Supporting Information for:

Macrocyclic Complexes Based on [N···I···N]⁺ Halogen Bond

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1. General Experimental Section

All reagents and solvents were purchased from commercial suppliers and used without further purification. Ligands L1-L3 and iodonium complex bis(1-methyl-1H-1,2,3-triazole)iodine(I) hexafluorophosphate ([I(mtz)₂]PF₆) were prepared according to literature procedures.^{1–4} ¹H and ¹³C NMR spectra, and the ¹H-¹⁵N NMR correlation were recorded at 298 K on a Bruker Avance III 500 MHz instrument in CD₂Cl₂. Signals in the ¹H-NMR spectra of the complexes were assigned with the aid of two-dimensional NMR experiments (COSY HMQC and ¹H-¹⁵N HMBC). Chemical shifts are reported on the δ scale in ppm using the residual solvent signal as internal standard, or for ¹H-¹⁵N NMR spectroscopy, to an external d_3 -MeNO₂ standard. Abbreviations of coupling patterns are as follows: br, broad; s, singlet; d, doublet; t, triplet; m, multiplet. Coupling constants (*J*) are expressed in Hz.

2. Synthetic and Spectroscopic Data

Synthesis of complex 1



To a solution of $[I(mtz)_2]PF_6$ (21.4 mg, 0.049 mmol, 1.0 eq.) in dichloromethane (2 mL), a solution of L1 (13.7 mg, 0.049mmol, 1 eq.) in dichloromethane (1 mL) was added. The reaction mixture was stirred for 5 mins and a white solid was precipitated from the colorless solution, which was filtered and washed with Et₂O. The product was dried under reduced pressure to obtain complex 1 (21.4 mg, 79.0%). ¹H NMR (500 MHz, CD₃CN): δ 8.81 (s, 4H, *H*_A), 8.51 (d, *J* = 5.5 Hz, 4H, *H*_B), 8.15 (d, *J* = 8.4 Hz, 4H, *H*_D), 7.73 (s, 2H, *H*_E), 7.58-7.47 (m, 8H, *H*_C and *H*_F), 7.43 (t, *J* = 7.6 Hz, 2H, *H*_G); ¹³C NMR (125 MHz, CD₃CN): δ 150.8, 148.3, 143.6, 134.3, 132.9, 129.3, 127.3, 123.3, 121.6, 94.1, 53.4; ¹H-¹⁵N HMBC NMR (500 MHz, CD₃CN): δ -173.3; ¹H 2D DOSY NMR (500 MHz, CD₃CN) of complex 1: Recorded diffusion coefficient for assigned peaks 1.33e⁻⁹ m²s⁻¹, Calculated hydrodynamic radius 4.9 Å; HRMS (ESI+) calcd for C₄₀H₂₄F₆I₂N₄P [M – PF₆]⁺ 958.9732, found 958.9719.





Figure S2. The ¹H-¹⁵N-HMBC spectrum of L1 (CD₃CN, 500 MHz, 25 °C).





Figure S6. The ¹³C NMR spectrum of complex 1 (CD₃CN, 125 MHz, 25 °C).



Figure S7. The stacked ¹H-¹⁵N-HMBC spectra of complex 1 (red) and ligand L1 (green) (CD₃CN, 500 MHz, 25 °C).



25 °C).

Synthesis of complex 2



To a solution of $[I(mtz)_2]PF_6$ (22.4 mg, 0.051 mmol, 1.0 eq.) in dichloromethane (2 mL), a solution of L2 (15.9 mg, 0.051 mmol, 1 eq.) in dichloromethane (1 mL) was added. The reaction mixture was stirred for 5 mins and a white solid was precipitated from the colorless solution, which was filtered and washed with Et₂O. The product was dried under reduced pressure to obtain complex 2 (25.9 mg, 87%). ¹H NMR (500 MHz, CD₃CN): δ 7.87 (s, 4H, H_A), 7.31 (s, 4H, H_B or H_C), 7.19 (s, 4H, H_C or H_B), 5.39 (s, 4H, H_D); ¹³C NMR (125 MHz, CD₃CN): δ 144.8 (CF), 138.2, 127.4, 122.8, 114.5, 39.2; ¹H-¹⁵N HMBC NMR (500 MHz, CD₃CN): δ -216.1 (N_E), -204.5 (N_F); ¹H 2D DOSY NMR (500 MHz, CD₃CN) of complex 2: Recorded diffusion coefficient for assigned peaks 1.33e⁻⁹ m²s⁻¹, Calculated hydrodynamic radius 4.9 Å; HRMS (ESI+) calcd for C₂₈H₂₀F₁₄I₂N₈P [M – PF₆]⁺ 1018.9403, found 1018.9424.





Figure S10. The 1 H- 15 N-HMBC spectrum of L2 (CD₃CN, 500 MHz, 25 °C).







Figure S14. The stacked ¹H-¹⁵N-HMBC spectra of complex 2 and ligand L2 (CD₃CN, 500 MHz, 25 °C).



Figure S15. The stacked ¹H DOSY spectra of complex **2** (blue) and ligand L**2** (green) (CD₃CN, 500 MHz, 25 °C).



Figure S16. Selected ¹H NMR spectra (500 MHz, CD₃CN, 25 °C) of pure $[I(mtz)_2]PF_6$ (a) and $[I(mtz)_2]PF_6$ in the presence of 0.2 (b), 0.4 (c), 0.6 (d), 0.8 (e) and 1.0 (f) equivalents of **L2** and 1-methyl-1H-1,2,3-triazole (g), showing the self-assembly of macrocycle **2** from the ligand exchange between **L2** and iodine(I) complex $[I(mtz)_2]PF_6$.

Synthesis of complex 3



To a solution of $[I(mtz)_2]PF_6$ (12.7 mg, 0.029 mmol, 1.0 eq.) in dichloromethane (2 mL), a solution of L3 (7.7 mg, 0.029 mmol, 1 eq.) in dichloromethane (1 mL) was added. The reaction mixture was stirred for 5 mins and a white solid was precipitated from the colorless solution, which was filtered and washed with Et₂O.

¹**H 2D DOSY NMR** (500 MHz, CD₃CN) of reaction **3**: Recorded diffusion coefficient for assigned peaks 1.78e⁻⁹ and 1.93e⁻⁹ m²s⁻¹, Calculated hydrodynamic radius 3.7 and 3.4 Å;

HRMS (ESI+) calcd for $C_{32}H_{36}F_6I_2N_8P [M - PF_6]^+$ 931.0794, found 931.0797.





Figure S18. The 1 H- 15 N-HMBC spectrum of L3 (CD₃CN, 500 MHz, 25 °C).



Figure S19. The ¹H DOSY spectrum of L3 (CD₃CN, 500 MHz, 25 °C).





Figure S21. The ¹H-¹⁵N-HMBC spectrum of reaction 3 (CD₃CN, 500 MHz, 25 °C).



Figure S22. The stacked ¹H 2D DOSY spectra of reaction **3** (blue) and ligand L**3** (green) (CD₃CN, 500 MHz, 25 °C).

Synthesis of [I(1-methylimidazole)₂]PF₆



To a solution of silver hexafluorophosphate (5.7 mg, 0.023 mmol, 1.0 eq) in CD₂Cl₂ (1.0 mL), a solution of 1-methylimidazole (3.7 mg, 0.045 mmol, 2.0 eq) in CD₂Cl₂ (0.8 mL) was added. After the solution was stirred for 3 mins at room temperature, the elementary I₂ (5.7 mg, 0.023 mmol, 1.0 eq) in CD₂Cl₂ (0.2 mL) was added. The mixture was centrifuged for 5 mins and was filtered, then the solution of [I(1-methylimidazole)₂]PF₆ (96%, determined by ¹H NMR integration of the crude reaction mixture) was stored in an 4 mL vial in fridge. ¹H NMR (500 MHz, CD₂Cl₂): δ 7.87 (s, 2H, *H*_F), 7.15 (s, 2H, *H*_D), 6.97 (s, 2H, *H*_C), 3.83 (s, 6H, *H*_A); ¹³C NMR (125 MHz, CD₂Cl₂): δ 138.6, 128.2, 122.7, 35.0; ¹H-¹⁵N HMBC NMR (500 MHz, CD₂Cl₂): δ 7.40 (s, 1H, *H*_F), 6.98 (s, 1H, *H*_C), 6.91 (s, 1H, *H*_D), 3.68 (s, 3H, *H*_A); ¹H-¹⁵N HMBC NMR (500 MHz, CD₃CN): δ -221.3 (*N*_B), -122.7 (*N*_E).





Figure S24. The ¹³C NMR spectrum of [I(1-methylimidazole)₂]PF₆ (CD₂Cl₂, 125 MHz, 25 °C).



Figure S25. The ¹H-¹⁵N-HMBC spectrum of [I(1-methylimidazole)₂]PF₆ (CD₂Cl₂, 500 MHz, 25 °C).



Figure S26. ¹H NMR spectrum of 1-methylimidazole (CD₂Cl₂, 500 MHz, 25 °C).



Figure S27. The ¹H-¹⁵N-HMBC spectrum of 1-methylimidazole (CD₂Cl₂, 500 MHz, 25 °C).

Table S1. The diffusion coefficient $(m^2 \cdot s^{-1})$ and calculated dynamic radius (in parentheses) of ligands L1-L3 and complexes 1-3.

Х	1	2	3
Ligand LX	15.0 × 10 ⁻¹⁰ (4.23 Å)	17.70 × 10 ⁻¹⁰ (3.59 Å)	17.9 × 10 ⁻¹⁰ (3.55 Å)
Complex X	6.95 × 10 ⁻¹⁰ (9.13 Å)	9.25 × 10 ⁻¹⁰ (6.86 Å)	1.026 × 10 ⁻¹⁰ (6.19 Å); 8.15 × 10 ⁻¹⁰ (7.79 Å)

3. Ion Mobility Mass Spectrometry (ESI-QTOF, ESI-IMMS)

Ion mobility mass spectrometry experiments were performed with Agilent 6560 IM-QTOF-MS instrument, which was equipped with a dual ESI ion source. The samples used for analyses were dissolved in MeCN (1 mg/ml, \sim 1 mM) and then diluted in MeCN (\sim 50 μ M). Samples were injected by direct infusion with syringe pump using flow rates from 5 to 9 μ l/min.

The parameters were optimized to get maximum abundance of the ions under study. Following ion source parameters were used: Drying gas temperature 150 °C, drying gas flow 2 l/min, nebulizer pressure 20 psi, fragmentor voltage 350 V, capillary voltage of 5000 V and nozzle voltage 2000 V. Nitrogen from N_2 generator was used as drying gas. Mass spectra were externally calibrated by ESI Tuning mix (Agilent Technologies). The charge states and composition of the ions were determined by comparison of experimental and theoretical isotopic distributions, which was calculated on basis of natural abundances of elements. The compositions of the ions were finally verified by comparing experimental m/z values with the theoretical ones. MS/MS (CID) experiments were performed for isolated selected ions. N_2 (99.9999%) was used collision gas and activation (lab frame) voltage (CE) was 10V. Mass spectra was recorded and analysed using Mass Hunter B.08.00 software package (Acquisition and Qualitative Analysis).

In IM-TOF experiments, either N_2 (99.999%) or He (99.9996%) from gas cylinders were used as drift gas. When N_2 was used as a drift gas, the drift tube entrance and exit voltages were set as 1574V and 224V, respectively. As a trap filling time 5000 μ s and trap release time 350 μ s were used. For He drift gas 875 V and 224 V were used as the drift tube entrance and exit voltages. Before introduction of samples, ES tuning mix (Agilent technologies) was measured as a reference for CCS values and to ensure stabile conditions for CCS determination.¹ For stepped-field measurements, the drift tube entrance voltage was varied in N_2 measurements from 1074 V to 1674 V with 100 V increments and in He measurements from 563 V to 875 V with 52 V increments. Data was analyzed using MassHunter IM-MS Browser (Version B08.00, Agilent Technologies, USA).

Theoretical ^{TMLJ}CCS_{He} values were calculated with IMoS.² Theoretical CCS values were obtained using the trajectory method (with Lennard Jones 4-6-12 parameters) with diffuse scattering in He gas. The number of rotations was 3 with 300000 gas molecules per rotations. Calculations were carried out using experimental parameters (gas, temperature and pressure) and coordinates for calculations were obtained from DFT-calculated structures optimized at M06-2X/def2-TZVP level of theory using Gaussian 16 program (see details below, 4. Computational Studies). This theoretical method for CCS calculation and drift gas was chosen to get the best fit for experimental data. Other tested methods were project approximation, elastic/diffuse hard sphere scattering, and diatomic trajectory method. All methods were also tested using N₂ as a drift gas.



Figure S28. ESI-TOF mass spectra measured from iodine(I) complex 1 in MeCN. a) Profile mass spectrum. Inset show comparison between theoretical and experimental isotopic distributions for ion $[1-PF_6]^+$ at m/z 958.97; b) MS/MS for ion $[1-PF_6]^+$ at m/z 958.97 (isolated ion marked with asterisk).



Figure S29. ESI-TOF mass spectra measured from iodine(I) complex 2 in MeCN. a) Profile mass spectrum. Inset shows comparison between theoretical and experimental isotopic distributions for ion $[2-PF_6]^+$ at m/z 1018.94; b) MS/MS for ion $[2-PF_6]^+$ at m/z 1018.94 (isolated ion marked with asterisk).



Figure S30. ESI-TOF mass spectra measured from iodonium complex **3** in MeCN. a) Profile mass spectrum. Inset shows comparison between theoretical and experimental isotopic distributions for ion $[3-PF_6]^+$ at m/z 1018.94; b) MS/MS for ion $[3-PF_6]^+$ at m/z 931.08 (isolated ion marked with asterisk).

sample	ion	formula	Charge state	$m/z_{\rm theor}$	m/z_{exp}	absolute mass accuracy (mDa)
	$[L1+H]^{+}$	$C_{20}H_{12}N_2 + H^+$	1	281.1073	281.1079	-0.6
Complay 1	$[L1+I]^+$	$C_{20}H_{12}N_2$ +I	1	407.0040	407.0053	-1.3
Complex 1	$[1-I-(PF_6)_2]^+$	C40H24N4+I	1	687.1040	687.1039	0.1
	[1- PF ₆] ⁺	$C_{40}H_{24}N_4I_2PF_6$	1	958.9727	958.9733	-0.6
	$[L2+H]^{+}$	$C_{14}H_{10}N_4F_4{+}H^+$	1	311.0914	311.0938	-2.4
	[L2 +I] ⁺	$C_{14}H_{10}N_4F_4\!+\!I^+$	1	436.9881	436.9903	-2.2
Complex 2	[2- PF ₆] ⁺	$C_{28}H_{20}N_8F_{14}PI_2{}^+$	1	1018.9409	1018.9405	0.4
	$[2-H-(PF_6)_2]^+$	$C_{28}H_{19}N_8F_8I_2^+$	1	562.8853	562.8842	1.1
	$[L3+H]^{+}$	$C_{16}H_{18}N_4\text{+}H^+$	1	267.1604	267.1615	-1.1
Complex 3	[L3 +I] ⁺	$C_{16}H_{18}N_4\!\!+\!I^+$	1	393,0571	393,0590	-1,9
	[3- PF ₆] ⁺	$C_{32}H_{36}N_8F_6PI_2{}^+$	1	931,0789	931,0845	-5.6

Table S2. Ions observed, their formulas, charge states and comparison to theoretical values.



Figure S31. Comparison on arrival time distributions (ATD) for ions $[1-PF_6]^+$, $[2-PF_6]^+$ and $[3-PF_6]^+$. ATDs measured in N₂ drift gas and extracted ^{DT}CCS_{N2} values and drift times are indicated in figure.

sample	ion	formula	Charge state	DTCCS _{N2} (Å ²)	DTCCS _{He} (Å2)	TMLJCC (Å ² /9	CS _{He} %)	Model		
	$[L1+H]^{+}$	$C_{20}H_{12}N_2 + H^+$	1	194.8	114.9					
	$[L1+I]^+$	C20H12N2+I	1	203.9	126.2					
	$[1-I-(PF_6)_2]^+$	C40H24N4+I	1	301.5	215.7					
Commissi 1				321.3	237.8	231.8	-2.5	PF6 out		
Complex I		C40H24N4I2PF6	C40H24N4I2PF6	C40H24N4I2PF6		299	219.3	228.8	4.3	PF ₆ in
	$[1-PF_6]^+$ C ₄₀ H ₂₄ N ₄ I2PF ₆				$C_{40}H_{24}N_4I2PF_6$	1	276.7	199.1		
				259.4	196.6					
			248.1	na						
	$[L2+H]^{+}$	$C_{14}H_{10}N_4F_4+H^+$	1	170.7	97.4					
Commission 2	[L2 +I] ⁺	$C_{14}H_{10}N_4F_4+I^+$	1	179.8	104.9					
Complex 2	$[2-PF_6]^+$	$C_{28}H_{20}N_8F_{14}PI_2^+$	1	259.5	184.4	180.9	-1.9			
	$[L2-H+2I]^+$	$C_{28}H19N_8F_8I_2{}^+$	1	193.7	114					
	$[L3+H]^{+}$	$C_{16}H_{18}N_4 + H^+$	1	174.4	108.6					
Complay 3	[L3 +I] ⁺	$C_{16}H_{18}N_4\!\!+\!I^+$	1	189.7	112.1					
Complex 3	[2 DE.]+	C. H. N.E.DI. ⁺	1	250.5	102.2	185.3	1.6	3b up-down-up-down		
l	$\begin{bmatrix} 3 - \mathbf{PF6} \end{bmatrix}^{\top} \qquad \mathbf{C}_{32}\mathbf{H}_{36}\mathbf{N}_{8}\mathbf{F6}\mathbf{PI2}^{\top}$	1	238.3	182.3	184.3	1.1	3a up-up-down-down			

Table S3. Experimental DT CCS values using N₂ and He as drift gas, theoretical TMLJ CCS_{He} (trajectory method with Lennard Jones 4-6-12 potential) and their comparison.

4. Computational Studies

4.1 General

The energetic features of the adducts analyzed in this work were calculated at the M06- $2X^5$ /def2-TZVP⁶ level of theory using the crystallographic coordinates of the corresponding Ag complexes as starting points for the optimizations, replacing the Ag ions by I. For iodine, the inner shell electrons are modelled by ECPs (ECP-60 scheme),⁷ which also accounts for scalar relativistic effects. The GAUSSIAN-16 program has been used for the geometry optimizations and energetic calculations.⁸



Figure S32. Optimized geometries of compounds $[1-PF_6]^+$ (a), $[2-PF_6]^+$ (b) and $[3-PF_6]^+$ (c) at the M06-2X/def2-TZVP level of theory.

4.2 X-ray coordinates

Complex 1			
1	-5.958142	-6.083171	-0.001441
6	-5.971301	-5.001602	-0.001148
7	-5.987332	-2.256929	-0.000375
6	-4.762970	-4.298125	-0.000729
6	-7.167482	-4.307729	-0.001172
6	-7.144468	-2.925545	-0.000781
6	-4.825126	-2.906772	-0.000339
1	-8.115244	-4.826707	-0.001493
1	-8.049221	-2.332399	-0.000791
1	-3.924898	-2.306547	0.00009
6	-3.504546	-4.961775	-0.000701
6	-2.447803	-5.537922	-0.000702
6	-1.206463	-6.244648	-0.000679
6	1.200808	-7.643026	-0.000665
6	-1.201087	-7.643024	-0.001150
6	-0.000136	-5.547154	-0.000200
6	1.206189	-6.244648	-0.000190
6	-0.000139	-8.332348	-0.001142
1	-2.141010	-8.177766	-0.001523
1	-0.000135	-4.466076	0.000167
1	-0.000141	-9.413686	-0.001508
1	2.140732	-8.177768	-0.000658

6	2.447531	-5.537927	0.000326
6	3.504322	-4.961868	0.000718
6	4.762770	-4.298258	0.000875
6	7.144325	-2.925778	0.001221
6	5.971070	-5.001784	0.001325
6	4.824984	-2.906903	0.000603
7	5.987221	-2.257109	0.000778
6	7.167277	-4.307962	0.001498
1	5.957866	-6.083352	0.001536
1	3.924781	-2.306639	0.000235
1	8.115017	-4.826981	0.001851
1	8.049106	-2.332675	0.001355
1	-5.957894	6.083359	0.002214
6	-5.971106	5.001792	0.001833
7	-5.987274	2.257119	0.000865
6	-4.762810	4.298256	0.000832
6	-7.167321	4.307976	0.002335
6	-7.144377	2.925791	0.001839
6	-4.825035	2.906905	0.000361
1	-8.115058	4.827000	0.003113
1	-8.049159	2.332689	0.002207
1	-3.924838	2.306636	-0.000446
6	-3.504354	4.961846	0.000298
6	-2.447573	5.537924	-0.000122
6	-1.206220	6.244626	-0.000496
6	1.201075	7.642965	-0.001245
6	-1.200820	7.643002	-0.001066
6	0.000097	5.547112	-0.000305
6	1.206432	6.244587	-0.000676
6	0.000138	8.332307	-0.001439
1	-2.140736	8.177758	-0.001225
1	0.000079	4.466034	0.000139
1	0.000153	9.413645	-0.001880
1	2.141008	8.177691	-0.001527
6	2.447765	5.537849	-0.000456
6	3.504559	4.961792	-0.000316
6	4.762983	4.298138	-0.000500
6	/.144493	2.925580	-0.000/84
6	5.971306	5.001625	-0.001071
6	4.825151	2.906782	-0.000082
	5.98/369	2.256949	-0.000230
6	/.16/491	4.307763	-0.001211
1	5.958137	6.083193	-0.001395
1	3.924929	2.30654/	0.000391
1	8.115248	4.826/50	-0.00164/
1 5 2	8.049254	2.332446	-0.000871
<u> つ </u>	5.993619	-0.000079	0.000326
53	-5.9935/1	0.000095	0.000197

Complex 2

6	0.00000	5.603958	-1.408650
6	0.095364	5.602829	1.408390
6	-1.159654	5.614065	-0.649692
6	1.211295	5.587937	-0.733616
6	1.255015	5.595789	0.649441
6	-1.116052	5.605132	0.733349
53	0.00000	-0.000000	3.902561
6	-0.069331	5.592141	-2.913614
1	-0.771437	6.344795	-3.267138
1	0.907610	5.809419	-3.339415
6	0.164566	5.589683	2.913341
1	0.879097	6.330567	3.266841
1	-0.808604	5.823047	3.339250
7	0.605522	4.288816	3.419589
6	-0.106112	3.153439	3.372617
7	0.607007	2.159363	3.862769
6	1.823356	2.668324	4.243547
1	2.586644	2.051839	4.685109
6	1.831747	3.998744	3.966660
1	2.585980	4.753562	4.105139
7	-0.531866	4.298847	-3.419978
6	0.160171	3.151454	-3.372164
7	-0.569612	2.169584	-3.862446
6	-1.776782	2.699224	-4.244193
1	-2.550364	2.095828	-4.685933
6	-1.762541	4.029672	-3.967661

1	-2.503670	4.797283	-4.106601	
6	-0.095364	-5.602829	1.408390	
6	-0.000000	-5.603958	-1.408650	
6	-1.255015	-5.595789	0.649441	
6	1.116052	-5.605132	0.733349	
6	1.159654	-5.614065	-0.649692	
6	-1.211295	-5.587937	-0.733616	
53	-0.00000	0.000000	-3.901803	
6	-0.164566	-5.589683	2.913341	
1	-0.879097	-6.330567	3.266841	
1	0.808604	-5.823047	3.339250	
6	0.069331	-5.592141	-2.913614	
1	0.771437	-6.344795	-3.267138	
1	-0.907610	-5.809419	-3.339415	
7	0.531866	-4.298847	-3.419978	
6	-0.160171	-3.151454	-3.372164	
7	0.569612	-2.169584	-3.862446	
6	1.776782	-2.699224	-4.244193	
1	2.550364	-2.095828	-4.685933	
6	1.762541	-4.029672	-3.967661	
1	2.503670	-4.797283	-4.106601	
7	-0.605522	-4.288816	3.419589	
6	0.106112	-3.153439	3.372617	
7	-0.607007	-2.159363	3.862769	
6	-1.823356	-2.668324	4.243547	
1	-2.586644	-2.051839	4.685109	
6	-1.831747	-3.998744	3.966660	
1	-2.585980	-4.753562	4.105139	
9	2.431799	5.585192	1.266000	
9	2.349785	5.554685	-1.417244	
9	-2.254876	5.588647	1.417048	
9	-2.336444	5.621207	-1.266302	
9	-2.431799	-5.585192	1.266000	
9	-2.349785	-5.554685	-1.417244	
9	2.336444	-5.621207	-1.266302	
9	2.254876	-5.588647	1.417048	
1	1.164505	3.065475	-2.988644	
1	-1.164505	-3.065475	-2.988644	
1	-1.112007	3.084664	2.989699	
T	1.112007	-3.084664	2.989699	
Complex 3	Ba			

6	1.344686	-0.378593	5.529437
6	-1.344686	0.378593	5.529437
6	0.992786	0.966664	5.533831
6	0.342031	-1.341831	5.535690
6	-0.992786	-0.966664	5.533831
6	-0.342031	1.341831	5.535690
1	1.763950	1.728657	5.537024
1	0.603485	-2.393558	5.546436
1	-0.603485	2.393558	5.546436
53	-4.025520	0.000083	-0.00008
1	-1.763950	-1.728657	5.537024
6	2.800578	-0.782067	5.514479
1	3.326592	-0.376742	6.378252
1	2.901327	-1.866740	5.548487
6	-2.800578	0.782067	5.514479
1	-3.326592	0.376742	6.378252
1	-2.901327	1.866740	5.548487
7	-3.494774	0.280104	4.328197
6	-3.260534	0.673598	3.062082
7	-4.017221	-0.044106	2.243969
6	-4.756131	-0.919856	3.002464
1	-5.458391	-1.604530	2.560111
6	-4.434942	-0.724280	4.305090
1	-4.794623	-1.188548	5.206655
7	3.494774	-0.280104	4.328197
6	3.260534	-0.673598	3.062082
7	4.017221	0.044106	2.243969
6	4.756131	0.919856	3.002464
1	5.458391	1.604530	2.560111
6	4.434942	0.724280	4.305090
1	4.794623	1.188548	5.206655
6	-1.344747	-0.378382	-5.529350
6	1.344747	0.378382	-5.529350
6	-0.992638	0.966820	-5.533705

6	-0 342241	_1 3/1777	_5 535505
0	0.042241	1.341///	5.555505
6	0.992638	-0.966820	-5.533705
6	0.342241	1.341777	-5.535585
1	-1 763680	1 728936	-5 536920
1	1.705000	1.720550	5.550520
1	-0.603852	-2.393465	-5.546353
1	0.603852	2.393465	-5.546353
E 2	4 025520	0 000002	0 000000
55	4.025520	-0.000083	-0.000008
1	1.763680	-1.728936	-5.536920
6	-2.800699	-0.781631	-5.514518
1	2 226570	0 276140	C 270200
1	-3.326579	-0.3/6149	-6.3/8299
1	-2.901596	-1.866285	-5.548660
6	2.800699	0.781631	-5.514518
1	2 226570	0.27(140	C 270200
1	3.320379	0.3/0149	-0.3/0299
1	2.901596	1.866285	-5.548660
7	3.494915	0.279684	-4.328229
, C	2 200000	0 (72212	2 0 0 2 1 2 0
6	3.260866	0.6/3313	-3.062120
7	4.017571	-0.044396	-2.244018
6	4 756245	-0 920337	-3 002509
1	1.730213	1 00001	0.002000
1	5.458485	-1.605041	-2.560172
6	4.434942	-0.724832	-4.305122
1	4 794472	-1 189226	-5 206681
-	1./911/2	1.109220	1.200001
/	-3.494915	-0.2/9684	-4.328229
6	-3.260866	-0.673313	-3.062120
7	-4.017571	0.044396	-2.244018
ć	1.01/1/1	0.000000	2.211010
ю	-4./56245	0.920337	-3.002509
1	-5.458485	1.605041	-2.560172
6	-4 13/0/0	0 70/000	-4 305100
1	1.404942	1 100000	T.JUJIZZ
Ţ	-4.794472	1.189226	-5.206681
6	2.298996	1.736515	-2.678246
1	2 301000	2 503110	-3 3/7100
1	2.304990	2.393110	-3.34/100
1	2.502699	2.068559	-1.663508
1	1,272636	1.369042	-2.733293
6	2 200006	1 726515	2 670246
0	-2.290990	-1./30313	-2.0/0240
1	-1.272636	-1.369042	-2.733293
1	-2.384998	-2.593110	-3.347108
1	2 502500	2.000110	1 (()=00
1	-2.302899	-2.000559	-1.003300
6	-2.298519	1.736685	2.678253
1	-2.501521	2.068069	1,663162
=	1 070156	1 200200	0 704000
1			/ / 34 30 3
1	-1.2/2156	1.309300	2.751505
1 1	-2.385135	2.593692	3.346517
1 1 6	-1.2/2156 -2.385135 2 298519	2.593692	3.346517
1 1 6	-1.2/2156 -2.385135 2.298519	2.593692	3.346517 2.678253
1 1 6 1	-1.272156 -2.385135 2.298519 1.272156	2.593692 -1.736685 -1.369380	3.346517 2.678253 2.734303
1 1 6 1 1	-1.272156 -2.385135 2.298519 1.272156 2.385135	2.593692 -1.736685 -1.369380 -2.593692	3.346517 2.678253 2.734303 3.346517
1 1 6 1 1	-1.272156 -2.385135 2.298519 1.272156 2.385135 2.501521	2.593692 -1.736685 -1.369380 -2.593692 -2.068069	3.346517 2.678253 2.734303 3.346517 1.663162
1 1 6 1 1	-1.272156 -2.385135 2.298519 1.272156 2.385135 2.501521	2.593692 -1.736685 -1.369380 -2.593692 -2.068069	3.346517 2.678253 2.734303 3.346517 1.663162
1 1 6 1 1 1	-1.272156 -2.385135 2.298519 1.272156 2.385135 2.501521	2.593692 -1.736685 -1.369380 -2.593692 -2.068069	3.346517 2.678253 2.734303 3.346517 1.663162
1 1 6 1 1 1 Complex 3b	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521	2.593692 -1.736685 -1.369380 -2.593692 -2.068069	3.346517 2.678253 2.734303 3.346517 1.663162
1 1 6 1 1 1 Complex 3b	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521	2.593692 -1.736685 -1.369380 -2.593692 -2.068069	3.346517 2.678253 2.734303 3.346517 1.663162
1 1 6 1 1 1 Complex 3b 7	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923
1 1 6 1 1 1 Complex 3b 7 7	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582
1 1 6 1 1 1 Complex 3b 7 7 6	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424
1 1 6 1 1 1 Complex 3b 7 7 6	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424
1 1 6 1 1 1 Complex 3b 7 7 6 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745
1 1 6 1 1 1 Complex 3b 7 7 6 1 6	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.00306	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6 1	-1.2/2136 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205 1.632661	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791 2.233188	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6	-1.2/2136 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482 -1 158561	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791 2.233188 6.235791	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819 0.694317
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 1 1 1 1 1 1 1 1 1 1 1 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482 -1.158561	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791 2.233188 6.235791 6.747227	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819 0.694317
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 1 1 1 1 1 1 1 1 1 1 1 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482 -1.158561 -1.950506	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791 2.233188 6.235791 6.747337	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819 0.694317 1.228488
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 7 7 7 6 1 1 6 1 1 7 7 7 6 1 1 1 1 1 1 1 1 1 1 1 1 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482 -1.158561 -1.950506 -0.157425	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791 2.233188 6.235791 6.747337 5.579584	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819 0.694317 1.228488 1.397624
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 1 1 1 1 1 1 1 1 1 1 1 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482 -1.158561 -1.950506 -0.157425 -0.154839	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791 2.233188 6.235791 6.747337 5.579584 5.603852	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819 0.694317 1.228488 1.397624 2.909538
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 1 1 1 1 1 1 1 1 1 1 1 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482 -1.158561 -1.950506 -0.157425 -0.154839 0.54262	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.919446 4.400306 2.799791 2.233188 6.235791 6.747337 5.579584 5.603852 6.71201	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819 0.694317 1.228488 1.397624 2.909538 2.201012
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 1 6 1 1 1 1 1 1 1 1 1 1 1 1 1	-1.2/2136 -2.385135 2.298519 1.272156 2.385135 2.501521 0.380591 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482 -1.158561 -1.950506 -0.157425 -0.154839 0.524299	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791 2.233188 6.235791 6.747337 5.579584 5.603852 6.371291	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819 0.694317 1.228488 1.397624 2.909538 3.281913
1 1 6 1 1 1 2 2 2 2 3 3 5 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 1 1 2 3 5 1 1 1 1 1 1 1 1 1 1 1 1 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482 -1.158561 -1.950506 -0.157425 -0.154839 0.524299 -1.149243	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791 2.233188 6.235791 6.747337 5.579584 5.603852 6.371291 5.839903	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819 0.694317 1.228488 1.397624 2.909538 3.281913 3.289591
1 1 6 1 1 1 Complex 3b 7 7 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 6 1 1 1 1 1 1 1 1 1 1 1 1 1	-1.2/2156 -2.385135 2.298519 1.272156 2.385135 2.501521 0.287139 1.454583 2.124575 0.845205 1.632661 1.504262 2.244482 -1.158561 -1.950506 -0.157425 -0.154839 0.524299 -1.149243 -1.633266	2.593692 -1.736685 -1.369380 -2.593692 -2.068069 2.211872 4.337572 4.127009 4.932344 4.919446 4.400306 2.799791 2.233188 6.235791 6.747337 5.579584 5.603852 6.371291 5.839903 2.978870	3.346517 2.678253 2.734303 3.346517 1.663162 3.923923 3.484582 4.181424 4.426745 0.692629 1.227383 4.453621 4.990819 0.694317 1.228488 1.397624 2.909538 3.281913 3.289591
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7	3.484840	0.780074	-4.196728
6	3.390176	1.072314	-2.883753
7	4.244829	0.309303	-2.218790
6	4.898333	-0.493287	-3.121759
1	5.646057	-1.201736	-2.811795
6	4.430957	-0.205963	-4.360669
1	4,683881	-0.595671	-5.330964
7	-3.484840	-0.780074	-4.196728
6	-3 390176	-1 072314	-2 883753
7	-4 244829	-0 309303	-2 218790
6	-/ 808333	0.303303	-3 121759
1	F. CACOE7	1 2017207	0.011705
1 C	-3.646037	1.201/30	-2.011/95
0	-4.430957	0.205963	-4.360669
1	-4.683881	0.5956/1	-5.330964
6	2.49/92/	2.125254	-2.339065
1	2.814585	3.105040	-2.703299
1	2.528712	2.117739	-1.253576
1	1.464869	1.945004	-2.636037
6	-2.497927	-2.125254	-2.339065
1	-1.464869	-1.945004	-2.636037
1	-2.814585	-3.105040	-2.703299
1	-2.528712	-2.117739	-1.253576
6	-2,498476	2,124699	2.338179
1	-2 529116	2 116719	1 252695
1	-1 /653/3	1 9/5183	2 635387
1	2 015751	2 104465	2.033307
Ĺ	-2.013/31	3.104403	2.701930
0	2.4984/0	-2.124699	2.3381/9
1	1.465343	-1.945183	2.63538/
1	2.815751	-3.104465	2.701938
1	2.529116	-2.116719	1.252695
15	0.00000	0.000000	0.001074
9	-0.000987	1.607682	0.001096
9	-1.137487	0.015487	-1.142123
9	1.137487	-0.015487	-1.142123
9	1.137505	0.016879	1.144290
9	-1.137505	-0.016879	1.144290
9	0.000987	-1.607682	0.001096

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