

Supporting Information

Direct Evidence for Neutral N-Pyrazolyl Radicals: Paddlewheel Dibismuthanes Bearing Pyrazolato Ligands with Very Short Bismuth-Bismuth Single Bonds

Ming-Gang Zhao,[†] Ting-Ting Hao,[†] Xiang Zhang,[†] Jian-Ping Ma,[§] Ji-Hu Su,[‡] and Wenjun Zheng^{*,†,‡}

[†]Institute of Organic Chemistry & College of Chemical and Materials Science, Shanxi Normal University, Linfen, Shanxi 041004, China

[‡]Key Laboratory of Magnetic Molecules and Magnetic Information Material, Ministry of Education, Linfen, Shanxi 041004, China

[§]College of Chemistry, Chemical Engineering and Materials Science, Shandong Normal University, Jinan, Shandong 250014, China

^{*}CAS Key Laboratory of Microscale Magnetic Resonance, Department of Modern Physics, University of Science and Technology of China, Hefei 230026, China

Email: wjzheng@sxnu.edu.cn, wjzheng_sxnu@qq.com

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General information

Experimental condition, reagents and materials.

All manipulations were carried out in a nitrogen atmosphere under anaerobic conditions using standard Schlenk, vacuum line and glove box techniques. The solvents were thoroughly dried, deoxygenated and distilled in a nitrogen atmosphere prior to use. THF-*d*₈ and C₆D₆ were dried with metallic potassium before the use. DMSO-*d*₆ was dried over 4Å molecular sieve before the use. 3,5-Di-*tert*-butylpyrazolatopotassium [K(3,5-*t*Bu₂pz)] and 3,5-di-phenylpyrazolatopotassium [K(3,5-Ph₂pz)] were prepared according to the literatures.^[1, 2] BiCl₃ and SbCl₃ were purchased from Aldrich.

Spectroscopy Measurements.

The ¹H NMR and ¹³C{¹H} NMR spectra were recorded with a Bruker DRX-600 spectrometer. IR measurements were carried out on a NICOLET 360 FT-IR spectrometer from Nujol mulls prepared in a dry box. Melting points were measured in sealed argon-filled capillaries without temperature correction with an apparatus XT4-100A (Electronic and Optical Instruments, Beijing).

The EPR measurements were performed using a Bruker A-300 apparatus (Germany), operating at the X-band. Typical spectrometer settings were microwave frequency, 9.45 GHz; modulation amplitude, 2.0 G; modulation frequency, 100 kHz; microwave power, 2.31 mW; conversion time, 160 ms; time constant, 655.36 ms, and receiver gain, 100–104. The solutions of DMPO (200 mM), [K(3,5-*t*Bu₂pz)] (2.18 mg) and BiCl₃ (3.15 mg) were prepared using anhydrous THF. BiCl₃ solution (0.2 mL) was fast added into the mixture of DMPO (0.1 mL) and [K(3,5-*t*Bu₂pz)](0.2 mL). The mixture was immediately loaded into a paramagnetic tube (NORELL S EPR 250S), and then cooled soon at -40 °C for 15 min. Subsequently, the EPR singal was detected by raising temperature slowly to room temperature in 20–30 min.

Cyclic voltammeries were performed on a CHI660E electrochemical work station (CH Instrumental Co., China) with a conventional three-electrode system consisted of a glassy carbon electrode(GCE, 3 mm in diameter) as the working electrode, the Ag/AgNO₃(a silver wire in a 0.1 M AgNO₃, acetonitrile solution) reference electrode and a platinum wire as the auxiliary electrode at room temperature under nitrogen. Cyclic voltammeries were carried out with a scan rate of 100 mv/s in a 0.04 M Bu₄NPF₆-CH₃CN solution. Ferrocene was added to the electrolyte solution at the end of a series of experiments. The Fc/Fc⁺ couple served as internal standard. Bu₄NPF₆ was recrystallized three times from dried ethanol and dried at 125 °C in vacuo for 24 h prior to use.

Computational aspects.

All calculations were performed using Gaussian 09 package.^[3] Cartesian coordinates of the optimized geometries of complexes **5**, **6**, [Bi(*t*Bu₂pz)₃](I), [Bi(*t*Bu₂pz)₂][•] (II), [_{3,5-t}Bu₂pz][•] (III), the dimer III(N)-III(N) and III(N)-III(C) by B₃LYP method with the combination of 6-31G(d) basis set for C, N, and H atoms and Lanl2dz basis set and pseudopotential for Bi atoms,^[4] SMD solvation model of THF, respectively.^[5] We also analyzed the orbital components of some key molecular orbitals that made the dominant contributions to the bonds between the (Bi₂)⁴⁺ unit (denoted by F₁) and the four coordinating pyrazolato {4[_{3,5-t}Bu₂pz]}⁴⁻ (denoted by F₂) by the charge decomposition analysis (CDA) method^[6] implemented in the Multiwfn 3.3.7 software packages,^[7] with the limited geometry of **5** in D₄ symmetry.

Synthesis.

{η¹,η¹-3,5-*t*Bu₂pz}₂(Bi-Bi){η¹,η¹-3,5-*t*Bu₂pz}₂ (**5α**, **5β**, **5γ**):

To a mixture of BiCl₃ (0.315 g, 1.0 mmol) and K[3,5-*t*Bu₂pz] (**3**, 0.655 g, 3.0 mmol) was added 30 mL tetrahydrofuran (THF) via a syringe. After the mixture was stirred for 72 hours the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (4 × 10 mL) and the solution was filtered through Celite. The filtrate was concentrated under the reduced pressure to about 25 mL to give **5** as orange crystals at room temperature. The mother liquid was further concentrated to afford another portion of **5** and a group of colorless free ligand H[3,5-*t*Bu₂pz] (0.06 g, 11.1 %) at -20°C. The total yield of **5** is 0.22 g (38.7 %). M.p.: 267°C, turn black, > 280°C decomp.. ¹H NMR (600 MHz, C₆D₆, 23 °C): δ = 4.88 (s, 4 H, -CH for pz ring), 1.32 (s, 72 H, -CH₃) ppm; ¹³C{¹H} NMR (150 MHz, C₆D₆, 23 °C): δ = 167.79 (s, CC(CH₃)₃), 97.05, 93.15 (s, -CH for pz ring), 31.83, 31.37 (CCH₃), 30.70, 29.85 (-CH₃) ppm; IR(Nujol mull, cm⁻¹): 2960(s), 2924(vs), 2853(s), 1461(m), 1377(w), 1260(s), 1092(s), 1019(s), 863(vw), 798(vs), 701(vw); Anal. calcd for C₄₄H₇₆Bi₂N₈: C 46.56, H 6.75, N 9.87; Found: C 46.43, H 6.65, N 9.78.

{η¹,η¹-3,5-Ph₂pz}₂(Bi-Bi){η¹,η¹-3,5-Ph₂pz}₂ (**6**):

To a mixture of BiCl₃ (0.315 g, 1.0 mmol) and K[3,5-Ph₂pz]·THF (**4**, 0.991 g, 3.0 mmol) was added THF (30 mL) via a syringe. After the mixture was stirred for 72 hours the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (4 × 10 mL). The solution was filtered through Celite and the filtrate was concentrated to about 30 mL to give a small amount of free ligand H[3,5-Ph₂pz]. The mother liquid was transferred to another Schlenk flask, further concentrated to about 22 mL, and then kept at about 30°C to afford **6** as orange crystals (0.09 g, 13.9%). The mother liquid was further concentrated to about 15 mL to afford the mixture of **6** and free ligand H[3,5-Ph₂pz], which were difficultly separated. M.p.: 256°C, turn black, >280°C

decomp.. ^1H NMR (600 MHz, THF- d_8 , 23°C): δ = 7.91, 7.90 (d, $^3J_{\text{H-H}} = 7.2$ Hz, 16 H, CH for -Ph), 7.24-7.21 (t, $^3J_{\text{H-H}} = 7.8$ Hz, 16 H, CH for -Ph), 7.01-6.99 (t, 8 H, $^3J_{\text{H-H}} = 7.8$ Hz, CH for -Ph), 6.76 (s, 4 H, -CH for pz ring) ppm; $^{13}\text{C}\{\text{H}\}$ NMR (150 MHz, C₆D₆, 23°C): δ = 151.12 (CHCN for pz ring), 127.47 (C for Ph ring), 124.18, 123.54 (CH for Ph ring), 96.51 (CH for pz ring) ppm; IR(Nujol mull, cm⁻¹): 2960(s), 2924(vs), 2854(s), 1464(m), 1412(vw), 1377(w), 1260(s), 1092(s), 1019(s), 864(w), 798(vs), 700(vw). Anal. calcd for C₆₀H₄₄Bi₂N₈: C 55.65, H 3.42, N 8.65; Found: C 55.53, H 3.34, N 8.54.

Sb[3,5-tBu₂pz]₃ (**10**)·toluene:

To a mixture of K[3,5-tBu₂pz] (**3**, 0.655 g, 3.0 mmol) and SbCl₃ (0.228 g, 1.0 mmol) 20 mL of THF was added via a syringe. After the solution was stirred for 72 h at room temperature the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (**3** × 10 mL) and the solution was filtered through Celite. The filtrate was concentrated under the reduced pressure to about 10 mL, and then kept at -20°C to afford [**10**·toluene] as colorless crystals (0.24 g, 32%). M.p. 246–247°C. ^1H NMR (600 MHz, DMSO- d_6 , 23 °C): δ = 5.82 (s, 3 H, -CH for pz ring), 1.24, 1.21 (2s, 54 H, -CH₃ for tBu) ppm. $^{13}\text{C}\{\text{H}\}$ NMR (150 MHz, C₆D₆, 23°C) : δ = 160.22, 160.16 (-CC(CH₃)₃), 152.53, 152.34(-CC(CH₃)₃), 96.84(-CH for pz ring), 32.09 (-CCH₃), 30.91 (-CH₃) ppm; IR(Nujol mull, cm⁻¹): 2959(s), 2923(vs), 2853(s), 1529(m), 1461(m), 1377(m), 1260(s), 1091(s), 1020(s), 798(vs), 727(w), 694(w), 463(m); Anal. calcd for C₃₃H₅₇SbN₆: C 60.09, H 8.71, N 12.74; Found: C 60.01, H 8.63, N 12.65 (The toluene molecule in the lattice was removed under high vacuum.).

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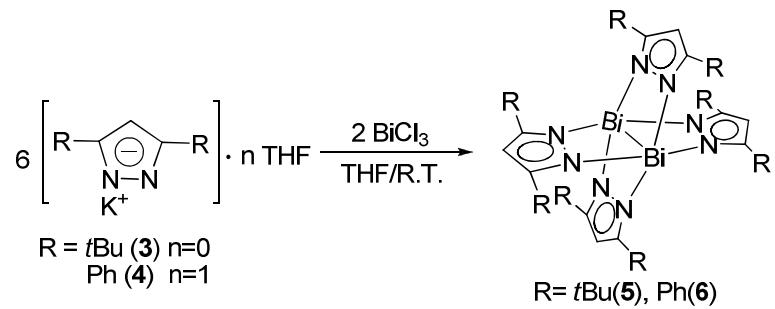
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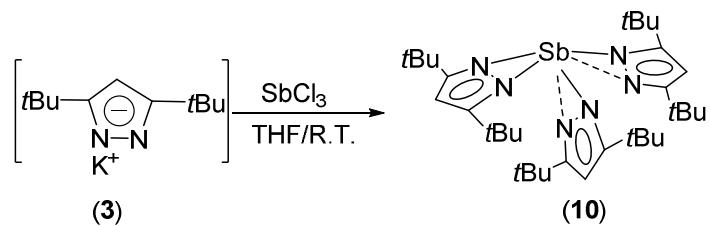
Full citation for Gaussian:

Gaussian 09, Revision C.01., M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.

Scheme S1. Preparation of the Compounds 5 and 6



Scheme S2. Preparation of the Compound 10



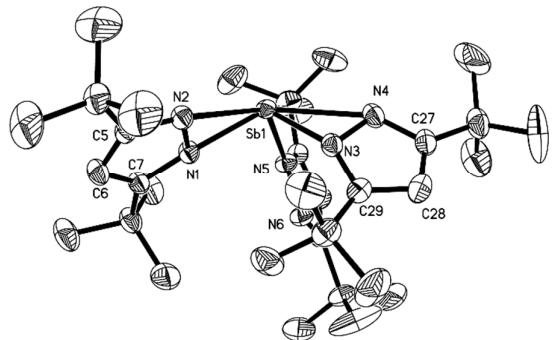


Figure S1. X-ray crystal structures of **10**. Drawn with ellipsoids at 30% probability, toluene and hydrogen atoms omitted for clarity. Selected bond distances [Å] and angles (deg). N₁-Sb₁ 2.096(2), N₃-Sb₁ 2.071(2), N₅-Sb₁ 2.074(2), N₂…Sb₁ 2.590(2), N₄-Sb₁ 2.475(2); N₃-Sb₁-N₅ 93.19(9), N₃-Sb₁-N₁ 101.90(9), N₅-Sb₁-N₁ 98.33(9).

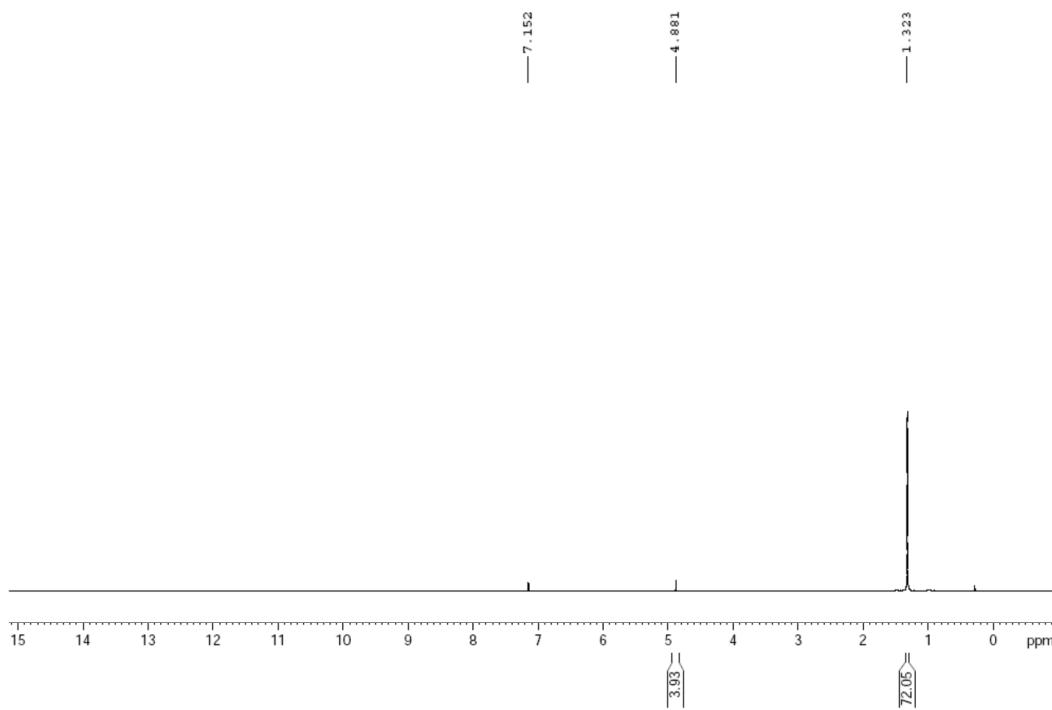


Figure S2. The ¹H NMR spectrum of **5** in C_6D_6 .

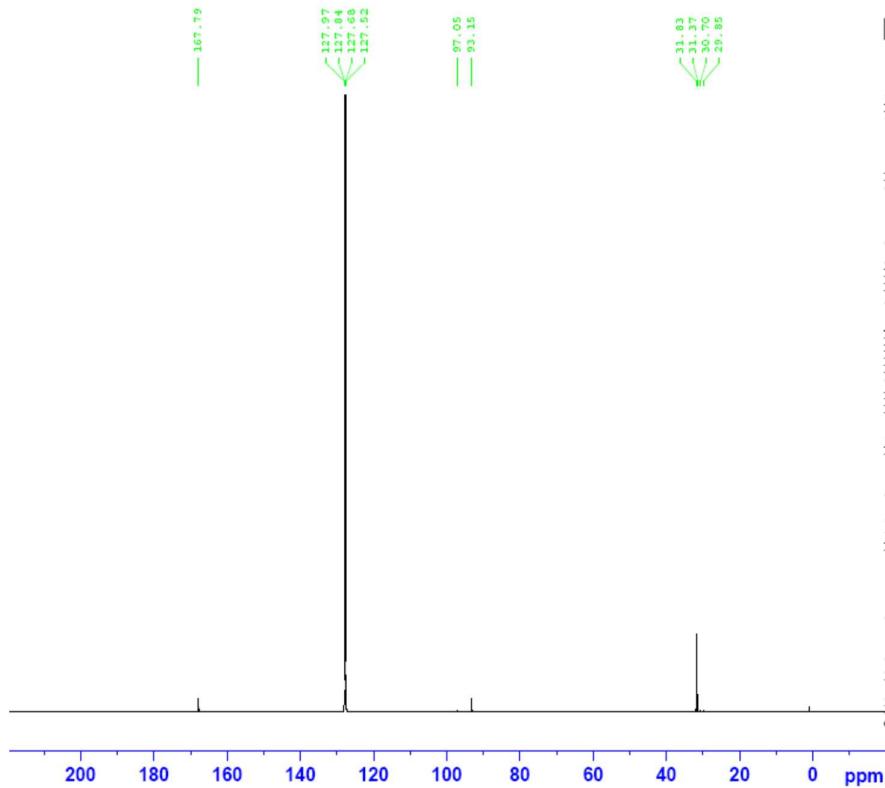


Figure S3. The ¹³C{¹H} NMR spectrum of **5** in C_6D_6 .

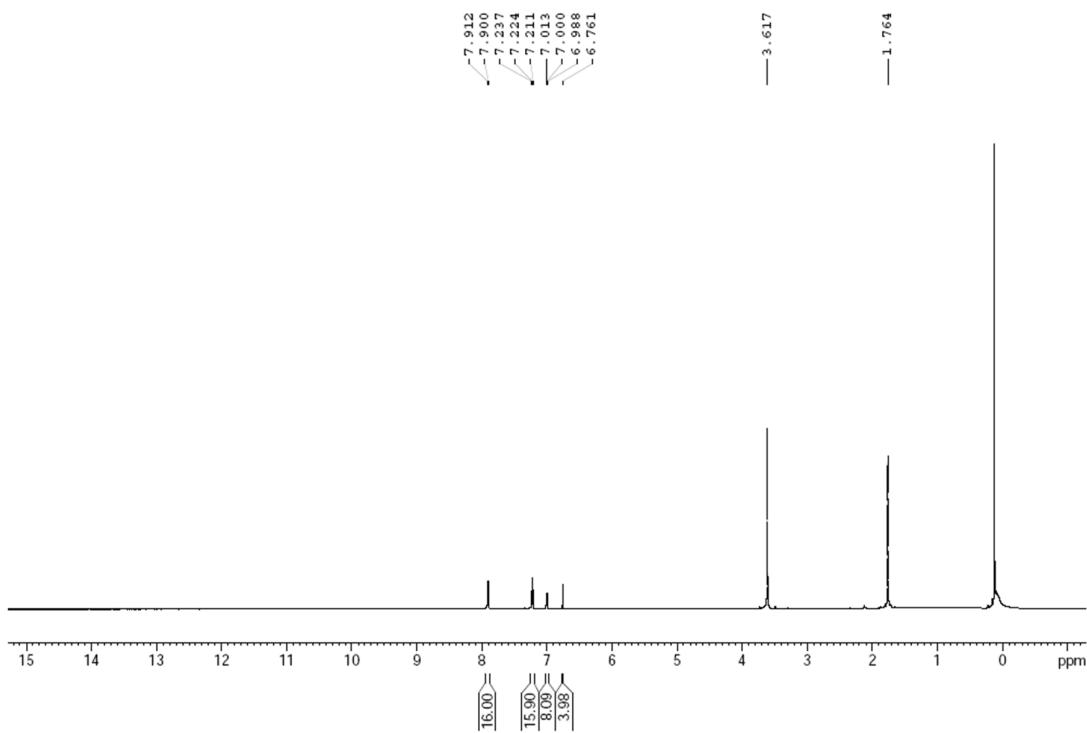


Figure S4. The ^1H NMR spectrum of **6** in $\text{THF}-d_8$.

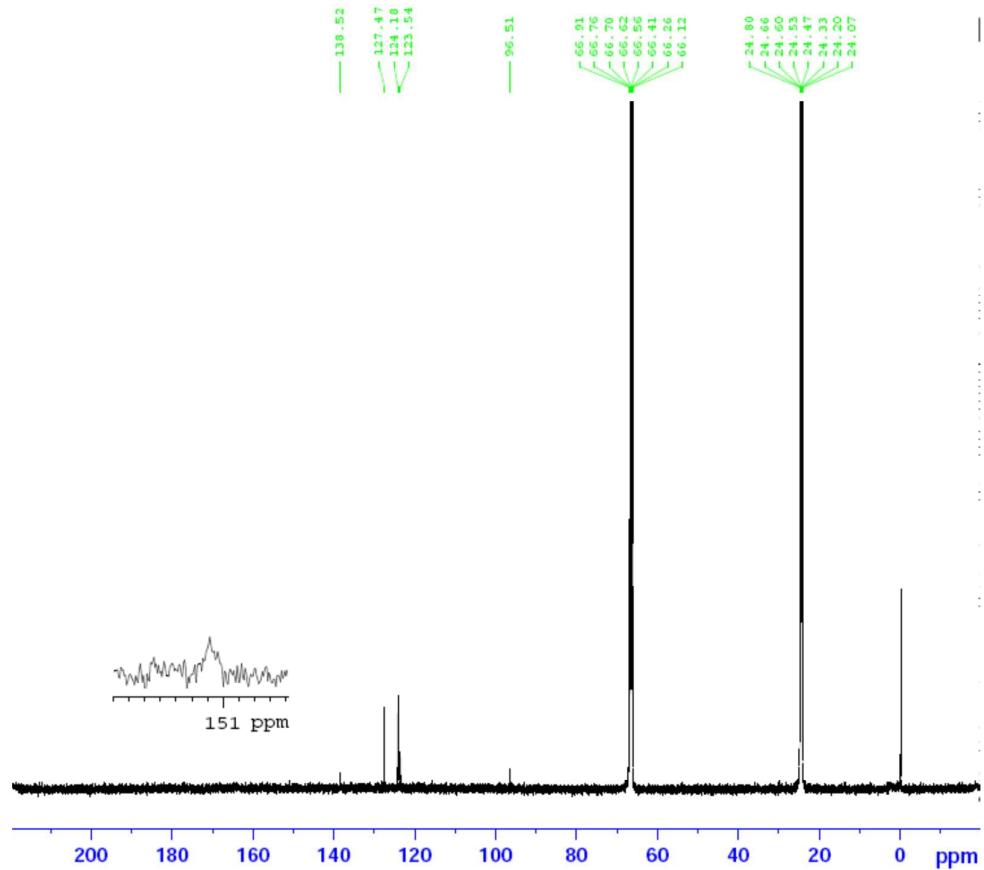


Figure S5. The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6** in $\text{THF}-d_8$.

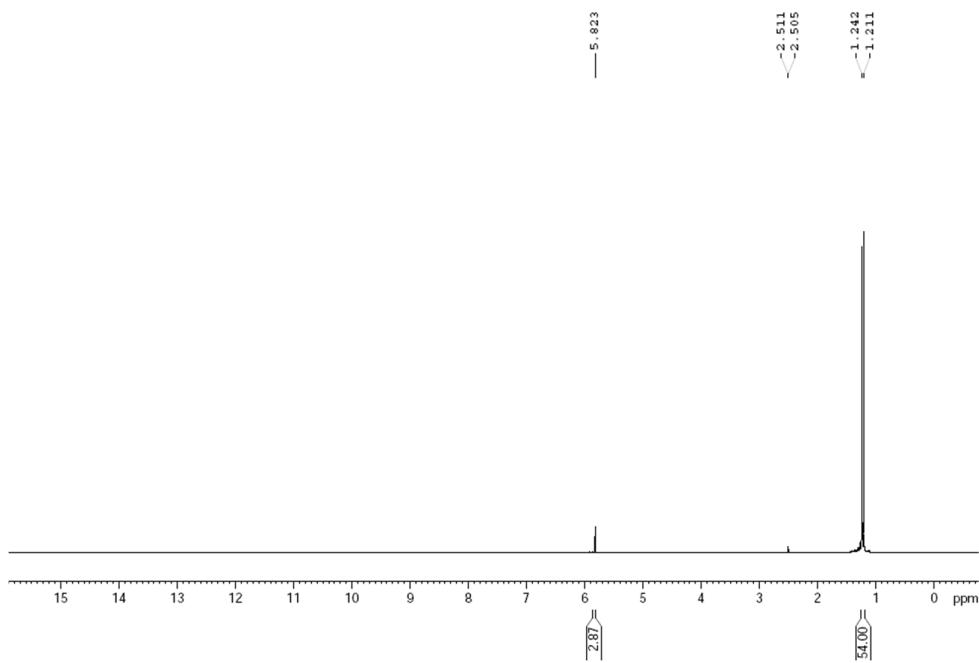


Figure S6. The ^1H NMR spectrum of **10** in $\text{DMSO}-d_6$.

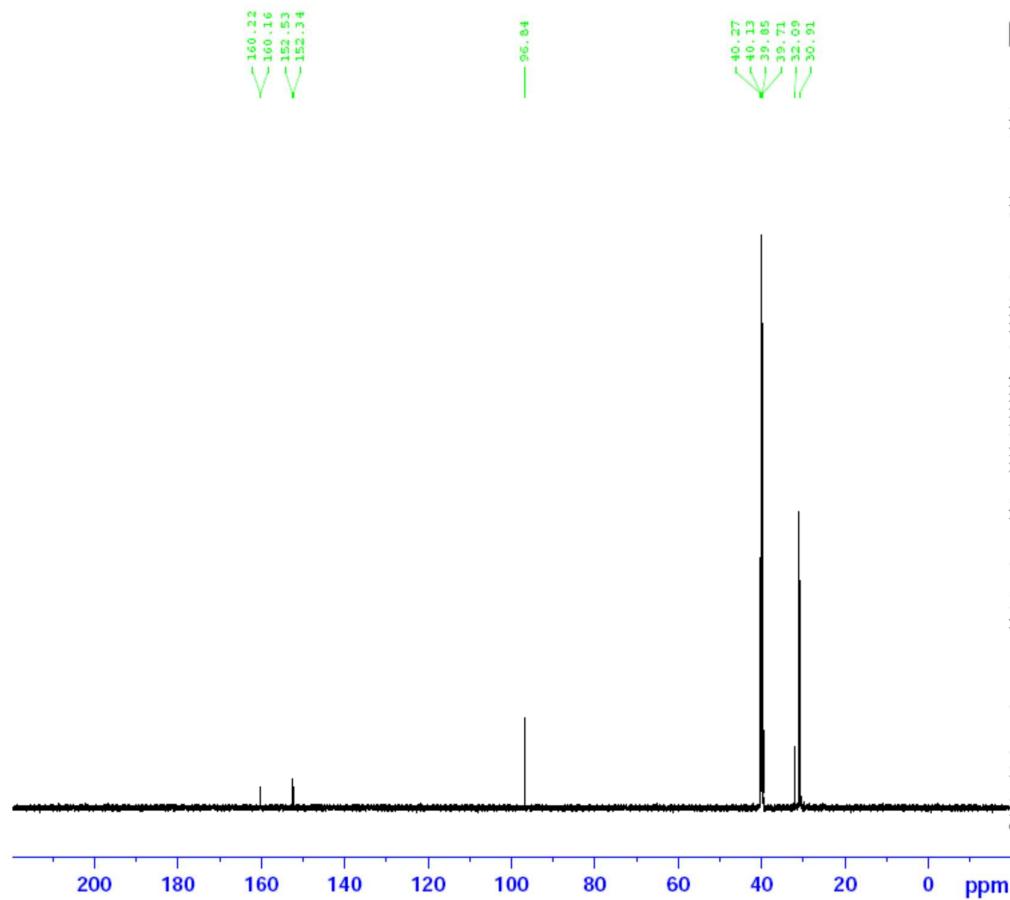


Figure S7. The $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **10** in $\text{DMSO}-d_6$.

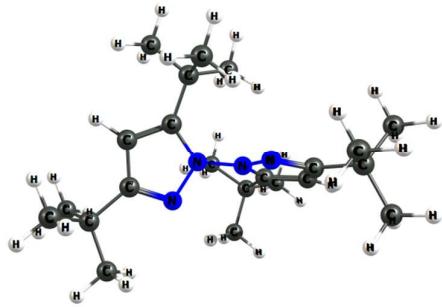


Figure S8. Molecular structure of the Dimer III(N)-III(N).

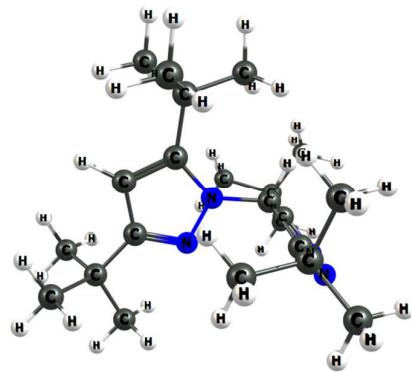


Figure S9. Molecular structure of the dimer III(N)-III(C).

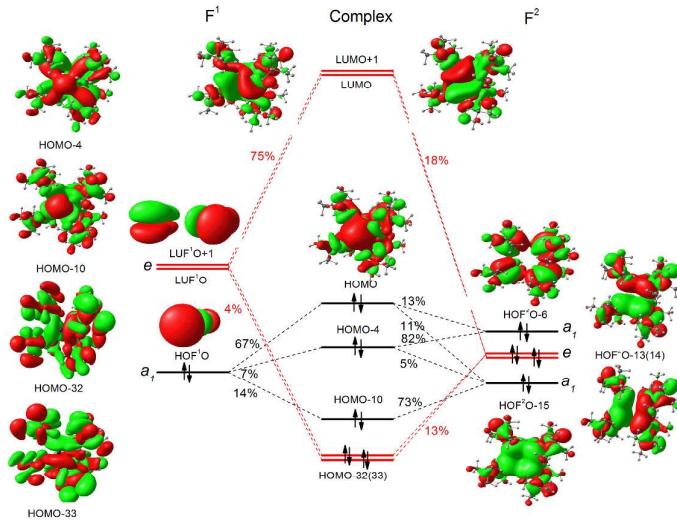


Figure S10. MO-FO interaction diagram for the main interaction between $[Bi-Bi]^{4+}$ unit (F^1) and the four coordinating pyrazolato $\{4[3,5-tBu_2pz]\}^{4-}$ (F^2) in **5**. The orbital energy levels of F^1 were shifted with a vshift of 24 eV, while the orbital energy levels of F^2 were shifted with a vshift of -11 eV.

Description for Figure S10: We provided the simplified fragmentorbital interaction diagrams for the key molecular orbitals of $[Bi_2(3,5-tBu_2pz)_4](5)$, based on the results of B₃LYP method. For comparison, the similar fragment orbital interaction diagrams of $[Bi_2(3,5-tBu_2dp)_4](A)$ were provided in Ref.^[8] Generally, the FO interactions in those selected MOs are similar to those of A, due to the similarity between 1,2,4-diazaphospholide and pyrazolatoligands. However, somewhat great difference on the e -irreducible orbitals can be seen: for complex **5**, many occupied e - F^2 Os have similar contributions to the 2-electron occupied e -MOs (HOMO-13/HOMO-14), among which the greatest contribution comes from HOFO-13/HOFO-14 (about 13%, for clarity, other e - F^2 Os were omitted), while for complex **A**, e - F^2 O of surrounding ligand HOFO-13/HOFO-14 contribute about 61% component of the e -MO HOMO-12/HOMO-13. Despite this difference, similar bonding patterns for **5** and **A** certainly result in similar effect on the shortening of Bi-Bi single bond.

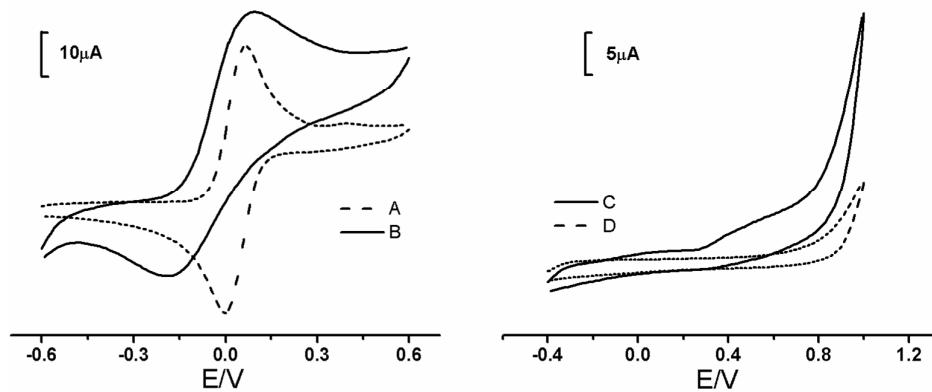


Figure S11. The cyclic voltammograms of Fc/Fc^+ (A), $\text{K}^+[\text{3,5-tBu}_2\text{pz}]^-$ (3) plus Fc/Fc^+ (B), $\text{K}^+[\text{3,5-tBu}_2\text{pz}]^-$ (3) (C), 2.0×10^{-3} M in $\text{CH}_3\text{CN}-\text{Bu}_4\text{NPF}_6$ (0.04 M), and Bu_4NPF_6 (D, 0.04 M) in acetonitrile as blank (D), were measured at 100 mV s^{-1} at 23°C vs. AgNO_3/Ag .

Table S1. Crystal Data Collection Parameters of Complexes 5, 6 and 10

Complexes	5	6	10
formula	C ₁₃₂ H ₂₂₈ Bi ₆ N ₂₄	C ₆₀ H ₄₄ Bi ₂ N ₈	C ₄₀ H ₆₅ N ₆ Sb
fw	3405.26	1294.99	751.73
Cryst. size (mm)	0.24 × 0.13 × 0.08	0.24 × 0.11 × 0.04	0.27 × 0.06 × 0.05
Cryst. Syst.	Triclinic	Triclinic	Triclinic
Space group	P -1	P -1	P -1
<i>a</i> (Å)	11.3961(3)	10.0946(3)	10.2592(4)
<i>b</i> (Å)	23.0746(6)	10.8077(4)	12.1257(5)
<i>c</i> (Å)	28.8497(8)	12.0343(4)	18.7258(7)
α (deg)	83.923(2)	84.304(3)	96.494(3)
β (deg)	83.961(2)	88.640(3)	101.694(3)
γ (deg)	89.818(2)	74.429(3)	107.308(3)
<i>V</i> (Å ³)	7501.6(3)	1258.50(7)	2140.06(15)
<i>Z</i>	2	1	2
<i>D_c</i> (g cm ⁻³)	1.508	1.709	1.167
Absorp. Coeffi. (mm ⁻¹)	7.063	7.030	0.676
<i>F</i> (000)	3372	626	796
<i>T</i> (K)	293(2)	298(2)	293(2)
range (deg)	2.86 – 25.65	2.88 – 25.68	3.08 – 25.68
reflns measured	87195	14652	25148
unique reflns	28436	4769	8127
θ_{max} (deg)	25.65	25.68	25.68
<i>R</i> _{int}	0.0539	0.0808	0.0319
Max and min Transmn	1.0000 and 0.0819	1.0000 and 0.2426	1.0000 and 0.31307
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)] ^a	0.0676, 0.1477	0.0514, 0.0627	0.0341, 0.0815
<i>R</i> ₁ , <i>wR</i> ₂ (all data) ^b	0.1050, 0.1670	0.0983, 0.0713	0.0450, 0.0859
GOF	1.037	0.957	1.067
Δ□(max) (eÅ ⁻³)	3.031	1.122	0.550
Δ□(min) (eÅ ⁻³)	-2.383	-1.175	-0.450

^a*R*₁ = Σ|*F*_o| - |*F*_c| / Σ|*F*_o|. ^b*wR*₂ = [Σ*w*(*F*_o² - *F*_c²)² / Σ*w*(*F*_o²)²]^{0.5}.

*Structure refinement description for complex 5:

All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93 and 0.97 Å for aromatic and methyl H, respectively, and *U*_{iso}(H)=1.5*U*_{eq}(C) for methyl H, and *U*_{iso}(H)=1.2*U*_{eq}(C) for all other H atoms. The C-C bond lengths involving the C₉, C₁₀, C₁₁, C₃₄, C₃₅, C₃₆, C₁₀₈, C₁₀₉ and C₁₁₀ were restrained to be the same within a standard deviation of 0.01 Å, C-C distances refined to values between 1.451 and 1.562 Å. The ADPs of C₁₄, C₃₄, C₃₅, C₃₆, C₈₆, C₈₇, C₈₈, C₆₆, C₆₅ and C₆₃ were restrained to be isotropic within a standard deviation of 0.002 Å². The ADPs of

C_{34} , C_{35} , C_{36} , C_{37} and C_8 , C_9 , C_{10} , C_{11} were restrained to be the same within a standard deviation of 0.005 Å. The atoms C_8 were constrained to have the same ADPs as atoms C_7 . Total 134 restraints were used to model this structure.

Table S2. Selected Bond Distances [Å] and Angles (deg) of Complex 5

Complex 5			
Bi(1)-N(3)	2.441(8)	Bi(3)-N(9)	2.451(8)
Bi(1)-N(7)	2.452(8)	Bi(3)-N(15)	2.479(8)
Bi(1)-N(1)	2.463(9)	Bi(4)-N(10)	2.452(8)
Bi(2)-N(6)	2.446(8)	Bi(4)-N(16)	2.456(9)
Bi(2)-N(8)	2.454(8)	Bi(4)-N(14)	2.490(8)
Bi(2)-N(4)	2.450(8)	Bi(5)-N(21)	2.445(9)
Bi(3)-N(13)	2.441(8)	Bi(5)-N(17)	2.453(8)
Bi(6)-N(24)	2.442(9)	Bi(6)-N(22)	2.470(8)
Bi(1)-Bi(2)	2.8189(6)	Bi(6)-N(20)	2.467(8)
Bi(5)-Bi(6)	2.8183(6)	Bi(3)-Bi(4)	2.8185(6)
N(3)-Bi(1)-N(1)	83.9(3)	N(3)-Bi(1)-N(5)	85.3(3)
N(7)-Bi(1)-N(1)	84.2(3)	N(1)-Bi(1)-N(5)	143.1(3)
N(6)-Bi(2)-N(8)	83.8(3)	N(6)-Bi(2)-N(4)	85.0(3)
N(4)-Bi(2)-N(2)	84.0(3)	N(13)-Bi(3)-N(11)	83.6(3)
N(13)-Bi(3)-N(15)	85.3(3)	N(9)-Bi(3)-N(15)	83.2(3)
N(10)-Bi(4)-N(12)	85.1(3)	N(10)-Bi(4)-N(16)	84.0(3)
N(12)-Bi(4)-N(14)	83.0(3)	N(16)-Bi(4)-N(14)	84.8(3)
N(21)-Bi(5)-N(19)	84.9(3)	N(17)-Bi(5)-N(19)	83.6(3)
N(21)-Bi(5)-N(23)	83.5(3)	N(17)-Bi(5)-N(23)	85.3(3)
N(24)-Bi(6)-N(18)	85.3(3)	N(18)-Bi(6)-N(20)	83.1(3)
N(24)-Bi(6)-N(22)	84.1(3)	N(20)-Bi(6)-N(22)	84.6(3)

Table S3. Selected Bond Distances [Å] and Angles (deg) of Complex 6

Complex 6			
Bi(1)-Bi(1A)	2.8705(6)	Bi(1)-N(1)	2.331(5)
Bi(1)-N(5A)	2.406(5)	Bi(1)-N(3A)	2.579(6)
Bi(1)-N(4)	2.488(5)	N(3)-Bi(1A)	2.579(6)
N(1)-Bi(1)-N(5A)	82.70(18)	N(1)-Bi(1)-N(4)	87.55(18)
N(5) ^{#1} -Bi(1)-N(3A)	83.76(18)	N(4)-Bi(1)-N(3a)	84.33(17)
N(1)-Bi(1)-Bi(1A)	74.42(15)	N(5A) ¹ -Bi(1)-Bi(1A)	73.55(13)

Table S4. Selected Bond Distances [Å] and Angles (deg) of Complex 10

Complex 10			
N(1)-Sb(1)	2.096(2)	N(2)-Sb(1)	2.590(2)
N(3)-Sb(1)	2.071(2)	N(4)-Sb(1)	2.475(2)
N(5)-Sb(1)	2.074(2)	N(3)-Sb(1)-N(5)	93.19(9)
N(3)-Sb(1)-N(1)	101.90(9)	N(5)-Sb(1)-N(1)	98.33(9)
N(5)-Sb(1)-N(4)	83.59(9)	N(1)-Sb(1)-N(4)	135.81(8)
N(4)-Sb(1)-N(2)	122.69(8)	N(5)-Sb(1)-N(2)	130.26(8)
N(3)-Sb(1)-N(2)	91.87(8)	N(1)-Sb(1)-N(2)	32.59(7)

Table S5. Cartesian Coordinates of Complex 5

Bi	0.000281000	-0.000035000	1.406748000
Bi	-0.000383000	0.000032000	-1.406935000
C	-3.079740000	3.190213000	0.000666000
C	3.190441000	3.079424000	-0.000879000
C	-3.190287000	-3.079697000	0.000654000
C	3.079859000	-3.190055000	-0.000660000
N	-1.497299000	1.782107000	0.660321000
N	-1.729385000	1.558366000	-0.659362000
N	1.558125000	1.729240000	-0.660123000
N	1.782159000	1.497474000	0.659569000
N	-1.781982000	-1.497457000	0.660383000
N	-1.558638000	-1.729132000	-0.659443000
N	1.728919000	-1.558478000	-0.660191000
N	1.497552000	-1.782098000	0.659644000
C	-2.300631000	2.772246000	1.078627000
C	-2.690094000	2.396786000	-1.077447000
C	-3.262431000	2.435316000	-2.476774000
C	-4.780613000	2.224604000	-2.388433000
C	-2.981921000	3.806297000	-3.105541000
C	-2.318864000	3.344916000	2.478170000
C	-2.056824000	4.855124000	2.390239000
C	-3.698231000	3.110793000	3.107574000
C	2.396671000	2.689641000	-1.078689000
C	2.772516000	2.300763000	1.077423000
C	3.345367000	2.319408000	2.476884000
C	4.855495000	2.056933000	2.388892000
C	3.111668000	3.699091000	3.105757000
C	2.434942000	3.261644000	-2.478163000
C	2.224424000	4.779870000	-2.390115000
C	3.805746000	2.980845000	-3.107185000
C	-2.771895000	-2.301035000	1.078771000
C	-2.397229000	-2.689662000	-1.077588000
C	-2.436257000	-3.261457000	-2.477123000
C	-3.807481000	-2.980753000	-3.105273000
C	-2.225449000	-4.779664000	-2.389461000
C	-3.343996000	-2.319895000	2.478538000
C	-4.854157000	-2.057333000	2.391375000
C	-3.110051000	-3.699701000	3.107049000
C	2.689464000	-2.396877000	-1.078688000
C	2.301405000	-2.771922000	1.077705000
C	2.320610000	-3.344246000	2.477376000
C	2.057857000	-4.854367000	2.390047000
C	3.700613000	-3.110547000	3.105545000

C	3.260902000	-2.435679000	-2.478374000
C	4.779103000	-2.224687000	-2.391085000
C	2.980207000	-3.806876000	-3.106590000
H	-5.230995000	2.261586000	-3.386216000
H	-5.257947000	2.995039000	-1.777505000
H	-5.016333000	1.253903000	-1.943262000
H	-1.907111000	3.993782000	-3.182386000
H	-3.417482000	4.613539000	-2.510661000
H	-3.408839000	3.862113000	-4.112657000
H	-1.079205000	5.057960000	1.944024000
H	-2.077413000	5.306208000	3.388154000
H	-2.811270000	5.358575000	1.780317000
H	-4.490425000	3.574375000	2.513645000
H	-3.738882000	3.538203000	4.115233000
H	-3.922451000	2.042986000	3.183293000
H	5.058023000	1.079073000	1.943067000
H	5.306694000	2.077823000	3.386748000
H	5.359080000	2.810990000	1.778599000
H	3.575382000	4.490928000	2.511456000
H	3.539203000	3.740038000	4.113351000
H	2.043924000	3.923610000	3.181507000
H	1.253842000	5.015802000	-1.944797000
H	2.261256000	5.230028000	-3.388006000
H	2.995040000	5.257245000	-1.779449000
H	4.613174000	3.416457000	-2.512596000
H	3.861371000	3.407530000	-4.114410000
H	3.993102000	1.9059999000	-3.183833000
H	-4.614488000	-3.416572000	-2.510263000
H	-3.863655000	-3.407286000	-4.112533000
H	-3.995032000	-1.905921000	-3.181635000
H	-2.995616000	-5.257270000	-1.778408000
H	-1.254557000	-5.015520000	-1.944781000
H	-2.262822000	-5.229654000	-3.387407000
H	-5.056870000	-1.079377000	1.945845000
H	-5.304847000	-2.078399000	3.389458000
H	-5.358087000	-2.811246000	1.781190000
H	-3.574125000	-4.491405000	2.512850000
H	-3.537065000	-3.740800000	4.114858000
H	-2.042285000	-3.924305000	3.182206000
H	1.079748000	-5.056901000	1.944772000
H	2.079165000	-5.305218000	3.388052000
H	2.811537000	-5.358281000	1.779560000
H	3.741940000	-3.537732000	4.113270000
H	3.925347000	-2.042816000	3.180818000

H	4.492109000	-3.574603000	2.511056000
H	5.014954000	-1.253802000	-1.946386000
H	5.228844000	-2.261926000	-3.389148000
H	5.256960000	-2.994844000	-1.780216000
H	3.406483000	-3.862891000	-4.113967000
H	1.905377000	-3.994551000	-3.182690000
H	3.416282000	-4.613888000	-2.511776000
H	3.830428000	-3.967836000	-0.000816000
H	3.968454000	3.829752000	-0.001124000
H	-3.830209000	3.968091000	0.000812000
H	-3.968162000	-3.830169000	0.000801000
C	-2.677563000	1.346243000	-3.370825000
H	-2.824461000	0.354112000	-2.934397000
H	-3.173809000	1.357498000	-4.346192000
H	-1.609205000	1.493130000	-3.552234000
C	-1.347542000	-2.676175000	-3.371341000
H	-1.359116000	-3.172041000	-4.346897000
H	-1.494566000	-1.607755000	-3.552279000
H	-0.355245000	-2.823172000	-2.935325000
C	2.675243000	-1.346961000	-3.372337000
H	3.170829000	-1.358407000	-4.348037000
H	1.606786000	-1.494085000	-3.552972000
H	2.822270000	-0.354683000	-2.936292000
C	1.345596000	2.676701000	-3.371832000
H	1.492313000	1.608285000	-3.553033000
H	0.353584000	2.823815000	-2.935210000
H	1.356688000	3.172724000	-4.347313000
C	2.723187000	1.250699000	3.370382000
H	3.219195000	1.244620000	4.345906000
H	1.660430000	1.434125000	3.551608000
H	2.836058000	0.254253000	2.933582000
C	-1.249616000	2.722936000	3.371161000
H	-1.243304000	3.218815000	4.346749000
H	-1.432643000	1.660100000	3.552316000
H	-0.253379000	2.836175000	2.933980000
C	-2.721298000	-1.251382000	3.371905000
H	-2.834256000	-0.254863000	2.935299000
H	-3.216861000	-1.245394000	4.347655000
H	-1.658479000	-1.434957000	3.552625000
C	1.252411000	-2.721562000	3.371132000
H	1.436182000	-1.658800000	3.551992000
H	0.255762000	-2.834297000	2.934765000
H	1.246609000	-3.217296000	4.346797000

Table S6. Cartesian Coordinates of Complex 6

Bi	1.431779000	0.000092000	0.000189000
Bi	-1.431868000	-0.000125000	-0.000229000
C	0.074889000	-3.469951000	2.746746000
C	-0.075695000	3.470219000	2.746524000
C	-0.074252000	-3.470341000	-2.746489000
C	0.075193000	3.469864000	-2.746855000
N	0.661728000	-1.581135000	1.703593000
N	-0.684945000	-1.726875000	1.566515000
N	-0.662282000	1.581579000	1.702925000
N	0.684417000	1.727355000	1.566154000
N	0.685172000	-1.727270000	-1.565996000
N	-0.661516000	-1.581753000	-1.703159000
N	-0.684752000	1.726761000	-1.566722000
N	0.661972000	1.581178000	-1.703453000
C	1.141189000	-2.624453000	2.421471000
C	-1.064213000	-2.866710000	2.192573000
C	-1.141917000	2.624779000	2.420854000
C	1.063498000	2.867217000	2.192280000
C	1.064686000	-2.867001000	-2.192097000
C	-1.140737000	-2.625102000	-2.421154000
C	-1.063942000	2.866669000	-2.192698000
C	1.141496000	2.624476000	-2.421314000
H	0.111725000	4.355500000	-3.365139000
H	-0.112322000	4.355775000	3.364917000
H	0.111373000	-4.355611000	3.364998000
H	-0.110533000	-4.355942000	-3.364838000
C	2.458875000	-3.335013000	-2.244252000
C	2.730566000	-4.711001000	-2.342589000
C	3.545311000	-2.444958000	-2.208223000
C	4.041658000	-5.179328000	-2.401232000
C	4.857350000	-2.914633000	-2.255822000
C	5.112518000	-4.283606000	-2.354541000
H	1.904132000	-5.415831000	-2.353805000
H	3.362118000	-1.376308000	-2.164682000
H	4.227570000	-6.247728000	-2.474337000
H	5.681672000	-2.206891000	-2.224906000
H	6.135028000	-4.648899000	-2.395699000
C	-2.560875000	-2.735038000	-2.788023000
C	-3.303684000	-1.592071000	-3.129632000
C	-3.196480000	-3.986782000	-2.825930000
C	-4.648821000	-1.696860000	-3.482736000
C	-4.539439000	-4.090493000	-3.185250000
C	-5.272163000	-2.946281000	-3.510527000

H	-2.804660000	-0.627787000	-3.155223000
H	-2.635613000	-4.876067000	-2.552206000
H	-5.205410000	-0.802971000	-3.752427000
H	-5.017367000	-5.066449000	-3.204037000
H	-6.319165000	-3.028936000	-3.789524000
C	2.561741000	2.734211000	-2.787828000
C	3.304529000	1.591113000	-3.129053000
C	3.197492000	3.985881000	-2.825724000
C	4.649778000	1.695711000	-3.481789000
C	4.540564000	4.089398000	-3.184680000
C	5.273258000	2.945063000	-3.509590000
H	2.805427000	0.626865000	-3.154612000
H	2.636650000	4.875265000	-2.552268000
H	5.206354000	0.801722000	-3.751176000
H	5.018602000	5.065300000	-3.203466000
H	6.320347000	3.027568000	-3.788304000
C	-2.458040000	3.334925000	-2.245047000
C	-2.729483000	4.710969000	-2.343302000
C	-3.544631000	2.445050000	-2.209263000
C	-4.040487000	5.179521000	-2.402114000
C	-4.856584000	2.914952000	-2.257027000
C	-5.111505000	4.283976000	-2.355669000
H	-1.902927000	5.415660000	-2.354323000
H	-3.361620000	1.376369000	-2.165770000
H	-4.226206000	6.247960000	-2.475156000
H	-5.681030000	2.207346000	-2.226295000
H	-6.133946000	4.649445000	-2.396955000
C	2.457551000	3.335609000	2.244685000
C	3.544235000	2.445854000	2.208748000
C	2.728852000	4.711665000	2.343156000
C	4.856139000	2.915884000	2.256579000
C	4.039808000	5.180345000	2.402032000
C	5.110919000	4.284919000	2.355439000
H	3.361340000	1.377160000	2.165080000
H	1.902225000	5.416269000	2.354295000
H	5.680659000	2.208368000	2.225726000
H	4.225416000	6.248791000	2.475241000
H	6.133323000	4.650488000	2.396776000
C	-2.562175000	2.734356000	2.787369000
C	-3.198063000	3.985956000	2.825280000
C	-3.304835000	1.591171000	3.128582000
C	-4.541145000	4.089320000	3.184242000
C	-4.650096000	1.695616000	3.481319000
C	-5.273712000	2.944899000	3.509135000

H	-2.637313000	4.875404000	2.551846000
H	-2.805623000	0.626980000	3.154132000
H	-5.019291000	5.065170000	3.203042000
H	-5.206574000	0.801564000	3.750694000
H	-6.320813000	3.027284000	3.787843000
C	2.561370000	-2.734117000	2.788252000
C	3.197205000	-3.985745000	2.826167000
C	3.304002000	-1.590998000	3.129740000
C	4.540209000	-4.089196000	3.185393000
C	4.649185000	-1.695529000	3.482749000
C	5.272751000	-2.944838000	3.510563000
H	2.636484000	-4.875144000	2.552514000
H	2.804818000	-0.626795000	3.155299000
H	5.018314000	-5.065066000	3.204191000
H	5.205636000	-0.801525000	3.752343000
H	6.319787000	-3.027293000	3.789491000
C	-2.458329000	-3.334913000	2.244877000
C	-3.544885000	-2.444993000	2.209107000
C	-2.729827000	-4.710949000	2.343094000
C	-4.856857000	-2.914845000	2.256830000
C	-4.040850000	-5.179451000	2.401858000
C	-5.111833000	-4.283863000	2.355416000
H	-3.361832000	-1.376313000	2.165685000
H	-1.903300000	-5.415673000	2.354112000
H	-5.681275000	-2.207205000	2.226117000
H	-4.226613000	-6.247885000	2.474864000
H	-6.134289000	-4.649294000	2.396671000

Table S7. Cartesian Coordinates of Complex [Bi(tBu₂pz)₃](I)

symmetry c1

C	-5.809998000	0.538451000	-1.993686000
C	-6.491844000	1.002506000	0.382868000
C	-4.884941000	2.540474000	-0.783677000
C	-5.326828000	1.073047000	-0.623932000
C	-4.169626000	0.206310000	-0.147258000
C	-4.213462000	-0.992596000	0.600356000
C	-2.903737000	-1.454455000	0.701827000
C	-2.391963000	-2.719415000	1.374101000
C	-1.647263000	-3.595136000	0.343124000
C	-1.435073000	-2.369300000	2.534112000
C	-3.580437000	-3.523237000	1.937128000
C	3.214407000	-3.556612000	2.946732000
C	4.839137000	-1.789595000	2.193552000
C	2.778297000	-1.136946000	3.469129000

C	3.343771000	-2.109260000	2.419430000
C	2.605224000	-1.986252000	1.094444000
C	2.898900000	-2.665372000	-0.114551000
C	1.974711000	-2.215497000	-1.044293000
C	1.852350000	-2.580923000	-2.519134000
C	2.826611000	-3.731628000	-2.844103000
C	2.229713000	-1.371423000	-3.406744000
C	0.424651000	-3.058174000	-2.867225000
C	3.682524000	2.751436000	-2.348514000
C	4.797873000	2.867407000	-0.097898000
C	3.582840000	4.875015000	-1.008729000
C	3.578539000	3.332490000	-0.927145000
C	2.305843000	2.864980000	-0.239244000
C	1.789294000	3.270291000	1.015350000
C	0.614425000	2.553798000	1.218773000
C	-0.388632000	2.649557000	2.354739000
C	-0.678765000	1.254556000	2.941975000
C	-1.702423000	3.265712000	1.820123000
C	0.169689000	3.554794000	3.469199000
N	-2.122025000	-0.538946000	0.046933000
N	-2.903812000	0.468385000	-0.482004000
N	0.455628000	1.766052000	0.111892000
N	1.490987000	1.957323000	-0.776789000
N	1.164036000	-1.317972000	-0.379764000
N	1.561114000	-1.174770000	0.926566000
Bi	-0.346886000	0.133164000	-1.085196000
H	-6.657232000	1.131251000	-2.361623000
H	-6.135376000	-0.506184000	-1.919750000
H	-5.009333000	0.589766000	-2.741124000
H	-7.318053000	1.642231000	0.049412000
H	-6.181941000	1.343199000	1.377912000
H	-6.883744000	-0.016455000	0.481016000
H	-4.048237000	2.634978000	-1.483273000
H	-4.571490000	2.969590000	0.175081000
H	-5.717336000	3.143541000	-1.166818000
H	-5.090450000	-1.467822000	1.014049000
H	-2.299019000	-3.854004000	-0.500247000
H	-1.312697000	-4.529059000	0.811563000
H	-0.764011000	-3.082342000	-0.046856000
H	-0.550155000	-1.836759000	2.174747000
H	-1.096673000	-3.289058000	3.028559000
H	-1.935651000	-1.747824000	3.285957000
H	-4.133923000	-2.953527000	2.692574000
H	-3.211790000	-4.438567000	2.414552000

H	-4.283008000	-3.817058000	1.148435000
H	2.165614000	-3.818516000	3.131240000
H	3.762612000	-3.671406000	3.890708000
H	3.621455000	-4.283249000	2.233612000
H	5.291703000	-2.470740000	1.463603000
H	5.397372000	-1.887986000	3.133354000
H	4.973118000	-0.765419000	1.825506000
H	2.844970000	-0.098229000	3.128411000
H	3.346404000	-1.226951000	4.403452000
H	1.727929000	-1.351256000	3.692515000
H	3.686655000	-3.384498000	-0.285357000
H	3.867886000	-3.439955000	-2.668661000
H	2.732128000	-4.009946000	-3.900178000
H	2.613918000	-4.621245000	-2.240643000
H	1.542582000	-0.526840000	-3.279537000
H	2.202400000	-1.654952000	-4.466022000
H	3.239258000	-1.014988000	-3.174555000
H	0.147460000	-3.941515000	-2.282306000
H	0.365245000	-3.320632000	-3.930304000
H	-0.337381000	-2.288909000	-2.686780000
H	3.696058000	1.656354000	-2.335621000
H	4.607564000	3.097115000	-2.825653000
H	2.840780000	3.068153000	-2.974981000
H	4.765946000	3.269718000	0.921399000
H	5.731566000	3.206526000	-0.564613000
H	4.830987000	1.773913000	-0.026537000
H	2.730876000	5.244899000	-1.591773000
H	4.502054000	5.227944000	-1.492969000
H	3.532904000	5.332846000	-0.014076000
H	2.209048000	4.008701000	1.683348000
H	-1.110532000	0.588812000	2.191864000
H	-1.395770000	1.337978000	3.768477000
H	0.234594000	0.788095000	3.325769000
H	-1.532656000	4.270966000	1.415937000
H	-2.439479000	3.344813000	2.629263000
H	-2.136006000	2.648253000	1.027371000
H	1.105275000	3.158688000	3.880947000
H	-0.555575000	3.621557000	4.288682000
H	0.358358000	4.572846000	3.109419000

Table S8. Cartesian Coordinates of Complex [Bi(tBu₂pz)₂][•] (II)

C	-6.012924000	0.414119000	-0.631080000
C	-5.113586000	2.041849000	1.064223000
C	-4.454934000	2.250622000	-1.352076000
C	-4.781800000	1.255666000	-0.224552000
C	-3.607453000	0.327088000	0.043839000
C	-3.527221000	-0.715495000	1.001033000
C	-2.265575000	-1.277164000	0.862713000
C	-1.650907000	-2.448205000	1.619202000
C	-2.636887000	-2.932407000	2.701624000
C	-0.335701000	-2.028585000	2.313344000
C	-1.375186000	-3.626561000	0.656438000
C	5.293063000	-1.482637000	-0.558481000
C	5.638288000	-0.439818000	1.703542000
C	6.112974000	0.886809000	-0.380192000
C	5.185662000	-0.176511000	0.248856000
C	3.756034000	0.341814000	0.257070000
C	3.271822000	1.562022000	0.790638000
C	1.900011000	1.574184000	0.567789000
C	0.877724000	2.641315000	0.929827000
C	0.128423000	3.130722000	-0.330221000
C	1.596600000	3.847903000	1.565191000
C	-0.136156000	2.075937000	1.949780000
N	1.602129000	0.386301000	-0.050884000
N	2.744235000	-0.358610000	-0.255151000
N	-1.637538000	-0.568839000	-0.135674000
N	-2.467002000	0.407230000	-0.641127000
Bi	0.188071000	-0.679503000	-1.338623000
H	-5.820109000	-0.153022000	-1.549850000
H	-6.879294000	1.063840000	-0.809493000
H	-6.286995000	-0.300895000	0.153409000
H	-5.372190000	1.369231000	1.890321000
H	-5.967425000	2.710759000	0.897063000
H	-4.261501000	2.653512000	1.384089000
H	-3.604170000	2.888938000	-1.090233000
H	-5.319661000	2.898511000	-1.541479000
H	-4.206630000	1.733793000	-2.285472000
H	-4.291834000	-1.018605000	1.701709000
H	-2.863786000	-2.140911000	3.424902000
H	-2.197828000	-3.773279000	3.250961000
H	-3.581248000	-3.275829000	2.264113000
H	0.432469000	-1.720141000	1.596453000
H	0.069759000	-2.870639000	2.887914000
H	-0.502291000	-1.195061000	3.005116000

H	-2.292100000	-3.943849000	0.145835000
H	-0.982191000	-4.485950000	1.213498000
H	-0.634901000	-3.364622000	-0.108472000
H	4.663482000	-2.271713000	-0.133624000
H	6.330598000	-1.838482000	-0.557542000
H	4.985731000	-1.336533000	-1.600246000
H	5.588600000	0.472631000	2.309089000
H	6.674428000	-0.801089000	1.723872000
H	5.006054000	-1.196556000	2.183282000
H	5.828765000	1.099688000	-1.417847000
H	7.152608000	0.535262000	-0.380072000
H	6.080891000	1.830212000	0.177189000
H	3.848075000	2.333025000	1.281537000
H	0.828549000	3.483843000	-1.096810000
H	-0.534068000	3.965471000	-0.068992000
H	-0.498745000	2.347799000	-0.768752000
H	2.137770000	3.563724000	2.474836000
H	0.860707000	4.612789000	1.839252000
H	2.311742000	4.304333000	0.870962000
H	-0.672356000	1.213639000	1.544593000
H	-0.876267000	2.842529000	2.211722000
H	0.369086000	1.763847000	2.871682000

Table S9. Cartesian Coordinates of [3,5-tBu₂pz][•] (III)

C	3.201869000	-0.481797000	-1.262625000
C	3.201877000	-0.481808000	1.262615000
C	2.866939000	1.679772000	0.000006000
C	2.580741000	0.169191000	0.000000000
C	1.104247000	-0.103439000	0.000003000
C	0.000000000	0.745726000	0.000004000
C	-1.104247000	-0.103439000	0.000003000
C	-2.580741000	0.169191000	0.000000000
C	-3.201878000	-0.481808000	1.262615000
C	-3.201868000	-0.481797000	-1.262625000
C	-2.866939000	1.679772000	0.000006000
N	-0.643679000	-1.456091000	0.000001000
N	0.643679000	-1.456091000	0.000001000
H	3.006051000	-1.558241000	-1.291798000
H	4.287591000	-0.327421000	-1.259358000
H	2.796469000	-0.034862000	-2.177762000
H	2.796482000	-0.034883000	2.177759000
H	4.287599000	-0.327431000	1.259343000
H	3.006061000	-1.558253000	1.291779000

H	2.450245000	2.168999000	-0.888160000
H	3.949024000	1.854468000	0.000003000
H	2.450251000	2.168991000	0.888178000
H	0.000000000	1.825167000	0.000005000
H	-3.006062000	-1.558253000	1.291779000
H	-4.287599000	-0.327430000	1.259344000
H	-2.796482000	-0.034883000	2.177759000
H	-2.796470000	-0.034861000	-2.177762000
H	-4.287590000	-0.327422000	-1.259358000
H	-3.006049000	-1.558241000	-1.291799000
H	-2.450252000	2.168991000	0.888179000
H	-3.949024000	1.854468000	0.000001000
H	-2.450244000	2.168999000	-0.888159000

Table S10. Cartesian Coordinates of The Dimer III(N)-III(N)

C	4.517508000	0.715152000	-2.220265000
C	5.000930000	-0.809005000	-0.275560000
C	3.640359000	-1.639807000	-2.221651000
C	3.948839000	-0.418898000	-1.338195000
C	2.694020000	0.079893000	-0.639067000
C	2.569342000	1.208757000	0.213923000
C	1.244866000	1.277855000	0.606704000
C	0.550166000	2.366570000	1.418213000
C	-0.043260000	3.409631000	0.439096000
C	-0.571976000	1.839030000	2.337051000
C	1.603130000	3.065145000	2.305605000
C	-3.640242000	1.639688000	-2.221836000
C	-5.000758000	0.809402000	-0.275496000
C	-4.517793000	-0.715129000	-2.220015000
C	-3.948839000	0.418955000	-1.338182000
C	-2.694018000	-0.079910000	-0.639103000
C	-2.569334000	-1.208862000	0.213782000
C	-1.244891000	-1.277921000	0.606654000
C	-0.550177000	-2.366616000	1.418171000
C	0.571837000	-1.838995000	2.337124000
C	0.043433000	-3.409581000	0.439069000
C	-1.603155000	-3.065318000	2.305446000
N	0.658941000	0.185276000	-0.004141000
N	1.522575000	-0.532259000	-0.779929000
N	-0.658948000	-0.185341000	-0.004190000
N	-1.522561000	0.532211000	-0.779981000
H	5.434437000	0.381982000	-2.721839000
H	4.765240000	1.603210000	-1.627355000

H	3.798565000	1.014716000	-2.991799000
H	5.922395000	-1.153971000	-0.760883000
H	4.634170000	-1.617440000	0.368141000
H	5.260017000	0.040812000	0.366819000
H	2.896294000	-1.401396000	-2.989367000
H	3.255261000	-2.478251000	-1.631454000
H	4.554911000	-1.973250000	-2.726410000
H	3.352802000	1.895616000	0.496892000
H	0.740109000	3.846040000	-0.190953000
H	-0.519626000	4.221230000	1.002888000
H	-0.792971000	2.953232000	-0.213388000
H	-1.411408000	1.418232000	1.778413000
H	-0.961134000	2.674146000	2.931035000
H	-0.200938000	1.082227000	3.035855000
H	2.072768000	2.362388000	3.003362000
H	1.117941000	3.852821000	2.893123000
H	2.392128000	3.537871000	1.711431000
H	-3.254916000	2.478131000	-1.631784000
H	-4.554800000	1.973243000	-2.726509000
H	-2.896323000	1.401035000	-2.989619000
H	-5.259956000	-0.040290000	0.366999000
H	-5.922192000	1.154500000	-0.760785000
H	-4.633768000	1.617836000	0.368072000
H	-3.798958000	-1.015037000	-2.991516000
H	-5.434666000	-0.381847000	-2.721618000
H	-4.765723000	-1.603022000	-1.626933000
H	-3.352789000	-1.895777000	0.496627000
H	1.411225000	-1.417997000	1.778571000
H	0.961092000	-2.674118000	2.931031000
H	0.200633000	-1.082328000	3.035986000
H	-0.739839000	-3.846054000	-0.191060000
H	0.519840000	-4.221153000	1.002867000
H	0.793151000	-2.953081000	-0.213332000
H	-2.072910000	-2.362626000	3.003192000
H	-1.117962000	-3.852983000	2.892977000
H	-2.392068000	-3.538082000	1.711880000

Table S11. Cartesian Coordinates of The Dimer III(N)-III(C)

C	-2.229150000	3.088286000	0.325412000
C	-0.119697000	2.956864000	-1.054881000
C	-2.348814000	3.182300000	-2.180445000
C	-1.610178000	2.549974000	-0.985775000
C	-1.767360000	1.037781000	-1.022555000
C	-1.289361000	0.022529000	0.024657000
C	-1.837475000	-1.253775000	-0.629432000
C	-1.817111000	-2.672159000	-0.076061000
C	-0.439809000	-3.054909000	0.501796000
C	-2.183943000	-3.671942000	-1.189527000
C	-2.884614000	-2.758191000	1.044213000
C	2.811534000	-0.752387000	-2.798385000
C	4.222209000	-1.517075000	-0.863113000
C	4.154350000	0.920159000	-1.486539000
C	3.322855000	-0.379567000	-1.395721000
C	2.166196000	-0.162890000	-0.433049000
C	2.226601000	0.123303000	0.949660000
C	0.917124000	0.236188000	1.400187000
C	0.516196000	0.563859000	2.844922000
C	-0.956326000	0.300655000	3.215812000
C	0.831970000	2.054707000	3.118631000
C	1.384801000	-0.304727000	3.788203000
N	0.141859000	0.023242000	0.278070000
N	0.898068000	-0.224150000	-0.831411000
N	-2.484249000	-0.969223000	-1.704393000
N	-2.444712000	0.451741000	-1.945527000
H	-3.285484000	2.808076000	0.413908000
H	-2.169893000	4.183013000	0.338835000
H	-1.700948000	2.718402000	1.210161000
H	0.453077000	2.591421000	-0.198027000
H	-0.047234000	4.051186000	-1.062996000
H	0.352857000	2.579424000	-1.967622000
H	-1.949498000	2.823712000	-3.134417000
H	-2.228820000	4.271494000	-2.146321000
H	-3.419314000	2.953940000	-2.160643000
H	-1.823530000	0.200850000	0.958311000
H	0.346770000	-2.984223000	-0.256065000
H	-0.475474000	-4.091322000	0.857489000
H	-0.153771000	-2.424536000	1.348919000
H	-3.172929000	-3.466777000	-1.608476000
H	-2.186254000	-4.689127000	-0.780554000
H	-1.457861000	-3.635676000	-2.009098000
H	-2.666329000	-2.073863000	1.871681000

H	-2.911575000	-3.775914000	1.451726000
H	-3.881661000	-2.519756000	0.656889000
H	2.228987000	-1.680056000	-2.781555000
H	3.661340000	-0.897708000	-3.476120000
H	2.172817000	0.032324000	-3.217475000
H	4.624561000	-1.282565000	0.129254000
H	5.071355000	-1.678373000	-1.538743000
H	3.666450000	-2.459382000	-0.787381000
H	3.550806000	1.750632000	-1.871578000
H	5.007665000	0.779652000	-2.161821000
H	4.547256000	1.215753000	-0.506609000
H	3.115808000	0.230693000	1.553339000
H	-1.650399000	0.996173000	2.733833000
H	-1.074378000	0.443721000	4.295906000
H	-1.266321000	-0.725138000	2.989514000
H	1.889815000	2.276678000	2.941659000
H	0.602192000	2.301723000	4.162486000
H	0.236240000	2.714761000	2.478439000
H	1.199343000	-1.373239000	3.629584000
H	1.143566000	-0.069362000	4.831395000
H	2.454020000	-0.121768000	3.646931000

Table S12. Comparison of the Selected Bond Distances (Å) and angles (°) for 5 α , 5 β , 5 γ , 5(calcu.) and A {[L₂(Bi-Bi) L₂] (L=3,5-tBu₂dp)}

complexes	5 α	5 β	5 γ	5(calcu.)	A ^[8]
Bi-Bi	2.8189(6)	2.8185(6)	2.8183(6)	2.814	2.7964(4)
Bi-N(avg.)	2.455(9)	2.460(8)	2.458(9)	2.447	2.481(8)
N-Bi-N(avg.)	84.26(7)	84.24(5)	84.30(5)	84.64	84.3(8)

Calc. = calculated value

Table S13. Comparison of the Selected Bond Distances (Å) and angles (°) for 6, 6(calcu.), B, 10 and [Sb(tBu₂dp)₃]

complexes	6(Bi)	6(calc.)	B	10(Sb)	[Sb(tBu ₂ dp) ₃] ^[9]
M-M	2.8705(6)	2.864	2.8873(3)	-	-
M-N(avg.)	2.464(8)	2.448	2.447(8)	2.261(2)	2.261(6)
				2.929 ^a	2.928 ^a
N-M-N(avg.)	84.58(18)	84.49	84.35(11)	107.2(8)	108.23(10)

B= {[L₂(Bi-Bi) L₂] (L=3,5-Ph₂dp)}; ^a Sb...N; Calc. = calculated value

Table S14. EPR Data of the DMPO[3,5-tBu₂pz][•] Adduct (9)**G:**

File List Date: 16.06.2017 Time: 18:25

File Name: Spectrum send from WinEPR ACQUISITION --- picked at 18:24

Data Point	Value[G]	Intensity
0	3221.9963	1.5173e+003
1	3222.2894	1.5293e+003
2	3222.5826	1.3183e+003
3	3222.8758	1.1923e+003
4	3223.1690	1.4623e+003
5	3223.4622	1.4193e+003
6	3223.7554	1.1763e+003
7	3224.0485	5.3433e+002
8	3224.3417	-2.1667e+002
9	3224.6349	-7.9967e+002
10	3224.9281	-1.2147e+003
11	3225.2213	-8.8467e+002
12	3225.5145	-5.0667e+002
13	3225.8076	-6.5367e+002
14	3226.1008	-1.0067e+003
15	3226.3940	-1.1947e+003
16	3226.6872	-6.4167e+002
17	3226.9804	-1.0297e+003
18	3227.2736	-1.1907e+003
19	3227.5667	-1.1737e+003
20	3227.8599	-1.1817e+003
21	3228.1531	-1.0727e+003
22	3228.4463	-4.7267e+002
23	3228.7395	5.3333e+002
24	3229.0327	4.8533e+002
25	3229.3258	-1.2867e+002
26	3229.6190	-1.3967e+002
27	3229.9122	-9.6367e+002
28	3230.2054	-1.6857e+003
29	3230.4986	-1.5277e+003
30	3230.7918	-1.4567e+003
31	3231.0849	-1.0737e+003
32	3231.3781	-6.4467e+002
33	3231.6713	8.6333e+002
34	3231.9645	2.0563e+003
35	3232.2577	2.1163e+003

36	3232.5509	1.4963e+003
37	3232.8440	6.9733e+002
38	3233.1372	1.8333e+002
39	3233.4304	7.8133e+002
40	3233.7236	9.8233e+002
41	3234.0168	9.8533e+002
42	3234.3100	7.8933e+002
43	3234.6031	2.2433e+002
44	3234.8963	7.9433e+002
45	3235.1895	1.0633e+003
46	3235.4827	1.2403e+003
47	3235.7759	1.4353e+003
48	3236.0691	1.8513e+003
49	3236.3622	2.2733e+003
50	3236.6554	1.8723e+003
51	3236.9486	1.1313e+003
52	3237.2418	1.0523e+003
53	3237.5350	1.6273e+003
54	3237.8282	2.5893e+003
55	3238.1213	2.9903e+003
56	3238.4145	2.6063e+003
57	3238.7077	1.5403e+003
58	3239.0009	3.8833e+002
59	3239.2941	1.3733e+002
60	3239.5873	5.4833e+002
61	3239.8804	1.1383e+003
62	3240.1736	2.1783e+003
63	3240.4668	1.8953e+003
64	3240.7600	1.4163e+003
65	3241.0532	8.3133e+002
66	3241.3464	-7.9668e+001
67	3241.6395	-5.4967e+002
68	3241.9327	-4.9367e+002
69	3242.2259	3.8733e+002
70	3242.5191	1.7463e+003
71	3242.8123	2.4663e+003
72	3243.1055	2.4693e+003
73	3243.3986	1.7513e+003
74	3243.6918	1.2603e+003
75	3243.9850	1.0373e+003
76	3244.2782	8.8633e+002
77	3244.5714	7.3933e+002
78	3244.8646	1.7933e+002
79	3245.1577	-1.1967e+002

80	3245.4509	-5.6467e+002
81	3245.7441	-3.9767e+002
82	3246.0373	3.1533e+002
83	3246.3305	9.1133e+002
84	3246.6237	1.3513e+003
85	3246.9168	1.8173e+003
86	3247.2100	2.7283e+003
87	3247.5032	3.1493e+003
88	3247.7964	2.8443e+003
89	3248.0896	2.4123e+003
90	3248.3828	1.8753e+003
91	3248.6760	1.2633e+003
92	3248.9691	1.5313e+003
93	3249.2623	1.7893e+003
94	3249.5555	9.0533e+002
95	3249.8487	-9.4567e+002
96	3250.1419	-1.9467e+003
97	3250.4351	-1.6807e+003
98	3250.7282	-7.0467e+002
99	3251.0214	5.5633e+002
100	3251.3146	8.1933e+002
101	3251.6078	9.5933e+002
102	3251.9010	1.2343e+003
103	3252.1942	1.0193e+003
104	3252.4873	7.5133e+002
105	3252.7805	5.6733e+002
106	3253.0737	9.0433e+002
107	3253.3669	7.6033e+002
108	3253.6601	6.6233e+002
109	3253.9533	8.5833e+002
110	3254.2464	1.4543e+003
111	3254.5396	1.6763e+003
112	3254.8328	9.0133e+002
113	3255.1260	7.6133e+002
114	3255.4192	8.0833e+002
115	3255.7124	1.0163e+003
116	3256.0055	1.4993e+003
117	3256.2987	1.6543e+003
118	3256.5919	1.7063e+003
119	3256.8851	3.5833e+002
120	3257.1783	-3.7067e+002
121	3257.4715	-5.2867e+002
122	3257.7646	-5.1267e+002
123	3258.0578	-2.7867e+002

124	3258.3510	-2.4767e+002
125	3258.6442	-4.5667e+002
126	3258.9374	-2.4967e+002
127	3259.2306	6.8933e+002
128	3259.5237	1.4253e+003
129	3259.8169	1.7103e+003
130	3260.1101	8.4833e+002
131	3260.4033	-1.2067e+002
132	3260.6965	-9.9767e+002
133	3260.9897	-8.5567e+002
134	3261.2828	-8.6967e+002
135	3261.5760	-7.7067e+002
136	3261.8692	-7.4467e+002
137	3262.1624	-7.4167e+002
138	3262.4556	-1.0157e+003
139	3262.7488	-1.7457e+003
140	3263.0419	-1.7877e+003
141	3263.3351	-1.7607e+003
142	3263.6283	-1.7287e+003
143	3263.9215	-1.7697e+003
144	3264.2147	-4.4267e+002
145	3264.5079	-1.9267e+002
146	3264.8010	-2.1567e+002
147	3265.0942	-6.0467e+002
148	3265.3874	-1.0807e+003
149	3265.6806	-3.4367e+002
150	3265.9738	4.7233e+002
151	3266.2670	1.3533e+002
152	3266.5601	-3.7067e+002
153	3266.8533	-1.3397e+003
154	3267.1465	-1.5917e+003
155	3267.4397	-5.8867e+002
156	3267.7329	6.6533e+002
157	3268.0261	1.6813e+003
158	3268.3192	2.5133e+003
159	3268.6124	1.9343e+003
160	3268.9056	1.7013e+003
161	3269.1988	2.0043e+003
162	3269.4920	1.5983e+003
163	3269.7852	1.4853e+003
164	3270.0783	1.1213e+003
165	3270.3715	-1.4967e+002
166	3270.6647	-1.3757e+003
167	3270.9579	-2.1577e+003

168	3271.2511	-2.3807e+003
169	3271.5443	-1.6607e+003
170	3271.8374	-6.7667e+002
171	3272.1306	8.2233e+002
172	3272.4238	2.0063e+003
173	3272.7170	2.3043e+003
174	3273.0102	2.3933e+003
175	3273.3034	2.6373e+003
176	3273.5965	2.5313e+003
177	3273.8897	2.0973e+003
178	3274.1829	1.0063e+003
179	3274.4761	1.8933e+002
180	3274.7693	-6.2867e+002
181	3275.0625	-8.5267e+002
182	3275.3557	-3.3267e+002
183	3275.6488	6.5133e+002
184	3275.9420	9.6733e+002
185	3276.2352	1.0733e+002
186	3276.5284	-6.6567e+002
187	3276.8216	-1.8717e+003
188	3277.1148	-2.4147e+003
189	3277.4079	-1.6197e+003
190	3277.7011	-1.7157e+003
191	3277.9943	-2.2137e+003
192	3278.2875	-1.5317e+003
193	3278.5807	-6.9067e+002
194	3278.8739	-5.6667e+002
195	3279.1670	-1.8467e+002
196	3279.4602	2.0833e+002
197	3279.7534	5.1033e+002
198	3280.0466	4.0533e+002
199	3280.3398	4.3333e+002
200	3280.6330	9.7332e+001
201	3280.9261	-2.2867e+002
202	3281.2193	-6.6668e+001
203	3281.5125	-8.5067e+002
204	3281.8057	-1.4517e+003
205	3282.0989	-1.5857e+003
206	3282.3921	-1.5527e+003
207	3282.6852	-8.6567e+002
208	3282.9784	8.0332e+001
209	3283.2716	9.1733e+002
210	3283.5648	8.7733e+002
211	3283.8580	-9.4668e+001

212	3284.1512	-1.1537e+003
213	3284.4443	-7.7767e+002
214	3284.7375	-4.3467e+002
215	3285.0307	-7.4867e+002
216	3285.3239	-4.3667e+002
217	3285.6171	-1.1867e+002
218	3285.9103	1.4033e+002
219	3286.2034	3.3633e+002
220	3286.4966	-2.4567e+002
221	3286.7898	-7.2067e+002
222	3287.0830	-2.5668e+001
223	3287.3762	9.5233e+002
224	3287.6694	1.5033e+003
225	3287.9625	1.9403e+003
226	3288.2557	1.7603e+003
227	3288.5489	8.2933e+002
228	3288.8421	-7.4767e+002
229	3289.1353	-1.6627e+003
230	3289.4285	-2.1707e+003
231	3289.7216	-1.3227e+003
232	3290.0148	-7.3668e+001
233	3290.3080	1.0333e+003
234	3290.6012	1.4033e+003
235	3290.8944	1.3033e+003
236	3291.1876	1.3243e+003
237	3291.4807	7.6533e+002
238	3291.7739	9.2233e+002
239	3292.0671	1.0273e+003
240	3292.3603	3.3332e+001
241	3292.6535	-7.7267e+002
242	3292.9467	-8.5767e+002
243	3293.2398	-3.3467e+002
244	3293.5330	4.9833e+002
245	3293.8262	7.8633e+002
246	3294.1194	3.2533e+002
247	3294.4126	-1.4767e+002
248	3294.7058	-5.2367e+002
249	3294.9989	-5.3967e+002
250	3295.2921	-1.2977e+003
251	3295.5853	-1.9587e+003
252	3295.8785	-1.7657e+003
253	3296.1717	-1.1627e+003
254	3296.4649	-9.4267e+002
255	3296.7580	-3.0767e+002

256	3297.0512	-1.1867e+002
257	3297.3444	1.1163e+003
258	3297.6376	2.1943e+003
259	3297.9308	2.4463e+003
260	3298.2240	2.3053e+003
261	3298.5171	1.7273e+003
262	3298.8103	1.3203e+003
263	3299.1035	6.3933e+002
264	3299.3967	4.5433e+002
265	3299.6899	6.9633e+002
266	3299.9831	3.6833e+002
267	3300.2762	3.5733e+002
268	3300.5694	-7.6667e+002
269	3300.8626	-1.1297e+003
270	3301.1558	-6.2467e+002
271	3301.4490	-3.3667e+002
272	3301.7422	-7.8767e+002
273	3302.0354	-1.1457e+003
274	3302.3285	-1.5737e+003
275	3302.6217	-1.6637e+003
276	3302.9149	-1.8917e+003
277	3303.2081	-2.1237e+003
278	3303.5013	-2.5387e+003
279	3303.7945	-2.2997e+003
280	3304.0876	-1.8927e+003
281	3304.3808	-9.1767e+002
282	3304.6740	6.2332e+001
283	3304.9672	2.3933e+002
284	3305.2604	-3.0967e+002
285	3305.5536	-2.7667e+002
286	3305.8467	-3.2367e+002
287	3306.1399	-2.8467e+002
288	3306.4331	-2.6867e+002
289	3306.7263	5.5233e+002
290	3307.0195	2.0113e+003
291	3307.3127	3.3963e+003
292	3307.6058	3.0053e+003
293	3307.8990	2.9403e+003
294	3308.1922	3.9423e+003
295	3308.4854	4.6673e+003
296	3308.7786	4.0193e+003
297	3309.0718	3.6213e+003
298	3309.3649	3.9603e+003
299	3309.6581	4.0153e+003

300	3309.9513	3.3403e+003
301	3310.2445	2.6073e+003
302	3310.5377	2.0143e+003
303	3310.8309	9.8033e+002
304	3311.1240	4.4433e+002
305	3311.4172	2.0833e+002
306	3311.7104	-2.8767e+002
307	3312.0036	-1.4447e+003
308	3312.2968	-1.4617e+003
309	3312.5900	-1.1307e+003
310	3312.8831	-7.7467e+002
311	3313.1763	-3.6467e+002
312	3313.4695	-4.1367e+002
313	3313.7627	3.7133e+002
314	3314.0559	1.2283e+003
315	3314.3491	1.3043e+003
316	3314.6422	9.6133e+002
317	3314.9354	1.7413e+003
318	3315.2286	2.9443e+003
319	3315.5218	3.8253e+003
320	3315.8150	4.1163e+003
321	3316.1082	4.0113e+003
322	3316.4013	3.1073e+003
323	3316.6945	2.0633e+003
324	3316.9877	1.2823e+003
325	3317.2809	3.7433e+002
326	3317.5741	-2.5567e+002
327	3317.8673	-1.6267e+002
328	3318.1604	2.9233e+002
329	3318.4536	1.2933e+003
330	3318.7468	2.2443e+003
331	3319.0400	2.1913e+003
332	3319.3332	7.7433e+002
333	3319.6264	-5.6267e+002
334	3319.9195	-1.0177e+003
335	3320.2127	-7.4767e+002
336	3320.5059	-2.4167e+002
337	3320.7991	4.5433e+002
338	3321.0923	8.7433e+002
339	3321.3855	9.8033e+002
340	3321.6786	7.8833e+002
341	3321.9718	-9.9668e+001
342	3322.2650	-7.4167e+002
343	3322.5582	-1.2087e+003

344	3322.8514	-1.2457e+003
345	3323.1446	-6.4067e+002
346	3323.4377	3.7633e+002
347	3323.7309	1.2763e+003
348	3324.0241	2.0263e+003
349	3324.3173	1.8093e+003
350	3324.6105	2.0223e+003
351	3324.9037	1.5523e+003
352	3325.1968	7.5633e+002
353	3325.4900	4.9033e+002
354	3325.7832	-2.3867e+002
355	3326.0764	-9.4767e+002
356	3326.3696	-8.2067e+002
357	3326.6628	-7.6067e+002
358	3326.9559	-1.1547e+003
359	3327.2491	-1.1187e+003
360	3327.5423	-1.2317e+003
361	3327.8355	-1.5877e+003
362	3328.1287	-3.8067e+002
363	3328.4219	8.9133e+002
364	3328.7151	1.7793e+003
365	3329.0082	1.8353e+003
366	3329.3014	2.1663e+003
367	3329.5946	1.8103e+003
368	3329.8878	1.6563e+003
369	3330.1810	1.5543e+003
370	3330.4742	7.4233e+002
371	3330.7673	-1.5267e+002
372	3331.0605	9.6332e+001
373	3331.3537	9.5033e+002
374	3331.6469	1.4303e+003
375	3331.9401	2.4423e+003
376	3332.2333	3.6963e+003
377	3332.5264	4.8683e+003
378	3332.8196	6.5993e+003
379	3333.1128	9.3003e+003
380	3333.4060	1.2156e+004
381	3333.6992	1.5330e+004
382	3333.9924	1.8321e+004
383	3334.2855	2.2429e+004
384	3334.5787	2.8149e+004
385	3334.8719	3.5459e+004
386	3335.1651	4.4739e+004
387	3335.4583	5.4832e+004

388	3335.7515	6.2268e+004
389	3336.0446	6.4199e+004
390	3336.3378	5.7790e+004
391	3336.6310	4.1689e+004
392	3336.9242	1.7817e+004
393	3337.2174	-9.3867e+003
394	3337.5106	-3.3103e+004
395	3337.8037	-4.9068e+004
396	3338.0969	-5.4967e+004
397	3338.3901	-5.1951e+004
398	3338.6833	-4.2733e+004
399	3338.9765	-2.8746e+004
400	3339.2697	-1.1493e+004
401	3339.5628	5.6713e+003
402	3339.8560	1.9697e+004
403	3340.1492	2.7276e+004
404	3340.4424	2.6610e+004
405	3340.7356	1.8207e+004
406	3341.0288	3.7973e+003
407	3341.3219	-1.1640e+004
408	3341.6151	-2.4740e+004
409	3341.9083	-3.2229e+004
410	3342.2015	-3.2552e+004
411	3342.4947	-2.7214e+004
412	3342.7879	-1.7798e+004
413	3343.0810	-4.4677e+003
414	3343.3742	1.0827e+004
415	3343.6674	2.5627e+004
416	3343.9606	3.6447e+004
417	3344.2538	3.9148e+004
418	3344.5470	3.3406e+004
419	3344.8401	1.9777e+004
420	3345.1333	3.4463e+003
421	3345.4265	-1.1524e+004
422	3345.7197	-2.1670e+004
423	3346.0129	-2.6177e+004
424	3346.3061	-2.5845e+004
425	3346.5992	-2.1348e+004
426	3346.8924	-1.4764e+004
427	3347.1856	-6.8767e+003
428	3347.4788	1.3493e+003
429	3347.7720	1.0523e+004
430	3348.0652	2.2123e+004
431	3348.3583	3.9305e+004

432	3348.6515	6.1667e+004
433	3348.9447	8.5627e+004
434	3349.2379	1.0381e+005
435	3349.5311	1.0929e+005
436	3349.8243	9.8006e+004
437	3350.1174	6.8886e+004
438	3350.4106	2.8686e+004
439	3350.7038	-1.2954e+004
440	3350.9970	-4.6976e+004
441	3351.2902	-6.7560e+004
442	3351.5834	-7.2919e+004
443	3351.8765	-6.4473e+004
444	3352.1697	-4.5202e+004
445	3352.4629	-1.7779e+004
446	3352.7561	1.2835e+004
447	3353.0493	4.1867e+004
448	3353.3425	6.2164e+004
449	3353.6357	6.7666e+004
450	3353.9288	5.5817e+004
451	3354.2220	3.2149e+004
452	3354.5152	4.1243e+003
453	3354.8084	-1.8946e+004
454	3355.1016	-3.2234e+004
455	3355.3948	-3.3397e+004
456	3355.6879	-2.4811e+004
457	3355.9811	-8.8097e+003
458	3356.2743	1.2803e+004
459	3356.5675	3.6545e+004
460	3356.8607	5.6170e+004
461	3357.1539	6.7695e+004
462	3357.4470	6.6445e+004
463	3357.7402	5.1170e+004
464	3358.0334	2.4057e+004
465	3358.3266	-8.8637e+003
466	3358.6198	-4.0339e+004
467	3358.9130	-6.4514e+004
468	3359.2061	-7.6804e+004
469	3359.4993	-7.6904e+004
470	3359.7925	-6.7266e+004
471	3360.0857	-5.1791e+004
472	3360.3789	-3.5639e+004
473	3360.6721	-1.9979e+004
474	3360.9652	-4.7217e+003
475	3361.2584	1.1399e+004

476	3361.5516	2.9869e+004
477	3361.8448	5.1575e+004
478	3362.1380	7.4868e+004
479	3362.4312	9.3974e+004
480	3362.7243	1.0272e+005
481	3363.0175	9.7683e+004
482	3363.3107	7.8549e+004
483	3363.6039	4.9321e+004
484	3363.8971	1.6479e+004
485	3364.1903	-1.2657e+004
486	3364.4834	-3.2965e+004
487	3364.7766	-4.3086e+004
488	3365.0698	-4.2516e+004
489	3365.3630	-3.3683e+004
490	3365.6562	-1.6839e+004
491	3365.9494	5.9723e+003
492	3366.2425	2.8781e+004
493	3366.5357	4.4584e+004
494	3366.8289	4.7346e+004
495	3367.1221	3.4229e+004
496	3367.4153	8.8543e+003
497	3367.7085	-1.9025e+004
498	3368.0016	-4.3200e+004
499	3368.2948	-5.9470e+004
500	3368.5880	-6.4460e+004
501	3368.8812	-5.8906e+004
502	3369.1744	-4.3273e+004
503	3369.4676	-1.7691e+004
504	3369.7607	1.3531e+004
505	3370.0539	4.3123e+004
506	3370.3471	6.4039e+004
507	3370.6403	7.0042e+004
508	3370.9335	5.7549e+004
509	3371.2267	2.8649e+004
510	3371.5198	-1.0203e+004
511	3371.8130	-4.9420e+004
512	3372.1062	-7.9994e+004
513	3372.3994	-9.7271e+004
514	3372.6926	-1.0063e+005
515	3372.9858	-9.3197e+004
516	3373.2789	-8.0962e+004
517	3373.5721	-6.6953e+004
518	3373.8653	-5.3067e+004
519	3374.1585	-4.1392e+004

520	3374.4517	-3.0974e+004
521	3374.7449	-2.0065e+004
522	3375.0380	-7.3997e+003
523	3375.3312	5.2423e+003
524	3375.6244	1.6024e+004
525	3375.9176	2.2726e+004
526	3376.2108	2.2174e+004
527	3376.5040	1.4384e+004
528	3376.7971	8.9133e+002
529	3377.0903	-1.4249e+004
530	3377.3835	-2.7696e+004
531	3377.6767	-3.5691e+004
532	3377.9699	-3.7868e+004
533	3378.2631	-3.4979e+004
534	3378.5562	-2.7057e+004
535	3378.8494	-1.4884e+004
536	3379.1426	-9.4767e+002
537	3379.4358	1.2533e+004
538	3379.7290	2.2955e+004
539	3380.0222	2.7400e+004
540	3380.3154	2.4748e+004
541	3380.6085	1.4794e+004
542	3380.9017	7.1533e+002
543	3381.1949	-1.3411e+004
544	3381.4881	-2.3376e+004
545	3381.7813	-2.8356e+004
546	3382.0745	-2.6902e+004
547	3382.3676	-1.9062e+004
548	3382.6608	-6.0517e+003
549	3382.9540	9.1563e+003
550	3383.2472	2.6392e+004
551	3383.5404	4.2414e+004
552	3383.8336	5.2780e+004
553	3384.1267	5.4129e+004
554	3384.4199	4.4602e+004
555	3384.7131	2.6405e+004
556	3385.0063	4.3133e+003
557	3385.2995	-1.7060e+004
558	3385.5927	-3.4540e+004
559	3385.8858	-4.6007e+004
560	3386.1790	-5.0580e+004
561	3386.4722	-4.9504e+004
562	3386.7654	-4.5733e+004
563	3387.0586	-4.0566e+004

564	3387.3518	-3.4962e+004
565	3387.6449	-3.0433e+004
566	3387.9381	-2.6390e+004
567	3388.2313	-2.2113e+004
568	3388.5245	-1.8261e+004
569	3388.8177	-1.4876e+004
570	3389.1109	-1.2771e+004
571	3389.4040	-1.1948e+004
572	3389.6972	-1.0450e+004
573	3389.9904	-8.5637e+003
574	3390.2836	-7.2247e+003
575	3390.5768	-6.3487e+003
576	3390.8700	-5.7447e+003
577	3391.1631	-4.1967e+003
578	3391.4563	-3.2897e+003
579	3391.7495	-3.4167e+003
580	3392.0427	-3.3537e+003
581	3392.3359	-3.1917e+003
582	3392.6291	-2.6137e+003
583	3392.9222	-1.8837e+003
584	3393.2154	-1.3977e+003
585	3393.5086	-9.6167e+002
586	3393.8018	-1.2477e+003
587	3394.0950	-1.5917e+003
588	3394.3882	-1.4007e+003
589	3394.6813	-5.9067e+002
590	3394.9745	2.3320e+000
591	3395.2677	4.1833e+002
592	3395.5609	-5.5668e+001
593	3395.8541	-2.5567e+002
594	3396.1473	-7.3867e+002
595	3396.4404	-1.7557e+003
596	3396.7336	-2.7307e+003
597	3397.0268	-3.1497e+003
598	3397.3200	-2.4637e+003
599	3397.6132	-1.2927e+003
600	3397.9064	-8.2667e+002
601	3398.1995	-3.0967e+002
602	3398.4927	-7.3967e+002
603	3398.7859	-1.5817e+003
604	3399.0791	-2.4717e+003
605	3399.3723	-3.4717e+003
606	3399.6655	-3.1077e+003
607	3399.9586	-2.3707e+003

608	3400.2518	-2.0667e+003
609	3400.5450	-1.8857e+003
610	3400.8382	-2.2107e+003
611	3401.1314	-2.9377e+003
612	3401.4246	-2.4597e+003
613	3401.7177	-1.8857e+003
614	3402.0109	-1.3917e+003
615	3402.3041	-8.0167e+002
616	3402.5973	-1.7567e+002
617	3402.8905	3.2033e+002
618	3403.1837	3.8033e+002
619	3403.4768	2.4233e+002
620	3403.7700	-4.4867e+002
621	3404.0632	-7.3367e+002
622	3404.3564	-2.9967e+002
623	3404.6496	1.1133e+002
624	3404.9428	-2.8668e+001
625	3405.2359	-7.8967e+002
626	3405.5291	-1.1757e+003
627	3405.8223	-1.0957e+003
628	3406.1155	-1.2587e+003
629	3406.4087	-8.9567e+002
630	3406.7019	-7.8767e+002
631	3406.9951	-1.0257e+003
632	3407.2882	-1.5877e+003
633	3407.5814	-8.5467e+002
634	3407.8746	-2.6967e+002
635	3408.1678	-3.9367e+002
636	3408.4610	-3.1667e+002
637	3408.7542	-3.8567e+002
638	3409.0473	-5.8067e+002
639	3409.3405	-6.4967e+002
640	3409.6337	2.7033e+002
641	3409.9269	3.5533e+002
642	3410.2201	-5.8668e+001
643	3410.5133	-6.0567e+002
644	3410.8064	-7.2667e+002
645	3411.0996	-1.1337e+003
646	3411.3928	-1.3147e+003
647	3411.6860	-9.7867e+002
648	3411.9792	-1.4197e+003
649	3412.2724	-2.0617e+003
650	3412.5655	-2.7077e+003
651	3412.8587	-3.7687e+003

652	3413.1519	-4.5597e+003
653	3413.4451	-4.7547e+003
654	3413.7383	-4.9957e+003
655	3414.0315	-4.2217e+003
656	3414.3246	-3.2717e+003
657	3414.6178	-2.4107e+003
658	3414.9110	-1.7627e+003
659	3415.2042	-9.6867e+002
660	3415.4974	-7.2967e+002
661	3415.7906	-7.2167e+002
662	3416.0837	-8.3467e+002
663	3416.3769	-8.9967e+002
664	3416.6701	-1.0377e+003
665	3416.9633	-9.9167e+002
666	3417.2565	-6.6667e+002
667	3417.5497	-4.0267e+002
668	3417.8428	-1.0837e+003
669	3418.1360	-8.0767e+002
670	3418.4292	-9.8867e+002
671	3418.7224	-8.2567e+002
672	3419.0156	-5.8167e+002
673	3419.3088	-4.6867e+002
674	3419.6019	-2.3667e+002
675	3419.8951	-2.9668e+001
676	3420.1883	6.4533e+002
677	3420.4815	1.4563e+003
678	3420.7747	1.2903e+003
679	3421.0679	8.3633e+002
680	3421.3610	1.5313e+003
681	3421.6542	2.4713e+003
682	3421.9474	3.2143e+003
683	3422.2406	3.1343e+003
684	3422.5338	2.4253e+003
685	3422.8270	2.3263e+003
686	3423.1201	2.5093e+003
687	3423.4133	2.4553e+003
688	3423.7065	2.0283e+003
689	3423.9997	1.9903e+003
690	3424.2929	1.9173e+003
691	3424.5861	2.0813e+003
692	3424.8792	1.9723e+003
693	3425.1724	1.4143e+003
694	3425.4656	1.4473e+003
695	3425.7588	1.5663e+003

696	3426.0520	6.7833e+002
697	3426.3452	4.0533e+002
698	3426.6383	5.0133e+002
699	3426.9315	4.9833e+002
700	3427.2247	-2.9667e+002
701	3427.5179	-7.8667e+002
702	3427.8111	-7.0367e+002
703	3428.1043	-5.8367e+002
704	3428.3974	-6.4867e+002
705	3428.6906	-3.8367e+002
706	3428.9838	-3.0367e+002
707	3429.2770	-5.2567e+002
708	3429.5702	-4.3267e+002
709	3429.8634	-5.6067e+002
710	3430.1565	-6.7467e+002
711	3430.4497	-9.9867e+002
712	3430.7429	-1.0707e+003
713	3431.0361	-1.1847e+003
714	3431.3293	-8.9667e+002
715	3431.6225	5.4332e+001
716	3431.9156	5.3833e+002
717	3432.2088	-4.6867e+002
718	3432.5020	-9.7467e+002
719	3432.7952	-1.3997e+003
720	3433.0884	-1.4717e+003
721	3433.3816	-2.1937e+003
722	3433.6748	-2.1107e+003
723	3433.9679	-1.5297e+003
724	3434.2611	-1.4697e+003
725	3434.5543	-1.7187e+003
726	3434.8475	-2.3967e+003
727	3435.1407	-2.7357e+003
728	3435.4339	-2.8767e+003
729	3435.7270	-2.0087e+003
730	3436.0202	-9.4167e+002
731	3436.3134	5.4133e+002
732	3436.6066	8.0633e+002
733	3436.8998	6.8433e+002
734	3437.1930	4.8333e+002
735	3437.4861	4.3933e+002
736	3437.7793	6.6733e+002
737	3438.0725	5.6133e+002
738	3438.3657	-1.4668e+001
739	3438.6589	-9.0967e+002

740	3438.9521	-1.3407e+003
741	3439.2452	-2.1587e+003
742	3439.5384	-2.7277e+003
743	3439.8316	-2.2417e+003
744	3440.1248	-1.0137e+003
745	3440.4180	6.0533e+002
746	3440.7112	1.2853e+003
747	3441.0043	1.2553e+003
748	3441.2975	6.8533e+002
749	3441.5907	-1.5467e+002
750	3441.8839	-2.6367e+002
751	3442.1771	1.2233e+002
752	3442.4703	9.3332e+001
753	3442.7634	-2.3668e+001
754	3443.0566	3.9332e+001
755	3443.3498	-6.5667e+002
756	3443.6430	-1.3567e+003
757	3443.9362	-9.9467e+002
758	3444.2294	2.4133e+002
759	3444.5225	7.0233e+002
760	3444.8157	7.8533e+002
761	3445.1089	-6.3668e+001
762	3445.4021	-1.2737e+003
763	3445.6953	-1.7467e+003
764	3445.9885	-1.6077e+003
765	3446.2816	-1.5197e+003
766	3446.5748	-8.7367e+002
767	3446.8680	-6.2667e+002
768	3447.1612	-8.3767e+002
769	3447.4544	-1.1937e+003
770	3447.7476	-1.1197e+003
771	3448.0407	-8.8067e+002
772	3448.3339	-6.8667e+002
773	3448.6271	-7.3967e+002
774	3448.9203	-1.3407e+003
775	3449.2135	-1.2917e+003
776	3449.5067	-1.1157e+003
777	3449.7998	-5.2767e+002
778	3450.0930	-7.0667e+002
779	3450.3862	-3.1967e+002
780	3450.6794	-3.0967e+002
781	3450.9726	-9.0067e+002
782	3451.2658	-1.1977e+003
783	3451.5589	-8.1467e+002

784	3451.8521	-1.7367e+002
785	3452.1453	-3.1668e+001
786	3452.4385	5.2433e+002
787	3452.7317	1.6263e+003
788	3453.0249	1.7873e+003
789	3453.3180	1.3993e+003
790	3453.6112	8.1733e+002
791	3453.9044	3.8233e+002
792	3454.1976	-1.9267e+002
793	3454.4908	-3.1668e+001
794	3454.7840	2.3733e+002
795	3455.0771	7.5533e+002
796	3455.3703	7.5433e+002
797	3455.6635	5.2332e+001
798	3455.9567	-5.2867e+002
799	3456.2499	-4.9667e+002
800	3456.5431	-3.9668e+001
801	3456.8362	-5.5667e+002
802	3457.1294	-1.3007e+003
803	3457.4226	-1.5177e+003
804	3457.7158	-1.5077e+003
805	3458.0090	-1.2527e+003
806	3458.3022	-1.0807e+003
807	3458.5953	-3.5367e+002
808	3458.8885	-4.8467e+002
809	3459.1817	-5.2467e+002
810	3459.4749	-7.8267e+002
811	3459.7681	-5.0167e+002
812	3460.0613	-6.8668e+001
813	3460.3545	-4.5567e+002
814	3460.6476	-1.0747e+003
815	3460.9408	-9.0967e+002
816	3461.2340	2.1433e+002
817	3461.5272	8.5033e+002
818	3461.8204	5.9033e+002
819	3462.1136	-1.9668e+001
820	3462.4067	4.3533e+002
821	3462.6999	8.1033e+002
822	3462.9931	7.3333e+002
823	3463.2863	1.3783e+003
824	3463.5795	1.4333e+003
825	3463.8727	6.2333e+002
826	3464.1658	1.8233e+002
827	3464.4590	3.8833e+002

828	3464.7522	3.5833e+002
829	3465.0454	2.9633e+002
830	3465.3386	8.7733e+002
831	3465.6318	1.1923e+003
832	3465.9249	8.1333e+002
833	3466.2181	6.2333e+002
834	3466.5113	1.0793e+003
835	3466.8045	1.7623e+003
836	3467.0977	8.6533e+002
837	3467.3909	1.0233e+002
838	3467.6840	-1.6367e+002
839	3467.9772	-2.9668e+001
840	3468.2704	-2.0867e+002
841	3468.5636	1.9633e+002
842	3468.8568	1.7423e+003
843	3469.1500	3.1083e+003
844	3469.4431	3.5983e+003
845	3469.7363	3.2573e+003
846	3470.0295	2.1623e+003
847	3470.3227	8.4833e+002
848	3470.6159	-6.2668e+001
849	3470.9091	-1.1367e+003
850	3471.2022	-1.5897e+003
851	3471.4954	-2.2247e+003
852	3471.7886	-1.9347e+003
853	3472.0818	-1.8217e+003
854	3472.3750	-2.2517e+003
855	3472.6682	-2.4737e+003
856	3472.9613	-2.7367e+003
857	3473.2545	-3.1247e+003
858	3473.5477	-2.8917e+003
859	3473.8409	-2.9867e+003
860	3474.1341	-2.6197e+003
861	3474.4273	-2.1047e+003
862	3474.7204	-1.3797e+003
863	3475.0136	-5.0867e+002
864	3475.3068	-8.6680e+000
865	3475.6000	7.4933e+002
866	3475.8932	2.4833e+002
867	3476.1864	-2.1667e+002
868	3476.4795	-4.7668e+001
869	3476.7727	-1.9567e+002
870	3477.0659	3.8933e+002
871	3477.3591	6.2633e+002

872	3477.6523	9.4233e+002
873	3477.9455	5.3033e+002
874	3478.2386	-6.2667e+002
875	3478.5318	-1.0007e+003
876	3478.8250	-2.2667e+002
877	3479.1182	3.3233e+002
878	3479.4114	2.8233e+002
879	3479.7046	3.0433e+002
880	3479.9977	2.9933e+002
881	3480.2909	6.9133e+002
882	3480.5841	8.0533e+002
883	3480.8773	7.7333e+002
884	3481.1705	1.3813e+003
885	3481.4637	1.7493e+003
886	3481.7568	1.2453e+003
887	3482.0500	2.7332e+001
888	3482.3432	-6.5167e+002
889	3482.6364	-4.3668e+001
890	3482.9296	6.8333e+002
891	3483.2228	8.6333e+002
892	3483.5159	1.4143e+003
893	3483.8091	3.3133e+003
894	3484.1023	4.1953e+003
895	3484.3955	4.1903e+003
896	3484.6887	3.5923e+003
897	3484.9819	2.8353e+003
898	3485.2751	2.4683e+003
899	3485.5682	2.2363e+003
900	3485.8614	2.0373e+003
901	3486.1546	1.9583e+003
902	3486.4478	1.7463e+003
903	3486.7410	4.9833e+002
904	3487.0342	-4.3367e+002
905	3487.3273	-8.6567e+002
906	3487.6205	-1.0017e+003
907	3487.9137	-1.0327e+003
908	3488.2069	-8.4067e+002
909	3488.5001	-1.1547e+003
910	3488.7933	-1.0877e+003
911	3489.0864	-7.0067e+002
912	3489.3796	-5.3867e+002
913	3489.6728	-4.2967e+002
914	3489.9660	3.5433e+002
915	3490.2592	1.8933e+002

916	3490.5524	6.9733e+002
917	3490.8455	9.4133e+002
918	3491.1387	1.2333e+003
919	3491.4319	1.5553e+003
920	3491.7251	1.1733e+003
921	3492.0183	6.7133e+002
922	3492.3115	9.8733e+002
923	3492.6046	1.9383e+003
924	3492.8978	2.7433e+003
925	3493.1910	2.5053e+003
926	3493.4842	2.4863e+003
927	3493.7774	2.5793e+003
928	3494.0706	1.7103e+003
929	3494.3637	1.8323e+003
930	3494.6569	1.9193e+003
931	3494.9501	1.4933e+003
932	3495.2433	1.3033e+003
933	3495.5365	1.2153e+003
934	3495.8297	3.4333e+002
935	3496.1228	-8.0467e+002
936	3496.4160	-2.2607e+003
937	3496.7092	-3.0437e+003
938	3497.0024	-2.9477e+003
939	3497.2956	-2.4227e+003
940	3497.5888	-1.5487e+003
941	3497.8819	-1.3167e+003
942	3498.1751	-8.4167e+002
943	3498.4683	4.9332e+001
944	3498.7615	5.1733e+002
945	3499.0547	4.1933e+002
946	3499.3479	5.0933e+002
947	3499.6410	6.2033e+002
948	3499.9342	4.6733e+002
949	3500.2274	6.0533e+002
950	3500.5206	1.4733e+002
951	3500.8138	-5.5167e+002
952	3501.1070	-5.2067e+002
953	3501.4001	-4.6867e+002
954	3501.6933	-5.3167e+002
955	3501.9865	-7.0267e+002
956	3502.2797	-8.1267e+002
957	3502.5729	-1.1527e+003
958	3502.8661	-1.3117e+003
959	3503.1592	-1.4247e+003

960	3503.4524	-7.9967e+002
961	3503.7456	-9.9668e+001
962	3504.0388	6.2333e+002
963	3504.3320	1.1443e+003
964	3504.6252	1.5733e+003
965	3504.9183	2.5603e+003
966	3505.2115	3.0413e+003
967	3505.5047	2.6473e+003
968	3505.7979	2.2803e+003
969	3506.0911	3.2933e+002
970	3506.3843	-1.6687e+003
971	3506.6774	-2.6997e+003
972	3506.9706	-3.4987e+003
973	3507.2638	-2.7017e+003
974	3507.5570	-2.4677e+003
975	3507.8502	-2.7427e+003
976	3508.1434	-2.4587e+003
977	3508.4365	-1.5847e+003
978	3508.7297	-1.1477e+003
979	3509.0229	-8.4667e+002
980	3509.3161	7.1332e+001
981	3509.6093	3.4933e+002
982	3509.9025	5.0133e+002
983	3510.1956	4.3033e+002
984	3510.4888	1.3332e+001
985	3510.7820	-2.7367e+002
986	3511.0752	-5.3167e+002
987	3511.3684	-1.0587e+003
988	3511.6616	-1.2057e+003
989	3511.9548	-1.1977e+003
990	3512.2479	-1.1837e+003
991	3512.5411	-1.8477e+003
992	3512.8343	-2.2917e+003
993	3513.1275	-2.2717e+003
994	3513.4207	-1.2357e+003
995	3513.7139	-2.5967e+002
996	3514.0070	6.7433e+002
997	3514.3002	1.5253e+003
998	3514.5934	2.0313e+003
999	3514.8866	1.6033e+003
1000	3515.1798	1.0303e+003
1001	3515.4730	-3.3867e+002
1002	3515.7661	-1.9247e+003
1003	3516.0593	-2.8357e+003

1004	3516.3525	-2.4797e+003
1005	3516.6457	-2.3557e+003
1006	3516.9389	-2.9437e+003
1007	3517.2321	-3.4477e+003
1008	3517.5252	-2.8717e+003
1009	3517.8184	-2.2657e+003
1010	3518.1116	-1.7287e+003
1011	3518.4048	-1.4407e+003
1012	3518.6980	-1.2707e+003
1013	3518.9912	-7.5967e+002
1014	3519.2843	-5.4267e+002
1015	3519.5775	-2.5767e+002
1016	3519.8707	4.4033e+002
1017	3520.1639	1.1033e+003
1018	3520.4571	1.1933e+003
1019	3520.7503	3.5333e+002
1020	3521.0434	-7.4567e+002
1021	3521.3366	-6.9667e+002
1022	3521.6298	1.0833e+002
1023	3521.9230	2.4133e+002

***g* factor:**

File List Date: 16.06.2017 Time: 18:25

File Name: Spectrum send from WinEPR ACQUISITION --- picked at 18:24

Data Point Value[g-Factor] Intensity

0	2.09559	1.5173e+003
1	2.09540	1.5293e+003
2	2.09521	1.3183e+003
3	2.09502	1.1923e+003
4	2.09483	1.4623e+003
5	2.09464	1.4193e+003
6	2.09445	1.1763e+003
7	2.09426	5.3433e+002
8	2.09407	-2.1667e+002
9	2.09388	-7.9967e+002
10	2.09369	-1.2147e+003
11	2.09350	-8.8467e+002
12	2.09331	-5.0667e+002
13	2.09312	-6.5367e+002
14	2.09293	-1.0067e+003

15	2.09274	-1.1947e+003
16	2.09255	-6.4167e+002
17	2.09236	-1.0297e+003
18	2.09217	-1.1907e+003
19	2.09198	-1.1737e+003
20	2.09179	-1.1817e+003
21	2.09160	-1.0727e+003
22	2.09141	-4.7267e+002
23	2.09122	5.3333e+002
24	2.09103	4.8533e+002
25	2.09084	-1.2867e+002
26	2.09065	-1.3967e+002
27	2.09046	-9.6367e+002
28	2.09027	-1.6857e+003
29	2.09008	-1.5277e+003
30	2.08989	-1.4567e+003
31	2.08970	-1.0737e+003
32	2.08951	-6.4467e+002
33	2.08932	8.6333e+002
34	2.08913	2.0563e+003
35	2.08894	2.1163e+003
36	2.08875	1.4963e+003
37	2.08856	6.9733e+002
38	2.08837	1.8333e+002
39	2.08818	7.8133e+002
40	2.08799	9.8233e+002
41	2.08780	9.8533e+002
42	2.08761	7.8933e+002
43	2.08742	2.2433e+002
44	2.08724	7.9433e+002
45	2.08705	1.0633e+003
46	2.08686	1.2403e+003
47	2.08667	1.4353e+003
48	2.08648	1.8513e+003
49	2.08629	2.2733e+003
50	2.08610	1.8723e+003
51	2.08591	1.1313e+003
52	2.08572	1.0523e+003
53	2.08553	1.6273e+003
54	2.08535	2.5893e+003
55	2.08516	2.9903e+003
56	2.08497	2.6063e+003
57	2.08478	1.5403e+003
58	2.08459	3.8833e+002

59	2.08440	1.3733e+002
60	2.08421	5.4833e+002
61	2.08402	1.1383e+003
62	2.08384	2.1783e+003
63	2.08365	1.8953e+003
64	2.08346	1.4163e+003
65	2.08327	8.3133e+002
66	2.08308	-7.9668e+001
67	2.08289	-5.4967e+002
68	2.08271	-4.9367e+002
69	2.08252	3.8733e+002
70	2.08233	1.7463e+003
71	2.08214	2.4663e+003
72	2.08195	2.4693e+003
73	2.08176	1.7513e+003
74	2.08158	1.2603e+003
75	2.08139	1.0373e+003
76	2.08120	8.8633e+002
77	2.08101	7.3933e+002
78	2.08082	1.7933e+002
79	2.08064	-1.1967e+002
80	2.08045	-5.6467e+002
81	2.08026	-3.9767e+002
82	2.08007	3.1533e+002
83	2.07988	9.1133e+002
84	2.07970	1.3513e+003
85	2.07951	1.8173e+003
86	2.07932	2.7283e+003
87	2.07913	3.1493e+003
88	2.07895	2.8443e+003
89	2.07876	2.4123e+003
90	2.07857	1.8753e+003
91	2.07838	1.2633e+003
92	2.07820	1.5313e+003
93	2.07801	1.7893e+003
94	2.07782	9.0533e+002
95	2.07763	-9.4567e+002
96	2.07745	-1.9467e+003
97	2.07726	-1.6807e+003
98	2.07707	-7.0467e+002
99	2.07688	5.5633e+002
100	2.07670	8.1933e+002
101	2.07651	9.5933e+002
102	2.07632	1.2343e+003

103	2.07613	1.0193e+003
104	2.07595	7.5133e+002
105	2.07576	5.6733e+002
106	2.07557	9.0433e+002
107	2.07539	7.6033e+002
108	2.07520	6.6233e+002
109	2.07501	8.5833e+002
110	2.07482	1.4543e+003
111	2.07464	1.6763e+003
112	2.07445	9.0133e+002
113	2.07426	7.6133e+002
114	2.07408	8.0833e+002
115	2.07389	1.0163e+003
116	2.07370	1.4993e+003
117	2.07352	1.6543e+003
118	2.07333	1.7063e+003
119	2.07314	3.5833e+002
120	2.07296	-3.7067e+002
121	2.07277	-5.2867e+002
122	2.07258	-5.1267e+002
123	2.07240	-2.7867e+002
124	2.07221	-2.4767e+002
125	2.07202	-4.5667e+002
126	2.07184	-2.4967e+002
127	2.07165	6.8933e+002
128	2.07147	1.4253e+003
129	2.07128	1.7103e+003
130	2.07109	8.4833e+002
131	2.07091	-1.2067e+002
132	2.07072	-9.9767e+002
133	2.07053	-8.5567e+002
134	2.07035	-8.6967e+002
135	2.07016	-7.7067e+002
136	2.06998	-7.4467e+002
137	2.06979	-7.4167e+002
138	2.06960	-1.0157e+003
139	2.06942	-1.7457e+003
140	2.06923	-1.7877e+003
141	2.06905	-1.7607e+003
142	2.06886	-1.7287e+003
143	2.06867	-1.7697e+003
144	2.06849	-4.4267e+002
145	2.06830	-1.9267e+002
146	2.06812	-2.1567e+002

147	2.06793	-6.0467e+002
148	2.06775	-1.0807e+003
149	2.06756	-3.4367e+002
150	2.06737	4.7233e+002
151	2.06719	1.3533e+002
152	2.06700	-3.7067e+002
153	2.06682	-1.3397e+003
154	2.06663	-1.5917e+003
155	2.06645	-5.8867e+002
156	2.06626	6.6533e+002
157	2.06608	1.6813e+003
158	2.06589	2.5133e+003
159	2.06571	1.9343e+003
160	2.06552	1.7013e+003
161	2.06534	2.0043e+003
162	2.06515	1.5983e+003
163	2.06496	1.4853e+003
164	2.06478	1.1213e+003
165	2.06459	-1.4967e+002
166	2.06441	-1.3757e+003
167	2.06422	-2.1577e+003
168	2.06404	-2.3807e+003
169	2.06385	-1.6607e+003
170	2.06367	-6.7667e+002
171	2.06348	8.2233e+002
172	2.06330	2.0063e+003
173	2.06311	2.3043e+003
174	2.06293	2.3933e+003
175	2.06275	2.6373e+003
176	2.06256	2.5313e+003
177	2.06238	2.0973e+003
178	2.06219	1.0063e+003
179	2.06201	1.8933e+002
180	2.06182	-6.2867e+002
181	2.06164	-8.5267e+002
182	2.06145	-3.3267e+002
183	2.06127	6.5133e+002
184	2.06108	9.6733e+002
185	2.06090	1.0733e+002
186	2.06072	-6.6567e+002
187	2.06053	-1.8717e+003
188	2.06035	-2.4147e+003
189	2.06016	-1.6197e+003
190	2.05998	-1.7157e+003

191	2.05979	-2.2137e+003
192	2.05961	-1.5317e+003
193	2.05943	-6.9067e+002
194	2.05924	-5.6667e+002
195	2.05906	-1.8467e+002
196	2.05887	2.0833e+002
197	2.05869	5.1033e+002
198	2.05850	4.0533e+002
199	2.05832	4.3333e+002
200	2.05814	9.7332e+001
201	2.05795	-2.2867e+002
202	2.05777	-6.6668e+001
203	2.05759	-8.5067e+002
204	2.05740	-1.4517e+003
205	2.05722	-1.5857e+003
206	2.05703	-1.5527e+003
207	2.05685	-8.6567e+002
208	2.05667	8.0332e+001
209	2.05648	9.1733e+002
210	2.05630	8.7733e+002
211	2.05612	-9.4668e+001
212	2.05593	-1.1537e+003
213	2.05575	-7.7767e+002
214	2.05556	-4.3467e+002
215	2.05538	-7.4867e+002
216	2.05520	-4.3667e+002
217	2.05501	-1.1867e+002
218	2.05483	1.4033e+002
219	2.05465	3.3633e+002
220	2.05446	-2.4567e+002
221	2.05428	-7.2067e+002
222	2.05410	-2.5668e+001
223	2.05392	9.5233e+002
224	2.05373	1.5033e+003
225	2.05355	1.9403e+003
226	2.05337	1.7603e+003
227	2.05318	8.2933e+002
228	2.05300	-7.4767e+002
229	2.05282	-1.6627e+003
230	2.05263	-2.1707e+003
231	2.05245	-1.3227e+003
232	2.05227	-7.3668e+001
233	2.05208	1.0333e+003
234	2.05190	1.4033e+003

235	2.05172	1.3033e+003
236	2.05154	1.3243e+003
237	2.05135	7.6533e+002
238	2.05117	9.2233e+002
239	2.05099	1.0273e+003
240	2.05081	3.3332e+001
241	2.05062	-7.7267e+002
242	2.05044	-8.5767e+002
243	2.05026	-3.3467e+002
244	2.05008	4.9833e+002
245	2.04989	7.8633e+002
246	2.04971	3.2533e+002
247	2.04953	-1.4767e+002
248	2.04935	-5.2367e+002
249	2.04916	-5.3967e+002
250	2.04898	-1.2977e+003
251	2.04880	-1.9587e+003
252	2.04862	-1.7657e+003
253	2.04843	-1.1627e+003
254	2.04825	-9.4267e+002
255	2.04807	-3.0767e+002
256	2.04789	-1.1867e+002
257	2.04771	1.1163e+003
258	2.04752	2.1943e+003
259	2.04734	2.4463e+003
260	2.04716	2.3053e+003
261	2.04698	1.7273e+003
262	2.04680	1.3203e+003
263	2.04661	6.3933e+002
264	2.04643	4.5433e+002
265	2.04625	6.9633e+002
266	2.04607	3.6833e+002
267	2.04589	3.5733e+002
268	2.04571	-7.6667e+002
269	2.04552	-1.1297e+003
270	2.04534	-6.2467e+002
271	2.04516	-3.3667e+002
272	2.04498	-7.8767e+002
273	2.04480	-1.1457e+003
274	2.04462	-1.5737e+003
275	2.04443	-1.6637e+003
276	2.04425	-1.8917e+003
277	2.04407	-2.1237e+003
278	2.04389	-2.5387e+003

279	2.04371	-2.2997e+003
280	2.04353	-1.8927e+003
281	2.04335	-9.1767e+002
282	2.04316	6.2332e+001
283	2.04298	2.3933e+002
284	2.04280	-3.0967e+002
285	2.04262	-2.7667e+002
286	2.04244	-3.2367e+002
287	2.04226	-2.8467e+002
288	2.04208	-2.6867e+002
289	2.04190	5.5233e+002
290	2.04172	2.0113e+003
291	2.04153	3.3963e+003
292	2.04135	3.0053e+003
293	2.04117	2.9403e+003
294	2.04099	3.9423e+003
295	2.04081	4.6673e+003
296	2.04063	4.0193e+003
297	2.04045	3.6213e+003
298	2.04027	3.9603e+003
299	2.04009	4.0153e+003
300	2.03991	3.3403e+003
301	2.03973	2.6073e+003
302	2.03955	2.0143e+003
303	2.03936	9.8033e+002
304	2.03918	4.4433e+002
305	2.03900	2.0833e+002
306	2.03882	-2.8767e+002
307	2.03864	-1.4447e+003
308	2.03846	-1.4617e+003
309	2.03828	-1.1307e+003
310	2.03810	-7.7467e+002
311	2.03792	-3.6467e+002
312	2.03774	-4.1367e+002
313	2.03756	3.7133e+002
314	2.03738	1.2283e+003
315	2.03720	1.3043e+003
316	2.03702	9.6133e+002
317	2.03684	1.7413e+003
318	2.03666	2.9443e+003
319	2.03648	3.8253e+003
320	2.03630	4.1163e+003
321	2.03612	4.0113e+003
322	2.03594	3.1073e+003

323	2.03576	2.0633e+003
324	2.03558	1.2823e+003
325	2.03540	3.7433e+002
326	2.03522	-2.5567e+002
327	2.03504	-1.6267e+002
328	2.03486	2.9233e+002
329	2.03468	1.2933e+003
330	2.03450	2.2443e+003
331	2.03432	2.1913e+003
332	2.03414	7.7433e+002
333	2.03396	-5.6267e+002
334	2.03378	-1.0177e+003
335	2.03360	-7.4767e+002
336	2.03342	-2.4167e+002
337	2.03324	4.5433e+002
338	2.03306	8.7433e+002
339	2.03288	9.8033e+002
340	2.03270	7.8833e+002
341	2.03253	-9.9668e+001
342	2.03235	-7.4167e+002
343	2.03217	-1.2087e+003
344	2.03199	-1.2457e+003
345	2.03181	-6.4067e+002
346	2.03163	3.7633e+002
347	2.03145	1.2763e+003
348	2.03127	2.0263e+003
349	2.03109	1.8093e+003
350	2.03091	2.0223e+003
351	2.03073	1.5523e+003
352	2.03055	7.5633e+002
353	2.03037	4.9033e+002
354	2.03020	-2.3867e+002
355	2.03002	-9.4767e+002
356	2.02984	-8.2067e+002
357	2.02966	-7.6067e+002
358	2.02948	-1.1547e+003
359	2.02930	-1.1187e+003
360	2.02912	-1.2317e+003
361	2.02894	-1.5877e+003
362	2.02877	-3.8067e+002
363	2.02859	8.9133e+002
364	2.02841	1.7793e+003
365	2.02823	1.8353e+003
366	2.02805	2.1663e+003

367	2.02787	1.8103e+003
368	2.02769	1.6563e+003
369	2.02751	1.5543e+003
370	2.02734	7.4233e+002
371	2.02716	-1.5267e+002
372	2.02698	9.6332e+001
373	2.02680	9.5033e+002
374	2.02662	1.4303e+003
375	2.02644	2.4423e+003
376	2.02627	3.6963e+003
377	2.02609	4.8683e+003
378	2.02591	6.5993e+003
379	2.02573	9.3003e+003
380	2.02555	1.2156e+004
381	2.02538	1.5330e+004
382	2.02520	1.8321e+004
383	2.02502	2.2429e+004
384	2.02484	2.8149e+004
385	2.02466	3.5459e+004
386	2.02448	4.4739e+004
387	2.02431	5.4832e+004
388	2.02413	6.2268e+004
389	2.02395	6.4199e+004
390	2.02377	5.7790e+004
391	2.02360	4.1689e+004
392	2.02342	1.7817e+004
393	2.02324	-9.3867e+003
394	2.02306	-3.3103e+004
395	2.02288	-4.9068e+004
396	2.02271	-5.4967e+004
397	2.02253	-5.1951e+004
398	2.02235	-4.2733e+004
399	2.02217	-2.8746e+004
400	2.02200	-1.1493e+004
401	2.02182	5.6713e+003
402	2.02164	1.9697e+004
403	2.02146	2.7276e+004
404	2.02129	2.6610e+004
405	2.02111	1.8207e+004
406	2.02093	3.7973e+003
407	2.02075	-1.1640e+004
408	2.02058	-2.4740e+004
409	2.02040	-3.2229e+004
410	2.02022	-3.2552e+004

411	2.02005	-2.7214e+004
412	2.01987	-1.7798e+004
413	2.01969	-4.4677e+003
414	2.01951	1.0827e+004
415	2.01934	2.5627e+004
416	2.01916	3.6447e+004
417	2.01898	3.9148e+004
418	2.01881	3.3406e+004
419	2.01863	1.9777e+004
420	2.01845	3.4463e+003
421	2.01828	-1.1524e+004
422	2.01810	-2.1670e+004
423	2.01792	-2.6177e+004
424	2.01774	-2.5845e+004
425	2.01757	-2.1348e+004
426	2.01739	-1.4764e+004
427	2.01721	-6.8767e+003
428	2.01704	1.3493e+003
429	2.01686	1.0523e+004
430	2.01668	2.2123e+004
431	2.01651	3.9305e+004
432	2.01633	6.1667e+004
433	2.01615	8.5627e+004
434	2.01598	1.0381e+005
435	2.01580	1.0929e+005
436	2.01563	9.8006e+004
437	2.01545	6.8886e+004
438	2.01527	2.8686e+004
439	2.01510	-1.2954e+004
440	2.01492	-4.6976e+004
441	2.01474	-6.7560e+004
442	2.01457	-7.2919e+004
443	2.01439	-6.4473e+004
444	2.01422	-4.5202e+004
445	2.01404	-1.7779e+004
446	2.01386	1.2835e+004
447	2.01369	4.1867e+004
448	2.01351	6.2164e+004
449	2.01333	6.7666e+004
450	2.01316	5.5817e+004
451	2.01298	3.2149e+004
452	2.01281	4.1243e+003
453	2.01263	-1.8946e+004
454	2.01246	-3.2234e+004

455	2.01228	-3.3397e+004
456	2.01210	-2.4811e+004
457	2.01193	-8.8097e+003
458	2.01175	1.2803e+004
459	2.01158	3.6545e+004
460	2.01140	5.6170e+004
461	2.01122	6.7695e+004
462	2.01105	6.6445e+004
463	2.01087	5.1170e+004
464	2.01070	2.4057e+004
465	2.01052	-8.8637e+003
466	2.01035	-4.0339e+004
467	2.01017	-6.4514e+004
468	2.01000	-7.6804e+004
469	2.00982	-7.6904e+004
470	2.00965	-6.7266e+004
471	2.00947	-5.1791e+004
472	2.00929	-3.5639e+004
473	2.00912	-1.9979e+004
474	2.00894	-4.7217e+003
475	2.00877	1.1399e+004
476	2.00859	2.9869e+004
477	2.00842	5.1575e+004
478	2.00824	7.4868e+004
479	2.00807	9.3974e+004
480	2.00789	1.0272e+005
481	2.00772	9.7683e+004
482	2.00754	7.8549e+004
483	2.00737	4.9321e+004
484	2.00719	1.6479e+004
485	2.00702	-1.2657e+004
486	2.00684	-3.2965e+004
487	2.00667	-4.3086e+004
488	2.00649	-4.2516e+004
489	2.00632	-3.3683e+004
490	2.00614	-1.6839e+004
491	2.00597	5.9723e+003
492	2.00579	2.8781e+004
493	2.00562	4.4584e+004
494	2.00545	4.7346e+004
495	2.00527	3.4229e+004
496	2.00510	8.8543e+003
497	2.00492	-1.9025e+004
498	2.00475	-4.3200e+004

499	2.00457	-5.9470e+004
500	2.00440	-6.4460e+004
501	2.00422	-5.8906e+004
502	2.00405	-4.3273e+004
503	2.00387	-1.7691e+004
504	2.00370	1.3531e+004
505	2.00353	4.3123e+004
506	2.00335	6.4039e+004
507	2.00318	7.0042e+004
508	2.00300	5.7549e+004
509	2.00283	2.8649e+004
510	2.00266	-1.0203e+004
511	2.00248	-4.9420e+004
512	2.00231	-7.9994e+004
513	2.00213	-9.7271e+004
514	2.00196	-1.0063e+005
515	2.00178	-9.3197e+004
516	2.00161	-8.0962e+004
517	2.00144	-6.6953e+004
518	2.00126	-5.3067e+004
519	2.00109	-4.1392e+004
520	2.00092	-3.0974e+004
521	2.00074	-2.0065e+004
522	2.00057	-7.3997e+003
523	2.00039	5.2423e+003
524	2.00022	1.6024e+004
525	2.00005	2.2726e+004
526	1.99987	2.2174e+004
527	1.99970	1.4384e+004
528	1.99953	8.9133e+002
529	1.99935	-1.4249e+004
530	1.99918	-2.7696e+004
531	1.99900	-3.5691e+004
532	1.99883	-3.7868e+004
533	1.99866	-3.4979e+004
534	1.99848	-2.7057e+004
535	1.99831	-1.4884e+004
536	1.99814	-9.4767e+002
537	1.99796	1.2533e+004
538	1.99779	2.2955e+004
539	1.99762	2.7400e+004
540	1.99744	2.4748e+004
541	1.99727	1.4794e+004
542	1.99710	7.1533e+002

543	1.99692	-1.3411e+004
544	1.99675	-2.3376e+004
545	1.99658	-2.8356e+004
546	1.99641	-2.6902e+004
547	1.99623	-1.9062e+004
548	1.99606	-6.0517e+003
549	1.99589	9.1563e+003
550	1.99571	2.6392e+004
551	1.99554	4.2414e+004
552	1.99537	5.2780e+004
553	1.99519	5.4129e+004
554	1.99502	4.4602e+004
555	1.99485	2.6405e+004
556	1.99468	4.3133e+003
557	1.99450	-1.7060e+004
558	1.99433	-3.4540e+004
559	1.99416	-4.6007e+004
560	1.99399	-5.0580e+004
561	1.99381	-4.9504e+004
562	1.99364	-4.5733e+004
563	1.99347	-4.0566e+004
564	1.99330	-3.4962e+004
565	1.99312	-3.0433e+004
566	1.99295	-2.6390e+004
567	1.99278	-2.2113e+004
568	1.99261	-1.8261e+004
569	1.99243	-1.4876e+004
570	1.99226	-1.2771e+004
571	1.99209	-1.1948e+004
572	1.99192	-1.0450e+004
573	1.99174	-8.5637e+003
574	1.99157	-7.2247e+003
575	1.99140	-6.3487e+003
576	1.99123	-5.7447e+003
577	1.99105	-4.1967e+003
578	1.99088	-3.2897e+003
579	1.99071	-3.4167e+003
580	1.99054	-3.3537e+003
581	1.99037	-3.1917e+003
582	1.99019	-2.6137e+003
583	1.99002	-1.8837e+003
584	1.98985	-1.3977e+003
585	1.98968	-9.6167e+002
586	1.98951	-1.2477e+003

587	1.98933	-1.5917e+003
588	1.98916	-1.4007e+003
589	1.98899	-5.9067e+002
590	1.98882	2.3320e+000
591	1.98865	4.1833e+002
592	1.98848	-5.5668e+001
593	1.98830	-2.5567e+002
594	1.98813	-7.3867e+002
595	1.98796	-1.7557e+003
596	1.98779	-2.7307e+003
597	1.98762	-3.1497e+003
598	1.98745	-2.4637e+003
599	1.98727	-1.2927e+003
600	1.98710	-8.2667e+002
601	1.98693	-3.0967e+002
602	1.98676	-7.3967e+002
603	1.98659	-1.5817e+003
604	1.98642	-2.4717e+003
605	1.98625	-3.4717e+003
606	1.98608	-3.1077e+003
607	1.98590	-2.3707e+003
608	1.98573	-2.0667e+003
609	1.98556	-1.8857e+003
610	1.98539	-2.2107e+003
611	1.98522	-2.9377e+003
612	1.98505	-2.4597e+003
613	1.98488	-1.8857e+003
614	1.98471	-1.3917e+003
615	1.98453	-8.0167e+002
616	1.98436	-1.7567e+002
617	1.98419	3.2033e+002
618	1.98402	3.8033e+002
619	1.98385	2.4233e+002
620	1.98368	-4.4867e+002
621	1.98351	-7.3367e+002
622	1.98334	-2.9967e+002
623	1.98317	1.1133e+002
624	1.98300	-2.8668e+001
625	1.98283	-7.8967e+002
626	1.98266	-1.1757e+003
627	1.98248	-1.0957e+003
628	1.98231	-1.2587e+003
629	1.98214	-8.9567e+002
630	1.98197	-7.8767e+002

631	1.98180	-1.0257e+003
632	1.98163	-1.5877e+003
633	1.98146	-8.5467e+002
634	1.98129	-2.6967e+002
635	1.98112	-3.9367e+002
636	1.98095	-3.1667e+002
637	1.98078	-3.8567e+002
638	1.98061	-5.8067e+002
639	1.98044	-6.4967e+002
640	1.98027	2.7033e+002
641	1.98010	3.5533e+002
642	1.97993	-5.8668e+001
643	1.97976	-6.0567e+002
644	1.97959	-7.2667e+002
645	1.97942	-1.1337e+003
646	1.97925	-1.3147e+003
647	1.97908	-9.7867e+002
648	1.97891	-1.4197e+003
649	1.97874	-2.0617e+003
650	1.97857	-2.7077e+003
651	1.97840	-3.7687e+003
652	1.97823	-4.5597e+003
653	1.97806	-4.7547e+003
654	1.97789	-4.9957e+003
655	1.97772	-4.2217e+003
656	1.97755	-3.2717e+003
657	1.97738	-2.4107e+003
658	1.97721	-1.7627e+003
659	1.97704	-9.6867e+002
660	1.97687	-7.2967e+002
661	1.97670	-7.2167e+002
662	1.97653	-8.3467e+002
663	1.97636	-8.9967e+002
664	1.97619	-1.0377e+003
665	1.97602	-9.9167e+002
666	1.97585	-6.6667e+002
667	1.97568	-4.0267e+002
668	1.97551	-1.0837e+003
669	1.97534	-8.0767e+002
670	1.97517	-9.8867e+002
671	1.97500	-8.2567e+002
672	1.97483	-5.8167e+002
673	1.97467	-4.6867e+002
674	1.97450	-2.3667e+002

675	1.97433	-2.9668e+001
676	1.97416	6.4533e+002
677	1.97399	1.4563e+003
678	1.97382	1.2903e+003
679	1.97365	8.3633e+002
680	1.97348	1.5313e+003
681	1.97331	2.4713e+003
682	1.97314	3.2143e+003
683	1.97297	3.1343e+003
684	1.97280	2.4253e+003
685	1.97264	2.3263e+003
686	1.97247	2.5093e+003
687	1.97230	2.4553e+003
688	1.97213	2.0283e+003
689	1.97196	1.9903e+003
690	1.97179	1.9173e+003
691	1.97162	2.0813e+003
692	1.97145	1.9723e+003
693	1.97129	1.4143e+003
694	1.97112	1.4473e+003
695	1.97095	1.5663e+003
696	1.97078	6.7833e+002
697	1.97061	4.0533e+002
698	1.97044	5.0133e+002
699	1.97027	4.9833e+002
700	1.97010	-2.9667e+002
701	1.96994	-7.8667e+002
702	1.96977	-7.0367e+002
703	1.96960	-5.8367e+002
704	1.96943	-6.4867e+002
705	1.96926	-3.8367e+002
706	1.96909	-3.0367e+002
707	1.96893	-5.2567e+002
708	1.96876	-4.3267e+002
709	1.96859	-5.6067e+002
710	1.96842	-6.7467e+002
711	1.96825	-9.9867e+002
712	1.96808	-1.0707e+003
713	1.96792	-1.1847e+003
714	1.96775	-8.9667e+002
715	1.96758	5.4332e+001
716	1.96741	5.3833e+002
717	1.96724	-4.6867e+002
718	1.96708	-9.7467e+002

719	1.96691	-1.3997e+003
720	1.96674	-1.4717e+003
721	1.96657	-2.1937e+003
722	1.96640	-2.1107e+003
723	1.96624	-1.5297e+003
724	1.96607	-1.4697e+003
725	1.96590	-1.7187e+003
726	1.96573	-2.3967e+003
727	1.96556	-2.7357e+003
728	1.96540	-2.8767e+003
729	1.96523	-2.0087e+003
730	1.96506	-9.4167e+002
731	1.96489	5.4133e+002
732	1.96473	8.0633e+002
733	1.96456	6.8433e+002
734	1.96439	4.8333e+002
735	1.96422	4.3933e+002
736	1.96406	6.6733e+002
737	1.96389	5.6133e+002
738	1.96372	-1.4668e+001
739	1.96355	-9.0967e+002
740	1.96339	-1.3407e+003
741	1.96322	-2.1587e+003
742	1.96305	-2.7277e+003
743	1.96288	-2.2417e+003
744	1.96272	-1.0137e+003
745	1.96255	6.0533e+002
746	1.96238	1.2853e+003
747	1.96222	1.2553e+003
748	1.96205	6.8533e+002
749	1.96188	-1.5467e+002
750	1.96171	-2.6367e+002
751	1.96155	1.2233e+002
752	1.96138	9.3332e+001
753	1.96121	-2.3668e+001
754	1.96105	3.9332e+001
755	1.96088	-6.5667e+002
756	1.96071	-1.3567e+003
757	1.96054	-9.9467e+002
758	1.96038	2.4133e+002
759	1.96021	7.0233e+002
760	1.96004	7.8533e+002
761	1.95988	-6.3668e+001
762	1.95971	-1.2737e+003

763	1.95954	-1.7467e+003
764	1.95938	-1.6077e+003
765	1.95921	-1.5197e+003
766	1.95904	-8.7367e+002
767	1.95888	-6.2667e+002
768	1.95871	-8.3767e+002
769	1.95854	-1.1937e+003
770	1.95838	-1.1197e+003
771	1.95821	-8.8067e+002
772	1.95804	-6.8667e+002
773	1.95788	-7.3967e+002
774	1.95771	-1.3407e+003
775	1.95755	-1.2917e+003
776	1.95738	-1.1157e+003
777	1.95721	-5.2767e+002
778	1.95705	-7.0667e+002
779	1.95688	-3.1967e+002
780	1.95671	-3.0967e+002
781	1.95655	-9.0067e+002
782	1.95638	-1.1977e+003
783	1.95622	-8.1467e+002
784	1.95605	-1.7367e+002
785	1.95588	-3.1668e+001
786	1.95572	5.2433e+002
787	1.95555	1.6263e+003
788	1.95538	1.7873e+003
789	1.95522	1.3993e+003
790	1.95505	8.1733e+002
791	1.95489	3.8233e+002
792	1.95472	-1.9267e+002
793	1.95455	-3.1668e+001
794	1.95439	2.3733e+002
795	1.95422	7.5533e+002
796	1.95406	7.5433e+002
797	1.95389	5.2332e+001
798	1.95373	-5.2867e+002
799	1.95356	-4.9667e+002
800	1.95339	-3.9668e+001
801	1.95323	-5.5667e+002
802	1.95306	-1.3007e+003
803	1.95290	-1.5177e+003
804	1.95273	-1.5077e+003
805	1.95257	-1.2527e+003
806	1.95240	-1.0807e+003

807	1.95224	-3.5367e+002
808	1.95207	-4.8467e+002
809	1.95190	-5.2467e+002
810	1.95174	-7.8267e+002
811	1.95157	-5.0167e+002
812	1.95141	-6.8668e+001
813	1.95124	-4.5567e+002
814	1.95108	-1.0747e+003
815	1.95091	-9.0967e+002
816	1.95075	2.1433e+002
817	1.95058	8.5033e+002
818	1.95042	5.9033e+002
819	1.95025	-1.9668e+001
820	1.95009	4.3533e+002
821	1.94992	8.1033e+002
822	1.94976	7.3333e+002
823	1.94959	1.3783e+003
824	1.94943	1.4333e+003
825	1.94926	6.2333e+002
826	1.94910	1.8233e+002
827	1.94893	3.8833e+002
828	1.94877	3.5833e+002
829	1.94860	2.9633e+002
830	1.94844	8.7733e+002
831	1.94827	1.1923e+003
832	1.94811	8.1333e+002
833	1.94794	6.2333e+002
834	1.94778	1.0793e+003
835	1.94761	1.7623e+003
836	1.94745	8.6533e+002
837	1.94728	1.0233e+002
838	1.94712	-1.6367e+002
839	1.94695	-2.9668e+001
840	1.94679	-2.0867e+002
841	1.94662	1.9633e+002
842	1.94646	1.7423e+003
843	1.94630	3.1083e+003
844	1.94613	3.5983e+003
845	1.94597	3.2573e+003
846	1.94580	2.1623e+003
847	1.94564	8.4833e+002
848	1.94547	-6.2668e+001
849	1.94531	-1.1367e+003
850	1.94514	-1.5897e+003

851	1.94498	-2.2247e+003
852	1.94482	-1.9347e+003
853	1.94465	-1.8217e+003
854	1.94449	-2.2517e+003
855	1.94432	-2.4737e+003
856	1.94416	-2.7367e+003
857	1.94400	-3.1247e+003
858	1.94383	-2.8917e+003
859	1.94367	-2.9867e+003
860	1.94350	-2.6197e+003
861	1.94334	-2.1047e+003
862	1.94318	-1.3797e+003
863	1.94301	-5.0867e+002
864	1.94285	-8.6680e+000
865	1.94268	7.4933e+002
866	1.94252	2.4833e+002
867	1.94236	-2.1667e+002
868	1.94219	-4.7668e+001
869	1.94203	-1.9567e+002
870	1.94186	3.8933e+002
871	1.94170	6.2633e+002
872	1.94154	9.4233e+002
873	1.94137	5.3033e+002
874	1.94121	-6.2667e+002
875	1.94105	-1.0007e+003
876	1.94088	-2.2667e+002
877	1.94072	3.3233e+002
878	1.94056	2.8233e+002
879	1.94039	3.0433e+002
880	1.94023	2.9933e+002
881	1.94007	6.9133e+002
882	1.93990	8.0533e+002
883	1.93974	7.7333e+002
884	1.93958	1.3813e+003
885	1.93941	1.7493e+003
886	1.93925	1.2453e+003
887	1.93909	2.7332e+001
888	1.93892	-6.5167e+002
889	1.93876	-4.3668e+001
890	1.93860	6.8333e+002
891	1.93843	8.6333e+002
892	1.93827	1.4143e+003
893	1.93811	3.3133e+003
894	1.93794	4.1953e+003

895	1.93778	4.1903e+003
896	1.93762	3.5923e+003
897	1.93745	2.8353e+003
898	1.93729	2.4683e+003
899	1.93713	2.2363e+003
900	1.93696	2.0373e+003
901	1.93680	1.9583e+003
902	1.93664	1.7463e+003
903	1.93648	4.9833e+002
904	1.93631	-4.3367e+002
905	1.93615	-8.6567e+002
906	1.93599	-1.0017e+003
907	1.93583	-1.0327e+003
908	1.93566	-8.4067e+002
909	1.93550	-1.1547e+003
910	1.93534	-1.0877e+003
911	1.93517	-7.0067e+002
912	1.93501	-5.3867e+002
913	1.93485	-4.2967e+002
914	1.93469	3.5433e+002
915	1.93452	1.8933e+002
916	1.93436	6.9733e+002
917	1.93420	9.4133e+002
918	1.93404	1.2333e+003
919	1.93387	1.5553e+003
920	1.93371	1.1733e+003
921	1.93355	6.7133e+002
922	1.93339	9.8733e+002
923	1.93323	1.9383e+003
924	1.93306	2.7433e+003
925	1.93290	2.5053e+003
926	1.93274	2.4863e+003
927	1.93258	2.5793e+003
928	1.93241	1.7103e+003
929	1.93225	1.8323e+003
930	1.93209	1.9193e+003
931	1.93193	1.4933e+003
932	1.93177	1.3033e+003
933	1.93160	1.2153e+003
934	1.93144	3.4333e+002
935	1.93128	-8.0467e+002
936	1.93112	-2.2607e+003
937	1.93096	-3.0437e+003
938	1.93079	-2.9477e+003

939	1.93063	-2.4227e+003
940	1.93047	-1.5487e+003
941	1.93031	-1.3167e+003
942	1.93015	-8.4167e+002
943	1.92999	4.9332e+001
944	1.92982	5.1733e+002
945	1.92966	4.1933e+002
946	1.92950	5.0933e+002
947	1.92934	6.2033e+002
948	1.92918	4.6733e+002
949	1.92902	6.0533e+002
950	1.92885	1.4733e+002
951	1.92869	-5.5167e+002
952	1.92853	-5.2067e+002
953	1.92837	-4.6867e+002
954	1.92821	-5.3167e+002
955	1.92805	-7.0267e+002
956	1.92788	-8.1267e+002
957	1.92772	-1.1527e+003
958	1.92756	-1.3117e+003
959	1.92740	-1.4247e+003
960	1.92724	-7.9967e+002
961	1.92708	-9.9668e+001
962	1.92692	6.2333e+002
963	1.92676	1.1443e+003
964	1.92659	1.5733e+003
965	1.92643	2.5603e+003
966	1.92627	3.0413e+003
967	1.92611	2.6473e+003
968	1.92595	2.2803e+003
969	1.92579	3.2933e+002
970	1.92563	-1.6687e+003
971	1.92547	-2.6997e+003
972	1.92531	-3.4987e+003
973	1.92515	-2.7017e+003
974	1.92498	-2.4677e+003
975	1.92482	-2.7427e+003
976	1.92466	-2.4587e+003
977	1.92450	-1.5847e+003
978	1.92434	-1.1477e+003
979	1.92418	-8.4667e+002
980	1.92402	7.1332e+001
981	1.92386	3.4933e+002
982	1.92370	5.0133e+002

983	1.92354	4.3033e+002
984	1.92338	1.3332e+001
985	1.92322	-2.7367e+002
986	1.92306	-5.3167e+002
987	1.92289	-1.0587e+003
988	1.92273	-1.2057e+003
989	1.92257	-1.1977e+003
990	1.92241	-1.1837e+003
991	1.92225	-1.8477e+003
992	1.92209	-2.2917e+003
993	1.92193	-2.2717e+003
994	1.92177	-1.2357e+003
995	1.92161	-2.5967e+002
996	1.92145	6.7433e+002
997	1.92129	1.5253e+003
998	1.92113	2.0313e+003
999	1.92097	1.6033e+003
1000	1.92081	1.0303e+003
1001	1.92065	-3.3867e+002
1002	1.92049	-1.9247e+003
1003	1.92033	-2.8357e+003
1004	1.92017	-2.4797e+003
1005	1.92001	-2.3557e+003
1006	1.91985	-2.9437e+003
1007	1.91969	-3.4477e+003
1008	1.91953	-2.8717e+003
1009	1.91937	-2.2657e+003
1010	1.91921	-1.7287e+003
1011	1.91905	-1.4407e+003
1012	1.91889	-1.2707e+003
1013	1.91873	-7.5967e+002
1014	1.91857	-5.4267e+002
1015	1.91841	-2.5767e+002
1016	1.91825	4.4033e+002
1017	1.91809	1.1033e+003
1018	1.91793	1.1933e+003
1019	1.91777	3.5333e+002
1020	1.91761	-7.4567e+002
1021	1.91745	-6.9667e+002
1022	1.91729	1.0833e+002
1023	1.91713	2.4133e+002