chloro-4'-fluoro-1,1'-biphenyl (5). The product was purified by column chromatography using mixture of EtOAc/petroleum ether =1/10 as an eluent. White solid. Yeild = 73%. ^{1}H NMR (500 MHz, 0.55CCl_4/0.1CD_2Cl_2): δ 7.57-7.54(m, 2H), 7.52-7.50(d, J = 8.6 Hz, 2H), 7.46-7.44(d, 2H), 7.19-7.16(t, 2H)ppm. ^{19}F NMR (282 MHz, 0.55CCl_4/0.1CD_2Cl_2): δ −115.04 ppm. ^{13}C NMR (126 MHz, 0.55CCl_4/0.1CD_2Cl_2): δ 163.87, 161.90, 139.01, 136.48, 133.85, 129.28, 128.85, 128.78, 128.48, 116.17, 116.00 ppm.

4-bromo-4'-fluoro-1,1'-biphenyl (6). The product was purified by column chromatography using mixture of EtOAc/petroleum ether =1/10 as an eluent. White solid. Yeild = 67%. ^{1}H NMR (500 MHz, 0.55CCl_4/0.1CD_2Cl_2): δ 7.61-7.60(d, 2H), 7.57-7.54(m, 2H), 7.46-7.44(d, 2H), 7.19-7.16(t, 2H) ppm. ^{19}F NMR (282 MHz, 0.55CCl_4/0.1CD_2Cl_2): δ –115 ppm. ^{13}C NMR (126 MHz, 0.55CCl_4/0.1CD_2Cl_2): δ 163.91, 161.93, 139.48, 136.48, 133.42, 132.23, 128.76, 121.95, 116.20, 116.03 ppm.

Complexes 1-7.

Initial trinuclear silver complex $[AgL]_3$ was obtained according to a previously published procedure.[S9]

General procedure for complexes 1Ag-7Ag.

The solution of $[AgL]_3$ (0.03 mmol) and corresponding biphenyl (0.03 mmol) was dissolved in a mixture of CH_2Cl_2 (1 mL) and CCl_4(1 mL). Crystals have been obtained at -10°C and dried under reduced pressure at 40°.

Elemental analysis for complexes obtained

1Ag. Calc. for $C_{27}H_{13}Ag_3F_{18}N_6$ (%): C, 29.83; H, 1.21; N, 7.73. Found (%): C, 29.58; H, 1.38; N, 8.00.

2Ag. Calc. for $C_{27}H_{11}Ag_3F_{20}N_6$ (%): C, 28.88; H, 0.99; N, 7.48. Found (%): C, 28.69; H, 1.28; N, 7.49.

3Ag. Calc. for $C_{27}H_{11}Ag_3F_{18}Cl_2N_6$ (%): C, 28.06; H, 0.96; N, 7.27. Found (%): C, 27.89; H, 1.15; N, 7.39.

4Ag. Calc. for $C_{27}H_{11}Ag_3F_{18}Br_2N_6$ (%): C, 26.05; H, 0.89; N, 6.75. Found (%): C, 25.98; H, 1.07; N, 6.98.

3/4Ag. Calc. for $C_{54}H_{22}Ag_6Br_2Cl_2F_{36}N_{12}$ (%): C, 27.02; H, 0.92; N, 7.00. Found (%): C, 27.24; H, 1.12; N, 6.84.

5Ag. Calc. for $C_{27}H_{11}Ag_3F_{19}ClN_6$ (%): C, 28.46; H, 0.97; N, 7.38. Found (%): C, 28.50; H, 1.13; N, 7.51.

6Ag. Calc. for $C_{27}H_{11}Ag_3F_{19}BrN_6$ (%): C, 27.39; H, 0.94; N, 7.10. Found (%): C, 27.52; H, 1.05; N, 7.02.

7Ag. Calc. for $C_{27}H_{11}Ag_3F_{18}I_2N_6$ (%): C, 24.22; H, 0.83; N, 6.28. Found (%): C, 24.08; H, 1.00; N, 6.31.

3. Computational details.

Calculations were performed with ORCA 5.04 software package[S10,S11] applying ωB97X-D3 functional[S12] and ZORA Hamiltonian. The applied basis set was SARC-ZORA-TZVP[S13] for silver atoms and ZORA-TZVP for H, C, N, F and Cu atoms. The geometry taken from the crystal structures were partially optimized, freezing positions of Ag atoms. All possible configurations of partially optimized $[AgL]_3\{BP\}[AgL]_3$ fragments are gathered in the Table S3. Electronic transitions were calculated under the TD-DFT approach utilizing the same computation level as the Tamm-Dankoff approximation considering 20 lowest energy singlet and triplet excitations. If symmetry forbidden dark states were not considered it stated in the corresponding part of discussion. Analysis of natural transition orbitals (NTO) and contributions from certain atomic orbitals to the electronic transitions were performed with the Multiwfn 3.8 package[S14].

Table S3. Principal geometry of calculated $[AgL]_3\{BP\}[AgL]_3$ complexes

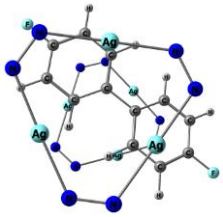
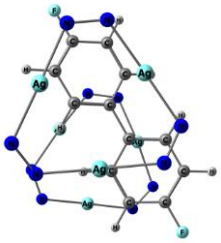
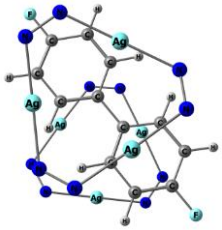
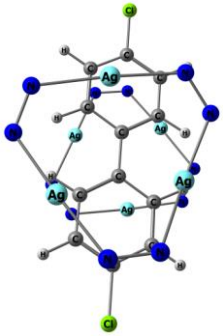
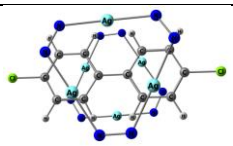
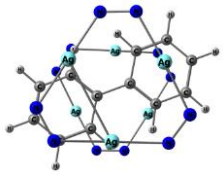
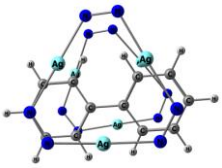
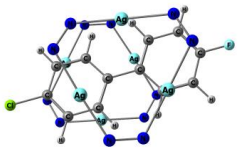
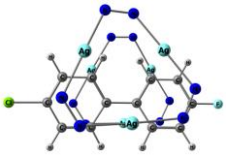
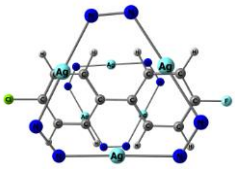
				
$2Ag^{3}$	$2Ag^{2}$	$2Ag^{1}$	$3Ag^{axial}/4Ag^{axial}$	$3Ag^{nonaxial}/4Ag^{nonaxial}$
				
$1Ag^{h2t}$	$1Ag^{h2h}$	$5Ag^{displaced}$	$5Ag^{h2h}$	$5Ag^{h2t}$

Table S4. Data for allowed singlet-triplet intersystem crossing pathways. S_1 and S_2 are lowest symmetry allowed LC^{BP} (S_1) and BP→$[AgL]_3$ CT type state (S_2).

complex	E S_1, eV LC^{BP} symmetry allowed	E S_2, eV $[AgL]_3$ involved	E T_1, eV	SOC $\langle S_0\|T_1\rangle$	SOC $\langle S_1\|T_1\rangle$	SOC $\langle S_2\|T_1\rangle$	SOC $\langle S_n\|T_1\rangle$; % of CT [a]
$1Ag^{h2t}$	4.983	5.142	3.498	0.8	2.5	17.0	S_9; 22.1; 69%
$1Ag^{h2h}$	5.037	5.104	3.517	5.8	0.8	17.3	S_8; 25.5; 55%
$2Ag^{1}$	4.977	5.131	3.464	9.1	3.6	15.9	S_8; 14.5; 42%
$2Ag^{2}$	5.131	5.177	3.563	10.3	2.5	17.7	S_8; 20.0; 46%
$2Ag^{3}$	5.045	5.104	3.527	7.0	9.2	12.4	S_8; 15.9; 47%
$3Ag^{axial}$	4.759	n/a[b]	3.327	0.02	3.5	n/a[b]	S_9; 22.5; 71%
$3Ag^{nonaxial}$	4.811	n/a[b]	3.367	0.02	2.5	n/a[b]	S_{10}; 23.1; 80%
$4Ag^{axial}$	4.691	n/a[b]	3.310	0.02	2.5	n/a[b]	S_9; 29.4; 71%
$4Ag^{nonaxial}$	4.735	n/a[b]	3.344	0.1	2.3	n/a[b]	S_9; 27.5; 79%
$5Ag^{displaced}$	4.882	5.159	3.404	4.2	2.1	12.4	S_9; 23.3; 73%
$5Ag^{h2h}$	5.003	5.132	3.486	6.9	1.6	15.5	S_8; 23.2; 52%
$5Ag^{h2t}$	4.876	5.148	3.401	2.6	3.0	17.5	S_9; 26.4; 65%

[a] data for second possible CT singlet state, singlet number is absolute, CT impact value calculated as a difference between hole and electron distribution on the biphenyl fragment of the complex [b] For centrosymmetric **3Ag** and **4Ag** there are no low lying CT type states

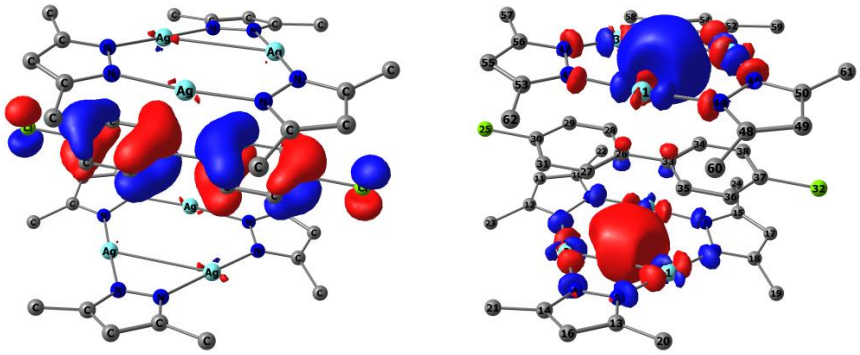


Figure S2. Typical view of high lying CT type state on the example of S_{10} for **$3Ag^{nonaxial}$**. HONTO (left) LUNTO (right) as isosurfaces as 0.04 a.u, 0.92 fraction of transition electron density.

Table S5. Main characteristics calculated for excited states of free biphenyls

	triplets			singlets			SOCME	
	λ, nm	K_{phos}	%FC	λ, nm	$K_{fluor}*10^7$	%FC	$\langle S_0\|T_1\rangle$	$\langle S_1\|T_1\rangle$
1	317.5	0.1	0	228.2	2.2	0.24	0.4	0.2
2	316.2	0.7	0.01	230.5	4185.4	0.04	0.4	0.0
5	323.7	5.9	38.38	233.4	4.9	2.61	0.5	0.2
3	327.4	8.4	0.06	233.2	138.1	0.17	0.6	0.4
4	328.4	229.2	23.41	233.9	42.8	0.39	1.5	3.4
7	330.4	1182.7	0.12	256.6	54.7	0.02	2.4	95.2

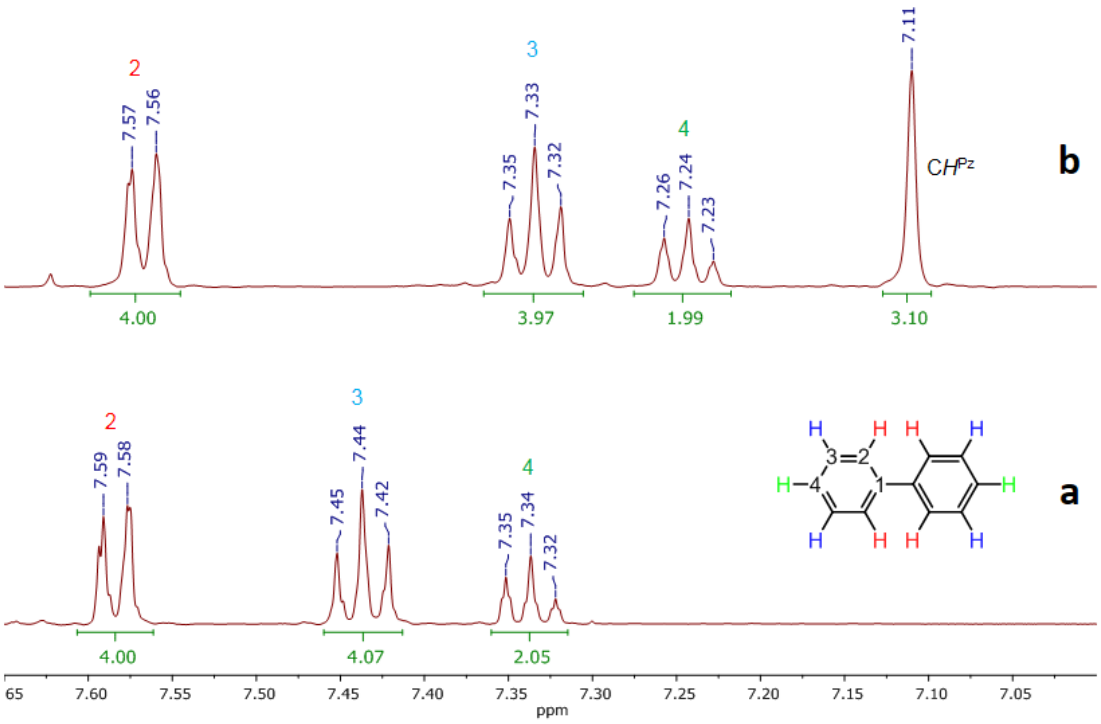


Figure S3. ^{1}H NMR spectra of **1** (a) and **1** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

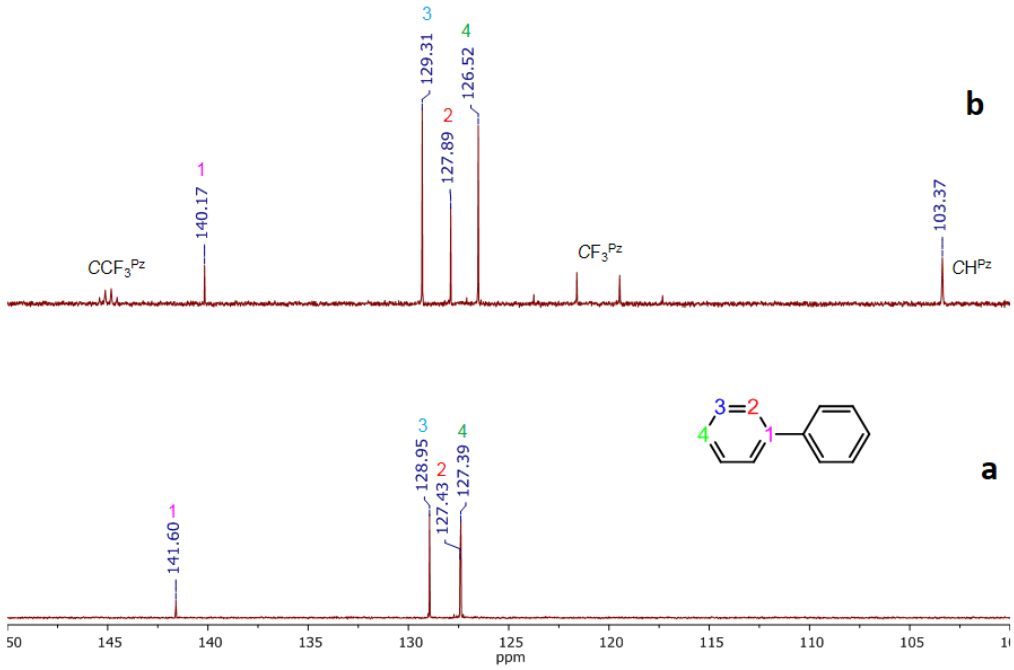


Figure S4. ^{1}H NMR spectra of **1** (a) and **1** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

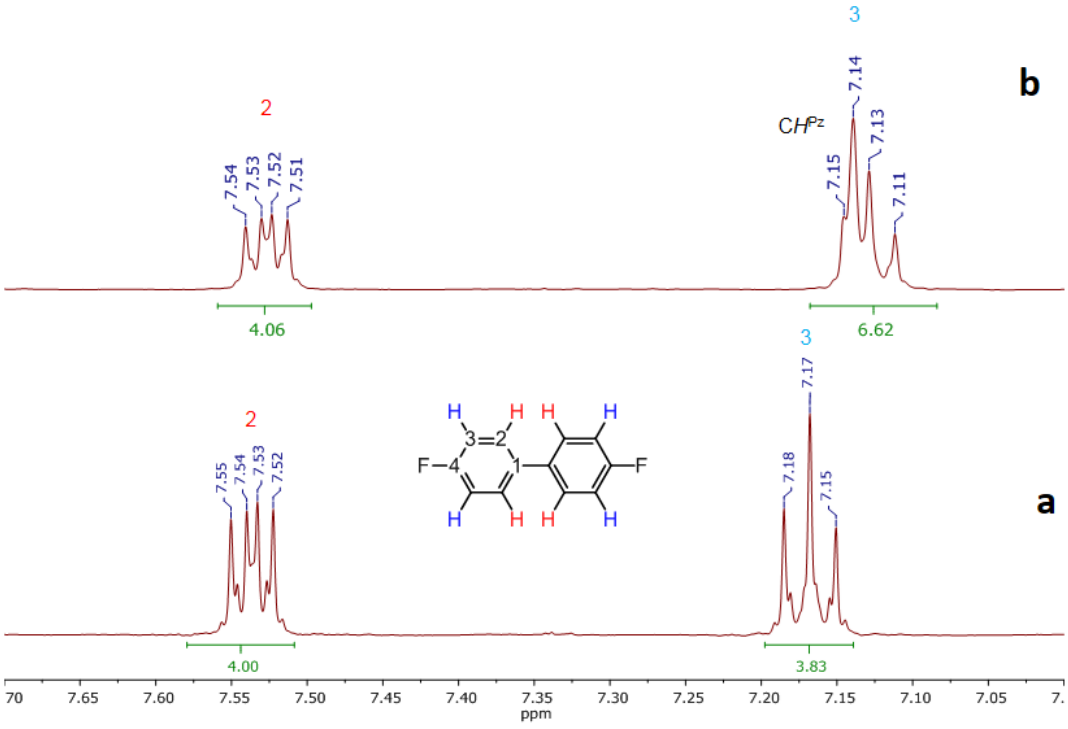


Figure S5. ^{1}H NMR spectra of **2** (a) and **2** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

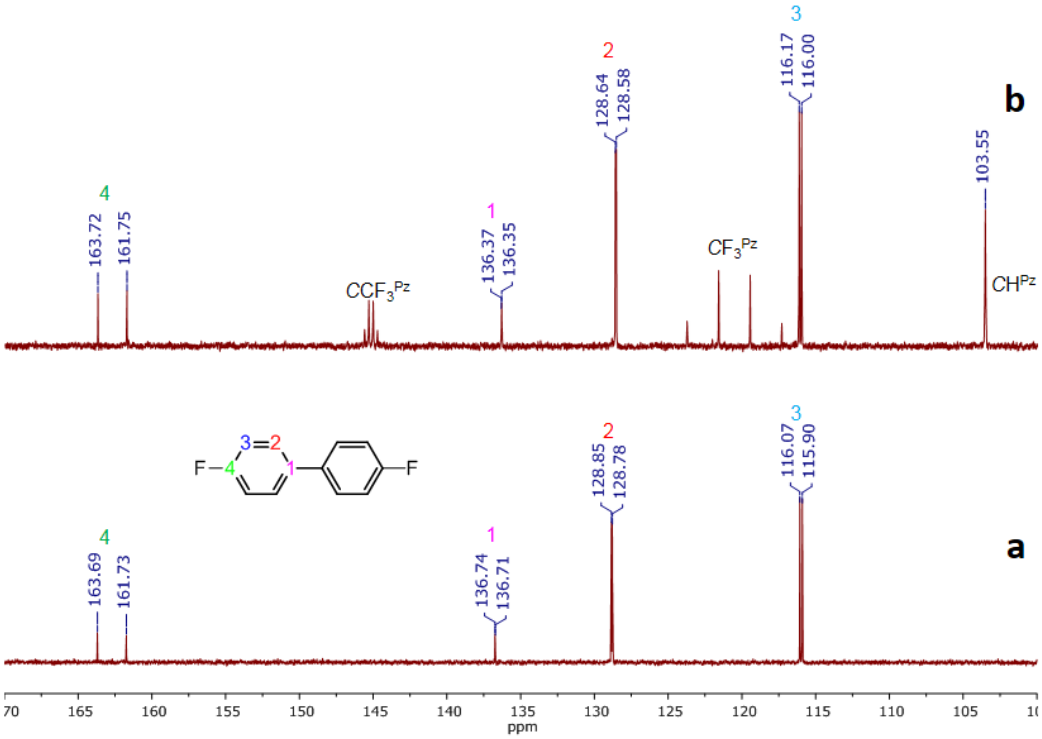


Figure S6. ^{13}C NMR spectra of **2** (a) and **2** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

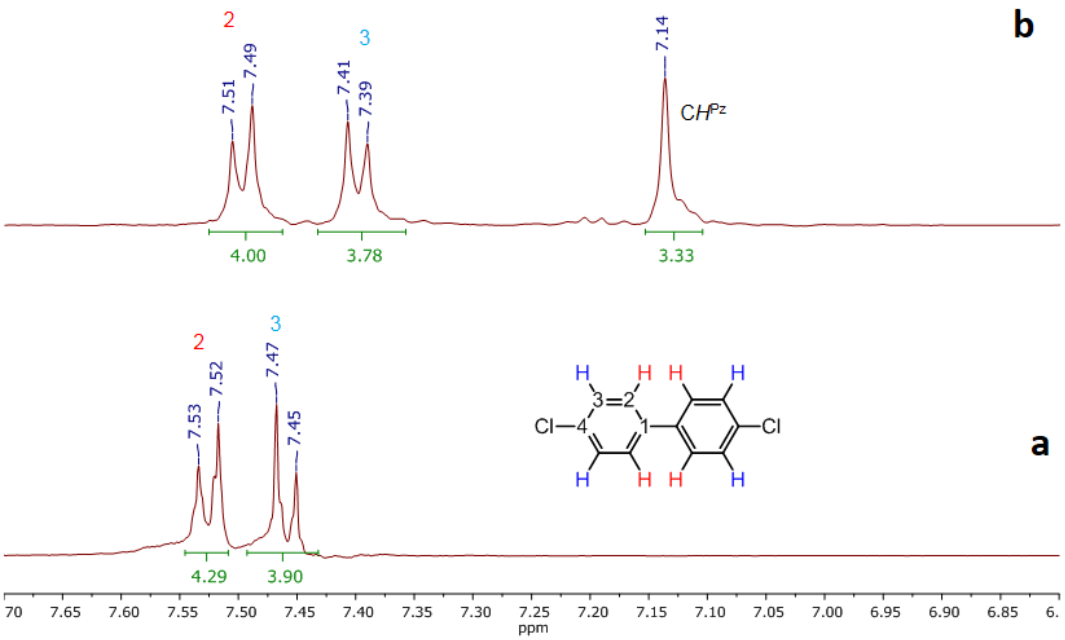


Figure S7. ^{1}H NMR spectra of **3** (a) and **3** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

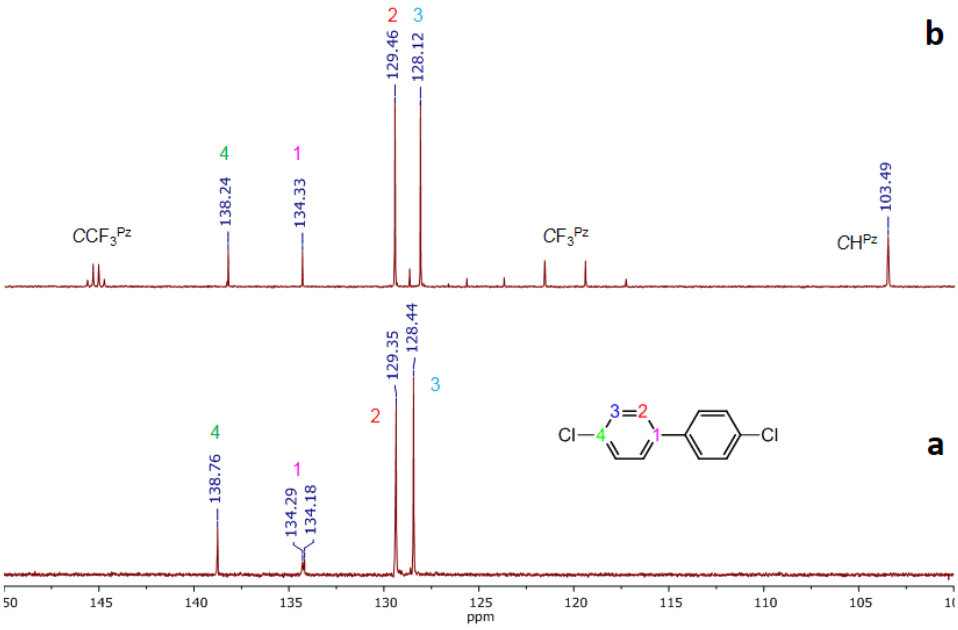


Figure S8. ^{13}C NMR spectra of **3** (a) and **3** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

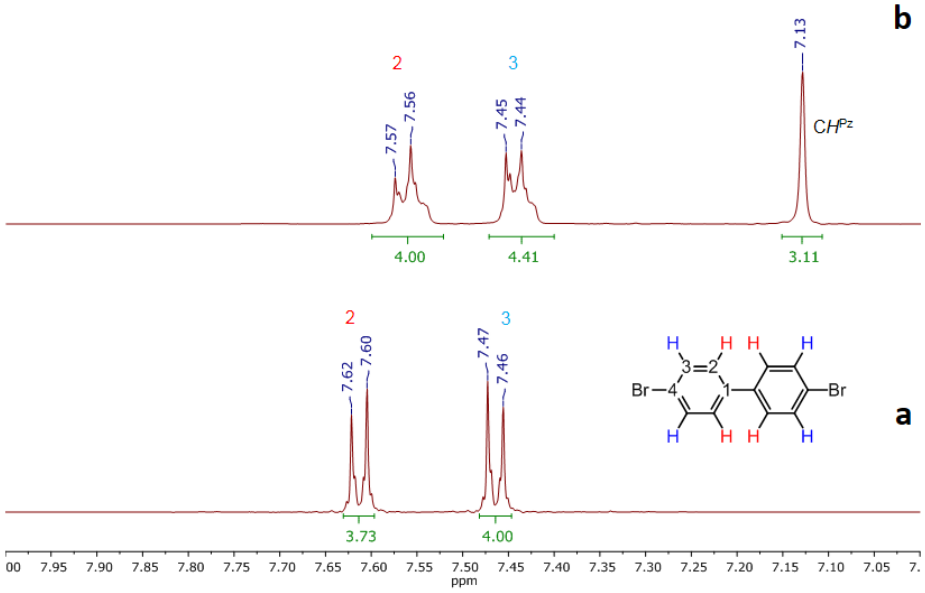


Figure S9. ^{1}H NMR spectra of 4 (a) and 4 in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

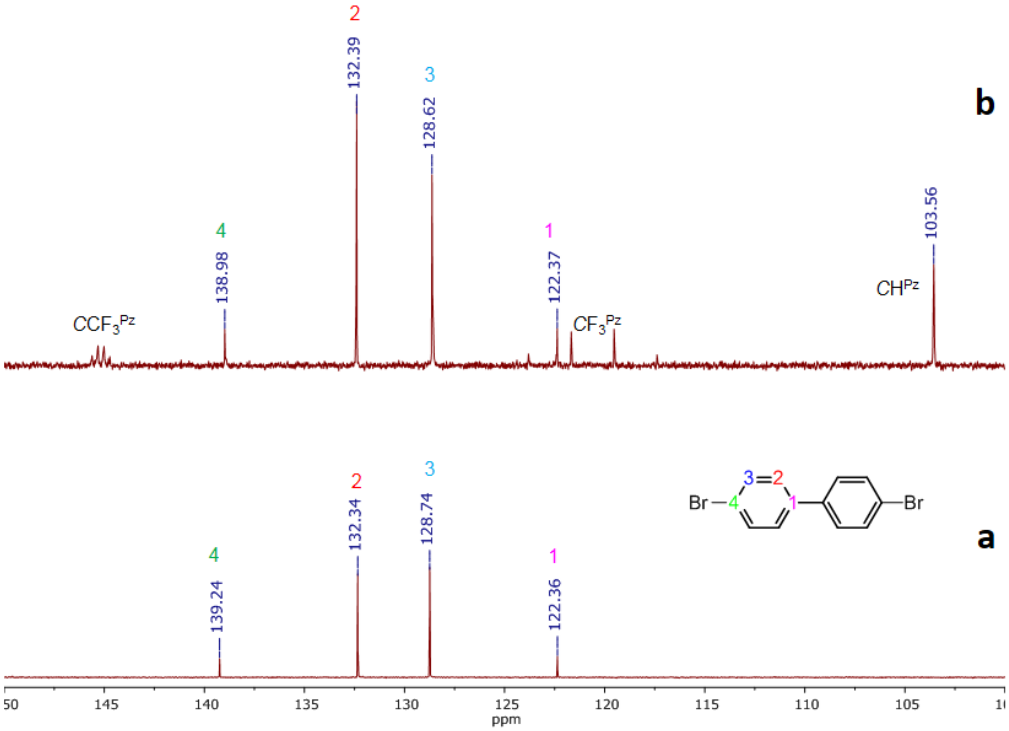


Figure S10. ^{13}C NMR spectra of **4** (a) and **4** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

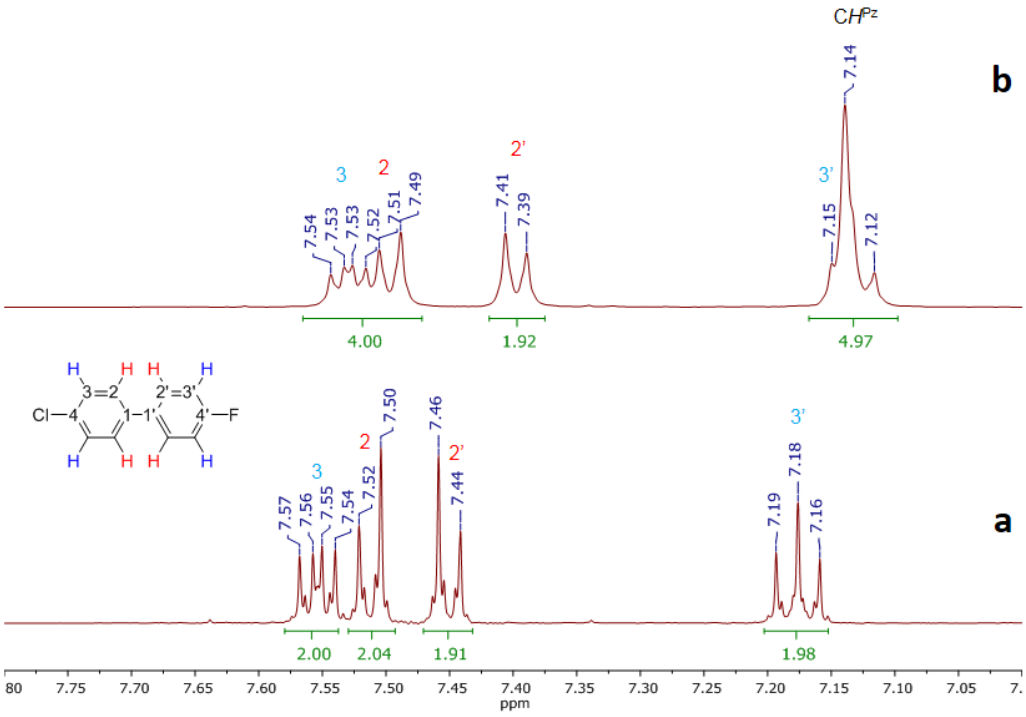


Figure S11. ^{1}H NMR spectra of **5** (a) and **5** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

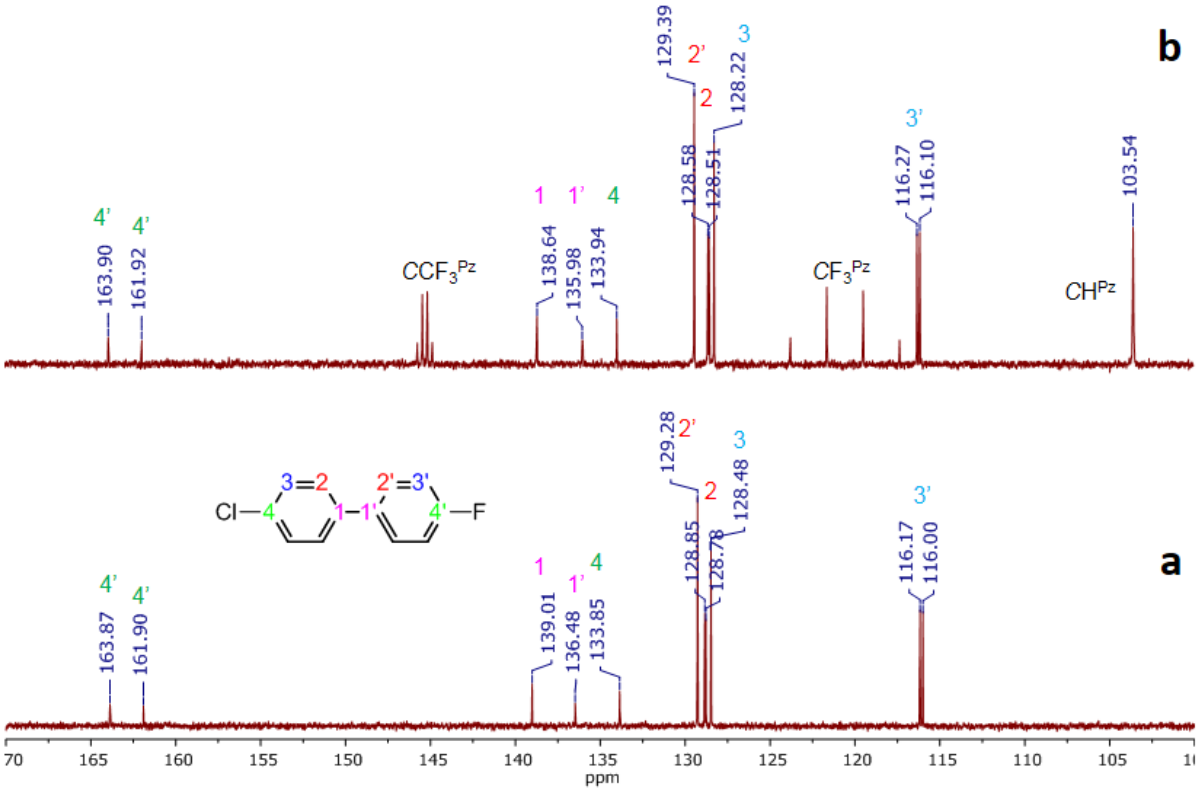


Figure S12. ^{13}C NMR spectra of **5** (a) and **5** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

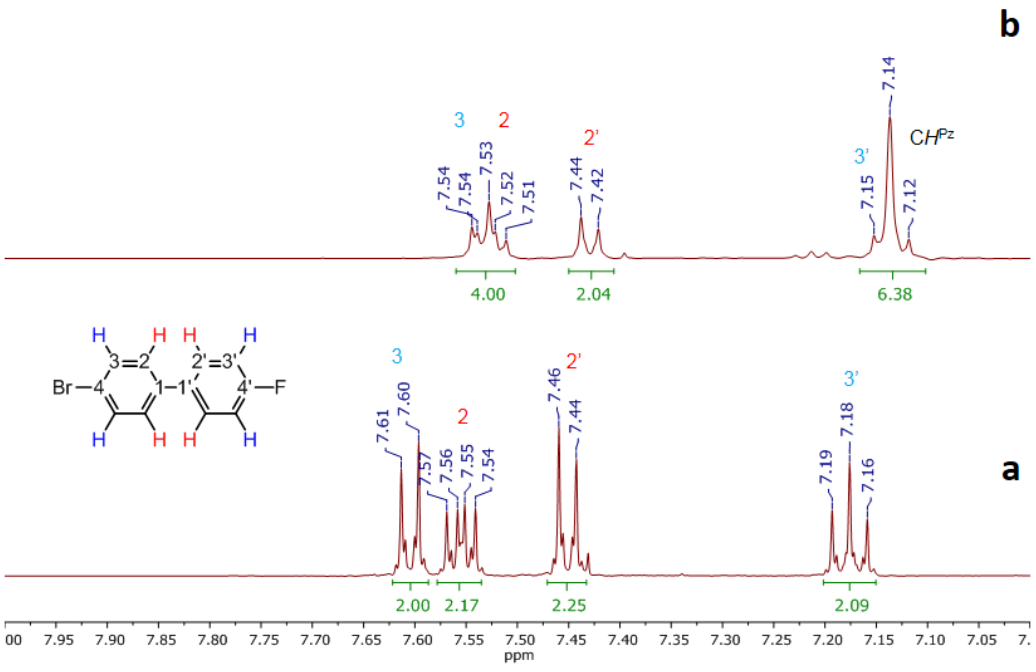


Figure S13. ^{1}H NMR spectra of **6** (a) and **6** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

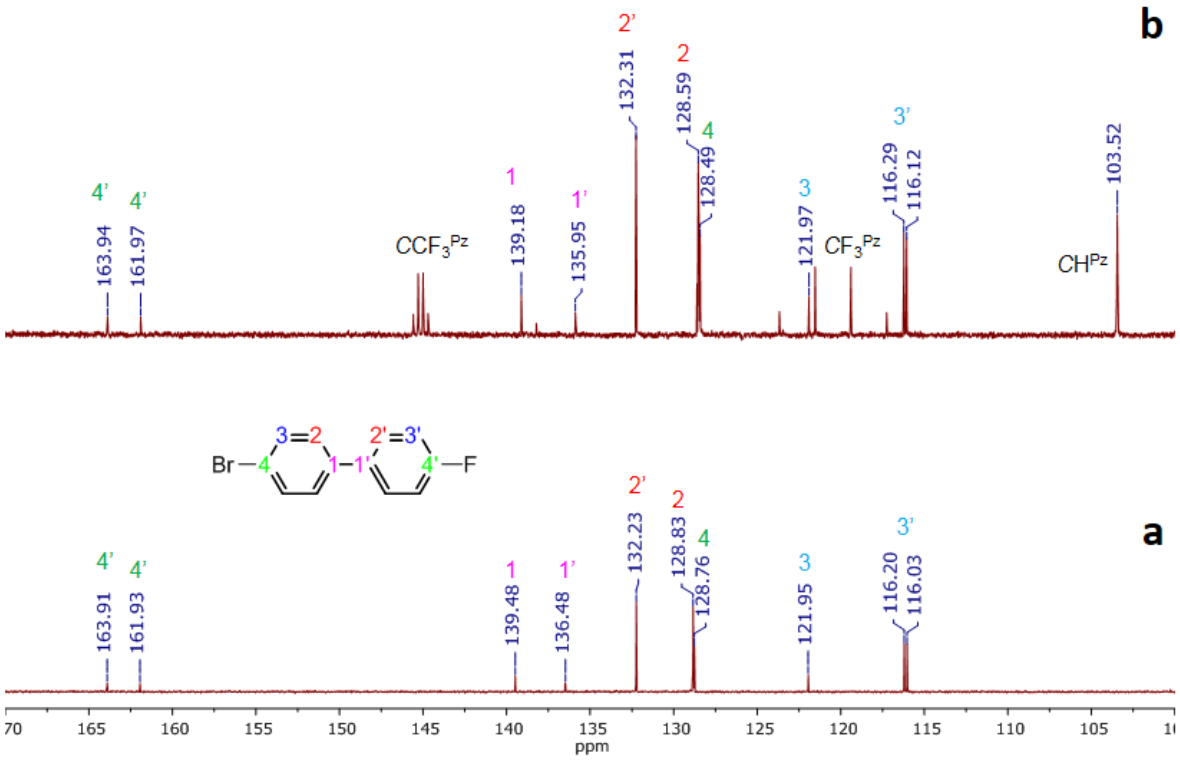


Figure S14. ^{13}C NMR spectra of **6** (a) and **6** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

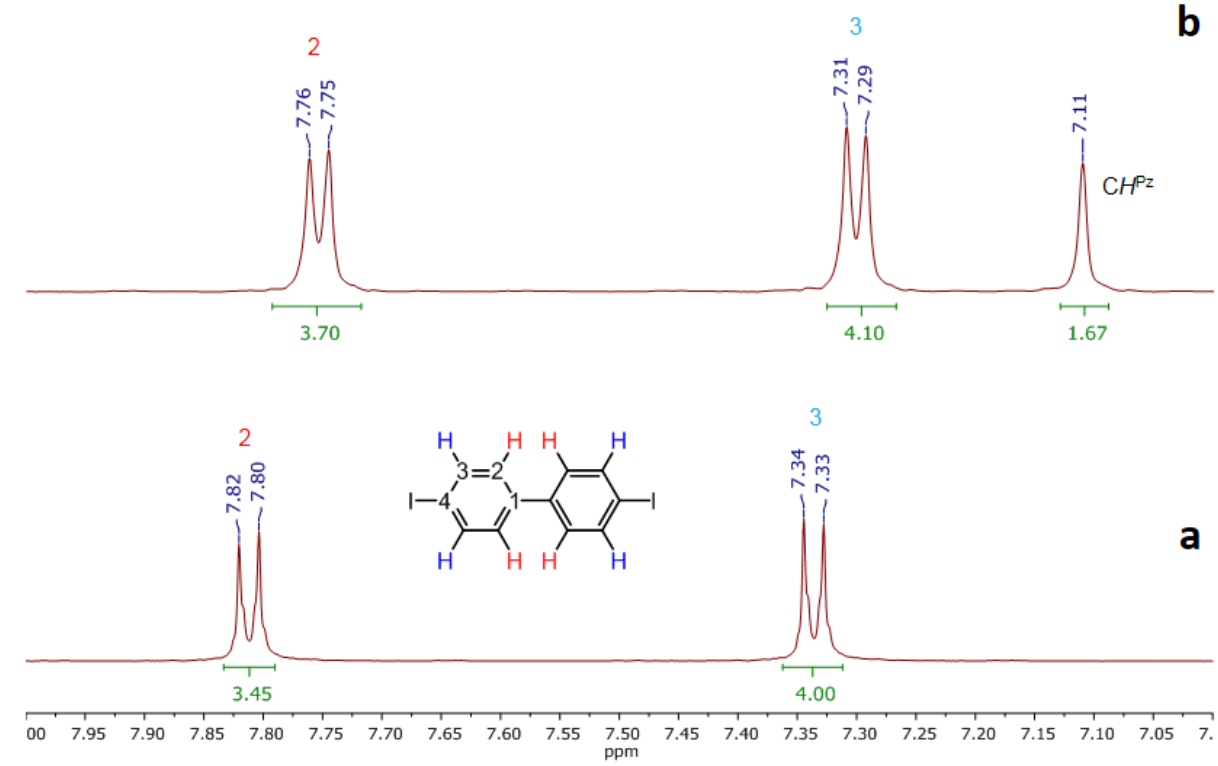


Figure S15. ^{13}H NMR spectra of **7** (a) and **7** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

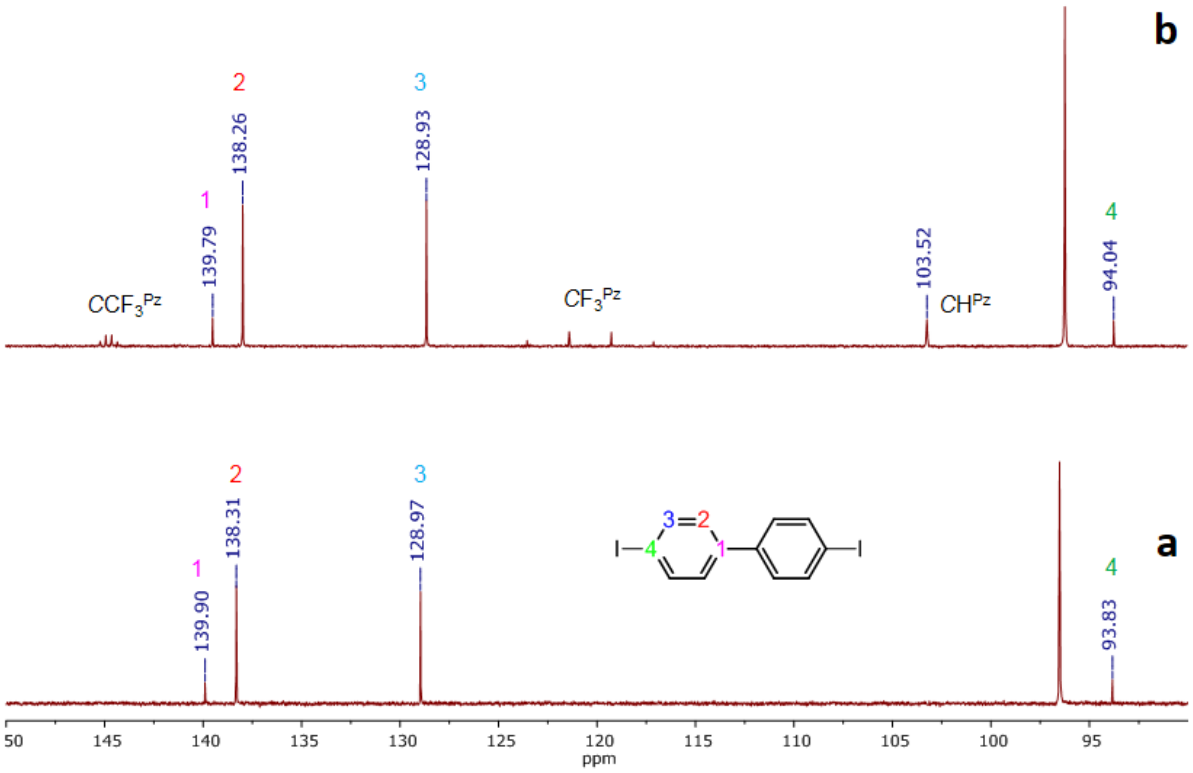
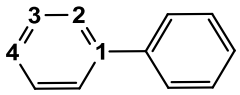
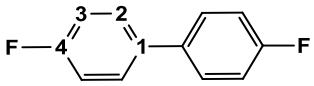


Figure S16. ^{13}C NMR spectra of **7** (a) and **7** in the presence of 1 eq. of $[AgL]_3$ (b) ($0.55CCl_4/0.1CD_2Cl_2$).

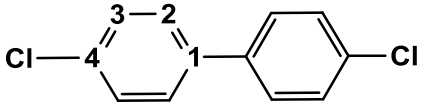
Table S6. ^{13}C NMR data for initial biphenyls and in the presence of $[AgL]_3$.



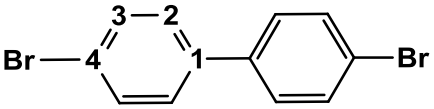
	1	2	3	4
L	141.60	127.43	128.95	127.39
+1 eq. [AgL]3	141.17	127.89	129.31	126.52
Δδ, ppm	-0.43	+0.46	+0.64	-0.87



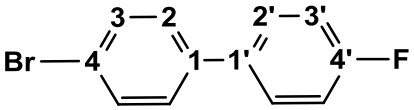
L	136.73	128.82	115.99	162.71
+1 eq. [AgL]3	136.36	129.61	116.09	162.74
Δδ, ppm	-0.37	-0.21	+0.1	+0.03



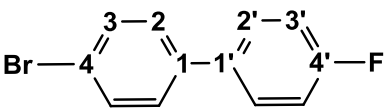
L	134.24	129.35	128.44	138.76
+1 eq. [AgL]3	134.33	129.46	128.12	138.24
Δδ, ppm	+0.09	+0.11	-0.32	-0.52



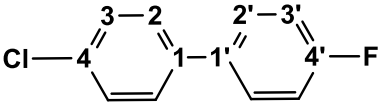
L	122.36	132.34	128.74	139.24
+1 eq. [AgL]3	122.37	132.39	128.62	138.98
Δδ, ppm	+0.01	+0.04	-0.12	-0.26



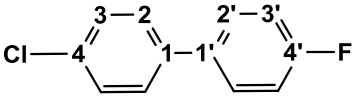
L	139.48	128.83	121.95	128.76
+1 eq. [AgL]3	139.18	128.59	121.97	128.49
Δδ, ppm	-0.3	-0.24	+0.02	-0.27



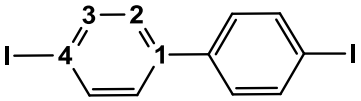
	1'	2'	3'	4'
L	136.48	132.23	116.12	162.92
+1 eq. [AgL]3	135.95	132.31	116.21	162.96
Δδ, ppm	-0.53	+0.08	+0.09	+0.04



L	139.01	128.85	128.48	133.85
+1 eq. [AgL]3	138.64	128.55	128.22	133.94
Δδ, ppm	-0.65	-0.3	-0.26	+0.09



	1'	2'	3'	4'
L	136.48	129.28	116.09	162.89
+1 eq. [AgL]3	135.98	129.39	116.19	162.91
Δδ, ppm	-0.5	+0.11	+0.1	+0.02



L	139.9	138.31	128.97	93.83
+1 eq. [AgL]3	139.79	138.26	128.93	94.04
Δδ, ppm	-0.11	-0.05	-0.04	+0.21

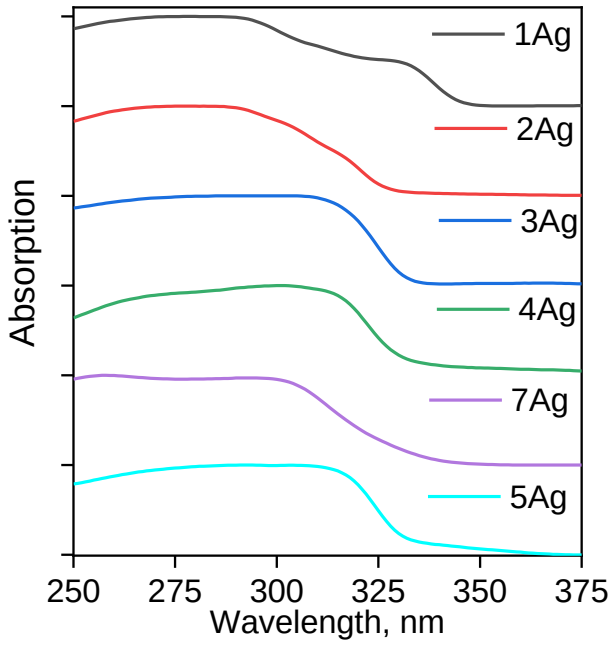


Figure S17. Diffuse reflectance spectra of investigated crystalline compounds.

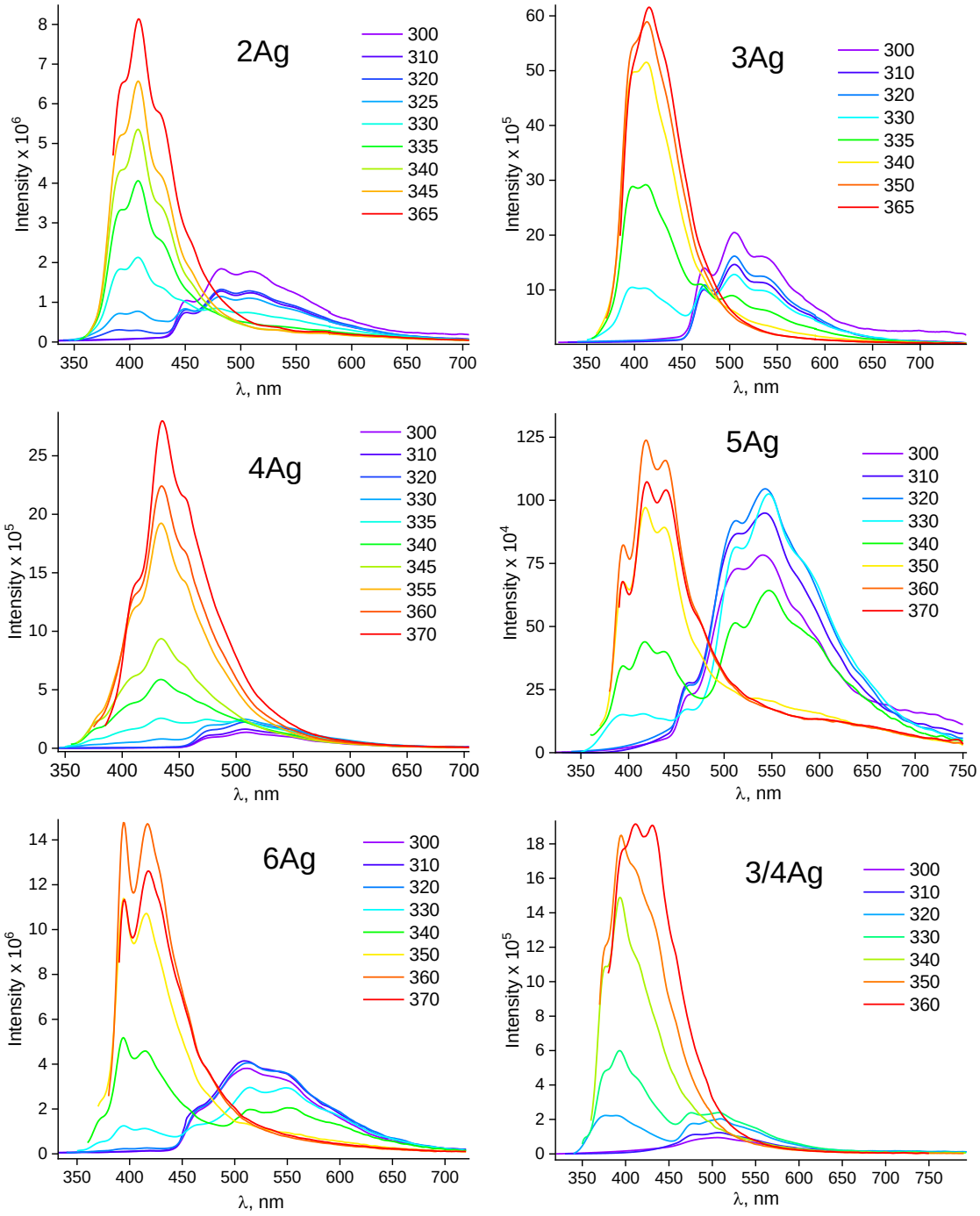


Figure S18. Emission spectra of solid samples of **2Ag-6Ag** and **3/4Ag** measured at different excitations (300-370 nm) at 300K.

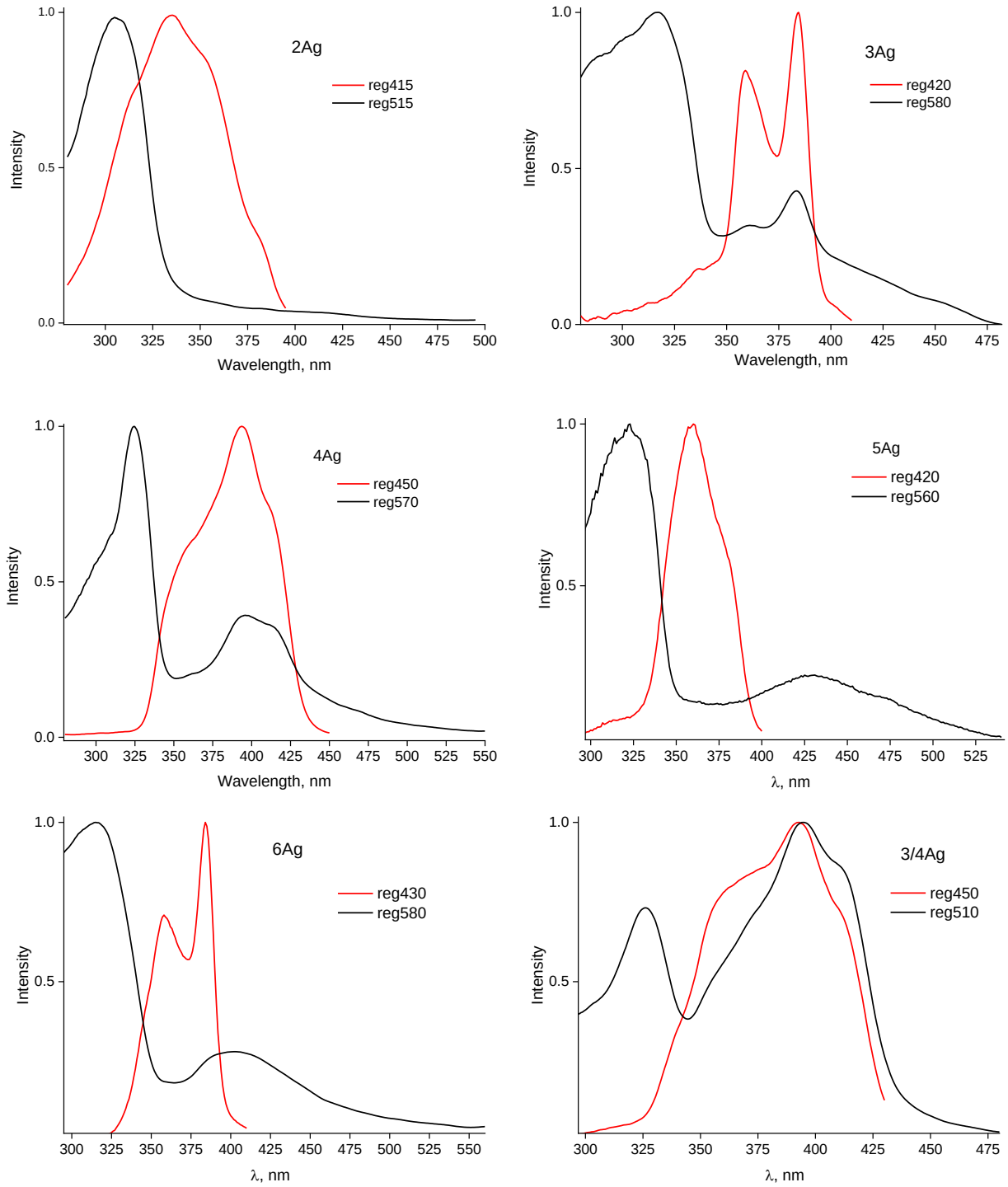


Figure S19. Optical excitation spectra of solid samples of **2Ag-6Ag** and **3/4Ag** registered at phosphorescence maxima (black curve) and fluorescence maxima (red curve) at 300K.

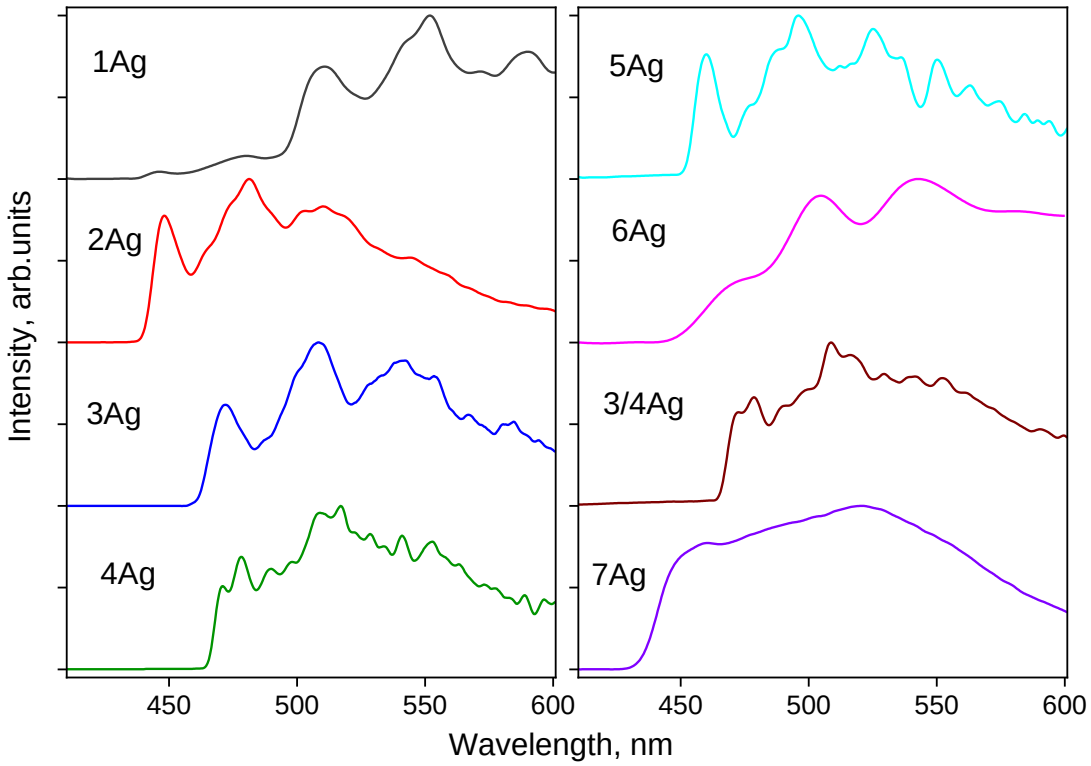


Figure S20. Phosphorescence spectra of solid samples of complexes obtained (λ_{exc}=320 nm) (time delay 10 μs).

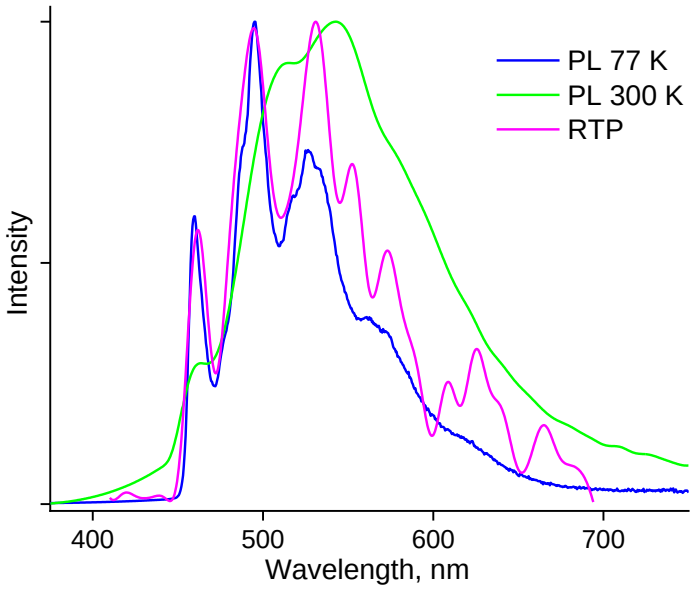


Figure S21. Photoluminescence spectra registered at 77 K (blue curve) and 300 K (green curve) and room temperature phosphorescence of **5Ag** compound upon excitation at 310 nm.

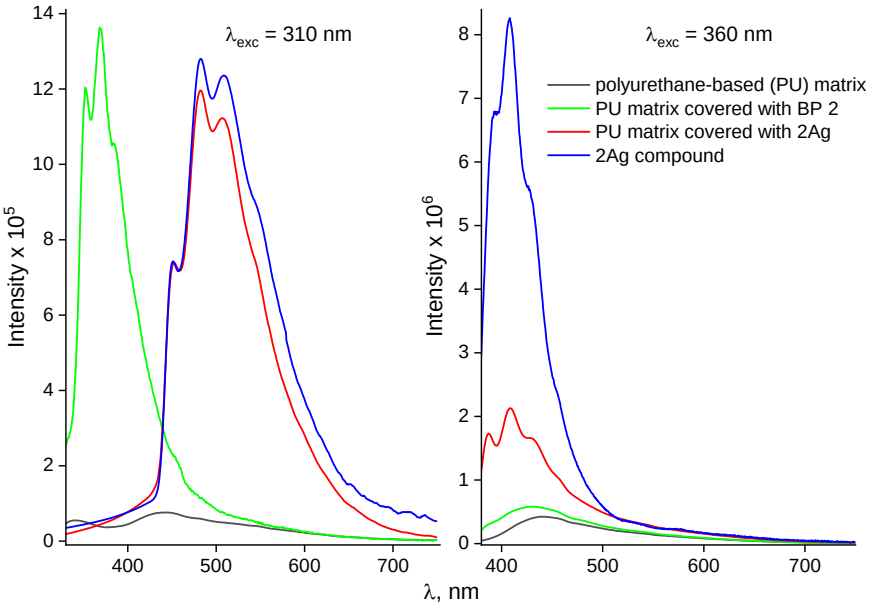


Figure S22. The PL spectra of free polyurethane-based matrix (grey curve) and polyurethane-based matrix covered with **BP 2** (green curve) and **2Ag** (red curve) under excitation at 360 and 310 nm at 300 K. PL spectra of **2Ag** compounds in crystalline powder at the same excitation conditions are for reference.

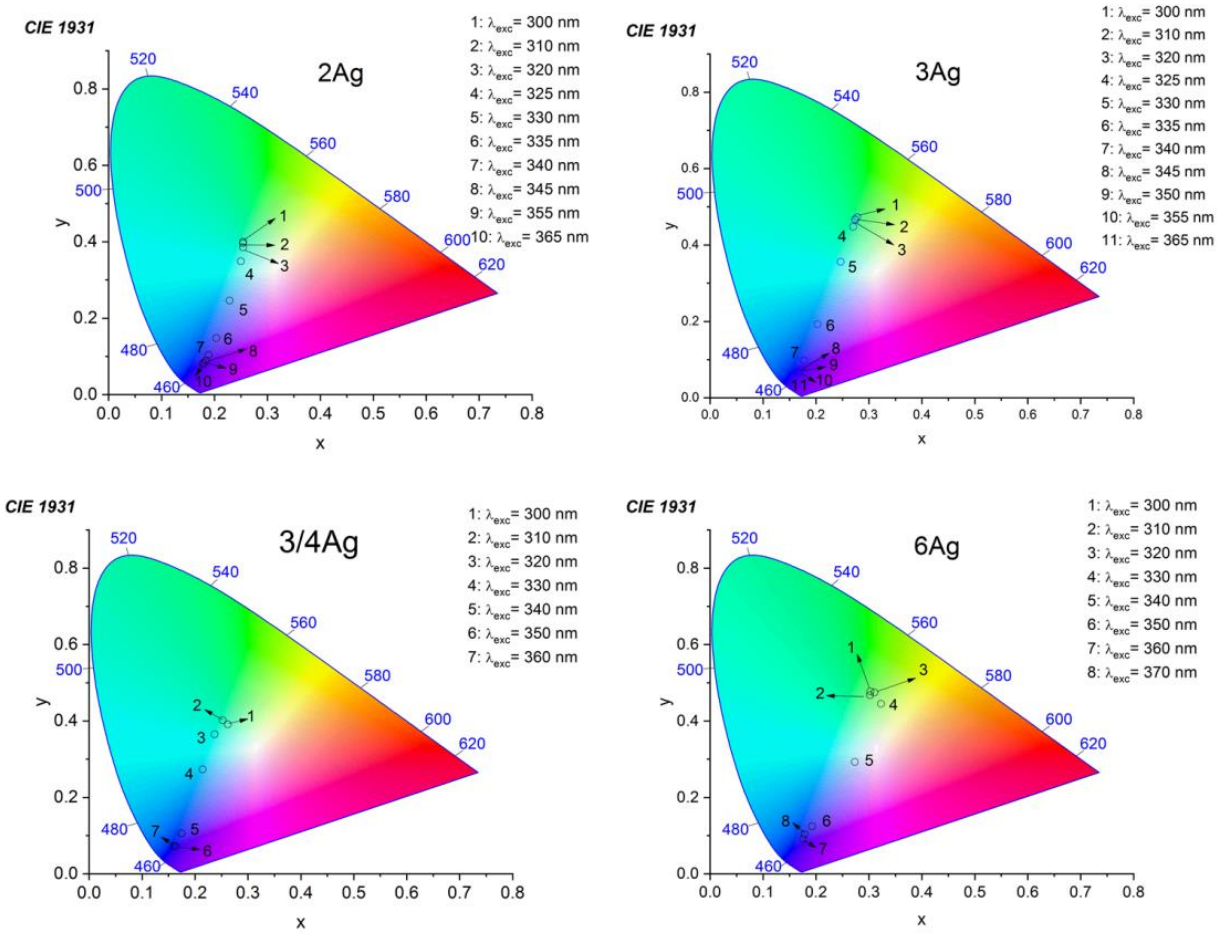


Figure S23. The CIE 1931 coordinates for **2Ag, 3Ag, 6Ag** and **3/4Ag**.

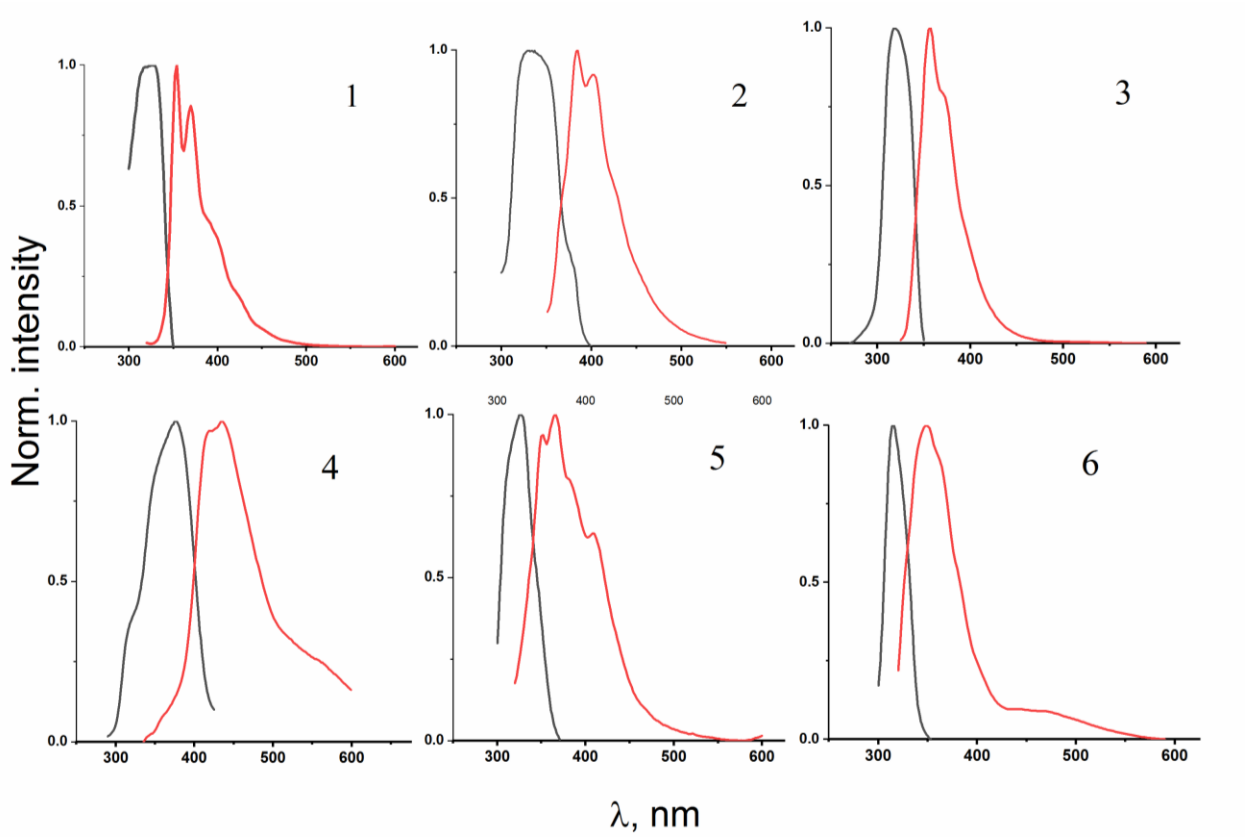


Figure S24. The normalized emission (red curves, λ_{exc}=310 nm) and excitation (black lines, recorded on the corresponding emission maxima) spectra of free BPs **1-6**.

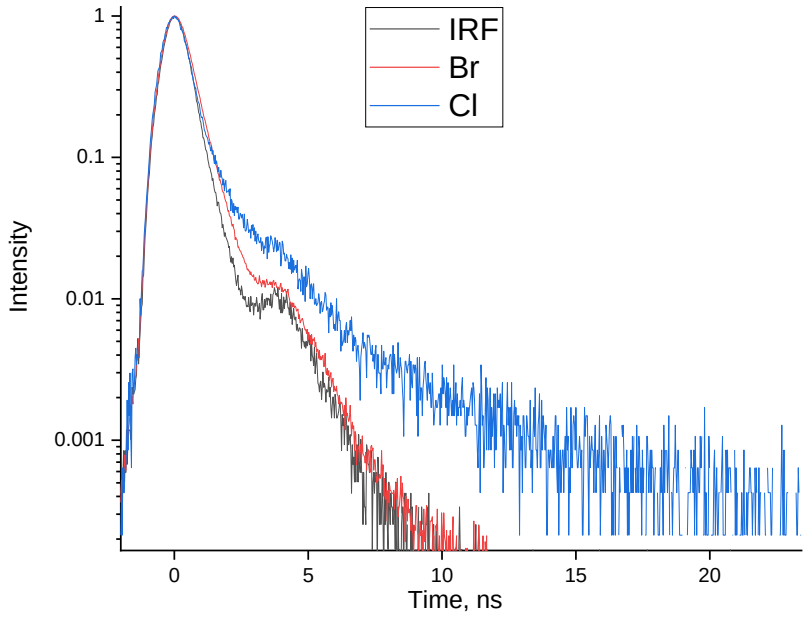


Figure S25. PL decays recorded for **3Ag** and **4Ag** with a pulsed laser excitation at 376 nm.

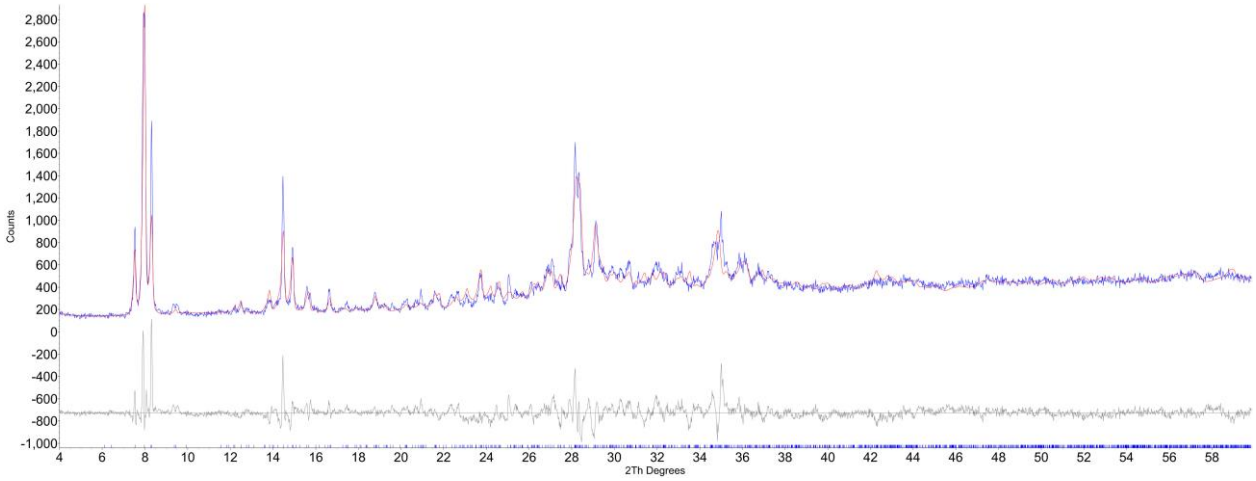


Figure S26. The XRPD patterns (blue) and result of Rietveld refinement (red) for **1Ag**. Difference curve is shown by grey line.

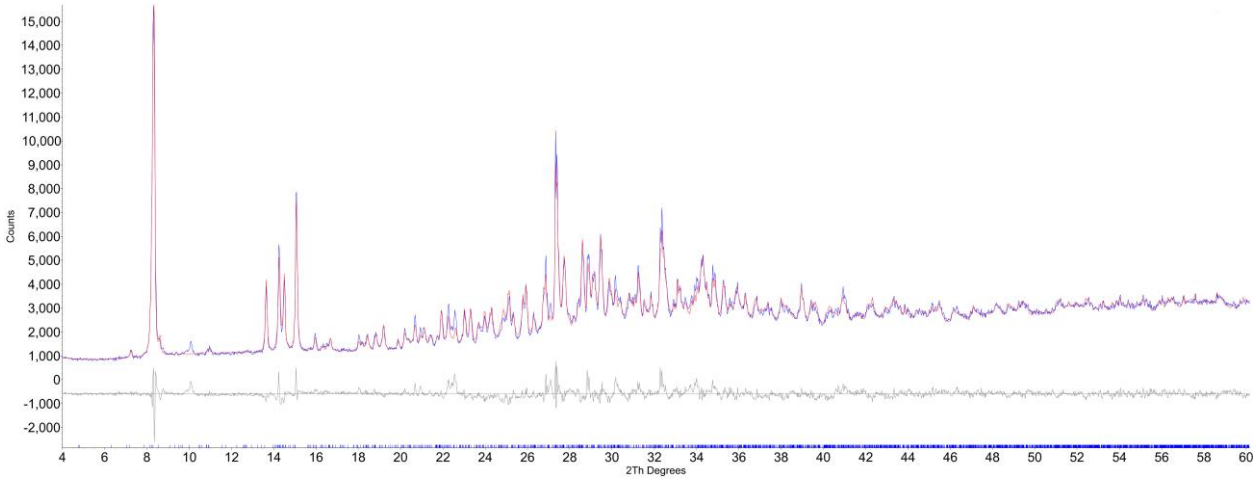


Figure S27. The XRPD patterns (blue) and result of Rietveld refinement (red) for **2Ag**. Difference curve is shown by grey line.

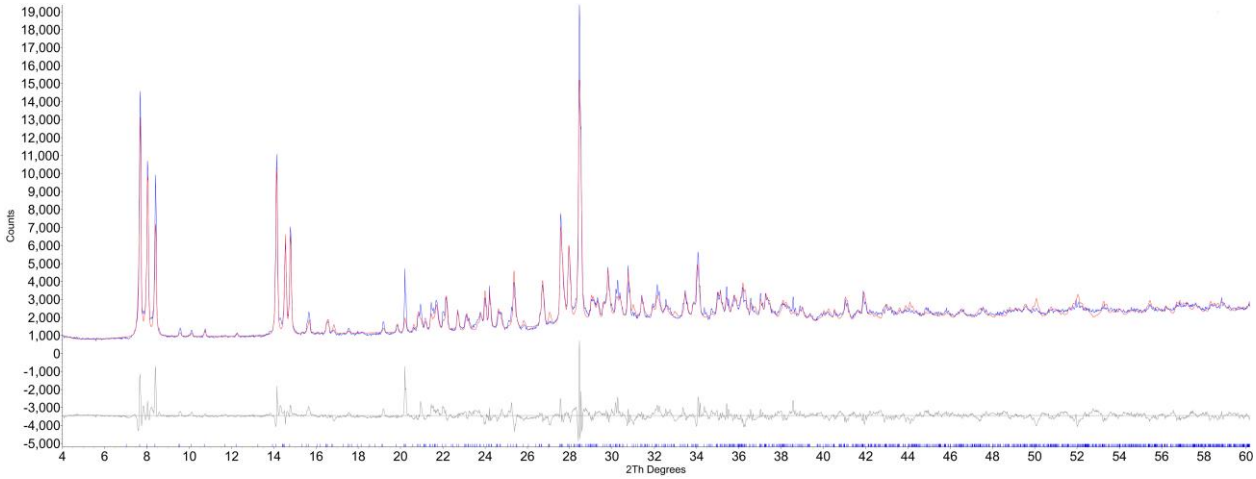


Figure S28. The XRPD patterns (blue) and result of Rietveld refinement (red) for **3Ag**. Difference curve is shown by grey line.

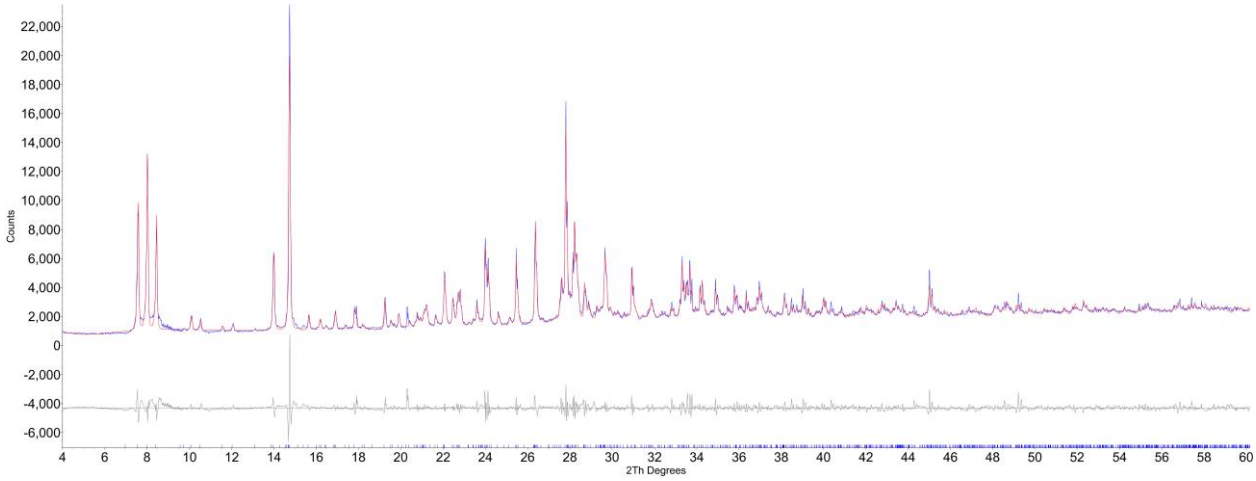


Figure S29. The XRPD patterns (blue) and result of Rietveld refinement (red) for **4Ag**. Difference curve is shown by grey line.

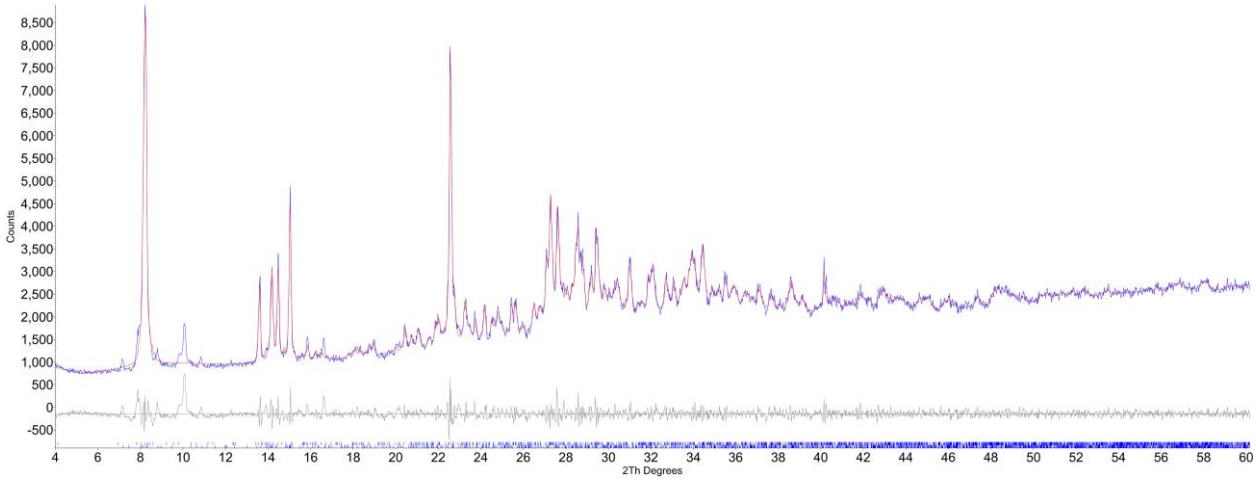


Figure S30. The XRPD patterns (blue) and result of Rietveld refinement (red) for **5Ag**. Difference curve is shown by grey line.

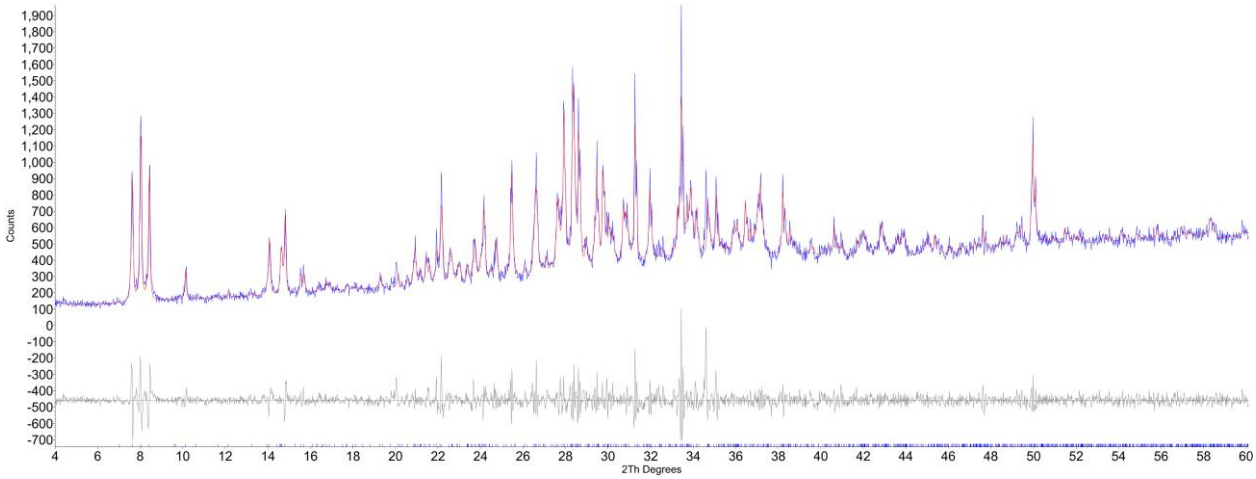


Figure S31. The XRPD patterns (blue) and result of Rietveld refinement (red) for **3/4Ag**. Difference curve is shown by grey line.

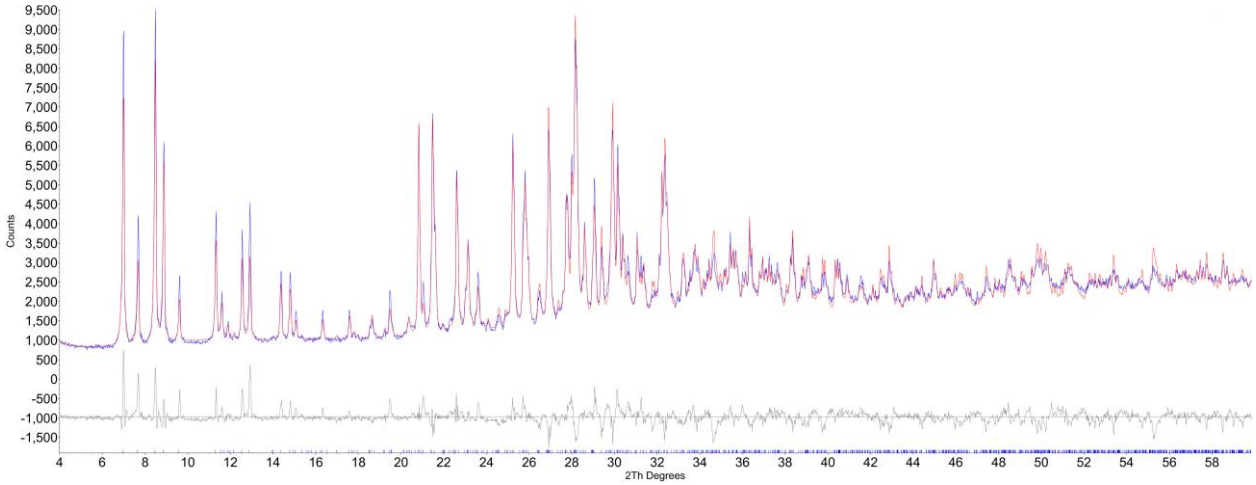


Figure S32. The XRPD patterns (blue) and result of Rietveld refinement (red) for **7Ag**. Difference curve is shown by grey line.

Table S7. Energetic characteristics of 10 lowest singlet excittions (without symmetry restrictions) and fragment (Ag_3^1 and L_3^1 from one macrocycle, Ag_3^2 and L_3^2 from second macrocycle, and biphenyl) contributions to the transition electron density for all possible units of complexes **1Ag**-**5Ag**. Lowest symmetry allowed transition marked as italic, MLCT states market with bold.

1Ag, head-to-tail

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	4.977	40140.8	249.1	0.00002	4	3	5	3	85	5	4	5	4	81
S2	*4.983*	*40193.6*	*248.8*	*0.23517*	*5*	*3*	*5*	*3*	*84*	*6*	*4*	*6*	*4*	*80*
S3	**5.142**	**41475.4**	**241.1**	**0.00988**	**19**	**10**	**20**	**11**	**39**	**21**	**9**	**23**	**9**	**38**
S4	5.175	41736.1	239.6	0.00009	19	10	19	10	42	33	13	33	13	8
S5	5.197	41913.6	238.6	0.00016	28	14	28	15	15	32	13	32	13	9
S6	5.264	42461.0	235.5	0.03791	17	10	17	10	47	18	9	18	9	45
S7	5.300	42743.5	234.0	0.07420	26	14	25	13	22	29	13	27	12	19
S8	5.475	44156.8	226.5	0.00000	17	8	17	8	49	33	13	33	13	8
S9	5.794	46734.3	214.0	0.00952	9	4	9	4	76	35	12	34	12	6
S10	5.856	47231.4	211.7	0.00013	11	9	12	9	60	9	9	8	9	65

1Ag, head-to-head

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	4.902	39534.0	252.9	0.00624	4	4	4	3	85	8	4	8	4	75
S2	*5.037*	*40622.3*	*246.2*	*0.24658*	*4*	*4*	*3*	*3*	*86*	*4*	*4*	*4*	*4*	*84*
S3	**5.104**	**41166.8**	**242.9**	**0.00186**	**41**	**21**	**7**	**4**	**27**	**51**	**20**	**11**	**5**	**13**
S4	5.167	41672.9	240.0	0.00255	13	7	44	21	16	14	7	50	19	10
S5	5.187	41839.6	239.0	0.00473	9	6	7	5	73	10	6	8	5	72
S6	5.237	42240.7	236.7	0.01954	47	23	10	5	15	53	21	12	5	8
S7	5.264	42459.1	235.5	0.00932	7	4	51	26	12	7	4	57	22	9
S8	5.477	44176.8	226.4	0.01144	8	6	8	5	73	32	12	27	11	18
S9	5.706	46020.7	217.3	0.04021	7	7	6	5	75	19	8	23	9	41
S10	5.928	47809.9	209.2	0.00246	35	39	6	5	15	53	21	6	4	15

2Ag; iso1

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	4.831	38964.0	256.6	0.00666	4	3	3	2	88	9	5	5	4	77
S2	*4.977*	*40144.3*	*249.1*	*0.24114*	*4*	*3*	*5*	*3*	*86*	*5*	*4*	*7*	*4*	*80*
S3	**5.131**	**41388.1**	**241.6**	**0.01656**	**19**	**10**	**13**	**7**	**51**	**32**	**12**	**27**	**11**	**18**
S4	5.222	42118.3	237.4	0.01184	9	5	40	20	27	10	5	43	17	24
S5	5.228	42165.4	237.2	0.01909	54	26	5	3	11	60	23	6	4	7
S6	5.260	42421.1	235.7	0.02423	25	13	31	16	16	27	12	34	14	12
S7	5.275	42548.3	235.0	0.00311	5	3	21	11	60	5	3	22	10	59
S8	5.460	44034.2	227.1	0.00062	14	7	18	9	52	27	10	38	15	10
S9	5.726	46187.0	216.5	0.01776	9	5	6	3	77	34	12	25	9	20
S10	5.951	47996.7	208.3	0.00639	5	4	34	46	12	4	4	54	22	16

2Ag; iso2

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP

S1	4.872	39295.2	254.5	0.01346	3	2	3	2	89	9	5	6	4	76
S2	*5.131*	*41380.8*	*241.7*	*0.24874*	*3*	*3*	*3*	*2*	*89*	*4*	*4*	*4*	*3*	*85*
S3	**5.177**	**41759.2**	**239.5**	**0.00035**	**10**	**6**	**9**	**5**	**70**	**20**	**9**	**19**	**8**	**45**
S4	5.304	42777.5	233.8	0.01139	58	28	2	2	10	60	25	2	2	10
S5	5.333	43013.2	232.5	0.01123	41	19	16	9	15	43	18	18	8	13
S6	5.352	43167.2	231.7	0.01675	6	4	34	18	37	7	4	38	17	34
S7	5.368	43298.9	231.0	0.01981	6	3	54	27	10	6	4	56	24	11
S8	5.586	45057.7	221.9	0.01002	10	6	13	7	65	30	12	28	12	18
S9	5.786	46663.5	214.3	0.05336	5	4	7	5	80	29	11	34	13	13
S10	5.948	47975.6	208.4	0.00257	41	55	1	1	2	66	25	1	2	7

2Ag; iso3

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	4.835	38996.4	256.4	0.01200	3	2	4	3	88	4	3	15	6	71
S2	*5.045*	*40689.2*	*245.8*	*0.15716*	*10*	*6*	*4*	*3*	*77*	*18*	*7*	*6*	*4*	*65*
S3	**5.104**	**41162.7**	**242.9**	**0.06955**	**12**	**7**	**15**	**8**	**58**	**22**	**10**	**20**	**8**	**40**
S4	5.186	41825.7	239.1	0.02807	19	10	36	18	17	21	10	39	16	14
S5	5.254	42373.7	236.0	0.01094	24	12	5	3	55	26	12	6	4	52
S6	5.315	42869.5	233.3	0.00757	6	4	56	27	7	7	4	58	24	8
S7	5.319	42902.0	233.1	0.02222	52	25	8	5	10	56	23	8	5	8
S8	5.476	44168.9	226.4	0.00208	10	5	6	3	75	35	14	16	7	28
S9	5.733	46236.1	216.3	0.01653	4	3	7	4	81	21	7	39	14	19
S10	5.913	47690.8	209.7	0.00009	1	1	40	56	2	1	2	66	24	7

3Ag; axial

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	*4.759*	*38386.8*	*260.5*	*0.46504*	*3*	*2*	*3*	*2*	*89*	*4*	*3*	*4*	*3*	*86*
S2	4.834	38991.3	256.5	0.00000	4	2	4	2	88	6	4	6	4	82
S3	5.111	41220.2	242.6	0.00352	9	5	9	5	73	7	4	7	4	78
S4	5.156	41583.3	240.5	0.00000	24	12	24	12	27	32	13	32	13	10
S5	5.212	42037.7	237.9	0.03398	26	13	26	13	21	29	13	29	13	16
S6	5.262	42444.0	235.6	0.00000	26	14	26	14	21	32	14	32	14	9
S7	5.288	42646.8	234.5	0.03794	28	14	28	14	14	32	14	32	14	7
S8	5.518	44503.8	224.7	0.00000	15	7	15	7	56	31	12	31	12	14
S9	5.743	46323.9	215.9	0.02329	7	4	7	4	78	34	12	34	12	7
S10	5.747	46356.5	215.7	0.00000	14	9	14	9	55	8	7	8	7	70

3Ag; non-axial

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	4.759	38384.6	260.5	0.00000	3	2	3	2	89	6	4	6	4	79
S2	*4.811*	*38803.9*	*257.7*	*0.43444*	*3*	*2*	*3*	*2*	*90*	*4*	*3*	*4*	*3*	*86*
S3	5.132	41396.2	241.6	0.00264	7	4	6	4	79	5	4	5	4	82
S4	5.205	41979.8	238.2	0.00009	27	13	22	12	26	35	14	29	12	10
S5	5.209	42011.0	238.0	0.03938	28	14	31	15	13	30	13	34	14	10
S6	5.290	42664.9	234.4	0.00000	30	15	29	14	12	33	14	33	13	7
S7	5.336	43039.5	232.3	0.02601	30	15	29	14	12	32	13	31	13	10
S8	5.458	44018.8	227.2	0.00000	11	5	11	5	68	32	12	32	12	13
S9	5.756	46423.5	215.4	0.00000	12	9	12	9	59	7	8	7	8	70

S10	5.796	46746.5	213.9	0.00777	5	2	4	2	87	35	12	35	12	6

4Ag; axial

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	*4.691*	*37836.6*	*264.3*	*0.56559*	*3*	*2*	*3*	*2*	*90*	*4*	*3*	*4*	*3*	*87*
S2	4.823	38904.1	257.0	0.00000	4	2	4	2	88	5	4	5	4	82
S3	5.101	41146.3	243.0	0.00106	7	4	6	4	79	5	3	5	3	84
S4	5.203	41966.8	238.3	0.00000	24	12	24	12	27	32	13	32	13	9
S5	5.241	42269.9	236.6	0.03180	28	14	28	14	15	32	13	32	13	10
S6	5.276	42555.3	235.0	0.00000	25	13	24	13	26	31	14	31	14	10
S7	5.324	42941.7	232.9	0.03147	28	14	28	14	16	32	14	32	14	7
S8	5.543	44710.7	223.7	0.00000	16	8	16	8	50	30	12	30	12	15
S9	5.758	46441.6	215.3	0.02245	7	4	7	5	77	34	13	34	13	7
S10	5.766	46502.1	215.0	0.00000	12	8	12	8	59	8	7	8	7	70

4Ag; non-axial

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	4.720	38070.6	262.7	0.00000	3	2	3	2	90	7	4	7	4	78
S2	*4.735*	*38194.0*	*261.8*	*0.52374*	*3*	*2*	*3*	*2*	*91*	*4*	*3*	*4*	*3*	*87*
S3	5.093	41073.8	243.5	0.00238	5	4	5	4	82	4	3	4	3	85
S4	5.218	42083.8	237.6	0.02089	30	14	30	14	12	32	14	32	14	9
S5	5.222	42122.2	237.4	0.00001	25	13	25	13	24	31	13	31	13	11
S6	5.294	42696.8	234.2	0.00000	29	15	29	15	12	33	13	33	13	8
S7	5.335	43027.9	232.4	0.02405	30	15	30	15	10	32	14	32	14	8
S8	5.494	44313.5	225.7	0.00000	10	5	10	5	69	30	11	29	11	19
S9	5.714	46083.1	217.0	0.00000	11	8	11	8	63	9	8	9	8	66
S10	5.800	46779.5	213.8	0.01371	5	2	5	2	86	34	12	35	12	6

5Ag; head-to-head

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	4.810	38797.5	257.7	0.01310	3	2	3	2	89	7	4	8	4	76
S2	*5.003*	*40352.5*	*247.8*	*0.34006*	*3*	*3*	*3*	*2*	*89*	*4*	*3*	*4*	*3*	*85*
S3	**5.132**	**41394.5**	**241.6**	**0.00220**	**7**	**4**	**4**	**3**	**82**	**15**	**7**	**13**	**6**	**60**
S4	5.226	42148.2	237.3	0.00262	3	2	52	26	17	3	3	57	23	15
S5	5.273	42531.7	235.1	0.00951	54	26	5	3	12	58	23	5	3	11
S6	5.292	42685.6	234.3	0.01989	50	25	4	3	19	54	22	4	3	17
S7	5.316	42880.0	233.2	0.01643	3	2	58	29	8	3	2	62	24	8
S8	5.497	44339.8	225.5	0.00792	12	6	6	4	72	25	10	33	12	20
S9	5.769	46532.2	214.9	0.03451	6	4	5	4	81	32	12	21	8	27
S10	5.934	47863.2	208.9	0.00205	2	3	38	52	5	2	3	62	24	10

5Ag; head-to-tail displaced

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	4.763	38418.5	260.3	0.00230	4	2	4	3	87	8	4	10	5	73
S2	*4.882*	*39372.3*	*254.0*	*0.35960*	*3*	*3*	*3*	*2*	*88*	*5*	*4*	*4*	*3*	*85*
S3	**5.159**	**41609.2**	**240.3**	**0.00040**	**15**	**8**	**11**	**6**	**60**	**16**	**8**	**12**	**5**	**59**
S4	5.185	41818.2	239.1	0.00891	23	12	22	12	32	26	11	25	11	27
S5	5.224	42131.3	237.4	0.01573	24	12	32	16	16	27	11	36	16	11

S6	5.261	42435.3	235.7	0.01165	12	7	42	21	19	13	7	46	19	16
S7	5.297	42720.2	234.1	0.01141	40	20	14	7	19	48	20	15	7	10
S8	5.486	44247.6	226.0	0.00661	14	7	9	5	64	25	10	33	13	19
S9	5.723	46162.2	216.6	0.02097	7	4	5	3	80	42	14	27	10	7
S10	5.798	46764.9	213.8	0.02973	18	11	9	6	55	9	10	8	7	65

5Ag; head-to-tail

	E				GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	f	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
S1	4.745	38270.0	261.3	0.00290	4	3	3	3	87	8	4	8	5	75
S2	*4.876*	*39328.2*	*254.3*	*0.34047*	*3*	*3*	*3*	*2*	*89*	*4*	*3*	*5*	*3*	*84*
S3	**5.148**	**41517.5**	**240.9**	**0.01243**	**19**	**10**	**19**	**11**	**41**	**21**	**9**	**23**	**10**	**37**
S4	5.164	41648.2	240.1	0.00913	35	18	6	4	37	40	16	6	4	34
S5	5.187	41836.8	239.0	0.00272	14	8	28	14	36	17	8	35	14	25
S6	5.202	41955.9	238.3	0.00298	21	11	35	17	17	26	11	40	16	8
S7	5.270	42503.7	235.3	0.03014	23	12	29	15	22	27	12	31	13	16
S8	5.438	43858.5	228.0	0.00106	15	8	11	6	60	31	12	32	12	13
S9	5.714	46088.0	217.0	0.01102	8	5	6	3	78	36	13	28	10	13
S10	5.750	46380.9	215.6	0.00861	14	10	10	8	59	8	8	13	10	61

Table S8. Energetic characteristics of 10 lowest triplet excitations (without symmetry restrictions) and fragment (Ag_3^1 and L_3^1 from one macrocycle, Ag_3^2 and L_3^2 from second macrocycle, and biphenyl) contributions to the transition electron density for all possible units of complexes **1Ag**-**5Ag**.

1Ag, head-to-tail

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.498	28215.8	354.4	3	2	3	2	91	3	3	3	3	87
T2	4.331	34931.9	286.3	4	4	4	4	85	4	5	4	5	83
T3	4.442	35828.1	279.1	3	2	3	2	89	4	4	4	4	85
T4	4.582	36960.3	270.6	4	4	4	4	84	4	4	4	5	83
T5	4.621	37270.3	268.3	7	5	7	5	77	6	4	6	4	79
T6	4.682	37762.5	264.8	28	14	28	14	17	29	14	29	13	15
T7	4.701	37917.7	263.7	27	17	28	17	12	27	17	28	17	11
T8	4.710	37990.4	263.2	22	20	28	24	7	23	20	28	24	5
T9	4.722	38085.6	262.6	10	44	9	33	5	11	42	10	33	5
T10	4.730	38147.3	262.1	10	32	11	42	4	11	31	13	41	4

1Ag, head-to-head

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.517	28363.5	352.6	3	3	2	3	90	3	4	3	4	86
T2	4.283	34542.9	289.5	5	4	5	4	82	5	5	5	5	82
T3	4.387	35380.9	282.6	3	3	3	3	89	5	4	5	4	82
T4	4.501	36303.2	275.5	9	6	7	5	72	10	6	8	5	71
T5	4.627	37317.1	268.0	15	8	11	6	59	16	8	11	6	60
T6	4.644	37459.8	267.0	37	17	9	5	31	38	16	9	6	31
T7	4.678	37731.0	265.0	9	12	37	20	22	9	12	39	20	21
T8	4.712	38004.8	263.1	14	66	3	5	12	17	64	3	5	12

T9	4.717	38045.8	262.8	26	48	6	6	14	28	46	6	6	14
T10	4.724	38100.0	262.5	3	6	11	76	4	3	7	13	73	4

2Ag; iso1

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.464	27936.7	358.0	3	2	3	2	90	4	3	3	3	87
T2	4.157	33524.7	298.3	3	2	2	2	91	5	4	4	4	84
T3	4.324	34877.5	286.7	5	4	4	4	84	4	5	4	4	83
T4	4.557	36753.4	272.1	3	2	3	2	90	4	3	3	4	86
T5	4.562	36795.7	271.8	9	5	5	3	78	8	5	5	4	78
T6	4.701	37916.5	263.7	24	14	34	18	10	26	13	36	17	7
T7	4.713	38009.6	263.1	15	10	40	29	6	15	10	41	28	6
T8	4.721	38075.7	262.6	39	34	10	9	8	40	34	11	9	7
T9	4.728	38132.1	262.2	5	59	12	20	4	7	57	13	19	4
T10	4.734	38183.8	261.9	4	22	7	65	3	5	21	8	63	3

2Ag; iso2

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.563	28741.0	347.9	2	2	3	2	91	3	3	3	3	87
T2	4.205	33919.0	294.8	2	2	2	2	92	5	3	5	3	84
T3	4.334	34959.0	286.0	3	4	4	3	85	4	4	4	4	84
T4	4.526	36503.1	273.9	3	2	3	2	90	5	4	4	3	84
T5	4.626	37313.1	268.0	5	4	5	3	83	6	4	5	4	80
T6	4.711	37996.4	263.2	6	90	1	2	1	8	86	1	3	2
T7	4.722	38085.5	262.6	1	2	6	89	1	1	3	8	86	2
T8	4.732	38169.6	262.0	12	82	1	2	3	14	79	1	2	4
T9	4.740	38232.0	261.6	1	2	7	89	1	1	2	8	86	2
T10	4.745	38269.2	261.3	7	88	1	2	3	8	85	1	2	3

2Ag; iso3

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.527	28447.2	351.5	2	2	2	2	91	3	3	3	4	87
T2	4.175	33672.8	297.0	2	2	2	2	92	4	4	6	4	82
T3	4.330	34921.1	286.4	5	4	5	4	83	4	5	5	5	82
T4	4.524	36492.2	274.0	3	3	4	3	87	5	4	5	4	81
T5	4.572	36877.9	271.2	9	5	10	5	70	9	6	10	6	69
T6	4.651	37509.0	266.6	13	7	46	19	14	14	7	47	19	13
T7	4.680	37748.5	264.9	43	21	12	7	16	45	20	12	7	16
T8	4.725	38105.7	262.4	1	2	6	89	2	1	2	9	84	3
T9	4.730	38152.8	262.1	7	87	1	2	3	9	83	1	2	4
T10	4.736	38200.6	261.8	7	87	1	2	2	9	84	1	2	3

3Ag; axial

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.327	26834.0	372.7	2	2	2	2	92	3	3	3	3	89
T2	4.229	34109.7	293.2	4	3	4	3	87	4	4	4	4	85
T3	4.286	34568.4	289.3	2	2	2	2	92	3	3	3	3	87
T4	4.572	36873.0	271.2	6	4	6	4	81	5	4	5	4	83

T5	4.589	37008.8	270.2	3	2	3	2	89	3	3	3	3	88
T6	4.682	37764.4	264.8	26	13	26	13	22	27	13	27	13	19
T7	4.703	37933.0	263.6	19	28	19	28	6	20	27	20	27	6
T8	4.712	38004.6	263.1	6	20	6	20	50	6	19	6	19	50
T9	4.715	38030.3	262.9	7	33	7	33	19	8	32	8	32	19
T10	4.721	38074.9	262.6	15	33	15	33	5	16	32	16	32	4

3Ag; non-axial

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.367	27160.2	368.2	2	2	2	2	92	3	3	3	3	89
T2	4.190	33795.7	295.9	3	2	3	2	90	5	4	5	4	83
T3	4.244	34234.2	292.1	3	3	3	3	88	4	4	4	4	85
T4	4.501	36306.4	275.4	5	4	5	4	81	5	5	5	5	80
T5	4.590	37023.5	270.1	3	3	3	3	88	4	3	3	3	87
T6	4.674	37695.9	265.3	29	14	28	13	16	29	14	28	13	16
T7	4.687	37801.3	264.5	26	21	26	20	7	26	21	26	20	7
T8	4.701	37912.3	263.8	6	34	6	34	20	7	33	7	33	20
T9	4.718	38053.1	262.8	9	38	9	38	7	10	36	10	36	7
T10	4.733	38173.0	262.0	4	26	4	26	39	5	25	5	26	39

4Ag; axial

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.310	26697.8	374.6	2	2	2	2	91	3	3	3	3	88
T2	4.223	34062.7	293.6	3	3	3	3	87	3	4	3	4	86
T3	4.283	34546.9	289.5	2	2	2	2	92	3	3	3	3	86
T4	4.574	36894.5	271.0	5	3	5	3	83	4	4	4	4	84
T5	4.584	36972.5	270.5	4	3	4	3	87	3	4	3	4	86
T6	4.695	37869.2	264.1	17	10	17	10	47	17	10	17	10	45
T7	4.712	38003.7	263.1	9	11	9	11	60	9	10	9	10	62
T8	4.714	38017.3	263.0	7	42	7	42	3	8	41	8	40	3
T9	4.718	38051.6	262.8	4	40	4	40	12	5	38	5	38	13
T10	4.736	38199.5	261.8	7	85	1	2	4	9	82	1	3	5

4Ag; non-axial

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.344	26973.2	370.7	2	2	2	2	92	3	3	3	3	89
T2	4.166	33602.8	297.6	4	2	4	2	88	5	4	5	4	82
T3	4.223	34059.2	293.6	2	3	2	3	90	4	4	4	4	84
T4	4.472	36065.2	277.3	5	4	5	4	81	6	4	6	4	80
T5	4.563	36806.8	271.7	3	3	3	3	88	3	3	3	3	87
T6	4.664	37619.6	265.8	4	10	4	10	73	5	10	5	10	71
T7	4.692	37840.1	264.3	28	12	28	12	21	28	12	28	12	21
T8	4.699	37897.8	263.9	19	28	19	28	6	20	27	20	27	7
T9	4.717	38048.8	262.8	4	37	4	37	18	4	36	4	36	19
T10	4.725	38110.4	262.4	11	35	11	35	8	12	34	12	34	8

5Ag; head-to-head

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP

T1	3.486	28115.9	355.7	3	3	2	2	90	3	4	3	4	86
T2	4.202	33891.0	295.1	3	2	2	2	91	6	4	5	4	81
T3	4.258	34339.8	291.2	4	4	4	4	85	4	4	4	5	83
T4	4.530	36537.5	273.7	5	4	8	5	78	5	4	8	5	77
T5	4.547	36674.2	272.7	3	3	3	3	89	5	4	5	4	82
T6	4.698	37891.1	263.9	3	3	32	55	7	3	4	34	52	7
T7	4.713	38008.9	263.1	7	77	2	10	4	10	74	2	10	4
T8	4.714	38019.0	263.0	2	10	6	77	5	2	10	8	74	6
T9	4.720	38070.8	262.7	9	75	3	10	3	11	73	3	10	3
T10	4.727	38123.0	262.3	6	17	25	46	6	7	17	26	44	7

5Ag; head-to-tail displaced

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.404	27457.9	364.2	3	2	3	2	90	4	3	3	3	86
T2	4.164	33585.7	297.7	3	2	3	2	91	6	4	5	4	81
T3	4.278	34504.5	289.8	5	4	5	4	83	4	5	5	5	82
T4	4.521	36461.2	274.3	7	4	8	5	76	7	5	8	5	76
T5	4.563	36807.1	271.7	3	3	3	2	89	3	3	4	4	85
T6	4.698	37889.5	263.9	35	19	14	13	19	36	19	15	12	18
T7	4.707	37962.7	263.4	15	10	29	37	10	16	9	30	35	10
T8	4.721	38079.1	262.6	4	4	22	64	6	4	5	24	61	6
T9	4.734	38181.0	261.9	5	60	4	25	5	6	59	5	25	6
T10	4.738	38214.5	261.7	5	27	10	52	5	6	26	11	50	6

5Ag; head-to-tail

	E			GS (hole)					ES (electron)				
	eV	cm^{-1}	nm	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP	Ag_3^1	L_3^1	Ag_3^2	L_3^2	BP
T1	3.401	27430.9	364.6	3	2	2	2	90	3	3	3	3	87
T2	4.147	33448.5	299.0	3	2	3	2	90	5	4	5	4	82
T3	4.261	34364.8	291.0	5	4	4	4	83	4	4	4	5	83
T4	4.487	36188.1	276.3	6	4	7	5	77	6	4	7	5	77
T5	4.569	36852.0	271.4	4	3	3	3	86	5	4	4	4	84
T6	4.667	37644.4	265.6	11	6	45	26	11	12	6	47	25	10
T7	4.678	37727.2	265.1	48	22	6	14	10	49	21	7	13	10
T8	4.698	37894.9	263.9	5	11	12	62	11	5	11	14	59	11
T9	4.707	37962.8	263.4	2	6	10	77	5	2	7	12	74	5
T10	4.715	38026.7	263.0	20	65	2	7	5	22	63	2	8	5

Table S9. XYZ coordinates of optimized complexes.

1Ag^{h2t}; E=-38149.187294210853

47	15.229808000	4.977655000	13.299648000
47	17.649406000	4.613838000	10.806689000
47	16.029450000	1.871135000	11.976449000
9	18.578286000	4.468394000	7.408915000
9	14.823931000	7.453335000	14.779144000
9	15.918946000	-0.495817000	14.155234000
9	20.262349000	3.947582000	8.647888000
9	15.487690000	-0.654305000	9.541833000
9	11.801484000	3.748505000	16.547033000
9	13.986434000	-0.906678000	13.290152000
9	14.244566000	-1.010072000	15.432010000
9	11.994290000	4.903716000	14.725746000
9	17.298470000	-1.541926000	8.752016000
9	17.133971000	-1.087440000	10.863037000
9	13.509323000	5.044945000	16.250421000
9	15.078026000	9.432937000	13.952918000
7	14.242997000	3.228900000	13.985563000
7	14.754442000	2.036229000	13.652757000
9	19.888188000	2.842660000	6.827549000
7	17.459413000	6.428344000	11.878789000
7	17.733432000	2.820990000	9.683854000
7	16.464555000	6.623306000	12.754568000
9	19.103560000	7.729574000	9.736813000
7	17.090498000	1.743816000	10.147524000
9	16.421440000	8.730748000	15.484213000
9	20.221237000	8.634767000	11.351048000
9	20.228862000	6.483558000	11.086657000
6	18.265523000	1.101535000	8.359581000
6	19.292790000	3.431164000	7.869701000
6	14.591313000	-0.330008000	14.337880000
6	15.738835000	8.353487000	14.390063000
6	14.237059000	1.115947000	14.473199000
6	16.662960000	7.806080000	13.346902000
6	17.399004000	0.705310000	9.363688000
6	12.673715000	4.190264000	15.635081000
6	13.361293000	1.707176000	15.368041000
6	18.444452000	2.451097000	8.613119000
6	18.271263000	7.492055000	11.924870000
6	17.808211000	8.409675000	12.849686000
6	16.826381000	-0.649175000	9.626980000
6	13.405605000	3.044467000	15.013090000
6	19.459847000	7.590743000	11.021941000
6	18.963664000	2.894622000	13.595795000
6	19.524366000	0.901238000	12.326446000
6	20.394304000	1.624500000	11.527864000
6	19.837706000	3.609267000	12.768337000
6	18.821104000	1.526160000	13.347123000
6	20.549976000	2.983108000	11.758397000
6	18.214868000	3.570654000	14.696468000
6	17.658400000	5.563606000	15.968387000
6	16.786976000	4.841093000	16.766077000
6	17.339026000	2.856940000	15.522560000
6	18.360783000	4.938454000	14.947346000
6	16.628496000	3.483081000	16.533897000
47	21.921794000	1.447945000	15.010124000
47	19.502196000	1.811762000	17.503082000
47	21.122152000	4.554465000	16.333323000
9	18.566364000	1.954084000	20.899203000
9	22.314042000	-1.015916000	13.517695000
9	21.246062000	6.921897000	14.140554000
9	16.890888000	2.480694000	19.650969000
9	21.681085000	7.069746000	18.788043000
9	25.377026000	2.672496000	11.789717000
9	23.171480000	7.336579000	15.020051000
9	22.930662000	7.430432000	12.875665000
9	25.177266000	1.524013000	13.614635000
9	19.868117000	7.963519000	19.565330000
9	20.045720000	7.507979000	17.455356000
9	23.670924000	1.373061000	12.082102000
9	22.059971000	-2.997392000	14.339571000
7	22.916110000	3.196134000	14.332263000
7	22.403561000	4.389833000	14.659883000
9	17.256480000	3.581358000	21.476092000
7	19.682694000	0.003310000	16.418653000
7	19.422265000	3.602855000	18.628542000
7	20.679901000	-0.194947000	15.546793000
9	18.004959000	-1.264465000	18.542549000
7	20.069778000	4.678486000	18.167947000
9	20.718497000	-2.293224000	12.807352000
9	16.901866000	-2.183429000	16.925707000
9	16.898176000	-0.029207000	17.167574000
6	18.894470000	5.321431000	19.955514000
6	17.856695000	2.993724000	20.436260000
6	22.575146000	6.755102000	13.970176000
6	21.399100000	-1.917698000	13.903149000
6	22.930006000	5.308635000	13.843412000
6	20.473149000	-1.371550000	14.945039000
6	19.763951000	5.716503000	18.953345000
6	24.500937000	2.232090000	12.698678000
6	23.813026000	4.715485000	12.957083000
6	18.710871000	3.973104000	19.698882000
6	18.860480000	-1.051716000	16.360578000
6	19.319290000	-1.967348000	15.431727000
6	20.343087000	7.068964000	18.693775000
6	23.763334000	3.378585000	13.312359000
6	17.662901000	-1.138671000	17.252169000
1	18.691723000	0.507845000	7.569851000
1	18.234851000	9.360725000	13.118753000
1	12.785652000	1.239906000	16.147948000
1	18.884307000	-2.911775000	15.152904000
1	24.396591000	5.181286000	12.182173000
1	18.469116000	5.915156000	20.745691000
1	21.221976000	3.568867000	11.144005000
1	19.997409000	4.667346000	12.921664000
1	20.949207000	1.134668000	10.737841000
1	19.382367000	-0.158795000	12.158958000
1	18.177465000	0.913904000	13.965933000
1	17.176058000	1.799633000	15.367011000
1	15.954957000	2.897958000	17.147239000
1	16.232721000	5.331005000	17.556513000
1	17.802219000	6.623232000	16.136726000
1	19.006165000	5.549893000	14.329792000

1Ag^{h2h}; E=-38149.187681373842 Ha

47	24.856194000	12.743329000	7.995782000
47	26.271959000	9.703055000	7.069907000
47	27.687723000	12.743329000	6.144032000
9	21.009957000	11.293793000	10.536303000
9	24.995140000	6.891324000	8.354295000
9	22.912302000	12.076860000	11.199478000
7	25.682310000	14.595324000	7.377447000
9	23.759366000	7.300260000	6.636679000
7	23.994089000	10.895636000	8.625089000
7	24.414246000	9.750301000	8.072813000
9	24.001722000	17.554764000	8.451154000
9	22.859160000	6.554602000	8.459925000
6	22.594395000	9.278406000	9.280365000
1	21.775413000	8.756957000	9.744369000
9	22.933599000	15.747933000	7.934419000
9	24.299903000	15.742454000	9.600546000
6	22.903471000	10.627185000	9.349924000
6	22.209544000	11.705425000	10.118343000
6	23.585132000	8.773144000	8.457488000
6	25.238709000	15.854317000	7.447133000
6	25.943399000	16.661698000	6.569196000
1	25.827504000	17.716891000	6.392515000
6	23.799902000	7.373334000	7.982451000
6	24.116704000	16.225642000	8.363812000
7	26.668276000	14.552389000	6.474602000
9	27.595607000	17.186859000	4.278840000
9	29.098642000	16.197923000	5.476976000
9	27.958950000	15.065435000	4.038003000
6	26.833897000	15.781765000	5.976479000
6	27.876981000	16.060155000	4.941887000
9	22.031753000	12.810242000	9.371760000
9	30.724407000	12.843483000	5.082116000
9	31.756811000	11.307984000	3.954635000
9	27.631212000	6.926792000	5.910874000
9	29.874056000	12.097712000	3.244339000
9	28.834465000	7.262591000	7.665781000
7	28.700896000	10.928308000	5.764740000
7	28.227425000	9.776587000	6.255343000
9	29.764571000	6.574934000	5.834996000
6	30.116713000	9.308877000	5.157739000
1	30.953008000	8.783992000	4.730044000
6	29.830912000	10.662425000	5.100458000
6	30.553437000	11.732678000	4.349240000
6	29.066670000	8.797999000	5.901363000
6	28.824408000	7.385784000	6.330129000
6	22.780781000	13.194176000	5.632384000
1	22.004168000	13.122248000	6.384408000
6	24.522757000	12.117216000	4.324277000
6	23.519380000	12.066348000	5.300387000
1	23.308681000	11.140767000	5.821588000
6	27.181060000	9.843631000	2.852244000
1	28.095491000	9.946971000	2.280744000
6	24.854822000	9.621438000	4.325286000
6	25.293436000	10.897841000	3.948200000
6	26.476800000	10.982390000	3.214009000
1	26.873756000	11.945503000	2.919090000
6	23.033265000	14.404035000	5.002695000
1	22.455692000	15.281887000	5.262191000
6	25.568183000	8.483206000	3.978360000
1	25.210399000	7.510853000	4.295765000
6	24.760327000	13.345285000	3.706644000
1	25.514245000	13.435921000	2.934803000
6	26.733713000	8.590030000	3.232717000
1	27.286095000	7.700614000	2.957649000
6	24.031284000	14.474746000	4.045204000
1	24.238592000	15.409928000	3.539441000
47	23.718335000	11.422719000	0.850651000
47	21.298549000	11.057263000	3.343783000
47	22.919773000	8.311645000	2.176117000
9	20.751480000	10.764715000	6.883892000
9	24.051732000	13.846691000	-0.716494000
9	23.791952000	5.726818000	0.320509000
9	18.933267000	10.628687000	5.735633000
9	22.979493000	5.551901000	4.125956000
9	27.746926000	10.371835000	-1.635847000
9	25.424180000	5.862173000	1.722207000
9	25.825608000	5.384977000	-0.347281000
9	26.704434000	11.737055000	-0.315831000
9	21.185734000	4.796388000	5.078212000
9	21.164735000	5.341360000	2.983144000
9	25.830697000	11.190316000	-2.210360000
9	24.435360000	15.451346000	0.674627000
7	24.792093000	9.706316000	0.249275000
7	24.389851000	8.497099000	0.656604000
9	19.235742000	9.318233000	7.431727000
7	21.434926000	12.848560000	2.202419000
7	21.113745000	9.226247000	4.388866000
7	22.450840000	13.028032000	1.351459000
9	19.710954000	13.556446000	4.341885000
7	21.584486000	8.113668000	3.810008000
9	22.953565000	15.709573000	-0.872143000
9	19.195375000	15.391824000	3.311242000
9	18.484539000	13.488218000	2.569597000
6	20.530394000	7.497553000	5.680802000
1	20.121832000	6.905142000	6.480760000
6	19.843235000	9.896594000	6.392104000
6	25.062849000	6.134662000	0.454257000
6	23.460100000	14.824009000	-0.009393000
6	25.219729000	7.586655000	0.136311000
6	22.405812000	14.286128000	0.903549000
6	21.243025000	7.071217000	4.572755000
6	26.539179000	10.714718000	-1.175448000
6	26.190292000	8.203785000	-0.633932000
1	26.996218000	7.749640000	-1.183677000
6	20.479708000	8.870741000	5.512716000
6	20.760233000	14.000627000	2.285698000
6	21.336935000	14.959659000	1.471727000
1	21.027558000	15.978776000	1.316090000
6	21.642876000	5.682456000	4.189462000
6	25.870025000	9.546527000	-0.526084000
6	19.532831000	14.110657000	3.129681000
1	23.938700000	9.502050000	4.890537000

2Ag[1]; E=-38347.984855971896 Ha

47	17.533257000	6.885894000	-0.528058000
47	14.402702000	5.903562000	-1.543253000
47	16.761070000	3.484418000	-0.670392000
9	18.270238000	10.171033000	-1.101476000
9	17.030955000	11.700879000	-0.201758000
9	17.668661000	9.986577000	0.959045000
9	12.559316000	8.355048000	-3.019171000
9	11.869596000	8.185133000	-0.985319000
9	12.065150000	10.139485000	-1.897429000
9	12.460541000	5.026121000	-4.003285000
9	11.185220000	3.274297000	-3.998401000
9	11.155777000	4.645873000	-2.327381000
9	16.021017000	0.157034000	-2.271942000
9	15.633935000	0.561744000	-0.188045000
9	14.198115000	-0.560143000	-1.360823000
9	18.940763000	1.328608000	-0.179057000
9	20.942180000	1.472795000	0.637212000
9	19.222624000	1.791295000	1.908140000
7	19.011484000	5.428090000	-0.159316000
7	15.996999000	8.321235000	-0.738771000
7	14.778312000	7.939677000	-1.136724000
7	14.050859000	3.865295000	-1.952739000
7	14.863399000	2.924385000	-1.454988000
7	18.672621000	4.141695000	-0.004830000
6	20.855450000	4.322309000	0.446490000
1	21.871261000	4.086936000	0.712505000
6	20.316380000	5.550283000	0.107442000
6	21.003103000	6.870865000	-0.018667000
6	17.247073000	10.384278000	-0.250743000
6	16.012109000	9.657076000	-0.673910000
6	14.779186000	10.171204000	-1.037629000
1	14.472026000	11.201048000	-1.088534000
6	14.037901000	9.037469000	-1.323211000
6	12.626650000	8.932422000	-1.805411000
6	11.951099000	4.049061000	-3.225116000
6	13.036113000	3.253424000	-2.575037000
6	13.173210000	1.880321000	-2.483505000
1	12.530003000	1.115863000	-2.883312000
6	14.347517000	1.730111000	-1.765241000
6	15.050510000	0.466202000	-1.391632000
6	19.718953000	2.007964000	0.679923000
6	19.769529000	3.467052000	0.356145000
9	21.077867000	7.271175000	-1.304886000
9	20.356926000	7.841063000	0.644667000
9	22.249222000	6.805784000	0.453481000
9	15.418845000	9.403331000	-4.462765000
9	20.525804000	1.237630000	-2.974428000
6	18.167717000	7.203817000	-3.700023000
1	19.210228000	7.300031000	-3.427245000
6	17.454019000	8.370378000	-3.921451000
1	17.919808000	9.340904000	-3.811344000
6	16.120189000	8.282164000	-4.265145000
6	15.492753000	7.061416000	-4.407681000
1	14.446831000	7.023205000	-4.681126000
6	17.578140000	5.941450000	-3.839336000
6	19.732325000	4.726398000	-3.374734000
1	20.262599000	5.667400000	-3.347161000
6	20.464648000	3.573964000	-3.148318000
1	21.529728000	3.615749000	-2.963522000
6	19.818604000	2.355438000	-3.182113000
6	18.462863000	2.263644000	-3.419582000
1	17.978937000	1.296107000	-3.434426000
6	17.742314000	3.430768000	-3.633497000
1	16.676136000	3.335885000	-3.799308000
6	18.356482000	4.688895000	-3.618307000
6	16.226078000	5.903514000	-4.196509000
1	15.716972000	4.958227000	-4.334416000
47	17.487106000	2.851932000	-6.720998000
47	20.228468000	4.868062000	-6.633463000
47	17.116314000	6.264254000	-7.303143000
9	14.707973000	0.890041000	-7.202662000
9	14.991165000	1.531897000	-5.165976000
9	12.993452000	1.435471000	-6.000666000
9	18.345215000	-0.515173000	-8.020481000
9	19.395429000	-1.574385000	-6.455134000
9	17.776965000	-0.220939000	-5.962440000
9	23.855812000	1.627802000	-6.237349000
9	23.262814000	3.312271000	-7.461953000
9	23.022203000	3.403849000	-5.322139000
9	18.065041000	10.002134000	-8.892387000
9	16.683552000	9.230506000	-7.426027000
9	17.947752000	10.922504000	-6.942875000
9	13.789251000	6.703956000	-9.200248000
9	12.283741000	6.643558000	-7.648613000
9	14.209867000	7.557773000	-7.267451000
7	15.583365000	3.714290000	-6.910947000
7	19.414144000	1.984612000	-6.733145000
7	20.491289000	2.772020000	-6.642513000
7	19.966163000	6.954271000	-6.647554000
7	18.835208000	7.500285000	-7.111436000
7	15.422798000	4.973148000	-7.331841000
6	13.386533000	4.089153000	-7.039530000
1	12.318487000	3.966606000	-6.991266000
6	14.374766000	3.170817000	-6.731264000
6	14.259686000	1.751367000	-6.279145000
6	18.834153000	-0.406362000	-6.775103000
6	19.819424000	0.712496000	-6.660070000
6	21.195567000	0.654584000	-6.518468000
1	21.822696000	-0.215183000	-6.430024000
6	21.567690000	1.988146000	-6.511559000
6	22.933451000	2.581908000	-6.384803000
6	22.160172000	7.635665000	-5.761493000
6	20.808202000	7.941809000	-6.323962000
6	20.224224000	9.170388000	-6.576217000
1	20.640655000	10.151897000	-6.428704000
6	18.974962000	8.829755000	-7.071657000
6	17.911400000	9.748808000	-7.584362000
6	13.593658000	6.534626000	-7.885306000
6	14.108273000	5.213120000	-7.410052000
9	22.881450000	6.853682000	-6.578339000
9	22.851840000	8.754670000	-5.542768000
9	22.068691000	6.979972000	-4.585913000

$2Ag^2$; E=-38347.978198833756 Ha

47	17.487106000	2.851932000	-6.720998000
47	20.228468000	4.868062000	-6.633463000
47	17.116314000	6.264254000	-7.303143000
9	14.990992000	0.904350000	-8.152826000
9	14.690613000	1.195065000	-6.040128000
9	12.992338000	1.226632000	-7.386546000
9	17.897280000	-0.369748000	-7.267278000
9	19.466085000	-1.578965000	-6.392064000
9	18.230937000	-0.320559000	-5.137212000
9	23.839688000	1.604126000	-7.189025000
9	22.936087000	3.270559000	-8.234077000
9	23.308536000	3.408595000	-6.118563000
9	17.409032000	9.546720000	-8.383025000
9	16.618979000	9.442754000	-6.377774000
9	18.035314000	10.994965000	-6.899798000
9	14.216950000	6.932935000	-9.455981000
9	12.415084000	6.612291000	-8.305391000
9	14.172537000	7.469504000	-7.369125000
7	15.600330000	3.661563000	-7.218766000
7	19.417375000	1.991920000	-6.540093000
7	20.488230000	2.773378000	-6.738928000
7	19.905426000	6.946552000	-6.396802000
7	18.757896000	7.496002000	-6.810154000
7	15.468119000	4.963723000	-7.496644000
6	13.486908000	3.996130000	-7.861822000
1	12.452636000	3.835437000	-8.111115000
6	14.422124000	3.068266000	-7.437326000
6	14.269377000	1.592563000	-7.252770000
6	18.852979000	-0.394423000	-6.323544000
6	19.831789000	0.721875000	-6.506860000
6	21.203874000	0.656992000	-6.681901000
1	21.831703000	-0.216513000	-6.708042000
6	21.566180000	1.985116000	-6.826336000
6	22.919011000	2.565608000	-7.082271000
6	22.068097000	7.641839000	-5.427569000
6	20.724018000	7.932746000	-6.015863000
6	20.105251000	9.162028000	-6.177625000
1	20.497429000	10.141329000	-5.964763000
6	18.863196000	8.823017000	-6.684178000
6	17.728460000	9.709050000	-7.082790000
6	13.747703000	6.551994000	-8.253036000
6	14.205305000	5.179715000	-7.878774000
9	22.682309000	6.625099000	-6.057746000
9	22.862315000	8.712118000	-5.500646000
9	21.974991000	7.294096000	-4.133907000
9	15.379854000	3.168462000	-11.004638000
9	23.415058000	8.291836000	-9.029165000
6	17.661056000	5.946309000	-10.770430000
1	17.695684000	6.983669000	-11.077263000
6	16.518855000	5.217823000	-11.056557000
1	15.669161000	5.674959000	-11.545416000
6	16.477722000	3.880343000	-10.717752000
6	17.540080000	3.256819000	-10.096893000
1	17.481862000	2.202860000	-9.856751000
6	18.672364000	4.004251000	-9.806654000
1	19.493838000	3.506997000	-9.305563000
6	18.761997000	5.360358000	-10.140110000
6	20.002259000	6.139243000	-9.871885000
6	19.980168000	7.535130000	-9.801988000
1	19.050563000	8.073906000	-9.930265000
6	21.123411000	8.263716000	-9.522335000
1	21.100778000	9.343525000	-9.465295000
6	22.308490000	7.589654000	-9.306311000
6	22.380189000	6.213428000	-9.362608000
1	23.320659000	5.711599000	-9.173606000
6	21.226326000	5.499140000	-9.651992000
1	21.299343000	4.420653000	-9.708624000
47	20.904146000	6.853781000	-12.953792000
47	20.305421000	3.459961000	-12.476618000
47	23.526817000	4.737907000	-12.235006000
9	23.175697000	11.176883000	-13.083979000
9	21.785104000	9.975872000	-14.229003000
9	21.557778000	10.133889000	-12.093265000
9	18.843718000	8.381614000	-15.447568000
9	16.732266000	8.259533000	-14.999517000
9	18.166334000	8.637997000	-13.417542000
9	18.046819000	2.292989000	-15.412983000
9	17.707890000	2.162292000	-13.288943000
9	16.104124000	2.788934000	-14.607380000
9	19.778847000	0.383607000	-11.693734000
9	20.790851000	-0.815407000	-10.199252000
9	19.810154000	1.024665000	-9.636085000
9	25.957556000	2.320515000	-11.862836000
9	25.565818000	3.250441000	-9.959528000
9	25.905040000	1.116010000	-10.064441000
9	26.616384000	6.112655000	-13.828346000
9	27.346247000	7.661625000	-12.509074000
9	26.410953000	5.882871000	-11.696631000
7	22.869596000	7.627603000	-12.768554000
7	19.113495000	5.963996000	-13.661482000
7	18.970516000	4.635510000	-13.613796000
7	21.829344000	2.356597000	-11.473147000
7	23.093550000	2.802964000	-11.496978000
7	23.894693000	6.770644000	-12.678009000
6	24.755867000	8.820722000	-12.889643000
1	25.448760000	9.640018000	-12.969968000
6	23.371487000	8.860084000	-12.900385000
6	22.471528000	10.041621000	-13.076687000
6	17.949695000	7.941719000	-14.550531000
6	18.062131000	6.469921000	-14.315244000
6	17.203007000	5.456372000	-14.705309000
1	16.272333000	5.535727000	-15.239949000
6	17.829064000	4.315059000	-14.230583000
6	17.416903000	2.885435000	-14.385867000
6	20.550491000	0.434179000	-10.600302000
6	21.823352000	1.176941000	-10.839672000
6	23.102481000	0.838626000	-10.433287000
1	23.427194000	-0.037312000	-9.899420000
6	23.864781000	1.906813000	-10.872669000
6	25.330962000	2.147156000	-10.689710000
6	26.357905000	6.782681000	-12.693454000
6	25.031460000	7.472187000	-12.742803000

2Ag^3; E=-38347.981171924846 Ha

47	20.904146000	6.853781000	-12.953792000
47	20.305421000	3.459961000	-12.476618000
47	23.526817000	4.737907000	-12.235006000
9	23.198325000	11.164416000	-13.177097000
9	21.854433000	10.006099000	-14.411111000
9	21.541744000	10.096803000	-12.278641000
9	18.809881000	8.732624000	-13.995314000
9	16.735015000	8.465446000	-14.561962000
9	17.284171000	8.580770000	-12.477439000
9	17.783958000	2.463417000	-14.912306000
9	17.356472000	2.300808000	-12.804866000
9	15.822900000	2.995498000	-14.170175000
9	20.296360000	-0.012708000	-12.846772000
9	20.923986000	-1.135207000	-11.105086000
9	19.661208000	0.609322000	-10.881774000
9	25.976929000	2.664407000	-11.880273000
9	25.451482000	2.870310000	-9.799710000
9	25.994554000	0.929398000	-10.584285000
9	26.451870000	5.927708000	-14.063599000
9	27.353463000	7.641146000	-13.102157000
9	26.576577000	6.008334000	-11.911281000
7	22.880098000	7.627288000	-12.800381000
7	18.956898000	6.055413000	-13.194568000
7	18.797706000	4.727133000	-13.223576000
7	21.872320000	2.247647000	-11.765241000
7	23.098829000	2.760114000	-11.607824000
7	23.902819000	6.762598000	-12.745693000
6	24.758049000	8.785986000	-13.160889000
1	25.447927000	9.587351000	-13.358966000
6	23.379494000	8.843663000	-13.050217000
6	22.489827000	10.033502000	-13.223110000
6	17.663901000	8.105387000	-13.673868000
6	17.831316000	6.617958000	-13.646570000
6	16.905487000	5.642134000	-13.980421000
1	15.910287000	5.769609000	-14.369799000
6	17.573564000	4.464597000	-13.694136000
6	17.126685000	3.052831000	-13.892964000
6	20.697035000	0.097286000	-11.564376000
6	21.919620000	0.949395000	-11.447963000
6	23.202160000	0.593287000	-11.067128000
1	23.564507000	-0.369073000	-10.750408000
6	23.906334000	1.779567000	-11.188855000
6	25.339919000	2.057833000	-10.863901000
6	26.359298000	6.756715000	-13.001310000
6	25.034281000	7.445394000	-12.961194000
9	25.294003000	0.990160000	-14.410703000
9	18.808555000	7.791263000	-16.949001000
6	22.171587000	2.569977000	-15.256618000
1	21.129620000	2.286515000	-15.336356000
6	23.080598000	1.588582000	-14.900447000
1	22.762934000	0.572020000	-14.709174000
6	24.411983000	1.928245000	-14.772023000
6	24.854717000	3.216653000	-14.997221000
1	25.904081000	3.452807000	-14.885273000
6	23.930590000	4.184339000	-15.363794000
1	24.296728000	5.187235000	-15.546245000
6	22.570368000	3.886785000	-15.500350000
6	21.585322000	4.930890000	-15.893251000
6	20.307543000	4.577335000	-16.335544000
1	20.024940000	3.538183000	-16.418606000
6	19.367958000	5.529307000	-16.687051000
1	18.383638000	5.242905000	-17.031502000
6	19.713865000	6.863208000	-16.609777000
6	20.963132000	7.263996000	-16.184655000
1	21.203143000	8.317086000	-16.127727000
6	21.889502000	6.293950000	-15.825904000
1	22.859302000	6.624877000	-15.473414000
47	24.790828000	3.747706000	-18.319773000
47	21.660273000	4.730038000	-19.334968000
47	24.018640000	7.149182000	-18.462107000
9	24.834604000	-0.652894000	-19.093684000
9	24.177657000	-0.656781000	-17.042075000
9	25.494078000	0.907009000	-17.755614000
9	19.596029000	2.492589000	-20.436878000
9	19.115901000	2.337220000	-18.340608000
9	19.250004000	0.549055000	-19.546707000
9	19.400978000	5.781596000	-21.567851000
9	18.109427000	7.475373000	-21.161811000
9	18.387598000	5.933622000	-19.672759000
9	23.349585000	10.404350000	-19.700738000
9	22.788669000	9.993407000	-17.659920000
9	21.496337000	11.197920000	-18.916316000
9	26.279227000	9.311108000	-18.144017000
9	28.083260000	9.209019000	-16.947734000
9	26.144866000	8.939470000	-16.026448000
7	26.257509000	5.224630000	-17.906628000
7	23.290568000	2.274521000	-18.657467000
7	22.061235000	2.683689000	-18.998995000
7	21.279374000	6.783927000	-19.670637000
7	22.139450000	7.704278000	-19.221504000
7	25.900682000	6.508232000	-17.774007000
6	28.063698000	6.360218000	-17.236304000
1	29.066219000	6.608365000	-16.934094000
6	27.551261000	5.121378000	-17.586096000
6	28.241563000	3.794926000	-17.610567000
6	24.445926000	0.140968000	-18.086494000
6	23.244582000	0.953396000	-18.457793000
6	21.960437000	0.477188000	-18.674429000
1	21.601241000	-0.535141000	-18.603278000
6	21.254421000	1.615767000	-19.014696000
6	19.801122000	1.746929000	-19.341759000
6	19.012119000	6.652223000	-20.623657000
6	20.172640000	7.418062000	-20.075129000
6	20.302526000	8.783955000	-19.890312000
1	19.589091000	9.558663000	-20.110407000
6	21.567749000	8.906437000	-19.343283000
6	22.300408000	10.134226000	-18.909298000
6	26.875905000	8.670698000	-17.124977000
6	26.974141000	7.200822000	-17.376481000
9	27.937375000	3.098967000	-18.717071000
9	27.888718000	3.029872000	-16.562281000
9	29.567221000	3.948315000	-17.569405000

3Ag^{axial}; E=-39072.931567094573 Ha

47	6.366500000	-2.025788000	5.975201000
47	8.661979000	-2.544564000	8.455404000
47	9.584260000	-2.897967000	5.078021000
9	10.696398000	-3.513791000	10.765475000
9	12.255208000	-4.811470000	4.354915000
7	6.890563000	-1.514502000	8.916917000
9	4.254917000	-1.085074000	3.457854000
9	14.016113000	-4.936022000	5.605734000
9	13.269736000	-3.009964000	4.958496000
7	5.981020000	-1.329471000	7.952185000
9	4.086280000	-3.234886000	3.522013000
9	10.466083000	-3.253951000	2.311721000
7	10.900361000	-3.507076000	6.636882000
7	8.152246000	-2.449078000	3.592118000
7	10.405596000	-3.594535000	7.880175000
7	6.862070000	-2.331204000	3.929640000
9	4.030878000	0.281085000	6.563450000
9	4.136742000	-2.212779000	1.615062000
9	9.833765000	-5.390252000	10.148878000
9	3.068513000	-1.507194000	7.291637000
9	11.942373000	-5.279135000	10.632810000
9	2.858467000	0.351541000	8.381847000
9	10.052816000	-1.391497000	1.304713000
9	9.440803000	-3.255706000	0.402616000
6	12.065891000	-4.167011000	6.614656000
6	12.343865000	-4.704079000	7.860611000
6	11.256494000	-4.312159000	8.621348000
6	4.924920000	-0.716685000	8.497937000
6	6.397712000	-1.024290000	10.058555000
6	8.230487000	-2.525593000	2.260413000
9	6.468858000	-0.664198000	12.361595000
6	5.137377000	-0.494162000	9.847808000
6	6.965795000	-2.451535000	1.699192000
6	6.139679000	-2.329731000	2.803056000
9	7.566879000	-2.365095000	11.593856000
9	8.310990000	-0.368865000	11.265061000
6	4.650919000	-2.208715000	2.845377000
6	3.717379000	-0.392904000	7.681319000
6	7.187486000	-1.103207000	11.325336000
6	12.905510000	-4.228703000	5.377900000
6	10.940607000	-4.621839000	10.049570000
6	9.552471000	-2.608619000	1.565597000
17	4.435737000	-4.243760000	10.105364000
6	6.792298000	-5.347634000	6.383593000
6	7.357798000	-5.441932000	7.657968000
6	5.464093000	-4.911702000	6.304784000
6	4.737467000	-4.580367000	7.438084000
6	6.639469000	-5.125238000	8.799769000
6	5.333016000	-4.682404000	8.682555000
17	9.925070000	-6.800682000	1.438525000
6	7.568411000	-5.696500000	5.160147000
6	7.002819000	-5.602663000	3.885782000
6	8.896709000	-6.132131000	5.238978000
6	9.623370000	-6.463563000	4.105731000
6	7.721197000	-5.919369000	2.744007000
6	9.027757000	-6.361890000	2.861257000
47	7.995441000	-9.019073000	5.567067000
47	5.699961000	-8.500297000	3.086864000
47	4.777681000	-8.146895000	6.464247000
9	3.665164000	-7.531351000	0.776799000
9	2.106700000	-6.233757000	7.187527000
7	7.471495000	-9.530156000	2.625315000
9	10.107173000	-9.959727000	8.084259000
9	0.345842000	-6.108761000	5.936675000
9	1.091892000	-8.035012000	6.583681000
7	8.380977000	-9.715240000	3.590093000
9	10.275552000	-7.809888000	8.020295000
9	3.896814000	-7.788879000	9.230849000
7	3.461550000	-7.537789000	4.905449000
7	6.209741000	-8.596112000	7.950006000
7	3.956253000	-7.450377000	3.662122000
7	7.499940000	-8.713736000	7.612552000
9	10.331061000	-11.326004000	4.978758000
9	10.225218000	-8.832180000	9.927156000
9	4.527803000	-5.654842000	1.393255000
9	11.293324000	-9.537491000	4.250997000
9	2.419157000	-5.766031000	0.909512000
9	11.503675000	-11.396009000	3.160475000
9	4.307262000	-9.653972000	10.234052000
9	4.921130000	-7.792478000	11.140534000
6	2.295969000	-6.877943000	4.927694000
6	2.017887000	-6.340992000	3.681716000
6	3.105240000	-6.732897000	2.920946000
6	9.437132000	-10.327955000	3.044362000
6	7.964450000	-10.020225000	1.483666000
6	6.131413000	-8.519894000	9.281715000
9	7.893667000	-10.379627000	-0.819482000
6	9.224787000	-10.550337000	1.694452000
6	7.396061000	-8.593905000	9.843019000
6	8.222269000	-8.715354000	8.739171000
9	6.795153000	-8.679218000	-0.051342000
9	6.051460000	-10.675730000	0.276721000
6	9.711044000	-8.836185000	8.696842000
6	10.644617000	-10.651774000	3.861046000
6	7.174802000	-9.941114000	0.216821000
6	1.456337000	-6.816278000	6.164448000
6	3.420993000	-6.423285000	1.492682000
6	4.809247000	-8.436899000	9.976117000
1	4.477337000	-0.032633000	10.561077000
1	13.198226000	-5.284559000	8.162140000
1	6.690797000	-2.482294000	0.659060000
1	7.670978000	-8.563321000	10.883176000
1	9.884909000	-11.011741000	0.981177000
1	1.163467000	-5.760600000	3.380190000
1	10.644116000	-6.808127000	4.193235000
1	9.399808000	-6.209361000	6.193931000
1	7.261116000	-5.830478000	1.768000000
1	5.986731000	-5.257464000	3.754391000
1	4.961053000	-4.834136000	5.349826000
1	3.716792000	-4.235583000	7.350636000
1	7.099516000	-5.214404000	9.775769000
1	8.373774000	-5.787466000	7.789344000

3Ag^{nonaxial}; E=-39072.930155365495 Ha

47	11.567529000	3.158635000	5.567067000
47	9.272050000	3.677412000	3.086864000
47	8.349769000	4.030814000	6.464247000
9	7.234191000	3.884132000	0.865189000
9	5.548270000	5.164215000	7.223911000
7	11.182915000	2.921158000	2.597237000
9	13.713288000	2.477161000	7.745899000
9	3.678336000	5.011082000	6.138037000
9	4.764639000	3.226421000	6.698280000
7	12.055551000	2.637904000	3.572693000
9	13.911950000	4.612489000	7.920799000
9	7.802469000	5.087314000	9.537537000
7	6.957520000	4.333802000	4.917468000
7	9.844642000	3.848217000	7.947604000
7	7.347942000	4.372541000	3.638367000
7	11.112129000	3.678181000	7.556223000
9	13.952303000	0.961930000	4.935947000
9	13.951819000	3.383894000	9.700149000
9	6.875418000	5.998029000	1.092020000
9	15.007133000	2.709505000	4.237738000
9	5.208761000	4.653794000	0.804585000
9	15.122760000	0.863456000	3.116766000
9	7.793878000	2.967275000	9.939524000
9	8.765795000	4.319984000	11.319477000
6	5.637823000	4.544041000	4.957418000
6	5.140298000	4.726114000	3.678416000
6	6.268526000	4.607059000	2.884143000
6	13.115595000	2.038970000	3.015901000
6	11.700345000	2.500063000	1.438924000
6	9.834085000	3.935871000	9.282279000
9	11.694221000	2.295966000	-0.883261000
6	12.942034000	1.925482000	1.647113000
6	11.119850000	3.822360000	9.784486000
6	11.888556000	3.661562000	8.644071000
9	10.585210000	3.950554000	-0.034516000
9	9.820175000	1.941202000	0.139726000
6	13.372776000	3.532178000	8.508547000
6	14.305288000	1.642728000	3.829647000
6	10.949820000	2.674536000	0.158038000
6	4.901855000	4.493521000	6.256749000
6	6.393696000	4.783940000	1.404404000
6	8.547165000	4.083995000	10.024455000
17	5.542481000	1.080988000	1.772022000
6	8.486310000	0.653825000	5.205734000
6	8.890811000	0.510069000	3.875768000
6	7.140115000	0.960080000	5.431178000
6	6.238316000	1.102861000	4.389606000
6	6.672713000	0.934050000	3.087491000
6	8.000763000	0.646743000	2.822992000
17	12.390911000	0.053741000	9.768296000
6	9.446642000	0.479554000	6.334779000
6	9.042124000	0.623085000	7.664775000
6	10.792847000	0.173384000	6.109288000
6	11.694706000	0.030638000	7.150825000
6	11.260393000	0.199615000	8.452941000
6	9.932256000	0.486516000	8.717521000
47	6.366500000	-2.025788000	5.975201000
47	8.661979000	-2.544564000	8.455404000
47	9.584260000	-2.897967000	5.078021000
9	10.701852000	-2.750173000	10.677603000
9	12.385911000	-4.028177000	4.317797000
7	6.751198000	-1.788347000	8.944989000
9	4.220355000	-1.345348000	3.796343000
9	14.255942000	-3.876073000	5.403597000
9	13.170040000	-2.090834000	4.844596000
7	5.878687000	-1.504436000	7.969596000
9	4.022081000	-3.480726000	3.622330000
9	10.130513000	-3.956712000	2.004850000
7	10.976825000	-3.200005000	6.624702000
7	8.089184000	-2.716131000	3.594728000
7	10.586289000	-3.239107000	7.903785000
7	6.821773000	-2.545685000	3.986137000
9	3.982592000	0.175492000	6.608278000
9	3.981719000	-2.252890000	1.842458000
9	11.059306000	-4.864247000	10.449784000
9	2.928502000	-1.574150000	7.302454000
9	12.726929000	-3.520887000	10.736662000
9	2.811362000	0.269663000	8.427109000
9	10.140509000	-1.836691000	1.602881000
9	9.167756000	-3.188744000	0.222869000
6	12.296634000	-3.409417000	6.584692000
6	12.794284000	-3.591257000	7.863583000
6	11.666026000	-3.473022000	8.657935000
6	4.818995000	-0.905037000	8.526569000
6	6.234030000	-1.367225000	10.103403000
6	8.099630000	-2.804121000	2.260084000
9	6.239876000	-1.164414000	12.425707000
6	4.992648000	-0.791933000	9.895371000
6	6.813791000	-2.690840000	1.757960000
6	6.045197000	-2.529762000	2.898413000
9	7.349847000	-2.817963000	11.576113000
9	8.113765000	-0.808059000	11.403040000
6	4.560966000	-2.400563000	3.034040000
6	3.629521000	-0.507783000	7.713007000
6	6.984547000	-1.542037000	11.384245000
6	13.032516000	-3.358205000	5.285337000
6	11.541501000	-3.650289000	10.137620000
6	9.386478000	-2.952899000	1.517910000
1	11.443214000	3.848065000	10.810452000
1	4.125653000	4.917943000	3.375459000
1	13.613130000	1.499639000	0.921799000
1	4.321777000	-0.365903000	10.620781000
1	13.809055000	-3.782554000	8.166452000
1	6.490305000	-2.716959000	0.732042000
1	8.339453000	0.519448000	1.803417000
1	9.917925000	0.275814000	3.629247000
1	6.760262000	1.103261000	6.434421000
1	5.203081000	1.336851000	4.596354000
1	8.014953000	0.857030000	7.911339000
1	9.593602000	0.613762000	9.737121000
1	12.729939000	-0.203256000	6.943979000
1	11.172648000	0.030213000	5.106024000

4Ag^{axial}; E=-43396.907474603431 Ha

47	11.092861000	3.085206000	5.197100000
47	10.073737000	3.303799000	8.586437000
47	7.828223000	3.910675000	6.084918000
9	13.913442000	1.506363000	4.498053000
9	15.686284000	1.621570000	5.733264000
9	14.661342000	3.428795000	5.121695000
9	13.566080000	0.799757000	10.732647000
9	11.454131000	0.656513000	10.269304000
9	12.285145000	2.534648000	10.922248000
9	8.771410000	3.129414000	11.659285000
9	9.629865000	5.101696000	11.518875000
9	7.737173000	4.820362000	12.532683000
9	4.452610000	4.415616000	7.375661000
9	5.484582000	6.186381000	6.702451000
9	4.292354000	6.253049000	8.508672000
9	5.573599000	3.586730000	1.812141000
9	5.644582000	2.279123000	3.532269000
9	5.639635000	4.415365000	3.811759000
9	10.889829000	2.502142000	0.548323000
9	11.980035000	2.782932000	2.401044000
9	11.389590000	4.489419000	1.220842000
7	12.412493000	2.605958000	6.785495000
7	11.914651000	2.431627000	8.016662000
7	8.254117000	4.244609000	9.047226000
7	7.384241000	4.522403000	8.068983000
7	8.349927000	3.530999000	4.060018000
7	9.639135000	3.463731000	3.700243000
6	13.647722000	2.091298000	6.764383000
6	13.972879000	1.560814000	8.002007000
1	14.886076000	1.079487000	8.305769000
6	12.836328000	1.803321000	8.754252000
6	7.728077000	4.650977000	10.205996000
6	6.484843000	5.219936000	9.994469000
1	5.804260000	5.631194000	10.719107000
6	6.317923000	5.109059000	8.624325000
6	7.605564000	3.446826000	2.950583000
6	8.414612000	3.319938000	1.835316000
1	8.121411000	3.230739000	0.803444000
6	9.692746000	3.335255000	2.370620000
6	14.483290000	2.162374000	5.525359000
6	12.543449000	1.449163000	10.176770000
6	8.466882000	4.429202000	11.485771000
6	5.134093000	5.495794000	7.799485000
6	6.112707000	3.441894000	3.022273000
6	10.994425000	3.276707000	1.633868000
35	12.123670000	-0.828546000	1.692638000
6	10.991273000	-0.411908000	3.144063000
6	9.678255000	-0.034680000	2.914869000
1	9.296039000	0.031293000	1.903868000
6	8.848460000	0.246735000	3.989443000
1	7.831679000	0.542252000	3.769112000
6	9.307414000	0.184943000	5.308086000
6	10.641392000	-0.189896000	5.502279000
1	11.061611000	-0.244854000	6.496934000
6	11.479084000	-0.484429000	4.437653000
1	12.504807000	-0.774363000	4.620969000
35	5.600515000	1.512022000	10.075738000
6	6.732913000	1.095646000	8.624248000
6	8.045857000	0.718155000	8.853427000
1	8.427976000	0.651842000	9.864439000
6	8.875666000	0.436864000	7.778838000
1	9.892397000	0.141160000	7.999163000
6	8.416820000	0.499150000	6.460176000
6	7.082888000	0.874186000	6.265993000
1	6.662726000	0.929470000	5.271330000
6	6.245152000	1.168481000	7.330658000
1	5.219458000	1.458546000	7.147375000
47	6.631853000	-2.400971000	6.571429000
47	7.650977000	-2.619564000	3.182093000
47	9.896491000	-3.226440000	5.683611000
9	3.811029000	-0.822010000	7.270432000
9	2.038284000	-0.937555000	6.035110000
9	3.063524000	-2.744583000	6.646771000
9	4.158927000	-0.115219000	1.035920000
9	6.270787000	0.028350000	1.499553000
9	5.440185000	-1.849884000	0.846393000
9	8.952305000	-2.446210000	0.109130000
9	8.095111000	-4.419049000	0.249658000
9	9.987676000	-4.136589000	-0.764060000
9	13.272127000	-3.733181000	4.392857000
9	12.238997000	-5.503126000	5.066454000
9	13.431206000	-5.570962000	3.260242000
9	12.151209000	-2.901623000	9.956267000
9	12.079995000	-1.593926000	8.236227000
9	12.085297000	-3.730169000	7.956617000
9	6.835161000	-1.816923000	11.220177000
9	5.744875000	-2.097619000	9.367489000
9	6.335025000	-3.804142000	10.547786000
7	5.312220000	-1.921667000	4.983067000
7	5.810149000	-1.747242000	3.751950000
7	9.470421000	-3.560719000	2.721352000
7	10.340305000	-3.838539000	3.699589000
7	9.374808000	-2.846362000	7.708470000
7	8.085606000	-2.779168000	8.068313000
6	4.077017000	-1.406942000	5.004143000
6	3.751975000	-0.876308000	3.766551000
1	2.838818000	-0.394914000	3.462774000
6	4.888564000	-1.118801000	3.014358000
6	9.996500000	-3.967071000	1.562592000
6	11.239539000	-4.536416000	1.774179000
1	11.919987000	-4.947982000	1.049590000
6	11.406380000	-4.425711000	3.144340000
6	10.119217000	-2.761947000	8.817861000
6	9.310216000	-2.634925000	9.933147000
1	9.603460000	-2.545499000	10.964987000
6	8.032062000	-2.650337000	9.397899000
6	3.241368000	-1.478132000	6.243103000
6	5.181584000	-0.764488000	1.591902000
6	9.257644000	-3.745778000	0.282772000
6	12.589951000	-4.813015000	3.969271000
6	11.612072000	-2.756808000	8.746146000
6	6.730404000	-2.591534000	10.134677000

4Ag^{nonaxial}; E=-43396.904035228559 Ha

47	11.092861000	3.085206000	5.197100000
47	10.073737000	3.303799000	8.586437000
47	7.828223000	3.910675000	6.084918000
9	13.888077000	1.899668000	4.481658000
9	15.735607000	2.065160000	5.602849000
9	14.638841000	3.842040000	5.037780000
9	14.133019000	2.231828000	10.888287000
9	12.425120000	0.949366000	10.560000000
9	12.132835000	3.066669000	10.845224000
9	8.766538000	3.004961000	11.700114000
9	9.466309000	5.038719000	11.536999000
9	7.601886000	4.619478000	12.553270000
9	4.302400000	4.142318000	7.453632000
9	5.346636000	5.872067000	6.697522000
9	4.176160000	6.021648000	8.514217000
9	5.543161000	3.553826000	1.858864000
9	5.659915000	2.216210000	3.552666000
9	5.622251000	4.345982000	3.874287000
9	10.854085000	2.825670000	0.420141000
9	11.922625000	2.638671000	2.296843000
9	11.458162000	4.590825000	1.509925000
7	12.429916000	2.711330000	6.775716000
7	12.016796000	2.635650000	8.046796000
7	8.155810000	4.050291000	9.069460000
7	7.282563000	4.319321000	8.090885000
7	8.341341000	3.431250000	4.079378000
7	9.626680000	3.368007000	3.709503000
6	13.749471000	2.496225000	6.751497000
6	14.224219000	2.270780000	8.031561000
1	15.232707000	2.065843000	8.345890000
6	13.083707000	2.371293000	8.809921000
6	7.610744000	4.428221000	10.229973000
6	6.349427000	4.957664000	10.020032000
1	5.656621000	5.345356000	10.746367000
6	6.194093000	4.864339000	8.647358000
6	7.590634000	3.417345000	2.971962000
6	8.393321000	3.351010000	1.845908000
1	8.092639000	3.328852000	0.812822000
6	9.673317000	3.321575000	2.373539000
6	14.508272000	2.569672000	5.466416000
6	12.945158000	2.156133000	10.282679000
6	8.361236000	4.269771000	11.512698000
6	4.998576000	5.225729000	7.826158000
6	6.097638000	3.387229000	3.060844000
6	10.978748000	3.336381000	1.646779000
35	6.751412000	7.121460000	1.851293000
6	8.006465000	6.955445000	3.254202000
6	7.588520000	7.051061000	4.569340000
1	6.550337000	7.241974000	4.803659000
6	8.511344000	6.890505000	5.591541000
1	8.143491000	6.976286000	6.605982000
6	9.862664000	6.635930000	5.332148000
6	10.251055000	6.573322000	3.991567000
1	11.280578000	6.382041000	3.719635000
6	9.340762000	6.731485000	2.959185000
1	9.672264000	6.662468000	1.931577000
35	13.955783000	5.938164000	9.916759000
6	12.700911000	6.104565000	8.513739000
6	13.118861000	6.008637000	7.198619000
1	14.157036000	5.817607000	6.964359000
6	12.196029000	6.169075000	6.176380000
1	12.563830000	6.082962000	5.161953000
6	10.844733000	6.423798000	6.435716000
6	10.456360000	6.486686000	7.776272000
1	9.426857000	6.678127000	8.048187000
6	11.366616000	6.328599000	8.808691000
1	11.035139000	6.397953000	9.836299000
47	9.614413000	9.974700000	6.571429000
47	10.633537000	9.756107000	3.182093000
47	12.879052000	9.149231000	5.683611000
9	6.819173000	11.158777000	7.287288000
9	4.971537000	10.993047000	6.166349000
9	6.068869000	9.216311000	6.730764000
9	6.572262000	10.823533000	0.880931000
9	8.278987000	12.108200000	1.206935000
9	8.573545000	9.991106000	0.923390000
9	11.940808000	10.055243000	0.068515000
9	11.240925000	8.021484000	0.231400000
9	13.105321000	8.440747000	-0.784868000
9	16.404800000	8.917648000	4.314824000
9	15.360861000	7.187640000	5.070780000
9	16.531263000	7.038461000	3.254019000
9	15.164178000	9.506187000	9.909473000
9	15.047009000	10.844262000	8.216037000
9	15.085086000	8.714543000	7.893899000
9	9.852624000	10.233869000	11.348217000
9	8.784369000	10.420453000	9.471309000
9	9.249395000	8.468453000	10.258415000
7	8.277158000	10.347907000	4.992825000
7	8.690165000	10.423718000	3.721644000
7	12.551452000	9.009605000	2.699040000
7	13.424702000	8.740493000	3.677601000
7	12.365837000	9.628683000	7.689183000
7	11.080507000	9.691840000	8.059081000
6	6.957589000	10.562729000	5.017261000
6	6.482444000	10.787447000	3.737312000
1	5.473772000	10.991730000	3.423162000
6	7.622817000	10.687236000	2.958675000
6	13.096526000	8.631739000	1.538481000
6	14.357775000	8.102144000	1.748432000
1	15.050555000	7.714416000	1.022088000
6	14.513167000	8.195511000	3.121084000
6	13.116570000	9.642513000	8.796584000
6	12.313905000	9.708412000	9.922674000
1	12.614600000	9.730348000	10.955761000
6	11.033898000	9.738177000	9.395034000
6	6.199030000	10.488833000	6.302454000
6	7.760448000	10.901121000	1.485658000
6	12.346038000	8.790371000	0.255768000
6	15.708760000	7.834171000	3.942215000
6	14.609559000	9.672999000	8.707597000
6	9.728363000	9.723076000	10.121589000

5Ag^{disp}; E=-38710.456606188767 Ha

47	-1.116141000	-8.587579000	-4.227673000
47	1.201109000	-7.034052000	-2.237232000
47	-2.106348000	-5.922106000	-2.273799000
7	1.827842000	-8.459105000	-3.668018000
7	-3.545982000	-7.054965000	-3.331656000
7	-3.172127000	-8.170318000	-3.969337000
7	-0.599839000	-4.849169000	-1.198164000
7	0.943261000	-8.955821000	-4.541659000
7	0.593694000	-5.428576000	-1.011415000
6	-4.270134000	-8.772102000	-4.436374000
6	3.034911000	-8.942360000	-3.980072000
6	-4.878333000	-6.962227000	-3.408241000
9	-5.364315000	-10.515793000	-5.535932000
6	-4.159589000	-10.056642000	-5.193630000
9	-3.436413000	-9.913962000	-6.314562000
9	-3.548740000	-11.009059000	-4.461767000
6	2.950872000	-9.772132000	-5.084545000
1	3.740935000	-10.310948000	-5.577629000
6	-5.398118000	-8.039906000	-4.105928000
1	-6.426922000	-8.254835000	-4.336794000
6	1.602650000	-9.744252000	-5.396558000
6	-0.646355000	-3.753374000	-0.431570000
6	4.239533000	-8.558592000	-3.183649000
9	4.556810000	-7.263840000	-3.345478000
9	5.300712000	-9.286104000	-3.539937000
9	4.039511000	-8.744437000	-1.865202000
9	-2.980407000	-3.498055000	-0.578795000
6	-1.824061000	-2.832419000	-0.432675000
9	-1.757024000	-1.938892000	-1.430877000
9	-1.885306000	-2.147112000	0.714212000
6	1.285843000	-4.691225000	-0.135449000
9	1.738174000	-10.988323000	-7.364686000
6	0.877451000	-10.474123000	-6.480735000
9	0.036926000	-9.664285000	-7.144965000
9	0.137834000	-11.485402000	-5.996213000
6	0.537903000	-3.601482000	0.270943000
1	0.806273000	-2.826628000	0.968069000
6	-5.595653000	-5.813651000	-2.775920000
9	-6.861302000	-5.752028000	-3.192900000
9	-5.004661000	-4.644845000	-3.064866000
9	-5.616431000	-5.915596000	-1.432862000
6	2.640174000	-5.119188000	0.329778000
9	3.428155000	-5.505008000	-0.684263000
9	3.256671000	-4.132810000	0.982050000
9	2.561288000	-6.171992000	1.174000000
47	-3.433392000	-10.141104000	2.161667000
47	-1.116142000	-8.587579000	4.152107000
47	-0.125935000	-11.253052000	2.198233000
7	-4.072173000	-8.744160000	3.602789000
7	1.300538000	-10.198950000	3.355398000
7	0.935439000	-9.036480000	3.909009000
7	-1.631155000	-12.258276000	1.059586000
7	-3.181017000	-8.207395000	4.444056000
7	-2.798400000	-11.639821000	0.840530000
6	2.038792000	-8.418219000	4.344126000
6	-5.276245000	-8.239628000	3.892355000
6	2.629743000	-10.304455000	3.450614000
6	1.938076000	-7.092322000	5.026443000
9	1.164229000	-6.240469000	4.323181000
9	1.386257000	-7.194837000	6.244477000
9	3.139392000	-6.530511000	5.166327000
6	-5.183210000	-7.352317000	4.950448000
1	-5.969037000	-6.788574000	5.422014000
6	3.158599000	-9.187867000	4.078484000
1	4.188102000	-8.971946000	4.305784000
6	-3.834022000	-7.373126000	5.260419000
6	-1.560520000	-13.304153000	0.228315000
6	-6.484846000	-8.656504000	3.118079000
9	-6.306520000	-8.486220000	1.793605000
9	-7.552801000	-7.940175000	3.477188000
9	-6.777329000	-9.953147000	3.301699000
9	-0.358361000	-15.007423000	-0.817116000
6	-0.420956000	-14.270164000	0.295023000
9	0.758060000	-13.648402000	0.451938000
9	-0.554185000	-15.111704000	1.332496000
6	-3.449889000	-12.298002000	-0.124566000
6	-3.106587000	-6.608644000	6.318509000
9	-2.377992000	-5.604733000	5.801452000
9	-2.255517000	-7.395707000	6.997319000
9	-3.963805000	-6.078184000	7.195059000
6	-2.700177000	-13.377605000	-0.557249000
1	-2.942507000	-14.101049000	-1.316295000
9	3.398625000	-11.453124000	1.544781000
6	3.339825000	-11.495935000	2.889993000
9	2.720640000	-12.640487000	3.210966000
9	4.592994000	-11.560433000	3.344466000
6	-4.779673000	-11.814612000	-0.607623000
9	-5.280646000	-12.632448000	-1.533285000
9	-5.673566000	-11.713592000	0.387307000
9	-4.687038000	-10.584117000	-1.160796000
6	-0.917597000	-8.656256000	-0.082264000
6	0.428244000	-8.951006000	0.165533000
1	0.984714000	-8.403822000	0.915371000
6	1.098287000	-9.948057000	-0.530425000
1	2.141918000	-10.148025000	-0.328550000
17	1.254226000	-11.911059000	-2.392429000
6	0.422993000	-10.677387000	-1.494518000
6	-0.910515000	-10.418156000	-1.759248000
1	-1.445353000	-11.008152000	-2.494060000
6	-1.561575000	-9.410299000	-1.065481000
1	-2.601172000	-9.235815000	-1.302915000
6	-1.636254000	-7.588632000	0.670523000
6	-3.010149000	-7.376270000	0.506981000
1	-3.596323000	-7.997402000	-0.159282000
6	-3.678606000	-6.373484000	1.191077000
1	-4.739985000	-6.218192000	1.055746000
6	-2.967876000	-5.572045000	2.059148000
9	-3.606651000	-4.601383000	2.722792000
6	-1.611780000	-5.744164000	2.254842000
1	-1.076593000	-5.098995000	2.939247000
6	-0.959354000	-6.750333000	1.561901000
1	0.106970000	-6.848833000	1.710679000

5Ag^{h2t}; E=-38710.457750595509 Ha

47	2.706228000	-7.023796000	-6.614844000
47	0.442521000	-9.483895000	-7.516387000
47	2.953941000	-10.176720000	-5.239844000
7	0.539256000	-7.668428000	-8.606944000
7	1.263551000	-6.656600000	-8.110642000
7	4.224037000	-7.447931000	-5.221199000
7	4.443178000	-8.710854000	-4.830928000
7	0.454756000	-11.343048000	-6.481666000
7	1.444544000	-11.607131000	-5.619869000
1	-0.399164000	-14.304892000	-5.364806000
6	0.051154000	-13.353996000	-5.590439000
6	0.909835000	-5.538168000	-8.753675000
6	1.216880000	-12.810490000	-5.080705000
1	6.826011000	-7.094443000	-3.262217000
6	5.992245000	-7.423272000	-3.857842000
6	-0.258284000	-7.177195000	-9.562167000
6	-0.387793000	-12.381561000	-6.472836000
6	5.143456000	-6.665724000	-4.644328000
9	6.785440000	-10.662507000	-4.295519000
6	6.043037000	-9.972262000	-3.417253000
9	6.816157000	-9.698666000	-2.362678000
9	5.063056000	-10.795324000	-3.007690000
6	-0.061025000	-5.813630000	-9.700602000
1	-0.551968000	-5.132557000	-10.373615000
6	5.500896000	-8.709711000	-4.011002000
9	-1.342157000	-12.068571000	-8.595922000
6	-1.616968000	-12.379699000	-7.321962000
9	-2.517994000	-11.476857000	-6.886604000
9	-2.206581000	-13.577327000	-7.305021000
9	2.836487000	-4.184633000	-8.730231000
6	1.535464000	-4.226239000	-8.407397000
9	0.921997000	-3.224397000	-9.041949000
9	1.460284000	-3.978720000	-7.083670000
6	-1.143450000	-8.071003000	-10.372735000
9	-0.450898000	-8.720467000	-11.322237000
9	-2.100964000	-7.368218000	-10.984046000
9	-1.739814000	-9.011165000	-9.620296000
6	2.145929000	-13.379998000	-4.058559000
9	3.428812000	-13.269605000	-4.432494000
9	1.886179000	-14.671127000	-3.844312000
9	2.031758000	-12.742816000	-2.876537000
6	5.115078000	-5.183588000	-4.835895000
9	5.151920000	-4.838227000	-6.130588000
9	6.145833000	-4.601287000	-4.220899000
9	3.986083000	-4.643965000	-4.328720000
6	0.004168000	-6.298722000	-4.803928000
6	0.122195000	-7.596138000	-4.293018000
1	0.677796000	-5.512102000	-4.487516000
6	-0.964075000	-5.966743000	-5.739686000
1	-1.028826000	-4.957398000	-6.120334000
6	-1.845581000	-6.935640000	-6.180930000
17	-3.068644000	-6.533932000	-7.351951000
6	-1.757589000	-8.231508000	-5.701557000
1	-2.454146000	-8.987937000	-6.039654000
6	-0.782983000	-8.548264000	-4.769682000
1	-0.757263000	-9.567695000	-4.411937000
6	1.153179000	-7.952124000	-3.274330000
6	1.249218000	-9.248350000	-2.755280000
1	0.557044000	-10.023157000	-3.058497000
6	2.218480000	-9.594268000	-1.827464000
1	2.285224000	-10.600579000	-1.437973000
6	3.108130000	-8.630308000	-1.405278000
9	4.050335000	-8.955810000	-0.512296000
6	3.052228000	-7.336115000	-1.883507000
1	3.766327000	-6.600020000	-1.538288000
6	2.078641000	-7.010061000	-2.813507000
1	2.069216000	-5.995691000	-3.188005000
47	0.686565000	-5.912400000	-0.193009000
47	-1.824856000	-5.219575000	-2.469552000
47	-1.577142000	-8.372499000	-1.094552000
7	-3.311466000	-6.682123000	-2.862615000
7	-0.125171000	-8.758683000	0.385389000
7	0.657000000	-7.766283000	0.826663000
7	-3.090612000	-7.952987000	-2.500091000
7	0.704440000	-4.078377000	-1.257675000
7	-0.275039000	-3.812964000	-2.131967000
1	1.690358000	-1.218610000	-2.521192000
6	1.197295000	-2.134739000	-2.246591000
6	0.260970000	-9.889281000	0.987536000
6	0.008031000	-2.649712000	-2.730395000
6	-4.836093000	-7.949372000	-3.895176000
1	-5.658322000	-8.266442000	-4.512780000
6	1.524916000	-8.280614000	1.705078000
6	1.593746000	-3.080774000	-1.317234000
6	-3.996428000	-8.723797000	-3.113625000
9	-5.706407000	-5.603799000	-5.277031000
6	-4.891058000	-5.379043000	-4.244887000
9	-3.905908000	-4.565441000	-4.663685000
9	-5.584452000	-4.697604000	-3.319679000
6	1.315826000	-9.641127000	1.848709000
1	1.848900000	-10.335823000	2.473879000
6	-4.355570000	-6.665493000	-3.699022000
6	2.830209000	-3.093885000	-0.478132000
9	3.712867000	-4.016200000	-0.910939000
9	2.562876000	-3.384059000	0.802559000
9	3.439994000	-1.907014000	-0.515873000
6	-0.405467000	-11.190353000	0.680271000
9	-0.384925000	-11.454255000	-0.642703000
9	-1.692496000	-11.201173000	1.052618000
9	0.212489000	-12.197625000	1.302387000
6	2.529273000	-7.410575000	2.391246000
9	3.327926000	-8.139300000	3.173993000
9	1.939598000	-6.477920000	3.155366000
9	3.303843000	-6.749809000	1.512241000
6	-0.899082000	-2.078869000	-3.771588000
9	-0.930723000	-2.848151000	-4.877426000
9	-2.162230000	-1.980101000	-3.334776000
9	-0.490644000	-0.864130000	-4.141898000
6	-3.967393000	-10.211512000	-2.969273000
9	-2.868932000	-10.744586000	-3.545181000
9	-5.028562000	-10.768924000	-3.554693000
9	-3.947299000	-10.596295000	-1.685371000

5Ag^{h2h}; E=-38710.456836038276

47	-0.709686000	0.000000000	-6.603906000
47	-2.367008000	-2.872988000	-5.609690000
47	-3.904164000	0.197502000	-5.290059000
7	0.334692000	-1.827782000	-6.415794000
7	-0.349369000	-2.967487000	-6.242083000
7	-4.281230000	-2.722121000	-4.713915000
7	-4.837105000	-1.521573000	-4.507841000
7	-1.862184000	1.751511000	-6.873150000
7	-3.058171000	1.849165000	-6.283864000
1	-2.716384000	4.830821000	-7.599359000
6	-2.632975000	3.813612000	-7.258177000
6	0.517482000	-3.983362000	-6.295515000
6	-3.532450000	3.079463000	-6.504063000
6	-6.081850000	-3.031271000	-3.428344000
1	-6.847106000	-3.490560000	-2.827601000
6	1.625615000	-2.141338000	-6.578088000
6	-1.592562000	2.921334000	-7.461288000
6	-5.013564000	-3.635675000	-4.067418000
9	-7.706542000	-0.929468000	-2.460354000
6	-6.776665000	-0.535655000	-3.336085000
9	-7.404366000	0.020811000	-4.381761000
9	-6.059831000	0.444578000	-2.753485000
6	1.801234000	-3.512332000	-6.512046000
1	2.713405000	-4.076451000	-6.596164000
6	-5.919169000	-1.692169000	-3.740039000
6	-0.348923000	3.101866000	-8.271357000
9	-0.467060000	2.541158000	-9.486441000
9	0.714056000	2.526543000	-7.683280000
9	-0.076381000	4.395615000	-8.450333000
6	0.055044000	-5.393943000	-6.112035000
9	-0.869362000	-5.735723000	-7.022899000
9	-0.503466000	-5.577957000	-4.904808000
9	1.077829000	-6.244652000	-6.224734000
6	2.647738000	-1.074211000	-6.796165000
9	3.880179000	-1.589272000	-6.818227000
9	2.609151000	-0.151084000	-5.814470000
9	2.455616000	-0.414909000	-7.945191000
6	-4.870140000	3.478580000	-5.970642000
9	-5.870593000	2.827127000	-6.582897000
9	-5.077437000	4.787436000	-6.129949000
9	-4.977440000	3.201413000	-4.655855000
6	-4.623665000	-5.079127000	-4.086111000
9	-4.664045000	-5.590282000	-5.326748000
9	-5.437872000	-5.804316000	-3.316679000
9	-3.367950000	-5.256903000	-3.636320000
1	-0.350462000	-1.457176000	-3.603771000
6	-1.204244000	-1.271238000	-2.963213000
1	-3.149587000	1.195990000	-1.703562000
6	-2.772201000	0.204987000	-1.921165000
6	-1.659612000	0.035320000	-2.748517000
6	-0.963584000	1.209705000	-3.343618000
6	0.347095000	1.115835000	-3.821548000
1	0.886540000	0.177799000	-3.768024000
6	1.003301000	2.213063000	-4.360558000
1	2.015119000	2.120757000	-4.733998000
6	0.348414000	3.431182000	-4.419813000
6	-0.952894000	3.553426000	-3.965632000
1	-1.463487000	4.505623000	-4.026770000
6	-1.598626000	2.447879000	-3.443689000
1	-2.624174000	2.568221000	-3.120848000
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1	-1.463119000	-3.369741000	-2.525061000
6	-3.412858000	-0.872858000	-1.335212000
1	-4.271533000	-0.730853000	-0.692576000
9	-3.525680000	-3.185531000	-0.979239000
6	-2.924079000	-2.140973000	-1.565285000
17	1.161269000	4.822063000	-5.080918000
47	1.046030000	-1.256925000	-0.653996000
47	2.667451000	1.608968000	-1.604049000
47	-0.395092000	1.795757000	0.058172000
7	3.381116000	-0.275216000	-2.272700000
7	-1.103194000	0.053921000	1.007095000
7	-0.518775000	-1.127548000	0.772958000
7	0.524992000	3.532318000	-0.706758000
7	2.604190000	-1.349433000	-2.077461000
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9	-1.752835000	-4.277157000	1.916940000
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9	-0.562973000	-3.918286000	0.142061000
9	0.329821000	-3.729133000	2.095410000
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1	4.903759000	-2.541366000	-4.085552000
6	-2.254582000	-1.493460000	2.133423000
1	-2.984444000	-1.979046000	2.757256000
6	3.120920000	-2.368068000	-2.774875000
6	0.120590000	4.805411000	-0.778572000
6	5.406106000	0.369996000	-3.520709000
9	4.881413000	1.311256000	-4.322744000
9	6.394835000	-0.230763000	-4.188414000
9	5.943713000	1.010647000	-2.471808000
9	-1.455771000	4.956575000	0.961073000
6	-1.255024000	5.194603000	-0.343895000
9	-2.203773000	4.504548000	-1.007664000
9	-1.473513000	6.493186000	-0.564047000
6	2.166646000	4.709216000	-1.492114000
9	3.028801000	-4.542925000	-3.624105000
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6	1.134416000	5.606632000	-1.275302000
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6	-3.027140000	0.980851000	2.235633000
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6	3.554769000	4.968352000	-1.987097000
9	3.922525000	4.081941000	-2.930451000
9	3.656236000	6.191708000	-2.510038000
9	4.459113000	4.869805000	-0.998890000

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