New Aryl α-Diimine Pd(II) Catalysts in the Stereocontrolled CO/Vinyl Arene Copolymerization

Carla Carfagna,[†] Giuseppe Gatti,[†] Paola Paoli,[‡] Barbara Binotti,[†] Francesco Fini,[†] Alessandra Passeri,[†] Patrizia Rossi,[‡] and Bartolo Gabriele[§]*

† Dipartimento di Scienze Biomolecolari, Università di Urbino "Carlo Bo", Piazza Rinascimento, 6, 61029 Urbino, Italy. ‡ Dipartimento di Ingegneria Industriale, Università di Firenze, Via S. Marta 3, 50139 Firenze, Italy. § Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Via P. Bucci, 12/C, 87036 Arcavacata di Rende (CS), Italy

carla.carfagna@uniurb.it

SUPPORTING INFORMATION

Table S1. Crystallographic data and refinement parameters for **2g** and **4g**.

	2g	**4g**
Chemical Formula	$C_{35}H_{30}N_3F_6PPd$ $0.5(CH_3CN)\cdot 0.5(CH_3OH)$	$C_{75}H_{49}N_2OBF_{24}Pd$
M	780.54	1567.37
T (K)	150	150
λ (Å)	0.71073	0.71073
Cryst. Syst., Space group	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$
Cell parameters (Å, °)	a = 8.8765(3)	a = 17.9701(5)
	b = 16.4479(7), β = 98.804(3)	b = 23.8667(5), β = 110.376(4)
	c = 23.5600(8)	c = 17.0081(6)
V ($Å^3$)	3399.2(2)	6838.1(3)
Z, $d_c(g/cm^3)$	4, 1.525	4, 1.522
$\mu(mm^{-1})$	0.660	0.384
F(000)	1584	3152
Reflections collected /unique	21064 / 6171	36861 / 14265
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / parameters	6171 / 435	14265 / 908
Residual electron density (max/min)	1.008/-0.452	1.277/-1.674
Final R indices[$I>2\sigma(I)$]	R1 = 0.0524, wR2 = 0.1017	R1 = 0.0817, wR^2 = 0.1681
R indices (all data)	R1 = 0.1150, wR^2 = 0.1206	R1 = 0.1268, wR^2 = 0.1898

Table S2. Selected bond lengths (Å) and angles (°) for **2g** and **4g**.

	Bond lengths (Å)		Angles (°)	
2g	Pd(1)-N(1)	2.111(4)	N(1)-Pd(1)-N(2)	77.7(2)
	Pd(1)-N(2)	2.033(4)	N(1)-Pd(1)-N(3)	97.1(2)
	Pd(1)-N(3)	1.993(4)	N(1)-Pd(1)-C(33)	174.3(2)
	Pd(1)-C(33)	2.002(6)	N(2)-Pd(1)-N(3)	174.3(2)
			N(2)-Pd(1)-C(33)	96.6(2)
			N(3)-Pd(1)-C(33)	88.6(2)
4g	Pd(1)-N(1)	2.103(4)	N(1)-Pd(1)-N(2)	76.4(2)
	Pd(1)-N(2)	2.085(4)	N(1)-Pd(1)-C(1a)	139.0(3)
	Pd(1)-C(1a)	2.146(9)	N(1)-Pd(1)-C(2a)	107.9(3)
	Pd(1)-C(2a)	2.27(1)	N(1)-Pd(1)-C(8a)	171.2(3)
	Pd(1)-C(8a)	2.043(8)	N(2)-Pd(1)-C(1a)	144.2(3)
	Pd(1)-C(1b	2.27(2)	N(2)-Pd(1)-C(2a)	160.8(4)
	Pd(1)-C(2b)	2.27(1)	N(2)-Pd(1)-C(8a)	106.8(3)
	Pd(1)-C(8b)	2.22(2)	C(1a)-Pd(1)-C(2a)	37.6(4)
			C(1a)-Pd(1)-C8a)	39.5(3)
			C(2a)-Pd(1)-C(8a)	66.4(4)
			N(1)-Pd(1)-C(1b)	132.8(4)
			N(1)-Pd(1)-C(2b)	111.6(4)
			N(1)-Pd(1)-C(8b)	160.5(4)
			N(2)-Pd(1)-C(1b)	142.4(4)
			N(2)-Pd(1)-C(2b)	169.3(3)

	N(2)-Pd(1)-C(8b)	106.5(4)
	C(1b)-Pd(1)-C(2b)	36.0(5)
	C(1b)-Pd(1)-C(8b)	37.5(5)
	C(2b)-Pd(1)-C(8b)	68.5(5)

Table S3. Comparison among selected chemical shifts (δ, ppm) for complexes [Pd(η^3-$C_{21}H_{23}O_2$)((9-$C_{14}H_9$)$_2$DABMe$_2$)]$^+$[BAr'$_4$]$^-$ (**6g**) and [Pd(η^3-$C_{11}H_{13}O$)((9-$C_{14}H_9$)$_2$DABMe$_2$)]$^+$[BAr'$_4$]$^-$ (**4g**) (Scheme 5).

	Complex 6g[a]	**Complex 4g**[b]	**Δδ**
H10	8.32	8.70	0.38
H8	7.98	8.29	0.31
H12	7.84	8.29	0.31
H10'	8.68	8.68	0.00
H8'	8.18	8.19	0.01
H12'	8.30	8.28	-0.02

[a] CD_2Cl_2, 4°C, [b] $CDCl_3$, 4°C

Table S4. Cartesian coordinates of compounds **5c'** and **5g'** as created by GaussView 3.09.

5c'

```
5c'cartesian coordinates

Created by GaussView 3.09
 73 74  0  0  0  0  0  0  0  0  0    0
    5.3610    2.4296    2.1907 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.1256    1.8129    1.3276 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.9205   -2.9381    1.8563 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.0129    0.9662    1.3854 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.9097    2.0142   -0.7744 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3596    0.4145   -1.1513 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.7806    2.5431    0.1598 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9535   -2.4663    1.1391 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2406   -3.0061    1.0118 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.9239    1.8767    0.1871 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.5460    0.1307   -0.4233 Pd  0  0  0  0  0  0  0  0  0  0  0  0
    3.7365    0.1719    0.2562 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5520   -0.6411    0.2644 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.2114   -1.9529    0.1012 N   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6513   -4.0344   -0.2477 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0957   -2.5609    0.0274 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6518   -3.6167   -0.1706 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5634   -1.8851    0.5879 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2357   -2.6117    0.5299 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.6174    1.0896   -0.9215 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.5181    0.2234   -0.9142 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.2348    1.1452   -1.8139 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7791   -3.6925   -1.2570 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4865   -3.1634   -1.1856 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2931    3.0684   -0.9669 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5464    0.0992   -2.2863 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3786    0.9688   -0.1556 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1473    0.5439    0.8249 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2019    2.4814   -0.0689 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3015    3.2833   -1.2170 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9561    3.0899    1.1700 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1590    4.6681   -1.1251 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4899    2.8257   -2.1855 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8186    4.4766    1.2606 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9022    2.4781    2.0664 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9163    5.2672    0.1138 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2381    5.2785   -2.0200 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6410    4.9380    2.2277 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8085    6.3456    0.1847 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8131    0.5366   -0.5204 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2390    1.1753   -1.3005 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8142   -0.4860   -0.9236 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7149    0.5134    0.7192 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2461    0.3782    1.8354 O   0  0  0  0  0  0  0  0  0  0  0  0
   -6.2016    0.6338    0.4738 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.7535    0.4135    1.3895 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.4346    1.6571    0.1507 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.5248   -0.0349   -0.3332 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5244   -1.8274    2.4403 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0203   -2.5499    3.0965 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8306   -0.9938    2.2848 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3935   -1.4398    2.9777 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.1846   -0.6143   -2.1269 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.3173   -1.6878   -1.9390 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.1453   -0.4705   -2.4493 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   4.8331   -0.3506   -2.9664 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.1473    0.9028    2.6218 C   0  0  0  0  0  0  0  0  0  0  0  0
   2.0863    1.0534    2.3844 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.2254   -0.0670    3.1307 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.4432    1.6718    3.3401 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.1861   -4.0447    0.9805 C   0  0  0  0  0  0  0  0  0  0  0  0
   1.4238   -4.1135    2.0495 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.2014   -4.4810    0.8161 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.9347   -4.6431    0.4499 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.7886   -2.6476    1.0124 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.6320   -3.1315    1.9827 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.0166   -3.4424    0.2916 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.6525   -1.9862    1.0826 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.1004   -4.1678   -2.1796 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.5504   -3.2405   -2.3683 C   0  0  0  0  0  0  0  0  0  0  0  0
  -0.2195   -2.2438   -2.6832 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.3477   -3.8314   -2.1475 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.0481   -3.7099   -3.2208 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 2  4  4  0  0  0  0
 2 10  4  0  0  0  0
 3  9  1  0  0  0  0
 4 12  4  0  0  0  0
 4 57  1  0  0  0  0
 5 11  1  0  0  0  0
 5 25  3  0  0  0  0
 6 11  1  0  0  0  0
 6 26  2  0  0  0  0
 6 27  1  0  0  0  0
 7 10  1  0  0  0  0
 8  9  4  0  0  0  0
 8 16  4  0  0  0  0
 8 49  1  0  0  0  0
 9 17  4  0  0  0  0
10 20  4  0  0  0  0
12 13  1  0  0  0  0
12 21  4  0  0  0  0
13 18  2  0  0  0  0
14 16  1  0  0  0  0
14 19  2  0  0  0  0
15 17  1  0  0  0  0
16 24  4  0  0  0  0
17 23  4  0  0  0  0
18 19  1  0  0  0  0
18 65  1  0  0  0  0
19 61  1  0  0  0  0
20 21  4  0  0  0  0
20 22  1  0  0  0  0
21 53  1  0  0  0  0
23 24  4  0  0  0  0
23 69  1  0  0  0  0
24 70  1  0  0  0  0
27 28  1  0  0  0  0
27 29  1  0  0  0  0
27 40  1  0  0  0  0
29 30  4  0  0  0  0
29 31  4  0  0  0  0
30 32  4  0  0  0  0
30 33  1  0  0  0  0
31 34  4  0  0  0  0
31 35  1  0  0  0  0
32 36  4  0  0  0  0
32 37  1  0  0  0  0
```

```
 34 36  4  0  0  0  0
 34 38  1  0  0  0  0
 36 39  1  0  0  0  0
 40 41  1  0  0  0  0
 40 42  1  0  0  0  0
 40 43  1  0  0  0  0
 43 44  2  0  0  0  0
 43 45  1  0  0  0  0
 45 46  1  0  0  0  0
 45 47  1  0  0  0  0
 45 48  1  0  0  0  0
 49 50  1  0  0  0  0
 49 51  1  0  0  0  0
 49 52  1  0  0  0  0
 53 54  1  0  0  0  0
 53 55  1  0  0  0  0
 53 56  1  0  0  0  0
 57 58  1  0  0  0  0
 57 59  1  0  0  0  0
 57 60  1  0  0  0  0
 61 62  1  0  0  0  0
 61 63  1  0  0  0  0
 61 64  1  0  0  0  0
 65 66  1  0  0  0  0
 65 67  1  0  0  0  0
 65 68  1  0  0  0  0
 70 71  1  0  0  0  0
 70 72  1  0  0  0  0
 70 73  1  0  0  0  0
```

5g’

```
5g' cartesian coordinates

Created by GaussView 3.09
 85 90  0  0  0  0  0  0  0  0  0    0
    5.1493    1.2138    0.9858 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8161    0.6928    1.1618 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2374    1.6835   -1.1422 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3591    0.6339   -1.3411 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.0543    0.9315    0.0301 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7007   -1.3388    1.5279 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.1268   -1.5692    1.4714 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.0492    0.5360    0.1547 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.3817    0.1048   -0.3786 Pd  0  0  0  0  0  0  0  0  0  0  0  0
    3.4589   -0.5055    0.4976 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.1187   -0.9542    0.6368 N   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4761   -1.6573    0.5563 N   0  0  0  0  0  0  0  0  0  0  0  0
   -5.7304   -2.5384    0.4179 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8890   -1.9280    0.5362 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6580   -2.3607    0.4464 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.8028   -2.0803    1.1877 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.3407   -2.4421    1.1853 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.6900   -0.6312   -0.5271 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.3593   -1.1748   -0.3699 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8470   -2.9375   -0.5381 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4191   -2.7144   -0.5076 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.8949    2.5100   -1.5676 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6075    0.0506   -2.3505 O   0  0  0  0  0  0  0  0  0  0  0  0
```

```
 -2.2008    1.7166   -0.6602 C   0  0  0  0  0  0  0  0  0  0  0  0
 -2.1057    1.5851    0.4214 H   0  0  0  0  0  0  0  0  0  0  0  0
 -1.6192    3.0779   -1.0303 C   0  0  0  0  0  0  0  0  0  0  0  0
 -1.4648    3.4496   -2.3753 C   0  0  0  0  0  0  0  0  0  0  0  0
 -1.2482    3.9822   -0.0253 C   0  0  0  0  0  0  0  0  0  0  0  0
 -0.9478    4.7022   -2.7073 C   0  0  0  0  0  0  0  0  0  0  0  0
 -1.7452    2.7581   -3.1666 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.7345    5.2365   -0.3598 C   0  0  0  0  0  0  0  0  0  0  0  0
 -1.3953    3.7128    1.0165 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.5797    5.5975   -1.6998 C   0  0  0  0  0  0  0  0  0  0  0  0
 -0.8324    4.9780   -3.7515 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.4619    5.9337    0.4274 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.1791    6.5733   -1.9587 H   0  0  0  0  0  0  0  0  0  0  0  0
 -3.6886    1.5679   -1.0319 C   0  0  0  0  0  0  0  0  0  0  0  0
 -3.8780    1.9009   -2.0580 H   0  0  0  0  0  0  0  0  0  0  0  0
 -3.9892    0.5111   -0.9973 H   0  0  0  0  0  0  0  0  0  0  0  0
 -4.5891    2.3243   -0.0501 C   0  0  0  0  0  0  0  0  0  0  0  0
 -4.1767    2.6896    1.0345 O   0  0  0  0  0  0  0  0  0  0  0  0
 -6.0131    2.5708   -0.5018 C   0  0  0  0  0  0  0  0  0  0  0  0
 -6.6160    2.9204    0.3385 H   0  0  0  0  0  0  0  0  0  0  0  0
 -6.0179    3.3376   -1.2877 H   0  0  0  0  0  0  0  0  0  0  0  0
 -6.4568    1.6668   -0.9357 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.0893   -3.6834    1.9171 C   0  0  0  0  0  0  0  0  0  0  0  0
  0.0681   -3.5594    2.9959 H   0  0  0  0  0  0  0  0  0  0  0  0
 -1.1420   -3.9029    1.7458 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.5101   -4.5439    1.6017 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.7855   -3.0119    1.8432 C   0  0  0  0  0  0  0  0  0  0  0  0
  2.3922   -3.3980    2.7875 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.0013   -3.8743    1.1995 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.7295   -2.4987    2.0335 H   0  0  0  0  0  0  0  0  0  0  0  0
  5.5210    2.4099    1.6724 C   0  0  0  0  0  0  0  0  0  0  0  0
  2.9244    1.3925    2.0313 C   0  0  0  0  0  0  0  0  0  0  0  0
  4.0144   -2.3297   -1.1383 C   0  0  0  0  0  0  0  0  0  0  0  0
  6.6146   -1.2967   -1.3916 C   0  0  0  0  0  0  0  0  0  0  0  0
 -4.9588   -0.9811    2.4750 C   0  0  0  0  0  0  0  0  0  0  0  0
 -2.1847   -0.5257    2.5867 C   0  0  0  0  0  0  0  0  0  0  0  0
 -4.3942   -3.7518   -1.5782 C   0  0  0  0  0  0  0  0  0  0  0  0
 -1.6162   -3.3051   -1.5329 C   0  0  0  0  0  0  0  0  0  0  0  0
 -3.5905   -4.3070   -2.5379 C   0  0  0  0  0  0  0  0  0  0  0  0
 -4.0187   -4.9234   -3.3225 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.1857   -4.0742   -2.5151 C   0  0  0  0  0  0  0  0  0  0  0  0
 -1.5611   -4.5092   -3.2899 H   0  0  0  0  0  0  0  0  0  0  0  0
 -4.4277   -0.2028    3.4686 C   0  0  0  0  0  0  0  0  0  0  0  0
 -3.0236    0.0278    3.5204 C   0  0  0  0  0  0  0  0  0  0  0  0
 -2.6157    0.6497    4.3119 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.3185    2.5483    2.6622 C   0  0  0  0  0  0  0  0  0  0  0  0
  4.6313    3.0649    2.4843 C   0  0  0  0  0  0  0  0  0  0  0  0
  4.9255    3.9737    3.0001 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.9305   -2.9307   -1.9653 C   0  0  0  0  0  0  0  0  0  0  0  0
  4.6417   -3.8043   -2.5428 H   0  0  0  0  0  0  0  0  0  0  0  0
  6.2528   -2.4194   -2.0866 C   0  0  0  0  0  0  0  0  0  0  0  0
  6.9629   -2.9141   -2.7419 H   0  0  0  0  0  0  0  0  0  0  0  0
  6.5304    2.7893    1.5376 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.9292    0.9961    2.2029 H   0  0  0  0  0  0  0  0  0  0  0  0
  7.6138   -0.8813   -1.4913 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.0060   -2.7266   -1.0884 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.6242    3.0695    3.3152 H   0  0  0  0  0  0  0  0  0  0  0  0
 -6.0288   -1.1668    2.4296 H   0  0  0  0  0  0  0  0  0  0  0  0
 -1.1165   -0.3425    2.6460 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.5457   -3.1288   -1.5397 H   0  0  0  0  0  0  0  0  0  0  0  0
 -5.4677   -3.9211   -1.5886 H   0  0  0  0  0  0  0  0  0  0  0  0
 -5.0716    0.2434    4.2200 H   0  0  0  0  0  0  0  0  0  0  0  0
1  2  4  0  0  0  0
```

1	8	4	0	0	0	0
1	54	4	0	0	0	0
2	10	4	0	0	0	0
2	55	4	0	0	0	0
3	9	1	0	0	0	0
3	22	3	0	0	0	0
4	9	1	0	0	0	0
4	23	2	0	0	0	0
4	24	1	0	0	0	0
5	8	1	0	0	0	0
6	7	4	0	0	0	0
6	14	4	0	0	0	0
6	59	4	0	0	0	0
7	15	4	0	0	0	0
7	58	4	0	0	0	0
8	18	4	0	0	0	0
10	11	1	0	0	0	0
10	19	4	0	0	0	0
11	16	2	0	0	0	0
12	14	1	0	0	0	0
12	17	2	0	0	0	0
13	15	1	0	0	0	0
14	21	4	0	0	0	0
15	20	4	0	0	0	0
16	17	1	0	0	0	0
16	50	1	0	0	0	0
17	46	1	0	0	0	0
18	19	4	0	0	0	0
18	57	4	0	0	0	0
19	56	4	0	0	0	0
20	21	4	0	0	0	0
20	60	4	0	0	0	0
21	61	4	0	0	0	0
24	25	1	0	0	0	0
24	26	1	0	0	0	0
24	37	1	0	0	0	0
26	27	4	0	0	0	0
26	28	4	0	0	0	0
27	29	4	0	0	0	0
27	30	1	0	0	0	0
28	31	4	0	0	0	0
28	32	1	0	0	0	0
29	33	4	0	0	0	0
29	34	1	0	0	0	0
31	33	4	0	0	0	0
31	35	1	0	0	0	0
33	36	1	0	0	0	0
37	38	1	0	0	0	0
37	39	1	0	0	0	0
37	40	1	0	0	0	0
40	41	2	0	0	0	0
40	42	1	0	0	0	0
42	43	1	0	0	0	0
42	44	1	0	0	0	0
42	45	1	0	0	0	0
46	47	1	0	0	0	0
46	48	1	0	0	0	0
46	49	1	0	0	0	0
50	51	1	0	0	0	0
50	52	1	0	0	0	0
50	53	1	0	0	0	0
54	70	2	0	0	0	0
54	76	1	0	0	0	0

55	69	2	0	0	0	0
55	77	1	0	0	0	0
56	72	2	0	0	0	0
56	79	1	0	0	0	0
57	74	2	0	0	0	0
57	78	1	0	0	0	0
58	66	2	0	0	0	0
58	81	1	0	0	0	0
59	67	2	0	0	0	0
59	82	1	0	0	0	0
60	62	2	0	0	0	0
60	84	1	0	0	0	0
61	64	2	0	0	0	0
61	83	1	0	0	0	0
62	63	1	0	0	0	0
62	64	4	0	0	0	0
64	65	1	0	0	0	0
66	67	4	0	0	0	0
66	85	1	0	0	0	0
67	68	1	0	0	0	0
69	70	4	0	0	0	0
69	80	1	0	0	0	0
70	71	1	0	0	0	0
72	73	1	0	0	0	0
72	74	4	0	0	0	0
74	75	1	0	0	0	0