### **Supporting Information**

#### for

*Cis* and *Trans*-bis(Tetrathiafulvalene-Acetylide) Platinum(II) Complexes : Syntheses, Crystal Structures, and Influence of the Ancillary Ligands on their Electronic Properties

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Fig. S1 ORTEP drawing of the second crystallographically independent molecule of complex2 with the main numbering scheme. Thermal ellipsoids drawn at the 50 % probability level.



Fig. S2 ORTEP drawing of the second crystallographically independent molecule of complex3 with the main numbering scheme. Thermal ellipsoids drawn at the 50 % probability level.



Fig. S3 UV-vis absorption spectra of complexes 3 and 4 in dichloromethane at room temperature,  $(c \sim 10^{-5} \text{ mol.L}^{-1})$ .



**Fig. S4** UV-visible absorption spectra of complex **3**, the alkynyl-TTF precursor and the  $Pt(dppe)Cl_2$  precursor in dichloromethane at room temperature, (c ~ 10<sup>-5</sup> mol.L<sup>-1</sup>).

#### **Computational Details**

DFT calculations (spin unrestricted for all open shell systems) were performed on gas phase molecules using the Gaussian 03, Revision D.02 program package, the B3LYP functional and the LanL2DZ basis set. The latter employs the Dunning/Huzinaga valence double zeta D95V[1] basis set for first row atoms and the Los Alamos Effective Core Potential plus DZ on atoms from Na-Bi.[2–4]

- 1 T. H. Dunning Jr and P. J. Hay, Modern Theoretical Chemistry, Plenum, New York, 1976.
- 2 P. J. Hay and W. R. Wadt, J. Chem. Phys., 1985, 82, 270.
- 3 W. R. Wadt and P. J. Hay, J. Chem. Phys., 1985, 82, 284.
- 4 P. J. Hay and W. R. Wadt, J. Chem. Phys., 1985, 82, 299.

Full parameters for common bases sets are available at https://bse.pnl.gov/bse/portal Parameters for the LanL2DZ basis set are reproduced next.

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#### LanL2DZ basis set

# When publishing results obtained from use of the Basis Set Exchange (BSE) software and the EMSL Basis Set Library, please cite:

The Role of Databases in Support of Computational Chemistry Calculations Feller, D., J. Comp. Chem., 17(13), 1571-1586, 1996.

Basis Set Exchange: A Community Database for Computational Sciences

Schuchardt, K.L., Didier, B.T., Elsethagen, T., Sun, L., Gurumoorthi, V., Chase, J., Li, J., and Windus, T.L. J. Chem. Inf. Model., 47(3), 1045-1052, 2007, doi:10.1021/ci600510j.

! LANL2DZ ECP EMSL Basis Set Exchange Library 4/26/11 8:55 AM ! Elements References ! ------! H - Ne: T. H. Dunning Jr. and P. J. Hay, in Methods of Electronic Structure ! Theory, Vol. 2, H. F. Schaefer III, ed., PLENUM PRESS (1977) ! Na - Hg: P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 270 (1985). ! P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 284 (1985). ! P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 299 (1985). ! P. J. Hay and W. R. Wadt, J. Chem. Phys. 82, 299 (1985).

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л с	2	1 00	
D	Ξ.	19 2384000	0 0328280
	-	2 8987000	0 2312040
		0.6535000	0.8172260
S	1	1.00	0.01/2200
2	-	0.1776000	1.0000000
* * *	*		
С		0	
S	7	1.00	
	423	33.000000	0.0012200
	63	34.9000000	0.0093420
	14	46.1000000	0.0454520
	4	42.5000000	0.1546570
	-	14.1900000	0.3588660
		5.1480000	0.4386320
		1.9670000	0.1459180
S	2	1.00	
		5.1480000	-0.1683670
		0.4962000	1.0600910
S	1	1.00	
P		0.1533000	1.0000000
Ρ	4.	1.00	0 0105300
		18.1600000	0.0185390
		1 1420000	0.1154360
		0.2594000	0.3801880
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		0 1 4 6 0 0 0	1 0000000
***	*	0.1146000	1.0000000
*** P	*	0.1146000	1.0000000
*** P S	* 2	0.1146000	1.0000000
*** P S	* 2	0.1146000 0 1.00 1.5160000	-0.5862089
*** P S	* 2	0 1.00 1.5160000 0.3369000	1.0000000 -0.5862089 1.2994376
*** P S S	* 2 1	0 1.00 1.5160000 0.3369000 1.00	-0.5862089 1.2994376
*** P S S	* 2 1	0.1146000 0 1.00 1.5160000 0.3369000 1.00 0.1211000	-0.5862089 1.2994376 1.0000000
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*** P S S P	* 2 1 2	0.1146000 0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000	-0.5862089 1.2994376 1.0000000 -0.0691472
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*** S S P P	* 1 2 1	0.1146000 0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000 0.3934000 1.00 0.1190000	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000
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*** P S P P *** S	* 1 2 1 * 2	0.1146000 0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000 0.3934000 1.00 0.1190000 0 1.00 1.00 1.00 1.00 1.00	-0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000
*** P S P P *** S S	* 1 2 1 * 2	0.1146000 0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000 0.3934000 1.00 0.1190000 0 1.00 1.8500000 0.4035000 1.00	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801
*** P S P P *** S S	* 1 2 1 * 2 1	0.1146000 0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 0.3934000 1.00 0.1190000 0 1.00 1.850000 0.4035000 1.00 0.4035000 0.1438000	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801
*** P S P P *** S S S	* 2 1 2 1 * 2 1 2	0.1146000 0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 0.3934000 1.00 0.1190000 0 1.00 1.850000 0.4035000 1.00 0.4438000 1.00	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000
*** P S P P *** S S P	* 2 1 2 1 * 2 1 2	0.1146000 0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000 0.3934000 1.00 0.1190000 0 1.00 1.00 1.850000 0.4035000 1.00 0.4435000 1.00 0.1438000 1.00	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000 -0.0608116
*** P S P P *** S S S P	* 2 1 2 1 * 2 1 2	0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000 0.3934000 1.00 0.1190000 0 1.00 1.00 1.8500000 0.4035000 1.00 0.1438000 1.00 0.44350000 0.44350000 0.44350000 0.44350000 0.44470000	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000 -0.0608116 1.0132686
*** P S P P *** S S S P P	* 1 2 1 * 2 1 2 1 2	0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000 0.3934000 1.00 0.1190000 0 1.00 1.8500000 0.4035000 0.4035000 0.1438000 1.00 4.9450000 0.4870000 1.00	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000 -0.0608116 1.0132686
**** P S P P *** S S P P P	* 1 2 1 * 2 1 2 1	0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 0.3934000 1.00 0.1190000 0 1.00 1.8500000 0.4035000 1.00 0.438000 1.00 0.1438000 1.00 0.4870000 0.1379000	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000 -0.0608116 1.0132686 1.0000000
**** S S P P *** S S P P *** S S P P ***	* 2 1 2 1 * 2 1 2 1 *	0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000 0.3934000 1.00 0.1190000 0 1.00 1.850000 0.4035000 1.00 0.435000 1.00 4.9450000 0.4870000 1.00 0.1379000	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000 -0.0608116 1.0132686 1.0000000
**** S P P P **** S S S P P P ***	* 2 1 2 1 * 2 1 2 1	0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000 0.3934000 1.00 0.1190000 0 1.00 1.00 1.438000 1.00 0.4435000 0.4435000 0.44870000 1.00 0.1379000 0	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000 -0.0608116 1.0132686 1.0000000
**** P S P P **** S S P P P *** Ru S	* 2 1 2 1 * 2 1 2 1 2 1 2 1 3	0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 3.7050000 0.3934000 1.00 0.1190000 0 1.00 1.8500000 0.4035000 1.00 0.1438000 1.00 0.1438000 0.00 1.00 0.1379000 0 1.00	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000 -0.0608116 1.0132686 1.0000000
**** P P P S S S P P P Ru S	* 2 1 2 1 * 2 1 2 1 2 1 2 1 3	0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 0.3934000 1.00 0.1190000 0 1.00 1.8500000 0.4035000 0.4035000 0.4438000 1.00 0.1438000 1.00 0.1379000 0 1.00 2.5650000	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000 -0.0608116 1.0132686 1.0000000 -1.0431056
*** P P P S S S P P Ru S	* 2 1 2 1 * 2 1 2 1 2 1 3	0 1.00 1.5160000 0.3369000 1.00 0.1211000 1.00 0.3934000 1.00 0.1190000 0 1.00 1.8500000 0.4035000 1.00 0.438000 1.00 0.4870000 0.1379000 0 1.00 2.5650000 1.5080000	1.0000000 -0.5862089 1.2994376 1.0000000 -0.0691472 1.0161988 1.0000000 -0.5324335 1.2763801 1.0000000 -0.608116 1.0132686 1.0000000 -1.0431056 1.3314786

0.512 S 4 1.0 2.565 1.508 0.512 0.136 S 1 1.0 0.041 P 3 1.0 4.859 1.219 0.441 P 2 1.0 0.572 0.083 P 1 1.0 0.025 D 3 1.0 4.195 1.377 0.482 D 1 1.0 0.150	9000 0 0000 2000 2000 0 0 0 0 0 0 0 0 0	0.5613065 0.8770128 -1.2634660 -0.8384987 1.0637773 1.0000000 -0.0945755 0.7434798 0.3668144 -0.0880864 1.0283970 1.0000000 0.0485729 0.5105223 0.5730028 1.0000000	
! Elements		References	
!	P.T. Hav and W	R Wadt J Chem Phys 82 2	70
!	P. J. Hay and W.	. R. Wadt, J. Chem. Phys. 82, 2	284
! !	P. J. Hay and W.	. R. Wadt, J. Chem. Phys. 82, 2	299
P 0 P-ECP 2 d potenti 5	al 10		
1 462.12	11423	-10.000000	
2 21.23	49094	-28.3668251	
2 6.33 2 2.06	88415 520684	-9.8577589 -1.0163783	
s-d potenti 5	al		
0 78.08 1 58.95	31823 576810	3.0000000 12.9104154	
2 36.05	71255	150.0250298	
2 2.67	57561	23.0397012	
p-d potenti 6	.al		
0 75.16	17880	5.000000	
2 47.94	81748	198.5585104	
2 18.45 2 5.94	14190	40.3944144	
2 1.84 S 0	87507	6.4483233	
S-ECP 2 d potenti	10 al		
5		10,000000	
2 108.13	42248	-10.0000000	
2 24.56 2 7.37	97664 02438	-30.4513290 -10.3745886	
2 2.37	12569 al	-0.9899295	
5	26201	2 000000	
0 106.31 1 100.82	./6/81 45833	10.6284036	
2 53.58 2 15.37	58472 06332	223.6360469 93.6460845	
2 3.17	78402	28.7609065	
p-u potenti 6	.a.		
0 101.97 1 93.28	09185 08973	5.000000 6.0969842	
2 65.14	31772	285.4425500 147 1448413	
2 7.81	.20535	53.6569778	
2 2.31 RU 0	. 12/30	8.9249559	
RU-ECP f potential	3 28		
5 0 554.37 1 155.10	'96303 166871	-0.0515270 -20.1816536	

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# Electronic Supplementary Material (ESI) for Dalton Transactions This journal is The Royal Society of Chemistry 2012

2	48.4976263	-105.9966915	
2	14.7701594	-42.2166788	
2	5.2077363	-3.7675024	
s-f	potential		
5	-		
0	66.7118060	2.9578344	
1	77.3503632	25.3748707	
2	18.3571445	536.1262372	
2	11.8404727	-651.2057221	
2	8.1179479	381.3816943	
p-f	potential		
5	L		
0	54.9937915	4.9651557	
1	13.9399212	23.8861501	
2	15,2118246	464,4631344	
2	10.5460691	-714.4451788	
2	7 5539486	377 5503594	
d-f	notential	37710000001	
4	poconcia		
0	60.3444595	3,0352988	
1	45.2100305	23,2901723	
2	19,1190074	146.0926620	
2	4 2712090	28 9129770	
4	4.2712090	20.9129770	

### <u>Input Files,</u>

#### Cartesian Coordinates of Optimized Geometry,

#### And Selection of Distances and Angles in the Optimized Geometry

Geometry Optimization of Complex 2 : input file.

#B3LYP/LanL2DZ opt

cisPt bipyTbu TTF)2 neutre singulet

0	1		
Pt O	-1.165500	-0.061000	-2.131000
N 0	-2.640500	-0.097000	-3.571000
C 0	-3.971500	-0.145000	-3.327000
C 0	-4.903500	-0.112000	-4.329000
C 0	-4.482500	-0.050000	-5.687000
C 0	-3.120500	-0.044000	-5.890000
C 0	-2.229500	-0.057000	-4.853000
C 0	-5.523500	-0.024000	-6.799000
C 0	-4.846500	0.046000	-8.204000
C 0	-6.423500	1.189000	-6.618000
N 0	-0.063500	0.027000	-3.862000
C 0	-6.368500	-1.279000	-6.730000
C 0	1.285500	0.104000	-3.928000
C 0	1.962500	0.104000	-5.147000
C 0	1.271500	0.023000	-6.328000
C 0	-0.114500	-0.020000	-6.257000
C 0	-0.762500	-0.012000	-5.029000
C U	1.995500	0.003000	-7.665000
CO	2.935500	-1.223000	-7.673000
C U	2.823500	1.290000	-7.800000
C U	1.076500	-0.091000	-8.849000
CO	-2.404500	-0.142000	-0.625000
C U	-3.21/500	-0.1/7000	0.233000
0	-4.193500	-0.187000	1.312000
C U	-5.512500	-0.166000	1.191000
0 0	-6.289500	-0.1/5000	-0.09/000
SU	-6.468500	-0.085000	2.655000
50	-3.540500 E 110E00	-0.137000	2.952000
	-5.110500 E 226E00	-0.123000	5.772000 E 088000
C 0	-3.230500	-0.085000	5.088000
2 0 2 0	-3 833500	-0.083000	5.929000
	-6.065500		7 567000
	-7 072500	-0.078000	8 671000
	-4 771500	-0 059000	7 635000
C O	-3 930500	-0.067000	8 887000
CO	0.391500	-0.018000	-0.945000
C 0	1.389500	-0.020000	-0.310000
C 0	2.555500	-0.020000	0.506000
C 0	3.841500	0.014000	0.124000
C 0	4.320500	0.036000	-1.287000
S 0	2.265500	-0.041000	2.266000
S 0	5.068500	-0.003000	1.378000
C 0	3.959500	-0.016000	2.748000
C 0	4.369500	-0.022000	4.006000
S 0	3.217500	-0.080000	5.357000
S 0	6.029500	0.032000	4.503000
C 0	4.436500	-0.121000	6.646000
C 0	3.932500	-0.181000	8.049000
C 0	5.709500	-0.087000	6.241000
C 0	6.933500	-0.160000	7.120000
н О	-4.269500	-0.200000	-2.427000

Η	0	-5.827500	-0.132000	-4.119000
Н	0	-2.789500	-0.031000	-6.778000
Η	0	-5.537500	0.057000	-8.901000
Η	0	-4.270500	-0.736000	-8.330000
Η	0	-4.307500	0.863000	-8.265000
Η	0	-7.090500	1.210000	-7.334000
Η	0	-5.882500	2.006000	-6.653000
Η	0	-6.875500	1.133000	-5.751000
Η	0	-7.030500	-1.266000	-7.451000
Η	0	-6.826500	-1.315000	-5.865000
Η	0	-5.792500	-2.066000	-6.828000
Η	0	1.785500	0.162000	-3.123000
Η	0	2.911500	0.158000	-5.158000
Η	0	-0.625500	-0.057000	-7.056000
Η	0	3.557500	-1.163000	-6.919000
Η	0	3.441500	-1.242000	-8.513000
Η	0	2.404500	-2.042000	-7.592000
Η	0	3.439500	1.363000	-7.041000
Η	0	2.222500	2.066000	-7.809000
Η	0	3.334500	1.264000	-8.634000
Η	0	0.538500	-0.908000	-8.779000
Η	0	1.606500	-0.119000	-9.673000
Η	0	0.484500	0.689000	-8.866000
Η	0	-6.475500	0.747000	-0.373000
Η	0	-7.132500	-0.655000	0.034000
Η	0	-5.764500	-0.623000	-0.791000
Η	0	-7.518500	-0.949000	8.715000
Η	0	-7.738500	0.621000	8.502000
Н	0	-6.623500	0.102000	9.521000
H	0	-3.390500	0.749000	8.924000
H	0	-3.339500	-0.850000	8.878000
H	0	-4.513500	-0.108000	9.6/3000
H	0	4.679500	-0.846000	-1.525000
Н	0	5.023500	0.711000	-1.384000
H	0	3.5/1500	0.254000	-1.883000
H	0	3.351500	-0.966000	8.152000
H	0	3.423500	0.632000	8.24/000
H	0	4.690500	-0.252000	8.665000
H	0	6.963500	0.625000	/./0/000
H	0	/./38500	-0.1/9000	6.558000
Н	υ	6.896500	-0.9/4000	/.665000

### Cartesians Coordinates for the Optimized Geometry of Complex 2 (-1858.598128 Hartrees)

Pt	0.00020	1.06621	-0.00279
N	-1.31734	2.68722	-0.07442
С	-2.67150	2.59227	-0.15755
С	-3.49003	3.72100	-0.21252
С	-2.92840	5.02173	-0.18490
С	-1.52462	5.09592	-0.09920
С	-0.73651	3.93102	-0.04464
С	-3.83709	6.26406	-0.25037
С	-3.03376	7.58694	-0.20121
С	-4.82048	6.23872	0.95804
N	1.31941	2.68575	0.07164
С	-4.64925	6.22817	-1.57970
С	2.67348	2.58928	0.15442
С	3.49314	3.71707	0.21172
С	2.93279	5.01841	0.18705
С	1.52908	5.09419	0.10160
С	0.73982	3.93020	0.04453
С	3.84272	6.25970	0.25527
С	4.82594	6.23616	-0.95333
С	4.65503	6.21991	1.58439
С	3.04069	7.58348	0.20927
С	-1.37974	-0.31577	-0.06357

С	-2.30142	-1.14371	-0.09861
C	-3 36490	-2 07429	-0 13297
a	3.30120	2.07125	0.15257
C	-3.28832	-3.39333	-0.45936
С	-2.03519	-4.13199	-0.84797
S	-4.82771	-4.38631	-0.42262
S	-5 04505	-1 41321	0 32867
5	5.04505	1.41521	0.52007
C	-5.93834	-2.98414	0.00780
С	-7.27827	-3.11029	0.09243
S	-8 16837	-4 69296	-0 20634
a	0.2003/	1 71700	0.20051
S	-8.39639	-1./1/23	0.53265
С	-9.85855	-3.97493	-0.03483
C	-10 97273	-4 96427	-0 27359
a		2 6 6 7 2 1	0.20007
C	-9.95956	-2.00/21	0.28987
С	-11.21278	-1.85313	0.49831
С	1.37877	-0.31721	0.05675
c	2 20074	1 1/505	0 00104
C	2.29974	-1.14595	0.09104
С	3.36260	-2.07724	0.12624
С	3.28568	-3.39558	0.45531
C	2 02271	_1 12272	0 8/727
Č	2.03271	-4.13273	0.04/2/
S	5.04240	-1.41839	-0.34006
S	4.82437	-4.38971	0.41750
C	5 93556	-2 98818	-0 01343
c	5.55550	2.00010	0.01040
C	1.2/5/1	-3.11408	-0.09488
S	8.39437	-1.72181	-0.53612
S	8 16572	-4 69580	0 20904
5	0.10572	4.00000	0.20004
C	9.95/35	-2.66856	-0.2/945
С	11.21075	-1.85308	-0.48116
C	9 85605	-3 97558	0 04797
a	10.07001	1.00050	0.01727
Ċ	10.97001	-4.96256	0.29/2/
Н	-3.07280	1.58628	-0.18025
Н	-4.56229	3,57129	-0.27716
тт	1 02574	6 06069	0 07507
н	-1.03574	0.00000	-0.0/56/
Н	-3.72587	8.43580	-0.25521
Н	-2.33881	7.67604	-1.04681
U	2 46472	7 69622	0 72072
н	-2.40472	7.00032	0.75275
Н	-5.48373	7.11219	0.91690
Н	-4.27639	6.26647	1.91074
ч	-5 45030	5 3/1/1	0 05533
	-3.43030	J. J. J. I.	0.9000
Н	-5.31604	7.09828	-1.63230
Н	-5.26905	5.32717	-1.65596
н	-3 98262	6 25410	-2 45110
	3.90202	1 50004	2.15110
н	3.0/3/8	1.58284	0.1/498
Н	4.56525	3.56616	0.27589
н	1 04116	6 05948	0 08045
 		F 22012	0.00013
н	5.454/4	5.33813	-0.95283
Н	5.49019	7.10877	-0.91019
н	4.28176	6.26680	-1.90589
ч	E 07401	E 21020	1 65020
11	J. Z/ HZI	5.51049	T.02020
H	3.98854	6.24412	2.45594
Н	5.32244	7.08942	1.63908
н	2 47160	7 68555	-0 72434
 TT	2.1/100	,.00000	0.72454
н	3./3364	8.43154	0.26508
Η	2.34596	7.67132	1.05518
н	-2 12344	-4 56591	-1 85343
11 77	1 00265	1.00001	0 1 4 7 1 0
н	-1.82365	-4.95200	-0.14/18
Η	-1.18595	-3.44223	-0.84279
Н	-10.89601	-5.81533	0.41661
17	10 02001	E 26040	1 20620
п	-10.93281	-5.30240	-1.29038
Η	-11.95386	-4.50226	-0.12943
Н	-11.26863	-1.02480	-0.22090
ч	-11 2358/	-1 41900	1 50715
11 TT	-11.23004	1.710 <i>99</i>	T. JU/TD
Н	-12.11054	-2.46626	0.37608
Η	2.12197	-4.56419	1.85370
н	1 81998	-4 95440	0 14878
 T T		2 44042	0.110
н	1.183/4	-3.44263	0.84137
Η	11.26173	-1.02458	0.23822
н	11 23883	-1,41907	-1.48993
<b>11</b>			
и Ц	12 1085/	-2 46518	-0 35300

Н	10.89789	-5.81690	-0.38937
Н	10.92507	-5.35599	1.32166
Н	11.95139	-4.50014	0.15615

Selection of distances (Å) for the Optimized Geometry of Complex 2

Pt-N : 2.090

Pt-C≡C-C : 1.954, 1.239, 1.414

TTF Central C-C distance : 1.349

Selection of angles (°) for the Optimized Geometry of Complex 2

Pt-C≡C : 176.9

C≡C-C : 179.2

Geometry Optimization of Complex  $2^+$ : input file.

#B3LYP/LanL2DZ opt

cisPt bipyTbu TTF)2 cation doublet

1 2

Рt	- 0	-1.165500	-0.061000	-2.131000
Ν	0	-2.640500	-0.097000	-3.571000
С	0	-3.971500	-0.145000	-3.327000
С	0	-4.903500	-0.112000	-4.329000
С	0	-4.482500	-0.050000	-5.687000
С	0	-3.120500	-0.044000	-5.890000
С	0	-2.229500	-0.057000	-4.853000
С	0	-5.523500	-0.024000	-6.799000
С	0	-4.846500	0.046000	-8.204000
С	0	-6.423500	1.189000	-6.618000
Ν	0	-0.063500	0.027000	-3.862000
С	0	-6.368500	-1.279000	-6.730000
С	0	1.285500	0.104000	-3.928000
С	0	1.962500	0.104000	-5.147000
С	0	1.271500	0.023000	-6.328000
С	0	-0.114500	-0.020000	-6.257000
С	0	-0.762500	-0.012000	-5.029000
С	0	1.995500	0.003000	-7.665000
С	0	2.935500	-1.223000	-7.673000
С	0	2.823500	1.290000	-7.800000
С	0	1.076500	-0.091000	-8.849000
С	0	-2.404500	-0.142000	-0.625000
С	0	-3.217500	-0.177000	0.233000
С	0	-4.193500	-0.187000	1.312000
С	0	-5.512500	-0.166000	1.191000
С	0	-6.289500	-0.175000	-0.097000
S	0	-6.468500	-0.085000	2.655000
S	0	-3.540500	-0.137000	2.952000
С	0	-5.110500	-0.123000	3.772000
С	0	-5.236500	-0.085000	5.088000
S	0	-6.764500	-0.085000	5.929000
S	0	-3.833500	-0.080000	6.153000
С	0	-6.065500	-0.087000	7.567000
С	0	-7.072500	-0.078000	8.671000
С	0	-4.771500	-0.059000	7.635000
С	0	-3.930500	-0.067000	8.887000
С	0	0.391500	-0.018000	-0.945000
С	0	1.389500	-0.020000	-0.310000
С	0	2.555500	-0.020000	0.506000
С	0	3.841500	0.014000	0.124000
С	0	4.320500	0.036000	-1.287000
S	0	2.265500	-0.041000	2.266000
S	0	5.068500	-0.003000	1.378000

С	0	3.959500	-0.016000	2.748000
С	0	4.369500	-0.022000	4.006000
S	0	3.217500	-0.080000	5.357000
S	0	6.029500	0.032000	4.503000
С	0	4.436500	-0.121000	6.646000
С	0	3.932500	-0.181000	8.049000
С	0	5,709500	-0.087000	6.241000
C	0	6.933500	-0.160000	7.120000
н	0	-4.269500	-0.200000	-2.427000
н	0	-5.827500	-0.132000	-4.119000
н	0	-2.789500	-0.031000	-6.778000
н	0	-5 537500	0 057000	-8 901000
н	0	-4 270500	-0 736000	-8 330000
н	0	-4 307500	0 863000	-8 265000
н	0	-7 090500	1 210000	-7 334000
н	0	-5 882500	2 006000	-6 653000
н	0	-6 875500	1 133000	-5 751000
ч	0	-7 030500	-1 266000	-7 451000
и П	0	-6 826500	-1 315000	-5 865000
и Ц	0	-5 792500	-2 066000	-6 828000
и Ц	0	1 785500	0 162000	-3 123000
и 11	0	2 911500	0.158000	-5 158000
и 11	0	_0 625500	-0.057000	-7 056000
ц ц	0	2 557500	1 162000	-7.030000
и 11	0	3.337300	-1 242000	-8 513000
и 11	0	2 404500	-2.042000	-7 592000
ц ц	0	2.404500	1 262000	7 041000
п	0	2 222500	2 066000	7 808000
п	0	2.222500	2.066000	-7.809000
п	0	0 539500	1.204000	-8.034000
п	0	1 606500	-0.908000	-8.779000
п	0	1.000500	-0.119000	-9.073000
п	0	6 475500	0.089000	-8.800000
п	0	-0.4/5500	0.747000	-0.373000
п	0	-7.132500	-0.655000	0.034000
п	0	-5.764500	-0.623000	-0.791000
п u	0	-7.516500	-0.949000	8.715000
п	0	-7.738500	0.021000	0.502000
п	0	-0.023500	0.102000	9.521000
п	0	-3.390500	0.749000	0.924000
п	0	-3.339500	-0.850000	0.070000
H	0	-4.513500	-0.108000	9.673000
H	0	4.679500	-0.846000	-1.525000
H	0	5.023500	0.711000	-1.384000
H	0	3.5/1500	0.254000	-1.883000
H	0	3.351500	-0.966000	8.152000
H	0	3.423500	0.632000	8.24/000
H	U	4.690500	-0.252000	8.065000
H	0	6.963500	0.625000	/./0/000
H	U	/./38500	-U.1/9000	6.558000
Н	υ	6.896500	-0.974000	/.665000

### Cartesians Coordinates for the Optimized Geometry of Complex 2<sup>+</sup> (-1858.4071051 Hartrees)

Pt	-0.00001	1.45536	-0.00012
N	-1.30348	3.07714	-0.22945
С	-2.63751	2.98466	-0.47420
С	-3.44165	4.11455	-0.63180
С	-2.88507	5.41398	-0.54155
С	-1.50056	5.48441	-0.28571
С	-0.72832	4.31960	-0.13309
С	-3.77306	6.65848	-0.72399
С	-2.97577	7.97839	-0.58293
С	-4.89799	6.64190	0.35450
N	1.30346	3.07713	0.22936
С	-4.41378	6.61577	-2.14429
С	2.63748	2.98462	0.47409
С	3.44162	4.11450	0.63178
С	2.88504	5.41394	0.54163

C	1 50053	5 48439	0 28581
C	0 72920	4 21050	0 12200
	0.72029	4.31939	0.13309
C	3.//304	6.65842	0./241/
С	4.89801	6.64190	-0.35428
С	4.41372	6.61562	2.14449
С	2,97578	7,97836	0.58316
C	1 24606	0 06150	0 22220
C	-1.34606	0.00150	-0.23239
С	-2.20625	-0.81970	-0.38349
С	-3.16429	-1.83625	-0.55424
С	-3.00741	-2.98740	-1.28217
C	1 77066	2 2017/	2 04412
C	-1.77088	-3.301/4	-2.04412
S	-4.40623	-4.14584	-1.35361
S	-4.79832	-1.59957	0.28576
С	-5.52554	-3,15758	-0.30997
a	6 70171	2 56106	0 00140
C ~	-0.79171	-3.50100	-0.00140
S	-/.511/8	-5.12611	-0.59112
S	-7.91535	-2.58227	1.04345
С	-9,13835	-4.90074	0.23888
Ċ	10 11240	6 02046	0 01071
c	-10.11240		0.01071
C	-9.31/98	-3.//138	0.964/0
С	-10.53975	-3.34283	1.73809
С	1.34603	0.06149	0.23220
Ċ	2 20621	-0 81972	0 38331
c	2.20021	1 02602	0.50551
C	3.10427	-1.83623	0.55414
С	3.00746	-2.98726	1.28228
С	1.77079	-3.38148	2.04442
S	4 79823	-1 59968	-0 28604
0	1.79023	1 1 4 5 6 0	1 25270
S	4.40629	-4.14568	1.353/9
С	5.52554	-3.15756	0.30994
С	6.79171	-3.56103	0.00140
S	7,91527	-2.58238	-1.04367
c	7 51107	E 12EQ/	0 50126
5	7.51187	-5.12594	0.59130
С	9.31797	-3.77139	-0.96472
С	10.53971	-3.34289	-1.73819
С	9.13842	-4.90062	-0.23869
C	10 11254	-6 02925	-0 01032
	10.11254	1 00116	0.01032
н	-3.038/9	1.98116	-0.54330
н	-4.49844	3.96921	-0.82674
н	-1.01810	6.44901	-0.20638
н	-3 65336	8 82862	-0 72199
 	2.10533	0.02002	1 24024
н	-2.18533	8.06490	-1.34034
Н	-2.52356		
Н	2102000	8.08120	0.41251
	-5.54662	8.08120 7.51685	0.41251
н	-5.54662	8.08120 7.51685 6.67682	0.41251 0.22489 1.36754
H	-5.54662 -4.47747 5.52750	8.08120 7.51685 6.67682	0.41251 0.22489 1.36754
H H	-5.54662 -4.47747 -5.52750	8.08120 7.51685 6.67682 5.74727	0.41251 0.22489 1.36754 0.27926
H H H	-5.54662 -4.47747 -5.52750 -5.06217	8.08120 7.51685 6.67682 5.74727 7.48934	0.41251 0.22489 1.36754 0.27926 -2.28390
H H H H	-5.54662 -4.47747 -5.52750 -5.06217 -5.02702	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177
H H H H	-5.54662 -4.47747 -5.52750 -5.06217 -5.02702 -3.64484	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704
H H H H H	-5.54662 -4.47747 -5.52750 -5.06217 -5.02702 -3.64484 2.03877	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311
Н Н Н Н Н	-5.54662 -4.47747 -5.52750 -5.06217 -5.02702 -3.64484 3.03877	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311
Н Н Н Н Н Н	-5.54662 -4.47747 -5.52750 -5.06217 -5.02702 -3.64484 3.03877 4.49841	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670
H H H H H H	-5.54662 -4.47747 -5.52750 -5.06217 -5.02702 -3.64484 3.03877 4.49841 1.01807	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657
H H H H H H H	$\begin{array}{c} -5.54662 \\ -4.47747 \\ -5.52750 \\ -5.06217 \\ -5.02702 \\ -3.64484 \\ 3.03877 \\ 4.49841 \\ 1.01807 \\ 5.52752 \end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908
H H H H H H H H	-5.54662 -4.47747 -5.52750 -5.06217 -5.02702 -3.64484 3.03877 4.49841 1.01807 5.52752 5.52752	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908
H H H H H H H H	-5.54662 -4.47747 -5.52750 -5.06217 -5.02702 -3.64484 3.03877 4.49841 1.01807 5.52752 5.54664	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459
H H H H H H H H H	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734
H H H H H H H H H H H	-5.54662 -4.47747 -5.52750 -5.06217 -5.02702 -3.64484 3.03877 4.49841 1.01807 5.52752 5.54664 4.47752 5.02694	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193
H H H H H H H H H H H H H H H	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721
H H H H H H H H H H H H H H H H H H H	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417
H H H H H H H H H H H H H H H H H H H	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 0.00000000000000000000000000000000000$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417
H H H H H H H H H H H H H H H H H H H	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228
Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226
нннннннннн	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057
H H H H H H H H H H H H H H H H H H H	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\\ -1.97228\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485 -3.47964	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057 -3.11911
н н н н н н н н н н н н н н н н н н н	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\\ -1.97828\\ \end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485 -3.47964	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057 -3.11811
н н н н н н н н н н н н н н н н н н н	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\\ -1.97828\\ -1.37485\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485 -3.47964 -4.34358	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057 -3.11811 -1.69164
н н н н н н н н н н н н н н н н н н н	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\\ -1.97828\\ -1.37485\\ -0.99793\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485 -3.47964 -4.34358 -2.61967	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057 -3.11811 -1.69164 -1.91039
	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\\ -1.97828\\ -1.37485\\ -0.99793\\ -9.70771\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485 -3.47964 -4.34358 -2.61967 -6.98053	0.41251 0.22489 1.36754 0.27926 -2.283900 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057 -3.11811 -1.69164 -1.91039 0.38017
н н н н н н н н н н н н н н н н н н н	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\\ -1.97828\\ -1.37485\\ -0.99793\\ -9.70771\\ -10.33121\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485 -3.47964 -4.34358 -2.61967 -6.98053 -6.15165	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057 -3.11811 -1.69164 -1.91039 0.38017 -1.05726
н н н н н н н н н н н н н н н н н н н	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\\ -1.97828\\ -1.37485\\ -0.99793\\ -9.70771\\ -10.33121\\ 11.05027\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485 -3.47964 -4.34358 -2.61967 -6.98053 -6.15165 5.24524	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.224599 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057 -3.11811 -1.69164 -1.91039 0.38017 -1.05796
H H H H H H H H H H H H H H H H H H H	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\\ -1.97828\\ -1.37485\\ -0.99793\\ -9.70771\\ -10.33121\\ -11.05827\\ \end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485 -3.47964 -4.34358 -2.61967 -6.98053 -6.15165 -5.84524	0.41251 0.22489 1.36754 0.27926 -2.28390 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057 -3.11811 -1.69164 -1.91039 0.38017 -1.05796 0.52686
H H H H H H H H H H H H H H H H H H H	$\begin{array}{c} -5.54662\\ -4.47747\\ -5.52750\\ -5.06217\\ -5.02702\\ -3.64484\\ 3.03877\\ 4.49841\\ 1.01807\\ 5.52752\\ 5.54664\\ 4.47752\\ 5.02694\\ 3.64475\\ 5.06212\\ 2.52358\\ 3.65339\\ 2.18534\\ -1.97828\\ -1.37485\\ -0.99793\\ -9.70771\\ -10.33121\\ -11.05827\\ -10.93765\end{array}$	8.08120 7.51685 6.67682 5.74727 7.48934 5.71892 6.63355 1.98112 3.96916 6.44900 5.74726 7.51684 6.67688 5.71876 6.63337 7.48918 8.08122 8.82857 8.06485 -3.47964 -4.34358 -2.61967 -6.98053 -6.15165 -5.84524 -2.39448	0.41251 0.22489 1.36754 0.27926 -2.283900 -2.29177 -2.92704 0.54311 0.82670 0.20657 -0.27908 -0.22459 -1.36734 2.29193 2.92721 2.28417 -0.41228 0.72226 1.34057 -3.11811 -1.69164 -1.91039 0.38017 -1.05796 0.52686 1.35420

Н	-11.33341	-4.09133	1.66822
Н	1.97845	-3.47887	3.11845
Н	1.37514	-4.34354	1.69237
Н	0.99793	-2.61960	1.91038
Н	10.93744	-2.39436	-1.35460
Н	10.30443	-3.20206	-2.80103
Н	11.33348	-4.09125	-1.66805
Н	9.70782	-6.98044	-0.37943
Н	10.33152	-6.15109	1.05836
Н	11.05832	-5.84515	-0.52668

Selection of distances (Å) for the Optimized Geometry of Complex  $2^+$ 

Pt-N : 2.093

Pt-C≡C-C : 1.952, 1.241, 1.407

TTF Central C-C distance : 1.364

Selection of angles (°) for the Optimized Geometry of Complex 2<sup>+</sup>

Pt-C≡C : 179.7

C≡C-C : 179.0

#### Geometry Optimization of Complex 3 : input file.

#B3LYP/LanL2DZ opt

cisPt dppe TTF)2 neutre singulet

C	)	1		
Ρt	0	0.704500	-0.143000	0.384500
ΡC	)	1.751500	1.007000	2.070500
ΡC	)	2.306500	0.742000	-0.979500
СC	)	3.330500	-0.423000	-1,923500
CC	)	3.138500	-1.769000	-1.847500
CC	)	3.979500	-2.613000	-2.551500
CC	)	5.041500	-2.179000	-3.221500
CC	)	5.220500	-0.833000	-3.294500
CC	)	4.395500	0.066000	-2.683500
CC	)	1.713500	1,929000	-2.201500
CC	)	0.998500	1.523000	-3.281500
CC	)	0.500500	2.410000	-4.228500
CC	)	0.719500	3.702000	-4.119500
C (	)	1 473500	4 150000	-3 049500
C (	)	1 982500	3 280000	-2 101500
C (	)	0 822500	1 895000	3 343500
C (	)	0 930500	3 258000	3 569500
CC	)	0.209500	3.896000	4.582500
CC	)	-0.629500	3,166000	5.365500
CC	)	-0.763500	1.796000	5.157500
CC	)	-0.048500	1.184000	4.129500
CC	)	2.920500	0.037000	3.063500
CC	)	3.666500	0.625000	4.067500
C (	)	4.605500	-0.093000	4.757500
CC	)	4.793500	-1.404000	4.523500
CC	)	4.042500	-1.999000	3.565500
CC	)	3.118500	-1.302000	2.815500
СC	)	2.815500	2.249000	1.252500
СC	)	3.554500	1.594000	0.071500
s C	)	-2.984500	-3.808000	-4.569500
s C	)	-0.840500	-1.798000	-4.836500
s C	)	-3.580500	-3.599000	-7.753500
s C	)	-1.591500	-1.460000	-7.997500
СC	)	-0.128500	-1.105000	-1.151500
CC	)	-0.649500	-1.629000	-2.106500
CC	)	-1.335500	-2.243000	-3.192500
СC	)	-2.304500	-3.161000	-3.106500

С	0	-2.819500	-3.725000	-1.796500
С	0	-2.121500	-2.696000	-5.634500
С	0	-2.412500	-2.594000	-6.936500
С	0	-3.611500	-2.665000	-9.234500
С	0	-4.615500	-3.071000	-10.262500
С	0	-2.707500	-1.677000	-9.330500
С	0	-2.551500	-0.707000	-10.487500
S	0	-3.141500	-0.872000	4.412500
S	0	-4.121500	-3.640000	4.465500
S	0	-3.814500	-0.494000	7.524500
S	0	-4.722500	-3.282000	7.742500
C	0	-0.715500	-0.925000	1.566500
С	0	-1.583500	-1.425000	2,209500
С	0	-2.546500	-1,961000	3,135500
С	0	-3.046500	-3.187000	3,149500
C	0	-2 836500	-4 291000	2 066500
C	0	-3 802500	-2 167000	5 396500
C	0	_1 079500	-2 020000	6 693500
C	0	-4 150500	_1 101000	9 1/0500
C	0	2 052500	-1.101000	10 240500
C	0	-4 554500	-2 364000	0 230500
d	0	4 000500	2.304000	10 402500
	0	-4.980500	-3.120000	1 216600
п	0	2.435500	-2.125000	-1.315500
H	0	3.789500	-3.545000	-2.554500
H	0	5.64/500	-2.781000	-3.634500
H TT	0	5.958500	-0.501000	-3./92500
H	0	4.542500	0.999000	-2.775500
H	0	0.833500	0.594000	-3.396500
H	0	-0.005500	2.080000	-4.962500
Н	0	0.368500	4.311000	-4.757500
Н	0	1.644500	5.081000	-2.963500
н	0	2.514500	3.609000	-1.385500
Η	0	1.510500	3.773000	3.020500
Η	0	0.306500	4.830000	4.724500
Η	0	-1.125500	3.593000	6.055500
Η	0	-1.337500	1.282000	5.712500
Η	0	-0.165500	0.255000	3.971500
Η	0	3.527500	1.540000	4.278500
Η	0	5.134500	0.343000	5.414500
Η	0	5.436500	-1.900000	5.018500
Η	0	4.156500	-2.931000	3.403500
Η	0	2.622500	-1.741000	2.135500
Η	0	2.260500	3.000000	0.926500
Η	0	3.471500	2.607000	1.900500
Η	0	4.220500	0.945000	0.404500
Η	0	4.028500	2.287000	-0.457500
Η	0	-2.489500	-3.177000	-1.055500
Η	0	-2.499500	-4.644000	-1.689500
Η	0	-3.798500	-3.718000	-1.798500
Η	0	-5.514500	-2.843000	-9.949500
Η	0	-4.558500	-4.038000	-10.411500
Η	0	-4.431500	-2.601000	-11.101500
Η	0	-2.984500	-1.077000	-11.283500
Η	0	-1.598500	-0.567000	-10.669500
Н	0	-2.966500	0.148000	-10.256500
Н	0	-3.703500	-4.535000	1.676500
Н	0	-2.429500	-5.081000	2.475500
Н	0	-2.246500	-3.950000	1.359500
Н	0	-4.316500	-0.451000	11.075500
Н	0	-4.419500	0.736000	10.008500
Н	0	-2.996500	0.087000	10.349500
Н	0	-4.595500	-2.689000	11.283500
Н	0	-4.662500	-4.047000	10.438500
Н	0	-5.958500	-3.116000	10.560500

### Cartesians Coordinates for the Optimized Geometry of Complex 3 (-2066.8664987 Hartrees)

D+	0 01092	-1 48158	0 08916
10	1 (1005	2,20611	0.000000
Р	1.61205	-3.32611	0.04410
Ρ	-1.66788	-3.22032	-0.15903
С	-3,13578	-3.25883	1.00353
Ċ	_3 11917	-2 43621	2 1/95/
C	-3.1101/	-2.43021	2.14034
С	-4.19194	-2.47675	3.05763
С	-5.28500	-3.33200	2.82449
C	-5 30810	-1 11151	1 67375
Č	-5.50810	-1.11151	1.07373
C	-4.23758	-4.10686	0.76227
С	-2.37022	-3.38393	-1.89062
C	-2 69270	-2 19415	-2 58108
ä	2.00270	2.19113	2.50100
C	-3.24169	-2.25690	-3.8/435
С	-3.46269	-3.50259	-4.49311
С	-3,13576	-4.68950	-3.81072
a		4 62110	2 5101016
C	-2.59504	-4.03112	-2.51210
С	3.11616	-3.31930	-1.07196
С	3.40453	-4.38248	-1.95436
Ċ	1 55570	1 22650	2 76261
C	4.55579	-4.33050	-2.70301
С	5.42636	-3.23285	-2.69274
С	5.14004	-2.17095	-1.81278
C	3 98900	-2 21113	-1 00683
c	5.50500	2.21113	1.00000
C	2.27784	-3.78297	1.74019
С	3.22290	-4.82005	1.89762
C	3 68669	-5 16185	3 18030
c	3.00000	5.10105	1 21110
C	3.21426	-4.46523	4.31110
С	2.28287	-3.42211	4.15368
C	1 81546	-3 07818	2 87051
a	0 60101	4 07100	0 47634
C	0.62181	-4.8/120	-0.4/634
С	-0.76553	-4.85931	0.19205
S	-4.28435	4,40673	0.00066
с С	1 02062	1 40020	0 25072
5	-4.92902	1.40930	0.25975
S	-7.56419	5.10473	-0.19629
S	-8.22193	2.11274	0.05580
C	_1 353/8	_0 05194	0 11750
Č	-1.33340	-0.05194	0.11/30
C	-2.19128	0.86060	0.11047
С	-3.14228	1.90738	0.09746
C	-2 87484	3 23743	-0 01449
a	1 50686	3.25715	0.01110
C	-1.50676	3.85333	-0.14388
С	-5.58973	3.11123	0.06414
С	-6.90550	3,39585	-0.01622
a	0.20052	4 59700	0.01022
C	-9.32053	4.58/29	-0.42267
С	-10.26620	5.72916	-0.70369
С	-9.60995	3,27211	-0.31157
Ċ	10 05524	2 60057	0 12000
C	-10.95524	2.00057	-0.43808
S	4.64993	1./6639	-0.63613
S	4.64060	4.00317	1.46990
S	7 80412	2 58647	-1 49065
0	7.00112	2.50017	1.19009
5	/./8881	4.82989	0.60838
С	1.41013	-0.09463	0.29472
C	2 24862	0 80825	0 42619
a	2.21002	1 01714	0.12010
C	5.22944	1.01/14	0.5/2/4
С	3.23694	2.82256	1.48839
С	2.17849	3.07390	2.52956
Ċ	5 5021/	2 110/0	0 16764
	5.59314	3.11940	0.10/04
С	6.85392	3.45321	-0.17524
С	9.39706	3.45436	-1.14696
C	10 55810	2 96056	-1 07427
C	TO.22012	2.20030	1.2/43/
Ċ	9.38963	4.44101	-0.22436
С	10.54115	5.30809	0.22195
н	-2 28815	-1 75445	2 31174
 T7	4 10000	1 02054	2.211/1
н	-4.18062	-1.83054	3.93141
Η	-6.11766	-3.35486	3.52340
Н	-6.15797	-4.79509	1,48217
 U	A 0701C	1 71700	0 12610
п	-4.2/810	-4./1/98	-0.13012
Н	-2.51341	-1.22843	-2.11566

Н	-3.48970	-1.33586	-4.39516
Н	-3.88164	-3.54767	-5.49550
Н	-3.30129	-5.65480	-4.28326
Н	-2.35046	-5.56163	-2.00559
Н	2.74770	-5.24470	-2.02758
Н	4.76864	-5.15780	-3.44381
Н	6.31452	-3.19794	-3.31912
Н	5.79853	-1.30845	-1.75542
Н	3.76711	-1.37864	-0.34624
Η	3.61424	-5.34457	1.02833
Η	4.41756	-5.95848	3.29665
Н	3.57791	-4.72684	5.30195
Η	1.92771	-2.87165	5.02119
Η	1.11319	-2.25797	2.74264
Η	0.52248	-4.84746	-1.56825
Η	1.17647	-5.77427	-0.19558
Η	-0.67524	-4.92470	1.28291
Η	-1.36823	-5.71389	-0.13492
Η	-0.74380	3.06991	-0.11137
Н	-1.31268	4.56498	0.67096
Н	-1.40351	4.39781	-1.09253
Η	-10.00544	6.23364	-1.64376
Η	-10.22464	6.47943	0.09760
Н	-11.30007	5.38027	-0.78346
Н	-11.74979	3.33121	-0.61616
Н	-11.20522	2.04703	0.47732
Η	-10.96097	1.88432	-1.27069
Н	1.76394	4.08749	2.43774
Н	2.58448	2.97083	3.54533
Н	1.36325	2.35453	2.40658
Η	11.46317	3.54286	-1.77725
Η	10.33589	3.03692	-3.04741
Н	10.77912	1.90732	-1.75512
Н	11.45305	5.07796	-0.33688
Н	10.75241	5.16321	1.28982
Н	10.31245	6.37176	0.07068

Selection of distances (Å) for the Optimized Geometry of Complex 3

Pt-P: 2.430 or 2.443

Pt-C≡C-C : 1.976, 1.239, 1.414 or 1.981, 1.239, 1.415

TTF Central C-C distance : 1.349

Selection of angles (°) for the Optimized Geometry of Complex 3

Pt-C≡C : 178.4 or 176.6

C≡C-C : 179.6 or 178.7

Geometry Optimization of Complex  $3^+$ : input file.

#B3LYP/LanL2DZ opt

cisPt dppe TTF)2 cation doublet

1	2			
Ρt		0.01092	-1.48158	0.08916
Ρ		1.61205	-3.32611	0.04410
Ρ		-1.66788	-3.22032	-0.15903
С		-3.13578	-3.25883	1.00353
С		-3.11817	-2.43621	2.14854
С		-4.19194	-2.47675	3.05763
С		-5.28500	-3.33200	2.82449
С		-5.30810	-4.14454	1.67375
С		-4.23758	-4.10686	0.76227
С		-2.37022	-3.38393	-1.89062

С	-2.69270	-2.19415	-2.58108
С	-3.24169	-2.25690	-3.87435
С	-3,46269	-3.50259	-4,49311
C	-3 13576	-4 68950	-3 81072
C	-2 59504	-4 63112	-2 51216
d	2.35304	2 21020	1 07106
C	5.11010	-3.31930	-1.07196
С	3.40453	-4.38248	-1.95436
С	4.55579	-4.33650	-2.76361
С	5.42636	-3.23285	-2.69274
С	5.14004	-2.17095	-1.81278
С	3.98900	-2.21113	-1.00683
C	2 27784	-3 78297	1 74019
C	2.27701	4 92005	1 00762
C	3.22290	-4.82005	1.09702
C	3.68669	-5.16185	3.18030
С	3.21426	-4.46523	4.31110
С	2.28287	-3.42211	4.15368
С	1.81546	-3.07818	2.87051
С	0.62181	-4.87120	-0.47634
С	-0.76553	-4.85931	0.19205
S	-4,28435	4,40673	0.00066
g	-4 92962	1 40930	0 25973
0	7.52502	I.40000	0.20070
5	-7.56419	5.10473	-0.19629
S	-8.22193	2.112/4	0.05580
С	-1.35348	-0.05194	0.11750
С	-2.19128	0.86060	0.11047
С	-3.14228	1.90738	0.09746
С	-2.87484	3.23743	-0.01449
С	-1.50676	3,85333	-0.14388
C	-5 58973	3 11123	0 06414
d	6 00550	2 20595	0.00414
C	-0.90550	3.39383	-0.01022
C	-9.32053	4.58/29	-0.42267
С	-10.26620	5.72916	-0.70369
С	-9.60995	3.27211	-0.31157
С	-10.95524	2.60057	-0.43808
S	4.64993	1.76639	-0.63613
S	4,64060	4.00317	1,46990
S	7 80412	2 58647	-1 49065
c	7 70001	4 92090	0 60020
2	1.1012	4.02909	0.00030
C	1.41013	-0.09463	0.29472
С	2.24862	0.80825	0.42619
С	3.22944	1.81714	0.57274
С	3.23694	2.82256	1.48839
С	2.17849	3.07390	2.52956
С	5.59314	3.11940	0.16764
С	6.85392	3,45321	-0.17524
Ċ	9 39706	3 45436	-1 14696
C	10 55819	2 96056	_1 07/37
c	10.55819	2.90050	-1.97437
C	9.38963	4.44101	-0.22436
C	10.54115	5.30809	0.22195
Η	-2.28815	-1.75445	2.31174
Η	-4.18062	-1.83054	3.93141
Η	-6.11766	-3.35486	3.52340
Н	-6.15797	-4.79509	1.48217
н	-4.27816	-4.71798	-0.13612
н	-2 51341	-1 22843	-2 11566
и П	2.01041	1 22596	4 20516
п 			-4.39310 F 40550
H	-3.88164	-3.54/0/	-5.49550
Н	-3.30129	-5.65480	-4.28326
Η	-2.35046	-5.56163	-2.00559
Η	2.74770	-5.24470	-2.02758
Н	4.76864	-5.15780	-3.44381
Н	6.31452	-3.19794	-3.31912
н	5.79853	-1.30845	-1.75542
н	3 76711	-1 37864	-0 34604
IJ	2.70711 2.61707	-5 24457	1 0.023
п 	J.01424		1.04033
H	4.41/50		3.29005
H	3.5//91	-4./2684	5.30195
Η	1.92771	-2.87165	5.02119

н	1.11319	-2.25797	2.74264
Н	0.52248	-4.84746	-1.56825
Н	1.17647	-5.77427	-0.19558
Н	-0.67524	-4.92470	1.28291
Н	-1.36823	-5.71389	-0.13492
Н	-0.74380	3.06991	-0.11137
Н	-1.31268	4.56498	0.67096
Н	-1.40351	4.39781	-1.09253
Н	-10.00544	6.23364	-1.64376
Н	-10.22464	6.47943	0.09760
Н	-11.30007	5.38027	-0.78346
Н	-11.74979	3.33121	-0.61616
Н	-11.20522	2.04703	0.47732
Н	-10.96097	1.88432	-1.27069
Н	1.76394	4.08749	2.43774
Н	2.58448	2.97083	3.54533
Н	1.36325	2.35453	2.40658
Н	11.46317	3.54286	-1.77725
Н	10.33589	3.03692	-3.04741
Н	10.77912	1.90732	-1.75512
Н	11.45305	5.07796	-0.33688
Н	10.75241	5.16321	1.28982
Н	10.31245	6.37176	0.07068

## Cartesians Coordinates for the Optimized Geometry of Complex **3**<sup>+</sup> (-2066.6758857 Hartrees)

Pt	0.00005	-1.4/216	-0.00038
P	-1.63272	-3.26420	-0.22255
P	1.63259	-3.26432	0.22237
С	3.13306	-3.22721	-0.89622
С	2.95435	-2.75104	-2.21378
С	4.03673	-2.73950	-3.11085
С	5.30475	-3.18996	-2.69374
С	5.48709	-3.64629	-1.37491
С	4.40423	-3.66670	-0.47508
С	2.22711	-3.55877	1.97190
С	2.19185	-2.48384	2.88659
С	2.63553	-2.66823	4.20937
С	3.11038	-3.92507	4.62946
С	3.14465	-5.00040	3.72025
С	2.70854	-4.81804	2.39529
С	-3.13281	-3.22668	0.89653
С	-2.95340	-2.75099	2.21417
С	-4.03547	-2.73913	3.11162
С	-5.30387	-3.18879	2.69479
С	-5.48690	-3.64463	1.37590
С	-4.40435	-3.66536	0.47569
С	-2.22784	-3.55887	-1.97184
С	-2.70994	-4.81805	-2.39473
С	-3.14645	-5.00062	-3.71952
С	-3.11193	-3.92558	-4.62907
С	-2.63641	-2.66883	-4.20948
С	-2.19233	-2.48423	-2.88686
С	-0.71862	-4.86152	0.27583
С	0.71839	-4.86157	-0.27602
S	4.48180	4.17193	1.04472
S	4.93234	1.39907	-0.15507
S	7.68669	4.94399	0.49174
S	8.14889	2.17844	-0.71003
С	1.39005	-0.07940	0.18729
С	2.24796	0.80827	0.31392
С	3.22843	1.80863	0.44468
С	3.04742	3.05891	0.97733
С	1.75396	3.59809	1.52721
С	5.65785	3.00964	0.27944
С	6.96519	3.32982	0.05548
С	9.37909	4.55622	-0.11689
С	10.37170	5.67903	0.05259

С	9.58439	3,32835	-0.65052
С	10.86044	2.75893	-1.21825
C C	_4 93174	1 39941	0 15563
C C	1.00171	4 17120	1 04700
5	9 14700	2 17000	-1.04709
5	-0.14790	2.1/900	0./124/
S	-7.68691	4.94351	-0.49216
C	-1.38987	-0.07935	-0.18836
C	-2.24776	0.80830	-0.31518
С	-3.22838	1.80852	-0.44600
С	-3.04791	3.05833	-0.97994
С	-1.75495	3.59711	-1.53140
С	-5.65774	3.00952	-0.27976
С	-6.96492	3.32980	-0.05503
С	-9.58357	3.32871	0.65302
С	-10.85913	2.75966	1,22224
С	-9.37881	4.55612	0.11813
C	-10 37166	5 67866	-0.05161
U U	1 99/95	-2 37392	-2 53249
и 11	2 90206	2.37352	4 10252
и 11	5.09590	2.17650	2 20642
п 11	0.14242	-3.1/059	-3.30043
п 	0.40051	-3.90291	-1.04400
Н 	4.56274	-4.00667	0.54412
H	1.82344	-1.51309	2.56690
H	2.60694	-1.83513	4.90666
H	3.44900	-4.06679	5.65259
Н	3.51051	-5.97310	4.03855
H	2.74699	-5.66089	1.70923
Н	-1.98360	-2.37447	2.53268
Н	-3.89216	-2.37169	4.12436
Н	-6.14130	-3.17518	3.38778
Н	-6.46661	-3.98063	1.04607
Н	-4.56338	-4.00496	-0.54355
Н	-2.74861	-5.66067	-1.70839
Н	-3.51283	-5.97325	-4.03743
Н	-3.45085	-4.06747	-5.65207
Н	-2.60762	-1.83595	-4.90703
Н	-1.82343	-1.51355	-2.56755
н	-0 72260	-4 89338	1 37173
H	-1 27296	-5 73632	-0 08082
н	0 72237	-4 89339	-1 37192
u u	1 27266	-5 73643	0 08060
и П	0 96225	2 95467	1 20707
и 11	1 45500	2.03407	1 01220
п тт	1 94069	4.JZIZI 2.02744	1.01229
п 11	10 40201	5.02/44	2.59/69
H	10.48221	5.95160	1.11011
H 	10.04976	6.5/593	-0.49215
H	11.35/5/	5.39441	-0.32431
H	11.67766	3.48236	-1.15564
Н	10.73486	2.48495	-2.27379
Н	11.16763	1.85743	-0.67246
Н	-1.45629	4.52045	-1.01721
Н	-1.84272	3.82597	-2.60210
Н	-0.96328	2.85369	-1.40189
H	-11.67646	3.48295	1.15962
H	-10.73270	2.48661	2.27791
Н	-11.16665	1.85766	0.67746
Н	-11.35719	5.39433	0.32643
Н	-10.48311	5.95019	-1.10930
Н	-10.04934	6.57613	0.49197

Selection of distances (Å) for the Optimized Geometry of Complex  $\mathbf{3}^+$ 

#### Pt-P : 2.434

Pt-C≡C-C : 1.977, 1.241, 1.407

TTF Central C-C distance : 1.364

Selection of angles (°) for the Optimized Geometry of Complex  $\mathbf{3}^+$ 

Pt-C≡C : 179.0

C≡C-C : 179.3

### Geometry Optimization of Complex 4 : input file.

#B3LYP/LanL2DZ opt

Pt PPh3)2 TTF)2 neutre singulet

0 1

Pt O	0.00000	0.00000	0.00000
P 0	0.600000	-2.220000	0.148000
S 0	-2.497000	-1.024000	4.992000
S 0	-4.509000	1.086000	5.514000
S 0	-3.530000	-2.653000	7.614000
S 0	-5.428000	-0.489000	8.231000
C 0	-0.261000	-3.309000	1.348000
C 0	-0.147000	-3.015000	2.704000
C 0	-0.775000	-3.833000	3.638000
C 0	-1.519000	-4.924000	3.241000
C 0	-1.634000	-5.223000	1.893000
CO	-0.999000	-4.405000	0.950000
CU	0.326000	-3.062000	-1.44/000
	-0.8/5000	-2.773000	-2.104000
	-1.193000	-3.424000	-3.288000
	-0.318000	4.530000	2 202000
	1 207000	-3.984000	-2.009000
	2 357000	-2 402000	-2.009000
C O	2.910000	-3 653000	0.01000
C 0	4,245000	-3.750000	1,298000
C 0	5.017000	-2.621000	1.424000
C 0	4.472000	-1.371000	1.165000
C 0	3.145000	-1.266000	0.766000
C 0	-1.185000	-0.032000	1.609000
C 0	-1.931000	0.064000	2.570000
C 0	-2.761000	0.169000	3.721000
C 0	-3.695000	1.111000	3.955000
C 0	-4.097000	2.202000	3.011000
C 0	-3.791000	-0.439000	6.041000
C U	-4.197000	-1.101000	7.128000
C U	-5.5/1000	-1.978000	9.16/000
	-6.641000	-1.954000	10.235000
	-4.617000	-2.934000 -4.321000	9 536000
P 0	-0 600000	2 220000	-0 148000
S 0	2,497000	1.024000	-4.992000
S 0	4.509000	-1.086000	-5.514000
S 0	3.530000	2.653000	-7.614000
S 0	5.428000	0.489000	-8.231000
C 0	0.261000	3.309000	-1.348000
C 0	0.147000	3.015000	-2.704000
C 0	0.775000	3.833000	-3.638000
C 0	1.519000	4.924000	-3.241000
C 0	1.634000	5.223000	-1.893000
C U	0.999000	4.405000	-0.950000
C U	-0.326000	3.062000	1.44/000
	0.8/5000	2.773000	2.104000
	1.193000	3.424000	3.200000
	-0 884000	4 621000	3 203000
C 0	-1.207000	3.984000	2.009000
C 0	-2.357000	2.402000	-0.618000
C 0	-2.910000	3.653000	-0.901000
C 0	-4.245000	3.750000	-1.298000
C 0	-5.017000	2.621000	-1.424000

C	Ω	-1 172000	1 371000	-1 165000
a	0	4.472000	1.0000	1.105000
Ċ	0	-3.145000	1.266000	-0./66000
С	0	1.185000	0.032000	-1.609000
С	0	1.931000	-0.064000	-2.570000
С	0	2.761000	-0.169000	-3.721000
C	0	3 695000	_1 111000	-3 955000
c	0	3.095000	-1.111000	-3.955000
С	0	4.097000	-2.202000	-3.011000
С	0	3.791000	0.439000	-6.041000
С	0	4.197000	1.101000	-7.128000
C	0	5 571000	1 978000	-9 167000
a	0	6 641000	1 054000	10 225000
C	0	0.041000	1.954000	-10.235000
С	0	4.721000	2.954000	-8.887000
С	0	4.617000	4.321000	-9.536000
Н	0	0.356000	-2.261000	2.989000
н	0	-0 691000	-3 638000	4 564000
11 TT	0	1 052000	5.050000	2 000000
н	0	-1.952000	-5.467000	3.889000
Η	0	-2.138000	-5.977000	1.611000
Η	0	-1.077000	-4.608000	0.025000
Н	0	-1.474000	-2.132000	-1.738000
н	0	-2 013000	-3 233000	-3 729000
11 TT	0	2.015000	1 000000	4 624000
н	0	-0.545000	-4.800000	-4.634000
Η	0	1.490000	-5.242000	-3.589000
Η	0	2.029000	-4.179000	-1.576000
Н	0	2.379000	-4.436000	0.823000
н	0	4 622000	-4 602000	1 483000
11 TT	0	I.022000	2.002000	1 600000
п	0	5.920000	-2.095000	1.000000
Η	0	5.005000	-0.590000	1.261000
Η	0	2.773000	-0.410000	0.590000
Н	0	-3.561000	2.141000	2.194000
н	0	-3 949000	3 073000	3 436000
11 TT	0	5.919000 E 046000	2 106000	2 797000
п	0	-5.040000	2.106000	2.787000
Η	0	-6.724000	-2.845000	10.633000
Η	0	-7.497000	-1.695000	9.834000
Н	0	-6.396000	-1.307000	10.929000
н	0	-5 261000	-4 382000	10 274000
U	0	2 710000	1 110000	0 994000
п	0	-3.710000	-4.449000	9.884000
Н	0	-4.814000	-5.014000	8.872000
Η	0	-0.356000	2.261000	-2.989000
Η	0	0.691000	3.638000	-4.564000
Н	0	1.952000	5.467000	-3.889000
ч	0	2 138000	5 977000	-1 611000
11 TT	0	1 077000	1 600000	1.011000
п	0	1.077000	4.000000	-0.025000
Н	0	1.474000	2.132000	1.738000
Η	0	2.013000	3.233000	3.729000
Η	0	0.545000	4.800000	4.634000
Н	0	-1.490000	5,242000	3,589000
ч	0	-2 029000	4 179000	1 576000
11	0	2.020000	4.126000	1.570000
н	0	-2.3/9000	4.436000	-0.823000
Η	0	-4.622000	4.602000	-1.483000
Η	0	-5.926000	2.695000	-1.688000
Н	0	-5.005000	0.590000	-1.261000
н	0	-2 773000	0 410000	-0 590000
11 TT	0	2.775000	0.110000	0.350000
п	0	3.561000	-2.141000	-2.194000
Н	0	3.949000	-3.073000	-3.436000
Η	0	5.046000	-2.106000	-2.787000
Н	0	6.724000	2.845000	-10.633000
н	0	7,497000	1,695000	-9.834000
 ц	ñ	6 306000	1 307000	_10 929000
11	0	0.390000 F 0C1000	1 202000	10.929000
H	U	5.201UUU	4.382000	-10.2/4000
Η	0	3.710000	4.449000	-9.884000
Η	0	4.814000	5.014000	-8.872000

Cartesians Coordinates for the Optimized Geometry of Complex 4 (-2451.4764955 Hartrees)

Pt	0.00000	0.00000	0.00000
P	0.33848	-2.39836	0.08242

S	-2.30944	-0.77278	5.10353
S	-5.24568	0.13076	5.17255
S	-2.61942	-2.00718	8.22221
S	-5.55353	-1.09361	8,29240
C	-1 00178	-3 45076	0 87250
C	1 22121	2 25207	2 26104
	-1.23131	-3.35207	2.20194
C	-2.24821	-4.10911	2.86/29
С	-3.05060	-4.96654	2.08914
С	-2.82945	-5.06143	0.70281
С	-1.80906	-4.30549	0.09404
С	0.57352	-3.18681	-1.60520
С	-0.14616	-2.66904	-2.70193
Ċ	-0 02694	-3 26490	-3 97009
C	0 81824	-4 37640	-4 15226
C	1 54467	1 00010	2 06050
	1 40005	-4.00010	-3.00039
C a	1.42205	-4.296/5	-1./8899
С	1.88818	-2.80798	1.06218
С	2.04590	-4.05600	1.70310
С	3.22699	-4.34243	2.41246
С	4.25842	-3.38656	2.48483
С	4.10149	-2.14053	1.84812
С	2,92101	-1.84942	1,13994
C	-1 36231	-0 07598	1 47734
C	2 195291	0.07915	2 10607
C	-2.16528	-0.07915	2.40007
C	-3.05423	-0.11624	3.52257
C	-4.35207	0.28510	3.57760
С	-5.14515	0.86984	2.43913
С	-3.87005	-0.69899	6.06671
С	-3.99633	-1.18916	7.31687
С	-4.93490	-2.11304	9.70076
С	-5,96898	-2.37989	10.76687
C	-3 64511	-2 51452	9 67048
C	2 20207	2.31132	10 60572
	-2.89897	-3.33240	10.09573
P	-0.33848	2.39836	-0.08242
S	2.30944	0.77278	-5.10353
S	5.24568	-0.13076	-5.17255
S	2.61942	2.00718	-8.22221
S	5.55353	1.09361	-8.29240
С	1.00178	3.45076	-0.87250
С	1,23131	3.35207	-2.26194
C	2 24821	4 10911	-2 86729
C	2.21021	1.10511	2.00725
	3.03000	4.90034 F 0C142	-2.00914
C ~	2.82945	5.06143	-0./0281
C	1.80906	4.30549	-0.09404
С	-0.57352	3.18681	1.60520
С	0.14616	2.66904	2.70193
С	0.02694	3.26490	3.97009
С	-0.81824	4.37640	4.15226
С	-1.54467	4.88818	3.06059
С	-1.42205	4,29675	1.78899
C	-1 88818	2 80798	-1 06218
C	2 04500	4 05600	1 70210
	-2.04590	4.05000	-1.70310
C	-3.22699	4.34243	-2.41246
С	-4.25842	3.38656	-2.48483
С	-4.10149	2.14053	-1.84812
С	-2.92101	1.84942	-1.13994
С	1.36231	0.07598	-1.47734
С	2.18528	0.07915	-2.40687
С	3.05423	0.11624	-3.52257
C	4 35207	-0 28510	-3 57760
C	5 1/515	-0 86081	_2 /2012
C	2.07005	0.00904	-2.43913 6 06691
	3.8/005	0.09099	-0.066/1
C	3.99633	1.18916	-/.31687
С	4.93490	2.11304	-9.70076
С	5.96898	2.37989	-10.76687
С	3.64511	2.51452	-9.67048
С	2.89897	3.33246	-10.69573
Н	-0.63282	-2.68249	2.87193

Н	-2.42137	-4.00990	3.93523
Н	-3.84160	-5.54726	2.55790
Н	-3.44536	-5.71894	0.09383
Н	-1.64725	-4.39311	-0.97606
Н	-0.77296	-1.79084	-2.57332
Н	-0.57511	-2.85120	-4.81240
Н	0.92044	-4.82840	-5.13596
Н	2.20858	-5.73852	-3.19635
Н	1.99928	-4.69285	-0.95860
Н	1.24981	-4.79474	1.66843
Н	3.33748	-5.30434	2.90718
Н	5.16932	-3.60786	3.03613
Н	4.89013	-1.39433	1.90636
Н	2.79876	-0.88452	0.65605
H	-4.49889	0.99077	1.56499
H	-5.55430	1.85484	2.70368
H	-5.98790	0.22054	2.16326
H	-5.54677	-2.95406	11.59687
H	-6.81655	-2.94733	10.35969
H	-6.36470	-1.43953	11.17415
H	-3.53245	-3.56649	11.55641
H	-2.01763	-2.78989	11.06393
H	-2.54876	-4.28030	10.26533
Н	0.63282	2.68249	-2.87193
Н	2.42137	4.00990	-3.93523
Н	3.84160	5.54726	-2.55790
Н	3.44536	5.71894	-0.09383
Н	1.64725	4.39311	0.97606
Н	0.77296	1.79084	2.57332
Н	0.57511	2.85120	4.81240
Н	-0.92044	4.82840	5.13596
Н	-2.20858	5.73852	3.19635
Н	-1.99928	4.69285	0.95860
Н	-1.24981	4.79474	-1.66843
H	-3.33748	5.30434	-2.90718
H	-5.16932	3.60786	-3.03613
H	-4.89013	1.39433	-1.90636
H	-2.79876	0.88452	-0.65605
H	4.49889	-0.99077	-1.56499
H	5.55430	-1.85484	-2./0368
н	5.98/90	-0.22054	-2.10326
H	5.546//	2.95406	-11.59687
п т	0.01055	2.94/33 1 42052	-LU.35969
п u	0.304/U 2 E20/E	1.43903 2 56640	-11.1/415
п u	3.33243 2.01762	3.30049 3.70000	-11.06202
п u	2.U1/03 2 5/076	4.10909 1.00000	-TT.00393
п	2.540/0	4.28030	-IU.20033

Selection of distances (Å) for the Optimized Geometry of Complex 4

Pt-P : 2.424

Pt-C≡C-C : 2.011, 1.242, 1.415

TTF Central C-C distance : 1.349

Selection of angles (°) for the Optimized Geometry of Complex 4

Pt-C≡C : 177.7

C≡C-C : 176.1

Geometry Optimization of Complex  $4^+$ : input file.

#B3LYP/LanL2DZ opt

Pt PPh3)2 TTF)2 cation doublet

1	2		
DH	0 0000	0 00000	0 00000
F C	0.00000	0.00000	0.00000
Р	0.33848	-2.39836	0.08242
S	-2.30944	-0.77278	5.10353
c	E 04E60	0 12076	E 170EE
5	-5.24508	0.13076	5.1/255
S	-2.61942	-2.00718	8.22221
C	_5 55353	_1 09361	8 20240
5	-0.00000	-1.09301	0.29240
С	-1.00178	-3.45076	0.87250
C	-1 23131	-3 35207	2 26194
C	1.23131	5.55207	2.20194
С	-2.24821	-4.10911	2.86729
С	-3.05060	-4.96654	2.08914
a	2,02045	F 0(142	0 70001
Ċ	-2.82945	-5.06143	0./0281
С	-1.80906	-4.30549	0.09404
C	0 57352	-3 19691	-1 60520
C	0.57552	-3.10001	-1.00520
С	-0.14616	-2.66904	-2.70193
С	-0.02694	-3,26490	-3,97009
a	0.01001	4 20 4 4	4 1 5 0 0 5
C	0.81824	-4.37640	-4.15226
С	1.54467	-4.88818	-3.06059
a	1 40005	4 20675	1 70000
C	1.42205	-4.29075	-1./0099
С	1.88818	-2.80798	1.06218
C	2 04590	-4 05600	1 70310
0	2.01590	1.05000	1.70510
C	3.22699	-4.34243	2.41246
С	4.25842	-3.38656	2,48483
a	4 10140	2 14052	1 04010
Ċ	4.10149	-2.14053	1.84812
С	2.92101	-1.84942	1.13994
C	-1 36231	_0 07598	1 /772/
C	-1.30231	-0.07598	1.4//34
С	-2.18528	-0.07915	2.40687
C	-3 05423	-0 11624	3 52257
~	5.05125	0.11021	3.52257
C	-4.35207	0.28510	3.57760
С	-5.14515	0.86984	2,43913
a	2 97005	0 60900	6 06671
C	-3.87005	-0.09099	0.000/1
С	-3.99633	-1.18916	7.31687
C	-1 03/00	-2 11304	9 70076
C	-4.93490	-2.11304	9.70070
С	-5.96898	-2.37989	10.76687
С	-3.64511	-2.51452	9,67048
a	2 00007	2,02,102	10 00073
Ċ	-2.89897	-3.33246	10.695/3
Ρ	-0.33848	2.39836	-0.08242
C	2 20044	0 77270	E 102E2
5	2.30944	0.77278	-3.10353
S	5.24568	-0.13076	-5.17255
S	2,61942	2,00718	-8.22221
a		1 00261	0,00040
S	5.55353	1.09361	-8.29240
С	1.00178	3.45076	-0.87250
Ċ	1 22121	2 25207	2 26104
C	1.23131	5.55207	-2.20194
С	2.24821	4.10911	-2.86729
С	3,05060	4,96654	-2.08914
a	2.02045	F 0(142	0 70001
C	2.82945	5.06143	-0.70281
С	1.80906	4.30549	-0.09404
C	-0 57352	3 18681	1 60520
~	0.57552	5.10001	1.00520
C	0.14616	2.66904	2.70193
С	0.02694	3,26490	3,97009
a	0 01004	1 27610	4 15006
C	-0.01024	4.37040	4.15220
С	-1.54467	4.88818	3.06059
C	-1 42205	4 29675	1 78899
C	-1.42205	4.29075	1.70099
С	-1.88818	2.80798	-1.06218
С	-2.04590	4.05600	-1.70310
a	2 22600	4 24242	2 41246
Ċ	-3.22699	4.34243	-2.41246
С	-4.25842	3.38656	-2.48483
C	-1 10140	2 1/052	_1 0/010
	-4.10149	2.14033	-1.04012
С	-2.92101	1.84942	-1.13994
С	1.36231	0.07598	-1 47734
c	1.50251	0.07015	
C	2.18528	0.07915	-2.40687
С	3.05423	0.11624	-3.52257
C	1 25007	_0 20510	-3 57760
C	4.35207	-0.20510	-3.57760
С	5.14515	-0.86984	-2.43913
С	3 87005	0 69899	-6 06671
a	2.07003	1 10016	
Ċ	3.99633	1.18910	-/.31687
С	4.93490	2.11304	-9.70076
C	E OCOOO	2 22000	10 76607
C	5.90090	2.31909	-10.10001

C	2 64511	2 51452	0 67049
	2 20207	2.51452	-9.07040
	2.09097	3.33240	-10.095/3
н	-0.63282	-2.68249	2.8/193
н	-2.42137	-4.00990	3.93523
H	-3.84160	-5.54/26	2.55/90
Н	-3.44536	-5.71894	0.09383
H	-1.64725	-4.39311	-0.97606
Н	-0.77296	-1.79084	-2.57332
Н	-0.57511	-2.85120	-4.81240
Н	0.92044	-4.82840	-5.13596
Н	2.20858	-5.73852	-3.19635
Н	1.99928	-4.69285	-0.95860
H	1.24981	-4.79474	1.66843
H	3.33748	-5.30434	2.90718
Н	5.16932	-3.60786	3.03613
Н	4.89013	-1.39433	1.90636
Н	2.79876	-0.88452	0.65605
Н	-4.49889	0.99077	1.56499
Н	-5.55430	1.85484	2.70368
Н	-5.98790	0.22054	2.16326
н	-5.54677	-2.95406	11.59687
н	-6.81655	-2.94733	10.35969
н	-6.36470	-1,43953	11.17415
н	-3 53245	-3 56649	11 55641
н	-2 01763	-2 78989	11 06393
н	-2 54876	-4 28030	10 26533
и П	0 63282	2 68249	-2 87193
и П	2 42137	4 00990	-3 93523
и П	3 84160	5 54726	-2 55790
и П	3 44536	5 71894	-0 09383
и П	1 64725	4 39311	0.0000
и 11	0 77296	1 7909/	2 57222
и и	0.77290	2 95120	4 01040
п т	0.37511	2.05120	4.01240 E 12E06
п 11	-0.92044	4.02040	2 10625
H T	-2.20858	5./3852	3.19635
H	-1.99928	4.09285	0.95860
н	-1.24981	4./94/4	-1.66843
H	-3.33/48	5.30434	-2.90/18
Н	-5.16932	3.60786	-3.03613
H	-4.89013	1.39433	-1.90636
Н	-2.79876	0.88452	-0.65605
H	4.49889	-0.99077	-1.56499
Н	5.55430	-1.85484	-2.70368
Н	5.98790	-0.22054	-2.16326
Н	5.54677	2.95406	-11.59687
Н	6.81655	2.94733	-10.35969
Н	6.36470	1.43953	-11.17415
Н	3.53245	3.56649	-11.55641
Н	2.01763	2.78989	-11.06393
H	2.54876	4.28030	-10.26533

# Cartesians Coordinates for the Optimized Geometry of Complex **4**<sup>+</sup> (-2451.2846444 Hartrees)

Pt	0.00000	0.00000	0.00000
P	0.40055	-2.40197	0.01610
S	-2.39609	-1.05183	5.04600
S	-5.27338	-0.03219	5.08211
S	-2.75751	-2.15396	8.19379
S	-5.62890	-1.11870	8.22924
С	-0.92323	-3.48598	0.78873
С	-1.06799	-3.51308	2.19275
С	-2.06849	-4.30246	2.78449
С	-2.94092	-5.06117	1.97964
С	-2.80474	-5.02746	0.57978
С	-1.79923	-4.24254	-0.01622
С	0.61550	-3.12347	-1.70297
С	-0.16136	-2.59999	-2.75798
С	-0.06846	-3.15525	-4.04669

С	0.80764	-4.23052	-4.29127
a	1 E0142	4 74601	2 2/102
C	1.59145	-4.74621	-3.24102
С	1.49500	-4.19684	-1.94914
С	1.96168	-2.80623	0.97361
Ċ	2 18245	-1 09930	1 /07/1
C	2.10345	-4.09930	1.49/41
С	3.37215	-4.38452	2.19351
С	4,34643	-3.38309	2.37121
a	4 10500	2,00070	1 05220
C	4.12503	-2.09278	1.05330
С	2.93713	-1.80328	1.15660
C	-1 34092	-0 15524	1 47406
2		0.20202	2.17100
C	-2.16645	-0.20392	2.40348
С	-3.04887	-0.27139	3.49481
C	-4 34087	0 18726	3 53954
C a	4.54007	0.10720	5.55554
C	-5.07143	0.86493	2.41167
С	-3.93777	-0.86825	5.99697
C	-4 08710	-1 31125	7 27706
C	4.00710	1.01120	7.27700
С	-5.01159	-1.96244	9.74461
С	-6.02125	-2.04495	10.86205
Ċ	2 72021	2 42250	0 72025
C	-3.73034	-2.42250	9.72933
С	-2.99090	-3.14051	10.82505
Ρ	-0.40055	2.40197	-0.01610
-	2 20600	1 05102	F 04600
5	2.39609	1.05183	-5.04600
S	5.27338	0.03219	-5.08211
S	2 75751	2 15396	-8 19379
5	5.0000	1 11000	0.1000
S	5.62890	1.118/0	-8.22924
С	0.92323	3.48598	-0.78873
C	1 06799	3 51308	_2 10275
C	1.00799	5.51500	-2.19275
С	2.06849	4.30246	-2.78449
С	2.94092	5.06117	-1.97964
Ċ	2 90474	E 02746	0 57070
C	2.004/4	5.02740	-0.57978
С	1.79923	4.24254	0.01622
С	-0.61550	3.12347	1.70297
2	0 1 6 1 2 6	2 50000	2.70227
C	0.10130	2.59999	2./5/98
С	0.06846	3.15525	4.04669
C	-0 80764	4 23052	4 29127
ä	1 50142	1.23032	2 24102
C	-1.59143	4./4621	3.24182
С	-1.49500	4.19684	1.94914
C	-1 96168	2 80623	-0 97361
Č	-1.90108	2.00023	-0.97301
C	-2.18345	4.09930	-1.49741
С	-3.37215	4.38452	-2.19351
C	-1 31613	3 38300	_2 27121
C	-4.54045	5.50509	-2.3/121
С	-4.12503	2.09278	-1.85338
С	-2.93713	1.80328	-1.15660
a	1 24002	0 1 5 5 2 4	1 47406
C	1.34092	0.15524	-1.4/400
С	2.16645	0.20392	-2.40348
С	3.04887	0.27139	-3.49481
a	4 24097	0 19726	2 52054
C	4.34087	-0.18/20	-3.33934
С	5.07143	-0.86493	-2.41167
С	3,93777	0.86825	-5.99697
Ċ	1 00710	1 21105	
C	4.08/10	1.31125	-/.2//00
С	5.01159	1.96244	-9.74461
С	6.02125	2.04495	-10.86205
2	0.02123	2.01155	10.00205
C	3./3834	2.42250	-9.72935
С	2.99090	3.14051	-10.82505
ч	-0 40674	-2 92592	2 82411
	0.40074		2.02411
Н	-2.17007	-4.31614	3.86612
Н	-3.71533	-5.67079	2.43850
ч	-2 17106	-5 61100	-0 0/077
п	-3.4/180	-2.01102	-0.048//
Н	-1.69910	-4.23848	-1.09732
Н	-0.82045	-1.75400	-2.58079
 ц	0 66021	2 74460	1 0 5 1 5 7 5
п	-0.00031	-2./4458	-4.0545/
Н	0.88349	-4.65651	-5.28857
н	2 27435	-5 57183	-3 42529
**	2.2/133	3.37103	1 1 5 0 0 4
н	2.11197	-4.60064	-1.15204
Н	1.43139	-4.87541	1.38378
н	2 52204	-5 38115	2 59600
**	5.55527	2.20112	2.39000
Н	5.26267	-3.60463	2.91272
Н	4.86852	-1.31269	1.99663

Н	2.76506	-0.80403	0.76680
Н	-4.40341	0.97526	1.55367
Н	-5.42063	1.86327	2.70697
Н	-5.94811	0.28269	2.09718
Н	-5.60387	-2.55474	11.73438
Н	-6.91562	-2.59721	10.54587
Н	-6.34111	-1.04391	11.17912
Н	-3.62017	-3.27609	11.70870
Н	-2.10008	-2.57644	11.13060
Н	-2.66068	-4.13317	10.49253
H	0.40674	2.92592	-2.82411
Н	2.17007	4.31614	-3.86612
H	3.71533	5.67079	-2.43850
Н	3.47186	5.61182	0.04877
Н	1.69910	4.23848	1.09732
Н	0.82045	1.75400	2.58079
Н	0.66831	2.74458	4.85457
Н	-0.88349	4.65651	5.28857
Н	-2.27435	5.57183	3.42529
Н	-2.11197	4.60064	1.15204
H	-1.43139	4.87541	-1.38378
Н	-3.53394	5.38115	-2.59600
Н	-5.26267	3.60463	-2.91272
Н	-4.86852	1.31269	-1.99663
Н	-2.76506	0.80403	-0.76680
Н	4.40341	-0.97526	-1.55367
Н	5.42063	-1.86327	-2.70697
Н	5.94811	-0.28269	-2.09718
H	5.60387	2.55474	-11.73438
Н	6.91562	2.59721	-10.54587
Н	6.34111	1.04391	-11.17912
Н	3.62017	3.27609	-11.70870
Н	2.10008	2.57644	-11.13060
Н	2.66068	4.13317	-10.49253

Selection of distances (Å) for the Optimized Geometry of Complex 4<sup>+</sup>

Pt-P : 2.435

Pt-C≡C-C : 1.999, 1.244, 1.405

TTF Central C-C distance : 1.363

Selection of angles (°) for the Optimized Geometry of Complex 4<sup>+</sup>

Pt-C≡C : 177.7 C≡C-C : 177.3