Supplementary Material (ESI) for Chemical Communications

Supporting Information

Electronic communication between metal-organic electrophores in an organometallic ruthenium-acetylide-tetrathiafulvalene complex.

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General procedures : All reagents are commercially available and were used without further purification. Melting points were measured on a Kofler hot-stage apparatus and are uncorrected. Infrared spectra were recorded on a Varian 640 FT-IR spectrometer. ^{1}H NMR, ^{13}C NMR and ^{31} P NMR spectra were recorded on Bruker ARX 200 and AC 300P spectrometers. Chemical shifts are quoted in parts per million (ppm) referenced to tetramethylsilane for ^{1}H NMR, ^{13}C NMR spectra and to H_3PO_4 for ^{31}P NMR spectra. Mass spectra were recorded with Varian MAT 311 instrument by the Centre Régional de Mesures Physiques de l'Ouest, Rennes. Elemental analysis were performed at the Centre Régional de Mesures Physiques de l'Ouest, Rennes. All the reactions were performed under an argon atmosphere with the use of Schlenk techniques. Tetrahydrofuran and diethyl ether were distilled from sodium-benzophenone. Column chromatography was performed using silica gel Merck 60 (70-260 mesh). Cyclic voltammetry were carried out on a 10^{-3} M solution of TTF derivatives in CH_2Cl_2, containing 0.1 M nBu_4NPF_6 as supporting electrolyte. Voltammograms were recorded at 0.1 Vs^{-1} on a platinum disk electrode (A = $1mm^2$). The

potentials were measured *versus* Saturated Calomel Electrode. The spectroelectrochemical setup was realized versus SCE in 0.2 M nBu_4NPF_6/CH_2Cl_2. A Cary 5 spectrophotometer was employed to record the UV-visible-NIR spectra. The EPR measurements were performed on Bruker ESP-300E X-band spectrometer. The EPR study was carried out on a CH_2Cl_2 solution of **5** with one equivalent of the oxidizing agent $NOPF_6$. The EPR spectrum of [**5**][PF6] is shown in Figure S3.

Synthesis of trimethylsilylethynyltrimethyl TTF 2 : The iodo TTF **1** (200 mg, 0.54 mmol), $Pd(PPh_3)_2Cl_2$ (110 mg, 0.16 mmol), CuI (50 mg, 0.26 mmol), the trimethylsilylacetylene (0.43 mmol), diisopropylamine (0.185 mL, 1.3 mmol) were added to THF (20 mL). The reaction mixture was stirred at room temperature for 48 h. The solvent was removed in vacuo and the crude product was chromatographied on a silica gel column using CH_2Cl_2/petroleum ether (50/50) as eluent. The TTF 2 was obtained as orange crystals in 75 % yield. mp 142°C; ^{1}H NMR($CDCl_3$) : δ 0.25 (s, 9H, $SiMe_3$), 1.98 (s, 6H, Me), 2.16 (s, 3H, Me); ^{13}C NMR ($CDCl_3$) δ 139.29 (C), 123.12 (C), 122.72 (C), 111.26 (C), 110.25 (C), 101.88 (C), 95.21 (C), 83.84 (C), 15.97 (CH_3), 13.90 (CH_3), 13.88 (CH_3), 0.00 ($SiMe_3$); IR (KBr)**:** 2140 cm^{-1} ($\upsilon_{C\equiv C}$). Anal Calcd for $C_{14}H_{18}S_4Si$ C, 49.08; H, 5.30; S, 37.43. Found: C, 49.35; H, 5.27; S, 37.91.

Synthesis of ethynyltrimethyl TTF 3 : To a solution **2** (113 mg, 0.32 mmol) in 20 mL of MeOH was added KF (40 mg, 0.66 mmol). The solution was stirred for 15h at room temperature and the solvent was removed under vacuum. The product was purified by column chromatography using using CH_2Cl_2/petroleumether (50/50) as eluent. TTF **3** was obtained as red powder in quantitative yield. mp 140°C; ^{1}H NMR($CDCl_3$) δ 1.98 (s, 3H, H_1), 2.18 (s, 6H, H_2), 3.37 (s, 1H, H_3); ^{13}C NMR ($CDCl_3$) : δ 138.94 (C), 121.93 (C), 121.58 (C), 110.55 (C), 107.83 (C), 104.43 (C), 82.65 (C), 73.76 (≡C-H), 14.68 (CH_3), 12.71 (CH_3), 12.69 (CH_3); IR (KBr)**:** 2140 cm^{-1} ($\upsilon_{C\equiv C}$); Anal Calcd for $C_{11}H_{10}S_4$ C, 48.85; H, 3.73. Found: C, 49.05; H, 3.47.

Synthesis of the Ruthenium-acetylide-tetrathiafulvalene complex 5: A solution of **3** (190 mg, 0.7 mmol) in 15 mL of CH_2Cl_2 was added to a solution of $[ClRu(dppe)_2][OTf]$ (573 mg, 0.53 mmol) in 15 mL of CH_2Cl_2. After 24 h of stirring at room temperature, the solvent was removed in vacuo and the precipitate was washed with diethyl ether. Dissolution of the precipitate in the minimum of CH_2Cl_2 followed by the addition of pentane allowed the purification of the complex [**4**][TfO] which was obtained in 40 % yield as a dark green precipitate. Crystals were obtained by slow diffusion of pentane into a concentrated solution of [**4**][TfO] in CH_2Cl_2. This vinylidene derivative [**4**][TfO] is not stable and was used without other purification in the formation of the complex **5** ^{31}P NMR (121 MHz, $CDCl_3$) δ 43.5 (t, $^3J_{PP}$ = 21 Hz), 41.9 (t, $^3J_{PP}$ = 21 Hz). This vinylidene derivative [**4**][TfO] was dissolved in 25 mL of CH_2Cl_2 and an excess of NEt_3 was added. The reaction mixture was stirred at room temperature for 1 h and then distilled water was added to the medium (2x 20 mL). The light orange organic phase was dried over Na_2SO_4 and the solvent was removed in *vacuo.* The precipitate was washed with pentane and dissolved in minimum amount of CH_2Cl_2 and precipitated again by the addition of pentane. Complex **5** was obtained as a light brown powder in 70 % yield. ^{31}P NMR($CDCl_3$) δ 49.18 (s, 4P); ^{1}H NMR ($CDCl_3$) δ 7.72-6.72 (m, 40H, phényl), 2.78 (m, 4H, dppe), 2.58 (m, 4H, dppe), 2.00(s, 3H, Me), 1.97(s, 3H, Me); 1.06 (s, 3H, Me); ^{13}C NMR (CD_2Cl_2) δ 136.59-136.04 (C_{ipso} Ph dppe), 135.43-134.90 (C_{ipso} Ph dppe), 134.67-134.60 (CH Ph dppe), 134.06-134.00 (CH Ph dppe), 129.44 (CH Ph dppe), 128.54 (CH Ph dppe), 127.46-127.41 (CH Ph dppe), 126.83-126.77 (CH Ph dppe),122.86 (TTF), 122.50 (TTF),.115.39 (Cβ), 109.75 (TTF), 105.35 (TTF), 105.22 (TTF), 30.79 (CH_2 dppe, $|^1J_{PC}+^3J_{PC}|$ = 23.3 Hz). 22.33 (TTF), 14.05 (MeTTF), 13.84 (MeTTF), 13.79 (MeTTF); IR (KBr) 2029 cm^{-1} (s, $\nu_{C\equiv C}$); HRMS (EI): *m/z* calcd for $C_{63}H_{57}P_4S_4ClRu$: 1202.1026 found: 1202.1028.

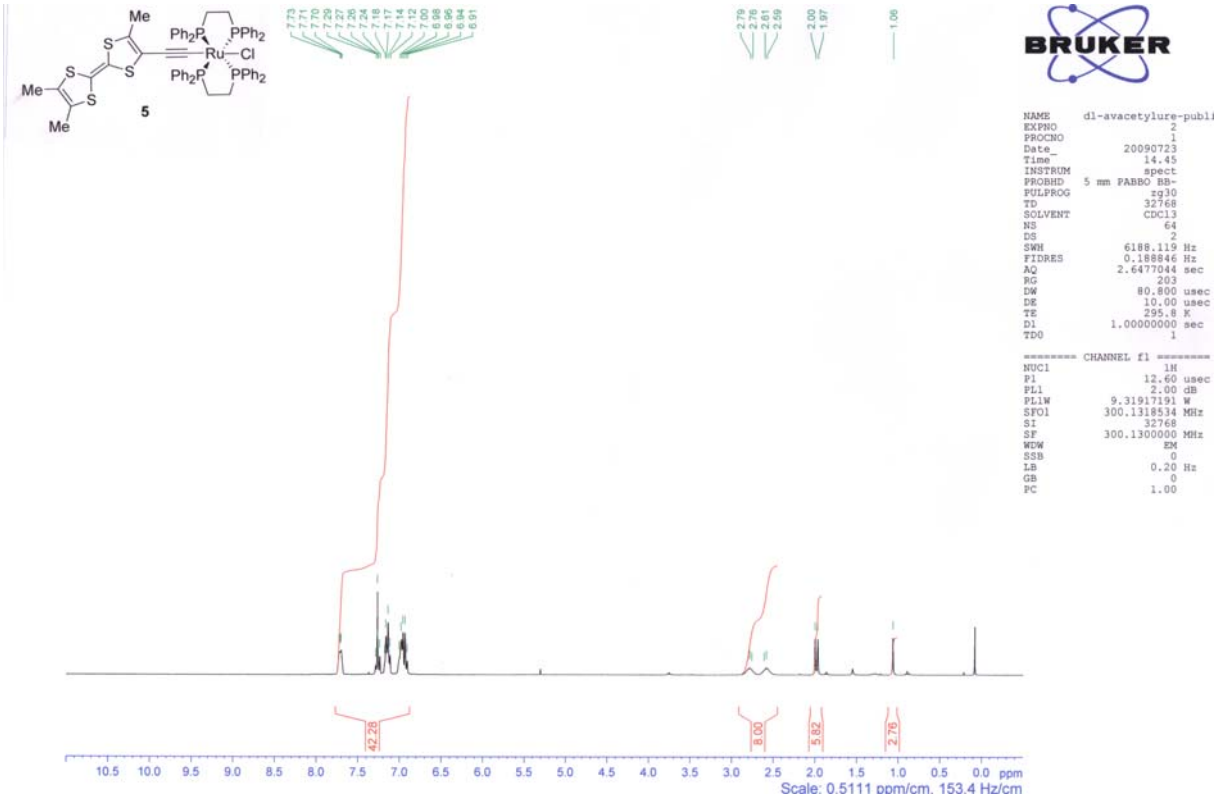

Fig S1 ^{1}H NMR spectrum of **5** in $CDCl_3$

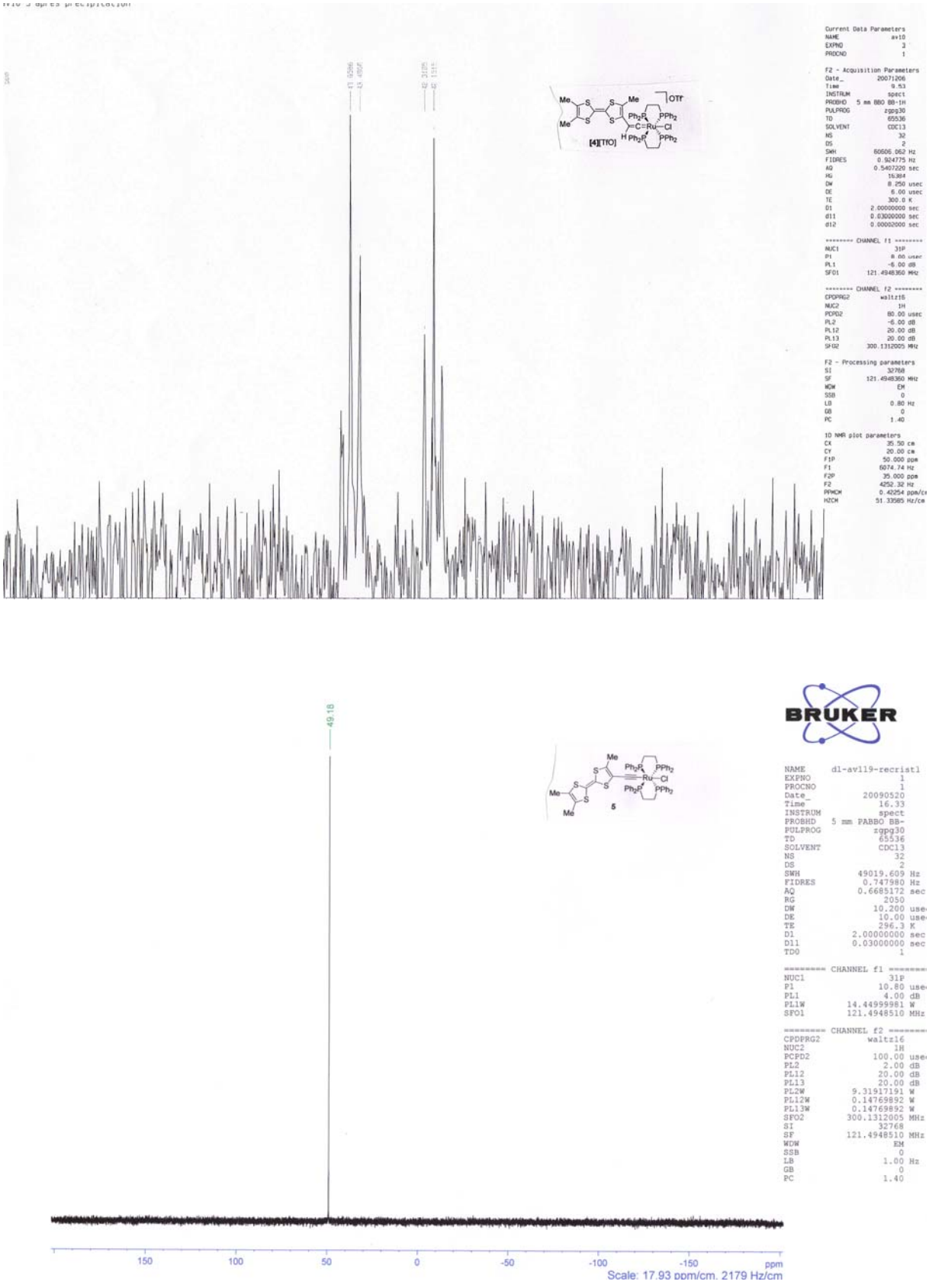

Fig S2. ^{31}P NMR spectra of vinylidene complex [**4**][TfO] (top) and complex **5** (bottom)

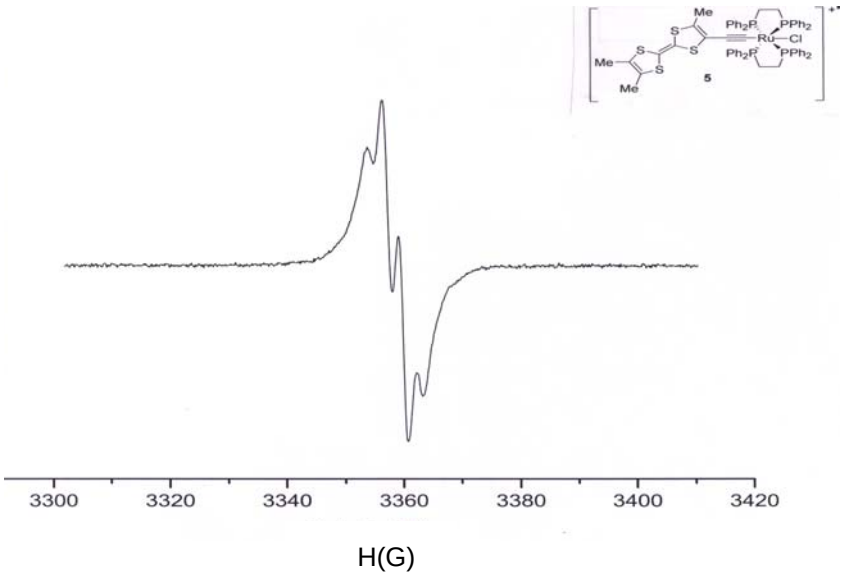

Fig S3. EPR spectrum of $\mathbf{5}^{+}$ ·recorded at room temperature (hyperfine coupling a_H = 2.7 G, g = 2.015)

Crystallography. Crystals were picked up with a cryo-loop and then freezed at T=100K under a stream of dry N_2 on a APEX II Brucker AXS diffractometer for X-ray data collection (Mo-Kα radiation, λ = 0.71073 Å). The structure was solved by direct methods using the SIR97 program [1], and then refined with full-matrix least-square methods based on F^2 (SHELX-97) [2] with the aid of the WINGX [3] program. The contribution of the disordered solvents to the calculated structure factors was estimated following the BYPASS algorithm [4], implemented as the SQUEEZE option in PLATON {5]. A new data set, free of solvent contribution, was then used in the final refinement. All non-hydrogen atoms were refined with anisotropic thermal parameters. H atoms were finally included in their calculated positions. (C63 H58 Cl P4 Ru S4, C F3 O3 S, 2(C H2 Cl2)); M = 1522.66. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å), T = 100(2) K; monoclinic C 2/c, a = 19.7287(11), b = 19.2039(9), c = 36.6357(19) Å, β = 101.699(2) °, V = 13591.8(12) $Å^3$, Z = 8, d = 1.488 $g.cm^{-3}$, μ = 0.729

mm^{-1} A final refinement on F^2 with 15532 unique intensities and 832 parameters converged at $\omega R(F^2)$ = 0.1211 (R(F) = 0.0609) for 14621 observed reflections with $I > 2\sigma(I)$.

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Computational Details.

Full geometry optimization of models of **5** and $\mathbf{5}^{\bullet+}$ with Density Functional Theory[1] calculations were performed with the hybrid Becke-3 parameter exchange functional[2] and the Lee-Yang-Parr nonlocal correlation functional[3] (B3LYP) implemented in the *Gaussian 03* (revision D.02) program suite[4] using the LANL2DZ basis set[5] and a quadratically convergent self-consistent field procedure[6] with the default convergence criteria implemented in the program. The figures were generated with Molekel 4.3.[7]

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Cartesian Coordinates of **5** and $\mathbf{5}^{\cdot+}$

Cartesian Coordinates of **5**
Neutral species\\\

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Stoichiometry    C63H57ClP4RuS4
 Framework group  C1[X(C63H57ClP4RuS4)]
 Deg. of freedom   384
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         44             0        1.585136    0.006068    0.238075
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    6          6             0       -0.334352   -2.555021   -2.825534
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   14          6             0        5.992100   -4.264027   -1.922163
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91	1	0	5.706188	3.540703	-4.629790
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127	1	0	-9.661398	-1.271569	2.389757
128	1	0	-11.180089	-0.118197	-1.732457
129	1	0	-10.970028	1.588089	-1.302000
130	1	0	-11.566195	0.435742	-0.093680

Cartesian Coordinates of **5**$^{\cdot+}$
Radical cation\\\

Stoichiometry C63H57ClP4RuS4(1+,2)
Framework group C1[X(C63H57ClP4RuS4)]
Deg. of freedom 384
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.548651	0.030734	0.182633
2	17	0	-3.936616	0.205250	1.044075
3	15	0	-1.994245	1.678944	-1.692134
4	15	0	-2.232909	-1.626416	-1.554475
5	6	0	-0.590341	2.842097	-2.188302
6	6	0	0.519621	2.365306	-2.918732
7	6	0	1.558431	3.239049	-3.290354
8	6	0	1.503639	4.598634	-2.928474
9	6	0	0.402086	5.077573	-2.194545
10	6	0	-0.638366	4.205597	-1.825310
11	6	0	-3.476092	2.842684	-1.807998
12	6	0	-4.324657	3.095990	-0.714949
13	6	0	-5.415330	3.977193	-0.860984
14	6	0	-5.665613	4.605645	-2.092774
15	6	0	-4.815718	4.354291	-3.189507
16	6	0	-3.725334	3.481093	-3.047491
17	6	0	-2.237674	0.633800	-3.285679
18	6	0	-1.674187	-0.789674	-3.168707
19	6	0	-4.045420	-2.030001	-1.864542
20	6	0	-4.832481	-2.497376	-0.791208
21	6	0	-6.177191	-2.851970	-0.997841
22	6	0	-6.755673	-2.736486	-2.275635
23	6	0	-5.977501	-2.266656	-3.349797
24	6	0	-4.629187	-1.918972	-3.146177
25	6	0	-1.396412	-3.318224	-1.695742
26	6	0	-2.010158	-4.359024	-2.426973
27	6	0	-1.371515	-5.606045	-2.562463
28	6	0	-0.115516	-5.828691	-1.965922
29	6	0	0.496301	-4.796111	-1.229617
30	6	0	-0.140645	-3.548094	-1.094301
31	15	0	-0.944454	1.715756	1.956352
32	15	0	-1.406560	-1.571336	2.125693
33	6	0	0.737794	2.567893	2.022610
34	6	0	1.221599	3.058083	3.258506
35	6	0	2.445489	3.745079	3.323483
36	6	0	3.197709	3.960732	2.151282
37	6	0	2.718382	3.480558	0.920310
38	6	0	1.495264	2.783946	0.855495
39	6	0	-2.091621	3.179808	2.290666
40	6	0	-1.733439	4.473323	1.852467
41	6	0	-2.572386	5.571337	2.116861
42	6	0	-3.777010	5.390436	2.821739
43	6	0	-4.139832	4.101729	3.256906
44	6	0	-3.305763	3.000653	2.988892
45	6	0	-0.951244	0.777812	3.631674
46	6	0	-1.836860	-0.475136	3.620123
47	6	0	-2.616677	-3.005444	2.256872
48	6	0	-3.875092	-2.846468	2.877201
49	6	0	-4.767265	-3.932117	2.963120
50	6	0	-4.418204	-5.183518	2.422001
51	6	0	-3.168248	-5.344007	1.793390
52	6	0	-2.272898	-4.263319	1.711705

53	6	0	0.213449	-2.336624	2.735289
54	6	0	1.457098	-1.824737	2.313336
55	6	0	2.657023	-2.331849	2.849308
56	6	0	2.625287	-3.356071	3.812526
57	6	0	1.385223	-3.868870	4.241950
58	6	0	0.186743	-3.361637	3.710087
59	6	0	0.266563	-0.163954	-0.446253
60	6	0	1.432951	-0.337937	-0.906967
61	6	0	2.762468	-0.507788	-1.263872
62	6	0	3.243450	-1.154639	-2.398316
63	6	0	2.393902	-1.773281	-3.476928
64	16	0	4.070536	0.171573	-0.118064
65	16	0	5.022402	-1.283092	-2.628045
66	6	0	5.493138	-0.440238	-1.081484
67	6	0	6.788929	-0.284873	-0.696721
68	16	0	7.260272	0.546429	0.854087
69	16	0	8.208805	-0.884043	-1.670833
70	6	0	9.077446	0.314057	0.639904
71	6	0	9.909151	0.874598	1.766251
72	6	0	9.497259	-0.319511	-0.478878
73	6	0	10.909862	-0.636288	-0.901757
74	1	0	0.583801	1.319440	-3.204239
75	1	0	2.402249	2.860425	-3.861885
76	1	0	2.302197	5.275645	-3.221076
77	1	0	0.347111	6.126933	-1.916248
78	1	0	-1.492176	4.595691	-1.279208
79	1	0	-4.163239	2.595773	0.230954
80	1	0	-6.065215	4.161797	-0.009894
81	1	0	-6.510357	5.281377	-2.201684
82	1	0	-4.998193	4.837851	-4.145864
83	1	0	-3.068264	3.316050	-3.898208
84	1	0	-3.317639	0.610424	-3.460504
85	1	0	-1.774341	1.169014	-4.121504
86	1	0	-0.581391	-0.782193	-3.128385
87	1	0	-1.966481	-1.402569	-4.028907
88	1	0	-4.413559	-2.568328	0.204577
89	1	0	-6.769910	-3.206611	-0.158953
90	1	0	-7.797486	-3.004719	-2.432126
91	1	0	-6.413089	-2.172600	-4.341335
92	1	0	-4.054538	-1.571959	-3.999812
93	1	0	-2.987728	-4.212245	-2.876559
94	1	0	-1.856323	-6.398953	-3.126403
95	1	0	0.374692	-6.793770	-2.067663
96	1	0	1.460524	-4.960526	-0.754652
97	1	0	0.339720	-2.764927	-0.519083
98	1	0	0.645803	2.926389	4.170584
99	1	0	2.803712	4.117526	4.279871
100	1	0	4.141219	4.498655	2.199641
101	1	0	3.288000	3.640675	0.009226
102	1	0	1.142318	2.421149	-0.101905
103	1	0	-0.794200	4.636579	1.331903
104	1	0	-2.280703	6.563453	1.781338
105	1	0	-4.420834	6.240734	3.031875
106	1	0	-5.068639	3.949544	3.800845
107	1	0	-3.618970	2.012593	3.307418
108	1	0	0.090312	0.507051	3.836391
109	1	0	-1.282647	1.469453	4.413354
110	1	0	-2.891781	-0.209113	3.533368
111	1	0	-1.683978	-1.062406	4.532931
112	1	0	-4.179133	-1.886723	3.278297
113	1	0	-5.729727	-3.795602	3.449420
114	1	0	-5.108139	-6.020805	2.489532
115	1	0	-2.888477	-6.304321	1.368485
116	1	0	-1.309996	-4.412104	1.233315
117	1	0	1.499063	-1.035823	1.571749
118	1	0	3.605988	-1.922594	2.512963
119	1	0	3.550993	-3.748685	4.225870
120	1	0	1.349678	-4.657886	4.988928

121	1	0	-0.759147	-3.771448	4.052750
122	1	0	1.366084	-1.882536	-3.125078
123	1	0	2.762871	-2.767436	-3.756696
124	1	0	2.391853	-1.153336	-4.384727
125	1	0	10.975455	0.714362	1.586225
126	1	0	9.654447	0.396934	2.721193
127	1	0	9.746620	1.954495	1.877860
128	1	0	11.149729	-0.163538	-1.862919
129	1	0	11.055012	-1.718328	-1.015430
130	1	0	11.631995	-0.277788	-0.163413