*Contribution from the School of Molecular Sciences, University of Sussex*

# The Crystal Structure of $[Pt(CH_3)_3(\textit{rac}\text{-diars})]I$; $(\text{diars}{=}C_6H_5CH_3AsCH_2CH_2AsCH_3C_6H_5)$

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*Crystals of $Pt(CH_3)_3(C_6H_5CH_3AsCH_2CH_2AsCH_3C_6H_5)I$ are monoclinic with* a = *17.008,* b = *15.736,* c = *8.393 Å, β = 101.37°, space group $P2_1/c$, Z=4. The definition of atomic parameters was by Fourier and least-squares analysis of 1976 independent reflections (MoKα, four circle diffractometry); convergence was to $R_1$ = 0.06 for the absorption corrected data.*

*The mean Pt-C(methyl) bond length is 2.11 Å, the Pt-As and Pt-I bond lengths being 2.455 and 2.771 Å The* trans-*influence of the methyl group on the Pt-As and Pt-I bonds is shown to be ca. 0.1 Å; the conformation of the chelate ring is a distorted envelope.*

## Introduction

During the course of their systematic studies of transitions metal-carbon bonds, Shaw and co-workers[1] have described oxidative addition reactions of $[PtMe_2(\textit{rac}\text{-diars})]$ or $[PtMe_2(\textit{meso}\text{-diars})]$, $(\text{diars}{=}C_6H_5CH_3AsCH_2CH_2AsCH_3C_6H_5)$; the complexes add methyl iodide stereospecifically but it was not initially clear what the conformation of the coordinated arsine was in the two adducts. An X-ray analysis provided clear information on the point but also allows some interesting conclusions on *cis*- and *trans*-influence in six coordinate complexes and on general conformational aspects of unsymmetrical coordinated diarsines.

## Experimental Section

Pale yellow prisms from benzene-light petroleum were shown to be monoclinic by Weissenberg and precession photographs (MoKα). A selected crystal of dimension 0.1×0.4×0.3 mm was used for intensity

**Table I.** $Pt(CH_3)_3(C_6H_5CH_3AsCH_2CH_2AsCH_3C_6H_5)I$.

(i) Heavy-atom parameters and their e.s.d's (multiplied by $10^4$). The temperature factor is in the form

$$\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)]$$

| | x | y | z | $\beta_{11}$ | $\beta_{22}$ | $\beta_{33}$ | $\beta_{12}$ | $\beta_{13}$ | $\beta_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| Pt | 2873(1) | 237(1) | 3989(1) | 37(0) | 41(0) | 113(1) | 2(0) | 11(1) | —2(1) |
| I | 1638(1) | —336(1) | 5428(2) | 64(1) | 67(1) | 193(3) | 0(1) | 59(1) | 18(2) |
| As(1) | 2800(2) | —1087(1) | 2407(3) | 41(1) | 31(1) | 127(4) | 1(1) | 19(2) | 7(2) |
| As(2) | 1887(1) | 729(1) | 1637(3) | 40(1) | 34(1) | 117(4) | 0(1) | 15(2) | 8(2) |

(ii) Carbon-atom parameters and their e.s.d's.

| | x | y | z | B |
|---|---|---|---|---|
| C(1) | 0.2904(19) | 0.1406(21) | 0.5255(38) | 5.1(7) |
| C(2) | 0.3749(19) | —0.0270(21) | 0.5919(38) | 6.8(7) |
| C(3) | 0.3903(17) | 0.0703(18) | 0.3276(34) | 5.5(6) |
| C(4) | 0.2535(18) | —0.2151(18) | 0.3425(35) | 6.7(6) |
| C(5) | 0.2327(16) | 0.1166(17) | —0.0282(31) | 5.6(5) |
| C(6) | 0.1948(16) | —0.0998(16) | 0.0482(31) | 5.0(5) |
| C(7) | 0.1350(14) | —0.0301(15) | 0.0652(27) | 4.6(4) |
| C(8) | 0.3758(14) | —0.1360(15) | 0.1577(28) | 4.1(5) |
| C(9) | 0.3945(15) | —0.0973(15) | 0.0267(29) | 3.8(5) |
| C(10) | 0.4682(17) | —0.1096(19) | —0.0199(34) | 5.7(6) |
| C(11) | 0.5214(19) | —0.1617(19) | 0.0674(37) | 6.0(6) |
| C(12) | 0.5027(21) | —0.2039(21) | 0.1914(40) | 7.2(8) |
| C(13) | 0.4329(17) | —0.1922(17) | 0.2481(33) | 5.6(6) |
| C(14) | 0.1038(14) | 0.1518(14) | 0.1798(27) | 4.0(4) |
| C(15) | 0.0357(16) | 0.1246(16) | 0.2356(31) | 5.6(5) |
| C(16) | —0.0232(17) | 0.1849(18) | 0.2524(34) | 6.2(6) |
| C(17) | —0.0152(17) | 0.2708(18) | 0.2177(34) | 5.8(6) |
| C(18) | 0.0544(16) | 0.2962(17) | 0.1570(32) | 5.3(5) |
| C(19) | 0.1154(17) | 0.2365(17) | 0.1487(34) | 5.9(6) |

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(1) A.J. Cheney and B.L. Shaw, *J. Chem. Soc. (A)*, 3549 (1971).

**Table II.** Observed and calculated structure factors. The values of $F_{obs}$ and $F_{cal}$ have been multiplied by 10.

| K | L | FO | FC |
|---|---|---|---|
| H | 0 | | |
| 0 | 2 | 696 | 545 |
| 0 | 4 | 757 | -571 |
| 0 | 6 | 1193 | -1009 |
| 1 | 1 | 3122 | -2810 |
| 1 | 3 | 786 | -840 |
| 1 | 4 | 982 | 879 |
| 1 | 5 | 2388 | 2036 |
| 1 | 7 | 613 | -538 |
| 1 | 9 | 625 | -587 |
| 2 | 0 | 5222 | 4896 |
| 2 | 1 | 279 | -215 |
| 2 | 2 | 2523 | 2482 |
| 2 | 3 | 1498 | -1513 |
| 2 | 4 | 1458 | -1298 |
| 2 | 5 | 881 | 896 |
| 2 | 6 | 961 | -958 |
| 2 | 7 | 414 | -388 |
| 3 | 1 | 3681 | -3718 |
| 3 | 2 | 1470 | 1461 |
| 3 | 4 | 1489 | 1485 |
| 3 | 5 | 1250 | 1269 |
| 3 | 7 | 585 | 558 |
| 3 | 8 | 476 | -513 |
| 3 | 9 | 426 | -467 |
| 4 | 0 | 1503 | 1511 |
| 4 | 1 | 2296 | -2242 |
| 4 | 2 | 1856 | 1970 |
| 4 | 3 | 2397 | -2183 |
| 4 | 4 | 1972 | -1918 |
| 4 | 5 | 338 | 374 |
| 4 | 6 | 736 | -736 |
| 5 | 1 | 3132 | -3090 |
| 5 | 2 | 1333 | 1368 |
| 5 | 3 | 727 | 697 |
| 5 | 4 | 1917 | 1926 |
| 5 | 5 | 639 | 668 |
| 5 | 8 | 409 | -470 |
| 6 | 0 | 481 | 435 |
| 6 | 1 | 2076 | -2126 |
| 6 | 2 | 1451 | 1429 |
| 6 | 3 | 1756 | -1819 |
| 6 | 4 | 859 | -852 |
| 6 | 5 | 791 | -816 |
| 6 | 6 | 878 | -932 |
| 6 | 7 | 457 | 511 |
| 7 | 1 | 1269 | -1247 |
| 7 | 2 | 2220 | 2264 |
| 7 | 3 | 627 | 617 |
| 7 | 4 | 1468 | 1508 |
| 7 | 5 | 615 | 619 |
| 7 | 6 | 289 | -276 |
| 8 | 0 | 587 | 600 |
| 8 | 1 | 1754 | -1774 |
| 8 | 3 | 1342 | -1411 |
| 8 | 5 | 961 | -1004 |
| 8 | 6 | 836 | -906 |
| 8 | 7 | 684 | 790 |
| 8 | 8 | 341 | 257 |
| 9 | 2 | 2289 | 2391 |
| 9 | 3 | 658 | 676 |
| 9 | 4 | 821 | 900 |
| 9 | 5 | 466 | 473 |
| 9 | 6 | 341 | -325 |
| 9 | 8 | 317 | -260 |
| 10 | 0 | 331 | 321 |
| 10 | 2 | 682 | -727 |
| 10 | 3 | 1801 | -1877 |
| 10 | 4 | 301 | 337 |
| 10 | 5 | 509 | -507 |
| 10 | 6 | 421 | -437 |
| 10 | 7 | 653 | 642 |
| 10 | 8 | 317 | 184 |
| 11 | 1 | 656 | 649 |
| 11 | 2 | 1927 | 1990 |
| 11 | 4 | 473 | 502 |
| 11 | 5 | 312 | 154 |
| 12 | 0 | 601 | -617 |
| 12 | 2 | 360 | -360 |
| 12 | 3 | 1458 | -1492 |
| 12 | 4 | 346 | -260 |
| 12 | 6 | 338 | 335 |
| 12 | 7 | 483 | 406 |
| 13 | 1 | 798 | 773 |
| 13 | 2 | 1129 | 1158 |
| 13 | 4 | 556 | 542 |
| 14 | 0 | 793 | -789 |
| 14 | 1 | 637 | -617 |
| 14 | 2 | 322 | -267 |
| 14 | 3 | 656 | -633 |
| 14 | 4 | 341 | -352 |
| 14 | 6 | 625 | 655 |
| 15 | 1 | 672 | 637 |
| 15 | 2 | 391 | 301 |
| 15 | 4 | 443 | 303 |
| 16 | 0 | 689 | -589 |
| 16 | 1 | 736 | -740 |
| 16 | 2 | 372 | -386 |
| 17 | 1 | 592 | 518 |
| 17 | 4 | 320 | 244 |
| 18 | 0 | 405 | -400 |
| 18 | 1 | 391 | -353 |
| 18 | 2 | 374 | -321 |
| H | 1 | | |
| 0 | -8 | 1060 | 1022 |
| 0 | -6 | 2601 | 2182 |
| 0 | -4 | 786 | -548 |
| 0 | -2 | 485 | -369 |
| 0 | 4 | 1787 | 1318 |
| 0 | 6 | 1356 | -1091 |
| 0 | 8 | 1785 | -1458 |
| 1 | -7 | 1491 | -1406 |
| 1 | -6 | 447 | -469 |
| 1 | -5 | 1468 | -1420 |
| 1 | -4 | 504 | 504 |
| 1 | -3 | 736 | -576 |
| 1 | -2 | 544 | 544 |
| 1 | -1 | 3723 | 3180 |
| 1 | 1 | 3806 | -3614 |
| 1 | 2 | 1567 | -1298 |
| 1 | 3 | 1844 | -1738 |
| 1 | 4 | 1626 | 1513 |
| 1 | 6 | 481 | -365 |
| 1 | 7 | 1484 | 1410 |
| 1 | 9 | 504 | 391 |
| 2 | -9 | 594 | 636 |
| 2 | -8 | 907 | 932 |
| 2 | -6 | 1697 | 1688 |
| 2 | -5 | 424 | -345 |
| 2 | -3 | 348 | -294 |
| 2 | -2 | 414 | -392 |
| 2 | -1 | 1155 | 1163 |
| 2 | 1 | 1101 | -1042 |
| 2 | 2 | 1669 | 1668 |
| 2 | 3 | 559 | 500 |
| 2 | 4 | 1150 | 1101 |
| 2 | 5 | 838 | -771 |
| 2 | 6 | 1023 | -994 |
| 2 | 7 | 540 | -540 |
| 2 | 8 | 1262 | -1280 |
| 3 | -7 | 1037 | -1046 |
| 3 | -6 | 769 | -793 |
| 3 | -5 | 1328 | -1336 |
| 3 | -4 | 1539 | 1565 |
| 3 | -3 | 1098 | 1040 |
| 3 | -2 | 521 | 431 |
| 3 | -1 | 902 | 859 |
| 3 | 0 | 353 | -145 |
| 3 | 3 | 2381 | -2404 |
| 3 | 4 | 2256 | 2315 |
| 3 | 5 | 407 | 433 |
| 3 | 7 | 914 | 950 |
| 3 | 9 | 580 | 603 |
| 4 | -9 | 691 | 778 |
| 4 | -8 | 705 | 745 |
| 4 | -6 | 930 | 947 |
| 4 | -5 | 1084 | -1114 |
| 4 | -4 | 632 | 677 |
| 4 | -2 | 1415 | -1291 |
| 4 | -1 | 433 | -322 |
| 4 | 0 | 533 | 543 |
| 4 | 2 | 2324 | 2262 |
| 4 | 3 | 348 | -327 |
| 4 | 4 | 592 | 527 |
| 4 | 5 | 1039 | -1149 |
| 4 | 6 | 620 | -618 |
| 4 | 7 | 710 | -720 |
| 4 | 8 | 798 | -810 |
| 5 | -8 | 462 | -484 |
| 5 | -7 | 736 | -781 |
| 5 | -5 | 1036 | -957 |
| 5 | -4 | 1112 | 1156 |
| 5 | -3 | 2036 | 1921 |
| 5 | -2 | 1343 | 1482 |
| 5 | -1 | 578 | -634 |
| 5 | 0 | 1044 | -1207 |
| 5 | 1 | 561 | 599 |
| 5 | 2 | 937 | 977 |
| 5 | 3 | 1567 | -1528 |
| 5 | 4 | 1830 | 1889 |
| 5 | 6 | 786 | 788 |
| 5 | 7 | 667 | 682 |
| 5 | 9 | 518 | 644 |
| 6 | -9 | 585 | 608 |
| 6 | -7 | 334 | 304 |
| 6 | -6 | 573 | 519 |
| 6 | -5 | 1131 | -1216 |
| 6 | -4 | 596 | 600 |
| 6 | -3 | 351 | -811 |
| 6 | -2 | 1572 | -1529 |
| 6 | -1 | 436 | -340 |
| 6 | 0 | 361 | -325 |
| 6 | 1 | 349 | 495 |
| 6 | 2 | 1737 | 1714 |
| 6 | 3 | 576 | -665 |
| 6 | 4 | 443 | 400 |
| 6 | 5 | 1444 | -1591 |
| 6 | 6 | 552 | -547 |
| 6 | 7 | 440 | -493 |
| 7 | -8 | 765 | -809 |
| 7 | -7 | 788 | -837 |
| 7 | -6 | 641 | 661 |
| 7 | -4 | 672 | 727 |
| 7 | -3 | 663 | 733 |
| 7 | -2 | 1139 | 1140 |
| 7 | 0 | 1425 | -1443 |
| 7 | 2 | 888 | 859 |
| 7 | 3 | 376 | -404 |
| 7 | 4 | 765 | 827 |
| 7 | 5 | 402 | -458 |
| 7 | 6 | 1299 | 1435 |
| 7 | 7 | 585 | 593 |
| 7 | 8 | 388 | -337 |
| 8 | -7 | 353 | 423 |
| 8 | -5 | 828 | -908 |
| 8 | -3 | 1219 | -1219 |
| 8 | -2 | 921 | -991 |
| 8 | -1 | 525 | 476 |
| 8 | 0 | 433 | -459 |
| 8 | 1 | 876 | 922 |
| 8 | 2 | 793 | 853 |
| 8 | 3 | 1157 | -1192 |
| 8 | 4 | 291 | 218 |
| 8 | 5 | 1292 | -1383 |
| 8 | 6 | 329 | -398 |
| 9 | -8 | 684 | -740 |
| 9 | -7 | 507 | -489 |
| 9 | -6 | 594 | 647 |
| 9 | -5 | 547 | 617 |
| 9 | -4 | 836 | 836 |
| 9 | -1 | 708 | 744 |
| 9 | 0 | 592 | -571 |
| 9 | 1 | 613 | -629 |
| 9 | 3 | 374 | 433 |
| 9 | 4 | 715 | 762 |
| 9 | 5 | 824 | -885 |
| 9 | 6 | 1139 | 1249 |
| 9 | 7 | 430 | 380 |
| 10 | -5 | 504 | -527 |
| 10 | -4 | 407 | -466 |
| 10 | -3 | 1397 | -1405 |
| 10 | -2 | 312 | -376 |
| 10 | -1 | 651 | 671 |
| 10 | 0 | 521 | -450 |
| 10 | 1 | 1231 | 1234 |
| 10 | 2 | 298 | 264 |
| 10 | 3 | 928 | -991 |
| 10 | 5 | 1025 | -997 |
| 11 | -6 | 369 | 345 |
| 11 | -5 | 488 | 427 |
| 11 | -4 | 1041 | 1117 |
| 11 | -2 | 767 | -826 |
| 11 | -1 | 431 | 434 |
| 11 | 0 | 360 | 294 |
| 11 | 2 | 708 | -749 |
| 11 | 4 | 944 | 973 |
| 11 | 6 | 667 | 715 |
| 12 | -4 | 447 | -452 |
| 12 | -3 | 1096 | -1110 |
| 12 | -1 | 717 | 774 |
| 12 | 1 | 982 | 991 |
| 12 | 2 | 549 | -572 |
| 12 | 3 | 417 | -435 |
| 12 | 5 | 795 | -845 |
| 12 | 6 | 362 | 329 |
| 13 | -7 | 641 | 652 |
| 13 | -4 | 885 | 893 |
| 13 | 0 | 376 | -349 |
| 13 | 1 | 372 | 353 |
| 13 | 2 | 391 | -397 |
| 13 | 3 | 296 | -266 |
| 13 | 4 | 620 | 620 |
| 13 | 5 | 473 | 496 |
| 13 | 6 | 402 | 402 |
| 14 | -6 | 445 | -393 |
| 14 | -5 | 559 | -576 |
| 14 | -4 | 360 | -295 |
| 14 | -1 | 450 | 413 |
| 14 | 1 | 600 | 662 |
| 14 | 2 | 717 | -681 |
| 14 | 5 | 424 | -512 |
| 14 | 6 | 374 | 369 |
| 15 | -2 | 383 | 360 |
| 15 | 0 | 959 | -998 |
| 15 | 1 | 341 | 313 |
| 16 | -5 | 440 | -481 |
| 16 | -2 | 348 | 372 |
| 16 | 1 | 353 | 304 |
| 16 | 2 | 509 | -470 |
| 17 | -3 | 436 | -345 |
| 17 | -2 | 370 | 275 |
| 17 | 0 | 845 | -824 |
| 17 | 3 | 485 | 446 |
| H | 2 | | |
| 0 | -6 | 1328 | 1205 |
| 0 | -4 | 2412 | 2031 |
| 0 | -2 | 2589 | 2111 |
| 0 | 0 | 5716 | -4612 |
| 0 | 2 | 4921 | -3818 |
| 0 | 6 | 1084 | 908 |
| 0 | 8 | 684 | -430 |
| 1 | -9 | 391 | 499 |
| 1 | -5 | 3058 | -2993 |
| 1 | -4 | 421 | 430 |
| 1 | -3 | 937 | -875 |
| 1 | -2 | 1273 | 1182 |
| 1 | -1 | 1969 | 1729 |
| 1 | 0 | 824 | -774 |
| 1 | 1 | 3418 | 3368 |
| 1 | 2 | 928 | 819 |
| 1 | 3 | 1702 | 1659 |
| 1 | 5 | 691 | -634 |
| 1 | 7 | 933 | -773 |
| 2 | -9 | 374 | 365 |
| 2 | -7 | 436 | -393 |
| 2 | -6 | 1146 | 1162 |
| 2 | -5 | 528 | 594 |
| 2 | -4 | 2336 | 2285 |
| 2 | -3 | 1186 | -1183 |
| 2 | -2 | 1579 | 1496 |
| 2 | -1 | 1508 | -1455 |
| 2 | 0 | 4755 | -4742 |
| 2 | 1 | 1766 | -1700 |
| 2 | 2 | 2234 | -2322 |
| 2 | 3 | 2081 | 2022 |
| 2 | 5 | 1139 | -1151 |
| 2 | 6 | 727 | 748 |
| 3 | -9 | 589 | 601 |
| 3 | -8 | 592 | -595 |
| 3 | -7 | 504 | -400 |
| 3 | -6 | 338 | -304 |
| 3 | -5 | 1823 | -1833 |
| 3 | -4 | 973 | 985 |
| 3 | -3 | 1939 | -1863 |
| 3 | -2 | 2197 | 2207 |
| 3 | -1 | 1598 | 1599 |
| 3 | 0 | 462 | 472 |
| 3 | 1 | 2334 | 2484 |
| 3 | 2 | 620 | 631 |
| 3 | 3 | 1210 | 1256 |
| 3 | 4 | 1096 | -1137 |
| 3 | 5 | 762 | -773 |
| 3 | 6 | 457 | -402 |
| 3 | 7 | 483 | -468 |
| 3 | 8 | 511 | 471 |
| 4 | -6 | 644 | 654 |
| 4 | -5 | 459 | 412 |
| 4 | -4 | 2672 | 2707 |
| 4 | -3 | 1468 | -1509 |
| 4 | -2 | 350 | -394 |
| 4 | -1 | 2682 | -2783 |
| 4 | 0 | 1157 | -1233 |
| 4 | 1 | 902 | -953 |
| 4 | 2 | 2819 | -2931 |
| 4 | 3 | 1718 | 1742 |
| 4 | 4 | 656 | 646 |
| 4 | 5 | 405 | -405 |
| 4 | 6 | 573 | 480 |
| 5 | -9 | 350 | 385 |
| 5 | -8 | 386 | -471 |
| 5 | -7 | 386 | -304 |
| 5 | -6 | 705 | -766 |
| 5 | -5 | 639 | -691 |
| 5 | -4 | 1709 | 1649 |
| 5 | -3 | 1950 | -1963 |
| 5 | -2 | 2088 | 2161 |
| 5 | -1 | 1337 | 1314 |
| 5 | 0 | 1572 | 1600 |
| 5 | 1 | 2618 | 2630 |
| 5 | 3 | 324 | 179 |
| 5 | 4 | 1094 | -1142 |
| 5 | 5 | 793 | -815 |
| 5 | 8 | 457 | 482 |
| 6 | -8 | 405 | -432 |
| 6 | -7 | 696 | 578 |
| 6 | -6 | 378 | 649 |
| 6 | -5 | 312 | -276 |
| 6 | -4 | 1697 | 1743 |
| 6 | -3 | 1233 | -1263 |
| 6 | -2 | 1139 | -1082 |
| 6 | -1 | 3633 | -3732 |
| 6 | 1 | 878 | 843 |
| 6 | 2 | 1361 | -1360 |
| 6 | 3 | 689 | 726 |
| 6 | 4 | 836 | 732 |
| 6 | 5 | 481 | 523 |
| 6 | 7 | 452 | -542 |
| 7 | -6 | 897 | -968 |
| 7 | -4 | 1101 | 1137 |
| 7 | -3 | 1169 | -1187 |
| 7 | -2 | 2294 | 2342 |
| 7 | -1 | 335 | 548 |
| 7 | 0 | 2336 | 2371 |
| 7 | 1 | 1834 | 1830 |
| 7 | 2 | 646 | -559 |
| 7 | 3 | 883 | -931 |
| 7 | 5 | 698 | -765 |
| 7 | 6 | 449 | 478 |
| 8 | -8 | 523 | -533 |
| 8 | -7 | 949 | 1325 |
| 8 | -5 | 615 | 643 |
| 8 | -5 | 289 | -263 |
| 8 | -4 | 353 | 297 |
| 8 | -3 | 1517 | -1570 |
| 8 | -1 | 2346 | -2403 |
| 8 | 0 | 786 | -808 |
| 8 | 2 | 368 | 343 |
| 8 | 3 | 812 | 848 |
| 8 | 4 | 575 | -590 |
| 8 | 5 | 1025 | 1085 |
| 8 | 6 | 847 | 854 |
| 8 | 7 | 516 | -530 |
| 9 | -8 | 376 | -372 |
| 9 | -5 | 530 | -550 |
| 9 | -2 | 2525 | 2577 |
| 9 | -1 | 353 | -309 |
| 9 | 0 | 1763 | 1799 |
| 9 | 1 | 727 | 593 |
| 9 | 2 | 1094 | -1164 |
| 9 | 3 | 452 | -435 |
| 9 | 4 | 753 | -743 |
| 9 | 5 | 398 | -404 |
| 10 | -7 | 810 | 855 |
| 10 | -5 | 296 | 298 |
| 10 | -3 | 1792 | -1889 |
| 10 | -1 | 956 | -983 |
| 10 | 1 | 689 | -509 |
| 10 | 2 | 684 | 669 |
| 10 | 3 | 914 | 965 |
| 10 | 4 | 554 | 589 |
| 10 | 5 | 523 | 505 |
| 11 | -8 | 443 | -451 |
| 11 | -4 | 286 | -201 |
| 11 | -2 | 2055 | 2106 |
| 11 | 0 | 1108 | 1372 |
| 11 | 1 | 443 | -895 |
| 11 | 2 | 1025 | -1088 |
| 11 | 4 | 959 | -991 |
| 11 | 7 | 336 | -176 |
| 12 | -7 | 589 | 562 |
| 12 | -6 | 362 | -407 |
| 12 | -5 | 459 | 504 |
| 12 | -4 | 372 | -358 |
| 12 | -3 | 1536 | -1571 |
| 12 | -1 | 463 | -393 |
| 12 | 0 | 355 | 327 |
| 12 | 1 | 405 | -428 |
| 12 | 2 | 312 | 244 |
| 12 | 3 | 911 | 872 |
| 12 | 4 | 575 | 548 |
| 13 | -6 | 386 | -415 |
| 13 | -3 | 391 | 387 |
| 13 | -2 | 1148 | 1153 |
| 13 | 0 | 646 | 589 |
| 13 | 1 | 1096 | -1074 |
| 13 | 2 | 662 | -598 |
| 13 | 4 | 751 | -753 |
| 14 | -6 | 606 | -567 |
| 14 | -4 | 334 | -331 |
| 14 | -3 | 341 | -403 |
| 14 | -1 | 838 | -830 |
| 14 | 0 | 608 | 604 |
| 14 | 3 | 651 | 651 |
| 14 | 4 | 578 | 590 |
| 14 | 6 | 440 | -441 |
| 15 | -5 | 391 | 363 |
| 15 | -4 | 405 | 313 |
| 15 | -3 | 466 | 436 |
| 15 | -2 | 346 | 381 |
| 15 | 0 | 294 | 217 |
| 15 | 1 | 899 | -855 |
| 15 | 4 | 419 | -425 |
| 16 | -4 | 391 | -423 |
| 16 | -1 | 793 | -853 |
| 16 | 0 | 388 | 439 |
| 16 | 1 | 473 | 463 |
| 16 | 2 | 483 | 364 |
| 16 | 3 | 341 | 327 |
| 17 | -4 | 336 | 273 |
| 17 | -3 | 400 | 419 |
| 17 | 1 | 516 | -504 |
| 18 | -1 | 409 | -330 |
| 18 | 2 | 658 | 545 |
| H | 3 | | |
| 0 | -5 | 2481 | -2338 |
| 0 | -4 | 564 | 635 |
| 0 | -2 | 613 | 415 |
| 0 | 2 | 4169 | -3411 |
| 0 | 4 | 2204 | -1755 |
| 0 | 5 | 698 | -581 |
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| 2 | -2 | 1967 | 1961 |
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| 3 | -5 | 485 | 477 |
| 3 | -2 | 386 | -307 |
| 3 | -1 | 1326 | -1461 |
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| 4 | -1 | 907 | -871 |
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| 4 | 2 | 1079 | 1163 |
| 4 | 3 | 712 | -745 |
| 4 | 4 | 1401 | -1483 |
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| 4 | 6 | 544 | -496 |
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| 5 | -1 | 1505 | -1540 |
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| 5 | 2 | 1844 | 1925 |
| 5 | 3 | 452 | 464 |
| 5 | 4 | 999 | 1072 |
| 5 | 5 | 516 | 544 |
| 5 | 6 | 497 | -468 |
| 5 | 7 | 447 | 526 |
| 6 | -8 | 367 | -232 |
| 6 | -7 | 705 | -663 |
| 6 | -5 | 395 | 427 |
| 6 | -4 | 452 | -452 |
| 6 | -3 | 386 | 454 |
| 6 | -1 | 630 | 594 |
| 6 | 0 | 1077 | 1157 |
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| 6 | 2 | 1079 | 1144 |
| 6 | 3 | 952 | -1026 |
| 6 | 4 | 1155 | -1245 |
| 6 | 5 | 537 | -504 |
| 6 | 7 | 549 | 549 |
| 7 | -5 | 978 | 996 |
| 7 | -4 | 570 | -634 |
| 7 | -2 | 1392 | -1378 |
| 7 | -1 | 1001 | -1072 |
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| 7 | 2 | 1373 | 1381 |
| 7 | 4 | 1155 | 1184 |
| 7 | 7 | 379 | 284 |
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| 8 | -6 | 398 | -379 |
| 8 | -5 | 341 | 473 |
| 8 | -3 | 374 | 314 |
| 8 | -2 | 847 | -899 |
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| 8 | 4 | 445 | -531 |
| 8 | 7 | 485 | 604 |
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| 9 | -5 | 658 | 664 |
| 9 | -4 | 952 | -992 |
| 9 | -2 | 985 | -977 |
| 9 | -1 | 400 | -337 |
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| 9 | 2 | 1075 | 1146 |
| 9 | 4 | 712 | 760 |
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| 10 | -3 | 727 | 798 |
| 10 | -2 | 587 | -617 |
| 10 | -1 | 724 | 736 |
| 10 | 0 | 317 | 306 |
| 10 | 1 | 604 | -599 |
| 10 | 2 | 521 | -499 |
| 10 | 3 | 1610 | -1647 |
| 11 | -7 | 310 | 267 |
| 11 | -6 | 386 | 423 |
| 11 | -4 | 722 | -793 |
| 11 | -3 | 308 | 330 |
| 11 | -2 | 769 | -759 |
| 11 | -1 | 393 | 351 |
| 11 | 0 | 308 | 340 |
| 11 | 2 | 1030 | 1077 |
| 11 | 4 | 338 | 464 |
| 12 | -4 | 374 | -373 |
| 12 | -3 | 885 | 913 |
| 12 | -1 | 322 | 347 |
| 12 | 0 | 613 | -596 |
| 12 | 3 | 1238 | -1267 |
| 13 | -5 | 308 | -224 |
| 13 | -4 | 483 | -509 |
| 13 | -2 | 791 | -732 |
| 13 | -1 | 578 | 578 |
| 13 | 2 | 663 | 662 |
| 14 | -3 | 440 | 497 |
| 14 | -2 | 338 | 388 |
| 14 | -1 | 355 | 336 |
| 14 | 0 | 968 | -918 |
| 14 | 1 | 405 | -385 |
| 14 | 3 | 578 | -509 |
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| 15 | -3 | 303 | 124 |
| 15 | -2 | 554 | -522 |
| 15 | -1 | 566 | 538 |
| 15 | 2 | 450 | 396 |
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| 17 | -1 | 393 | 346 |
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| 0 | 4 | 729 | 675 |
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| 1 | -1 | 2201 | 2180 |
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| 2 | -2 | 1264 | -1294 |
| 2 | 0 | 1288 | -1323 |
| 2 | 1 | 968 | 971 |
| 2 | 2 | 1001 | 1069 |
| 2 | 4 | 746 | 761 |
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| 8 | 1 | 488 | 531 |
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| 9 | -5 | 495 | 537 |
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| 12 | 1 | 417 | 411 |
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| 13 | -3 | 454 | 435 |
| 13 | -1 | 705 | -737 |
| 13 | 0 | 336 | -358 |
| 13 | 2 | 601 | -565 |
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| 16 | 1 | 443 | 464 |
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| 1 | -1 | 892 | 1007 |
| 1 | 0 | 544 | 498 |
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| 2 | 3 | 469 | 470 |
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| 3 | -6 | 573 | 536 |
| 3 | -5 | 658 | -707 |
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| 3 | 3 | 495 | 517 |
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| 6 | 2 | 1378 | -1491 |
| 6 | 3 | 696 | 722 |
| 6 | 4 | 559 | 539 |
| 6 | 5 | 672 | 721 |
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| 7 | -5 | 734 | -753 |
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| 7 | -3 | 478 | -493 |
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| 7 | 0 | 826 | 847 |
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| 8 | 2 | 331 | -337 |
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| 8 | 5 | 592 | 546 |
| 8 | 5 | 521 | 505 |
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| 9 | -5 | 627 | -635 |
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| 9 | -2 | 1723 | 1771 |
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| 9 | 4 | 570 | -592 |
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| 10 | 2 | 381 | 406 |
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| 11 | -2 | 1304 | 1372 |
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| 11 | 2 | 473 | -476 |
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| 12 | -3 | 684 | -722 |
| 12 | -1 | 554 | -556 |
| 12 | 0 | 426 | 428 |
| 12 | 1 | 376 | -321 |
| 12 | 3 | 1072 | 1398 |
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| 13 | -2 | 805 | 792 |
| 13 | -1 | 535 | -491 |
| 13 | 1 | 324 | -278 |
| 13 | 2 | 453 | -443 |
| 13 | 4 | 409 | -427 |
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| 14 | -1 | 514 | -559 |
| 14 | 0 | 551 | 565 |
| 14 | 2 | 376 | 327 |
| 14 | 3 | 388 | 387 |
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| 15 | -1 | 454 | -370 |
| 15 | 0 | 375 | 359 |
| 15 | 1 | 447 | -334 |
| 16 | -1 | 398 | -414 |
| H | 10 | | |
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| 1 | 5 | 499 | 569 |
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| 2 | -8 | 542 | -484 |
| 2 | -6 | 1259 | -1199 |
| 2 | -5 | 663 | -594 |
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| 2 | -3 | 438 | 361 |
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| 2 | 4 | 1086 | -1100 |
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| 4 | -6 | 954 | -983 |
| 4 | -4 | 852 | -879 |
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| 4 | -2 | 907 | 903 |
| 4 | -1 | 578 | 607 |
| 4 | 1 | 447 | -437 |
| 4 | 2 | 535 | -634 |
| 4 | 3 | 471 | -346 |
| 4 | 4 | 660 | -664 |
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| 5 | -3 | 381 | -350 |
| 5 | -2 | 710 | -766 |
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| 6 | -6 | 691 | -698 |
| 6 | -5 | 483 | 473 |
| 6 | -4 | 355 | -405 |
| 6 | -3 | 819 | 778 |
| 6 | -2 | 1034 | 1073 |
| 6 | -1 | 748 | 810 |
| 6 | 1 | 528 | -612 |
| 6 | 2 | 459 | -392 |
| 6 | 5 | 578 | 647 |
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| 7 | -2 | 1084 | -1079 |
| 7 | -1 | 488 | -633 |
| 7 | 0 | 982 | 1007 |
| 7 | -4 | 336 | -242 |
| 7 | 1 | 523 | -505 |
| 7 | 3 | 556 | 580 |
| 7 | 6 | 755 | -776 |
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| 8 | -6 | 537 | -555 |
| 8 | -5 | 553 | 592 |
| 8 | -3 | 932 | 970 |
| 8 | -2 | 601 | 633 |
| 8 | 1 | 492 | -560 |
| 8 | 5 | 379 | 361 |
| 9 | -8 | 566 | 648 |
| 9 | -5 | 365 | -472 |
| 9 | -4 | 395 | -415 |
| 9 | -2 | 391 | -495 |
| 9 | -1 | 620 | -587 |
| 9 | 0 | 320 | 163 |
| 9 | 2 | 783 | 750 |
| 9 | 4 | 374 | -279 |
| 9 | 5 | 381 | 346 |
| 9 | 6 | 630 | -679 |
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| 11 | -2 | 367 | -374 |
| 11 | 2 | 1015 | 1005 |
| 11 | 4 | 405 | -478 |
| 12 | -6 | 454 | 436 |
| 12 | -5 | 334 | 274 |
| 12 | -3 | 757 | 738 |
| 12 | -1 | 400 | -370 |
| 12 | 1 | 381 | -399 |
| 13 | -4 | 592 | -570 |
| 13 | -3 | 544 | -522 |
| 13 | 2 | 547 | 541 |
| 14 | -3 | 350 | 332 |
| 14 | 1 | 438 | -427 |
| 15 | -4 | 381 | -285 |
| 15 | 0 | 450 | 515 |
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| 0 | -2 | 1375 | -1449 |
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| 0 | 2 | 530 | 669 |
| 0 | 4 | 476 | 495 |
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| 1 | 7 | 457 | 464 |
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| 2 | -4 | 1669 | -1715 |
| 2 | -3 | 1148 | 1160 |
| 2 | -2 | 1155 | -1171 |
| 2 | -1 | 587 | 661 |
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| 2 | 2 | 1060 | 1137 |
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| 3 | 3 | 873 | -880 |
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| 4 | -2 | 471 | -465 |
| 4 | -1 | 1385 | 1400 |
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| 5 | -3 | 1586 | 1631 |
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| 5 | 1 | 585 | -701 |
| 5 | 3 | 447 | -451 |
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| 6 | -3 | 457 | 462 |
| 6 | -2 | 372 | -303 |
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**Table II.** (Continued)

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| 12 | 3 | 620 | -608 |
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| 13 | -3 | 379 | -389 |
| 13 | -2 | 596 | -547 |
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| 14 | -1 | 336 | 540 |
| 15 | -3 | 374 | -376 |
| 15 | 0 | 436 | -407 |
| 15 | 1 | 445 | 373 |
| H | 12 | | |
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| 3 | 3 | 866 | -846 |
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| 5 | 3 | 563 | -714 |
| 6 | -7 | 781 | 812 |
| 6 | -4 | 781 | 700 |
| 6 | -2 | 850 | -846 |
| 6 | -1 | 499 | -516 |
| 6 | 1 | 830 | 741 |
| 6 | 3 | 388 | 440 |
| 7 | -8 | 670 | -679 |
| 7 | -6 | 440 | -426 |
| 7 | -2 | 544 | 639 |
| 7 | 0 | 544 | -541 |
| 7 | 1 | 523 | 521 |
| 7 | 2 | 478 | -473 |
| 7 | 5 | 462 | -438 |
| 8 | -7 | 904 | 924 |
| 8 | -3 | 436 | -448 |
| 8 | 0 | 495 | -560 |
| 8 | 1 | 750 | 817 |
| 9 | -2 | 431 | 481 |
| 9 | 2 | 715 | -713 |
| 10 | -7 | 672 | 590 |
| 10 | -3 | 757 | -858 |
| 10 | 1 | 589 | 609 |
| 11 | 2 | 862 | -870 |
| 12 | -3 | 810 | -832 |
| 12 | 1 | 473 | 395 |
| 13 | 2 | 533 | -515 |
| 14 | -3 | 367 | -319 |
| H | 13 | | |
| 0 | -4 | 1082 | 1152 |
| 0 | -2 | 1955 | 2134 |
| 0 | 0 | 440 | -467 |
| 1 | -7 | 481 | 607 |
| 1 | -5 | 963 | -997 |
| 1 | -3 | 954 | -945 |
| 1 | -1 | 1332 | -1345 |
| 1 | 1 | 528 | 448 |
| 1 | 3 | 962 | 959 |
| 2 | -5 | 657 | 571 |
| 2 | -4 | 1037 | 1372 |
| 2 | -2 | 1569 | 1679 |
| 2 | -1 | 573 | -593 |
| 2 | 1 | 424 | -448 |
| 2 | 2 | 717 | -809 |
| 2 | 3 | 428 | 335 |
| 3 | -8 | 509 | -506 |
| 3 | -3 | 1508 | -1521 |
| 3 | -1 | 703 | -755 |
| 3 | 2 | 862 | 848 |
| 3 | 3 | 793 | 814 |
| 4 | -8 | 433 | -502 |
| 4 | -5 | 940 | 961 |
| 4 | -4 | 966 | 1312 |
| 4 | -2 | 762 | 744 |
| 4 | -1 | 904 | -852 |
| 4 | 2 | 933 | -946 |
| 5 | -5 | 743 | -690 |
| 5 | -3 | 1392 | -1483 |
| 5 | 0 | 952 | 918 |
| 5 | 2 | 436 | 438 |
| 5 | 3 | 492 | 473 |
| 6 | -8 | 502 | -409 |
| 6 | -7 | 471 | 409 |
| 6 | -5 | 734 | 783 |
| 6 | -4 | 447 | 341 |
| 6 | -3 | 362 | 317 |
| 6 | -1 | 1025 | -1042 |
| 6 | 0 | 419 | 378 |
| 6 | 1 | 646 | -591 |
| 6 | 2 | 601 | -629 |
| 7 | -6 | 873 | -887 |
| 7 | -4 | 490 | -439 |
| 7 | -3 | 741 | -816 |
| 7 | 0 | 1103 | 1130 |
| 7 | 1 | 568 | 576 |
| 8 | -7 | 485 | 599 |
| 8 | -5 | 618 | 624 |
| 8 | -1 | 881 | -895 |
| 8 | 1 | 556 | -716 |
| 9 | -6 | 573 | -625 |
| 9 | -4 | 727 | -716 |
| 9 | -2 | 490 | 432 |
| 9 | 0 | 888 | 848 |
| 9 | 1 | 530 | 452 |
| 10 | -5 | 620 | 544 |
| 10 | -1 | 445 | -429 |
| 10 | 0 | 350 | -218 |
| 10 | 1 | 854 | -827 |
| 11 | -4 | 907 | -930 |
| 11 | -2 | 615 | 626 |
| 11 | 0 | 627 | 610 |
| 12 | -5 | 457 | 506 |
| 12 | 1 | 596 | -627 |
| 13 | -4 | 478 | -466 |
| 13 | -3 | 381 | 307 |
| 13 | 0 | 471 | 397 |
| 13 | 1 | 511 | -523 |
| 14 | -2 | 433 | -315 |
| 14 | -1 | 402 | -373 |
| H | 14 | | |
| 0 | -8 | 630 | 641 |
| 0 | -6 | 499 | -596 |
| 0 | 0 | 769 | 849 |
| 0 | 4 | 485 | -531 |
| 1 | -7 | 556 | -496 |
| 1 | -6 | 395 | 235 |
| 1 | -5 | 393 | 365 |
| 1 | -1 | 1096 | -1214 |
| 1 | 1 | 454 | -487 |
| 1 | 5 | 620 | 552 |
| 2 | -8 | 504 | 456 |
| 2 | -1 | 445 | -455 |
| 2 | 0 | 748 | 762 |
| 2 | 3 | 552 | -655 |
| 2 | 4 | 599 | -553 |
| 3 | -6 | 528 | 546 |
| 3 | -5 | 478 | 539 |
| 3 | -1 | 554 | -613 |
| 3 | 1 | 585 | -510 |
| 3 | 2 | 665 | 534 |
| 3 | 3 | 464 | 391 |
| 3 | 5 | 575 | 448 |
| 4 | -8 | 421 | 196 |
| 4 | -4 | 547 | -633 |
| 4 | -2 | 473 | 480 |
| 4 | 0 | 658 | 584 |
| 4 | 3 | 637 | -686 |
| 4 | 4 | 464 | -547 |
| 5 | -6 | 587 | 599 |
| 5 | -5 | 407 | 433 |
| 5 | -2 | 476 | -536 |
| 5 | 0 | 424 | 377 |
| 5 | 1 | 563 | -633 |
| 5 | 2 | 717 | 588 |
| 5 | 4 | 481 | 397 |
| 6 | -7 | 623 | -548 |
| 6 | -4 | 663 | -696 |
| 6 | -2 | 511 | 537 |
| 6 | 0 | 492 | 587 |
| 6 | 1 | 518 | -539 |
| 6 | 3 | 471 | -426 |
| 7 | -2 | 405 | -420 |
| 7 | 1 | 481 | -404 |
| 7 | 2 | 514 | 541 |
| 7 | 4 | 443 | 467 |
| 8 | -7 | 563 | -541 |
| 8 | 0 | 424 | 523 |
| 8 | 1 | 684 | -651 |
| 9 | 2 | 630 | 567 |
| 10 | -5 | 497 | -458 |
| 10 | -3 | 623 | 598 |
| 10 | 1 | 466 | -486 |
| 11 | 2 | 618 | 489 |
| 12 | -3 | 587 | 608 |
| 13 | -2 | 417 | -269 |
| H | 15 | | |
| 0 | -6 | 786 | 814 |
| 0 | -2 | 1589 | -1497 |
| 0 | 0 | 433 | -391 |
| 0 | 2 | 547 | 620 |
| 1 | -7 | 890 | -1011 |
| 1 | -1 | 1053 | 1132 |
| 2 | -6 | 682 | 719 |
| 2 | -5 | 478 | -408 |
| 2 | -3 | 471 | -452 |
| 2 | -2 | 1167 | -1246 |
| 2 | 1 | 432 | 322 |
| 2 | 2 | 398 | 420 |
| 3 | -7 | 547 | -554 |
| 3 | -4 | 573 | 541 |
| 3 | -3 | 736 | 762 |
| 3 | -1 | 831 | 792 |
| 3 | 2 | 613 | -577 |
| 3 | 3 | 682 | -649 |
| 4 | -5 | 755 | -717 |
| 4 | -3 | 828 | -783 |
| 4 | -2 | 677 | -746 |
| 4 | 0 | 478 | -467 |
| 4 | 1 | 471 | 446 |
| 5 | -6 | 632 | 661 |
| 5 | -5 | 686 | -616 |
| 5 | -3 | 810 | 853 |
| 5 | -1 | 466 | 422 |
| 5 | 2 | 450 | -313 |
| 5 | 3 | 596 | -512 |
| 6 | -5 | 794 | -706 |
| 6 | -3 | 836 | -810 |
| 6 | 1 | 483 | 440 |
| 7 | -6 | 743 | 641 |
| 7 | -4 | 656 | 640 |
| 7 | -3 | 407 | 391 |
| 7 | -2 | 547 | 492 |
| 7 | -1 | 445 | 418 |
| 7 | 0 | 717 | -710 |
| 8 | -5 | 611 | -668 |
| 8 | -3 | 561 | -505 |
| 8 | 1 | 459 | 520 |
| 9 | -4 | 838 | 855 |
| 9 | -1 | 395 | 361 |
| 9 | 0 | 701 | -675 |
| 10 | -5 | 613 | -569 |
| 10 | -3 | 348 | -290 |
| 10 | 1 | 608 | 539 |
| 11 | -4 | 866 | 819 |
| H | 16 | | |
| 0 | 0 | 753 | -724 |
| 0 | 2 | 447 | -475 |
| 1 | -7 | 552 | 474 |
| 1 | -3 | 431 | -425 |
| 1 | -1 | 963 | 655 |
| 1 | 1 | 793 | 808 |
| 2 | 0 | 644 | -639 |
| 2 | 2 | 569 | -537 |
| 3 | -2 | 478 | 526 |
| 3 | 1 | 689 | 593 |
| 3 | 2 | 405 | -314 |
| 4 | -4 | 653 | -519 |
| 4 | 0 | 454 | -362 |
| 4 | 2 | 556 | -503 |
| 5 | -2 | 525 | 579 |
| 5 | 2 | 455 | -446 |
| 6 | -4 | 521 | 535 |
| 6 | -1 | 663 | -515 |
| 6 | 2 | 495 | -259 |
| 8 | -1 | 634 | -639 |
| 10 | -3 | 407 | -382 |
| H | 17 | | |
| 0 | -6 | 795 | -802 |
| 0 | -4 | 556 | -459 |
| 0 | -2 | 653 | 597 |
| 0 | 0 | 582 | 559 |
| 1 | -5 | 407 | 410 |
| 1 | -1 | 632 | -621 |
| 2 | -6 | 748 | -708 |
| 2 | -3 | 509 | 461 |
| 2 | -2 | 516 | 603 |
| 2 | 3 | 511 | 491 |
| 3 | -5 | 618 | 653 |
| 3 | -4 | 417 | -464 |
| 3 | -1 | 440 | -408 |
| 4 | -6 | 544 | -476 |
| 4 | -3 | 691 | 718 |
| 4 | -2 | 452 | 328 |
| 5 | -5 | 623 | 615 |
| 5 | -4 | 518 | -451 |
| 6 | -5 | 499 | 348 |
| 6 | -3 | 656 | 549 |
| 7 | -5 | 462 | 284 |
| 7 | -4 | 447 | -362 |
| 7 | -2 | 667 | -580 |
| 9 | -4 | 523 | -487 |
| 9 | -2 | 544 | -428 |
| H | 18 | | |
| 0 | 0 | 412 | 422 |
| 1 | -3 | 533 | 556 |
| 1 | -1 | 710 | -719 |
| 2 | -3 | 381 | 390 |
| 2 | 2 | 476 | 449 |
| 3 | -3 | 507 | 487 |
| 3 | -2 | 405 | -386 |
| 3 | 1 | 554 | -549 |
| 4 | -4 | 450 | -509 |
| 4 | 2 | 466 | 484 |
| 5 | -4 | 443 | 128 |
| 5 | -2 | 481 | -371 |
| 5 | 0 | 473 | -394 |
| 6 | -1 | 533 | 492 |
| 7 | -2 | 448 | -290 |
| 8 | -1 | 739 | 624 |
| H | 19 | | |
| 0 | -4 | 421 | 434 |
| 0 | 0 | 542 | -570 |
| 1 | -5 | 457 | -470 |
| 2 | -4 | 511 | 512 |
| 2 | 0 | 421 | -467 |
| 4 | -4 | 460 | 401 |
| 4 | -3 | 462 | -334 |
| H | 20 | | |
| 0 | -2 | 426 | 406 |
| 1 | -1 | 514 | -402 |

**Table III.** $Pt(CH_3)_3(C_6H_5CH_3AsCH_2CH_2AsCH_3C_6H_5)I$.

(i) Bond lengths (Å) and their e.s.d's.

| | | |
|---|---|---|
| Platinum-ligand bonds: | | |
| Pt-I | 2.771(2) | |
| Pt-As(1) | 2.461(3) | |
| Pt-As(2) | 2.450(3) | |
| Pt-C(1) | 2.12(3) | |
| Pt-C(2) | 2.13(3) | |
| Pt-C(3) | 2.09(3) | |
| Arsenic-carbon bonds: | | |
| As(1)-C(4) | 1.97(3) | |
| As(1)-C(6) | 1.95(3) | |
| As(1)-C(8) | 1.94(2) | |
| As(2)-C(5) | 2.02(3) | |
| As(2)-C(7) | 1.96(2) | |
| As(2)-C(14) | 1.93(2) | |
| Carbon-carbon bonds: | | |
| C(6)-C(7) | 1.52(4) | |
| C(8)-C(9) | 1.35(3) | |
| C(9)-C(10) | 1.40(3) | |
| C(10)-C11) | 1.33(4) | |
| C(11)-C(12) | 1.32(5) | |
| C(12)-C(13) | 1.38(5) | Mean value of the $(C-C)_{penyl}$ distance = 1.39 Å |
| C(13)-C(8) | 1.42(4) | |
| C(14)-C(15) | 1.40(4) | |
| C(15)-C(16) | 1.41(4) | |
| C(16)-C(17) | 1.40(4) | |
| C(17)-C(18) | 1.43(4) | |
| C(18)-C(19) | 1.41(4) | |
| C(19)-C(14) | 1.38(4) | |

(ii) Bond angles (degrees) and their e.s.d's.

| | | |
|---|---|---|
| I-Pt-As(1) | 89.9(1) | |
| I-Pt-As(2) | 89.9(1) | |
| I-Pt-C(1) | 90.6(9) | |
| I-Pt-C(2) | 91.4(9) | |
| I-Pt-C(3) | 171.0(8) | |
| As(1)-Pt-As(2) | 83.1(1) | |
| As(1)-Pt-C(1) | 177.3(8) | |
| As(1)-Pt-C(2) | 92.7(9) | |
| As(1)-Pt-C(3) | 95.6(8) | |
| As(2)-Pt-C(1) | 94.3(9) | |
| As(2)-Pt-C(2) | 175.6(9) | |
| As(2)-Pt-C(3) | 97.9(8) | |
| C(1)-Pt-C(2) | 90.0(12) | |
| C(1)-Pt-C(3) | 84.3(12) | |
| C(2)-Pt-C(3) | 81.3(12) | |
| Pt-As(1)-C(4) | 118.5(9) | |
| Pt-As(1)-C(6) | 109.6(8) | |
| Pt-As(1)-C(8) | 115.1(7) | |
| Pt-As(2)-C(5) | 116.5(8) | |
| Pt-As(2)-C(7) | 105.4(7) | |
| Pt-As(2)-C(14) | 123.3(7) | |
| C(4)-As(1)-C(6) | 103.0(12) | |
| C(4)-As(1)-C(8) | 104.3(11) | |
| C(6)-As(1)-C(8) | 104.9(11) | |
| C(5)-As(2)-C(7) | 99.2(10) | |
| C(5)-As(2)-C(14) | 103.7(10) | |
| C(7)-As(2)-C(14) | 105.6(10) | |
| As(1)-C(6)-C(7) | 112.1(17) | |
| As(2)-C(7)-C(6) | 111.8(17) | |
| $(C-C-C)_{penyl}$ | 120.0(30) | mean value |

measurements, the unit cell parameters being determined from four circle setting of 12 reflections (MoK$\alpha$ $\lambda = 0.7107$ Å). The unit cell is $a$ = 17.008(6), $b$ = 15.736(5), $c$ = 8.393(3) Å, $\beta$ = 101.37(3)°;* For $PtIAs_2C_{19}H_{29}$: M = 729.3, U = 2202 Å$^3$, $D_m$ = 2.183 g . cm$^{-3}$ (flotation), Z = 4, $D_c$ = 2.190 g . cm$^{-3}$, F(000) = 1360. The absorption coefficient $\mu$(Mo-K$\alpha$) = 111.7 cm$^{-1}$. The systematic absences {h0l} for l = 2n+1 and {0k0} for k = 2n+1 establish the space group $P2_1/c$.

Intensity measurements were based on an $\omega$-2$\theta$ scan routine, background measurements at each extremity of a scan being made with stationary crystal and counter. Each background count was over 25 or 50 seconds, each peak count being accumulated over 50 steps of 0.01° with 1 (or 2) second counts respectively at each step.

Of the 3876 independent reflections measured (4° ≤ 2$\theta$ ≤ 50°), 1998 were judged to be significant ($I \geq 3.0 \sigma(I)$). These were corrected for geometrical effects and, using the method of Wells, for absorption. Stability of the crystal and of the instrument was monitored by following the intensities of 3 reference reflections every 100 reflections.

The platinum, iodine and arsenic atoms were obtained, after some difficulties, from a Patterson synthesis after which the structure determination was based on a straightforward application of the difference Fourier method. Initial refinement of atomic para-

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(*) Here as elsewhere, the figures in parentheses refer to the e.s.d's of the observation referred to the last significant figure.

meters was via block-diagonal least-squares methods but refinement of atomic positions, anisotropic temperature factors for the platinum, iodine and arsenic atoms and isotropic temperature factors for the remaining non-hydrogen atoms was completed by three full-matrix least-squares cycles. 22 reflections, apparently suffering from extinction effects, were excluded from these terminal cycles and convergence was to $R_1 = 0.06$ and $R_2 = 0.08$. The weighting scheme was $w = (55.03-0.61 \,.\, |F_{obs}| + 0.005 \,.\, |F_{obs}|^2)^{-1}$ and was obtained from a least-squares fit of $(|F_{obs}|-|F_{cal}|)^2$ as a function of $|F_{obs}|$. In the structure factor calculations, the atomic scattering factors of Cromer and Waber[2] were used for platinum, iodine, arsenic and carbon atoms.

Atomic parameters and their e.s.d's are listed in Table I, observed and calculated structure factors being collected in Table II. Atom numbering and some important intramolecular bond lengths and bond angles are shown in Figure 1, a more complete listing of molecular parameters forming Table III.

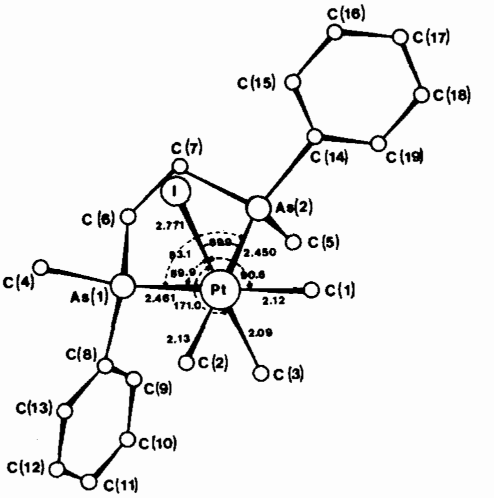


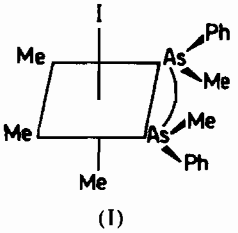
Figure 1. $Pt(CH_3)_3(C_6H_5CH_3AsCH_2CH_2AsCH_3C_6H_5)I$. Numbering of atoms and some bond lengths and bond angles. The molecule is viewed along the *c* axis.

## Discussion

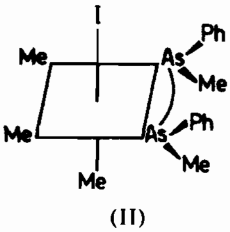
Two general features of the molecular geometry deserve emphasis.

(i) *The metal-ligand bond lengths.* There seem to be remarkably few (if any) really accurate measurements of the platinum(IV)-iodine bond length. In di-iodo-di-(*o*-phenylenebis(dimethylarsine)) platinum(II)[3] the platinum-arsenic and platinum-iodine bond lengths are 2.38Å and 3.50 Å respectively; the latter value is obviously not comparable with the present result, the bond being essentially "ionic" in the platinum(II) complex. The covalent radii of arsenic, platinum(II) and iodine atoms are *ca.* 1.20, 1.30 and 1.33 Å respectively; the platinum-carbon bond lengths are thus close to the sum of covalent radii (2.07 Å) and the mean value of 2.11 Å is not significantly different from those found in acetylacetonyl-2,2'-bipyridyltrimethylplatinum(IV)[4] (2.05 Å), in salicylaldehydatotrimethylplatinum(IV)[5] (2.03 Å), or indeed, the platinum(II)-carbon bond length of 2.11 Å in the bis-acetylacetonatochloroplatinate(II) anion.[6] That the platinum-arsenic bond length is also close to the sum of covalent radii is fortuitous; it is a general observation that the metal-arsenic and metal-phosphorus bond lengths are normally 0.10-0.15 Å shorter than the sum of covalent radii in the absence of strong *trans*-influencing ligands. Whatever the reason for the "normal" foreshortening of metal-arsenic bonds, it is offset in the present structure by the lengthening of the bonds *trans* to methyl groups. Elsewhere we have estimated the *trans*-influence of a σ-bonded carbon atom in planar and octahedral complexes as approximately 0.1 Å. This is essentially the difference between the sum of the platinum and iodine covalent radii (2.63 Å) and the observed value.

(ii) *The chelate ring geometry and the conformation of substituents.* The chelate ring has a distorted envelope conformation. The mean plane containing Pt, As(1), As(2), C(1) and C(2) atoms has direction cosines 0.8376, 0.3252, –0.5955 referred to the crystallographic axes *a, b,* and *c*; the r.m.s. deviation of these atoms from the plane is 0.01 Å. The C(6) atom is displaced –0.21 Å from the plane, C(7) being –0.79 Å (both are bent towards the iodine atom). The two methyl carbon atoms C(4) and C(5) are displaced –1.43 Å and 1.82 Å respectively, the phenyl carbon atoms C(8) and C(14) having equivalent displacements of 1.64 Å and –0.88 Å so that the *dl* form of the complex is established as (I), the *meso* form as (II):



(I)



(II)

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