

## Supporting Information

### The Solely Motif-Doped $\text{Au}_{36-x}\text{Ag}_x(\text{SPh-tBu})_{24}$ ( $x=1-8$ ) Nanoclusters:

#### X-ray Crystal Structure and Optical Properties

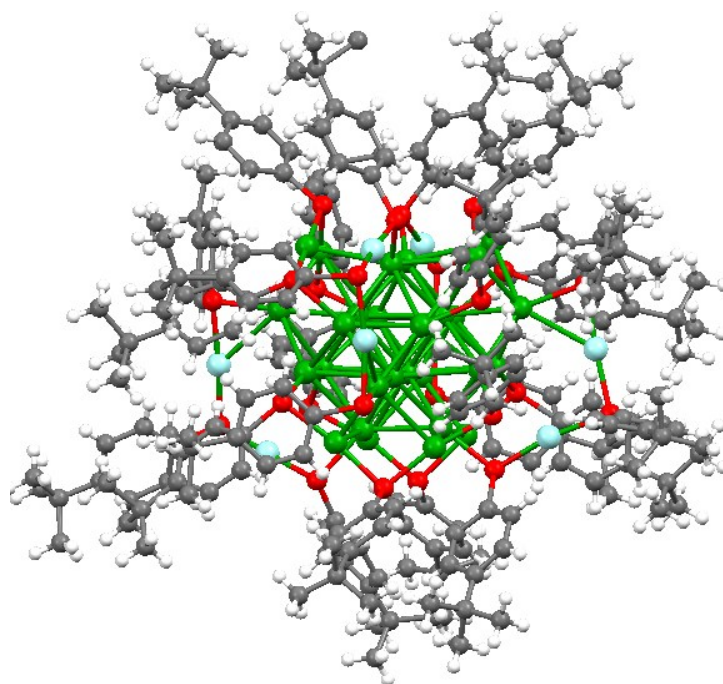
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#### Crystallization of $[\text{Au}_{36-x}\text{Ag}_x(\text{SPh-tBu})_{24}]$ nanocluster

Single crystal of  $[\text{Au}_{36-x}\text{Ag}_x(\text{SPh-tBu})_{24}]$  nanocluster was grown for 3-4 days in  $\text{CH}_2\text{Cl}_2$ /methanol. Dark crystals were collected and the structure of  $[\text{Au}_{36-x}\text{Ag}_x(\text{SPh-tBu})_{24}]$  was determined.



**Figure S1.** The total structure of the  $[\text{Au}_{36-x}\text{Ag}_x(\text{SPh-tBu})_{24}]$  nanocluster. Color labels: green = Au, red = S, light blue =  $\text{Au}_{0.5}\text{Ag}_{0.5}$ , gray C; white H, pure O.

**Table S1. Assignments of the peaks**

| Assigned Formula                                                                           | Experimental Mass |
|--------------------------------------------------------------------------------------------|-------------------|
| $\text{Au}_{35}\text{Ag}(\text{C}_{10}\text{H}_{13}\text{S})_{23}$                         | 10802.07          |
| $\text{Au}_{34}\text{Ag}_2(\text{C}_{10}\text{H}_{13}\text{S})_{23}$                       | 10713.44          |
| $\text{Au}_{34}\text{Ag}_2(\text{C}_{10}\text{H}_{13}\text{S})_{23} - 2(\cdot\text{CH}_3)$ | 10683.56          |
| $\text{Au}_{33}\text{Ag}_3(\text{C}_{10}\text{H}_{13}\text{S})_{23}$                       | 10624.54          |
| $\text{Au}_{33}\text{Ag}_3(\text{C}_{10}\text{H}_{13}\text{S})_{23} - 3(\cdot\text{CH}_3)$ | 10580.03          |
| $\text{Au}_{32}\text{Ag}_4(\text{C}_{10}\text{H}_{13}\text{S})_{23}$                       | 10535.38          |
| $\text{Au}_{32}\text{Ag}_4(\text{C}_{10}\text{H}_{13}\text{S})_{23} - 2(\cdot\text{CH}_3)$ | 10504.98          |
| $\text{Au}_{31}\text{Ag}_5(\text{C}_{10}\text{H}_{13}\text{S})_{23}$                       | 10446.60          |
| $\text{Au}_{30}\text{Ag}_6(\text{C}_{10}\text{H}_{13}\text{S})_{23}$                       | 10357.57          |
| $\text{Au}_{29}\text{Ag}_7(\text{C}_{10}\text{H}_{13}\text{S})_{23}$                       | 10268.29          |
| $\text{Au}_{28}\text{Ag}_8(\text{C}_{10}\text{H}_{13}\text{S})_{23}$                       | 10179.40          |

**Table S2: Crystal data and structure refinement for the  $[\text{Au}_{32}\text{Ag}_4(\text{SPh-tBu})_{24}]$  nanocluster.**

|                                   |                                                                          |                          |
|-----------------------------------|--------------------------------------------------------------------------|--------------------------|
| Compound reference                | $[\text{Au}_{32}\text{Ag}_4(\text{SPh-tBu})_{24}]$                       |                          |
| Empirical formula                 | $\text{C}_{240} \text{H}_{312} \text{Ag}_4 \text{Au}_{32} \text{S}_{24}$ |                          |
| Formula weight                    | 10700.73g/mol                                                            |                          |
| Temperature                       | 293.15 K                                                                 |                          |
| Wavelength                        | 0.71073 Å                                                                |                          |
| Crystal system                    | Monoclinic                                                               |                          |
| Space group                       | C 1 2/c 1                                                                |                          |
| Unit cell dimensions              | A=58.539(4) Å                                                            | $\alpha=90^\circ$        |
|                                   | B=34.472(2) Å                                                            | $\beta=91.2322(9)^\circ$ |
|                                   | C=41.488(3) Å                                                            | $\gamma=90^\circ$        |
| Volume                            | 83701(10) Å <sup>3</sup>                                                 |                          |
| Z                                 | 12                                                                       |                          |
| Density (calculated)              | 2.547 Mg m <sup>-3</sup>                                                 |                          |
| Absorption coefficient            | 17.244 mm <sup>-1</sup>                                                  |                          |
| F(000)                            | 58224                                                                    |                          |
| Crystal size                      | 0.18 × 0.1 × 0.02 mm <sup>3</sup>                                        |                          |
| Theta range for data collection   | 0.686 to 25.719°                                                         |                          |
| Index ranges                      | -71 ≤ h ≤ 71, -42 ≤ k ≤ 42, -50 ≤ l ≤ 50                                 |                          |
| Reflections collected             | 317544                                                                   |                          |
| Independent reflections           | 79435                                                                    |                          |
| Absorption correction             | Semi-empirical from equivalents                                          |                          |
| Refinement method                 | Full-matrix-block least-squares on F <sup>2</sup>                        |                          |
| Data / restraints / parameters    | 79435 / 2512 / 4158                                                      |                          |
| Goodness-of-fit on F <sup>2</sup> | 1.093                                                                    |                          |
| Final R indices [I > 2σ(I)]       | R1=0.0828, wR2=0.2137                                                    |                          |
| R indices (all data)              | R1=0.1859, wR2=0.2441                                                    |                          |
| Largest diff. peak and hole       | 6.558 and -6.293 e.Å <sup>-3</sup>                                       |                          |

**Table S3: Atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for  $[\text{Au}_{32}\text{Ag}_4(\text{SPh-tBu})_{24}]$ .  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.**

|        | x    | y     | z    | $U(\text{eq})$ |
|--------|------|-------|------|----------------|
| Au(1)  | 3383 | 9922  | 6229 | 23(1)          |
| Au(2)  | 3134 | 10553 | 5911 | 23(1)          |
| Au(3)  | 3321 | 9918  | 5514 | 23(1)          |
| Au(4)  | 3555 | 9349  | 5837 | 27(1)          |
| Au(5)  | 3634 | 10471 | 5828 | 22(1)          |
| Au(6)  | 3379 | 11043 | 5523 | 26(1)          |
| Au(7)  | 3087 | 10482 | 5174 | 31(1)          |
| Au(8)  | 3264 | 9842  | 4854 | 53(1)          |
| Au(9)  | 3546 | 10411 | 5090 | 29(1)          |
| Au(10) | 3904 | 11078 | 5358 | 31(1)          |
| Au(11) | 3836 | 9888  | 5459 | 31(1)          |
| Au(12) | 3545 | 9156  | 5112 | 33(1)          |
| Au(13) | 4095 | 10467 | 5745 | 54(1)          |
| Au(14) | 3956 | 11111 | 6183 | 33(1)          |
| Au(15) | 3445 | 11063 | 6180 | 27(1)          |
| Au(16) | 2935 | 11238 | 6366 | 33(1)          |
| Au(17) | 3230 | 10505 | 6644 | 32(1)          |
| Au(18) | 3441 | 9858  | 6884 | 55(1)          |
| Au(19) | 3684 | 10418 | 6546 | 32(1)          |
| Au(20) | 3913 | 9886  | 6111 | 29(1)          |
| Au(21) | 3665 | 9253  | 6563 | 31(1)          |
| Au(22) | 2880 | 11287 | 5533 | 30(1)          |
| Au(23) | 3083 | 9248  | 6628 | 32(1)          |
| Au(24) | 2881 | 10051 | 6293 | 31(1)          |
| Au(25) | 2679 | 10690 | 6005 | 53(1)          |
| Au(26) | 2799 | 10066 | 5642 | 30(1)          |
| Au(27) | 2970 | 9355  | 5202 | 31(1)          |
| Au(28) | 3090 | 9419  | 5920 | 25(1)          |
| Au(29) | 3636 | 10400 | 7405 | 33(1)          |
| Au(30) | 3606 | 11290 | 6993 | 23(1)          |
| Au(31) | 4510 | 9960  | 5674 | 25(1)          |
| Au(32) | 4174 | 9131  | 5753 | 32(1)          |
| Au(33) | 2451 | 9338  | 6026 | 31(1)          |

|        |      |       |      |       |
|--------|------|-------|------|-------|
| Au(34) | 2219 | 10270 | 6066 | 18(1) |
| Au(35) | 3307 | 11141 | 4614 | 26(1) |
| Au(36) | 3242 | 10256 | 4220 | 23(1) |
| Ag(29) | 3636 | 10400 | 7405 | 33(1) |
| Ag(30) | 3606 | 11290 | 6993 | 23(1) |
| Ag(31) | 4510 | 9960  | 5674 | 25(1) |
| Ag(32) | 4174 | 9131  | 5753 | 32(1) |
| Ag(33) | 2451 | 9338  | 6026 | 31(1) |
| Ag(34) | 2219 | 10270 | 6066 | 18(1) |
| Ag(35) | 3307 | 11141 | 4614 | 26(1) |
| Ag(36) | 3242 | 10256 | 4220 | 23(1) |
| S(1)   | 4014 | 10802 | 6677 | 37(2) |
| S(2)   | 3840 | 8864  | 5906 | 31(2) |
| S(3)   | 4496 | 10627 | 5667 | 41(2) |
| S(4)   | 4552 | 9296  | 5656 | 45(2) |
| S(5)   | 3920 | 11543 | 5756 | 34(2) |
| S(6)   | 3900 | 9416  | 5044 | 33(2) |
| S(7)   | 4003 | 9595  | 6621 | 32(2) |
| S(8)   | 3422 | 11578 | 6560 | 32(2) |
| S(9)   | 3811 | 10996 | 7408 | 55(3) |
| S(10)  | 3367 | 8809  | 6524 | 32(2) |
| S(11)  | 3516 | 9765  | 7451 | 44(2) |
| S(12)  | 2764 | 9621  | 6714 | 32(2) |
| S(13)  | 2761 | 9009  | 5859 | 31(2) |
| S(14)  | 3202 | 9601  | 4307 | 37(2) |
| S(15)  | 2688 | 9817  | 5135 | 28(2) |
| S(16)  | 2102 | 9631  | 6125 | 36(2) |
| S(17)  | 2810 | 10968 | 5049 | 28(2) |
| S(18)  | 2293 | 10922 | 6082 | 37(2) |
| S(19)  | 2904 | 10842 | 6811 | 32(2) |
| S(20)  | 2941 | 11696 | 5962 | 33(2) |
| S(21)  | 3417 | 11464 | 5074 | 31(2) |
| S(22)  | 3909 | 10643 | 4937 | 31(2) |
| S(23)  | 3248 | 10908 | 4095 | 38(2) |
| S(24)  | 3216 | 8837  | 5248 | 36(2) |
| C(1)   | 4282 | 10553 | 6678 | 36(8) |
| C(2)   | 4453 | 10631 | 6470 | 32(8) |

|       |      |       |      |        |
|-------|------|-------|------|--------|
| C(3)  | 4660 | 10455 | 6482 | 34(8)  |
| C(4)  | 4720 | 10207 | 6752 | 46(9)  |
| C(5)  | 4538 | 10116 | 6955 | 55(10) |
| C(6)  | 4318 | 10288 | 6948 | 66(12) |
| C(7)  | 4956 | 10004 | 6773 | 82(8)  |
| C(8)  | 5018 | 9831  | 6446 | 79(8)  |
| C(9)  | 5118 | 10340 | 6874 | 86(9)  |
| C(10) | 4966 | 9703  | 7039 | 87(9)  |
| C(11) | 3766 | 8453  | 5646 | 38(8)  |
| C(12) | 3881 | 8403  | 5368 | 44(9)  |
| C(13) | 3803 | 8100  | 5173 | 56(11) |
| C(14) | 3632 | 7831  | 5260 | 57(11) |
| C(15) | 3533 | 7908  | 5553 | 96(16) |
| C(16) | 3589 | 8238  | 5736 | 44(9)  |
| C(17) | 3554 | 7483  | 5055 | 34(8)  |
| C(18) | 3619 | 7533  | 4700 | 50(10) |
| C(19) | 3303 | 7409  | 5080 | 26(7)  |
| C(20) | 3691 | 7124  | 5218 | 36(8)  |
| C(21) | 4521 | 10767 | 5249 | 36(8)  |
| C(22) | 4534 | 11154 | 5186 | 43(9)  |
| C(23) | 4555 | 11284 | 4858 | 78(13) |
| C(24) | 4587 | 11014 | 4627 | 52(10) |
| C(25) | 4586 | 10611 | 4695 | 62(11) |
| C(26) | 4546 | 10471 | 5006 | 44(9)  |
| C(27) | 4630 | 11138 | 4273 | 60(11) |
| C(28) | 4613 | 11609 | 4222 | 87(15) |
| C(29) | 4875 | 11028 | 4196 | 88(15) |
| C(30) | 4454 | 10955 | 4030 | 76(13) |
| C(31) | 4598 | 9225  | 5235 | 40(9)  |
| C(32) | 4466 | 8972  | 5049 | 56(11) |
| C(33) | 4493 | 8871  | 4714 | 70(12) |
| C(34) | 4673 | 9075  | 4589 | 42(9)  |
| C(35) | 4823 | 9330  | 4760 | 56(11) |
| C(36) | 4776 | 9396  | 5085 | 62(11) |
| C(37) | 4712 | 9021  | 4232 | 84(8)  |
| C(38) | 4547 | 8771  | 4051 | 87(9)  |
| C(39) | 4959 | 8847  | 4168 | 81(9)  |

|       |      |       |      |         |
|-------|------|-------|------|---------|
| C(40) | 4702 | 9436  | 4040 | 89(9)   |
| C(41) | 4192 | 11754 | 5718 | 21(7)   |
| C(42) | 4239 | 12002 | 5443 | 26(7)   |
| C(43) | 4447 | 12179 | 5419 | 39(8)   |
| C(44) | 4617 | 12155 | 5667 | 27(7)   |
| C(45) | 4575 | 11924 | 5926 | 36(8)   |
| C(46) | 4362 | 11715 | 5967 | 33(8)   |
| C(47) | 4851 | 12382 | 5649 | 41(9)   |
| C(48) | 4977 | 12228 | 5314 | 48(10)  |
| C(49) | 4784 | 12825 | 5605 | 49(10)  |
| C(50) | 5010 | 12321 | 5933 | 49(10)  |
| C(51) | 3923 | 9580  | 4646 | 34(8)   |
| C(52) | 4105 | 9824  | 4549 | 23(7)   |
| C(53) | 4126 | 9891  | 4241 | 55(10)  |
| C(54) | 3985 | 9780  | 3990 | 32(8)   |
| C(55) | 3806 | 9537  | 4082 | 43(9)   |
| C(56) | 3767 | 9438  | 4391 | 60(11)  |
| C(57) | 4005 | 9876  | 3613 | 50(10)  |
| C(58) | 4107 | 9491  | 3454 | 59(11)  |
| C(59) | 3777 | 9995  | 3438 | 65(12)  |
| C(60) | 4179 | 10204 | 3581 | 69(12)  |
| C(61) | 4204 | 9206  | 6593 | 33(8)   |
| C(62) | 4151 | 8841  | 6693 | 40(9)   |
| C(63) | 4299 | 8551  | 6675 | 75(13)  |
| C(64) | 4522 | 8597  | 6554 | 66(12)  |
| C(65) | 4576 | 8983  | 6453 | 56(11)  |
| C(66) | 4417 | 9269  | 6456 | 35(8)   |
| C(67) | 4704 | 8259  | 6508 | 66(12)  |
| C(68) | 4731 | 8178  | 6137 | 112(19) |
| C(69) | 4920 | 8406  | 6669 | 78(13)  |
| C(70) | 4609 | 7907  | 6677 | 100(17) |
| C(71) | 3586 | 11973 | 6418 | 22(7)   |
| C(72) | 3807 | 12032 | 6504 | 40(9)   |
| C(73) | 3923 | 12348 | 6367 | 35(8)   |
| C(74) | 3824 | 12607 | 6148 | 32(8)   |
| C(75) | 3597 | 12547 | 6059 | 41(9)   |
| C(76) | 3470 | 12240 | 6202 | 39(9)   |

|        |      |       |      |         |
|--------|------|-------|------|---------|
| C(77)  | 3951 | 12947 | 5986 | 47(9)   |
| C(78)  | 3939 | 12903 | 5619 | 62(11)  |
| C(79)  | 4204 | 12972 | 6095 | 46(9)   |
| C(80)  | 3840 | 13330 | 6096 | 47(10)  |
| C(81)  | 3755 | 11202 | 7795 | 53(10)  |
| C(82)  | 3629 | 11035 | 8026 | 42(9)   |
| C(83)  | 3617 | 11202 | 8344 | 35(8)   |
| C(84)  | 3739 | 11571 | 8399 | 52(10)  |
| C(85)  | 3866 | 11747 | 8169 | 51(10)  |
| C(86)  | 3874 | 11565 | 7843 | 73(13)  |
| C(87)  | 3741 | 11744 | 8745 | 54(10)  |
| C(88)  | 3567 | 11551 | 8935 | 75(13)  |
| C(89)  | 3705 | 12198 | 8723 | 72(13)  |
| C(90)  | 3986 | 11623 | 8908 | 113(19) |
| C(91)  | 3419 | 8478  | 6856 | 52(10)  |
| C(92)  | 3617 | 8239  | 6824 | 42(9)   |
| C(93)  | 3663 | 7973  | 7054 | 47(10)  |
| C(94)  | 3538 | 7940  | 7310 | 52(10)  |
| C(95)  | 3346 | 8170  | 7357 | 45(9)   |
| C(96)  | 3289 | 8455  | 7132 | 45(9)   |
| C(97)  | 3604 | 7601  | 7572 | 66(12)  |
| C(98)  | 3410 | 7585  | 7850 | 49(10)  |
| C(99)  | 3590 | 7225  | 7413 | 71(13)  |
| C(100) | 3833 | 7706  | 7720 | 73(13)  |
| C(101) | 3790 | 9517  | 7486 | 45(9)   |
| C(102) | 3990 | 9710  | 7571 | 51(10)  |
| C(103) | 4183 | 9483  | 7628 | 72(13)  |
| C(104) | 4192 | 9093  | 7603 | 59(11)  |
| C(105) | 3988 | 8908  | 7500 | 55(10)  |
| C(106) | 3789 | 9115  | 7468 | 36(8)   |
| C(107) | 4414 | 8857  | 7654 | 62(11)  |
| C(108) | 4597 | 9025  | 7426 | 51(10)  |
| C(109) | 4475 | 8890  | 8009 | 73(13)  |
| C(110) | 4388 | 8412  | 7585 | 72(13)  |
| C(111) | 2801 | 9816  | 7111 | 45(9)   |
| C(112) | 2672 | 10134 | 7208 | 38(8)   |
| C(113) | 2699 | 10293 | 7513 | 35(8)   |

|        |      |       |      |        |
|--------|------|-------|------|--------|
| C(114) | 2838 | 10089 | 7740 | 42(9)  |
| C(115) | 2947 | 9756  | 7638 | 53(10) |
| C(116) | 2932 | 9628  | 7322 | 53(10) |
| C(117) | 2854 | 10246 | 8095 | 59(11) |
| C(118) | 3113 | 10340 | 8180 | 58(11) |
| C(119) | 2717 | 10617 | 8156 | 66(12) |
| C(120) | 2761 | 9905  | 8334 | 88(15) |
| C(121) | 2811 | 8548  | 6070 | 85(6)  |
| C(122) | 2658 | 8446  | 6330 | 88(6)  |
| C(123) | 2717 | 8088  | 6479 | 90(5)  |
| C(124) | 2892 | 7866  | 6389 | 91(5)  |
| C(125) | 3009 | 7982  | 6136 | 89(5)  |
| C(126) | 2990 | 8357  | 5971 | 86(6)  |
| C(127) | 2965 | 7464  | 6547 | 93(5)  |
| C(128) | 3044 | 7171  | 6211 | 99(7)  |
| C(129) | 2756 | 7215  | 6564 | 93(7)  |
| C(130) | 3153 | 7473  | 6735 | 94(7)  |
| C(131) | 2895 | 9531  | 4242 | 27(5)  |
| C(132) | 2844 | 9162  | 4138 | 53(10) |
| C(133) | 2599 | 9092  | 4083 | 41(9)  |
| C(134) | 2452 | 9385  | 4071 | 42(9)  |
| C(135) | 2517 | 9750  | 4170 | 29(5)  |
| C(136) | 2736 | 9826  | 4227 | 27(4)  |
| C(137) | 2187 | 9331  | 3955 | 57(11) |
| C(138) | 2026 | 9491  | 4201 | 69(12) |
| C(139) | 2132 | 8892  | 3902 | 66(12) |
| C(140) | 2154 | 9516  | 3614 | 72(13) |
| C(141) | 2445 | 9529  | 5134 | 31(8)  |
| C(142) | 2434 | 9184  | 4951 | 70(12) |
| C(143) | 2227 | 8973  | 4920 | 40(9)  |
| C(144) | 2035 | 9098  | 5069 | 39(9)  |
| C(145) | 2042 | 9426  | 5258 | 45(9)  |
| C(146) | 2235 | 9641  | 5289 | 30(8)  |
| C(147) | 1801 | 8873  | 5020 | 54(10) |
| C(148) | 1757 | 8669  | 5368 | 55(11) |
| C(149) | 1824 | 8561  | 4745 | 68(12) |
| C(150) | 1597 | 9141  | 4942 | 53(10) |



|        |      |       |      |         |
|--------|------|-------|------|---------|
| C(151) | 2065 | 9644  | 6565 | 50(10)  |
| C(152) | 2182 | 9374  | 6755 | 49(10)  |
| C(153) | 2146 | 9399  | 7101 | 53(10)  |
| C(154) | 2001 | 9661  | 7220 | 44(9)   |
| C(155) | 1868 | 9917  | 7012 | 45(9)   |
| C(156) | 1907 | 9882  | 6695 | 28(7)   |
| C(157) | 1958 | 9665  | 7614 | 95(9)   |
| C(158) | 1827 | 10009 | 7710 | 99(9)   |
| C(159) | 1883 | 9283  | 7713 | 95(9)   |
| C(160) | 2192 | 9776  | 7798 | 96(9)   |
| C(161) | 2523 | 10824 | 5043 | 24(4)   |
| C(162) | 2432 | 10579 | 4815 | 38(8)   |
| C(163) | 2202 | 10494 | 4814 | 28(7)   |
| C(164) | 2056 | 10635 | 5028 | 37(8)   |
| C(165) | 2134 | 10878 | 5278 | 23(4)   |
| C(166) | 2374 | 10966 | 5286 | 22(4)   |
| C(167) | 1796 | 10541 | 5039 | 37(8)   |
| C(168) | 1719 | 10411 | 5386 | 51(10)  |
| C(169) | 1726 | 10220 | 4793 | 51(10)  |
| C(170) | 1649 | 10929 | 4936 | 49(10)  |
| C(171) | 2260 | 11024 | 6495 | 43(9)   |
| C(172) | 2227 | 10747 | 6752 | 44(9)   |
| C(173) | 2170 | 10863 | 7057 | 61(11)  |
| C(174) | 2157 | 11259 | 7133 | 53(10)  |
| C(175) | 2213 | 11529 | 6885 | 56(11)  |
| C(176) | 2256 | 11419 | 6577 | 54(10)  |
| C(177) | 2103 | 11357 | 7493 | 109(10) |
| C(178) | 2133 | 11842 | 7527 | 110(10) |
| C(179) | 1850 | 11292 | 7510 | 112(11) |
| C(180) | 2258 | 11232 | 7703 | 110(10) |
| C(181) | 2938 | 11172 | 7146 | 43(9)   |
| C(182) | 3087 | 11076 | 7388 | 37(8)   |
| C(183) | 3088 | 11322 | 7670 | 58(11)  |
| C(184) | 2958 | 11641 | 7692 | 59(11)  |
| C(185) | 2827 | 11753 | 7410 | 104(17) |
| C(186) | 2813 | 11531 | 7142 | 45(9)   |
| C(187) | 2943 | 11926 | 7989 | 67(12)  |

|        |      |       |      |         |
|--------|------|-------|------|---------|
| C(188) | 2812 | 12304 | 7940 | 76(13)  |
| C(189) | 3198 | 12034 | 8119 | 115(19) |
| C(190) | 2821 | 11671 | 8268 | 94(16)  |
| C(191) | 2685 | 11940 | 6034 | 31(5)   |
| C(192) | 2686 | 12184 | 6319 | 32(5)   |
| C(193) | 2503 | 12414 | 6399 | 45(9)   |
| C(194) | 2295 | 12390 | 6196 | 54(10)  |
| C(195) | 2296 | 12146 | 5918 | 41(9)   |
| C(196) | 2483 | 11935 | 5841 | 32(5)   |
| C(197) | 2079 | 12656 | 6278 | 50(10)  |
| C(198) | 1878 | 12365 | 6301 | 73(13)  |
| C(199) | 2036 | 12932 | 6000 | 79(14)  |
| C(200) | 2117 | 12853 | 6599 | 85(14)  |
| C(201) | 3223 | 11883 | 5112 | 36(8)   |
| C(202) | 3276 | 12126 | 5388 | 30(8)   |
| C(203) | 3140 | 12449 | 5423 | 41(9)   |
| C(204) | 2978 | 12557 | 5200 | 41(9)   |
| C(205) | 2936 | 12301 | 4955 | 56(11)  |
| C(206) | 3052 | 11954 | 4905 | 33(8)   |
| C(207) | 2841 | 12926 | 5267 | 47(10)  |
| C(208) | 2686 | 13043 | 4958 | 71(12)  |
| C(209) | 3001 | 13268 | 5322 | 63(12)  |
| C(210) | 2676 | 12883 | 5543 | 46(9)   |
| C(211) | 3870 | 10933 | 4560 | 32(8)   |
| C(212) | 3816 | 10738 | 4293 | 40(9)   |
| C(213) | 3797 | 10937 | 3984 | 51(10)  |
| C(214) | 3834 | 11354 | 3997 | 40(9)   |
| C(215) | 3899 | 11536 | 4276 | 39(9)   |
| C(216) | 3926 | 11339 | 4559 | 54(10)  |
| C(217) | 3809 | 11551 | 3662 | 97(9)   |
| C(218) | 3611 | 11829 | 3705 | 99(10)  |
| C(219) | 3736 | 11265 | 3388 | 103(10) |
| C(220) | 4046 | 11762 | 3593 | 96(10)  |
| C(221) | 2964 | 10982 | 3968 | 47(9)   |
| C(222) | 2922 | 11043 | 3637 | 60(11)  |
| C(223) | 2703 | 11120 | 3504 | 83(14)  |
| C(224) | 2514 | 11137 | 3727 | 77(13)  |

|        |      |       |      |         |
|--------|------|-------|------|---------|
| C(225) | 2557 | 11078 | 4046 | 56(11)  |
| C(226) | 2787 | 11014 | 4179 | 36(8)   |
| C(227) | 2251 | 11219 | 3580 | 82(14)  |
| C(228) | 2154 | 11549 | 3782 | 106(18) |
| C(229) | 2139 | 10820 | 3597 | 91(15)  |
| C(230) | 2270 | 11317 | 3228 | 114(19) |
| C(231) | 3090 | 8511  | 4954 | 43(9)   |
| C(232) | 2887 | 8346  | 5055 | 48(10)  |
| C(233) | 2784 | 8077  | 4852 | 41(9)   |
| C(234) | 2879 | 7966  | 4550 | 46(9)   |
| C(235) | 3079 | 8132  | 4473 | 40(9)   |
| C(236) | 3195 | 8398  | 4667 | 54(10)  |
| C(237) | 2765 | 7646  | 4354 | 105(9)  |
| C(238) | 2725 | 7276  | 4543 | 103(10) |
| C(239) | 2889 | 7564  | 4064 | 108(10) |
| C(240) | 2502 | 7776  | 4291 | 112(10) |
| Au(37) | 250  | 9307  | 7562 | 24(1)   |
| Au(38) | 303  | 9366  | 6839 | 29(1)   |
| Au(39) | 38   | 9924  | 7155 | 25(1)   |
| Au(40) | 532  | 9869  | 7298 | 33(1)   |
| Au(41) | 548  | 8619  | 7232 | 30(1)   |
| Au(42) | 452  | 8628  | 8013 | 32(1)   |
| Au(43) | 155  | 9388  | 8269 | 33(1)   |
| Au(44) | -34  | 8760  | 7827 | 26(1)   |
| Au(45) | 492  | 9843  | 7943 | 31(1)   |
| Au(46) | -231 | 10477 | 7442 | 29(1)   |
| Au(47) | -210 | 10545 | 6684 | 33(1)   |
| Au(48) | 123  | 9983  | 6508 | 54(1)   |
| Au(49) | -59  | 8611  | 8736 | 21(1)   |
| Au(50) | -830 | 10659 | 7308 | 39(1)   |
| Au(51) | 170  | 9514  | 5895 | 24(1)   |
| Au(52) | 1153 | 9806  | 7606 | 27(1)   |
| Ag(49) | -59  | 8611  | 8736 | 21(1)   |
| Ag(50) | -830 | 10659 | 7308 | 39(1)   |
| Ag(51) | 170  | 9514  | 5895 | 24(1)   |
| Ag(52) | 1153 | 9806  | 7606 | 27(1)   |
| Au(53) | 369  | 10615 | 6852 | 33(1)   |

|        |      |       |      |         |
|--------|------|-------|------|---------|
| Au(54) | 718  | 9250  | 7616 | 56(1)   |
| S(25)  | -489 | 10971 | 7273 | 40(2)   |
| S(26)  | 59   | 11022 | 6785 | 36(2)   |
| S(27)  | 205  | 10171 | 5958 | 43(2)   |
| S(28)  | 714  | 10314 | 6953 | 34(2)   |
| S(29)  | 654  | 9032  | 6820 | 30(2)   |
| S(30)  | 1213 | 10467 | 7650 | 56(3)   |
| S(31)  | 502  | 8151  | 7627 | 30(2)   |
| S(32)  | 432  | 8957  | 8503 | 31(2)   |
| S(33)  | 1128 | 9142  | 7615 | 40(2)   |
| S(34)  | -98  | 8876  | 9246 | 37(2)   |
| S(35)  | 511  | 10145 | 8463 | 33(2)   |
| S(36)  | -118 | 8311  | 8246 | 32(2)   |
| C(241) | -499 | 11346 | 7572 | 26(7)   |
| C(242) | -664 | 11368 | 7807 | 47(9)   |
| C(243) | -653 | 11665 | 8032 | 65(12)  |
| C(244) | -479 | 11937 | 8036 | 55(10)  |
| C(245) | -317 | 11918 | 7789 | 85(14)  |
| C(246) | -323 | 11599 | 7562 | 45(9)   |
| C(247) | -474 | 12261 | 8267 | 56(11)  |
| C(248) | -231 | 12307 | 8426 | 74(13)  |
| C(249) | -659 | 12240 | 8542 | 82(14)  |
| C(250) | -528 | 12666 | 8065 | 62(11)  |
| C(251) | 87   | 11254 | 6403 | 35(8)   |
| C(252) | 286  | 11290 | 6238 | 32(8)   |
| C(253) | 307  | 11476 | 5964 | 61(11)  |
| C(254) | 124  | 11716 | 5823 | 115(9)  |
| C(255) | -89  | 11712 | 6005 | 33(8)   |
| C(256) | -104 | 11456 | 6284 | 63(11)  |
| C(257) | 162  | 11928 | 5501 | 117(9)  |
| C(258) | 403  | 11830 | 5381 | 122(10) |
| C(259) | 92   | 12382 | 5626 | 117(10) |
| C(260) | 6    | 11807 | 5273 | 122(10) |
| C(261) | -64  | 10314 | 5800 | 43(9)   |
| C(262) | -75  | 10712 | 5683 | 63(12)  |
| C(263) | -290 | 10826 | 5533 | 82(14)  |
| C(264) | -491 | 10628 | 5508 | 48(10)  |

|        |      |       |      |         |
|--------|------|-------|------|---------|
| C(265) | -473 | 10267 | 5673 | 53(10)  |
| C(266) | -263 | 10111 | 5799 | 54(10)  |
| C(267) | -705 | 10783 | 5329 | 69(12)  |
| C(268) | -920 | 10557 | 5464 | 100(17) |
| C(269) | -715 | 11213 | 5405 | 77(13)  |
| C(270) | -664 | 10764 | 4956 | 97(16)  |
| C(271) | 812  | 10092 | 6611 | 22(7)   |
| C(272) | 981  | 9780  | 6659 | 36(8)   |
| C(273) | 1093 | 9629  | 6399 | 39(9)   |
| C(274) | 1064 | 9780  | 6088 | 26(7)   |
| C(275) | 896  | 10083 | 6041 | 42(9)   |
| C(276) | 771  | 10211 | 6296 | 31(8)   |
| C(277) | 1200 | 9639  | 5805 | 45(9)   |
| C(278) | 1456 | 9711  | 5914 | 37(8)   |
| C(279) | 1160 | 9190  | 5743 | 68(12)  |
| C(280) | 1153 | 9843  | 5491 | 51(10)  |
| C(281) | 658  | 8702  | 6490 | 30(8)   |
| C(282) | 693  | 8335  | 6498 | 37(8)   |
| C(283) | 708  | 8112  | 6209 | 35(8)   |
| C(284) | 679  | 8273  | 5893 | 40(9)   |
| C(285) | 654  | 8674  | 5876 | 29(7)   |
| C(286) | 635  | 8899  | 6176 | 47(9)   |
| C(287) | 702  | 8033  | 5587 | 30(8)   |
| C(288) | 738  | 7609  | 5652 | 52(10)  |
| C(289) | 468  | 8106  | 5387 | 54(10)  |
| C(290) | 900  | 8220  | 5394 | 47(9)   |
| C(291) | 1264 | 10669 | 7260 | 54(10)  |
| C(292) | 1321 | 10436 | 6998 | 64(12)  |
| C(293) | 1356 | 10598 | 6702 | 54(10)  |
| C(294) | 1359 | 11004 | 6668 | 96(8)   |
| C(295) | 1317 | 11209 | 6942 | 65(12)  |
| C(296) | 1266 | 11061 | 7233 | 43(9)   |
| C(297) | 1401 | 11193 | 6346 | 98(8)   |
| C(298) | 1272 | 11034 | 6078 | 101(9)  |
| C(299) | 1652 | 11088 | 6214 | 104(9)  |
| C(300) | 1357 | 11620 | 6319 | 102(9)  |
| C(301) | 798  | 7992  | 7681 | 34(8)   |

|        |      |      |       |        |
|--------|------|------|-------|--------|
| C(302) | 917  | 8110 | 7942  | 38(8)  |
| C(303) | 1153 | 8018 | 7977  | 39(9)  |
| C(304) | 1261 | 7802 | 7748  | 45(9)  |
| C(305) | 1130 | 7654 | 7473  | 44(9)  |
| C(306) | 884  | 7742 | 7438  | 55(10) |
| C(307) | 1518 | 7694 | 7767  | 53(10) |
| C(308) | 1643 | 7863 | 8067  | 90(15) |
| C(309) | 1550 | 7248 | 7700  | 62(11) |
| C(310) | 1618 | 7931 | 7471  | 88(15) |
| C(311) | 709  | 9159 | 8586  | 28(5)  |
| C(312) | 735  | 9388 | 8866  | 30(5)  |
| C(313) | 948  | 9532 | 8938  | 32(5)  |
| C(314) | 1149 | 9440 | 8752  | 39(9)  |
| C(315) | 1110 | 9249 | 8463  | 30(8)  |
| C(316) | 892  | 9094 | 8388  | 25(7)  |
| C(317) | 1383 | 9619 | 8861  | 51(10) |
| C(318) | 1366 | 9952 | 9078  | 42(9)  |
| C(319) | 1502 | 9272 | 9024  | 50(10) |
| C(320) | 1527 | 9726 | 8528  | 65(12) |
| C(321) | 1244 | 8970 | 7251  | 27(7)  |
| C(322) | 1182 | 8603 | 7133  | 32(8)  |
| C(323) | 1278 | 8437 | 6867  | 46(9)  |
| C(324) | 1452 | 8623 | 6726  | 36(8)  |
| C(325) | 1526 | 9012 | 6820  | 40(9)  |
| C(326) | 1410 | 9169 | 7077  | 32(8)  |
| C(327) | 1585 | 8422 | 6441  | 51(10) |
| C(328) | 1720 | 8044 | 6602  | 64(12) |
| C(329) | 1754 | 8691 | 6294  | 73(13) |
| C(330) | 1404 | 8232 | 6178  | 53(10) |
| C(331) | 163  | 8937 | 9465  | 41(9)  |
| C(332) | 153  | 9123 | 9757  | 63(11) |
| C(333) | 361  | 9178 | 9952  | 66(12) |
| C(334) | 563  | 9016 | 9858  | 38(8)  |
| C(335) | 573  | 8806 | 9560  | 62(11) |
| C(336) | 366  | 8772 | 9360  | 32(8)  |
| C(337) | 788  | 9099 | 10036 | 41(9)  |
| C(338) | 742  | 9192 | 10395 | 71(13) |

|        |      |       |       |         |
|--------|------|-------|-------|---------|
| C(339) | 940  | 8703  | 10050 | 115(19) |
| C(340) | 923  | 9429  | 9866  | 85(14)  |
| C(341) | 744  | 10473 | 8502  | 79(5)   |
| C(342) | 714  | 10845 | 8633  | 80(5)   |
| C(343) | 886  | 11108 | 8649  | 82(5)   |
| C(344) | 1100 | 10998 | 8563  | 84(5)   |
| C(345) | 1143 | 10629 | 8443  | 82(5)   |
| C(346) | 968  | 10390 | 8411  | 80(5)   |
| C(347) | 1311 | 11312 | 8597  | 90(5)   |
| C(348) | 1388 | 11349 | 8937  | 95(7)   |
| C(349) | 1538 | 11143 | 8378  | 97(7)   |
| C(350) | 1278 | 11625 | 8377  | 98(7)   |
| C(351) | 48   | 7888  | 8191  | 28(7)   |
| C(352) | 252  | 7808  | 8351  | 41(9)   |
| C(353) | 378  | 7472  | 8292  | 39(9)   |
| C(354) | 309  | 7220  | 8059  | 35(8)   |
| C(355) | 86   | 7285  | 7909  | 66(12)  |
| C(356) | -44  | 7600  | 7982  | 66(12)  |
| C(357) | 430  | 6846  | 7975  | 35(8)   |
| C(358) | 681  | 6840  | 8082  | 46(9)   |
| C(359) | 306  | 6468  | 8107  | 94(16)  |
| C(360) | 440  | 6802  | 7617  | 64(12)  |

**Table S4. Anisotropic displacement parameters ( $\text{\AA}^2$ ) for  $[\text{Au}_{32}\text{Ag}_4(\text{SPh-tBu})_{24}]$ . The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$ .**

|        | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|--------|----------|----------|----------|----------|----------|----------|
| Au(1)  | 26(1)    | 19(1)    | 24(1)    | 0(1)     | 0(1)     | -2(1)    |
| Au(2)  | 23(1)    | 19(1)    | 26(1)    | 2(1)     | 1(1)     | -3(1)    |
| Au(3)  | 24(1)    | 21(1)    | 24(1)    | 3(1)     | 0(1)     | 0(1)     |
| Au(4)  | 29(1)    | 21(1)    | 31(1)    | 1(1)     | 4(1)     | 2(1)     |
| Au(5)  | 25(1)    | 17(1)    | 24(1)    | 2(1)     | 1(1)     | 1(1)     |
| Au(6)  | 28(1)    | 21(1)    | 29(1)    | 4(1)     | -1(1)    | 0(1)     |
| Au(7)  | 31(1)    | 28(1)    | 36(1)    | 1(1)     | 1(1)     | 1(1)     |
| Au(8)  | 58(1)    | 48(1)    | 55(1)    | -2(1)    | 2(1)     | -6(1)    |
| Au(9)  | 29(1)    | 26(1)    | 32(1)    | 3(1)     | 5(1)     | -4(1)    |
| Au(10) | 29(1)    | 27(1)    | 37(1)    | 1(1)     | -3(1)    | -3(1)    |
| Au(11) | 33(1)    | 29(1)    | 30(1)    | 0(1)     | 4(1)     | -2(1)    |

|        |       |       |       |       |       |        |
|--------|-------|-------|-------|-------|-------|--------|
| Au(12) | 37(1) | 27(1) | 35(1) | -1(1) | 3(1)  | 3(1)   |
| Au(13) | 53(1) | 52(1) | 59(1) | 2(1)  | 5(1)  | -6(1)  |
| Au(14) | 34(1) | 27(1) | 38(1) | -2(1) | 6(1)  | -4(1)  |
| Au(15) | 29(1) | 19(1) | 31(1) | 0(1)  | 0(1)  | -2(1)  |
| Au(16) | 30(1) | 27(1) | 41(1) | -3(1) | 0(1)  | 0(1)   |
| Au(17) | 34(1) | 27(1) | 34(1) | 1(1)  | 6(1)  | 2(1)   |
| Au(18) | 61(1) | 49(1) | 54(1) | 3(1)  | 4(1)  | 5(1)   |
| Au(19) | 32(1) | 27(1) | 36(1) | 1(1)  | 1(1)  | -2(1)  |
| Au(20) | 32(1) | 25(1) | 31(1) | 4(1)  | -1(1) | 0(1)   |
| Au(21) | 35(1) | 25(1) | 33(1) | 3(1)  | 5(1)  | 4(1)   |
| Au(22) | 27(1) | 23(1) | 39(1) | 0(1)  | 0(1)  | -1(1)  |
| Au(23) | 35(1) | 28(1) | 33(1) | 2(1)  | 3(1)  | 1(1)   |
| Au(24) | 33(1) | 24(1) | 34(1) | 3(1)  | 6(1)  | 1(1)   |
| Au(25) | 52(1) | 46(1) | 60(1) | -1(1) | 5(1)  | 4(1)   |
| Au(26) | 34(1) | 23(1) | 32(1) | -2(1) | -2(1) | -2(1)  |
| Au(27) | 35(1) | 25(1) | 32(1) | 0(1)  | 4(1)  | -2(1)  |
| Au(28) | 28(1) | 19(1) | 29(1) | 2(1)  | 4(1)  | -1(1)  |
| Au(29) | 42(1) | 25(1) | 32(1) | -6(1) | 1(1)  | 4(1)   |
| Au(30) | 28(1) | 20(1) | 21(1) | -2(1) | 2(1)  | -2(1)  |
| Au(31) | 20(1) | 29(1) | 27(2) | 2(1)  | -1(1) | 4(1)   |
| Au(32) | 23(1) | 45(2) | 29(2) | -3(1) | 4(1)  | -4(1)  |
| Au(33) | 26(1) | 37(2) | 31(2) | 2(1)  | 2(1)  | 7(1)   |
| Au(34) | 20(1) | 16(1) | 19(1) | 0(1)  | 0(1)  | -4(1)  |
| Au(35) | 20(2) | 29(2) | 28(2) | -2(2) | 0(2)  | 1(2)   |
| Au(36) | 23(2) | 22(2) | 24(2) | 2(3)  | 4(3)  | -2(3)  |
| Ag(29) | 42(1) | 25(1) | 32(1) | -6(1) | 1(1)  | 4(1)   |
| Ag(30) | 28(1) | 20(1) | 21(1) | -2(1) | 2(1)  | -2(2)  |
| Ag(31) | 20(1) | 29(1) | 27(1) | 2(1)  | -1(2) | 4(2)   |
| Ag(32) | 23(1) | 45(1) | 29(1) | -3(1) | 4(2)  | -4(2)  |
| Ag(33) | 26(1) | 37(1) | 31(1) | 2(1)  | 2(1)  | 7(1)   |
| Ag(34) | 20(1) | 16(1) | 19(1) | 0(2)  | 0(2)  | -4(2)  |
| Ag(35) | 20(2) | 29(2) | 28(2) | -2(2) | 0(2)  | 1(2)   |
| Ag(36) | 23(3) | 22(3) | 24(3) | 2(5)  | 4(5)  | -2(5)  |
| S(1)   | 42(5) | 41(5) | 29(5) | -8(4) | 5(4)  | -14(4) |
| S(2)   | 33(5) | 29(5) | 30(5) | -2(4) | -1(4) | 9(4)   |
| S(3)   | 45(5) | 42(5) | 36(5) | -2(4) | 1(4)  | -6(4)  |
| S(4)   | 31(5) | 54(6) | 50(6) | 10(5) | 6(4)  | 6(4)   |



|       |        |        |        |        |       |       |
|-------|--------|--------|--------|--------|-------|-------|
| S(5)  | 37(5)  | 29(5)  | 36(5)  | -4(4)  | -2(4) | 0(4)  |
| S(6)  | 36(5)  | 26(5)  | 36(5)  | 3(4)   | 8(4)  | 5(4)  |
| S(7)  | 38(5)  | 34(5)  | 24(5)  | 7(4)   | 0(4)  | 6(4)  |
| S(8)  | 33(5)  | 20(4)  | 42(5)  | -5(4)  | 1(4)  | -4(4) |
| S(9)  | 82(8)  | 40(6)  | 42(6)  | -11(5) | 8(5)  | 13(5) |
| S(10) | 34(5)  | 27(5)  | 35(5)  | 2(4)   | 7(4)  | 2(4)  |
| S(11) | 55(6)  | 50(6)  | 27(5)  | -3(4)  | 9(4)  | 5(5)  |
| S(12) | 35(5)  | 28(5)  | 32(5)  | 3(4)   | 2(4)  | -4(4) |
| S(13) | 34(5)  | 18(4)  | 41(5)  | 3(4)   | -6(4) | 3(4)  |
| S(14) | 39(5)  | 43(5)  | 29(5)  | -3(4)  | -3(4) | 4(4)  |
| S(15) | 28(4)  | 29(5)  | 27(5)  | -1(4)  | -4(4) | -2(4) |
| S(16) | 33(5)  | 30(5)  | 45(6)  | -9(4)  | 6(4)  | -6(4) |
| S(17) | 28(4)  | 17(4)  | 38(5)  | 0(4)   | 2(4)  | 4(3)  |
| S(18) | 38(5)  | 41(5)  | 33(5)  | 6(4)   | 14(4) | 3(4)  |
| S(19) | 36(5)  | 33(5)  | 27(5)  | 0(4)   | 10(4) | -1(4) |
| S(20) | 33(5)  | 21(4)  | 45(6)  | 0(4)   | -3(4) | -5(4) |
| S(21) | 29(5)  | 25(4)  | 39(5)  | 12(4)  | 1(4)  | 1(4)  |
| S(22) | 39(5)  | 18(4)  | 37(5)  | -2(4)  | 9(4)  | -6(4) |
| S(23) | 36(5)  | 48(6)  | 29(5)  | 0(4)   | -1(4) | -7(4) |
| S(24) | 44(5)  | 25(5)  | 40(5)  | 2(4)   | -1(4) | 2(4)  |
| C(1)  | 36(9)  | 35(9)  | 37(9)  | 0(5)   | 2(5)  | -3(5) |
| C(2)  | 34(9)  | 30(9)  | 31(9)  | 0(5)   | 2(5)  | 0(5)  |
| C(3)  | 33(9)  | 35(9)  | 33(9)  | 0(5)   | 5(5)  | -1(5) |
| C(4)  | 44(10) | 47(10) | 47(10) | 0(5)   | 1(5)  | 0(5)  |
| C(5)  | 55(11) | 55(11) | 54(11) | 0(5)   | 1(5)  | 0(5)  |
| C(6)  | 68(13) | 66(13) | 65(13) | 0(5)   | -1(5) | -1(5) |
| C(7)  | 81(8)  | 82(8)  | 82(8)  | 2(4)   | 2(4)  | -1(4) |
| C(8)  | 78(10) | 78(10) | 82(10) | 7(7)   | 2(7)  | -1(7) |
| C(9)  | 85(10) | 88(11) | 85(11) | -1(7)  | -1(7) | 0(7)  |
| C(10) | 85(11) | 89(11) | 88(11) | 4(7)   | -1(7) | 1(7)  |
| C(11) | 36(9)  | 37(9)  | 40(9)  | -2(5)  | 3(5)  | -1(5) |
| C(12) | 44(10) | 45(10) | 43(10) | 1(5)   | 1(5)  | -2(5) |
| C(13) | 56(11) | 57(11) | 55(11) | -2(5)  | 3(5)  | -1(5) |
| C(14) | 57(11) | 57(11) | 56(11) | 1(5)   | 4(5)  | -1(5) |
| C(15) | 97(17) | 96(17) | 96(17) | 0(5)   | 4(5)  | 0(5)  |
| C(16) | 43(10) | 44(10) | 45(10) | 0(5)   | 3(5)  | 1(5)  |
| C(17) | 34(9)  | 32(9)  | 35(9)  | 0(5)   | 2(5)  | 1(5)  |

|       |        |        |        |        |        |        |
|-------|--------|--------|--------|--------|--------|--------|
| C(18) | 52(13) | 45(12) | 52(13) | 0(9)   | -1(9)  | 2(9)   |
| C(19) | 27(10) | 23(10) | 27(10) | -5(8)  | 5(8)   | -3(8)  |
| C(20) | 39(11) | 33(11) | 36(11) | -8(9)  | 6(9)   | 9(9)   |
| C(21) | 36(9)  | 35(9)  | 36(9)  | 2(5)   | -1(5)  | 0(5)   |
| C(22) | 43(10) | 43(10) | 43(10) | -2(5)  | 1(5)   | 2(5)   |
| C(23) | 77(14) | 79(14) | 78(14) | 1(5)   | 3(5)   | 0(5)   |
| C(24) | 50(11) | 53(11) | 51(11) | 2(5)   | 0(5)   | -1(5)  |
| C(25) | 61(12) | 62(12) | 62(12) | 0(5)   | 3(5)   | 0(5)   |
| C(26) | 45(10) | 42(10) | 44(10) | 0(5)   | 0(5)   | -2(5)  |
| C(27) | 61(12) | 61(12) | 59(12) | 1(5)   | 2(5)   | -1(5)  |
| C(28) | 89(17) | 89(17) | 84(17) | 4(10)  | 5(10)  | 0(10)  |
| C(29) | 83(17) | 93(17) | 88(17) | 3(10)  | 3(10)  | 3(10)  |
| C(30) | 76(15) | 78(16) | 76(16) | -3(10) | -4(10) | 0(10)  |
| C(31) | 39(10) | 40(10) | 40(10) | -1(5)  | 2(5)   | -1(5)  |
| C(32) | 56(11) | 56(11) | 57(11) | -1(5)  | 1(5)   | -2(5)  |
| C(33) | 70(13) | 70(13) | 70(13) | 1(5)   | 2(5)   | -2(5)  |
| C(34) | 40(10) | 44(10) | 41(10) | 0(5)   | 3(5)   | -1(5)  |
| C(35) | 57(11) | 56(11) | 56(11) | -1(5)  | 1(5)   | -2(5)  |
| C(36) | 62(12) | 63(12) | 62(12) | 0(5)   | 3(5)   | -3(5)  |
| C(37) | 85(9)  | 85(9)  | 83(9)  | 0(4)   | 2(4)   | 0(4)   |
| C(38) | 86(11) | 90(11) | 84(11) | -4(7)  | 5(7)   | -4(7)  |
| C(39) | 81(10) | 80(10) | 82(11) | -3(7)  | 3(7)   | 0(7)   |
| C(40) | 89(11) | 90(11) | 86(11) | 2(7)   | 3(7)   | 2(7)   |
| C(41) | 21(8)  | 20(8)  | 21(8)  | -3(5)  | 1(5)   | 2(5)   |
| C(42) | 26(8)  | 26(8)  | 25(8)  | 2(5)   | -1(5)  | 0(5)   |
| C(43) | 38(9)  | 40(9)  | 38(9)  | 0(5)   | 1(5)   | 0(5)   |
| C(44) | 28(8)  | 26(8)  | 27(8)  | 0(5)   | 3(5)   | -2(5)  |
| C(45) | 37(9)  | 36(9)  | 34(9)  | 0(5)   | 0(5)   | 1(5)   |
| C(46) | 33(9)  | 33(9)  | 32(9)  | 0(5)   | 1(5)   | -2(5)  |
| C(47) | 41(10) | 41(10) | 41(10) | -2(5)  | 3(5)   | -1(5)  |
| C(48) | 47(12) | 46(12) | 50(13) | 3(9)   | 9(9)   | -4(9)  |
| C(49) | 54(12) | 41(12) | 50(13) | -2(9)  | 9(9)   | -13(9) |
| C(50) | 50(12) | 49(12) | 49(13) | -5(9)  | -2(9)  | -8(9)  |
| C(51) | 36(9)  | 33(9)  | 34(9)  | -2(5)  | -1(5)  | 1(5)   |
| C(52) | 23(8)  | 22(8)  | 23(8)  | 0(5)   | 1(5)   | -1(5)  |
| C(53) | 54(11) | 55(11) | 55(11) | -1(5)  | 2(5)   | 2(5)   |
| C(54) | 33(9)  | 30(9)  | 31(9)  | 1(5)   | -3(5)  | 0(5)   |

|       |         |         |         |        |        |        |
|-------|---------|---------|---------|--------|--------|--------|
| C(55) | 43(10)  | 43(10)  | 44(10)  | -1(5)  | 0(5)   | -1(5)  |
| C(56) | 60(12)  | 59(12)  | 62(12)  | -2(5)  | 0(5)   | -1(5)  |
| C(57) | 50(11)  | 50(11)  | 48(11)  | -1(5)  | 2(5)   | 1(5)   |
| C(58) | 60(14)  | 62(14)  | 56(14)  | 1(9)   | -6(9)  | -4(9)  |
| C(59) | 70(14)  | 62(14)  | 63(14)  | -8(9)  | 0(9)   | -1(9)  |
| C(60) | 72(15)  | 71(15)  | 63(15)  | 5(9)   | 4(9)   | 6(9)   |
| C(61) | 34(9)   | 31(9)   | 35(9)   | 1(5)   | 2(5)   | -1(5)  |
| C(62) | 38(10)  | 39(10)  | 42(10)  | 0(5)   | 1(5)   | 1(5)   |
| C(63) | 74(14)  | 73(14)  | 76(14)  | 0(5)   | 2(5)   | 0(5)   |
| C(64) | 65(13)  | 67(13)  | 66(13)  | 0(5)   | 2(5)   | 1(5)   |
| C(65) | 56(11)  | 57(11)  | 56(11)  | 1(5)   | 2(5)   | 1(5)   |
| C(66) | 35(9)   | 34(9)   | 34(9)   | 2(5)   | -2(5)  | -3(5)  |
| C(67) | 66(13)  | 66(13)  | 66(13)  | -1(5)  | 1(5)   | 0(5)   |
| C(68) | 110(20) | 110(20) | 110(20) | -6(10) | 4(10)  | 1(10)  |
| C(69) | 77(16)  | 78(16)  | 78(16)  | 1(10)  | 3(10)  | 10(10) |
| C(70) | 101(19) | 96(19)  | 103(19) | 7(10)  | 2(10)  | 0(10)  |
| C(71) | 23(8)   | 21(8)   | 24(8)   | 0(5)   | 0(5)   | -3(5)  |
| C(72) | 39(10)  | 40(10)  | 40(10)  | 1(5)   | 2(5)   | -1(5)  |
| C(73) | 34(9)   | 34(9)   | 36(9)   | 3(5)   | 2(5)   | 1(5)   |
| C(74) | 32(9)   | 32(9)   | 32(9)   | -1(5)  | 2(5)   | 2(5)   |
| C(75) | 42(10)  | 40(10)  | 41(10)  | -2(5)  | 0(5)   | -1(5)  |
| C(76) | 38(9)   | 40(10)  | 38(10)  | 0(5)   | 0(5)   | 0(5)   |
| C(77) | 48(10)  | 45(10)  | 47(10)  | 0(5)   | 3(5)   | 0(5)   |
| C(78) | 61(14)  | 61(14)  | 63(14)  | -2(9)  | -4(9)  | 0(9)   |
| C(79) | 47(12)  | 44(12)  | 47(12)  | 9(9)   | 2(9)   | -3(9)  |
| C(80) | 46(12)  | 48(12)  | 48(12)  | 3(9)   | 7(9)   | -1(9)  |
| C(81) | 54(11)  | 52(11)  | 53(11)  | -1(5)  | 1(5)   | 2(5)   |
| C(82) | 43(10)  | 43(10)  | 41(10)  | 0(5)   | 1(5)   | 1(5)   |
| C(83) | 35(9)   | 35(9)   | 34(9)   | -1(5)  | -1(5)  | -1(5)  |
| C(84) | 52(11)  | 53(11)  | 50(11)  | 0(5)   | 0(5)   | 0(5)   |
| C(85) | 51(11)  | 50(11)  | 51(11)  | 0(5)   | 2(5)   | -1(5)  |
| C(86) | 73(13)  | 73(13)  | 73(13)  | 0(5)   | 2(5)   | -2(5)  |
| C(87) | 54(11)  | 53(11)  | 53(11)  | -1(5)  | 0(5)   | 0(5)   |
| C(88) | 79(15)  | 73(15)  | 73(15)  | -1(10) | 8(10)  | -2(10) |
| C(89) | 78(15)  | 68(15)  | 70(15)  | -1(9)  | -1(9)  | 4(9)   |
| C(90) | 110(20) | 120(20) | 110(20) | -2(10) | -6(10) | 1(10)  |
| C(91) | 51(11)  | 54(11)  | 50(11)  | 0(5)   | 1(5)   | 1(5)   |

|        |        |        |         |       |       |       |
|--------|--------|--------|---------|-------|-------|-------|
| C(92)  | 42(10) | 41(10) | 42(10)  | 1(5)  | 1(5)  | -1(5) |
| C(93)  | 48(10) | 47(10) | 46(10)  | -2(5) | 0(5)  | 0(5)  |
| C(94)  | 52(11) | 52(11) | 53(11)  | 2(5)  | 2(5)  | 1(5)  |
| C(95)  | 46(10) | 44(10) | 46(10)  | 0(5)  | 1(5)  | 2(5)  |
| C(96)  | 45(10) | 45(10) | 46(10)  | 0(5)  | 2(5)  | 2(5)  |
| C(97)  | 65(13) | 66(13) | 66(13)  | 1(5)  | 1(5)  | -1(5) |
| C(98)  | 55(13) | 43(12) | 49(13)  | 9(9)  | 1(9)  | 6(9)  |
| C(99)  | 75(15) | 67(15) | 71(15)  | 0(9)  | -6(9) | 4(9)  |
| C(100) | 74(15) | 75(15) | 72(15)  | 9(9)  | -3(9) | 1(9)  |
| C(101) | 44(10) | 46(10) | 45(10)  | 0(5)  | 3(5)  | -1(5) |
| C(102) | 51(11) | 51(11) | 52(11)  | 1(5)  | -1(5) | 0(5)  |
| C(103) | 72(13) | 73(13) | 71(13)  | 1(5)  | 3(5)  | -1(5) |
| C(104) | 59(12) | 59(12) | 58(12)  | 1(5)  | 0(5)  | 1(5)  |
| C(105) | 55(11) | 54(11) | 55(11)  | 1(5)  | 2(5)  | -1(5) |
| C(106) | 37(9)  | 35(9)  | 35(9)   | 1(5)  | 2(5)  | -1(5) |
| C(107) | 62(12) | 62(12) | 61(12)  | -3(5) | 2(5)  | 0(5)  |
| C(108) | 53(13) | 51(13) | 48(13)  | 0(9)  | -3(9) | -5(9) |
| C(109) | 71(15) | 80(15) | 68(15)  | 7(9)  | 3(9)  | 0(9)  |
| C(110) | 70(15) | 66(15) | 78(15)  | 4(9)  | -1(9) | 3(9)  |
| C(111) | 44(10) | 44(10) | 47(10)  | 0(5)  | 1(5)  | 3(5)  |
| C(112) | 39(9)  | 37(9)  | 40(9)   | 2(5)  | 2(5)  | 3(5)  |
| C(113) | 35(9)  | 34(9)  | 35(9)   | 0(5)  | 2(5)  | 0(5)  |
| C(114) | 41(10) | 41(10) | 43(10)  | 1(5)  | 0(5)  | -1(5) |
| C(115) | 56(11) | 52(11) | 52(11)  | 1(5)  | 0(5)  | -1(5) |
| C(116) | 54(11) | 53(11) | 52(11)  | 2(5)  | 0(5)  | 0(5)  |
| C(117) | 59(12) | 60(12) | 59(12)  | -1(5) | 4(5)  | 0(5)  |
| C(118) | 62(13) | 57(13) | 54(13)  | -1(9) | 4(9)  | -2(9) |
| C(119) | 72(14) | 65(14) | 62(14)  | 0(9)  | 0(9)  | 5(9)  |
| C(120) | 88(15) | 88(15) | 87(15)  | 0(4)  | 3(4)  | 0(4)  |
| C(121) | 86(6)  | 85(6)  | 86(6)   | 0(3)  | 2(3)  | 0(3)  |
| C(122) | 88(6)  | 87(6)  | 88(6)   | 1(2)  | 2(2)  | 0(2)  |
| C(123) | 90(6)  | 90(6)  | 90(6)   | 2(3)  | 3(3)  | 0(3)  |
| C(124) | 90(6)  | 90(6)  | 91(6)   | 2(3)  | 3(3)  | 0(3)  |
| C(125) | 89(6)  | 88(6)  | 88(6)   | 1(3)  | 3(3)  | 2(3)  |
| C(126) | 86(6)  | 85(6)  | 87(6)   | 0(3)  | 3(3)  | 1(3)  |
| C(127) | 93(6)  | 93(6)  | 94(6)   | 3(4)  | 2(4)  | 0(4)  |
| C(128) | 99(10) | 97(10) | 100(10) | 3(7)  | 7(7)  | 0(7)  |

|        |        |         |        |       |       |       |
|--------|--------|---------|--------|-------|-------|-------|
| C(129) | 93(9)  | 90(9)   | 95(9)  | 6(7)  | 1(7)  | -1(7) |
| C(130) | 94(10) | 93(9)   | 95(10) | 7(7)  | -1(7) | -1(7) |
| C(131) | 28(6)  | 26(6)   | 27(6)  | -1(4) | 1(4)  | -2(4) |
| C(132) | 54(11) | 53(11)  | 53(11) | 1(5)  | 0(5)  | 0(5)  |
| C(133) | 42(10) | 40(10)  | 40(10) | 0(5)  | -1(5) | -1(5) |
| C(134) | 42(10) | 43(10)  | 42(10) | -1(5) | 1(5)  | 1(5)  |
| C(135) | 30(6)  | 28(6)   | 30(6)  | -1(4) | 1(4)  | 0(4)  |
| C(136) | 28(5)  | 26(5)   | 28(5)  | -2(3) | 1(3)  | -2(3) |
| C(137) | 57(11) | 56(11)  | 57(11) | -1(5) | 1(5)  | -3(5) |
| C(138) | 67(15) | 70(15)  | 71(15) | 1(9)  | 6(9)  | -2(9) |
| C(139) | 69(14) | 64(14)  | 66(14) | 4(9)  | 1(9)  | -4(9) |
| C(140) | 70(15) | 73(15)  | 74(15) | 7(9)  | -2(9) | -6(9) |
| C(141) | 32(9)  | 30(9)   | 31(9)  | -2(5) | 5(5)  | -1(5) |
| C(142) | 68(13) | 69(13)  | 72(13) | 0(5)  | 2(5)  | 0(5)  |
| C(143) | 41(10) | 40(10)  | 39(10) | -2(5) | 0(5)  | -2(5) |
| C(144) | 39(9)  | 38(9)   | 40(10) | -3(5) | -4(5) | -2(5) |
| C(145) | 44(10) | 45(10)  | 45(10) | -1(5) | 3(5)  | 2(5)  |
| C(146) | 30(9)  | 31(9)   | 30(9)  | -3(5) | 2(5)  | 0(5)  |
| C(147) | 54(11) | 54(11)  | 54(11) | 0(5)  | 3(5)  | -1(5) |
| C(148) | 58(13) | 52(13)  | 56(13) | 3(9)  | 2(9)  | -1(9) |
| C(149) | 70(14) | 66(14)  | 69(15) | -4(9) | 3(9)  | -9(9) |
| C(150) | 53(13) | 52(13)  | 53(13) | -1(9) | -8(9) | -7(9) |
| C(151) | 50(11) | 50(11)  | 50(11) | 2(5)  | 1(5)  | -3(5) |
| C(152) | 49(11) | 50(11)  | 49(11) | 0(5)  | 2(5)  | -1(5) |
| C(153) | 52(11) | 53(11)  | 53(11) | 1(5)  | 0(5)  | 0(5)  |
| C(154) | 43(10) | 43(10)  | 44(10) | -1(5) | 2(5)  | 2(5)  |
| C(155) | 44(10) | 46(10)  | 45(10) | 2(5)  | 1(5)  | -3(5) |
| C(156) | 27(8)  | 29(8)   | 27(8)  | 0(5)  | 3(5)  | 0(5)  |
| C(157) | 94(9)  | 95(9)   | 95(9)  | 2(4)  | 2(4)  | 0(4)  |
| C(158) | 98(11) | 101(11) | 98(11) | 1(7)  | 1(7)  | 0(7)  |
| C(159) | 94(11) | 95(11)  | 95(11) | 3(7)  | 3(7)  | -1(7) |
| C(160) | 92(11) | 98(11)  | 97(11) | 3(7)  | 1(7)  | 1(7)  |
| C(161) | 25(5)  | 23(5)   | 25(6)  | 2(4)  | 0(4)  | -1(4) |
| C(162) | 40(9)  | 36(9)   | 37(9)  | 2(5)  | 2(5)  | -1(5) |
| C(163) | 29(8)  | 28(8)   | 27(8)  | -1(5) | 0(5)  | 0(5)  |
| C(164) | 38(9)  | 34(9)   | 38(9)  | 3(5)  | 1(5)  | -1(5) |
| C(165) | 23(5)  | 22(5)   | 24(6)  | 1(4)  | -1(4) | 0(4)  |

|        |         |         |         |        |       |        |
|--------|---------|---------|---------|--------|-------|--------|
| C(166) | 22(5)   | 22(5)   | 23(5)   | 1(3)   | 0(3)  | 0(3)   |
| C(167) | 38(9)   | 37(9)   | 37(9)   | 1(5)   | 1(5)  | 0(5)   |
| C(168) | 53(13)  | 48(13)  | 51(13)  | -2(9)  | 6(9)  | -4(9)  |
| C(169) | 49(13)  | 52(13)  | 53(13)  | -1(9)  | 2(9)  | 0(9)   |
| C(170) | 45(12)  | 49(12)  | 53(13)  | 2(9)   | -7(9) | -1(9)  |
| C(171) | 43(10)  | 43(10)  | 43(10)  | -2(5)  | 1(5)  | 1(5)   |
| C(172) | 43(10)  | 44(10)  | 44(10)  | -3(5)  | 2(5)  | 0(5)   |
| C(173) | 61(12)  | 61(12)  | 60(12)  | 0(5)   | 2(5)  | 3(5)   |
| C(174) | 52(11)  | 54(11)  | 53(11)  | -1(5)  | 1(5)  | 0(5)   |
| C(175) | 57(11)  | 55(11)  | 56(11)  | 0(5)   | -1(5) | 1(5)   |
| C(176) | 54(11)  | 54(11)  | 55(11)  | 0(5)   | 1(5)  | 1(5)   |
| C(177) | 110(10) | 110(10) | 109(10) | 0(4)   | 3(4)  | 1(4)   |
| C(178) | 111(12) | 109(12) | 109(12) | 0(7)   | 3(7)  | 1(7)   |
| C(179) | 112(12) | 114(12) | 112(12) | 1(7)   | 5(7)  | 3(7)   |
| C(180) | 110(12) | 111(12) | 108(12) | -1(7)  | 2(7)  | 3(7)   |
| C(181) | 41(10)  | 44(10)  | 44(10)  | 0(5)   | 0(5)  | 0(5)   |
| C(182) | 38(9)   | 38(9)   | 37(9)   | 2(5)   | 1(5)  | -2(5)  |
| C(183) | 57(12)  | 58(12)  | 59(12)  | 0(5)   | 3(5)  | -1(5)  |
| C(184) | 59(12)  | 59(12)  | 59(12)  | 0(5)   | 2(5)  | 0(5)   |
| C(185) | 104(18) | 105(18) | 104(18) | -2(5)  | 3(5)  | 1(5)   |
| C(186) | 45(10)  | 44(10)  | 46(10)  | -2(5)  | 1(5)  | 0(5)   |
| C(187) | 66(13)  | 67(13)  | 68(13)  | -2(5)  | 2(5)  | 0(5)   |
| C(188) | 77(15)  | 75(15)  | 77(16)  | 3(10)  | 8(10) | 0(10)  |
| C(189) | 110(20) | 110(20) | 110(20) | -2(10) | 1(10) | -1(10) |
| C(190) | 96(18)  | 93(18)  | 93(18)  | -4(10) | 5(10) | 3(10)  |
| C(191) | 30(5)   | 30(5)   | 33(6)   | 1(3)   | -1(3) | -1(3)  |
| C(192) | 32(6)   | 31(6)   | 34(6)   | 1(4)   | -1(4) | 0(4)   |
| C(193) | 45(10)  | 45(10)  | 45(10)  | -1(5)  | 3(5)  | 0(5)   |
| C(194) | 54(11)  | 53(11)  | 56(11)  | 1(5)   | 3(5)  | -1(5)  |
| C(195) | 42(10)  | 40(10)  | 40(10)  | 0(5)   | -1(5) | 0(5)   |
| C(196) | 31(6)   | 31(6)   | 33(6)   | 0(4)   | -2(4) | -1(4)  |
| C(197) | 50(11)  | 49(11)  | 50(11)  | 3(5)   | 3(5)  | 1(5)   |
| C(198) | 75(15)  | 71(15)  | 72(15)  | 1(9)   | -2(9) | -3(9)  |
| C(199) | 79(16)  | 75(16)  | 84(16)  | 8(10)  | 7(10) | 12(10) |
| C(200) | 86(17)  | 81(16)  | 87(17)  | 0(10)  | 3(10) | 5(10)  |
| C(201) | 37(9)   | 34(9)   | 36(9)   | 0(5)   | 0(5)  | -1(5)  |
| C(202) | 31(9)   | 29(9)   | 30(9)   | 2(5)   | 2(5)  | -2(5)  |

|        |         |         |         |        |        |        |
|--------|---------|---------|---------|--------|--------|--------|
| C(203) | 41(10)  | 41(10)  | 41(10)  | 0(5)   | 1(5)   | 2(5)   |
| C(204) | 41(10)  | 39(10)  | 42(10)  | 1(5)   | 2(5)   | 1(5)   |
| C(205) | 55(11)  | 56(11)  | 57(11)  | 1(5)   | -2(5)  | 0(5)   |
| C(206) | 33(9)   | 32(9)   | 34(9)   | -3(5)  | -1(5)  | 0(5)   |
| C(207) | 47(10)  | 48(10)  | 48(10)  | 0(5)   | 0(5)   | 0(5)   |
| C(208) | 67(15)  | 73(15)  | 72(15)  | 8(9)   | 3(9)   | 8(9)   |
| C(209) | 67(14)  | 57(14)  | 66(14)  | 8(9)   | 3(9)   | 0(9)   |
| C(210) | 51(12)  | 43(12)  | 45(12)  | 1(9)   | 2(9)   | 0(9)   |
| C(211) | 32(8)   | 32(8)   | 33(8)   | 0(2)   | 0(2)   | 0(2)   |
| C(212) | 40(10)  | 39(10)  | 41(10)  | 1(5)   | 0(5)   | -1(5)  |
| C(213) | 51(11)  | 51(11)  | 51(11)  | -1(5)  | -1(5)  | 2(5)   |
| C(214) | 40(10)  | 40(10)  | 40(10)  | 0(5)   | 2(5)   | 1(5)   |
| C(215) | 39(9)   | 39(9)   | 38(9)   | 0(5)   | 0(5)   | 0(5)   |
| C(216) | 52(11)  | 54(11)  | 55(11)  | 0(5)   | 1(5)   | 0(5)   |
| C(217) | 98(10)  | 97(10)  | 97(10)  | 1(4)   | 2(4)   | 0(4)   |
| C(218) | 100(11) | 98(11)  | 100(11) | 3(7)   | 1(7)   | 4(7)   |
| C(219) | 105(11) | 103(11) | 101(12) | 1(7)   | -2(7)  | 1(7)   |
| C(220) | 95(11)  | 97(11)  | 96(11)  | 3(7)   | 1(7)   | -1(7)  |
| C(221) | 47(10)  | 46(10)  | 46(10)  | 1(5)   | 1(5)   | -1(5)  |
| C(222) | 60(12)  | 61(12)  | 59(12)  | 1(5)   | 0(5)   | 0(5)   |
| C(223) | 84(15)  | 83(15)  | 83(15)  | 0(5)   | 3(5)   | 0(5)   |
| C(224) | 76(14)  | 77(14)  | 77(14)  | 0(5)   | 1(5)   | 2(5)   |
| C(225) | 56(11)  | 57(11)  | 56(11)  | 1(5)   | 4(5)   | 1(5)   |
| C(226) | 38(9)   | 38(9)   | 34(9)   | 0(5)   | -1(5)  | 1(5)   |
| C(227) | 82(15)  | 82(15)  | 81(15)  | -2(5)  | 1(5)   | 0(5)   |
| C(228) | 106(19) | 105(19) | 107(19) | -2(10) | 2(10)  | 6(10)  |
| C(229) | 87(17)  | 92(17)  | 94(18)  | 4(10)  | 3(10)  | -4(10) |
| C(230) | 110(20) | 110(20) | 120(20) | 4(10)  | -1(10) | 0(10)  |
| C(231) | 42(10)  | 42(10)  | 43(10)  | 0(5)   | -1(5)  | -1(5)  |
| C(232) | 49(10)  | 49(10)  | 47(11)  | -1(5)  | 4(5)   | -2(5)  |
| C(233) | 39(10)  | 41(10)  | 43(10)  | -1(5)  | 1(5)   | -2(5)  |
| C(234) | 46(10)  | 46(10)  | 46(10)  | -1(5)  | -1(5)  | 1(5)   |
| C(235) | 41(10)  | 39(10)  | 40(10)  | 0(5)   | 2(5)   | 1(5)   |
| C(236) | 55(11)  | 54(11)  | 54(11)  | 0(5)   | 2(5)   | 0(5)   |
| C(237) | 106(10) | 105(10) | 105(10) | -1(4)  | 2(4)   | -1(4)  |
| C(238) | 103(12) | 103(12) | 103(12) | 2(7)   | 2(7)   | -3(7)  |
| C(239) | 110(12) | 107(12) | 108(12) | -1(7)  | 2(7)   | -5(7)  |

|        |         |         |         |        |        |        |
|--------|---------|---------|---------|--------|--------|--------|
| C(240) | 112(12) | 112(12) | 113(12) | -5(7)  | -2(7)  | -2(7)  |
| Au(37) | 22(1)   | 19(1)   | 30(1)   | -2(1)  | -1(1)  | -2(1)  |
| Au(38) | 27(1)   | 24(1)   | 35(1)   | 0(1)   | 1(1)   | 2(1)   |
| Au(39) | 25(1)   | 20(1)   | 30(1)   | -1(1)  | -1(1)  | 2(1)   |
| Au(40) | 33(1)   | 28(1)   | 38(1)   | 3(1)   | 3(1)   | 2(1)   |
| Au(41) | 30(1)   | 27(1)   | 33(1)   | 2(1)   | 0(1)   | -2(1)  |
| Au(42) | 26(1)   | 30(1)   | 40(1)   | 1(1)   | -1(1)  | 1(1)   |
| Au(43) | 30(1)   | 30(1)   | 38(1)   | -2(1)  | -3(1)  | 0(1)   |
| Au(44) | 27(1)   | 21(1)   | 31(1)   | 2(1)   | -1(1)  | 1(1)   |
| Au(45) | 34(1)   | 26(1)   | 33(1)   | -2(1)  | -3(1)  | -1(1)  |
| Au(46) | 29(1)   | 21(1)   | 38(1)   | 1(1)   | 3(1)   | 2(1)   |
| Au(47) | 32(1)   | 26(1)   | 40(1)   | 2(1)   | 1(1)   | 3(1)   |
| Au(48) | 56(1)   | 47(1)   | 58(1)   | 7(1)   | 2(1)   | 0(1)   |
| Au(49) | 19(1)   | 21(1)   | 24(2)   | -1(1)  | -1(1)  | 1(1)   |
| Au(50) | 39(2)   | 46(2)   | 33(2)   | -4(2)  | -6(2)  | -7(2)  |
| Au(51) | 21(1)   | 19(1)   | 32(2)   | -3(1)  | -2(1)  | 1(1)   |
| Au(52) | 26(1)   | 24(1)   | 31(2)   | -5(1)  | -6(1)  | 4(1)   |
| Ag(49) | 19(1)   | 21(1)   | 24(1)   | -1(2)  | -1(2)  | 1(2)   |
| Ag(50) | 39(2)   | 46(2)   | 33(2)   | -4(1)  | -6(1)  | -7(2)  |
| Ag(51) | 21(1)   | 19(1)   | 32(1)   | -3(1)  | -2(1)  | 1(2)   |
| Ag(52) | 26(1)   | 24(1)   | 31(1)   | -5(1)  | -6(1)  | 4(1)   |
| Au(53) | 35(1)   | 26(1)   | 38(1)   | 2(1)   | 0(1)   | -2(1)  |
| Au(54) | 48(1)   | 53(1)   | 65(1)   | -1(1)  | 2(1)   | 3(1)   |
| S(25)  | 43(5)   | 27(5)   | 50(6)   | 3(4)   | 10(4)  | 15(4)  |
| S(26)  | 38(5)   | 32(5)   | 39(5)   | 9(4)   | -2(4)  | -5(4)  |
| S(27)  | 41(5)   | 40(5)   | 47(6)   | -3(4)  | 4(4)   | -10(4) |
| S(28)  | 24(4)   | 33(5)   | 45(6)   | -6(4)  | 0(4)   | 0(4)   |
| S(29)  | 29(4)   | 27(4)   | 35(5)   | 0(4)   | 10(4)  | 4(4)   |
| S(30)  | 51(6)   | 47(6)   | 70(8)   | -15(5) | -13(5) | 1(5)   |
| S(31)  | 34(5)   | 27(4)   | 30(5)   | 1(4)   | 5(4)   | -1(4)  |
| S(32)  | 27(4)   | 23(4)   | 44(5)   | 2(4)   | 0(4)   | 3(4)   |
| S(33)  | 37(5)   | 40(5)   | 43(6)   | 6(4)   | -4(4)  | -2(4)  |
| S(34)  | 36(5)   | 46(6)   | 29(5)   | -2(4)  | 9(4)   | 2(4)   |
| S(35)  | 42(5)   | 22(4)   | 33(5)   | -12(4) | -7(4)  | 7(4)   |
| S(36)  | 31(5)   | 32(5)   | 32(5)   | 15(4)  | -1(4)  | 1(4)   |
| C(241) | 27(8)   | 25(8)   | 25(8)   | 2(5)   | -1(5)  | 0(5)   |
| C(242) | 47(10)  | 46(10)  | 48(10)  | 3(5)   | 5(5)   | -2(5)  |



|        |         |         |         |        |        |        |
|--------|---------|---------|---------|--------|--------|--------|
| C(243) | 65(12)  | 65(12)  | 64(12)  | 1(5)   | 3(5)   | -1(5)  |
| C(244) | 55(11)  | 54(11)  | 55(11)  | 0(5)   | 0(5)   | 1(5)   |
| C(245) | 85(15)  | 84(15)  | 86(15)  | 1(5)   | 2(5)   | -1(5)  |
| C(246) | 44(10)  | 45(10)  | 46(10)  | -1(5)  | 2(5)   | 1(5)   |
| C(247) | 56(11)  | 56(11)  | 55(11)  | 0(5)   | 0(5)   | 0(5)   |
| C(248) | 73(15)  | 74(15)  | 74(15)  | -6(10) | 0(9)   | -2(9)  |
| C(249) | 80(16)  | 82(16)  | 85(16)  | -4(10) | 3(10)  | -4(10) |
| C(250) | 60(14)  | 56(14)  | 68(14)  | -4(9)  | -10(9) | 5(9)   |
| C(251) | 35(9)   | 33(9)   | 36(9)   | -2(5)  | 0(5)   | 2(5)   |
| C(252) | 31(9)   | 32(9)   | 34(9)   | 4(5)   | -2(5)  | 3(5)   |
| C(253) | 61(12)  | 61(12)  | 61(12)  | 1(5)   | 0(5)   | -2(5)  |
| C(254) | 115(10) | 115(10) | 115(10) | 0(4)   | 3(4)   | 0(4)   |
| C(255) | 34(9)   | 31(9)   | 33(9)   | 1(5)   | 1(5)   | 2(5)   |
| C(256) | 63(12)  | 61(12)  | 64(12)  | 2(5)   | 2(5)   | 1(5)   |
| C(257) | 117(10) | 117(10) | 117(10) | 2(4)   | 2(4)   | 0(4)   |
| C(258) | 122(12) | 124(12) | 122(12) | 5(7)   | 6(7)   | -1(7)  |
| C(259) | 119(12) | 115(12) | 116(12) | 2(7)   | 2(7)   | -2(7)  |
| C(260) | 124(12) | 122(12) | 121(12) | 5(7)   | 1(7)   | 0(7)   |
| C(261) | 43(10)  | 42(10)  | 44(10)  | 0(5)   | 2(5)   | 0(5)   |
| C(262) | 63(12)  | 62(12)  | 65(12)  | 2(5)   | -1(5)  | -1(5)  |
| C(263) | 83(15)  | 81(15)  | 83(15)  | 0(5)   | 0(5)   | 0(5)   |
| C(264) | 49(10)  | 46(10)  | 50(11)  | 0(5)   | 0(5)   | -1(5)  |
| C(265) | 53(11)  | 52(11)  | 53(11)  | 3(5)   | 0(5)   | 0(5)   |
| C(266) | 52(11)  | 52(11)  | 56(11)  | 2(5)   | 1(5)   | -1(5)  |
| C(267) | 69(13)  | 69(13)  | 70(13)  | 0(5)   | 1(5)   | 0(5)   |
| C(268) | 101(19) | 96(18)  | 102(19) | 0(10)  | 2(10)  | 1(10)  |
| C(269) | 80(16)  | 70(15)  | 80(16)  | 6(10)  | -2(10) | 2(10)  |
| C(270) | 101(18) | 97(18)  | 94(18)  | -5(10) | -1(10) | 0(10)  |
| C(271) | 22(8)   | 20(8)   | 23(8)   | 2(5)   | 0(5)   | -3(5)  |
| C(272) | 35(9)   | 35(9)   | 37(9)   | 2(5)   | 2(5)   | 0(5)   |
| C(273) | 39(9)   | 39(9)   | 38(10)  | 1(5)   | 0(5)   | -2(5)  |
| C(274) | 28(8)   | 24(8)   | 27(8)   | -1(5)  | 0(5)   | -1(5)  |
| C(275) | 43(10)  | 41(10)  | 42(10)  | 4(5)   | 1(5)   | 1(5)   |
| C(276) | 32(9)   | 30(9)   | 32(9)   | 2(5)   | -3(5)  | 1(5)   |
| C(277) | 44(10)  | 46(10)  | 45(10)  | -1(5)  | 3(5)   | -3(5)  |
| C(278) | 36(11)  | 40(11)  | 34(11)  | 2(9)   | 3(9)   | -11(9) |
| C(279) | 69(14)  | 67(14)  | 68(15)  | -4(9)  | 10(9)  | 0(9)   |

|        |         |         |         |       |        |        |
|--------|---------|---------|---------|-------|--------|--------|
| C(280) | 56(13)  | 49(13)  | 48(13)  | 12(9) | -6(9)  | -1(9)  |
| C(281) | 30(9)   | 32(9)   | 28(9)   | -1(5) | -5(5)  | 0(5)   |
| C(282) | 37(9)   | 36(9)   | 39(9)   | 0(5)  | 1(5)   | 0(5)   |
| C(283) | 35(9)   | 34(9)   | 35(9)   | 3(5)  | 1(5)   | 2(5)   |
| C(284) | 40(10)  | 40(10)  | 40(10)  | 0(5)  | 0(5)   | 2(5)   |
| C(285) | 29(8)   | 29(9)   | 30(9)   | 1(5)  | 0(5)   | -2(5)  |
| C(286) | 45(10)  | 47(10)  | 49(10)  | 1(5)  | 1(5)   | -2(5)  |
| C(287) | 30(9)   | 32(9)   | 29(9)   | 0(5)  | 1(5)   | 3(5)   |
| C(288) | 48(13)  | 54(13)  | 53(13)  | -1(9) | 1(9)   | 5(9)   |
| C(289) | 55(13)  | 52(13)  | 55(13)  | -7(9) | 1(9)   | 5(9)   |
| C(290) | 50(12)  | 46(12)  | 45(12)  | -8(9) | 7(9)   | 5(9)   |
| C(291) | 53(11)  | 54(11)  | 55(11)  | 0(5)  | 1(5)   | -2(5)  |
| C(292) | 64(12)  | 64(12)  | 64(12)  | -2(5) | -1(5)  | -1(5)  |
| C(293) | 53(11)  | 54(11)  | 55(11)  | -1(5) | 1(5)   | 0(5)   |
| C(294) | 96(9)   | 96(9)   | 96(9)   | 0(4)  | 3(4)   | -1(4)  |
| C(295) | 64(12)  | 65(12)  | 66(12)  | -1(5) | 0(5)   | 0(5)   |
| C(296) | 43(10)  | 41(10)  | 45(10)  | -1(5) | 3(5)   | 2(5)   |
| C(297) | 98(8)   | 98(8)   | 98(8)   | 1(4)  | 3(4)   | -1(4)  |
| C(298) | 100(11) | 100(11) | 102(11) | 3(7)  | 2(7)   | -5(7)  |
| C(299) | 103(11) | 105(11) | 103(11) | 1(7)  | 3(7)   | 0(7)   |
| C(300) | 103(11) | 100(11) | 103(11) | 2(7)  | 3(7)   | 0(7)   |
| C(301) | 35(9)   | 35(9)   | 33(9)   | 0(5)  | 2(5)   | -3(5)  |
| C(302) | 37(9)   | 39(9)   | 37(9)   | 3(5)  | 0(5)   | 3(5)   |
| C(303) | 38(9)   | 41(10)  | 38(10)  | -2(5) | 0(5)   | 2(5)   |
| C(304) | 44(10)  | 46(10)  | 45(10)  | 3(5)  | 3(5)   | 0(5)   |
| C(305) | 43(10)  | 44(10)  | 44(10)  | -1(5) | 3(5)   | 1(5)   |
| C(306) | 55(11)  | 54(11)  | 55(11)  | 1(5)  | 1(5)   | 1(5)   |
| C(307) | 53(11)  | 53(11)  | 53(11)  | 3(5)  | 2(5)   | 1(5)   |
| C(308) | 86(17)  | 94(17)  | 90(17)  | 1(10) | -4(10) | 2(10)  |
| C(309) | 64(14)  | 60(14)  | 62(14)  | 3(9)  | 1(9)   | 11(9)  |
| C(310) | 85(17)  | 88(17)  | 91(17)  | 8(10) | 6(10)  | -6(10) |
| C(311) | 27(6)   | 29(6)   | 30(6)   | -2(4) | 1(4)   | 0(4)   |
| C(312) | 30(5)   | 30(5)   | 31(5)   | 0(3)  | 2(3)   | -1(3)  |
| C(313) | 32(6)   | 32(6)   | 32(6)   | 0(4)  | 1(4)   | -1(4)  |
| C(314) | 40(9)   | 37(9)   | 40(10)  | 2(5)  | 1(5)   | 0(5)   |
| C(315) | 31(9)   | 32(9)   | 28(9)   | 0(5)  | 0(5)   | -1(5)  |
| C(316) | 26(8)   | 23(8)   | 26(8)   | -1(5) | -1(5)  | 1(5)   |

|        |         |         |         |        |        |        |
|--------|---------|---------|---------|--------|--------|--------|
| C(317) | 50(11)  | 50(11)  | 52(11)  | 0(5)   | 0(5)   | 0(5)   |
| C(318) | 44(12)  | 37(12)  | 45(12)  | -8(9)  | -2(9)  | 1(9)   |
| C(319) | 45(12)  | 52(13)  | 54(13)  | 5(9)   | -3(9)  | 5(9)   |
| C(320) | 65(14)  | 65(14)  | 66(14)  | 0(9)   | -3(9)  | 4(9)   |
| C(321) | 24(8)   | 28(8)   | 28(8)   | 1(5)   | -2(5)  | 1(5)   |
| C(322) | 35(9)   | 30(9)   | 31(9)   | 3(5)   | -2(5)  | 1(5)   |
| C(323) | 46(10)  | 45(10)  | 47(10)  | 3(5)   | 1(5)   | 2(5)   |
| C(324) | 35(9)   | 35(9)   | 37(9)   | 1(5)   | 2(5)   | 1(5)   |
| C(325) | 40(10)  | 40(10)  | 41(10)  | 0(5)   | 0(5)   | 0(5)   |
| C(326) | 31(9)   | 31(9)   | 33(9)   | 2(5)   | 1(5)   | -1(5)  |
| C(327) | 51(11)  | 51(11)  | 50(11)  | 3(5)   | 0(5)   | 1(5)   |
| C(328) | 62(14)  | 66(14)  | 64(14)  | 2(9)   | 2(9)   | 3(9)   |
| C(329) | 75(15)  | 71(15)  | 72(15)  | 2(9)   | 5(9)   | -1(9)  |
| C(330) | 61(13)  | 47(13)  | 50(13)  | 4(9)   | -1(9)  | -2(9)  |
| C(331) | 41(10)  | 41(10)  | 41(10)  | -2(5)  | 2(5)   | -2(5)  |
| C(332) | 63(12)  | 64(12)  | 61(12)  | -3(5)  | -2(5)  | 1(5)   |
| C(333) | 66(13)  | 67(13)  | 66(13)  | -1(5)  | 1(5)   | 3(5)   |
| C(334) | 39(9)   | 38(9)   | 38(9)   | -4(5)  | 0(5)   | 1(5)   |
| C(335) | 64(12)  | 61(12)  | 61(12)  | 0(5)   | 0(5)   | 0(5)   |
| C(336) | 31(9)   | 32(9)   | 33(9)   | -1(5)  | 1(5)   | 1(5)   |
| C(337) | 41(10)  | 39(10)  | 41(10)  | 1(5)   | 1(5)   | 0(5)   |
| C(338) | 69(15)  | 69(15)  | 74(15)  | 1(9)   | -4(9)  | -3(9)  |
| C(339) | 110(20) | 110(20) | 120(20) | -1(10) | -3(10) | 4(10)  |
| C(340) | 84(16)  | 87(17)  | 83(17)  | -7(10) | -5(10) | -3(10) |
| C(341) | 79(6)   | 79(6)   | 80(6)   | 1(3)   | 2(3)   | -1(3)  |
| C(342) | 80(6)   | 80(6)   | 81(6)   | 0(3)   | 2(3)   | 0(3)   |
| C(343) | 83(6)   | 82(6)   | 82(6)   | 1(3)   | 2(3)   | -1(3)  |
| C(344) | 85(6)   | 85(6)   | 84(6)   | 1(3)   | 1(3)   | -1(3)  |
| C(345) | 82(6)   | 82(6)   | 82(6)   | 2(3)   | 1(3)   | -1(3)  |
| C(346) | 80(6)   | 80(6)   | 80(6)   | 2(3)   | 2(3)   | 0(3)   |
| C(347) | 90(6)   | 90(6)   | 90(6)   | 1(4)   | 1(4)   | -2(4)  |
| C(348) | 95(9)   | 96(9)   | 94(9)   | -1(7)  | -2(7)  | -3(7)  |
| C(349) | 96(9)   | 96(9)   | 99(9)   | 0(7)   | -1(7)  | -6(7)  |
| C(350) | 97(9)   | 98(9)   | 99(10)  | 3(7)   | 0(7)   | -4(7)  |
| C(351) | 27(8)   | 27(8)   | 29(8)   | 1(5)   | 1(5)   | 0(5)   |
| C(352) | 41(10)  | 42(10)  | 41(10)  | 1(5)   | 2(5)   | -1(5)  |
| C(353) | 39(10)  | 40(10)  | 39(10)  | 0(5)   | 0(5)   | 1(5)   |

|        |        |        |        |        |        |       |
|--------|--------|--------|--------|--------|--------|-------|
| C(354) | 35(9)  | 32(9)  | 37(9)  | 0(5)   | -1(5)  | -1(5) |
| C(355) | 66(13) | 66(13) | 65(13) | -3(5)  | 0(5)   | 0(5)  |
| C(356) | 65(13) | 66(13) | 66(13) | -2(5)  | -1(5)  | 1(5)  |
| C(357) | 34(9)  | 34(9)  | 35(9)  | -2(5)  | -1(5)  | 1(5)  |
| C(358) | 49(12) | 42(12) | 48(12) | 5(9)   | -1(9)  | 3(9)  |
| C(359) | 93(18) | 93(18) | 96(18) | -2(10) | -4(10) | 4(10) |
| C(360) | 64(14) | 64(14) | 65(14) | 4(9)   | 1(9)   | 4(9)  |

**Table S5. Bond lengths [Å] and angles [deg] for [Au<sub>32</sub>Ag<sub>4</sub>(SPh-tBu)<sub>24</sub>].**

|              |        |
|--------------|--------|
| Au(1)-Au(2)  | 2.9167 |
| Au(1)-Au(3)  | 2.9809 |
| Au(1)-Au(4)  | 2.7610 |
| Au(1)-Au(5)  | 2.9312 |
| Au(1)-Au(17) | 2.8053 |
| Au(1)-Au(18) | 2.7389 |
| Au(1)-Au(19) | 2.7641 |
| Au(1)-Au(20) | 3.1560 |
| Au(1)-Au(21) | 3.1424 |
| Au(1)-Au(23) | 3.3701 |
| Au(1)-Au(24) | 2.9882 |
| Au(1)-Au(28) | 2.7406 |
| Au(2)-Au(3)  | 2.9595 |
| Au(2)-Au(5)  | 2.9653 |
| Au(2)-Au(6)  | 2.7578 |
| Au(2)-Au(7)  | 3.0707 |
| Au(2)-Au(15) | 2.7489 |
| Au(2)-Au(16) | 3.2558 |
| Au(2)-Au(17) | 3.0876 |
| Au(2)-Au(22) | 3.3138 |
| Au(2)-Au(24) | 2.7922 |
| Au(2)-Au(25) | 2.7386 |
| Au(2)-Au(26) | 2.7931 |
| Au(3)-Au(4)  | 2.7280 |
| Au(3)-Au(5)  | 2.9283 |
| Au(3)-Au(7)  | 2.7483 |
| Au(3)-Au(8)  | 2.7643 |
| Au(3)-Au(9)  | 2.7976 |
| Au(3)-Au(11) | 3.0302 |

|               |        |
|---------------|--------|
| Au(3)-Au(26)  | 3.1506 |
| Au(3)-Au(27)  | 3.0930 |
| Au(3)-Au(28)  | 2.7789 |
| Au(4)-Au(11)  | 2.9547 |
| Au(4)-Au(12)  | 3.0824 |
| Au(4)-Au(20)  | 3.0027 |
| Au(4)-Au(21)  | 3.0826 |
| Au(4)-Au(28)  | 2.7588 |
| Au(4)-S(2)    | 2.3787 |
| Au(5)-Au(6)   | 2.7656 |
| Au(5)-Au(9)   | 3.1027 |
| Au(5)-Au(10)  | 3.2932 |
| Au(5)-Au(11)  | 2.8045 |
| Au(5)-Au(13)  | 2.7302 |
| Au(5)-Au(14)  | 3.2362 |
| Au(5)-Au(15)  | 2.7543 |
| Au(5)-Au(19)  | 2.9890 |
| Au(5)-Au(20)  | 2.8338 |
| Au(6)-Au(7)   | 2.9396 |
| Au(6)-Au(9)   | 3.0018 |
| Au(6)-Au(10)  | 3.1682 |
| Au(6)-Au(15)  | 2.7457 |
| Au(6)-Au(22)  | 3.0402 |
| Au(6)-S(21)   | 2.3735 |
| Au(7)-Au(8)   | 2.7885 |
| Au(7)-Au(9)   | 2.7271 |
| Au(7)-Au(26)  | 2.9671 |
| Au(7)-S(17)   | 2.3795 |
| Au(8)-Au(9)   | 2.7307 |
| Au(8)-Au(12)  | 3.0593 |
| Au(8)-Au(27)  | 2.8259 |
| Au(8)-Au(36)  | 2.9941 |
| Au(8)-S(14)   | 2.4392 |
| Au(9)-Au(10)  | 3.2894 |
| Au(9)-Au(11)  | 2.8930 |
| Au(9)-S(22)   | 2.3678 |
| Au(10)-Au(13) | 2.8613 |

|               |        |
|---------------|--------|
| Au(10)-S(5)   | 2.3032 |
| Au(10)-S(22)  | 2.3027 |
| Au(11)-Au(12) | 3.3524 |
| Au(11)-Au(13) | 2.7628 |
| Au(11)-Au(20) | 2.7316 |
| Au(11)-S(6)   | 2.4026 |
| Au(12)-S(6)   | 2.2886 |
| Au(12)-S(24)  | 2.2963 |
| Au(13)-Au(14) | 2.9898 |
| Au(13)-Au(20) | 2.7410 |
| Au(13)-Au(31) | 3.0154 |
| Au(13)-S(3)   | 2.4413 |
| Au(14)-Au(15) | 2.9975 |
| Au(14)-Au(19) | 3.2573 |
| Au(14)-S(1)   | 2.3276 |
| Au(14)-S(5)   | 2.3218 |
| Au(15)-Au(16) | 3.1537 |
| Au(15)-Au(17) | 3.0132 |
| Au(15)-Au(19) | 3.0169 |
| Au(15)-S(8)   | 2.3814 |
| Au(16)-Au(17) | 3.2579 |
| Au(16)-Au(25) | 2.8227 |
| Au(16)-S(19)  | 2.3075 |
| Au(16)-S(20)  | 2.3033 |
| Au(17)-Au(18) | 2.7283 |
| Au(17)-Au(19) | 2.7110 |
| Au(17)-Au(24) | 2.9360 |
| Au(17)-S(19)  | 2.3513 |
| Au(18)-Au(19) | 2.7917 |
| Au(18)-Au(21) | 2.8133 |
| Au(18)-Au(23) | 3.1410 |
| Au(18)-Au(29) | 3.0590 |
| Au(18)-S(11)  | 2.4064 |
| Au(19)-Au(20) | 2.9215 |
| Au(19)-S(1)   | 2.3967 |
| Au(20)-Au(21) | 3.2435 |
| Au(20)-Au(32) | 3.3762 |

|               |        |
|---------------|--------|
| Au(20)-S(7)   | 2.3917 |
| Au(21)-S(7)   | 2.3122 |
| Au(21)-S(10)  | 2.3212 |
| Au(22)-Au(25) | 3.0921 |
| Au(22)-S(17)  | 2.3179 |
| Au(22)-S(20)  | 2.2927 |
| Au(23)-Au(24) | 3.3048 |
| Au(23)-Au(28) | 2.9963 |
| Au(23)-S(10)  | 2.2969 |
| Au(23)-S(12)  | 2.3036 |
| Au(24)-Au(25) | 2.7576 |
| Au(24)-Au(26) | 2.7338 |
| Au(24)-Au(28) | 2.9536 |
| Au(24)-S(12)  | 2.4036 |
| Au(25)-Au(26) | 2.7251 |
| Au(25)-Au(34) | 3.0751 |
| Au(25)-S(18)  | 2.4288 |
| Au(26)-Au(27) | 3.2292 |
| Au(26)-Au(28) | 3.0196 |
| Au(26)-S(15)  | 2.3495 |
| Au(27)-Au(28) | 3.0553 |
| Au(27)-S(15)  | 2.3043 |
| Au(27)-S(24)  | 2.2981 |
| Au(28)-S(13)  | 2.3983 |
| Au(29)-S(9)   | 2.2940 |
| Au(29)-S(11)  | 2.3119 |
| Au(30)-S(8)   | 2.3003 |
| Au(30)-S(9)   | 2.3108 |
| Au(31)-S(3)   | 2.3006 |
| Au(31)-S(4)   | 2.3021 |
| Au(32)-S(2)   | 2.2615 |
| Au(32)-S(4)   | 2.3292 |
| Au(33)-S(13)  | 2.2611 |
| Au(33)-S(16)  | 2.3214 |
| Au(34)-S(16)  | 2.3205 |
| Au(34)-S(18)  | 2.2923 |
| Au(35)-S(21)  | 2.2898 |

|              |        |
|--------------|--------|
| Au(35)-S(23) | 2.3160 |
| Au(36)-S(14) | 2.3011 |
| Au(36)-S(23) | 2.3080 |
| S(1)-C(1)    | 1.7879 |
| S(2)-C(11)   | 1.8283 |
| S(3)-C(21)   | 1.8098 |
| S(4)-C(31)   | 1.7909 |
| S(5)-C(41)   | 1.7614 |
| S(6)-C(51)   | 1.7521 |
| S(7)-C(61)   | 1.7900 |
| S(8)-C(71)   | 1.7749 |
| S(9)-C(81)   | 1.7895 |
| S(10)-C(91)  | 1.8082 |
| S(11)-C(101) | 1.8213 |
| S(12)-C(111) | 1.7883 |
| S(13)-C(121) | 1.8335 |
| S(14)-C(131) | 1.8250 |
| S(15)-C(141) | 1.7352 |
| S(16)-C(151) | 1.8445 |
| S(17)-C(161) | 1.7524 |
| S(18)-C(171) | 1.7615 |
| S(19)-C(181) | 1.8037 |
| S(20)-C(191) | 1.7492 |
| S(21)-C(201) | 1.8455 |
| S(22)-C(211) | 1.8658 |
| S(23)-C(221) | 1.7524 |
| S(24)-C(231) | 1.8020 |
| C(1)-C(2)    | 1.3634 |
| C(1)-C(6)    | 1.4584 |
| C(2)-H(2)    | 0.9300 |
| C(2)-C(3)    | 1.3530 |
| C(3)-H(3)    | 0.9300 |
| C(3)-C(4)    | 1.4440 |
| C(4)-C(5)    | 1.4070 |
| C(4)-C(7)    | 1.5468 |
| C(5)-H(5)    | 0.9300 |
| C(5)-C(6)    | 1.4181 |



|              |        |
|--------------|--------|
| C(6)-H(6)    | 0.9300 |
| C(7)-C(8)    | 1.5333 |
| C(7)-C(9)    | 1.5524 |
| C(7)-C(10)   | 1.5142 |
| C(8)-H(8A)   | 0.9600 |
| C(8)-H(8B)   | 0.9600 |
| C(8)-H(8C)   | 0.9600 |
| C(9)-H(9A)   | 0.9600 |
| C(9)-H(9B)   | 0.9600 |
| C(9)-H(9C)   | 0.9600 |
| C(10)-H(10A) | 0.9600 |
| C(10)-H(10B) | 0.9600 |
| C(10)-H(10C) | 0.9600 |
| C(11)-C(12)  | 1.3561 |
| C(11)-C(16)  | 1.3371 |
| C(12)-H(12)  | 0.9300 |
| C(12)-C(13)  | 1.3923 |
| C(13)-H(13)  | 0.9300 |
| C(13)-C(14)  | 1.4208 |
| C(14)-C(15)  | 1.3829 |
| C(14)-C(17)  | 1.5323 |
| C(15)-H(15)  | 0.9300 |
| C(15)-C(16)  | 1.4009 |
| C(16)-H(16)  | 0.9300 |
| C(17)-C(18)  | 1.5388 |
| C(17)-C(19)  | 1.4971 |
| C(17)-C(20)  | 1.6137 |
| C(18)-H(18A) | 0.9600 |
| C(18)-H(18B) | 0.9600 |
| C(18)-H(18C) | 0.9600 |
| C(19)-H(19A) | 0.9600 |
| C(19)-H(19B) | 0.9600 |
| C(19)-H(19C) | 0.9600 |
| C(20)-H(20A) | 0.9600 |
| C(20)-H(20B) | 0.9600 |
| C(20)-H(20C) | 0.9600 |
| C(21)-C(22)  | 1.3613 |

|              |        |
|--------------|--------|
| C(21)-C(26)  | 1.4399 |
| C(22)-H(22)  | 0.9300 |
| C(22)-C(23)  | 1.4391 |
| C(23)-H(23)  | 0.9300 |
| C(23)-C(24)  | 1.3508 |
| C(24)-C(25)  | 1.4158 |
| C(24)-C(27)  | 1.5552 |
| C(25)-H(25)  | 0.9300 |
| C(25)-C(26)  | 1.4054 |
| C(26)-H(26)  | 0.9300 |
| C(27)-C(28)  | 1.6375 |
| C(27)-C(29)  | 1.5257 |
| C(27)-C(30)  | 1.5597 |
| C(28)-H(28A) | 0.9600 |
| C(28)-H(28B) | 0.9600 |
| C(28)-H(28C) | 0.9600 |
| C(29)-H(29A) | 0.9600 |
| C(29)-H(29B) | 0.9600 |
| C(29)-H(29C) | 0.9600 |
| C(30)-H(30A) | 0.9600 |
| C(30)-H(30B) | 0.9600 |
| C(30)-H(30C) | 0.9600 |
| C(31)-C(32)  | 1.3905 |
| C(31)-C(36)  | 1.3558 |
| C(32)-H(32)  | 0.9300 |
| C(32)-C(33)  | 1.4437 |
| C(33)-H(33)  | 0.9300 |
| C(33)-C(34)  | 1.3799 |
| C(34)-C(35)  | 1.4182 |
| C(34)-C(37)  | 1.5124 |
| C(35)-H(35)  | 0.9300 |
| C(35)-C(36)  | 1.4032 |
| C(36)-H(36)  | 0.9300 |
| C(37)-C(38)  | 1.4866 |
| C(37)-C(39)  | 1.5939 |
| C(37)-C(40)  | 1.6397 |
| C(38)-H(38A) | 0.9600 |

|              |        |
|--------------|--------|
| C(38)-H(38B) | 0.9600 |
| C(38)-H(38C) | 0.9600 |
| C(39)-H(39A) | 0.9600 |
| C(39)-H(39B) | 0.9600 |
| C(39)-H(39C) | 0.9600 |
| C(40)-H(40A) | 0.9600 |
| C(40)-H(40B) | 0.9600 |
| C(40)-H(40C) | 0.9600 |
| C(41)-C(42)  | 1.4581 |
| C(41)-C(46)  | 1.4247 |
| C(42)-H(42)  | 0.9300 |
| C(42)-C(43)  | 1.3718 |
| C(43)-H(43)  | 0.9300 |
| C(43)-C(44)  | 1.4167 |
| C(44)-C(45)  | 1.3632 |
| C(44)-C(47)  | 1.5796 |
| C(45)-H(45)  | 0.9300 |
| C(45)-C(46)  | 1.4525 |
| C(46)-H(46)  | 0.9300 |
| C(47)-C(48)  | 1.6722 |
| C(47)-C(49)  | 1.5852 |
| C(47)-C(50)  | 1.5032 |
| C(48)-H(48A) | 0.9600 |
| C(48)-H(48B) | 0.9600 |
| C(48)-H(48C) | 0.9600 |
| C(49)-H(49A) | 0.9600 |
| C(49)-H(49B) | 0.9600 |
| C(49)-H(49C) | 0.9600 |
| C(50)-H(50A) | 0.9600 |
| C(50)-H(50B) | 0.9600 |
| C(50)-H(50C) | 0.9600 |
| C(51)-C(52)  | 1.4249 |
| C(51)-C(56)  | 1.4652 |
| C(52)-H(52)  | 0.9300 |
| C(52)-C(53)  | 1.3085 |
| C(53)-H(53)  | 0.9300 |
| C(53)-C(54)  | 1.3663 |

|              |        |
|--------------|--------|
| C(54)-C(55)  | 1.4007 |
| C(54)-C(57)  | 1.6084 |
| C(55)-H(55)  | 0.9300 |
| C(55)-C(56)  | 1.3527 |
| C(56)-H(56)  | 0.9300 |
| C(57)-C(58)  | 1.6026 |
| C(57)-C(59)  | 1.5613 |
| C(57)-C(60)  | 1.5290 |
| C(58)-H(58A) | 0.9600 |
| C(58)-H(58B) | 0.9600 |
| C(58)-H(58C) | 0.9600 |
| C(59)-H(59A) | 0.9600 |
| C(59)-H(59B) | 0.9600 |
| C(59)-H(59C) | 0.9600 |
| C(60)-H(60A) | 0.9600 |
| C(60)-H(60B) | 0.9600 |
| C(60)-H(60C) | 0.9600 |
| C(61)-C(62)  | 1.3613 |
| C(61)-C(66)  | 1.4031 |
| C(62)-H(62)  | 0.9300 |
| C(62)-C(63)  | 1.3229 |
| C(63)-H(63)  | 0.9300 |
| C(63)-C(64)  | 1.4157 |
| C(64)-C(65)  | 1.4335 |
| C(64)-C(67)  | 1.5920 |
| C(65)-H(65)  | 0.9300 |
| C(65)-C(66)  | 1.3566 |
| C(66)-H(66)  | 0.9300 |
| C(67)-C(68)  | 1.5766 |
| C(67)-C(69)  | 1.5060 |
| C(67)-C(70)  | 1.5137 |
| C(68)-H(68A) | 0.9600 |
| C(68)-H(68B) | 0.9600 |
| C(68)-H(68C) | 0.9600 |
| C(69)-H(69A) | 0.9600 |
| C(69)-H(69B) | 0.9600 |
| C(69)-H(69C) | 0.9600 |

|              |        |
|--------------|--------|
| C(70)-H(70A) | 0.9600 |
| C(70)-H(70B) | 0.9600 |
| C(70)-H(70C) | 0.9600 |
| C(71)-C(72)  | 1.3475 |
| C(71)-C(76)  | 1.4445 |
| C(72)-H(72)  | 0.9300 |
| C(72)-C(73)  | 1.4094 |
| C(73)-H(73)  | 0.9300 |
| C(73)-C(74)  | 1.3930 |
| C(74)-C(75)  | 1.3869 |
| C(74)-C(77)  | 1.5451 |
| C(75)-H(75)  | 0.9300 |
| C(75)-C(76)  | 1.4308 |
| C(76)-H(76)  | 0.9300 |
| C(77)-C(78)  | 1.5330 |
| C(77)-C(79)  | 1.5442 |
| C(77)-C(80)  | 1.5423 |
| C(78)-H(78A) | 0.9600 |
| C(78)-H(78B) | 0.9600 |
| C(78)-H(78C) | 0.9600 |
| C(79)-H(79A) | 0.9600 |
| C(79)-H(79B) | 0.9600 |
| C(79)-H(79C) | 0.9600 |
| C(80)-H(80A) | 0.9600 |
| C(80)-H(80B) | 0.9600 |
| C(80)-H(80C) | 0.9600 |
| C(81)-C(82)  | 1.3516 |
| C(81)-C(86)  | 1.4449 |
| C(82)-H(82)  | 0.9300 |
| C(82)-C(83)  | 1.4418 |
| C(83)-H(83)  | 0.9300 |
| C(83)-C(84)  | 1.4717 |
| C(84)-C(85)  | 1.3642 |
| C(84)-C(87)  | 1.5552 |
| C(85)-H(85)  | 0.9300 |
| C(85)-C(86)  | 1.4931 |
| C(86)-H(86)  | 0.9300 |

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|---------------|--------|
| C(87)-C(88)   | 1.4637 |
| C(87)-C(89)   | 1.5794 |
| C(87)-C(90)   | 1.6239 |
| C(88)-H(88A)  | 0.9600 |
| C(88)-H(88B)  | 0.9600 |
| C(88)-H(88C)  | 0.9600 |
| C(89)-H(89A)  | 0.9600 |
| C(89)-H(89B)  | 0.9600 |
| C(89)-H(89C)  | 0.9600 |
| C(90)-H(90A)  | 0.9600 |
| C(90)-H(90B)  | 0.9600 |
| C(90)-H(90C)  | 0.9600 |
| C(91)-C(92)   | 1.4316 |
| C(91)-C(96)   | 1.3903 |
| C(92)-H(92)   | 0.9300 |
| C(92)-C(93)   | 1.3476 |
| C(93)-H(93)   | 0.9300 |
| C(93)-C(94)   | 1.3038 |
| C(94)-C(95)   | 1.3937 |
| C(94)-C(97)   | 1.6350 |
| C(95)-H(95)   | 0.9300 |
| C(95)-C(96)   | 1.3922 |
| C(96)-H(96)   | 0.9300 |
| C(97)-C(98)   | 1.6349 |
| C(97)-C(99)   | 1.4539 |
| C(97)-C(100)  | 1.5108 |
| C(98)-H(98A)  | 0.9600 |
| C(98)-H(98B)  | 0.9600 |
| C(98)-H(98C)  | 0.9600 |
| C(99)-H(99A)  | 0.9600 |
| C(99)-H(99B)  | 0.9600 |
| C(99)-H(99C)  | 0.9600 |
| C(100)-H(10D) | 0.9600 |
| C(100)-H(10E) | 0.9600 |
| C(100)-H(10F) | 0.9600 |
| C(101)-C(102) | 1.3865 |
| C(101)-C(106) | 1.3855 |

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|---------------|--------|
| C(102)-H(102) | 0.9300 |
| C(102)-C(103) | 1.3923 |
| C(103)-H(103) | 0.9300 |
| C(103)-C(104) | 1.3520 |
| C(104)-C(105) | 1.4112 |
| C(104)-C(107) | 1.5456 |
| C(105)-H(105) | 0.9300 |
| C(105)-C(106) | 1.3712 |
| C(106)-H(106) | 0.9300 |
| C(107)-C(108) | 1.5561 |
| C(107)-C(109) | 1.5147 |
| C(107)-C(110) | 1.5657 |
| C(108)-H(10G) | 0.9600 |
| C(108)-H(10H) | 0.9600 |
| C(108)-H(10I) | 0.9600 |
| C(109)-H(10J) | 0.9600 |
| C(109)-H(10K) | 0.9600 |
| C(109)-H(10L) | 0.9600 |
| C(110)-H(11A) | 0.9600 |
| C(110)-H(11B) | 0.9600 |
| C(110)-H(11C) | 0.9600 |
| C(111)-C(112) | 1.3944 |
| C(111)-C(116) | 1.3197 |
| C(112)-H(112) | 0.9300 |
| C(112)-C(113) | 1.3832 |
| C(113)-H(113) | 0.9300 |
| C(113)-C(114) | 1.4184 |
| C(114)-C(115) | 1.3846 |
| C(114)-C(117) | 1.5700 |
| C(115)-H(115) | 0.9300 |
| C(115)-C(116) | 1.3845 |
| C(116)-H(116) | 0.9300 |
| C(117)-C(118) | 1.5809 |
| C(117)-C(119) | 1.5344 |
| C(117)-C(120) | 1.6408 |
| C(118)-H(11D) | 0.9600 |
| C(118)-H(11E) | 0.9600 |

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| C(118)-H(11F) | 0.9600 |
| C(119)-H(11G) | 0.9600 |
| C(119)-H(11H) | 0.9600 |
| C(119)-H(11I) | 0.9600 |
| C(120)-H(12A) | 0.9600 |
| C(120)-H(12B) | 0.9600 |
| C(120)-H(12C) | 0.9600 |
| C(121)-C(122) | 1.4578 |
| C(121)-C(126) | 1.3097 |
| C(122)-H(122) | 0.9300 |
| C(122)-C(123) | 1.4185 |
| C(123)-H(123) | 0.9300 |
| C(123)-C(124) | 1.3391 |
| C(124)-C(125) | 1.3279 |
| C(124)-C(127) | 1.5896 |
| C(125)-H(125) | 0.9300 |
| C(125)-C(126) | 1.4663 |
| C(126)-H(126) | 0.9300 |
| C(127)-C(128) | 1.7902 |
| C(127)-C(129) | 1.4960 |
| C(127)-C(130) | 1.3379 |
| C(129)-H(12D) | 0.9600 |
| C(129)-H(12E) | 0.9600 |
| C(129)-H(12F) | 0.9600 |
| C(130)-H(13A) | 0.9600 |
| C(130)-H(13B) | 0.9600 |
| C(130)-H(13C) | 0.9600 |
| C(131)-C(132) | 1.3739 |
| C(131)-C(136) | 1.3817 |
| C(132)-H(132) | 0.9300 |
| C(132)-C(133) | 1.4660 |
| C(133)-H(133) | 0.9300 |
| C(133)-C(134) | 1.3268 |
| C(134)-C(135) | 1.3756 |
| C(134)-C(137) | 1.6281 |
| C(135)-H(135) | 0.9300 |
| C(135)-C(136) | 1.3239 |



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|---------------|--------|
| C(136)-H(136) | 0.9300 |
| C(137)-C(138) | 1.5051 |
| C(137)-C(139) | 1.5617 |
| C(137)-C(140) | 1.5620 |
| C(138)-H(13D) | 0.9600 |
| C(138)-H(13E) | 0.9600 |
| C(138)-H(13F) | 0.9600 |
| C(139)-H(13G) | 0.9600 |
| C(139)-H(13H) | 0.9600 |
| C(139)-H(13I) | 0.9600 |
| C(140)-H(14A) | 0.9600 |
| C(140)-H(14B) | 0.9600 |
| C(140)-H(14C) | 0.9600 |
| C(141)-C(142) | 1.4104 |
| C(141)-C(146) | 1.4530 |
| C(142)-H(142) | 0.9300 |
| C(142)-C(143) | 1.4188 |
| C(143)-H(143) | 0.9300 |
| C(143)-C(144) | 1.3632 |
| C(144)-C(145) | 1.3749 |
| C(144)-C(147) | 1.5857 |
| C(145)-H(145) | 0.9300 |
| C(145)-C(146) | 1.3517 |
| C(146)-H(146) | 0.9300 |
| C(147)-C(148) | 1.6316 |
| C(147)-C(149) | 1.5750 |
| C(147)-C(150) | 1.5401 |
| C(148)-H(14D) | 0.9600 |
| C(148)-H(14E) | 0.9600 |
| C(148)-H(14F) | 0.9600 |
| C(149)-H(14G) | 0.9600 |
| C(149)-H(14H) | 0.9600 |
| C(149)-H(14I) | 0.9600 |
| C(150)-H(15A) | 0.9600 |
| C(150)-H(15B) | 0.9600 |
| C(150)-H(15C) | 0.9600 |
| C(151)-C(152) | 1.3915 |

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|---------------|--------|
| C(151)-C(156) | 1.3543 |
| C(152)-H(152) | 0.9300 |
| C(152)-C(153) | 1.4576 |
| C(153)-H(153) | 0.9300 |
| C(153)-C(154) | 1.3428 |
| C(154)-C(155) | 1.4507 |
| C(154)-C(157) | 1.6569 |
| C(155)-H(155) | 0.9300 |
| C(155)-C(156) | 1.3442 |
| C(156)-H(156) | 0.9300 |
| C(157)-C(158) | 1.4718 |
| C(157)-C(159) | 1.4503 |
| C(157)-C(160) | 1.6002 |
| C(158)-H(15D) | 0.9600 |
| C(158)-H(15E) | 0.9600 |
| C(158)-H(15F) | 0.9600 |
| C(159)-H(15G) | 0.9600 |
| C(159)-H(15H) | 0.9600 |
| C(159)-H(15I) | 0.9600 |
| C(160)-H(16A) | 0.9600 |
| C(160)-H(16B) | 0.9600 |
| C(160)-H(16C) | 0.9600 |
| C(161)-C(162) | 1.3673 |
| C(161)-C(166) | 1.4338 |
| C(162)-H(162) | 0.9300 |
| C(162)-C(163) | 1.3776 |
| C(163)-H(163) | 0.9300 |
| C(163)-C(164) | 1.3361 |
| C(164)-C(165) | 1.4060 |
| C(164)-C(167) | 1.5550 |
| C(165)-H(165) | 0.9300 |
| C(165)-C(166) | 1.4318 |
| C(166)-H(166) | 0.9300 |
| C(167)-C(168) | 1.5801 |
| C(167)-C(169) | 1.5549 |
| C(167)-C(170) | 1.6440 |
| C(168)-H(16D) | 0.9600 |

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| C(168)-H(16E) | 0.9600 |
| C(168)-H(16F) | 0.9600 |
| C(169)-H(16G) | 0.9600 |
| C(169)-H(16H) | 0.9600 |
| C(169)-H(16I) | 0.9600 |
| C(170)-H(17A) | 0.9600 |
| C(170)-H(17B) | 0.9600 |
| C(170)-H(17C) | 0.9600 |
| C(171)-C(172) | 1.4466 |
| C(171)-C(176) | 1.4041 |
| C(172)-H(172) | 0.9300 |
| C(172)-C(173) | 1.3764 |
| C(173)-H(173) | 0.9300 |
| C(173)-C(174) | 1.4036 |
| C(174)-C(175) | 1.4327 |
| C(174)-C(177) | 1.5688 |
| C(175)-H(175) | 0.9300 |
| C(175)-C(176) | 1.3604 |
| C(176)-H(176) | 0.9300 |
| C(177)-C(178) | 1.6878 |
| C(177)-C(179) | 1.5012 |
| C(177)-C(180) | 1.3140 |
| C(178)-H(17D) | 0.9600 |
| C(178)-H(17E) | 0.9600 |
| C(178)-H(17F) | 0.9600 |
| C(179)-H(17G) | 0.9600 |
| C(179)-H(17H) | 0.9600 |
| C(179)-H(17I) | 0.9600 |
| C(180)-H(18D) | 0.9600 |
| C(180)-H(18E) | 0.9600 |
| C(180)-H(18F) | 0.9600 |
| C(181)-C(182) | 1.3557 |
| C(181)-C(186) | 1.4373 |
| C(182)-H(182) | 0.9300 |
| C(182)-C(183) | 1.4464 |
| C(183)-H(183) | 0.9300 |
| C(183)-C(184) | 1.3418 |

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|---------------|--------|
| C(184)-C(185) | 1.4369 |
| C(184)-C(187) | 1.5813 |
| C(185)-H(185) | 0.9300 |
| C(185)-C(186) | 1.3511 |
| C(186)-H(186) | 0.9300 |
| C(187)-C(188) | 1.5229 |
| C(187)-C(189) | 1.6216 |
| C(187)-C(190) | 1.6294 |
| C(188)-H(18G) | 0.9600 |
| C(188)-H(18H) | 0.9600 |
| C(188)-H(18I) | 0.9600 |
| C(189)-H(18J) | 0.9600 |
| C(189)-H(18K) | 0.9600 |
| C(189)-H(18L) | 0.9600 |
| C(190)-H(19D) | 0.9600 |
| C(190)-H(19E) | 0.9600 |
| C(190)-H(19F) | 0.9600 |
| C(191)-C(192) | 1.4487 |
| C(191)-C(196) | 1.4157 |
| C(192)-H(192) | 0.9300 |
| C(192)-C(193) | 1.3805 |
| C(193)-H(193) | 0.9300 |
| C(193)-C(194) | 1.4705 |
| C(194)-C(195) | 1.4253 |
| C(194)-C(197) | 1.6038 |
| C(195)-H(195) | 0.9300 |
| C(195)-C(196) | 1.3549 |
| C(196)-H(196) | 0.9300 |
| C(197)-C(198) | 1.5519 |
| C(197)-C(199) | 1.5122 |
| C(197)-C(200) | 1.5035 |
| C(198)-H(19G) | 0.9600 |
| C(198)-H(19H) | 0.9600 |
| C(198)-H(19I) | 0.9600 |
| C(199)-H(19J) | 0.9600 |
| C(199)-H(19K) | 0.9600 |
| C(199)-H(19L) | 0.9600 |

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| C(200)-H(20D) | 0.9600 |
| C(200)-H(20E) | 0.9600 |
| C(200)-H(20F) | 0.9600 |
| C(201)-C(202) | 1.4462 |
| C(201)-C(206) | 1.3271 |
| C(202)-H(202) | 0.9300 |
| C(202)-C(203) | 1.3756 |
| C(203)-H(203) | 0.9300 |
| C(203)-C(204) | 1.3599 |
| C(204)-C(205) | 1.3654 |
| C(204)-C(207) | 1.5314 |
| C(205)-H(205) | 0.9300 |
| C(205)-C(206) | 1.3977 |
| C(206)-H(206) | 0.9300 |
| C(207)-C(208) | 1.6040 |
| C(207)-C(209) | 1.5189 |
| C(207)-C(210) | 1.5217 |
| C(208)-H(20G) | 0.9600 |
| C(208)-H(20H) | 0.9600 |
| C(208)-H(20I) | 0.9600 |
| C(209)-H(20J) | 0.9600 |
| C(209)-H(20K) | 0.9600 |
| C(209)-H(20L) | 0.9600 |
| C(210)-H(21A) | 0.9600 |
| C(210)-H(21B) | 0.9600 |
| C(210)-H(21C) | 0.9600 |
| C(211)-C(212) | 1.3270 |
| C(211)-C(216) | 1.4373 |
| C(212)-H(212) | 0.9300 |
| C(212)-C(213) | 1.4534 |
| C(213)-H(213) | 0.9300 |
| C(213)-C(214) | 1.4539 |
| C(214)-C(215) | 1.3631 |
| C(214)-C(217) | 1.5510 |
| C(215)-H(215) | 0.9300 |
| C(215)-C(216) | 1.3631 |
| C(216)-H(216) | 0.9300 |

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|---------------|--------|
| C(217)-C(218) | 1.5177 |
| C(217)-C(219) | 1.5568 |
| C(217)-C(220) | 1.5945 |
| C(218)-H(21D) | 0.9600 |
| C(218)-H(21E) | 0.9600 |
| C(218)-H(21F) | 0.9600 |
| C(219)-H(21G) | 0.9600 |
| C(219)-H(21H) | 0.9600 |
| C(219)-H(21I) | 0.9600 |
| C(220)-H(22A) | 0.9600 |
| C(220)-H(22B) | 0.9600 |
| C(220)-H(22C) | 0.9600 |
| C(221)-C(222) | 1.4054 |
| C(221)-C(226) | 1.3767 |
| C(222)-H(222) | 0.9300 |
| C(222)-C(223) | 1.4126 |
| C(223)-H(223) | 0.9300 |
| C(223)-C(224) | 1.4547 |
| C(224)-C(225) | 1.3603 |
| C(224)-C(227) | 1.6691 |
| C(225)-H(225) | 0.9300 |
| C(225)-C(226) | 1.4579 |
| C(226)-H(226) | 0.9300 |
| C(227)-C(228) | 1.5302 |
| C(227)-C(229) | 1.5245 |
| C(227)-C(230) | 1.5077 |
| C(228)-H(22D) | 0.9600 |
| C(228)-H(22E) | 0.9600 |
| C(228)-H(22F) | 0.9600 |
| C(229)-H(22G) | 0.9600 |
| C(229)-H(22H) | 0.9600 |
| C(229)-H(22I) | 0.9600 |
| C(230)-H(23A) | 0.9600 |
| C(230)-H(23B) | 0.9600 |
| C(230)-H(23C) | 0.9600 |
| C(231)-C(232) | 1.3884 |
| C(231)-C(236) | 1.4073 |

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| C(232)-H(232)   | 0.9300 |
| C(232)-C(233)   | 1.3850 |
| C(233)-H(233)   | 0.9300 |
| C(233)-C(234)   | 1.4309 |
| C(234)-C(235)   | 1.3470 |
| C(234)-C(237)   | 1.5155 |
| C(235)-H(235)   | 0.9300 |
| C(235)-C(236)   | 1.3926 |
| C(236)-H(236)   | 0.9300 |
| C(237)-C(238)   | 1.5200 |
| C(237)-C(239)   | 1.4419 |
| C(237)-C(240)   | 1.6220 |
| C(238)-H(23D)   | 0.9600 |
| C(238)-H(23E)   | 0.9600 |
| C(238)-H(23F)   | 0.9600 |
| C(239)-H(23G)   | 0.9600 |
| C(239)-H(23H)   | 0.9600 |
| C(239)-H(23I)   | 0.9600 |
| C(240)-H(24A)   | 0.9600 |
| C(240)-H(24B)   | 0.9600 |
| C(240)-H(24C)   | 0.9600 |
| Au(37)-Au(37)#1 | 2.9553 |
| Au(37)-Au(38)   | 3.0326 |
| Au(37)-Au(39)#1 | 2.9694 |
| Au(37)-Au(39)   | 2.9705 |
| Au(37)-Au(40)   | 2.7863 |
| Au(37)-Au(41)   | 3.2636 |
| Au(37)-Au(42)   | 3.2065 |
| Au(37)-Au(43)   | 3.0113 |
| Au(37)-Au(44)   | 2.7574 |
| Au(37)-Au(44)#1 | 2.7680 |
| Au(37)-Au(45)   | 2.7973 |
| Au(37)-Au(54)   | 2.7520 |
| Au(38)-Au(39)   | 2.8143 |
| Au(38)-Au(40)   | 2.8857 |
| Au(38)-Au(41)   | 3.3523 |
| Au(38)-Au(43)#1 | 2.7086 |

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| Au(38)-Au(44)#1 | 2.9769 |
| Au(38)-Au(48)   | 2.7291 |
| Au(38)-S(29)    | 2.3548 |
| Au(39)-Au(37)#1 | 2.9693 |
| Au(39)-Au(39)#1 | 2.9063 |
| Au(39)-Au(40)   | 2.9436 |
| Au(39)-Au(43)#1 | 2.7750 |
| Au(39)-Au(45)#1 | 3.1300 |
| Au(39)-Au(46)   | 2.7588 |
| Au(39)-Au(46)#1 | 2.7622 |
| Au(39)-Au(47)   | 3.2223 |
| Au(39)-Au(48)   | 2.7471 |
| Au(39)-Au(53)   | 3.3332 |
| Au(40)-Au(45)   | 2.6898 |
| Au(40)-Au(46)#1 | 2.9525 |
| Au(40)-Au(53)   | 3.2964 |
| Au(40)-Au(54)   | 2.7242 |
| Au(40)-S(28)    | 2.3682 |
| Au(41)-Au(42)   | 3.3018 |
| Au(41)-Au(44)#1 | 3.0483 |
| Au(41)-Au(54)   | 2.8640 |
| Au(41)-S(29)    | 2.3174 |
| Au(41)-S(31)    | 2.3222 |
| Au(42)-Au(43)   | 3.3326 |
| Au(42)-Au(44)   | 2.9692 |
| Au(42)-Au(54)   | 3.1363 |
| Au(42)-S(31)    | 2.3166 |
| Au(42)-S(32)    | 2.3317 |
| Au(43)-Au(38)#1 | 2.7084 |
| Au(43)-Au(39)#1 | 2.7749 |
| Au(43)-Au(44)   | 3.0307 |
| Au(43)-Au(45)   | 2.8828 |
| Au(43)-Au(48)#1 | 2.7869 |
| Au(43)-S(32)    | 2.3888 |
| Au(44)-Au(37)#1 | 2.7680 |
| Au(44)-Au(38)#1 | 2.9769 |
| Au(44)-Au(41)#1 | 3.0484 |



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| Au(44)-Au(44)#1 | 2.7540 |
| Au(44)-S(36)    | 2.3878 |
| Au(45)-Au(39)#1 | 3.1299 |
| Au(45)-Au(46)#1 | 3.0887 |
| Au(45)-Au(47)#1 | 3.3285 |
| Au(45)-Au(54)   | 2.8004 |
| Au(45)-S(35)    | 2.3957 |
| Au(46)-Au(39)#1 | 2.7620 |
| Au(46)-Au(40)#1 | 2.9521 |
| Au(46)-Au(45)#1 | 3.0887 |
| Au(46)-Au(46)#1 | 2.7381 |
| Au(46)-Au(47)   | 3.1582 |
| Au(46)-Au(53)#1 | 3.0921 |
| Au(46)-S(25)    | 2.3730 |
| Au(47)-Au(45)#1 | 3.3283 |
| Au(47)-Au(48)   | 2.8536 |
| Au(47)-S(26)    | 2.3106 |
| Au(47)-S(35)#1  | 2.3091 |
| Au(48)-Au(43)#1 | 2.7869 |
| Au(48)-Au(51)   | 3.0319 |
| Au(48)-Au(53)   | 2.9588 |
| Au(48)-S(27)    | 2.4331 |
| Au(49)-S(34)    | 2.3197 |
| Au(49)-S(36)    | 2.3001 |
| Au(50)-S(25)    | 2.2732 |
| Au(50)-S(30)#1  | 2.3453 |
| Au(51)-S(27)    | 2.2901 |
| Au(51)-S(34)#1  | 2.3104 |
| Au(52)-Au(54)   | 3.1876 |
| Au(52)-S(30)    | 2.3137 |
| Au(52)-S(33)    | 2.2930 |
| Au(53)-Au(46)#1 | 3.0922 |
| Au(53)-S(26)    | 2.3034 |
| Au(53)-S(28)    | 2.2995 |
| Au(54)-S(33)    | 2.4336 |
| S(25)-C(241)    | 1.7911 |
| S(26)-C(251)    | 1.7850 |

|                |        |
|----------------|--------|
| S(27)-C(261)   | 1.7631 |
| S(28)-C(271)   | 1.7195 |
| S(29)-C(281)   | 1.7818 |
| S(30)-Au(50)#1 | 2.3452 |
| S(30)-Ag(50)#1 | 2.3452 |
| S(30)-C(291)   | 1.7923 |
| S(31)-C(301)   | 1.8246 |
| S(32)-C(311)   | 1.7944 |
| S(33)-C(321)   | 1.7686 |
| S(34)-Au(51)#1 | 2.3104 |
| S(34)-Ag(51)#1 | 2.3104 |
| S(34)-C(331)   | 1.7740 |
| S(35)-Au(47)#1 | 2.3093 |
| S(35)-C(341)   | 1.7760 |
| S(36)-C(351)   | 1.7705 |
| C(241)-C(242)  | 1.3899 |
| C(241)-C(246)  | 1.3484 |
| C(242)-H(242)  | 0.9300 |
| C(242)-C(243)  | 1.3843 |
| C(243)-H(243)  | 0.9300 |
| C(243)-C(244)  | 1.3823 |
| C(244)-C(245)  | 1.4107 |
| C(244)-C(247)  | 1.4705 |
| C(245)-H(245)  | 0.9300 |
| C(245)-C(246)  | 1.4494 |
| C(246)-H(246)  | 0.9300 |
| C(247)-C(248)  | 1.5669 |
| C(247)-C(249)  | 1.5888 |
| C(247)-C(250)  | 1.6545 |
| C(248)-H(24D)  | 0.9600 |
| C(248)-H(24E)  | 0.9600 |
| C(248)-H(24F)  | 0.9600 |
| C(249)-H(24G)  | 0.9600 |
| C(249)-H(24H)  | 0.9600 |
| C(249)-H(24I)  | 0.9600 |
| C(250)-H(25A)  | 0.9600 |
| C(250)-H(25B)  | 0.9600 |

|               |        |
|---------------|--------|
| C(250)-H(25C) | 0.9600 |
| C(251)-C(252) | 1.3653 |
| C(251)-C(256) | 1.4013 |
| C(252)-H(252) | 0.9300 |
| C(252)-C(253) | 1.3118 |
| C(253)-H(253) | 0.9300 |
| C(253)-C(254) | 1.4652 |
| C(254)-C(255) | 1.4748 |
| C(254)-C(257) | 1.5426 |
| C(255)-H(255) | 0.9300 |
| C(255)-C(256) | 1.4604 |
| C(256)-H(256) | 0.9300 |
| C(257)-C(258) | 1.5435 |
| C(257)-C(259) | 1.7016 |
| C(257)-C(260) | 1.3658 |
| C(258)-H(25D) | 0.9600 |
| C(258)-H(25E) | 0.9600 |
| C(258)-H(25F) | 0.9600 |
| C(259)-H(25G) | 0.9600 |
| C(259)-H(25H) | 0.9600 |
| C(259)-H(25I) | 0.9600 |
| C(260)-H(26A) | 0.9600 |
| C(260)-H(26B) | 0.9600 |
| C(260)-H(26C) | 0.9600 |
| C(261)-C(262) | 1.4569 |
| C(261)-C(266) | 1.3575 |
| C(262)-H(262) | 0.9300 |
| C(262)-C(263) | 1.4429 |
| C(263)-H(263) | 0.9300 |
| C(263)-C(264) | 1.3633 |
| C(264)-C(265) | 1.4203 |
| C(264)-C(267) | 1.5404 |
| C(265)-H(265) | 0.9300 |
| C(265)-C(266) | 1.4309 |
| C(266)-H(266) | 0.9300 |
| C(267)-C(268) | 1.5922 |
| C(267)-C(269) | 1.5169 |

|               |        |
|---------------|--------|
| C(267)-C(270) | 1.5724 |
| C(268)-H(26D) | 0.9600 |
| C(268)-H(26E) | 0.9600 |
| C(268)-H(26F) | 0.9600 |
| C(269)-H(26G) | 0.9600 |
| C(269)-H(26H) | 0.9600 |
| C(269)-H(26I) | 0.9600 |
| C(270)-H(27A) | 0.9600 |
| C(270)-H(27B) | 0.9600 |
| C(270)-H(27C) | 0.9600 |
| C(271)-C(272) | 1.4727 |
| C(271)-C(276) | 1.3879 |
| C(272)-H(272) | 0.9300 |
| C(272)-C(273) | 1.3738 |
| C(273)-H(273) | 0.9300 |
| C(273)-C(274) | 1.4009 |
| C(274)-C(275) | 1.4483 |
| C(274)-C(277) | 1.5135 |
| C(275)-H(275) | 0.9300 |
| C(275)-C(276) | 1.3698 |
| C(276)-H(276) | 0.9300 |
| C(277)-C(278) | 1.5777 |
| C(277)-C(279) | 1.5860 |
| C(277)-C(280) | 1.5000 |
| C(278)-H(27D) | 0.9600 |
| C(278)-H(27E) | 0.9600 |
| C(278)-H(27F) | 0.9600 |
| C(279)-H(27G) | 0.9600 |
| C(279)-H(27H) | 0.9600 |
| C(279)-H(27I) | 0.9600 |
| C(280)-H(28D) | 0.9600 |
| C(280)-H(28E) | 0.9600 |
| C(280)-H(28F) | 0.9600 |
| C(281)-C(282) | 1.2841 |
| C(281)-C(286) | 1.4706 |
| C(282)-H(282) | 0.9300 |
| C(282)-C(283) | 1.4258 |

|               |        |
|---------------|--------|
| C(283)-H(283) | 0.9300 |
| C(283)-C(284) | 1.4305 |
| C(284)-C(285) | 1.3932 |
| C(284)-C(287) | 1.5236 |
| C(285)-H(285) | 0.9300 |
| C(285)-C(286) | 1.4707 |
| C(286)-H(286) | 0.9300 |
| C(287)-C(288) | 1.5006 |
| C(287)-C(289) | 1.6067 |
| C(287)-C(290) | 1.5627 |
| C(288)-H(28G) | 0.9600 |
| C(288)-H(28H) | 0.9600 |
| C(288)-H(28I) | 0.9600 |
| C(289)-H(28J) | 0.9600 |
| C(289)-H(28K) | 0.9600 |
| C(289)-H(28L) | 0.9600 |
| C(290)-H(29D) | 0.9600 |
| C(290)-H(29E) | 0.9600 |
| C(290)-H(29F) | 0.9600 |
| C(291)-C(292) | 1.3989 |
| C(291)-C(296) | 1.3553 |
| C(292)-H(292) | 0.9300 |
| C(292)-C(293) | 1.3679 |
| C(293)-H(293) | 0.9300 |
| C(293)-C(294) | 1.4096 |
| C(294)-C(295) | 1.3660 |
| C(294)-C(297) | 1.5094 |
| C(295)-H(295) | 0.9300 |
| C(295)-C(296) | 1.3532 |
| C(296)-H(296) | 0.9300 |
| C(297)-C(298) | 1.4388 |
| C(297)-C(299) | 1.6199 |
| C(297)-C(300) | 1.4968 |
| C(298)-H(29G) | 0.9600 |
| C(298)-H(29H) | 0.9600 |
| C(298)-H(29I) | 0.9600 |
| C(299)-H(29J) | 0.9600 |

|               |        |
|---------------|--------|
| C(299)-H(29K) | 0.9600 |
| C(299)-H(29L) | 0.9600 |
| C(300)-H(30D) | 0.9600 |
| C(300)-H(30E) | 0.9600 |
| C(300)-H(30F) | 0.9600 |
| C(301)-C(302) | 1.3393 |
| C(301)-C(306) | 1.4287 |
| C(302)-H(302) | 0.9300 |
| C(302)-C(303) | 1.4169 |
| C(303)-H(303) | 0.9300 |
| C(303)-C(304) | 1.3739 |
| C(304)-C(305) | 1.4525 |
| C(304)-C(307) | 1.5497 |
| C(305)-H(305) | 0.9300 |
| C(305)-C(306) | 1.4757 |
| C(306)-H(306) | 0.9300 |
| C(307)-C(308) | 1.5449 |
| C(307)-C(309) | 1.5759 |
| C(307)-C(310) | 1.5974 |
| C(308)-H(30G) | 0.9600 |
| C(308)-H(30H) | 0.9600 |
| C(308)-H(30I) | 0.9600 |
| C(309)-H(30J) | 0.9600 |
| C(309)-H(30K) | 0.9600 |
| C(309)-H(30L) | 0.9600 |
| C(310)-H(31A) | 0.9600 |
| C(310)-H(31B) | 0.9600 |
| C(310)-H(31C) | 0.9600 |
| C(311)-C(312) | 1.4091 |
| C(311)-C(316) | 1.3787 |
| C(312)-H(312) | 0.9300 |
| C(312)-C(313) | 1.3677 |
| C(313)-H(313) | 0.9300 |
| C(313)-C(314) | 1.4545 |
| C(314)-C(315) | 1.3851 |
| C(314)-C(317) | 1.5616 |
| C(315)-H(315) | 0.9300 |

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|---------------|--------|
| C(315)-C(316) | 1.4121 |
| C(316)-H(316) | 0.9300 |
| C(317)-C(318) | 1.4670 |
| C(317)-C(319) | 1.5319 |
| C(317)-C(320) | 1.6758 |
| C(318)-H(31D) | 0.9600 |
| C(318)-H(31E) | 0.9600 |
| C(318)-H(31F) | 0.9600 |
| C(319)-H(31G) | 0.9600 |
| C(319)-H(31H) | 0.9600 |
| C(319)-H(31I) | 0.9600 |
| C(320)-H(32A) | 0.9600 |
| C(320)-H(32B) | 0.9600 |
| C(320)-H(32C) | 0.9600 |
| C(321)-C(322) | 1.4015 |
| C(321)-C(326) | 1.4058 |
| C(322)-H(322) | 0.9300 |
| C(322)-C(323) | 1.3767 |
| C(323)-H(323) | 0.9300 |
| C(323)-C(324) | 1.3493 |
| C(324)-C(325) | 1.4623 |
| C(324)-C(327) | 1.5880 |
| C(325)-H(325) | 0.9300 |
| C(325)-C(326) | 1.3852 |
| C(326)-H(326) | 0.9300 |
| C(327)-C(328) | 1.6598 |
| C(327)-C(329) | 1.4955 |
| C(327)-C(330) | 1.6388 |
| C(328)-H(32D) | 0.9600 |
| C(328)-H(32E) | 0.9600 |
| C(328)-H(32F) | 0.9600 |
| C(329)-H(32G) | 0.9600 |
| C(329)-H(32H) | 0.9600 |
| C(329)-H(32I) | 0.9600 |
| C(330)-H(33A) | 0.9600 |
| C(330)-H(33B) | 0.9600 |
| C(330)-H(33C) | 0.9600 |

|               |        |
|---------------|--------|
| C(331)-C(332) | 1.3722 |
| C(331)-C(336) | 1.3963 |
| C(332)-H(332) | 0.9300 |
| C(332)-C(333) | 1.4607 |
| C(333)-H(333) | 0.9300 |
| C(333)-C(334) | 1.3678 |
| C(334)-C(335) | 1.4370 |
| C(334)-C(337) | 1.5220 |
| C(335)-H(335) | 0.9300 |
| C(335)-C(336) | 1.4602 |
| C(336)-H(336) | 0.9300 |
| C(337)-C(338) | 1.5544 |
| C(337)-C(339) | 1.6306 |
| C(337)-C(340) | 1.5651 |
| C(338)-H(33D) | 0.9600 |
| C(338)-H(33E) | 0.9600 |
| C(338)-H(33F) | 0.9600 |
| C(339)-H(33G) | 0.9600 |
| C(339)-H(33H) | 0.9600 |
| C(339)-H(33I) | 0.9600 |
| C(340)-H(34A) | 0.9600 |
| C(340)-H(34B) | 0.9600 |
| C(340)-H(34C) | 0.9600 |
| C(341)-C(342) | 1.4055 |
| C(341)-C(346) | 1.4000 |
| C(342)-H(342) | 0.9300 |
| C(342)-C(343) | 1.3571 |
| C(343)-H(343) | 0.9300 |
| C(343)-C(344) | 1.3671 |
| C(344)-C(345) | 1.3878 |
| C(344)-C(347) | 1.6460 |
| C(345)-H(345) | 0.9300 |
| C(345)-C(346) | 1.3181 |
| C(346)-H(346) | 0.9300 |
| C(347)-C(348) | 1.4751 |
| C(347)-C(349) | 1.7246 |
| C(347)-C(350) | 1.4227 |



|                    |        |
|--------------------|--------|
| C(348)-H(34D)      | 0.9600 |
| C(348)-H(34E)      | 0.9600 |
| C(348)-H(34F)      | 0.9600 |
| C(349)-H(34G)      | 0.9600 |
| C(349)-H(34H)      | 0.9600 |
| C(349)-H(34I)      | 0.9600 |
| C(350)-H(35A)      | 0.9600 |
| C(350)-H(35B)      | 0.9600 |
| C(350)-H(35C)      | 0.9600 |
| C(351)-C(352)      | 1.3844 |
| C(351)-C(356)      | 1.4143 |
| C(352)-H(352)      | 0.9300 |
| C(352)-C(353)      | 1.3943 |
| C(353)-H(353)      | 0.9300 |
| C(353)-C(354)      | 1.3564 |
| C(354)-C(355)      | 1.4499 |
| C(354)-C(357)      | 1.5198 |
| C(355)-H(355)      | 0.9300 |
| C(355)-C(356)      | 1.3634 |
| C(356)-H(356)      | 0.9300 |
| C(357)-C(358)      | 1.5222 |
| C(357)-C(359)      | 1.5965 |
| C(357)-C(360)      | 1.4968 |
| C(358)-H(35D)      | 0.9600 |
| C(358)-H(35E)      | 0.9600 |
| C(358)-H(35F)      | 0.9600 |
| C(359)-H(35G)      | 0.9600 |
| C(359)-H(35H)      | 0.9600 |
| C(359)-H(35I)      | 0.9600 |
| C(360)-H(36A)      | 0.9600 |
| C(360)-H(36B)      | 0.9600 |
| C(360)-H(36C)      | 0.9600 |
|                    |        |
| Au(2)-Au(1)-Au(3)  | 60.2   |
| Au(2)-Au(1)-Au(5)  | 60.9   |
| Au(2)-Au(1)-Au(20) | 116.3  |
| Au(2)-Au(1)-Au(21) | 178.3  |

|                     |       |
|---------------------|-------|
| Au(2)-Au(1)-Au(23)  | 118.4 |
| Au(2)-Au(1)-Au(24)  | 56.4  |
| Au(3)-Au(1)-Au(20)  | 86.8  |
| Au(3)-Au(1)-Au(21)  | 119.1 |
| Au(3)-Au(1)-Au(23)  | 115.5 |
| Au(3)-Au(1)-Au(24)  | 89.4  |
| Au(4)-Au(1)-Au(2)   | 116.8 |
| Au(4)-Au(1)-Au(3)   | 56.6  |
| Au(4)-Au(1)-Au(5)   | 86.3  |
| Au(4)-Au(1)-Au(17)  | 177.1 |
| Au(4)-Au(1)-Au(19)  | 119.1 |
| Au(4)-Au(1)-Au(20)  | 60.6  |
| Au(4)-Au(1)-Au(21)  | 62.6  |
| Au(4)-Au(1)-Au(23)  | 89.7  |
| Au(4)-Au(1)-Au(24)  | 121.9 |
| Au(5)-Au(1)-Au(3)   | 59.4  |
| Au(5)-Au(1)-Au(20)  | 55.3  |
| Au(5)-Au(1)-Au(21)  | 117.3 |
| Au(5)-Au(1)-Au(23)  | 174.8 |
| Au(5)-Au(1)-Au(24)  | 117.4 |
| Au(17)-Au(1)-Au(2)  | 65.3  |
| Au(17)-Au(1)-Au(3)  | 125.5 |
| Au(17)-Au(1)-Au(5)  | 93.2  |
| Au(17)-Au(1)-Au(20) | 116.9 |
| Au(17)-Au(1)-Au(21) | 115.3 |
| Au(17)-Au(1)-Au(23) | 91.0  |
| Au(17)-Au(1)-Au(24) | 60.8  |
| Au(18)-Au(1)-Au(2)  | 124.1 |
| Au(18)-Au(1)-Au(3)  | 175.1 |
| Au(18)-Au(1)-Au(4)  | 119.1 |
| Au(18)-Au(1)-Au(5)  | 124.2 |
| Au(18)-Au(1)-Au(17) | 58.9  |
| Au(18)-Au(1)-Au(19) | 61.0  |
| Au(18)-Au(1)-Au(20) | 92.8  |
| Au(18)-Au(1)-Au(21) | 56.7  |
| Au(18)-Au(1)-Au(23) | 60.8  |
| Au(18)-Au(1)-Au(24) | 91.5  |

|                     |       |
|---------------------|-------|
| Au(18)-Au(1)-Au(28) | 118.4 |
| Au(19)-Au(1)-Au(2)  | 93.5  |
| Au(19)-Au(1)-Au(3)  | 122.6 |
| Au(19)-Au(1)-Au(5)  | 63.2  |
| Au(19)-Au(1)-Au(17) | 58.2  |
| Au(19)-Au(1)-Au(20) | 58.7  |
| Au(19)-Au(1)-Au(21) | 85.5  |
| Au(19)-Au(1)-Au(23) | 121.8 |
| Au(19)-Au(1)-Au(24) | 118.9 |
| Au(20)-Au(1)-Au(23) | 125.0 |
| Au(21)-Au(1)-Au(20) | 62.0  |
| Au(21)-Au(1)-Au(23) | 63.3  |
| Au(24)-Au(1)-Au(20) | 172.7 |
| Au(24)-Au(1)-Au(21) | 125.3 |
| Au(24)-Au(1)-Au(23) | 62.3  |
| Au(28)-Au(1)-Au(2)  | 87.6  |
| Au(28)-Au(1)-Au(3)  | 57.9  |
| Au(28)-Au(1)-Au(4)  | 60.2  |
| Au(28)-Au(1)-Au(5)  | 117.3 |
| Au(28)-Au(1)-Au(17) | 122.5 |
| Au(28)-Au(1)-Au(19) | 178.9 |
| Au(28)-Au(1)-Au(20) | 120.6 |
| Au(28)-Au(1)-Au(21) | 93.3  |
| Au(28)-Au(1)-Au(23) | 57.6  |
| Au(28)-Au(1)-Au(24) | 61.9  |
| Au(1)-Au(2)-Au(3)   | 61.0  |
| Au(1)-Au(2)-Au(5)   | 59.8  |
| Au(1)-Au(2)-Au(7)   | 115.1 |
| Au(1)-Au(2)-Au(16)  | 117.3 |
| Au(1)-Au(2)-Au(17)  | 55.6  |
| Au(1)-Au(2)-Au(22)  | 176.6 |
| Au(3)-Au(2)-Au(5)   | 59.2  |
| Au(3)-Au(2)-Au(7)   | 54.2  |
| Au(3)-Au(2)-Au(16)  | 178.3 |
| Au(3)-Au(2)-Au(17)  | 116.6 |
| Au(3)-Au(2)-Au(22)  | 118.0 |
| Au(5)-Au(2)-Au(7)   | 86.8  |

|                     |       |
|---------------------|-------|
| Au(5)-Au(2)-Au(16)  | 120.1 |
| Au(5)-Au(2)-Au(17)  | 87.1  |
| Au(5)-Au(2)-Au(22)  | 116.9 |
| Au(6)-Au(2)-Au(1)   | 117.4 |
| Au(6)-Au(2)-Au(3)   | 85.8  |
| Au(6)-Au(2)-Au(5)   | 57.7  |
| Au(6)-Au(2)-Au(7)   | 60.3  |
| Au(6)-Au(2)-Au(16)  | 95.1  |
| Au(6)-Au(2)-Au(17)  | 121.4 |
| Au(6)-Au(2)-Au(22)  | 59.3  |
| Au(6)-Au(2)-Au(24)  | 178.9 |
| Au(6)-Au(2)-Au(26)  | 120.3 |
| Au(7)-Au(2)-Au(16)  | 127.5 |
| Au(7)-Au(2)-Au(17)  | 170.7 |
| Au(7)-Au(2)-Au(22)  | 63.9  |
| Au(15)-Au(2)-Au(1)  | 88.4  |
| Au(15)-Au(2)-Au(3)  | 116.7 |
| Au(15)-Au(2)-Au(5)  | 57.5  |
| Au(15)-Au(2)-Au(6)  | 59.8  |
| Au(15)-Au(2)-Au(7)  | 119.9 |
| Au(15)-Au(2)-Au(16) | 62.7  |
| Au(15)-Au(2)-Au(17) | 61.8  |
| Au(15)-Au(2)-Au(22) | 89.4  |
| Au(15)-Au(2)-Au(24) | 121.3 |
| Au(15)-Au(2)-Au(26) | 176.8 |
| Au(16)-Au(2)-Au(22) | 63.7  |
| Au(17)-Au(2)-Au(16) | 61.7  |
| Au(17)-Au(2)-Au(22) | 125.3 |
| Au(24)-Au(2)-Au(1)  | 63.1  |
| Au(24)-Au(2)-Au(3)  | 93.7  |
| Au(24)-Au(2)-Au(5)  | 122.8 |
| Au(24)-Au(2)-Au(7)  | 118.6 |
| Au(24)-Au(2)-Au(16) | 85.4  |
| Au(24)-Au(2)-Au(17) | 59.7  |
| Au(24)-Au(2)-Au(22) | 120.3 |
| Au(24)-Au(2)-Au(26) | 58.6  |
| Au(25)-Au(2)-Au(1)  | 122.8 |

|                     |       |
|---------------------|-------|
| Au(25)-Au(2)-Au(3)  | 125.3 |
| Au(25)-Au(2)-Au(5)  | 175.2 |
| Au(25)-Au(2)-Au(6)  | 119.8 |
| Au(25)-Au(2)-Au(7)  | 95.1  |
| Au(25)-Au(2)-Au(15) | 117.9 |
| Au(25)-Au(2)-Au(16) | 55.4  |
| Au(25)-Au(2)-Au(17) | 91.4  |
| Au(25)-Au(2)-Au(22) | 60.6  |
| Au(25)-Au(2)-Au(24) | 59.8  |
| Au(25)-Au(2)-Au(26) | 59.0  |
| Au(26)-Au(2)-Au(1)  | 94.2  |
| Au(26)-Au(2)-Au(3)  | 66.3  |
| Au(26)-Au(2)-Au(5)  | 125.6 |
| Au(26)-Au(2)-Au(7)  | 60.6  |
| Au(26)-Au(2)-Au(16) | 114.3 |
| Au(26)-Au(2)-Au(17) | 118.2 |
| Au(26)-Au(2)-Au(22) | 88.1  |
| Au(1)-Au(3)-Au(11)  | 88.6  |
| Au(1)-Au(3)-Au(26)  | 86.0  |
| Au(1)-Au(3)-Au(27)  | 119.1 |
| Au(2)-Au(3)-Au(1)   | 58.8  |
| Au(2)-Au(3)-Au(11)  | 116.6 |
| Au(2)-Au(3)-Au(26)  | 54.3  |
| Au(2)-Au(3)-Au(27)  | 116.6 |
| Au(4)-Au(3)-Au(1)   | 57.6  |
| Au(4)-Au(3)-Au(2)   | 116.4 |
| Au(4)-Au(3)-Au(5)   | 86.9  |
| Au(4)-Au(3)-Au(7)   | 178.6 |
| Au(4)-Au(3)-Au(8)   | 117.8 |
| Au(4)-Au(3)-Au(9)   | 120.5 |
| Au(4)-Au(3)-Au(11)  | 61.5  |
| Au(4)-Au(3)-Au(26)  | 120.7 |
| Au(4)-Au(3)-Au(27)  | 94.4  |
| Au(4)-Au(3)-Au(28)  | 60.1  |
| Au(5)-Au(3)-Au(1)   | 59.5  |
| Au(5)-Au(3)-Au(2)   | 60.5  |
| Au(5)-Au(3)-Au(11)  | 56.1  |

|                     |       |
|---------------------|-------|
| Au(5)-Au(3)-Au(26)  | 114.8 |
| Au(5)-Au(3)-Au(27)  | 177.0 |
| Au(7)-Au(3)-Au(1)   | 123.8 |
| Au(7)-Au(3)-Au(2)   | 65.0  |
| Au(7)-Au(3)-Au(5)   | 93.9  |
| Au(7)-Au(3)-Au(8)   | 60.8  |
| Au(7)-Au(3)-Au(9)   | 58.9  |
| Au(7)-Au(3)-Au(11)  | 118.1 |
| Au(7)-Au(3)-Au(26)  | 59.9  |
| Au(7)-Au(3)-Au(27)  | 84.9  |
| Au(7)-Au(3)-Au(28)  | 120.4 |
| Au(8)-Au(3)-Au(1)   | 174.8 |
| Au(8)-Au(3)-Au(2)   | 125.7 |
| Au(8)-Au(3)-Au(5)   | 124.3 |
| Au(8)-Au(3)-Au(9)   | 58.8  |
| Au(8)-Au(3)-Au(11)  | 91.1  |
| Au(8)-Au(3)-Au(26)  | 95.0  |
| Au(8)-Au(3)-Au(27)  | 57.4  |
| Au(8)-Au(3)-Au(28)  | 119.5 |
| Au(9)-Au(3)-Au(1)   | 125.0 |
| Au(9)-Au(3)-Au(2)   | 94.9  |
| Au(9)-Au(3)-Au(5)   | 65.6  |
| Au(9)-Au(3)-Au(11)  | 59.4  |
| Au(9)-Au(3)-Au(26)  | 118.6 |
| Au(9)-Au(3)-Au(27)  | 115.8 |
| Au(11)-Au(3)-Au(26) | 170.9 |
| Au(11)-Au(3)-Au(27) | 126.8 |
| Au(27)-Au(3)-Au(26) | 62.3  |
| Au(28)-Au(3)-Au(1)  | 56.7  |
| Au(28)-Au(3)-Au(2)  | 86.0  |
| Au(28)-Au(3)-Au(5)  | 116.2 |
| Au(28)-Au(3)-Au(9)  | 178.3 |
| Au(28)-Au(3)-Au(11) | 121.4 |
| Au(28)-Au(3)-Au(26) | 60.8  |
| Au(28)-Au(3)-Au(27) | 62.4  |
| Au(1)-Au(4)-Au(11)  | 94.4  |
| Au(1)-Au(4)-Au(12)  | 136.9 |

|                     |       |
|---------------------|-------|
| Au(1)-Au(4)-Au(20)  | 66.2  |
| Au(1)-Au(4)-Au(21)  | 64.8  |
| Au(3)-Au(4)-Au(1)   | 65.8  |
| Au(3)-Au(4)-Au(11)  | 64.3  |
| Au(3)-Au(4)-Au(12)  | 71.2  |
| Au(3)-Au(4)-Au(20)  | 94.7  |
| Au(3)-Au(4)-Au(21)  | 130.6 |
| Au(3)-Au(4)-Au(28)  | 60.9  |
| Au(11)-Au(4)-Au(12) | 67.4  |
| Au(11)-Au(4)-Au(20) | 54.6  |
| Au(11)-Au(4)-Au(21) | 118.6 |
| Au(12)-Au(4)-Au(21) | 158.3 |
| Au(20)-Au(4)-Au(12) | 120.0 |
| Au(20)-Au(4)-Au(21) | 64.4  |
| Au(28)-Au(4)-Au(1)  | 59.5  |
| Au(28)-Au(4)-Au(11) | 125.0 |
| Au(28)-Au(4)-Au(12) | 98.2  |
| Au(28)-Au(4)-Au(20) | 125.7 |
| Au(28)-Au(4)-Au(21) | 94.3  |
| S(2)-Au(4)-Au(1)    | 134.1 |
| S(2)-Au(4)-Au(3)    | 155.4 |
| S(2)-Au(4)-Au(11)   | 96.1  |
| S(2)-Au(4)-Au(12)   | 87.9  |
| S(2)-Au(4)-Au(20)   | 84.5  |
| S(2)-Au(4)-Au(21)   | 71.0  |
| S(2)-Au(4)-Au(28)   | 137.6 |
| Au(1)-Au(5)-Au(2)   | 59.3  |
| Au(1)-Au(5)-Au(9)   | 116.3 |
| Au(1)-Au(5)-Au(10)  | 178.1 |
| Au(1)-Au(5)-Au(14)  | 118.4 |
| Au(1)-Au(5)-Au(19)  | 55.7  |
| Au(2)-Au(5)-Au(9)   | 88.7  |
| Au(2)-Au(5)-Au(10)  | 119.7 |
| Au(2)-Au(5)-Au(14)  | 116.7 |
| Au(2)-Au(5)-Au(19)  | 88.1  |
| Au(3)-Au(5)-Au(1)   | 61.2  |
| Au(3)-Au(5)-Au(2)   | 60.3  |

|                     |       |
|---------------------|-------|
| Au(3)-Au(5)-Au(9)   | 55.2  |
| Au(3)-Au(5)-Au(10)  | 117.0 |
| Au(3)-Au(5)-Au(14)  | 176.9 |
| Au(3)-Au(5)-Au(19)  | 116.8 |
| Au(6)-Au(5)-Au(1)   | 116.7 |
| Au(6)-Au(5)-Au(2)   | 57.4  |
| Au(6)-Au(5)-Au(3)   | 86.2  |
| Au(6)-Au(5)-Au(9)   | 61.2  |
| Au(6)-Au(5)-Au(10)  | 62.3  |
| Au(6)-Au(5)-Au(11)  | 119.4 |
| Au(6)-Au(5)-Au(14)  | 91.4  |
| Au(6)-Au(5)-Au(19)  | 122.7 |
| Au(6)-Au(5)-Au(20)  | 176.6 |
| Au(9)-Au(5)-Au(10)  | 61.8  |
| Au(9)-Au(5)-Au(14)  | 125.2 |
| Au(11)-Au(5)-Au(1)  | 94.0  |
| Au(11)-Au(5)-Au(2)  | 124.1 |
| Au(11)-Au(5)-Au(3)  | 63.8  |
| Au(11)-Au(5)-Au(9)  | 58.4  |
| Au(11)-Au(5)-Au(10) | 85.3  |
| Au(11)-Au(5)-Au(14) | 119.2 |
| Au(11)-Au(5)-Au(19) | 117.9 |
| Au(11)-Au(5)-Au(20) | 58.0  |
| Au(13)-Au(5)-Au(1)  | 125.3 |
| Au(13)-Au(5)-Au(2)  | 174.7 |
| Au(13)-Au(5)-Au(3)  | 123.5 |
| Au(13)-Au(5)-Au(6)  | 118.0 |
| Au(13)-Au(5)-Au(9)  | 91.0  |
| Au(13)-Au(5)-Au(10) | 55.8  |
| Au(13)-Au(5)-Au(11) | 59.9  |
| Au(13)-Au(5)-Au(14) | 59.4  |
| Au(13)-Au(5)-Au(15) | 118.7 |
| Au(13)-Au(5)-Au(19) | 92.8  |
| Au(13)-Au(5)-Au(20) | 59.0  |
| Au(14)-Au(5)-Au(10) | 63.4  |
| Au(15)-Au(5)-Au(1)  | 88.0  |
| Au(15)-Au(5)-Au(2)  | 57.3  |



|                     |       |
|---------------------|-------|
| Au(15)-Au(5)-Au(3)  | 117.6 |
| Au(15)-Au(5)-Au(6)  | 59.7  |
| Au(15)-Au(5)-Au(9)  | 120.8 |
| Au(15)-Au(5)-Au(10) | 92.7  |
| Au(15)-Au(5)-Au(11) | 177.9 |
| Au(15)-Au(5)-Au(14) | 59.4  |
| Au(15)-Au(5)-Au(19) | 63.2  |
| Au(15)-Au(5)-Au(20) | 122.9 |
| Au(19)-Au(5)-Au(9)  | 171.8 |
| Au(19)-Au(5)-Au(10) | 126.2 |
| Au(19)-Au(5)-Au(14) | 63.0  |
| Au(20)-Au(5)-Au(1)  | 66.4  |
| Au(20)-Au(5)-Au(2)  | 125.6 |
| Au(20)-Au(5)-Au(3)  | 94.1  |
| Au(20)-Au(5)-Au(9)  | 116.3 |
| Au(20)-Au(5)-Au(10) | 114.6 |
| Au(20)-Au(5)-Au(14) | 88.4  |
| Au(20)-Au(5)-Au(19) | 60.2  |
| Au(2)-Au(6)-Au(5)   | 64.9  |
| Au(2)-Au(6)-Au(7)   | 65.1  |
| Au(2)-Au(6)-Au(9)   | 94.8  |
| Au(2)-Au(6)-Au(10)  | 132.0 |
| Au(2)-Au(6)-Au(22)  | 69.5  |
| Au(5)-Au(6)-Au(7)   | 93.3  |
| Au(5)-Au(6)-Au(9)   | 64.9  |
| Au(5)-Au(6)-Au(10)  | 67.0  |
| Au(5)-Au(6)-Au(22)  | 134.4 |
| Au(7)-Au(6)-Au(9)   | 54.6  |
| Au(7)-Au(6)-Au(10)  | 118.3 |
| Au(7)-Au(6)-Au(22)  | 68.9  |
| Au(9)-Au(6)-Au(10)  | 64.4  |
| Au(9)-Au(6)-Au(22)  | 122.3 |
| Au(15)-Au(6)-Au(2)  | 59.9  |
| Au(15)-Au(6)-Au(5)  | 60.0  |
| Au(15)-Au(6)-Au(7)  | 124.9 |
| Au(15)-Au(6)-Au(9)  | 124.8 |
| Au(15)-Au(6)-Au(10) | 95.6  |

|                     |       |
|---------------------|-------|
| Au(15)-Au(6)-Au(22) | 95.4  |
| Au(22)-Au(6)-Au(10) | 158.4 |
| S(21)-Au(6)-Au(2)   | 153.0 |
| S(21)-Au(6)-Au(5)   | 137.5 |
| S(21)-Au(6)-Au(7)   | 94.5  |
| S(21)-Au(6)-Au(9)   | 86.3  |
| S(21)-Au(6)-Au(10)  | 72.5  |
| S(21)-Au(6)-Au(15)  | 138.7 |
| S(21)-Au(6)-Au(22)  | 87.0  |
| Au(3)-Au(7)-Au(2)   | 60.8  |
| Au(3)-Au(7)-Au(6)   | 86.3  |
| Au(3)-Au(7)-Au(8)   | 59.9  |
| Au(3)-Au(7)-Au(26)  | 66.8  |
| Au(6)-Au(7)-Au(2)   | 54.6  |
| Au(6)-Au(7)-Au(26)  | 109.2 |
| Au(8)-Au(7)-Au(2)   | 120.7 |
| Au(8)-Au(7)-Au(6)   | 122.5 |
| Au(8)-Au(7)-Au(26)  | 98.7  |
| Au(9)-Au(7)-Au(2)   | 93.9  |
| Au(9)-Au(7)-Au(3)   | 61.5  |
| Au(9)-Au(7)-Au(6)   | 63.8  |
| Au(9)-Au(7)-Au(8)   | 59.3  |
| Au(9)-Au(7)-Au(26)  | 128.0 |
| Au(26)-Au(7)-Au(2)  | 55.1  |
| S(17)-Au(7)-Au(2)   | 102.0 |
| S(17)-Au(7)-Au(3)   | 159.8 |
| S(17)-Au(7)-Au(6)   | 91.8  |
| S(17)-Au(7)-Au(8)   | 135.3 |
| S(17)-Au(7)-Au(9)   | 134.7 |
| S(17)-Au(7)-Au(26)  | 95.1  |
| Au(3)-Au(8)-Au(7)   | 59.3  |
| Au(3)-Au(8)-Au(12)  | 71.1  |
| Au(3)-Au(8)-Au(27)  | 67.2  |
| Au(3)-Au(8)-Au(36)  | 145.8 |
| Au(7)-Au(8)-Au(12)  | 130.4 |
| Au(7)-Au(8)-Au(27)  | 89.4  |
| Au(7)-Au(8)-Au(36)  | 91.8  |

|                     |       |
|---------------------|-------|
| Au(9)-Au(8)-Au(3)   | 61.2  |
| Au(9)-Au(8)-Au(7)   | 59.2  |
| Au(9)-Au(8)-Au(12)  | 96.6  |
| Au(9)-Au(8)-Au(27)  | 127.9 |
| Au(9)-Au(8)-Au(36)  | 89.3  |
| Au(27)-Au(8)-Au(12) | 72.0  |
| Au(27)-Au(8)-Au(36) | 135.7 |
| Au(36)-Au(8)-Au(12) | 133.6 |
| S(14)-Au(8)-Au(3)   | 165.3 |
| S(14)-Au(8)-Au(7)   | 131.6 |
| S(14)-Au(8)-Au(9)   | 131.0 |
| S(14)-Au(8)-Au(12)  | 97.5  |
| S(14)-Au(8)-Au(27)  | 101.0 |
| S(14)-Au(8)-Au(36)  | 48.8  |
| Au(3)-Au(9)-Au(5)   | 59.2  |
| Au(3)-Au(9)-Au(6)   | 84.3  |
| Au(3)-Au(9)-Au(10)  | 121.2 |
| Au(3)-Au(9)-Au(11)  | 64.3  |
| Au(5)-Au(9)-Au(10)  | 61.9  |
| Au(6)-Au(9)-Au(5)   | 53.8  |
| Au(6)-Au(9)-Au(10)  | 60.3  |
| Au(7)-Au(9)-Au(3)   | 59.6  |
| Au(7)-Au(9)-Au(5)   | 90.5  |
| Au(7)-Au(9)-Au(6)   | 61.5  |
| Au(7)-Au(9)-Au(8)   | 61.5  |
| Au(7)-Au(9)-Au(10)  | 121.1 |
| Au(7)-Au(9)-Au(11)  | 123.8 |
| Au(8)-Au(9)-Au(3)   | 60.0  |
| Au(8)-Au(9)-Au(5)   | 119.1 |
| Au(8)-Au(9)-Au(6)   | 122.3 |
| Au(8)-Au(9)-Au(10)  | 177.4 |
| Au(8)-Au(9)-Au(11)  | 94.8  |
| Au(11)-Au(9)-Au(5)  | 55.6  |
| Au(11)-Au(9)-Au(6)  | 109.3 |
| Au(11)-Au(9)-Au(10) | 84.0  |
| S(22)-Au(9)-Au(3)   | 144.2 |
| S(22)-Au(9)-Au(5)   | 96.5  |

|                      |       |
|----------------------|-------|
| S(22)-Au(9)-Au(6)    | 102.8 |
| S(22)-Au(9)-Au(7)    | 153.6 |
| S(22)-Au(9)-Au(8)    | 133.2 |
| S(22)-Au(9)-Au(10)   | 44.4  |
| S(22)-Au(9)-Au(11)   | 80.4  |
| Au(6)-Au(10)-Au(5)   | 50.6  |
| Au(6)-Au(10)-Au(9)   | 55.4  |
| Au(9)-Au(10)-Au(5)   | 56.2  |
| Au(13)-Au(10)-Au(5)  | 52.1  |
| Au(13)-Au(10)-Au(6)  | 102.7 |
| Au(13)-Au(10)-Au(9)  | 85.1  |
| S(5)-Au(10)-Au(5)    | 91.7  |
| S(5)-Au(10)-Au(6)    | 83.9  |
| S(5)-Au(10)-Au(9)    | 138.0 |
| S(5)-Au(10)-Au(13)   | 95.8  |
| S(22)-Au(10)-Au(5)   | 92.8  |
| S(22)-Au(10)-Au(6)   | 99.6  |
| S(22)-Au(10)-Au(9)   | 46.0  |
| S(22)-Au(10)-Au(13)  | 86.4  |
| S(22)-Au(10)-S(5)    | 175.5 |
| Au(3)-Au(11)-Au(12)  | 64.0  |
| Au(4)-Au(11)-Au(3)   | 54.2  |
| Au(4)-Au(11)-Au(12)  | 58.1  |
| Au(5)-Au(11)-Au(3)   | 60.1  |
| Au(5)-Au(11)-Au(4)   | 85.0  |
| Au(5)-Au(11)-Au(9)   | 66.0  |
| Au(5)-Au(11)-Au(12)  | 123.9 |
| Au(9)-Au(11)-Au(3)   | 56.3  |
| Au(9)-Au(11)-Au(4)   | 110.3 |
| Au(9)-Au(11)-Au(12)  | 87.5  |
| Au(13)-Au(11)-Au(3)  | 118.7 |
| Au(13)-Au(11)-Au(4)  | 122.2 |
| Au(13)-Au(11)-Au(5)  | 58.7  |
| Au(13)-Au(11)-Au(9)  | 95.0  |
| Au(13)-Au(11)-Au(12) | 177.1 |
| Au(20)-Au(11)-Au(3)  | 94.0  |
| Au(20)-Au(11)-Au(4)  | 63.6  |

|                      |       |
|----------------------|-------|
| Au(20)-Au(11)-Au(5)  | 61.6  |
| Au(20)-Au(11)-Au(9)  | 127.5 |
| Au(20)-Au(11)-Au(12) | 119.7 |
| Au(20)-Au(11)-Au(13) | 59.8  |
| S(6)-Au(11)-Au(3)    | 104.4 |
| S(6)-Au(11)-Au(4)    | 93.1  |
| S(6)-Au(11)-Au(5)    | 161.9 |
| S(6)-Au(11)-Au(9)    | 98.1  |
| S(6)-Au(11)-Au(12)   | 43.0  |
| S(6)-Au(11)-Au(13)   | 134.8 |
| S(6)-Au(11)-Au(20)   | 133.0 |
| Au(4)-Au(12)-Au(11)  | 54.5  |
| Au(8)-Au(12)-Au(4)   | 99.9  |
| Au(8)-Au(12)-Au(11)  | 80.3  |
| S(6)-Au(12)-Au(4)    | 92.1  |
| S(6)-Au(12)-Au(8)    | 97.8  |
| S(6)-Au(12)-Au(11)   | 45.8  |
| S(6)-Au(12)-S(24)    | 170.6 |
| S(24)-Au(12)-Au(4)   | 82.1  |
| S(24)-Au(12)-Au(8)   | 90.5  |
| S(24)-Au(12)-Au(11)  | 132.5 |
| Au(5)-Au(13)-Au(10)  | 72.1  |
| Au(5)-Au(13)-Au(11)  | 61.4  |
| Au(5)-Au(13)-Au(14)  | 68.7  |
| Au(5)-Au(13)-Au(20)  | 62.4  |
| Au(5)-Au(13)-Au(31)  | 144.8 |
| Au(10)-Au(13)-Au(14) | 71.8  |
| Au(10)-Au(13)-Au(31) | 132.6 |
| Au(11)-Au(13)-Au(10) | 95.0  |
| Au(11)-Au(13)-Au(14) | 130.0 |
| Au(11)-Au(13)-Au(31) | 88.5  |
| Au(14)-Au(13)-Au(31) | 136.1 |
| Au(20)-Au(13)-Au(10) | 134.2 |
| Au(20)-Au(13)-Au(11) | 59.5  |
| Au(20)-Au(13)-Au(14) | 95.3  |
| Au(20)-Au(13)-Au(31) | 87.4  |
| S(3)-Au(13)-Au(5)    | 166.7 |

|                      |       |
|----------------------|-------|
| S(3)-Au(13)-Au(10)   | 97.1  |
| S(3)-Au(13)-Au(11)   | 128.8 |
| S(3)-Au(13)-Au(14)   | 100.9 |
| S(3)-Au(13)-Au(20)   | 128.6 |
| S(3)-Au(13)-Au(31)   | 48.5  |
| Au(5)-Au(14)-Au(19)  | 54.8  |
| Au(13)-Au(14)-Au(5)  | 51.8  |
| Au(13)-Au(14)-Au(15) | 104.0 |
| Au(13)-Au(14)-Au(19) | 83.1  |
| Au(15)-Au(14)-Au(5)  | 52.3  |
| Au(15)-Au(14)-Au(19) | 57.5  |
| S(1)-Au(14)-Au(5)    | 99.3  |
| S(1)-Au(14)-Au(13)   | 99.2  |
| S(1)-Au(14)-Au(15)   | 96.0  |
| S(1)-Au(14)-Au(19)   | 47.3  |
| S(5)-Au(14)-Au(5)    | 92.8  |
| S(5)-Au(14)-Au(13)   | 92.0  |
| S(5)-Au(14)-Au(15)   | 87.6  |
| S(5)-Au(14)-Au(19)   | 141.8 |
| S(5)-Au(14)-S(1)     | 167.0 |
| Au(2)-Au(15)-Au(5)   | 65.2  |
| Au(2)-Au(15)-Au(14)  | 133.5 |
| Au(2)-Au(15)-Au(16)  | 66.5  |
| Au(2)-Au(15)-Au(17)  | 64.6  |
| Au(2)-Au(15)-Au(19)  | 91.7  |
| Au(5)-Au(15)-Au(14)  | 68.3  |
| Au(5)-Au(15)-Au(16)  | 131.6 |
| Au(5)-Au(15)-Au(17)  | 92.5  |
| Au(5)-Au(15)-Au(19)  | 62.2  |
| Au(6)-Au(15)-Au(2)   | 60.3  |
| Au(6)-Au(15)-Au(5)   | 60.4  |
| Au(6)-Au(15)-Au(14)  | 97.1  |
| Au(6)-Au(15)-Au(16)  | 97.7  |
| Au(6)-Au(15)-Au(17)  | 124.6 |
| Au(6)-Au(15)-Au(19)  | 122.3 |
| Au(14)-Au(15)-Au(16) | 159.6 |
| Au(14)-Au(15)-Au(17) | 117.5 |

|                      |       |
|----------------------|-------|
| Au(14)-Au(15)-Au(19) | 65.6  |
| Au(17)-Au(15)-Au(16) | 63.7  |
| Au(17)-Au(15)-Au(19) | 53.4  |
| Au(19)-Au(15)-Au(16) | 116.7 |
| S(8)-Au(15)-Au(2)    | 134.5 |
| S(8)-Au(15)-Au(5)    | 158.8 |
| S(8)-Au(15)-Au(6)    | 131.8 |
| S(8)-Au(15)-Au(14)   | 91.5  |
| S(8)-Au(15)-Au(16)   | 68.2  |
| S(8)-Au(15)-Au(17)   | 91.3  |
| S(8)-Au(15)-Au(19)   | 104.4 |
| Au(2)-Au(16)-Au(17)  | 56.6  |
| Au(15)-Au(16)-Au(2)  | 50.8  |
| Au(15)-Au(16)-Au(17) | 56.0  |
| Au(25)-Au(16)-Au(2)  | 53.0  |
| Au(25)-Au(16)-Au(15) | 103.6 |
| Au(25)-Au(16)-Au(17) | 86.5  |
| S(19)-Au(16)-Au(2)   | 94.0  |
| S(19)-Au(16)-Au(15)  | 100.0 |
| S(19)-Au(16)-Au(17)  | 46.2  |
| S(19)-Au(16)-Au(25)  | 88.7  |
| S(20)-Au(16)-Au(2)   | 93.7  |
| S(20)-Au(16)-Au(15)  | 85.8  |
| S(20)-Au(16)-Au(17)  | 140.8 |
| S(20)-Au(16)-Au(25)  | 95.1  |
| S(20)-Au(16)-S(19)   | 172.2 |
| Au(1)-Au(17)-Au(2)   | 59.1  |
| Au(1)-Au(17)-Au(15)  | 85.5  |
| Au(1)-Au(17)-Au(16)  | 120.8 |
| Au(1)-Au(17)-Au(24)  | 62.7  |
| Au(2)-Au(17)-Au(16)  | 61.7  |
| Au(15)-Au(17)-Au(2)  | 53.5  |
| Au(15)-Au(17)-Au(16) | 60.2  |
| Au(18)-Au(17)-Au(1)  | 59.3  |
| Au(18)-Au(17)-Au(2)  | 118.3 |
| Au(18)-Au(17)-Au(15) | 124.2 |
| Au(18)-Au(17)-Au(16) | 174.9 |

|                      |       |
|----------------------|-------|
| Au(18)-Au(17)-Au(24) | 92.8  |
| Au(19)-Au(17)-Au(1)  | 60.1  |
| Au(19)-Au(17)-Au(2)  | 90.9  |
| Au(19)-Au(17)-Au(15) | 63.4  |
| Au(19)-Au(17)-Au(16) | 123.0 |
| Au(19)-Au(17)-Au(18) | 61.8  |
| Au(19)-Au(17)-Au(24) | 122.6 |
| Au(24)-Au(17)-Au(2)  | 55.2  |
| Au(24)-Au(17)-Au(15) | 108.5 |
| Au(24)-Au(17)-Au(16) | 83.1  |
| S(19)-Au(17)-Au(1)   | 143.7 |
| S(19)-Au(17)-Au(2)   | 97.6  |
| S(19)-Au(17)-Au(15)  | 103.0 |
| S(19)-Au(17)-Au(16)  | 45.1  |
| S(19)-Au(17)-Au(18)  | 131.4 |
| S(19)-Au(17)-Au(19)  | 154.6 |
| S(19)-Au(17)-Au(24)  | 81.3  |
| Au(1)-Au(18)-Au(19)  | 60.0  |
| Au(1)-Au(18)-Au(21)  | 68.9  |
| Au(1)-Au(18)-Au(23)  | 69.6  |
| Au(1)-Au(18)-Au(29)  | 133.4 |
| Au(17)-Au(18)-Au(1)  | 61.7  |
| Au(17)-Au(18)-Au(19) | 58.8  |
| Au(17)-Au(18)-Au(21) | 130.3 |
| Au(17)-Au(18)-Au(23) | 97.5  |
| Au(17)-Au(18)-Au(29) | 85.2  |
| Au(19)-Au(18)-Au(21) | 91.7  |
| Au(19)-Au(18)-Au(23) | 129.5 |
| Au(19)-Au(18)-Au(29) | 75.3  |
| Au(21)-Au(18)-Au(23) | 70.0  |
| Au(21)-Au(18)-Au(29) | 128.2 |
| Au(29)-Au(18)-Au(23) | 152.2 |
| S(11)-Au(18)-Au(1)   | 175.5 |
| S(11)-Au(18)-Au(17)  | 122.4 |
| S(11)-Au(18)-Au(19)  | 120.1 |
| S(11)-Au(18)-Au(21)  | 106.7 |
| S(11)-Au(18)-Au(23)  | 110.3 |



|                      |       |
|----------------------|-------|
| S(11)-Au(18)-Au(29)  | 48.2  |
| Au(1)-Au(19)-Au(5)   | 61.1  |
| Au(1)-Au(19)-Au(14)  | 123.1 |
| Au(1)-Au(19)-Au(15)  | 86.1  |
| Au(1)-Au(19)-Au(18)  | 59.1  |
| Au(1)-Au(19)-Au(20)  | 67.4  |
| Au(5)-Au(19)-Au(14)  | 62.2  |
| Au(5)-Au(19)-Au(15)  | 54.6  |
| Au(15)-Au(19)-Au(14) | 56.9  |
| Au(17)-Au(19)-Au(1)  | 61.6  |
| Au(17)-Au(19)-Au(5)  | 93.9  |
| Au(17)-Au(19)-Au(14) | 118.6 |
| Au(17)-Au(19)-Au(15) | 63.2  |
| Au(17)-Au(19)-Au(18) | 59.4  |
| Au(17)-Au(19)-Au(20) | 128.9 |
| Au(18)-Au(19)-Au(5)  | 120.1 |
| Au(18)-Au(19)-Au(14) | 176.5 |
| Au(18)-Au(19)-Au(15) | 121.8 |
| Au(18)-Au(19)-Au(20) | 97.0  |
| Au(20)-Au(19)-Au(5)  | 57.3  |
| Au(20)-Au(19)-Au(14) | 86.5  |
| Au(20)-Au(19)-Au(15) | 111.5 |
| S(1)-Au(19)-Au(1)    | 162.1 |
| S(1)-Au(19)-Au(5)    | 104.7 |
| S(1)-Au(19)-Au(14)   | 45.5  |
| S(1)-Au(19)-Au(15)   | 94.0  |
| S(1)-Au(19)-Au(17)   | 133.8 |
| S(1)-Au(19)-Au(18)   | 133.2 |
| S(1)-Au(19)-Au(20)   | 96.2  |
| Au(1)-Au(20)-Au(21)  | 58.8  |
| Au(1)-Au(20)-Au(32)  | 123.7 |
| Au(4)-Au(20)-Au(1)   | 53.2  |
| Au(4)-Au(20)-Au(21)  | 59.0  |
| Au(4)-Au(20)-Au(32)  | 71.2  |
| Au(5)-Au(20)-Au(1)   | 58.3  |
| Au(5)-Au(20)-Au(4)   | 83.6  |
| Au(5)-Au(20)-Au(19)  | 62.6  |

|                      |       |
|----------------------|-------|
| Au(5)-Au(20)-Au(21)  | 117.1 |
| Au(5)-Au(20)-Au(32)  | 129.0 |
| Au(11)-Au(20)-Au(1)  | 90.6  |
| Au(11)-Au(20)-Au(4)  | 61.8  |
| Au(11)-Au(20)-Au(5)  | 60.5  |
| Au(11)-Au(20)-Au(13) | 60.6  |
| Au(11)-Au(20)-Au(19) | 122.8 |
| Au(11)-Au(20)-Au(21) | 120.5 |
| Au(11)-Au(20)-Au(32) | 68.6  |
| Au(13)-Au(20)-Au(1)  | 116.9 |
| Au(13)-Au(20)-Au(4)  | 121.2 |
| Au(13)-Au(20)-Au(5)  | 58.6  |
| Au(13)-Au(20)-Au(19) | 94.1  |
| Au(13)-Au(20)-Au(21) | 175.0 |
| Au(13)-Au(20)-Au(32) | 97.9  |
| Au(19)-Au(20)-Au(1)  | 53.9  |
| Au(19)-Au(20)-Au(4)  | 107.0 |
| Au(19)-Au(20)-Au(21) | 81.2  |
| Au(19)-Au(20)-Au(32) | 166.8 |
| Au(21)-Au(20)-Au(32) | 87.0  |
| S(7)-Au(20)-Au(1)    | 94.4  |
| S(7)-Au(20)-Au(4)    | 102.4 |
| S(7)-Au(20)-Au(5)    | 141.0 |
| S(7)-Au(20)-Au(11)   | 155.0 |
| S(7)-Au(20)-Au(13)   | 135.7 |
| S(7)-Au(20)-Au(19)   | 79.1  |
| S(7)-Au(20)-Au(21)   | 45.4  |
| S(7)-Au(20)-Au(32)   | 88.5  |
| Au(1)-Au(21)-Au(20)  | 59.2  |
| Au(4)-Au(21)-Au(1)   | 52.6  |
| Au(4)-Au(21)-Au(20)  | 56.6  |
| Au(18)-Au(21)-Au(1)  | 54.4  |
| Au(18)-Au(21)-Au(4)  | 107.0 |
| Au(18)-Au(21)-Au(20) | 89.6  |
| S(7)-Au(21)-Au(1)    | 96.4  |
| S(7)-Au(21)-Au(4)    | 102.0 |
| S(7)-Au(21)-Au(18)   | 88.7  |

|                      |       |
|----------------------|-------|
| S(7)-Au(21)-Au(20)   | 47.4  |
| S(7)-Au(21)-S(10)    | 169.4 |
| S(10)-Au(21)-Au(1)   | 93.9  |
| S(10)-Au(21)-Au(4)   | 82.1  |
| S(10)-Au(21)-Au(18)  | 99.5  |
| S(10)-Au(21)-Au(20)  | 138.5 |
| Au(6)-Au(22)-Au(2)   | 51.2  |
| Au(6)-Au(22)-Au(25)  | 101.7 |
| Au(25)-Au(22)-Au(2)  | 50.5  |
| S(17)-Au(22)-Au(2)   | 96.6  |
| S(17)-Au(22)-Au(6)   | 90.5  |
| S(17)-Au(22)-Au(25)  | 99.8  |
| S(20)-Au(22)-Au(2)   | 92.4  |
| S(20)-Au(22)-Au(6)   | 92.7  |
| S(20)-Au(22)-Au(25)  | 88.4  |
| S(20)-Au(22)-S(17)   | 170.4 |
| Au(18)-Au(23)-Au(1)  | 49.6  |
| Au(18)-Au(23)-Au(24) | 79.1  |
| Au(24)-Au(23)-Au(1)  | 53.2  |
| Au(28)-Au(23)-Au(1)  | 50.6  |
| Au(28)-Au(23)-Au(18) | 100.2 |
| Au(28)-Au(23)-Au(24) | 55.6  |
| S(10)-Au(23)-Au(1)   | 88.6  |
| S(10)-Au(23)-Au(18)  | 91.3  |
| S(10)-Au(23)-Au(24)  | 136.7 |
| S(10)-Au(23)-Au(28)  | 85.5  |
| S(10)-Au(23)-S(12)   | 172.3 |
| S(12)-Au(23)-Au(1)   | 97.1  |
| S(12)-Au(23)-Au(18)  | 96.4  |
| S(12)-Au(23)-Au(24)  | 46.7  |
| S(12)-Au(23)-Au(28)  | 94.1  |
| Au(1)-Au(24)-Au(23)  | 64.5  |
| Au(2)-Au(24)-Au(1)   | 60.5  |
| Au(2)-Au(24)-Au(17)  | 65.2  |
| Au(2)-Au(24)-Au(23)  | 124.7 |
| Au(2)-Au(24)-Au(28)  | 85.9  |
| Au(17)-Au(24)-Au(1)  | 56.5  |

|                      |       |
|----------------------|-------|
| Au(17)-Au(24)-Au(23) | 90.0  |
| Au(17)-Au(24)-Au(28) | 111.3 |
| Au(25)-Au(24)-Au(1)  | 119.5 |
| Au(25)-Au(24)-Au(2)  | 59.1  |
| Au(25)-Au(24)-Au(17) | 94.4  |
| Au(25)-Au(24)-Au(23) | 175.3 |
| Au(25)-Au(24)-Au(28) | 122.7 |
| Au(26)-Au(24)-Au(1)  | 93.8  |
| Au(26)-Au(24)-Au(2)  | 60.7  |
| Au(26)-Au(24)-Au(17) | 125.9 |
| Au(26)-Au(24)-Au(23) | 119.0 |
| Au(26)-Au(24)-Au(25) | 59.5  |
| Au(26)-Au(24)-Au(28) | 64.0  |
| Au(28)-Au(24)-Au(1)  | 54.9  |
| Au(28)-Au(24)-Au(23) | 56.9  |
| S(12)-Au(24)-Au(1)   | 105.7 |
| S(12)-Au(24)-Au(2)   | 163.4 |
| S(12)-Au(24)-Au(17)  | 100.1 |
| S(12)-Au(24)-Au(23)  | 44.2  |
| S(12)-Au(24)-Au(25)  | 132.9 |
| S(12)-Au(24)-Au(26)  | 133.1 |
| S(12)-Au(24)-Au(28)  | 93.1  |
| Au(2)-Au(25)-Au(16)  | 71.7  |
| Au(2)-Au(25)-Au(22)  | 69.0  |
| Au(2)-Au(25)-Au(24)  | 61.1  |
| Au(2)-Au(25)-Au(34)  | 141.9 |
| Au(16)-Au(25)-Au(22) | 71.6  |
| Au(16)-Au(25)-Au(34) | 136.8 |
| Au(24)-Au(25)-Au(16) | 95.0  |
| Au(24)-Au(25)-Au(22) | 129.9 |
| Au(24)-Au(25)-Au(34) | 87.5  |
| Au(26)-Au(25)-Au(2)  | 61.5  |
| Au(26)-Au(25)-Au(16) | 133.0 |
| Au(26)-Au(25)-Au(22) | 94.0  |
| Au(26)-Au(25)-Au(24) | 59.8  |
| Au(26)-Au(25)-Au(34) | 84.8  |
| Au(34)-Au(25)-Au(22) | 135.3 |

|                      |       |
|----------------------|-------|
| S(18)-Au(25)-Au(2)   | 170.6 |
| S(18)-Au(25)-Au(16)  | 101.2 |
| S(18)-Au(25)-Au(22)  | 103.4 |
| S(18)-Au(25)-Au(24)  | 126.7 |
| S(18)-Au(25)-Au(26)  | 125.8 |
| S(18)-Au(25)-Au(34)  | 47.5  |
| Au(2)-Au(26)-Au(3)   | 59.4  |
| Au(2)-Au(26)-Au(7)   | 64.3  |
| Au(2)-Au(26)-Au(27)  | 117.3 |
| Au(2)-Au(26)-Au(28)  | 84.7  |
| Au(3)-Au(26)-Au(27)  | 58.0  |
| Au(7)-Au(26)-Au(3)   | 53.3  |
| Au(7)-Au(26)-Au(27)  | 79.1  |
| Au(7)-Au(26)-Au(28)  | 106.5 |
| Au(24)-Au(26)-Au(2)  | 60.7  |
| Au(24)-Au(26)-Au(3)  | 90.8  |
| Au(24)-Au(26)-Au(7)  | 124.4 |
| Au(24)-Au(26)-Au(27) | 119.7 |
| Au(24)-Au(26)-Au(28) | 61.5  |
| Au(25)-Au(26)-Au(2)  | 59.5  |
| Au(25)-Au(26)-Au(3)  | 118.8 |
| Au(25)-Au(26)-Au(7)  | 97.8  |
| Au(25)-Au(26)-Au(24) | 60.7  |
| Au(25)-Au(26)-Au(27) | 176.5 |
| Au(25)-Au(26)-Au(28) | 121.4 |
| Au(28)-Au(26)-Au(3)  | 53.5  |
| Au(28)-Au(26)-Au(27) | 58.4  |
| S(15)-Au(26)-Au(2)   | 139.1 |
| S(15)-Au(26)-Au(3)   | 92.4  |
| S(15)-Au(26)-Au(7)   | 75.1  |
| S(15)-Au(26)-Au(24)  | 156.4 |
| S(15)-Au(26)-Au(25)  | 135.5 |
| S(15)-Au(26)-Au(27)  | 45.5  |
| S(15)-Au(26)-Au(28)  | 102.4 |
| Au(3)-Au(27)-Au(26)  | 59.7  |
| Au(8)-Au(27)-Au(3)   | 55.5  |
| Au(8)-Au(27)-Au(26)  | 92.1  |

|                      |       |
|----------------------|-------|
| Au(8)-Au(27)-Au(28)  | 108.9 |
| Au(28)-Au(27)-Au(3)  | 53.7  |
| Au(28)-Au(27)-Au(26) | 57.4  |
| S(15)-Au(27)-Au(3)   | 94.7  |
| S(15)-Au(27)-Au(8)   | 88.4  |
| S(15)-Au(27)-Au(26)  | 46.6  |
| S(15)-Au(27)-Au(28)  | 102.4 |
| S(24)-Au(27)-Au(3)   | 92.5  |
| S(24)-Au(27)-Au(8)   | 96.6  |
| S(24)-Au(27)-Au(26)  | 138.0 |
| S(24)-Au(27)-Au(28)  | 81.0  |
| S(24)-Au(27)-S(15)   | 172.7 |
| Au(1)-Au(28)-Au(3)   | 65.4  |
| Au(1)-Au(28)-Au(4)   | 60.3  |
| Au(1)-Au(28)-Au(23)  | 71.8  |
| Au(1)-Au(28)-Au(24)  | 63.2  |
| Au(1)-Au(28)-Au(26)  | 93.0  |
| Au(1)-Au(28)-Au(27)  | 129.1 |
| Au(3)-Au(28)-Au(23)  | 137.1 |
| Au(3)-Au(28)-Au(24)  | 94.1  |
| Au(3)-Au(28)-Au(26)  | 65.7  |
| Au(3)-Au(28)-Au(27)  | 63.8  |
| Au(4)-Au(28)-Au(3)   | 59.0  |
| Au(4)-Au(28)-Au(23)  | 98.0  |
| Au(4)-Au(28)-Au(24)  | 123.3 |
| Au(4)-Au(28)-Au(26)  | 124.4 |
| Au(4)-Au(28)-Au(27)  | 94.6  |
| Au(23)-Au(28)-Au(26) | 120.0 |
| Au(23)-Au(28)-Au(27) | 159.1 |
| Au(24)-Au(28)-Au(23) | 67.5  |
| Au(24)-Au(28)-Au(26) | 54.5  |
| Au(24)-Au(28)-Au(27) | 118.4 |
| Au(26)-Au(28)-Au(27) | 64.2  |
| S(13)-Au(28)-Au(1)   | 156.3 |
| S(13)-Au(28)-Au(3)   | 134.6 |
| S(13)-Au(28)-Au(4)   | 136.7 |
| S(13)-Au(28)-Au(23)  | 87.6  |

|                     |       |
|---------------------|-------|
| S(13)-Au(28)-Au(24) | 98.6  |
| S(13)-Au(28)-Au(26) | 87.2  |
| S(13)-Au(28)-Au(27) | 71.8  |
| S(9)-Au(29)-Au(18)  | 135.3 |
| S(9)-Au(29)-S(11)   | 170.0 |
| S(11)-Au(29)-Au(18) | 50.9  |
| S(8)-Au(30)-S(9)    | 176.3 |
| S(3)-Au(31)-Au(13)  | 52.6  |
| S(3)-Au(31)-S(4)    | 175.2 |
| S(4)-Au(31)-Au(13)  | 131.7 |
| S(2)-Au(32)-Au(20)  | 77.8  |
| S(2)-Au(32)-S(4)    | 167.9 |
| S(4)-Au(32)-Au(20)  | 109.1 |
| S(13)-Au(33)-S(16)  | 170.5 |
| S(16)-Au(34)-Au(25) | 135.7 |
| S(18)-Au(34)-Au(25) | 51.3  |
| S(18)-Au(34)-S(16)  | 169.8 |
| S(21)-Au(35)-S(23)  | 167.6 |
| S(14)-Au(36)-Au(8)  | 52.9  |
| S(14)-Au(36)-S(23)  | 173.8 |
| S(23)-Au(36)-Au(8)  | 131.4 |
| Au(14)-S(1)-Au(19)  | 87.2  |
| C(1)-S(1)-Au(14)    | 109.4 |
| C(1)-S(1)-Au(19)    | 116.0 |
| Au(32)-S(2)-Au(4)   | 106.8 |
| C(11)-S(2)-Au(4)    | 108.4 |
| C(11)-S(2)-Au(32)   | 110.1 |
| Au(31)-S(3)-Au(13)  | 78.9  |
| C(21)-S(3)-Au(13)   | 106.6 |
| C(21)-S(3)-Au(31)   | 105.9 |
| Au(31)-S(4)-Au(32)  | 97.9  |
| C(31)-S(4)-Au(31)   | 100.6 |
| C(31)-S(4)-Au(32)   | 107.4 |
| Au(10)-S(5)-Au(14)  | 95.8  |
| C(41)-S(5)-Au(10)   | 104.1 |
| C(41)-S(5)-Au(14)   | 105.3 |
| Au(12)-S(6)-Au(11)  | 91.2  |

|                     |       |
|---------------------|-------|
| C(51)-S(6)-Au(11)   | 118.3 |
| C(51)-S(6)-Au(12)   | 109.3 |
| Au(21)-S(7)-Au(20)  | 87.2  |
| C(61)-S(7)-Au(20)   | 112.9 |
| C(61)-S(7)-Au(21)   | 99.8  |
| Au(30)-S(8)-Au(15)  | 99.4  |
| C(71)-S(8)-Au(15)   | 108.3 |
| C(71)-S(8)-Au(30)   | 110.1 |
| Au(29)-S(9)-Au(30)  | 99.4  |
| C(81)-S(9)-Au(29)   | 105.7 |
| C(81)-S(9)-Au(30)   | 113.1 |
| Au(23)-S(10)-Au(21) | 95.7  |
| C(91)-S(10)-Au(21)  | 104.4 |
| C(91)-S(10)-Au(23)  | 112.6 |
| Au(29)-S(11)-Au(18) | 80.8  |
| C(101)-S(11)-Au(18) | 106.3 |
| C(101)-S(11)-Au(29) | 100.5 |
| Au(23)-S(12)-Au(24) | 89.2  |
| C(111)-S(12)-Au(23) | 105.7 |
| C(111)-S(12)-Au(24) | 114.0 |
| Au(33)-S(13)-Au(28) | 108.7 |
| C(121)-S(13)-Au(28) | 110.0 |
| C(121)-S(13)-Au(33) | 114.2 |
| Au(36)-S(14)-Au(8)  | 78.3  |
| C(131)-S(14)-Au(8)  | 108.1 |
| C(131)-S(14)-Au(36) | 102.1 |
| Au(27)-S(15)-Au(26) | 87.9  |
| C(141)-S(15)-Au(26) | 115.0 |
| C(141)-S(15)-Au(27) | 101.0 |
| Au(34)-S(16)-Au(33) | 97.6  |
| C(151)-S(16)-Au(33) | 107.9 |
| C(151)-S(16)-Au(34) | 97.0  |
| Au(22)-S(17)-Au(7)  | 92.2  |
| C(161)-S(17)-Au(7)  | 117.0 |
| C(161)-S(17)-Au(22) | 107.3 |
| Au(34)-S(18)-Au(25) | 81.2  |
| C(171)-S(18)-Au(25) | 108.4 |



|                     |       |
|---------------------|-------|
| C(171)-S(18)-Au(34) | 101.6 |
| Au(16)-S(19)-Au(17) | 88.7  |
| C(181)-S(19)-Au(16) | 103.5 |
| C(181)-S(19)-Au(17) | 117.4 |
| Au(22)-S(20)-Au(16) | 98.0  |
| C(191)-S(20)-Au(16) | 100.3 |
| C(191)-S(20)-Au(22) | 108.1 |
| Au(35)-S(21)-Au(6)  | 109.2 |
| C(201)-S(21)-Au(6)  | 110.1 |
| C(201)-S(21)-Au(35) | 106.9 |
| Au(10)-S(22)-Au(9)  | 89.5  |
| C(211)-S(22)-Au(9)  | 108.2 |
| C(211)-S(22)-Au(10) | 106.5 |
| Au(36)-S(23)-Au(35) | 97.6  |
| C(221)-S(23)-Au(35) | 110.6 |
| C(221)-S(23)-Au(36) | 100.9 |
| Au(12)-S(24)-Au(27) | 97.8  |
| C(231)-S(24)-Au(12) | 117.7 |
| C(231)-S(24)-Au(27) | 100.5 |
| C(2)-C(1)-S(1)      | 124.2 |
| C(2)-C(1)-C(6)      | 120.7 |
| C(6)-C(1)-S(1)      | 114.6 |
| C(1)-C(2)-H(2)      | 118.1 |
| C(3)-C(2)-C(1)      | 123.9 |
| C(3)-C(2)-H(2)      | 118.1 |
| C(2)-C(3)-H(3)      | 120.1 |
| C(2)-C(3)-C(4)      | 119.9 |
| C(4)-C(3)-H(3)      | 120.1 |
| C(3)-C(4)-C(7)      | 121.0 |
| C(5)-C(4)-C(3)      | 114.9 |
| C(5)-C(4)-C(7)      | 123.2 |
| C(4)-C(5)-H(5)      | 116.9 |
| C(4)-C(5)-C(6)      | 126.3 |
| C(6)-C(5)-H(5)      | 116.9 |
| C(1)-C(6)-H(6)      | 123.3 |
| C(5)-C(6)-C(1)      | 113.4 |
| C(5)-C(6)-H(6)      | 123.3 |

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| C(4)-C(7)-C(9)      | 102.6 |
| C(8)-C(7)-C(4)      | 110.7 |
| C(8)-C(7)-C(9)      | 111.8 |
| C(10)-C(7)-C(4)     | 111.9 |
| C(10)-C(7)-C(8)     | 111.8 |
| C(10)-C(7)-C(9)     | 107.6 |
| C(7)-C(8)-H(8A)     | 109.5 |
| C(7)-C(8)-H(8B)     | 109.5 |
| C(7)-C(8)-H(8C)     | 109.5 |
| H(8A)-C(8)-H(8B)    | 109.5 |
| H(8A)-C(8)-H(8C)    | 109.5 |
| H(8B)-C(8)-H(8C)    | 109.5 |
| C(7)-C(9)-H(9A)     | 109.5 |
| C(7)-C(9)-H(9B)     | 109.5 |
| C(7)-C(9)-H(9C)     | 109.5 |
| H(9A)-C(9)-H(9B)    | 109.5 |
| H(9A)-C(9)-H(9C)    | 109.5 |
| H(9B)-C(9)-H(9C)    | 109.5 |
| C(7)-C(10)-H(10A)   | 109.5 |
| C(7)-C(10)-H(10B)   | 109.5 |
| C(7)-C(10)-H(10C)   | 109.5 |
| H(10A)-C(10)-H(10B) | 109.5 |
| H(10A)-C(10)-H(10C) | 109.5 |
| H(10B)-C(10)-H(10C) | 109.5 |
| C(12)-C(11)-S(2)    | 119.1 |
| C(16)-C(11)-S(2)    | 116.1 |
| C(16)-C(11)-C(12)   | 124.6 |
| C(11)-C(12)-H(12)   | 122.2 |
| C(11)-C(12)-C(13)   | 115.5 |
| C(13)-C(12)-H(12)   | 122.2 |
| C(12)-C(13)-H(13)   | 117.8 |
| C(12)-C(13)-C(14)   | 124.4 |
| C(14)-C(13)-H(13)   | 117.8 |
| C(13)-C(14)-C(17)   | 124.9 |
| C(15)-C(14)-C(13)   | 114.1 |
| C(15)-C(14)-C(17)   | 121.1 |
| C(14)-C(15)-H(15)   | 118.7 |

|                     |       |
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| C(14)-C(15)-C(16)   | 122.5 |
| C(16)-C(15)-H(15)   | 118.7 |
| C(11)-C(16)-C(15)   | 118.1 |
| C(11)-C(16)-H(16)   | 121.0 |
| C(15)-C(16)-H(16)   | 121.0 |
| C(14)-C(17)-C(18)   | 111.7 |
| C(14)-C(17)-C(20)   | 103.2 |
| C(18)-C(17)-C(20)   | 111.0 |
| C(19)-C(17)-C(14)   | 112.0 |
| C(19)-C(17)-C(18)   | 110.2 |
| C(19)-C(17)-C(20)   | 108.5 |
| C(17)-C(18)-H(18A)  | 109.5 |
| C(17)-C(18)-H(18B)  | 109.5 |
| C(17)-C(18)-H(18C)  | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18C) | 109.5 |
| H(18B)-C(18)-H(18C) | 109.5 |
| C(17)-C(19)-H(19A)  | 109.5 |
| C(17)-C(19)-H(19B)  | 109.5 |
| C(17)-C(19)-H(19C)  | 109.5 |
| H(19A)-C(19)-H(19B) | 109.5 |
| H(19A)-C(19)-H(19C) | 109.5 |
| H(19B)-C(19)-H(19C) | 109.5 |
| C(17)-C(20)-H(20A)  | 109.5 |
| C(17)-C(20)-H(20B)  | 109.5 |
| C(17)-C(20)-H(20C)  | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 |
| C(22)-C(21)-S(3)    | 116.8 |
| C(22)-C(21)-C(26)   | 123.6 |
| C(26)-C(21)-S(3)    | 119.4 |
| C(21)-C(22)-H(22)   | 120.3 |
| C(21)-C(22)-C(23)   | 119.5 |
| C(23)-C(22)-H(22)   | 120.3 |
| C(22)-C(23)-H(23)   | 121.0 |
| C(24)-C(23)-C(22)   | 118.1 |

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| C(24)-C(23)-H(23)   | 121.0 |
| C(23)-C(24)-C(25)   | 122.3 |
| C(23)-C(24)-C(27)   | 120.5 |
| C(25)-C(24)-C(27)   | 117.2 |
| C(24)-C(25)-H(25)   | 119.3 |
| C(26)-C(25)-C(24)   | 121.3 |
| C(26)-C(25)-H(25)   | 119.3 |
| C(21)-C(26)-H(26)   | 122.6 |
| C(25)-C(26)-C(21)   | 114.8 |
| C(25)-C(26)-H(26)   | 122.6 |
| C(24)-C(27)-C(28)   | 112.6 |
| C(24)-C(27)-C(30)   | 112.4 |
| C(29)-C(27)-C(24)   | 107.7 |
| C(29)-C(27)-C(28)   | 106.1 |
| C(29)-C(27)-C(30)   | 111.8 |
| C(30)-C(27)-C(28)   | 106.2 |
| C(27)-C(28)-H(28A)  | 109.5 |
| C(27)-C(28)-H(28B)  | 109.5 |
| C(27)-C(28)-H(28C)  | 109.5 |
| H(28A)-C(28)-H(28B) | 109.5 |
| H(28A)-C(28)-H(28C) | 109.5 |
| H(28B)-C(28)-H(28C) | 109.5 |
| C(27)-C(29)-H(29A)  | 109.5 |
| C(27)-C(29)-H(29B)  | 109.5 |
| C(27)-C(29)-H(29C)  | 109.5 |
| H(29A)-C(29)-H(29B) | 109.5 |
| H(29A)-C(29)-H(29C) | 109.5 |
| H(29B)-C(29)-H(29C) | 109.5 |
| C(27)-C(30)-H(30A)  | 109.5 |
| C(27)-C(30)-H(30B)  | 109.5 |
| C(27)-C(30)-H(30C)  | 109.5 |
| H(30A)-C(30)-H(30B) | 109.5 |
| H(30A)-C(30)-H(30C) | 109.5 |
| H(30B)-C(30)-H(30C) | 109.5 |
| C(32)-C(31)-S(4)    | 122.2 |
| C(36)-C(31)-S(4)    | 121.5 |
| C(36)-C(31)-C(32)   | 116.1 |

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| C(31)-C(32)-H(32)   | 116.1 |
| C(31)-C(32)-C(33)   | 127.9 |
| C(33)-C(32)-H(32)   | 116.1 |
| C(32)-C(33)-H(33)   | 125.0 |
| C(34)-C(33)-C(32)   | 109.9 |
| C(34)-C(33)-H(33)   | 125.0 |
| C(33)-C(34)-C(35)   | 126.6 |
| C(33)-C(34)-C(37)   | 116.0 |
| C(35)-C(34)-C(37)   | 117.4 |
| C(34)-C(35)-H(35)   | 121.6 |
| C(36)-C(35)-C(34)   | 116.7 |
| C(36)-C(35)-H(35)   | 121.6 |
| C(31)-C(36)-C(35)   | 122.7 |
| C(31)-C(36)-H(36)   | 118.7 |
| C(35)-C(36)-H(36)   | 118.7 |
| C(34)-C(37)-C(39)   | 111.5 |
| C(34)-C(37)-C(40)   | 111.3 |
| C(38)-C(37)-C(34)   | 117.1 |
| C(38)-C(37)-C(39)   | 106.3 |
| C(38)-C(37)-C(40)   | 104.2 |
| C(39)-C(37)-C(40)   | 105.6 |
| C(37)-C(38)-H(38A)  | 109.5 |
| C(37)-C(38)-H(38B)  | 109.5 |
| C(37)-C(38)-H(38C)  | 109.5 |
| H(38A)-C(38)-H(38B) | 109.5 |
| H(38A)-C(38)-H(38C) | 109.5 |
| H(38B)-C(38)-H(38C) | 109.5 |
| C(37)-C(39)-H(39A)  | 109.5 |
| C(37)-C(39)-H(39B)  | 109.5 |
| C(37)-C(39)-H(39C)  | 109.5 |
| H(39A)-C(39)-H(39B) | 109.5 |
| H(39A)-C(39)-H(39C) | 109.5 |
| H(39B)-C(39)-H(39C) | 109.5 |
| C(37)-C(40)-H(40A)  | 109.5 |
| C(37)-C(40)-H(40B)  | 109.5 |
| C(37)-C(40)-H(40C)  | 109.5 |
| H(40A)-C(40)-H(40B) | 109.5 |

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| H(40A)-C(40)-H(40C) | 109.5 |
| H(40B)-C(40)-H(40C) | 109.5 |
| C(42)-C(41)-S(5)    | 119.7 |
| C(46)-C(41)-S(5)    | 121.1 |
| C(46)-C(41)-C(42)   | 118.9 |
| C(41)-C(42)-H(42)   | 120.0 |
| C(43)-C(42)-C(41)   | 120.0 |
| C(43)-C(42)-H(42)   | 120.0 |
| C(42)-C(43)-H(43)   | 118.9 |
| C(42)-C(43)-C(44)   | 122.1 |
| C(44)-C(43)-H(43)   | 118.9 |
| C(43)-C(44)-C(47)   | 122.0 |
| C(45)-C(44)-C(43)   | 118.1 |
| C(45)-C(44)-C(47)   | 119.9 |
| C(44)-C(45)-H(45)   | 118.2 |
| C(44)-C(45)-C(46)   | 123.5 |
| C(46)-C(45)-H(45)   | 118.2 |
| C(41)-C(46)-C(45)   | 117.1 |
| C(41)-C(46)-H(46)   | 121.5 |
| C(45)-C(46)-H(46)   | 121.5 |
| C(44)-C(47)-C(48)   | 106.6 |
| C(44)-C(47)-C(49)   | 105.7 |
| C(49)-C(47)-C(48)   | 108.8 |
| C(50)-C(47)-C(44)   | 114.7 |
| C(50)-C(47)-C(48)   | 109.0 |
| C(50)-C(47)-C(49)   | 111.7 |
| C(47)-C(48)-H(48A)  | 109.5 |
| C(47)-C(48)-H(48B)  | 109.5 |
| C(47)-C(48)-H(48C)  | 109.5 |
| H(48A)-C(48)-H(48B) | 109.5 |
| H(48A)-C(48)-H(48C) | 109.5 |
| H(48B)-C(48)-H(48C) | 109.5 |
| C(47)-C(49)-H(49A)  | 109.5 |
| C(47)-C(49)-H(49B)  | 109.5 |
| C(47)-C(49)-H(49C)  | 109.5 |
| H(49A)-C(49)-H(49B) | 109.5 |
| H(49A)-C(49)-H(49C) | 109.5 |

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| H(49B)-C(49)-H(49C) | 109.5 |
| C(47)-C(50)-H(50A)  | 109.5 |
| C(47)-C(50)-H(50B)  | 109.5 |
| C(47)-C(50)-H(50C)  | 109.5 |
| H(50A)-C(50)-H(50B) | 109.5 |
| H(50A)-C(50)-H(50C) | 109.5 |
| H(50B)-C(50)-H(50C) | 109.5 |
| C(52)-C(51)-S(6)    | 122.0 |
| C(52)-C(51)-C(56)   | 116.8 |
| C(56)-C(51)-S(6)    | 120.9 |
| C(51)-C(52)-H(52)   | 121.1 |
| C(53)-C(52)-C(51)   | 117.9 |
| C(53)-C(52)-H(52)   | 121.1 |
| C(52)-C(53)-H(53)   | 115.6 |
| C(52)-C(53)-C(54)   | 128.7 |
| C(54)-C(53)-H(53)   | 115.6 |
| C(53)-C(54)-C(55)   | 113.9 |
| C(53)-C(54)-C(57)   | 128.8 |
| C(55)-C(54)-C(57)   | 117.3 |
| C(54)-C(55)-H(55)   | 118.3 |
| C(56)-C(55)-C(54)   | 123.4 |
| C(56)-C(55)-H(55)   | 118.3 |
| C(51)-C(56)-H(56)   | 120.5 |
| C(55)-C(56)-C(51)   | 119.0 |
| C(55)-C(56)-H(56)   | 120.5 |
| C(58)-C(57)-C(54)   | 105.4 |
| C(59)-C(57)-C(54)   | 115.2 |
| C(59)-C(57)-C(58)   | 110.4 |
| C(60)-C(57)-C(54)   | 107.5 |
| C(60)-C(57)-C(58)   | 108.8 |
| C(60)-C(57)-C(59)   | 109.3 |
| C(57)-C(58)-H(58A)  | 109.5 |
| C(57)-C(58)-H(58B)  | 109.5 |
| C(57)-C(58)-H(58C)  | 109.5 |
| H(58A)-C(58)-H(58B) | 109.5 |
| H(58A)-C(58)-H(58C) | 109.5 |
| H(58B)-C(58)-H(58C) | 109.5 |

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| C(57)-C(59)-H(59A)  | 109.5 |
| C(57)-C(59)-H(59B)  | 109.5 |
| C(57)-C(59)-H(59C)  | 109.5 |
| H(59A)-C(59)-H(59B) | 109.5 |
| H(59A)-C(59)-H(59C) | 109.5 |
| H(59B)-C(59)-H(59C) | 109.5 |
| C(57)-C(60)-H(60A)  | 109.5 |
| C(57)-C(60)-H(60B)  | 109.5 |
| C(57)-C(60)-H(60C)  | 109.5 |
| H(60A)-C(60)-H(60B) | 109.5 |
| H(60A)-C(60)-H(60C) | 109.5 |
| H(60B)-C(60)-H(60C) | 109.5 |
| C(62)-C(61)-S(7)    | 121.5 |
| C(62)-C(61)-C(66)   | 118.4 |
| C(66)-C(61)-S(7)    | 120.1 |
| C(61)-C(62)-H(62)   | 119.0 |
| C(63)-C(62)-C(61)   | 121.9 |
| C(63)-C(62)-H(62)   | 119.0 |
| C(62)-C(63)-H(63)   | 118.5 |
| C(62)-C(63)-C(64)   | 122.9 |
| C(64)-C(63)-H(63)   | 118.5 |
| C(63)-C(64)-C(65)   | 114.8 |
| C(63)-C(64)-C(67)   | 125.8 |
| C(65)-C(64)-C(67)   | 119.2 |
| C(64)-C(65)-H(65)   | 119.5 |
| C(66)-C(65)-C(64)   | 121.0 |
| C(66)-C(65)-H(65)   | 119.5 |
| C(61)-C(66)-H(66)   | 119.7 |
| C(65)-C(66)-C(61)   | 120.5 |
| C(65)-C(66)-H(66)   | 119.7 |
| C(68)-C(67)-C(64)   | 109.4 |
| C(69)-C(67)-C(64)   | 105.0 |
| C(69)-C(67)-C(68)   | 113.0 |
| C(69)-C(67)-C(70)   | 112.1 |
| C(70)-C(67)-C(64)   | 106.0 |
| C(70)-C(67)-C(68)   | 110.8 |
| C(67)-C(68)-H(68A)  | 109.5 |



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| C(67)-C(68)-H(68B)  | 109.5 |
| C(67)-C(68)-H(68C)  | 109.5 |
| H(68A)-C(68)-H(68B) | 109.5 |
| H(68A)-C(68)-H(68C) | 109.5 |
| H(68B)-C(68)-H(68C) | 109.5 |
| C(67)-C(69)-H(69A)  | 109.5 |
| C(67)-C(69)-H(69B)  | 109.5 |
| C(67)-C(69)-H(69C)  | 109.5 |
| H(69A)-C(69)-H(69B) | 109.5 |
| H(69A)-C(69)-H(69C) | 109.5 |
| H(69B)-C(69)-H(69C) | 109.5 |
| C(67)-C(70)-H(70A)  | 109.5 |
| C(67)-C(70)-H(70B)  | 109.5 |
| C(67)-C(70)-H(70C)  | 109.5 |
| H(70A)-C(70)-H(70B) | 109.5 |
| H(70A)-C(70)-H(70C) | 109.5 |
| H(70B)-C(70)-H(70C) | 109.5 |
| C(72)-C(71)-S(8)    | 123.4 |
| C(72)-C(71)-C(76)   | 120.3 |
| C(76)-C(71)-S(8)    | 116.3 |
| C(71)-C(72)-H(72)   | 120.7 |
| C(71)-C(72)-C(73)   | 118.6 |
| C(73)-C(72)-H(72)   | 120.7 |
| C(72)-C(73)-H(73)   | 117.9 |
| C(74)-C(73)-C(72)   | 124.1 |
| C(74)-C(73)-H(73)   | 117.9 |
| C(73)-C(74)-C(77)   | 125.0 |
| C(75)-C(74)-C(73)   | 117.3 |
| C(75)-C(74)-C(77)   | 117.6 |
| C(74)-C(75)-H(75)   | 119.8 |
| C(74)-C(75)-C(76)   | 120.4 |
| C(76)-C(75)-H(75)   | 119.8 |
| C(71)-C(76)-H(76)   | 120.5 |
| C(75)-C(76)-C(71)   | 119.0 |
| C(75)-C(76)-H(76)   | 120.5 |
| C(78)-C(77)-C(74)   | 110.2 |
| C(78)-C(77)-C(79)   | 108.6 |

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| C(78)-C(77)-C(80)   | 111.5 |
| C(79)-C(77)-C(74)   | 112.4 |
| C(80)-C(77)-C(74)   | 108.2 |
| C(80)-C(77)-C(79)   | 105.8 |
| C(77)-C(78)-H(78A)  | 109.5 |
| C(77)-C(78)-H(78B)  | 109.5 |
| C(77)-C(78)-H(78C)  | 109.5 |
| H(78A)-C(78)-H(78B) | 109.5 |
| H(78A)-C(78)-H(78C) | 109.5 |
| H(78B)-C(78)-H(78C) | 109.5 |
| C(77)-C(79)-H(79A)  | 109.5 |
| C(77)-C(79)-H(79B)  | 109.5 |
| C(77)-C(79)-H(79C)  | 109.5 |
| H(79A)-C(79)-H(79B) | 109.5 |
| H(79A)-C(79)-H(79C) | 109.5 |
| H(79B)-C(79)-H(79C) | 109.5 |
| C(77)-C(80)-H(80A)  | 109.5 |
| C(77)-C(80)-H(80B)  | 109.5 |
| C(77)-C(80)-H(80C)  | 109.5 |
| H(80A)-C(80)-H(80B) | 109.5 |
| H(80A)-C(80)-H(80C) | 109.5 |
| H(80B)-C(80)-H(80C) | 109.5 |
| C(82)-C(81)-S(9)    | 125.5 |
| C(82)-C(81)-C(86)   | 122.5 |
| C(86)-C(81)-S(9)    | 111.8 |
| C(81)-C(82)-H(82)   | 119.4 |
| C(81)-C(82)-C(83)   | 121.2 |
| C(83)-C(82)-H(82)   | 119.4 |
| C(82)-C(83)-H(83)   | 121.5 |
| C(82)-C(83)-C(84)   | 117.0 |
| C(84)-C(83)-H(83)   | 121.5 |
| C(83)-C(84)-C(87)   | 118.0 |
| C(85)-C(84)-C(83)   | 123.1 |
| C(85)-C(84)-C(87)   | 118.6 |
| C(84)-C(85)-H(85)   | 120.9 |
| C(84)-C(85)-C(86)   | 118.2 |
| C(86)-C(85)-H(85)   | 120.9 |

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| C(81)-C(86)-C(85)   | 117.9 |
| C(81)-C(86)-H(86)   | 121.1 |
| C(85)-C(86)-H(86)   | 121.1 |
| C(84)-C(87)-C(89)   | 109.3 |
| C(84)-C(87)-C(90)   | 106.0 |
| C(88)-C(87)-C(84)   | 109.2 |
| C(88)-C(87)-C(89)   | 112.7 |
| C(88)-C(87)-C(90)   | 106.1 |
| C(89)-C(87)-C(90)   | 113.2 |
| C(87)-C(88)-H(88A)  | 109.5 |
| C(87)-C(88)-H(88B)  | 109.5 |
| C(87)-C(88)-H(88C)  | 109.5 |
| H(88A)-C(88)-H(88B) | 109.5 |
| H(88A)-C(88)-H(88C) | 109.5 |
| H(88B)-C(88)-H(88C) | 109.5 |
| C(87)-C(89)-H(89A)  | 109.5 |
| C(87)-C(89)-H(89B)  | 109.5 |
| C(87)-C(89)-H(89C)  | 109.5 |
| H(89A)-C(89)-H(89B) | 109.5 |
| H(89A)-C(89)-H(89C) | 109.5 |
| H(89B)-C(89)-H(89C) | 109.5 |
| C(87)-C(90)-H(90A)  | 109.5 |
| C(87)-C(90)-H(90B)  | 109.5 |
| C(87)-C(90)-H(90C)  | 109.5 |
| H(90A)-C(90)-H(90B) | 109.5 |
| H(90A)-C(90)-H(90C) | 109.5 |
| H(90B)-C(90)-H(90C) | 109.5 |
| C(92)-C(91)-S(10)   | 114.5 |
| C(96)-C(91)-S(10)   | 125.1 |
| C(96)-C(91)-C(92)   | 120.3 |
| C(91)-C(92)-H(92)   | 120.9 |
| C(93)-C(92)-C(91)   | 118.3 |
| C(93)-C(92)-H(92)   | 120.9 |
| C(92)-C(93)-H(93)   | 119.0 |
| C(94)-C(93)-C(92)   | 122.0 |
| C(94)-C(93)-H(93)   | 119.0 |
| C(93)-C(94)-C(95)   | 122.2 |

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| C(93)-C(94)-C(97)    | 118.3 |
| C(95)-C(94)-C(97)    | 119.4 |
| C(94)-C(95)-H(95)    | 120.3 |
| C(96)-C(95)-C(94)    | 119.4 |
| C(96)-C(95)-H(95)    | 120.3 |
| C(91)-C(96)-C(95)    | 117.6 |
| C(91)-C(96)-H(96)    | 121.2 |
| C(95)-C(96)-H(96)    | 121.2 |
| C(98)-C(97)-C(94)    | 109.8 |
| C(99)-C(97)-C(94)    | 109.1 |
| C(99)-C(97)-C(98)    | 105.1 |
| C(99)-C(97)-C(100)   | 115.8 |
| C(100)-C(97)-C(94)   | 107.1 |
| C(100)-C(97)-C(98)   | 110.0 |
| C(97)-C(98)-H(98A)   | 109.5 |
| C(97)-C(98)-H(98B)   | 109.5 |
| C(97)-C(98)-H(98C)   | 109.5 |
| H(98A)-C(98)-H(98B)  | 109.5 |
| H(98A)-C(98)-H(98C)  | 109.5 |
| H(98B)-C(98)-H(98C)  | 109.5 |
| C(97)-C(99)-H(99A)   | 109.5 |
| C(97)-C(99)-H(99B)   | 109.5 |
| C(97)-C(99)-H(99C)   | 109.5 |
| H(99A)-C(99)-H(99B)  | 109.5 |
| H(99A)-C(99)-H(99C)  | 109.5 |
| H(99B)-C(99)-H(99C)  | 109.5 |
| C(97)-C(100)-H(10D)  | 109.5 |
| C(97)-C(100)-H(10E)  | 109.5 |
| C(97)-C(100)-H(10F)  | 109.5 |
| H(10D)-C(100)-H(10E) | 109.5 |
| H(10D)-C(100)-H(10F) | 109.5 |
| H(10E)-C(100)-H(10F) | 109.5 |
| C(102)-C(101)-S(11)  | 122.1 |
| C(106)-C(101)-S(11)  | 117.5 |
| C(106)-C(101)-C(102) | 119.8 |
| C(101)-C(102)-H(102) | 121.6 |
| C(101)-C(102)-C(103) | 116.8 |

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| C(103)-C(102)-H(102) | 121.6 |
| C(102)-C(103)-H(103) | 117.3 |
| C(104)-C(103)-C(102) | 125.4 |
| C(104)-C(103)-H(103) | 117.3 |
| C(103)-C(104)-C(105) | 116.0 |
| C(103)-C(104)-C(107) | 123.1 |
| C(105)-C(104)-C(107) | 120.7 |
| C(104)-C(105)-H(105) | 119.8 |
| C(106)-C(105)-C(104) | 120.5 |
| C(106)-C(105)-H(105) | 119.8 |
| C(101)-C(106)-H(106) | 119.6 |
| C(105)-C(106)-C(101) | 120.8 |
| C(105)-C(106)-H(106) | 119.6 |
| C(104)-C(107)-C(108) | 108.0 |
| C(104)-C(107)-C(110) | 114.2 |
| C(108)-C(107)-C(110) | 108.7 |
| C(109)-C(107)-C(104) | 105.8 |
| C(109)-C(107)-C(108) | 114.5 |
| C(109)-C(107)-C(110) | 105.8 |
| C(107)-C(108)-H(10G) | 109.5 |
| C(107)-C(108)-H(10H) | 109.5 |
| C(107)-C(108)-H(10I) | 109.5 |
| H(10G)-C(108)-H(10H) | 109.5 |
| H(10G)-C(108)-H(10I) | 109.5 |
| H(10H)-C(108)-H(10I) | 109.5 |
| C(107)-C(109)-H(10J) | 109.5 |
| C(107)-C(109)-H(10K) | 109.5 |
| C(107)-C(109)-H(10L) | 109.5 |
| H(10J)-C(109)-H(10K) | 109.5 |
| H(10J)-C(109)-H(10L) | 109.5 |
| H(10K)-C(109)-H(10L) | 109.5 |
| C(107)-C(110)-H(11A) | 109.5 |
| C(107)-C(110)-H(11B) | 109.5 |
| C(107)-C(110)-H(11C) | 109.5 |
| H(11A)-C(110)-H(11B) | 109.5 |
| H(11A)-C(110)-H(11C) | 109.5 |
| H(11B)-C(110)-H(11C) | 109.5 |

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| C(112)-C(111)-S(12)  | 120.4 |
| C(116)-C(111)-S(12)  | 118.9 |
| C(116)-C(111)-C(112) | 120.3 |
| C(111)-C(112)-H(112) | 119.2 |
| C(113)-C(112)-C(111) | 121.6 |
| C(113)-C(112)-H(112) | 119.2 |
| C(112)-C(113)-H(113) | 121.2 |
| C(112)-C(113)-C(114) | 117.5 |
| C(114)-C(113)-H(113) | 121.2 |
| C(113)-C(114)-C(117) | 118.3 |
| C(115)-C(114)-C(113) | 118.0 |
| C(115)-C(114)-C(117) | 123.7 |
| C(114)-C(115)-H(115) | 118.9 |
| C(116)-C(115)-C(114) | 122.2 |
| C(116)-C(115)-H(115) | 118.9 |
| C(111)-C(116)-C(115) | 119.7 |
| C(111)-C(116)-H(116) | 120.2 |
| C(115)-C(116)-H(116) | 120.2 |
| C(114)-C(117)-C(118) | 108.6 |
| C(114)-C(117)-C(120) | 107.8 |
| C(118)-C(117)-C(120) | 109.8 |
| C(119)-C(117)-C(114) | 114.9 |
| C(119)-C(117)-C(118) | 107.1 |
| C(119)-C(117)-C(120) | 108.5 |
| C(117)-C(118)-H(11D) | 109.5 |
| C(117)-C(118)-H(11E) | 109.5 |
| C(117)-C(118)-H(11F) | 109.5 |
| H(11D)-C(118)-H(11E) | 109.5 |
| H(11D)-C(118)-H(11F) | 109.5 |
| H(11E)-C(118)-H(11F) | 109.5 |
| C(117)-C(119)-H(11G) | 109.5 |
| C(117)-C(119)-H(11H) | 109.5 |
| C(117)-C(119)-H(11I) | 109.5 |
| H(11G)-C(119)-H(11H) | 109.5 |
| H(11G)-C(119)-H(11I) | 109.5 |
| H(11H)-C(119)-H(11I) | 109.5 |
| C(117)-C(120)-H(12A) | 109.5 |

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| C(117)-C(120)-H(12B) | 109.5 |
| C(117)-C(120)-H(12C) | 109.5 |
| H(12A)-C(120)-H(12B) | 109.5 |
| H(12A)-C(120)-H(12C) | 109.5 |
| H(12B)-C(120)-H(12C) | 109.5 |
| C(122)-C(121)-S(13)  | 117.8 |
| C(126)-C(121)-S(13)  | 114.0 |
| C(126)-C(121)-C(122) | 128.2 |
| C(121)-C(122)-H(122) | 123.7 |
| C(123)-C(122)-C(121) | 112.7 |
| C(123)-C(122)-H(122) | 123.7 |
| C(122)-C(123)-H(123) | 118.2 |
| C(124)-C(123)-C(122) | 123.7 |
| C(124)-C(123)-H(123) | 118.2 |
| C(123)-C(124)-C(127) | 125.7 |
| C(125)-C(124)-C(123) | 117.5 |
| C(125)-C(124)-C(127) | 116.7 |
| C(124)-C(125)-H(125) | 116.7 |
| C(124)-C(125)-C(126) | 126.7 |
| C(126)-C(125)-H(125) | 116.7 |
| C(121)-C(126)-C(125) | 110.5 |
| C(121)-C(126)-H(126) | 124.7 |
| C(125)-C(126)-H(126) | 124.7 |
| C(124)-C(127)-C(128) | 104.0 |
| C(129)-C(127)-C(124) | 107.9 |
| C(129)-C(127)-C(128) | 86.5  |
| C(130)-C(127)-C(124) | 115.4 |
| C(130)-C(127)-C(128) | 104.1 |
| C(130)-C(127)-C(129) | 130.7 |
| C(127)-C(129)-H(12D) | 109.5 |
| C(127)-C(129)-H(12E) | 109.5 |
| C(127)-C(129)-H(12F) | 109.5 |
| H(12D)-C(129)-H(12E) | 109.5 |
| H(12D)-C(129)-H(12F) | 109.5 |
| H(12E)-C(129)-H(12F) | 109.5 |
| C(127)-C(130)-H(13A) | 109.5 |
| C(127)-C(130)-H(13B) | 109.5 |

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| C(127)-C(130)-H(13C) | 109.5 |
| H(13A)-C(130)-H(13B) | 109.5 |
| H(13A)-C(130)-H(13C) | 109.5 |
| H(13B)-C(130)-H(13C) | 109.5 |
| C(132)-C(131)-S(14)  | 112.0 |
| C(132)-C(131)-C(136) | 121.8 |
| C(136)-C(131)-S(14)  | 124.8 |
| C(131)-C(132)-H(132) | 123.0 |
| C(131)-C(132)-C(133) | 113.9 |
| C(133)-C(132)-H(132) | 123.0 |
| C(132)-C(133)-H(133) | 119.6 |
| C(134)-C(133)-C(132) | 120.8 |
| C(134)-C(133)-H(133) | 119.6 |
| C(133)-C(134)-C(135) | 120.8 |
| C(133)-C(134)-C(137) | 122.6 |
| C(135)-C(134)-C(137) | 116.5 |
| C(134)-C(135)-H(135) | 120.3 |
| C(136)-C(135)-C(134) | 119.5 |
| C(136)-C(135)-H(135) | 120.3 |
| C(131)-C(136)-H(136) | 119.6 |
| C(135)-C(136)-C(131) | 120.8 |
| C(135)-C(136)-H(136) | 119.6 |
| C(138)-C(137)-C(134) | 111.4 |
| C(138)-C(137)-C(139) | 108.7 |
| C(138)-C(137)-C(140) | 113.5 |
| C(139)-C(137)-C(134) | 110.2 |
| C(139)-C(137)-C(140) | 104.3 |
| C(140)-C(137)-C(134) | 108.6 |
| C(137)-C(138)-H(13D) | 109.5 |
| C(137)-C(138)-H(13E) | 109.5 |
| C(137)-C(138)-H(13F) | 109.5 |
| H(13D)-C(138)-H(13E) | 109.5 |
| H(13D)-C(138)-H(13F) | 109.5 |
| H(13E)-C(138)-H(13F) | 109.5 |
| C(137)-C(139)-H(13G) | 109.5 |
| C(137)-C(139)-H(13H) | 109.5 |
| C(137)-C(139)-H(13I) | 109.5 |



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| H(13G)-C(139)-H(13H) | 109.5 |
| H(13G)-C(139)-H(13I) | 109.5 |
| H(13H)-C(139)-H(13I) | 109.5 |
| C(137)-C(140)-H(14A) | 109.5 |
| C(137)-C(140)-H(14B) | 109.5 |
| C(137)-C(140)-H(14C) | 109.5 |
| H(14A)-C(140)-H(14B) | 109.5 |
| H(14A)-C(140)-H(14C) | 109.5 |
| H(14B)-C(140)-H(14C) | 109.5 |
| C(142)-C(141)-S(15)  | 120.8 |
| C(142)-C(141)-C(146) | 115.6 |
| C(146)-C(141)-S(15)  | 123.4 |
| C(141)-C(142)-H(142) | 119.6 |
| C(141)-C(142)-C(143) | 120.8 |
| C(143)-C(142)-H(142) | 119.6 |
| C(142)-C(143)-H(143) | 119.9 |
| C(144)-C(143)-C(142) | 120.2 |
| C(144)-C(143)-H(143) | 119.9 |
| C(143)-C(144)-C(145) | 120.5 |
| C(143)-C(144)-C(147) | 120.1 |
| C(145)-C(144)-C(147) | 119.4 |
| C(144)-C(145)-H(145) | 119.4 |
| C(146)-C(145)-C(144) | 121.1 |
| C(146)-C(145)-H(145) | 119.4 |
| C(141)-C(146)-H(146) | 119.1 |
| C(145)-C(146)-C(141) | 121.7 |
| C(145)-C(146)-H(146) | 119.1 |
| C(144)-C(147)-C(148) | 104.5 |
| C(149)-C(147)-C(144) | 110.0 |
| C(149)-C(147)-C(148) | 111.3 |
| C(150)-C(147)-C(144) | 113.5 |
| C(150)-C(147)-C(148) | 107.8 |
| C(150)-C(147)-C(149) | 109.6 |
| C(147)-C(148)-H(14D) | 109.5 |
| C(147)-C(148)-H(14E) | 109.5 |
| C(147)-C(148)-H(14F) | 109.5 |
| H(14D)-C(148)-H(14E) | 109.5 |

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| H(14D)-C(148)-H(14F) | 109.5 |
| H(14E)-C(148)-H(14F) | 109.5 |
| C(147)-C(149)-H(14G) | 109.5 |
| C(147)-C(149)-H(14H) | 109.5 |
| C(147)-C(149)-H(14I) | 109.5 |
| H(14G)-C(149)-H(14H) | 109.5 |
| H(14G)-C(149)-H(14I) | 109.5 |
| H(14H)-C(149)-H(14I) | 109.5 |
| C(147)-C(150)-H(15A) | 109.5 |
| C(147)-C(150)-H(15B) | 109.5 |
| C(147)-C(150)-H(15C) | 109.5 |
| H(15A)-C(150)-H(15B) | 109.5 |
| H(15A)-C(150)-H(15C) | 109.5 |
| H(15B)-C(150)-H(15C) | 109.5 |
| C(152)-C(151)-S(16)  | 118.6 |
| C(156)-C(151)-S(16)  | 120.4 |
| C(156)-C(151)-C(152) | 120.6 |
| C(151)-C(152)-H(152) | 121.9 |
| C(151)-C(152)-C(153) | 116.1 |
| C(153)-C(152)-H(152) | 121.9 |
| C(152)-C(153)-H(153) | 119.7 |
| C(154)-C(153)-C(152) | 120.6 |
| C(154)-C(153)-H(153) | 119.7 |
| C(153)-C(154)-C(155) | 121.6 |
| C(153)-C(154)-C(157) | 118.6 |
| C(155)-C(154)-C(157) | 119.6 |
| C(154)-C(155)-H(155) | 122.4 |
| C(156)-C(155)-C(154) | 115.3 |
| C(156)-C(155)-H(155) | 122.4 |
| C(151)-C(156)-H(156) | 117.3 |
| C(155)-C(156)-C(151) | 125.3 |
| C(155)-C(156)-H(156) | 117.3 |
| C(158)-C(157)-C(154) | 111.3 |
| C(158)-C(157)-C(160) | 97.1  |
| C(159)-C(157)-C(154) | 109.0 |
| C(159)-C(157)-C(158) | 119.5 |
| C(159)-C(157)-C(160) | 110.1 |

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| C(160)-C(157)-C(154) | 109.0 |
| C(157)-C(158)-H(15D) | 109.5 |
| C(157)-C(158)-H(15E) | 109.5 |
| C(157)-C(158)-H(15F) | 109.5 |
| H(15D)-C(158)-H(15E) | 109.5 |
| H(15D)-C(158)-H(15F) | 109.5 |
| H(15E)-C(158)-H(15F) | 109.5 |
| C(157)-C(159)-H(15G) | 109.5 |
| C(157)-C(159)-H(15H) | 109.5 |
| C(157)-C(159)-H(15I) | 109.5 |
| H(15G)-C(159)-H(15H) | 109.5 |
| H(15G)-C(159)-H(15I) | 109.5 |
| H(15H)-C(159)-H(15I) | 109.5 |
| C(157)-C(160)-H(16A) | 109.5 |
| C(157)-C(160)-H(16B) | 109.5 |
| C(157)-C(160)-H(16C) | 109.5 |
| H(16A)-C(160)-H(16B) | 109.5 |
| H(16A)-C(160)-H(16C) | 109.5 |
| H(16B)-C(160)-H(16C) | 109.5 |
| C(162)-C(161)-S(17)  | 122.9 |
| C(162)-C(161)-C(166) | 117.5 |
| C(166)-C(161)-S(17)  | 119.6 |
| C(161)-C(162)-H(162) | 120.0 |
| C(161)-C(162)-C(163) | 120.0 |
| C(163)-C(162)-H(162) | 120.0 |
| C(162)-C(163)-H(163) | 118.0 |
| C(164)-C(163)-C(162) | 124.1 |
| C(164)-C(163)-H(163) | 118.0 |
| C(163)-C(164)-C(165) | 120.2 |
| C(163)-C(164)-C(167) | 125.8 |
| C(165)-C(164)-C(167) | 113.9 |
| C(164)-C(165)-H(165) | 121.8 |
| C(164)-C(165)-C(166) | 116.5 |
| C(166)-C(165)-H(165) | 121.8 |
| C(161)-C(166)-H(166) | 119.2 |
| C(165)-C(166)-C(161) | 121.6 |
| C(165)-C(166)-H(166) | 119.2 |

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| C(164)-C(167)-C(168) | 112.8 |
| C(164)-C(167)-C(170) | 109.2 |
| C(168)-C(167)-C(170) | 107.9 |
| C(169)-C(167)-C(164) | 111.9 |
| C(169)-C(167)-C(168) | 108.5 |
| C(169)-C(167)-C(170) | 106.2 |
| C(167)-C(168)-H(16D) | 109.5 |
| C(167)-C(168)-H(16E) | 109.5 |
| C(167)-C(168)-H(16F) | 109.5 |
| H(16D)-C(168)-H(16E) | 109.5 |
| H(16D)-C(168)-H(16F) | 109.5 |
| H(16E)-C(168)-H(16F) | 109.5 |
| C(167)-C(169)-H(16G) | 109.5 |
| C(167)-C(169)-H(16H) | 109.5 |
| C(167)-C(169)-H(16I) | 109.5 |
| H(16G)-C(169)-H(16H) | 109.5 |
| H(16G)-C(169)-H(16I) | 109.5 |
| H(16H)-C(169)-H(16I) | 109.5 |
| C(167)-C(170)-H(17A) | 109.5 |
| C(167)-C(170)-H(17B) | 109.5 |
| C(167)-C(170)-H(17C) | 109.5 |
| H(17A)-C(170)-H(17B) | 109.5 |
| H(17A)-C(170)-H(17C) | 109.5 |
| H(17B)-C(170)-H(17C) | 109.5 |
| C(172)-C(171)-S(18)  | 127.1 |
| C(176)-C(171)-S(18)  | 115.5 |
| C(176)-C(171)-C(172) | 117.3 |
| C(171)-C(172)-H(172) | 119.1 |
| C(173)-C(172)-C(171) | 121.8 |
| C(173)-C(172)-H(172) | 119.1 |
| C(172)-C(173)-H(173) | 119.9 |
| C(172)-C(173)-C(174) | 120.2 |
| C(174)-C(173)-H(173) | 119.9 |
| C(173)-C(174)-C(175) | 117.2 |
| C(173)-C(174)-C(177) | 115.8 |
| C(175)-C(174)-C(177) | 126.7 |
| C(174)-C(175)-H(175) | 118.5 |

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| C(176)-C(175)-C(174) | 123.0 |
| C(176)-C(175)-H(175) | 118.5 |
| C(171)-C(176)-H(176) | 120.0 |
| C(175)-C(176)-C(171) | 120.1 |
| C(175)-C(176)-H(176) | 120.0 |
| C(174)-C(177)-C(178) | 105.8 |
| C(179)-C(177)-C(174) | 103.4 |
| C(179)-C(177)-C(178) | 104.2 |
| C(180)-C(177)-C(174) | 114.4 |
| C(180)-C(177)-C(178) | 101.5 |
| C(180)-C(177)-C(179) | 125.7 |
| C(177)-C(178)-H(17D) | 109.5 |
| C(177)-C(178)-H(17E) | 109.5 |
| C(177)-C(178)-H(17F) | 109.5 |
| H(17D)-C(178)-H(17E) | 109.5 |
| H(17D)-C(178)-H(17F) | 109.5 |
| H(17E)-C(178)-H(17F) | 109.5 |
| C(177)-C(179)-H(17G) | 109.5 |
| C(177)-C(179)-H(17H) | 109.5 |
| C(177)-C(179)-H(17I) | 109.5 |
| H(17G)-C(179)-H(17H) | 109.5 |
| H(17G)-C(179)-H(17I) | 109.5 |
| H(17H)-C(179)-H(17I) | 109.5 |
| C(177)-C(180)-H(18D) | 109.5 |
| C(177)-C(180)-H(18E) | 109.5 |
| C(177)-C(180)-H(18F) | 109.5 |
| H(18D)-C(180)-H(18E) | 109.5 |
| H(18D)-C(180)-H(18F) | 109.5 |
| H(18E)-C(180)-H(18F) | 109.5 |
| C(182)-C(181)-S(19)  | 118.3 |
| C(182)-C(181)-C(186) | 122.6 |
| C(186)-C(181)-S(19)  | 119.0 |
| C(181)-C(182)-H(182) | 121.8 |
| C(181)-C(182)-C(183) | 116.5 |
| C(183)-C(182)-H(182) | 121.8 |
| C(182)-C(183)-H(183) | 118.5 |
| C(184)-C(183)-C(182) | 123.0 |

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| C(184)-C(183)-H(183) | 118.5 |
| C(183)-C(184)-C(185) | 117.2 |
| C(183)-C(184)-C(187) | 127.1 |
| C(185)-C(184)-C(187) | 115.5 |
| C(184)-C(185)-H(185) | 118.7 |
| C(186)-C(185)-C(184) | 122.7 |
| C(186)-C(185)-H(185) | 118.7 |
| C(181)-C(186)-H(186) | 121.4 |
| C(185)-C(186)-C(181) | 117.1 |
| C(185)-C(186)-H(186) | 121.4 |
| C(184)-C(187)-C(189) | 109.6 |
| C(184)-C(187)-C(190) | 104.6 |
| C(188)-C(187)-C(184) | 117.6 |
| C(188)-C(187)-C(189) | 107.8 |
| C(188)-C(187)-C(190) | 109.3 |
| C(189)-C(187)-C(190) | 107.6 |
| C(187)-C(188)-H(18G) | 109.5 |
| C(187)-C(188)-H(18H) | 109.5 |
| C(187)-C(188)-H(18I) | 109.5 |
| H(18G)-C(188)-H(18H) | 109.5 |
| H(18G)-C(188)-H(18I) | 109.5 |
| H(18H)-C(188)-H(18I) | 109.5 |
| C(187)-C(189)-H(18J) | 109.5 |
| C(187)-C(189)-H(18K) | 109.5 |
| C(187)-C(189)-H(18L) | 109.5 |
| H(18J)-C(189)-H(18K) | 109.5 |
| H(18J)-C(189)-H(18L) | 109.5 |
| H(18K)-C(189)-H(18L) | 109.5 |
| C(187)-C(190)-H(19D) | 109.5 |
| C(187)-C(190)-H(19E) | 109.5 |
| C(187)-C(190)-H(19F) | 109.5 |
| H(19D)-C(190)-H(19E) | 109.5 |
| H(19D)-C(190)-H(19F) | 109.5 |
| H(19E)-C(190)-H(19F) | 109.5 |
| C(192)-C(191)-S(20)  | 115.4 |
| C(196)-C(191)-S(20)  | 127.2 |
| C(196)-C(191)-C(192) | 117.4 |

|                      |       |
|----------------------|-------|
| C(191)-C(192)-H(192) | 118.7 |
| C(193)-C(192)-C(191) | 122.6 |
| C(193)-C(192)-H(192) | 118.7 |
| C(192)-C(193)-H(193) | 121.1 |
| C(192)-C(193)-C(194) | 117.8 |
| C(194)-C(193)-H(193) | 121.1 |
| C(193)-C(194)-C(197) | 119.4 |
| C(195)-C(194)-C(193) | 118.6 |
| C(195)-C(194)-C(197) | 121.9 |
| C(194)-C(195)-H(195) | 119.1 |
| C(196)-C(195)-C(194) | 121.8 |
| C(196)-C(195)-H(195) | 119.1 |
| C(191)-C(196)-H(196) | 119.2 |
| C(195)-C(196)-C(191) | 121.7 |
| C(195)-C(196)-H(196) | 119.2 |
| C(198)-C(197)-C(194) | 104.1 |
| C(199)-C(197)-C(194) | 108.4 |
| C(199)-C(197)-C(198) | 109.8 |
| C(200)-C(197)-C(194) | 110.3 |
| C(200)-C(197)-C(198) | 109.6 |
| C(200)-C(197)-C(199) | 114.2 |
| C(197)-C(198)-H(19G) | 109.5 |
| C(197)-C(198)-H(19H) | 109.5 |
| C(197)-C(198)-H(19I) | 109.5 |
| H(19G)-C(198)-H(19H) | 109.5 |
| H(19G)-C(198)-H(19I) | 109.5 |
| H(19H)-C(198)-H(19I) | 109.5 |
| C(197)-C(199)-H(19J) | 109.5 |
| C(197)-C(199)-H(19K) | 109.5 |
| C(197)-C(199)-H(19L) | 109.5 |
| H(19J)-C(199)-H(19K) | 109.5 |
| H(19J)-C(199)-H(19L) | 109.5 |
| H(19K)-C(199)-H(19L) | 109.5 |
| C(197)-C(200)-H(20D) | 109.5 |
| C(197)-C(200)-H(20E) | 109.5 |
| C(197)-C(200)-H(20F) | 109.5 |
| H(20D)-C(200)-H(20E) | 109.5 |

|                      |       |
|----------------------|-------|
| H(20D)-C(200)-H(20F) | 109.5 |
| H(20E)-C(200)-H(20F) | 109.5 |
| C(202)-C(201)-S(21)  | 113.8 |
| C(206)-C(201)-S(21)  | 122.9 |
| C(206)-C(201)-C(202) | 123.3 |
| C(201)-C(202)-H(202) | 122.0 |
| C(203)-C(202)-C(201) | 116.0 |
| C(203)-C(202)-H(202) | 122.0 |
| C(202)-C(203)-H(203) | 118.5 |
| C(204)-C(203)-C(202) | 123.1 |
| C(204)-C(203)-H(203) | 118.5 |
| C(203)-C(204)-C(205) | 116.3 |
| C(203)-C(204)-C(207) | 117.7 |
| C(205)-C(204)-C(207) | 125.6 |
| C(204)-C(205)-H(205) | 117.3 |
| C(204)-C(205)-C(206) | 125.5 |
| C(206)-C(205)-H(205) | 117.3 |
| C(201)-C(206)-C(205) | 115.3 |
| C(201)-C(206)-H(206) | 122.4 |
| C(205)-C(206)-H(206) | 122.4 |
| C(204)-C(207)-C(208) | 110.7 |
| C(209)-C(207)-C(204) | 110.4 |
| C(209)-C(207)-C(208) | 105.1 |
| C(209)-C(207)-C(210) | 111.0 |
| C(210)-C(207)-C(204) | 113.5 |
| C(210)-C(207)-C(208) | 105.7 |
| C(207)-C(208)-H(20G) | 109.5 |
| C(207)-C(208)-H(20H) | 109.5 |
| C(207)-C(208)-H(20I) | 109.5 |
| H(20G)-C(208)-H(20H) | 109.5 |
| H(20G)-C(208)-H(20I) | 109.5 |
| H(20H)-C(208)-H(20I) | 109.5 |
| C(207)-C(209)-H(20J) | 109.5 |
| C(207)-C(209)-H(20K) | 109.5 |
| C(207)-C(209)-H(20L) | 109.5 |
| H(20J)-C(209)-H(20K) | 109.5 |
| H(20J)-C(209)-H(20L) | 109.5 |



|                      |       |
|----------------------|-------|
| H(20K)-C(209)-H(20L) | 109.5 |
| C(207)-C(210)-H(21A) | 109.5 |
| C(207)-C(210)-H(21B) | 109.5 |
| C(207)-C(210)-H(21C) | 109.5 |
| H(21A)-C(210)-H(21B) | 109.5 |
| H(21A)-C(210)-H(21C) | 109.5 |
| H(21B)-C(210)-H(21C) | 109.5 |
| C(212)-C(211)-S(22)  | 116.8 |
| C(212)-C(211)-C(216) | 122.7 |
| C(216)-C(211)-S(22)  | 120.0 |
| C(211)-C(212)-H(212) | 119.7 |
| C(211)-C(212)-C(213) | 120.6 |
| C(213)-C(212)-H(212) | 119.7 |
| C(212)-C(213)-H(213) | 122.4 |
| C(212)-C(213)-C(214) | 115.2 |
| C(214)-C(213)-H(213) | 122.4 |
| C(213)-C(214)-C(217) | 112.9 |
| C(215)-C(214)-C(213) | 121.5 |
| C(215)-C(214)-C(217) | 125.4 |
| C(214)-C(215)-H(215) | 119.1 |
| C(214)-C(215)-C(216) | 121.9 |
| C(216)-C(215)-H(215) | 119.1 |
| C(211)-C(216)-H(216) | 121.2 |
| C(215)-C(216)-C(211) | 117.7 |
| C(215)-C(216)-H(216) | 121.2 |
| C(214)-C(217)-C(219) | 113.3 |
| C(214)-C(217)-C(220) | 107.1 |
| C(218)-C(217)-C(214) | 103.2 |
| C(218)-C(217)-C(219) | 106.8 |
| C(218)-C(217)-C(220) | 113.5 |
| C(219)-C(217)-C(220) | 112.7 |
| C(217)-C(218)-H(21D) | 109.5 |
| C(217)-C(218)-H(21E) | 109.5 |
| C(217)-C(218)-H(21F) | 109.5 |
| H(21D)-C(218)-H(21E) | 109.5 |
| H(21D)-C(218)-H(21F) | 109.5 |
| H(21E)-C(218)-H(21F) | 109.5 |

|                      |       |
|----------------------|-------|
| C(217)-C(219)-H(21G) | 109.5 |
| C(217)-C(219)-H(21H) | 109.5 |
| C(217)-C(219)-H(21I) | 109.5 |
| H(21G)-C(219)-H(21H) | 109.5 |
| H(21G)-C(219)-H(21I) | 109.5 |
| H(21H)-C(219)-H(21I) | 109.5 |
| C(217)-C(220)-H(22A) | 109.5 |
| C(217)-C(220)-H(22B) | 109.5 |
| C(217)-C(220)-H(22C) | 109.5 |
| H(22A)-C(220)-H(22B) | 109.5 |
| H(22A)-C(220)-H(22C) | 109.5 |
| H(22B)-C(220)-H(22C) | 109.5 |
| C(222)-C(221)-S(23)  | 117.4 |
| C(226)-C(221)-S(23)  | 123.0 |
| C(226)-C(221)-C(222) | 119.4 |
| C(221)-C(222)-H(222) | 118.5 |
| C(221)-C(222)-C(223) | 123.1 |
| C(223)-C(222)-H(222) | 118.5 |
| C(222)-C(223)-H(223) | 121.4 |
| C(222)-C(223)-C(224) | 117.2 |
| C(224)-C(223)-H(223) | 121.4 |
| C(223)-C(224)-C(227) | 118.9 |
| C(225)-C(224)-C(223) | 119.1 |
| C(225)-C(224)-C(227) | 122.0 |
| C(224)-C(225)-H(225) | 118.7 |
| C(224)-C(225)-C(226) | 122.6 |
| C(226)-C(225)-H(225) | 118.7 |
| C(221)-C(226)-C(225) | 118.4 |
| C(221)-C(226)-H(226) | 120.8 |
| C(225)-C(226)-H(226) | 120.8 |
| C(228)-C(227)-C(224) | 106.0 |
| C(229)-C(227)-C(224) | 103.0 |
| C(229)-C(227)-C(228) | 118.8 |
| C(230)-C(227)-C(224) | 107.7 |
| C(230)-C(227)-C(228) | 113.6 |
| C(230)-C(227)-C(229) | 106.8 |
| C(227)-C(228)-H(22D) | 109.5 |

|                      |       |
|----------------------|-------|
| C(227)-C(228)-H(22E) | 109.5 |
| C(227)-C(228)-H(22F) | 109.5 |
| H(22D)-C(228)-H(22E) | 109.5 |
| H(22D)-C(228)-H(22F) | 109.5 |
| H(22E)-C(228)-H(22F) | 109.5 |
| C(227)-C(229)-H(22G) | 109.5 |
| C(227)-C(229)-H(22H) | 109.5 |
| C(227)-C(229)-H(22I) | 109.5 |
| H(22G)-C(229)-H(22H) | 109.5 |
| H(22G)-C(229)-H(22I) | 109.5 |
| H(22H)-C(229)-H(22I) | 109.5 |
| C(227)-C(230)-H(23A) | 109.5 |
| C(227)-C(230)-H(23B) | 109.5 |
| C(227)-C(230)-H(23C) | 109.5 |
| H(23A)-C(230)-H(23B) | 109.5 |
| H(23A)-C(230)-H(23C) | 109.5 |
| H(23B)-C(230)-H(23C) | 109.5 |
| C(232)-C(231)-S(24)  | 113.1 |
| C(232)-C(231)-C(236) | 122.2 |
| C(236)-C(231)-S(24)  | 124.4 |
| C(231)-C(232)-H(232) | 121.4 |
| C(233)-C(232)-C(231) | 117.2 |
| C(233)-C(232)-H(232) | 121.4 |
| C(232)-C(233)-H(233) | 118.7 |
| C(232)-C(233)-C(234) | 122.6 |
| C(234)-C(233)-H(233) | 118.7 |
| C(233)-C(234)-C(237) | 119.4 |
| C(235)-C(234)-C(233) | 116.7 |
| C(235)-C(234)-C(237) | 123.5 |
| C(234)-C(235)-H(235) | 118.0 |
| C(234)-C(235)-C(236) | 124.1 |
| C(236)-C(235)-H(235) | 118.0 |
| C(231)-C(236)-H(236) | 121.5 |
| C(235)-C(236)-C(231) | 117.0 |
| C(235)-C(236)-H(236) | 121.5 |
| C(234)-C(237)-C(238) | 113.9 |
| C(234)-C(237)-C(240) | 106.7 |

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|--------------------------|-------|
| C(238)-C(237)-C(240)     | 99.0  |
| C(239)-C(237)-C(234)     | 111.6 |
| C(239)-C(237)-C(238)     | 110.6 |
| C(239)-C(237)-C(240)     | 114.4 |
| C(237)-C(238)-H(23D)     | 109.5 |
| C(237)-C(238)-H(23E)     | 109.5 |
| C(237)-C(238)-H(23F)     | 109.5 |
| H(23D)-C(238)-H(23E)     | 109.5 |
| H(23D)-C(238)-H(23F)     | 109.5 |
| H(23E)-C(238)-H(23F)     | 109.5 |
| C(237)-C(239)-H(23G)     | 109.5 |
| C(237)-C(239)-H(23H)     | 109.5 |
| C(237)-C(239)-H(23I)     | 109.5 |
| H(23G)-C(239)-H(23H)     | 109.5 |
| H(23G)-C(239)-H(23I)     | 109.5 |
| H(23H)-C(239)-H(23I)     | 109.5 |
| C(237)-C(240)-H(24A)     | 109.5 |
| C(237)-C(240)-H(24B)     | 109.5 |
| C(237)-C(240)-H(24C)     | 109.5 |
| H(24A)-C(240)-H(24B)     | 109.5 |
| H(24A)-C(240)-H(24C)     | 109.5 |
| H(24B)-C(240)-H(24C)     | 109.5 |
| Au(37)#1-Au(37)-Au(38)   | 87.2  |
| Au(37)#1-Au(37)-Au(39)   | 60.1  |
| Au(37)#1-Au(37)-Au(39)#1 | 60.2  |
| Au(37)#1-Au(37)-Au(41)   | 117.5 |
| Au(37)#1-Au(37)-Au(42)   | 117.0 |
| Au(37)#1-Au(37)-Au(43)   | 88.1  |
| Au(38)-Au(37)-Au(41)     | 64.2  |
| Au(38)-Au(37)-Au(42)     | 125.6 |
| Au(39)#1-Au(37)-Au(38)   | 114.5 |
| Au(39)-Au(37)-Au(38)     | 55.9  |
| Au(39)#1-Au(37)-Au(39)   | 58.6  |
| Au(39)-Au(37)-Au(41)     | 120.1 |
| Au(39)#1-Au(37)-Au(41)   | 177.6 |
| Au(39)-Au(37)-Au(42)     | 177.1 |
| Au(39)#1-Au(37)-Au(42)   | 119.9 |

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|--------------------------|-------|
| Au(39)-Au(37)-Au(43)     | 113.8 |
| Au(39)#1-Au(37)-Au(43)   | 55.3  |
| Au(40)-Au(37)-Au(37)#1   | 121.5 |
| Au(40)-Au(37)-Au(38)     | 59.3  |
| Au(40)-Au(37)-Au(39)     | 61.4  |
| Au(40)-Au(37)-Au(39)#1   | 90.1  |
| Au(40)-Au(37)-Au(41)     | 90.8  |
| Au(40)-Au(37)-Au(42)     | 121.5 |
| Au(40)-Au(37)-Au(43)     | 116.2 |
| Au(40)-Au(37)-Au(45)     | 57.6  |
| Au(42)-Au(37)-Au(41)     | 61.4  |
| Au(43)-Au(37)-Au(38)     | 169.7 |
| Au(43)-Au(37)-Au(41)     | 126.1 |
| Au(43)-Au(37)-Au(42)     | 64.7  |
| Au(44)-Au(37)-Au(37)#1   | 57.8  |
| Au(44)#1-Au(37)-Au(37)#1 | 57.5  |
| Au(44)-Au(37)-Au(38)     | 121.2 |
| Au(44)#1-Au(37)-Au(38)   | 61.6  |
| Au(44)-Au(37)-Au(39)     | 118.0 |
| Au(44)-Au(37)-Au(39)#1   | 88.9  |
| Au(44)#1-Au(37)-Au(39)   | 88.7  |
| Au(44)#1-Au(37)-Au(39)#1 | 117.6 |
| Au(44)#1-Au(37)-Au(40)   | 120.7 |
| Au(44)-Au(37)-Au(40)     | 179.0 |
| Au(44)-Au(37)-Au(41)     | 90.2  |
| Au(44)#1-Au(37)-Au(41)   | 60.0  |
| Au(44)-Au(37)-Au(42)     | 59.1  |
| Au(44)#1-Au(37)-Au(42)   | 90.1  |
| Au(44)#1-Au(37)-Au(43)   | 122.7 |
| Au(44)-Au(37)-Au(43)     | 63.2  |
| Au(44)-Au(37)-Au(44)#1   | 59.8  |
| Au(44)-Au(37)-Au(45)     | 121.9 |
| Au(44)#1-Au(37)-Au(45)   | 176.6 |
| Au(45)-Au(37)-Au(37)#1   | 125.8 |
| Au(45)-Au(37)-Au(38)     | 116.9 |
| Au(45)-Au(37)-Au(39)#1   | 65.7  |
| Au(45)-Au(37)-Au(39)     | 92.7  |

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|--------------------------|-------|
| Au(45)-Au(37)-Au(41)     | 116.6 |
| Au(45)-Au(37)-Au(42)     | 88.7  |
| Au(45)-Au(37)-Au(43)     | 59.4  |
| Au(54)-Au(37)-Au(37)#1   | 173.3 |
| Au(54)-Au(37)-Au(38)     | 87.8  |
| Au(54)-Au(37)-Au(39)     | 120.0 |
| Au(54)-Au(37)-Au(39)#1   | 126.2 |
| Au(54)-Au(37)-Au(40)     | 58.9  |
| Au(54)-Au(37)-Au(41)     | 56.1  |
| Au(54)-Au(37)-Au(42)     | 63.0  |
| Au(54)-Au(37)-Au(43)     | 97.6  |
| Au(54)-Au(37)-Au(44)#1   | 116.0 |
| Au(54)-Au(37)-Au(44)     | 121.8 |
| Au(54)-Au(37)-Au(45)     | 60.6  |
| Au(37)-Au(38)-Au(41)     | 61.2  |
| Au(39)-Au(38)-Au(37)     | 60.9  |
| Au(39)-Au(38)-Au(40)     | 62.2  |
| Au(39)-Au(38)-Au(41)     | 122.1 |
| Au(39)-Au(38)-Au(44)#1   | 87.7  |
| Au(40)-Au(38)-Au(37)     | 56.1  |
| Au(40)-Au(38)-Au(41)     | 87.3  |
| Au(40)-Au(38)-Au(44)#1   | 110.9 |
| Au(43)#1-Au(38)-Au(37)   | 92.4  |
| Au(43)#1-Au(38)-Au(39)   | 60.3  |
| Au(43)#1-Au(38)-Au(40)   | 122.4 |
| Au(43)#1-Au(38)-Au(41)   | 120.8 |
| Au(43)#1-Au(38)-Au(44)#1 | 64.2  |
| Au(43)#1-Au(38)-Au(48)   | 61.7  |
| Au(44)#1-Au(38)-Au(37)   | 54.8  |
| Au(44)#1-Au(38)-Au(41)   | 57.2  |
| Au(48)-Au(38)-Au(37)     | 120.2 |
| Au(48)-Au(38)-Au(39)     | 59.4  |
| Au(48)-Au(38)-Au(40)     | 91.8  |
| Au(48)-Au(38)-Au(41)     | 177.4 |
| Au(48)-Au(38)-Au(44)#1   | 125.3 |
| S(29)-Au(38)-Au(37)      | 96.2  |
| S(29)-Au(38)-Au(39)      | 147.1 |

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|--------------------------|-------|
| S(29)-Au(38)-Au(40)      | 85.7  |
| S(29)-Au(38)-Au(41)      | 43.7  |
| S(29)-Au(38)-Au(43)#1    | 150.1 |
| S(29)-Au(38)-Au(44)#1    | 98.1  |
| S(29)-Au(38)-Au(48)      | 133.8 |
| Au(37)#1-Au(39)-Au(37)   | 59.7  |
| Au(37)#1-Au(39)-Au(45)#1 | 54.5  |
| Au(37)-Au(39)-Au(45)#1   | 114.2 |
| Au(37)-Au(39)-Au(47)     | 175.9 |
| Au(37)#1-Au(39)-Au(47)   | 117.7 |
| Au(37)#1-Au(39)-Au(53)   | 178.7 |
| Au(37)-Au(39)-Au(53)     | 119.2 |
| Au(38)-Au(39)-Au(37)#1   | 91.0  |
| Au(38)-Au(39)-Au(37)     | 63.2  |
| Au(38)-Au(39)-Au(39)#1   | 123.9 |
| Au(38)-Au(39)-Au(40)     | 60.1  |
| Au(38)-Au(39)-Au(45)#1   | 115.7 |
| Au(38)-Au(39)-Au(47)     | 114.6 |
| Au(38)-Au(39)-Au(53)     | 88.9  |
| Au(39)#1-Au(39)-Au(37)   | 60.7  |
| Au(39)#1-Au(39)-Au(37)#1 | 60.7  |
| Au(39)#1-Au(39)-Au(40)   | 88.3  |
| Au(39)#1-Au(39)-Au(45)#1 | 87.5  |
| Au(39)#1-Au(39)-Au(47)   | 121.4 |
| Au(39)#1-Au(39)-Au(53)   | 118.3 |
| Au(40)-Au(39)-Au(37)#1   | 115.9 |
| Au(40)-Au(39)-Au(37)     | 56.2  |
| Au(40)-Au(39)-Au(45)#1   | 170.3 |
| Au(40)-Au(39)-Au(47)     | 126.3 |
| Au(40)-Au(39)-Au(53)     | 63.0  |
| Au(43)#1-Au(39)-Au(37)#1 | 63.1  |
| Au(43)#1-Au(39)-Au(37)   | 92.4  |
| Au(43)#1-Au(39)-Au(38)   | 58.0  |
| Au(43)#1-Au(39)-Au(39)#1 | 123.8 |
| Au(43)#1-Au(39)-Au(40)   | 118.0 |
| Au(43)#1-Au(39)-Au(45)#1 | 58.1  |
| Au(43)#1-Au(39)-Au(47)   | 83.5  |

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|--------------------------|-------|
| Au(43)#1-Au(39)-Au(53)   | 117.9 |
| Au(45)#1-Au(39)-Au(47)   | 63.2  |
| Au(45)#1-Au(39)-Au(53)   | 126.6 |
| Au(46)#1-Au(39)-Au(37)   | 89.4  |
| Au(46)-Au(39)-Au(37)     | 119.0 |
| Au(46)-Au(39)-Au(37)#1   | 89.5  |
| Au(46)#1-Au(39)-Au(37)#1 | 118.9 |
| Au(46)#1-Au(39)-Au(38)   | 122.1 |
| Au(46)-Au(39)-Au(38)     | 177.7 |
| Au(46)-Au(39)-Au(39)#1   | 58.3  |
| Au(46)#1-Au(39)-Au(39)#1 | 58.2  |
| Au(46)#1-Au(39)-Au(40)   | 62.2  |
| Au(46)-Au(39)-Au(40)     | 121.6 |
| Au(46)-Au(39)-Au(43)#1   | 120.4 |
| Au(46)#1-Au(39)-Au(43)#1 | 177.8 |
| Au(46)#1-Au(39)-Au(45)#1 | 122.1 |
| Au(46)-Au(39)-Au(45)#1   | 62.9  |
| Au(46)-Au(39)-Au(46)#1   | 59.5  |
| Au(46)-Au(39)-Au(47)     | 63.2  |
| Au(46)#1-Au(39)-Au(47)   | 94.7  |
| Au(46)-Au(39)-Au(53)     | 90.6  |
| Au(46)#1-Au(39)-Au(53)   | 60.1  |
| Au(47)-Au(39)-Au(53)     | 63.5  |
| Au(48)-Au(39)-Au(37)#1   | 123.7 |
| Au(48)-Au(39)-Au(37)     | 121.8 |
| Au(48)-Au(39)-Au(38)     | 58.8  |
| Au(48)-Au(39)-Au(39)#1   | 175.4 |
| Au(48)-Au(39)-Au(40)     | 90.2  |
| Au(48)-Au(39)-Au(43)#1   | 60.6  |
| Au(48)-Au(39)-Au(45)#1   | 94.6  |
| Au(48)-Au(39)-Au(46)     | 119.2 |
| Au(48)-Au(39)-Au(46)#1   | 117.4 |
| Au(48)-Au(39)-Au(47)     | 56.4  |
| Au(48)-Au(39)-Au(53)     | 57.3  |
| Au(37)-Au(40)-Au(38)     | 64.6  |
| Au(37)-Au(40)-Au(39)     | 62.4  |
| Au(37)-Au(40)-Au(46)#1   | 89.3  |



|                        |       |
|------------------------|-------|
| Au(37)-Au(40)-Au(53)   | 126.6 |
| Au(38)-Au(40)-Au(39)   | 57.7  |
| Au(38)-Au(40)-Au(46)#1 | 113.4 |
| Au(38)-Au(40)-Au(53)   | 88.4  |
| Au(39)-Au(40)-Au(46)#1 | 55.9  |
| Au(39)-Au(40)-Au(53)   | 64.3  |
| Au(45)-Au(40)-Au(37)   | 61.4  |
| Au(45)-Au(40)-Au(38)   | 126.0 |
| Au(45)-Au(40)-Au(39)   | 95.6  |
| Au(45)-Au(40)-Au(46)#1 | 66.2  |
| Au(45)-Au(40)-Au(53)   | 123.7 |
| Au(45)-Au(40)-Au(54)   | 62.3  |
| Au(46)#1-Au(40)-Au(53) | 59.0  |
| Au(54)-Au(40)-Au(37)   | 59.9  |
| Au(54)-Au(40)-Au(38)   | 91.3  |
| Au(54)-Au(40)-Au(39)   | 121.9 |
| Au(54)-Au(40)-Au(46)#1 | 127.9 |
| Au(54)-Au(40)-Au(53)   | 172.1 |
| S(28)-Au(40)-Au(37)    | 165.1 |
| S(28)-Au(40)-Au(38)    | 101.3 |
| S(28)-Au(40)-Au(39)    | 106.8 |
| S(28)-Au(40)-Au(45)    | 132.4 |
| S(28)-Au(40)-Au(46)#1  | 92.4  |
| S(28)-Au(40)-Au(53)    | 44.2  |
| S(28)-Au(40)-Au(54)    | 128.3 |
| Au(37)-Au(41)-Au(38)   | 54.5  |
| Au(37)-Au(41)-Au(42)   | 58.5  |
| Au(42)-Au(41)-Au(38)   | 113.0 |
| Au(44)#1-Au(41)-Au(37) | 51.9  |
| Au(44)#1-Au(41)-Au(38) | 55.2  |
| Au(44)#1-Au(41)-Au(42) | 83.7  |
| Au(54)-Au(41)-Au(37)   | 52.9  |
| Au(54)-Au(41)-Au(38)   | 80.0  |
| Au(54)-Au(41)-Au(42)   | 60.7  |
| Au(54)-Au(41)-Au(44)#1 | 104.7 |
| S(29)-Au(41)-Au(37)    | 91.0  |
| S(29)-Au(41)-Au(38)    | 44.6  |

|                          |       |
|--------------------------|-------|
| S(29)-Au(41)-Au(42)      | 140.5 |
| S(29)-Au(41)-Au(44)#1    | 97.0  |
| S(29)-Au(41)-Au(54)      | 81.3  |
| S(29)-Au(41)-S(31)       | 170.0 |
| S(31)-Au(41)-Au(37)      | 97.8  |
| S(31)-Au(41)-Au(38)      | 145.4 |
| S(31)-Au(41)-Au(42)      | 44.6  |
| S(31)-Au(41)-Au(44)#1    | 92.2  |
| S(31)-Au(41)-Au(54)      | 100.2 |
| Au(37)-Au(42)-Au(41)     | 60.2  |
| Au(37)-Au(42)-Au(43)     | 54.8  |
| Au(41)-Au(42)-Au(43)     | 114.9 |
| Au(44)-Au(42)-Au(37)     | 52.9  |
| Au(44)-Au(42)-Au(41)     | 85.9  |
| Au(44)-Au(42)-Au(43)     | 57.1  |
| Au(44)-Au(42)-Au(54)     | 104.0 |
| Au(54)-Au(42)-Au(37)     | 51.4  |
| Au(54)-Au(42)-Au(41)     | 52.8  |
| Au(54)-Au(42)-Au(43)     | 84.2  |
| S(31)-Au(42)-Au(37)      | 99.5  |
| S(31)-Au(42)-Au(41)      | 44.7  |
| S(31)-Au(42)-Au(43)      | 148.5 |
| S(31)-Au(42)-Au(44)      | 93.7  |
| S(31)-Au(42)-Au(54)      | 93.0  |
| S(31)-Au(42)-S(32)       | 163.0 |
| S(32)-Au(42)-Au(37)      | 97.4  |
| S(32)-Au(42)-Au(41)      | 150.8 |
| S(32)-Au(42)-Au(43)      | 45.8  |
| S(32)-Au(42)-Au(44)      | 94.9  |
| S(32)-Au(42)-Au(54)      | 99.2  |
| Au(37)-Au(43)-Au(42)     | 60.5  |
| Au(37)-Au(43)-Au(44)     | 54.3  |
| Au(38)#1-Au(43)-Au(37)   | 92.2  |
| Au(38)#1-Au(43)-Au(39)#1 | 61.7  |
| Au(38)#1-Au(43)-Au(42)   | 116.6 |
| Au(38)#1-Au(43)-Au(44)   | 62.2  |
| Au(38)#1-Au(43)-Au(45)   | 128.5 |

|                          |       |
|--------------------------|-------|
| Au(38)#1-Au(43)-Au(48)#1 | 59.5  |
| Au(39)#1-Au(43)-Au(37)   | 61.6  |
| Au(39)#1-Au(43)-Au(42)   | 121.9 |
| Au(39)#1-Au(43)-Au(44)   | 87.3  |
| Au(39)#1-Au(43)-Au(45)   | 67.1  |
| Au(39)#1-Au(43)-Au(48)#1 | 59.2  |
| Au(44)-Au(43)-Au(42)     | 55.4  |
| Au(45)-Au(43)-Au(37)     | 56.6  |
| Au(45)-Au(43)-Au(42)     | 84.8  |
| Au(45)-Au(43)-Au(44)     | 110.4 |
| Au(48)#1-Au(43)-Au(37)   | 120.8 |
| Au(48)#1-Au(43)-Au(42)   | 175.5 |
| Au(48)#1-Au(43)-Au(44)   | 121.2 |
| Au(48)#1-Au(43)-Au(45)   | 99.5  |
| S(32)-Au(43)-Au(37)      | 101.5 |
| S(32)-Au(43)-Au(38)#1    | 135.3 |
| S(32)-Au(43)-Au(39)#1    | 159.0 |
| S(32)-Au(43)-Au(42)      | 44.4  |
| S(32)-Au(43)-Au(44)      | 92.1  |
| S(32)-Au(43)-Au(45)      | 93.6  |
| S(32)-Au(43)-Au(48)#1    | 136.0 |
| Au(37)-Au(44)-Au(37)#1   | 64.7  |
| Au(37)-Au(44)-Au(38)#1   | 92.0  |
| Au(37)#1-Au(44)-Au(38)#1 | 63.6  |
| Au(37)#1-Au(44)-Au(41)#1 | 68.1  |
| Au(37)-Au(44)-Au(41)#1   | 132.7 |
| Au(37)#1-Au(44)-Au(42)   | 132.6 |
| Au(37)-Au(44)-Au(42)     | 68.0  |
| Au(37)#1-Au(44)-Au(43)   | 91.3  |
| Au(37)-Au(44)-Au(43)     | 62.5  |
| Au(38)#1-Au(44)-Au(41)#1 | 67.6  |
| Au(38)#1-Au(44)-Au(43)   | 53.6  |
| Au(42)-Au(44)-Au(38)#1   | 120.0 |
| Au(42)-Au(44)-Au(41)#1   | 159.2 |
| Au(42)-Au(44)-Au(43)     | 67.5  |
| Au(43)-Au(44)-Au(41)#1   | 120.6 |
| Au(44)#1-Au(44)-Au(37)   | 60.3  |

|                          |       |
|--------------------------|-------|
| Au(44)#1-Au(44)-Au(37)#1 | 59.9  |
| Au(44)#1-Au(44)-Au(38)#1 | 123.3 |
| Au(44)#1-Au(44)-Au(41)#1 | 94.9  |
| Au(44)#1-Au(44)-Au(42)   | 95.5  |
| Au(44)#1-Au(44)-Au(43)   | 122.5 |
| S(36)-Au(44)-Au(37)      | 150.4 |
| S(36)-Au(44)-Au(37)#1    | 140.2 |
| S(36)-Au(44)-Au(38)#1    | 89.8  |
| S(36)-Au(44)-Au(41)#1    | 74.7  |
| S(36)-Au(44)-Au(42)      | 85.6  |
| S(36)-Au(44)-Au(43)      | 95.8  |
| S(36)-Au(44)-Au(44)#1    | 139.0 |
| Au(37)-Au(45)-Au(39)#1   | 59.8  |
| Au(37)-Au(45)-Au(43)     | 64.0  |
| Au(37)-Au(45)-Au(46)#1   | 86.4  |
| Au(37)-Au(45)-Au(47)#1   | 119.5 |
| Au(37)-Au(45)-Au(54)     | 58.9  |
| Au(39)#1-Au(45)-Au(47)#1 | 59.8  |
| Au(40)-Au(45)-Au(37)     | 61.0  |
| Au(40)-Au(45)-Au(39)#1   | 88.6  |
| Au(40)-Au(45)-Au(43)     | 124.1 |
| Au(40)-Au(45)-Au(46)#1   | 61.0  |
| Au(40)-Au(45)-Au(47)#1   | 119.5 |
| Au(40)-Au(45)-Au(54)     | 59.5  |
| Au(43)-Au(45)-Au(39)#1   | 54.8  |
| Au(43)-Au(45)-Au(46)#1   | 107.0 |
| Au(43)-Au(45)-Au(47)#1   | 80.0  |
| Au(46)#1-Au(45)-Au(39)#1 | 52.7  |
| Au(46)#1-Au(45)-Au(47)#1 | 58.8  |
| Au(54)-Au(45)-Au(39)#1   | 118.6 |
| Au(54)-Au(45)-Au(43)     | 99.5  |
| Au(54)-Au(45)-Au(46)#1   | 120.0 |
| Au(54)-Au(45)-Au(47)#1   | 178.3 |
| S(35)-Au(45)-Au(37)      | 144.0 |
| S(35)-Au(45)-Au(39)#1    | 96.1  |
| S(35)-Au(45)-Au(40)      | 151.2 |
| S(35)-Au(45)-Au(43)      | 80.4  |

|                          |       |
|--------------------------|-------|
| S(35)-Au(45)-Au(46)#1    | 99.9  |
| S(35)-Au(45)-Au(47)#1    | 43.9  |
| S(35)-Au(45)-Au(54)      | 137.6 |
| Au(39)-Au(46)-Au(39)#1   | 63.5  |
| Au(39)#1-Au(46)-Au(40)#1 | 61.9  |
| Au(39)-Au(46)-Au(40)#1   | 91.0  |
| Au(39)#1-Au(46)-Au(45)#1 | 90.9  |
| Au(39)-Au(46)-Au(45)#1   | 64.4  |
| Au(39)#1-Au(46)-Au(47)   | 129.0 |
| Au(39)-Au(46)-Au(47)     | 65.6  |
| Au(39)-Au(46)-Au(53)#1   | 132.7 |
| Au(39)#1-Au(46)-Au(53)#1 | 69.1  |
| Au(40)#1-Au(46)-Au(45)#1 | 52.8  |
| Au(40)#1-Au(46)-Au(47)   | 116.9 |
| Au(40)#1-Au(46)-Au(53)#1 | 66.0  |
| Au(45)#1-Au(46)-Au(47)   | 64.4  |
| Au(45)#1-Au(46)-Au(53)#1 | 117.6 |
| Au(46)#1-Au(46)-Au(39)#1 | 60.2  |
| Au(46)#1-Au(46)-Au(39)   | 60.3  |
| Au(46)#1-Au(46)-Au(40)#1 | 122.0 |
| Au(46)#1-Au(46)-Au(45)#1 | 124.5 |
| Au(46)#1-Au(46)-Au(47)   | 96.6  |
| Au(46)#1-Au(46)-Au(53)#1 | 96.3  |
| Au(53)#1-Au(46)-Au(47)   | 161.5 |
| S(25)-Au(46)-Au(39)      | 137.3 |
| S(25)-Au(46)-Au(39)#1    | 157.5 |
| S(25)-Au(46)-Au(40)#1    | 103.7 |
| S(25)-Au(46)-Au(45)#1    | 92.9  |
| S(25)-Au(46)-Au(46)#1    | 132.3 |
| S(25)-Au(46)-Au(47)      | 72.1  |
| S(25)-Au(46)-Au(53)#1    | 89.5  |
| Au(39)-Au(47)-Au(45)#1   | 57.1  |
| Au(46)-Au(47)-Au(39)     | 51.2  |
| Au(46)-Au(47)-Au(45)#1   | 56.8  |
| Au(48)-Au(47)-Au(39)     | 53.3  |
| Au(48)-Au(47)-Au(45)#1   | 88.5  |
| Au(48)-Au(47)-Au(46)     | 104.2 |

|                         |       |
|-------------------------|-------|
| S(26)-Au(47)-Au(39)     | 93.8  |
| S(26)-Au(47)-Au(45)#1   | 140.9 |
| S(26)-Au(47)-Au(46)     | 85.1  |
| S(26)-Au(47)-Au(48)     | 93.6  |
| S(35)#1-Au(47)-Au(39)   | 95.4  |
| S(35)#1-Au(47)-Au(45)#1 | 46.0  |
| S(35)#1-Au(47)-Au(46)   | 99.9  |
| S(35)#1-Au(47)-Au(48)   | 92.9  |
| S(35)#1-Au(47)-S(26)    | 170.7 |
| Au(38)-Au(48)-Au(39)    | 61.8  |
| Au(38)-Au(48)-Au(43)#1  | 58.8  |
| Au(38)-Au(48)-Au(47)    | 131.2 |
| Au(38)-Au(48)-Au(51)    | 88.0  |
| Au(38)-Au(48)-Au(53)    | 98.8  |
| Au(39)-Au(48)-Au(43)#1  | 60.2  |
| Au(39)-Au(48)-Au(47)    | 70.2  |
| Au(39)-Au(48)-Au(51)    | 143.3 |
| Au(39)-Au(48)-Au(53)    | 71.4  |
| Au(43)#1-Au(48)-Au(47)  | 90.5  |
| Au(43)#1-Au(48)-Au(51)  | 87.0  |
| Au(43)#1-Au(48)-Au(53)  | 131.6 |
| Au(47)-Au(48)-Au(51)    | 130.6 |
| Au(47)-Au(48)-Au(53)    | 72.8  |
| Au(53)-Au(48)-Au(51)    | 138.2 |
| S(27)-Au(48)-Au(38)     | 126.7 |
| S(27)-Au(48)-Au(39)     | 168.7 |
| S(27)-Au(48)-Au(43)#1   | 129.5 |
| S(27)-Au(48)-Au(47)     | 102.0 |
| S(27)-Au(48)-Au(51)     | 48.0  |
| S(27)-Au(48)-Au(53)     | 98.8  |
| S(36)-Au(49)-S(34)      | 165.2 |
| S(25)-Au(50)-S(30)#1    | 168.1 |
| S(27)-Au(51)-Au(48)     | 52.2  |
| S(27)-Au(51)-S(34)#1    | 170.3 |
| S(34)#1-Au(51)-Au(48)   | 134.5 |
| S(30)-Au(52)-Au(54)     | 135.3 |
| S(33)-Au(52)-Au(54)     | 49.5  |

|                        |       |
|------------------------|-------|
| S(33)-Au(52)-S(30)     | 172.5 |
| Au(40)-Au(53)-Au(39)   | 52.7  |
| Au(46)#1-Au(53)-Au(39) | 50.8  |
| Au(46)#1-Au(53)-Au(40) | 54.9  |
| Au(48)-Au(53)-Au(39)   | 51.4  |
| Au(48)-Au(53)-Au(40)   | 80.1  |
| Au(48)-Au(53)-Au(46)#1 | 102.1 |
| S(26)-Au(53)-Au(39)    | 91.1  |
| S(26)-Au(53)-Au(40)    | 139.5 |
| S(26)-Au(53)-Au(46)#1  | 89.3  |
| S(26)-Au(53)-Au(48)    | 91.0  |
| S(28)-Au(53)-Au(39)    | 97.1  |
| S(28)-Au(53)-Au(40)    | 45.9  |
| S(28)-Au(53)-Au(46)#1  | 90.2  |
| S(28)-Au(53)-Au(48)    | 99.9  |
| S(28)-Au(53)-S(26)     | 169.0 |
| Au(37)-Au(54)-Au(41)   | 71.0  |
| Au(37)-Au(54)-Au(42)   | 65.6  |
| Au(37)-Au(54)-Au(45)   | 60.5  |
| Au(37)-Au(54)-Au(52)   | 138.7 |
| Au(40)-Au(54)-Au(37)   | 61.2  |
| Au(40)-Au(54)-Au(41)   | 101.2 |
| Au(40)-Au(54)-Au(42)   | 126.3 |
| Au(40)-Au(54)-Au(45)   | 58.3  |
| Au(40)-Au(54)-Au(52)   | 80.4  |
| Au(41)-Au(54)-Au(42)   | 66.6  |
| Au(41)-Au(54)-Au(52)   | 135.8 |
| Au(42)-Au(54)-Au(52)   | 145.4 |
| Au(45)-Au(54)-Au(41)   | 131.4 |
| Au(45)-Au(54)-Au(42)   | 90.0  |
| Au(45)-Au(54)-Au(52)   | 87.4  |
| S(33)-Au(54)-Au(37)    | 173.3 |
| S(33)-Au(54)-Au(40)    | 120.3 |
| S(33)-Au(54)-Au(41)    | 102.4 |
| S(33)-Au(54)-Au(42)    | 113.4 |
| S(33)-Au(54)-Au(45)    | 126.2 |
| S(33)-Au(54)-Au(52)    | 45.8  |

|                       |       |
|-----------------------|-------|
| Au(50)-S(25)-Au(46)   | 101.3 |
| C(241)-S(25)-Au(46)   | 110.0 |
| C(241)-S(25)-Au(50)   | 104.9 |
| Au(53)-S(26)-Au(47)   | 96.9  |
| C(251)-S(26)-Au(47)   | 103.5 |
| C(251)-S(26)-Au(53)   | 107.0 |
| Au(51)-S(27)-Au(48)   | 79.8  |
| C(261)-S(27)-Au(48)   | 103.3 |
| C(261)-S(27)-Au(51)   | 98.9  |
| Au(53)-S(28)-Au(40)   | 89.8  |
| C(271)-S(28)-Au(40)   | 112.0 |
| C(271)-S(28)-Au(53)   | 111.1 |
| Au(41)-S(29)-Au(38)   | 91.7  |
| C(281)-S(29)-Au(38)   | 111.3 |
| C(281)-S(29)-Au(41)   | 100.5 |
| Au(52)-S(30)-Au(50)#1 | 98.1  |
| C(291)-S(30)-Au(50)#1 | 97.9  |
| C(291)-S(30)-Au(52)   | 109.8 |
| C(291)-S(30)-Ag(50)#1 | 97.9  |
| Au(42)-S(31)-Au(41)   | 90.8  |
| C(301)-S(31)-Au(41)   | 99.8  |
| C(301)-S(31)-Au(42)   | 105.2 |
| Au(42)-S(32)-Au(43)   | 89.8  |
| C(311)-S(32)-Au(42)   | 107.1 |
| C(311)-S(32)-Au(43)   | 116.2 |
| Au(52)-S(33)-Au(54)   | 84.8  |
| C(321)-S(33)-Au(52)   | 107.2 |
| C(321)-S(33)-Au(54)   | 116.7 |
| Au(51)#1-S(34)-Au(49) | 99.6  |
| C(331)-S(34)-Au(49)   | 114.5 |
| C(331)-S(34)-Au(51)#1 | 99.6  |
| C(331)-S(34)-Ag(51)#1 | 99.6  |
| Au(47)#1-S(35)-Au(45) | 90.0  |
| C(341)-S(35)-Au(45)   | 112.4 |
| C(341)-S(35)-Au(47)#1 | 103.0 |
| Au(49)-S(36)-Au(44)   | 108.8 |
| C(351)-S(36)-Au(44)   | 108.5 |



|                      |       |
|----------------------|-------|
| C(351)-S(36)-Au(49)  | 114.4 |
| C(242)-C(241)-S(25)  | 123.9 |
| C(246)-C(241)-S(25)  | 114.2 |
| C(246)-C(241)-C(242) | 121.9 |
| C(241)-C(242)-H(242) | 120.4 |
| C(243)-C(242)-C(241) | 119.3 |
| C(243)-C(242)-H(242) | 120.4 |
| C(242)-C(243)-H(243) | 118.8 |
| C(244)-C(243)-C(242) | 122.4 |
| C(244)-C(243)-H(243) | 118.8 |
| C(243)-C(244)-C(245) | 117.5 |
| C(243)-C(244)-C(247) | 121.9 |
| C(245)-C(244)-C(247) | 120.3 |
| C(244)-C(245)-H(245) | 120.0 |
| C(244)-C(245)-C(246) | 120.1 |
| C(246)-C(245)-H(245) | 120.0 |
| C(241)-C(246)-C(245) | 118.6 |
| C(241)-C(246)-H(246) | 120.7 |
| C(245)-C(246)-H(246) | 120.7 |
| C(244)-C(247)-C(248) | 110.7 |
| C(244)-C(247)-C(249) | 115.4 |
| C(244)-C(247)-C(250) | 108.1 |
| C(248)-C(247)-C(249) | 109.3 |
| C(248)-C(247)-C(250) | 106.8 |
| C(249)-C(247)-C(250) | 106.0 |
| C(247)-C(248)-H(24D) | 109.5 |
| C(247)-C(248)-H(24E) | 109.5 |
| C(247)-C(248)-H(24F) | 109.5 |
| H(24D)-C(248)-H(24E) | 109.5 |
| H(24D)-C(248)-H(24F) | 109.5 |
| H(24E)-C(248)-H(24F) | 109.5 |
| C(247)-C(249)-H(24G) | 109.5 |
| C(247)-C(249)-H(24H) | 109.5 |
| C(247)-C(249)-H(24I) | 109.5 |
| H(24G)-C(249)-H(24H) | 109.5 |
| H(24G)-C(249)-H(24I) | 109.5 |
| H(24H)-C(249)-H(24I) | 109.5 |

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| C(247)-C(250)-H(25A) | 109.5 |
| C(247)-C(250)-H(25B) | 109.5 |
| C(247)-C(250)-H(25C) | 109.5 |
| H(25A)-C(250)-H(25B) | 109.5 |
| H(25A)-C(250)-H(25C) | 109.5 |
| H(25B)-C(250)-H(25C) | 109.5 |
| C(252)-C(251)-S(26)  | 125.6 |
| C(252)-C(251)-C(256) | 117.5 |
| C(256)-C(251)-S(26)  | 116.5 |
| C(251)-C(252)-H(252) | 117.4 |
| C(253)-C(252)-C(251) | 125.2 |
| C(253)-C(252)-H(252) | 117.4 |
| C(252)-C(253)-H(253) | 118.7 |
| C(252)-C(253)-C(254) | 122.7 |
| C(254)-C(253)-H(253) | 118.7 |
| C(253)-C(254)-C(255) | 114.2 |
| C(253)-C(254)-C(257) | 119.8 |
| C(255)-C(254)-C(257) | 126.0 |
| C(254)-C(255)-H(255) | 120.7 |
| C(256)-C(255)-C(254) | 118.6 |
| C(256)-C(255)-H(255) | 120.7 |
| C(251)-C(256)-C(255) | 121.2 |
| C(251)-C(256)-H(256) | 119.4 |
| C(255)-C(256)-H(256) | 119.4 |
| C(254)-C(257)-C(258) | 109.0 |
| C(254)-C(257)-C(259) | 97.5  |
| C(258)-C(257)-C(259) | 121.8 |
| C(260)-C(257)-C(254) | 110.4 |
| C(260)-C(257)-C(258) | 108.2 |
| C(260)-C(257)-C(259) | 109.3 |
| C(257)-C(258)-H(25D) | 109.5 |
| C(257)-C(258)-H(25E) | 109.5 |
| C(257)-C(258)-H(25F) | 109.5 |
| H(25D)-C(258)-H(25E) | 109.5 |
| H(25D)-C(258)-H(25F) | 109.5 |
| H(25E)-C(258)-H(25F) | 109.5 |
| C(257)-C(259)-H(25G) | 109.5 |

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| C(257)-C(259)-H(25H) | 109.5 |
| C(257)-C(259)-H(25I) | 109.5 |
| H(25G)-C(259)-H(25H) | 109.5 |
| H(25G)-C(259)-H(25I) | 109.5 |
| H(25H)-C(259)-H(25I) | 109.5 |
| C(257)-C(260)-H(26A) | 109.5 |
| C(257)-C(260)-H(26B) | 109.5 |
| C(257)-C(260)-H(26C) | 109.5 |
| H(26A)-C(260)-H(26B) | 109.5 |
| H(26A)-C(260)-H(26C) | 109.5 |
| H(26B)-C(260)-H(26C) | 109.5 |
| C(262)-C(261)-S(27)  | 114.8 |
| C(266)-C(261)-S(27)  | 128.2 |
| C(266)-C(261)-C(262) | 116.8 |
| C(261)-C(262)-H(262) | 122.1 |
| C(263)-C(262)-C(261) | 115.7 |
| C(263)-C(262)-H(262) | 122.1 |
| C(262)-C(263)-H(263) | 115.3 |
| C(264)-C(263)-C(262) | 129.5 |
| C(264)-C(263)-H(263) | 115.3 |
| C(263)-C(264)-C(265) | 110.5 |
| C(263)-C(264)-C(267) | 123.7 |
| C(265)-C(264)-C(267) | 125.9 |
| C(264)-C(265)-H(265) | 118.1 |
| C(264)-C(265)-C(266) | 123.9 |
| C(266)-C(265)-H(265) | 118.1 |
| C(261)-C(266)-C(265) | 122.6 |
| C(261)-C(266)-H(266) | 118.7 |
| C(265)-C(266)-H(266) | 118.7 |
| C(264)-C(267)-C(268) | 107.5 |
| C(264)-C(267)-C(270) | 108.7 |
| C(269)-C(267)-C(264) | 105.9 |
| C(269)-C(267)-C(268) | 111.8 |
| C(269)-C(267)-C(270) | 104.6 |
| C(270)-C(267)-C(268) | 117.7 |
| C(267)-C(268)-H(26D) | 109.5 |
| C(267)-C(268)-H(26E) | 109.5 |

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| C(267)-C(268)-H(26F) | 109.5 |
| H(26D)-C(268)-H(26E) | 109.5 |
| H(26D)-C(268)-H(26F) | 109.5 |
| H(26E)-C(268)-H(26F) | 109.5 |
| C(267)-C(269)-H(26G) | 109.5 |
| C(267)-C(269)-H(26H) | 109.5 |
| C(267)-C(269)-H(26I) | 109.5 |
| H(26G)-C(269)-H(26H) | 109.5 |
| H(26G)-C(269)-H(26I) | 109.5 |
| H(26H)-C(269)-H(26I) | 109.5 |
| C(267)-C(270)-H(27A) | 109.5 |
| C(267)-C(270)-H(27B) | 109.5 |
| C(267)-C(270)-H(27C) | 109.5 |
| H(27A)-C(270)-H(27B) | 109.5 |
| H(27A)-C(270)-H(27C) | 109.5 |
| H(27B)-C(270)-H(27C) | 109.5 |
| C(272)-C(271)-S(28)  | 116.8 |
| C(276)-C(271)-S(28)  | 126.3 |
| C(276)-C(271)-C(272) | 116.3 |
| C(271)-C(272)-H(272) | 119.9 |
| C(273)-C(272)-C(271) | 120.2 |
| C(273)-C(272)-H(272) | 119.9 |
| C(272)-C(273)-H(273) | 118.9 |
| C(272)-C(273)-C(274) | 122.1 |
| C(274)-C(273)-H(273) | 118.9 |
| C(273)-C(274)-C(275) | 117.5 |
| C(273)-C(274)-C(277) | 122.9 |
| C(275)-C(274)-C(277) | 119.7 |
| C(274)-C(275)-H(275) | 120.0 |
| C(276)-C(275)-C(274) | 120.0 |
| C(276)-C(275)-H(275) | 120.0 |
| C(271)-C(276)-H(276) | 118.3 |
| C(275)-C(276)-C(271) | 123.4 |
| C(275)-C(276)-H(276) | 118.3 |
| C(274)-C(277)-C(278) | 103.8 |
| C(274)-C(277)-C(279) | 111.1 |
| C(278)-C(277)-C(279) | 109.6 |

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| C(280)-C(277)-C(274) | 115.8 |
| C(280)-C(277)-C(278) | 109.5 |
| C(280)-C(277)-C(279) | 107.1 |
| C(277)-C(278)-H(27D) | 109.5 |
| C(277)-C(278)-H(27E) | 109.5 |
| C(277)-C(278)-H(27F) | 109.5 |
| H(27D)-C(278)-H(27E) | 109.5 |
| H(27D)-C(278)-H(27F) | 109.5 |
| H(27E)-C(278)-H(27F) | 109.5 |
| C(277)-C(279)-H(27G) | 109.5 |
| C(277)-C(279)-H(27H) | 109.5 |
| C(277)-C(279)-H(27I) | 109.5 |
| H(27G)-C(279)-H(27H) | 109.5 |
| H(27G)-C(279)-H(27I) | 109.5 |
| H(27H)-C(279)-H(27I) | 109.5 |
| C(277)-C(280)-H(28D) | 109.5 |
| C(277)-C(280)-H(28E) | 109.5 |
| C(277)-C(280)-H(28F) | 109.5 |
| H(28D)-C(280)-H(28E) | 109.5 |
| H(28D)-C(280)-H(28F) | 109.5 |
| H(28E)-C(280)-H(28F) | 109.5 |
| C(282)-C(281)-S(29)  | 127.9 |
| C(282)-C(281)-C(286) | 119.4 |
| C(286)-C(281)-S(29)  | 112.5 |
| C(281)-C(282)-H(282) | 119.3 |
| C(281)-C(282)-C(283) | 121.4 |
| C(283)-C(282)-H(282) | 119.3 |
| C(282)-C(283)-H(283) | 118.2 |
| C(282)-C(283)-C(284) | 123.6 |
| C(284)-C(283)-H(283) | 118.2 |
| C(283)-C(284)-C(287) | 122.9 |
| C(285)-C(284)-C(283) | 116.2 |
| C(285)-C(284)-C(287) | 120.5 |
| C(284)-C(285)-H(285) | 120.3 |
| C(284)-C(285)-C(286) | 119.3 |
| C(286)-C(285)-H(285) | 120.3 |
| C(281)-C(286)-C(285) | 119.9 |

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| C(281)-C(286)-H(286) | 120.1 |
| C(285)-C(286)-H(286) | 120.1 |
| C(284)-C(287)-C(289) | 105.0 |
| C(284)-C(287)-C(290) | 106.4 |
| C(288)-C(287)-C(284) | 113.2 |
| C(288)-C(287)-C(289) | 111.1 |
| C(288)-C(287)-C(290) | 112.9 |
| C(290)-C(287)-C(289) | 107.8 |
| C(287)-C(288)-H(28G) | 109.5 |
| C(287)-C(288)-H(28H) | 109.5 |
| C(287)-C(288)-H(28I) | 109.5 |
| H(28G)-C(288)-H(28H) | 109.5 |
| H(28G)-C(288)-H(28I) | 109.5 |
| H(28H)-C(288)-H(28I) | 109.5 |
| C(287)-C(289)-H(28J) | 109.5 |
| C(287)-C(289)-H(28K) | 109.5 |
| C(287)-C(289)-H(28L) | 109.5 |
| H(28J)-C(289)-H(28K) | 109.5 |
| H(28J)-C(289)-H(28L) | 109.5 |
| H(28K)-C(289)-H(28L) | 109.5 |
| C(287)-C(290)-H(29D) | 109.5 |
| C(287)-C(290)-H(29E) | 109.5 |
| C(287)-C(290)-H(29F) | 109.5 |
| H(29D)-C(290)-H(29E) | 109.5 |
| H(29D)-C(290)-H(29F) | 109.5 |
| H(29E)-C(290)-H(29F) | 109.5 |
| C(292)-C(291)-S(30)  | 121.7 |
| C(296)-C(291)-S(30)  | 117.6 |
| C(296)-C(291)-C(292) | 120.5 |
| C(291)-C(292)-H(292) | 119.8 |
| C(293)-C(292)-C(291) | 120.3 |
| C(293)-C(292)-H(292) | 119.8 |
| C(292)-C(293)-H(293) | 120.0 |
| C(292)-C(293)-C(294) | 120.1 |
| C(294)-C(293)-H(293) | 120.0 |
| C(293)-C(294)-C(297) | 121.5 |
| C(295)-C(294)-C(293) | 115.2 |

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| C(295)-C(294)-C(297) | 123.3 |
| C(294)-C(295)-H(295) | 116.7 |
| C(296)-C(295)-C(294) | 126.6 |
| C(296)-C(295)-H(295) | 116.7 |
| C(291)-C(296)-H(296) | 121.5 |
| C(295)-C(296)-C(291) | 116.9 |
| C(295)-C(296)-H(296) | 121.5 |
| C(294)-C(297)-C(299) | 111.6 |
| C(298)-C(297)-C(294) | 115.3 |
| C(298)-C(297)-C(299) | 96.6  |
| C(298)-C(297)-C(300) | 103.3 |
| C(300)-C(297)-C(294) | 117.4 |
| C(300)-C(297)-C(299) | 110.4 |
| C(297)-C(298)-H(29G) | 109.5 |
| C(297)-C(298)-H(29H) | 109.5 |
| C(297)-C(298)-H(29I) | 109.5 |
| H(29G)-C(298)-H(29H) | 109.5 |
| H(29G)-C(298)-H(29I) | 109.5 |
| H(29H)-C(298)-H(29I) | 109.5 |
| C(297)-C(299)-H(29J) | 109.5 |
| C(297)-C(299)-H(29K) | 109.5 |
| C(297)-C(299)-H(29L) | 109.5 |
| H(29J)-C(299)-H(29K) | 109.5 |
| H(29J)-C(299)-H(29L) | 109.5 |
| H(29K)-C(299)-H(29L) | 109.5 |
| C(297)-C(300)-H(30D) | 109.5 |
| C(297)-C(300)-H(30E) | 109.5 |
| C(297)-C(300)-H(30F) | 109.5 |
| H(30D)-C(300)-H(30E) | 109.5 |
| H(30D)-C(300)-H(30F) | 109.5 |
| H(30E)-C(300)-H(30F) | 109.5 |
| C(302)-C(301)-S(31)  | 119.1 |
| C(302)-C(301)-C(306) | 124.4 |
| C(306)-C(301)-S(31)  | 116.5 |
| C(301)-C(302)-H(302) | 119.8 |
| C(301)-C(302)-C(303) | 120.5 |
| C(303)-C(302)-H(302) | 119.8 |

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| C(302)-C(303)-H(303) | 119.6 |
| C(304)-C(303)-C(302) | 120.8 |
| C(304)-C(303)-H(303) | 119.6 |
| C(303)-C(304)-C(305) | 119.4 |
| C(303)-C(304)-C(307) | 123.8 |
| C(305)-C(304)-C(307) | 116.8 |
| C(304)-C(305)-H(305) | 119.9 |
| C(304)-C(305)-C(306) | 120.1 |
| C(306)-C(305)-H(305) | 119.9 |
| C(301)-C(306)-C(305) | 114.5 |
| C(301)-C(306)-H(306) | 122.7 |
| C(305)-C(306)-H(306) | 122.7 |
| C(304)-C(307)-C(309) | 110.2 |
| C(304)-C(307)-C(310) | 102.2 |
| C(308)-C(307)-C(304) | 113.2 |
| C(308)-C(307)-C(309) | 117.0 |
| C(308)-C(307)-C(310) | 104.6 |
| C(309)-C(307)-C(310) | 108.3 |
| C(307)-C(308)-H(30G) | 109.5 |
| C(307)-C(308)-H(30H) | 109.5 |
| C(307)-C(308)-H(30I) | 109.5 |
| H(30G)-C(308)-H(30H) | 109.5 |
| H(30G)-C(308)-H(30I) | 109.5 |
| H(30H)-C(308)-H(30I) | 109.5 |
| C(307)-C(309)-H(30J) | 109.5 |
| C(307)-C(309)-H(30K) | 109.5 |
| C(307)-C(309)-H(30L) | 109.5 |
| H(30J)-C(309)-H(30K) | 109.5 |
| H(30J)-C(309)-H(30L) | 109.5 |
| H(30K)-C(309)-H(30L) | 109.5 |
| C(307)-C(310)-H(31A) | 109.5 |
| C(307)-C(310)-H(31B) | 109.5 |
| C(307)-C(310)-H(31C) | 109.5 |
| H(31A)-C(310)-H(31B) | 109.5 |
| H(31A)-C(310)-H(31C) | 109.5 |
| H(31B)-C(310)-H(31C) | 109.5 |
| C(312)-C(311)-S(32)  | 117.2 |



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| C(316)-C(311)-S(32)  | 122.1 |
| C(316)-C(311)-C(312) | 120.8 |
| C(311)-C(312)-H(312) | 121.2 |
| C(313)-C(312)-C(311) | 117.7 |
| C(313)-C(312)-H(312) | 121.2 |
| C(312)-C(313)-H(313) | 118.4 |
| C(312)-C(313)-C(314) | 123.3 |
| C(314)-C(313)-H(313) | 118.4 |
| C(313)-C(314)-C(317) | 118.6 |
| C(315)-C(314)-C(313) | 116.1 |
| C(315)-C(314)-C(317) | 124.5 |
| C(314)-C(315)-H(315) | 119.8 |
| C(314)-C(315)-C(316) | 120.3 |
| C(316)-C(315)-H(315) | 119.8 |
| C(311)-C(316)-C(315) | 120.9 |
| C(311)-C(316)-H(316) | 119.6 |
| C(315)-C(316)-H(316) | 119.6 |
| C(314)-C(317)-C(320) | 107.6 |
| C(318)-C(317)-C(314) | 114.5 |
| C(318)-C(317)-C(319) | 112.1 |
| C(318)-C(317)-C(320) | 112.1 |
| C(319)-C(317)-C(314) | 102.1 |
| C(319)-C(317)-C(320) | 107.7 |
| C(317)-C(318)-H(31D) | 109.5 |
| C(317)-C(318)-H(31E) | 109.5 |
| C(317)-C(318)-H(31F) | 109.5 |
| H(31D)-C(318)-H(31E) | 109.5 |
| H(31D)-C(318)-H(31F) | 109.5 |
| H(31E)-C(318)-H(31F) | 109.5 |
| C(317)-C(319)-H(31G) | 109.5 |
| C(317)-C(319)-H(31H) | 109.5 |
| C(317)-C(319)-H(31I) | 109.5 |
| H(31G)-C(319)-H(31H) | 109.5 |
| H(31G)-C(319)-H(31I) | 109.5 |
| H(31H)-C(319)-H(31I) | 109.5 |
| C(317)-C(320)-H(32A) | 109.5 |
| C(317)-C(320)-H(32B) | 109.5 |

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| C(317)-C(320)-H(32C) | 109.5 |
| H(32A)-C(320)-H(32B) | 109.5 |
| H(32A)-C(320)-H(32C) | 109.5 |
| H(32B)-C(320)-H(32C) | 109.5 |
| C(322)-C(321)-S(33)  | 119.9 |
| C(322)-C(321)-C(326) | 116.1 |
| C(326)-C(321)-S(33)  | 123.8 |
| C(321)-C(322)-H(322) | 118.4 |
| C(323)-C(322)-C(321) | 123.1 |
| C(323)-C(322)-H(322) | 118.4 |
| C(322)-C(323)-H(323) | 120.7 |
| C(324)-C(323)-C(322) | 118.6 |
| C(324)-C(323)-H(323) | 120.7 |
| C(323)-C(324)-C(325) | 122.9 |
| C(323)-C(324)-C(327) | 120.2 |
| C(325)-C(324)-C(327) | 116.9 |
| C(324)-C(325)-H(325) | 122.7 |
| C(326)-C(325)-C(324) | 114.6 |
| C(326)-C(325)-H(325) | 122.7 |
| C(321)-C(326)-H(326) | 117.9 |
| C(325)-C(326)-C(321) | 124.2 |
| C(325)-C(326)-H(326) | 117.9 |
| C(324)-C(327)-C(328) | 106.1 |
| C(324)-C(327)-C(330) | 110.6 |
| C(329)-C(327)-C(324) | 111.8 |
| C(329)-C(327)-C(328) | 109.7 |
| C(329)-C(327)-C(330) | 113.5 |
| C(330)-C(327)-C(328) | 104.5 |
| C(327)-C(328)-H(32D) | 109.5 |
| C(327)-C(328)-H(32E) | 109.5 |
| C(327)-C(328)-H(32F) | 109.5 |
| H(32D)-C(328)-H(32E) | 109.5 |
| H(32D)-C(328)-H(32F) | 109.5 |
| H(32E)-C(328)-H(32F) | 109.5 |
| C(327)-C(329)-H(32G) | 109.5 |
| C(327)-C(329)-H(32H) | 109.5 |
| C(327)-C(329)-H(32I) | 109.5 |

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| H(32G)-C(329)-H(32H) | 109.5 |
| H(32G)-C(329)-H(32I) | 109.5 |
| H(32H)-C(329)-H(32I) | 109.5 |
| C(327)-C(330)-H(33A) | 109.5 |
| C(327)-C(330)-H(33B) | 109.5 |
| C(327)-C(330)-H(33C) | 109.5 |
| H(33A)-C(330)-H(33B) | 109.5 |
| H(33A)-C(330)-H(33C) | 109.5 |
| H(33B)-C(330)-H(33C) | 109.5 |
| C(332)-C(331)-S(34)  | 117.0 |
| C(332)-C(331)-C(336) | 121.4 |
| C(336)-C(331)-S(34)  | 121.3 |
| C(331)-C(332)-H(332) | 120.1 |
| C(331)-C(332)-C(333) | 119.8 |
| C(333)-C(332)-H(332) | 120.1 |
| C(332)-C(333)-H(333) | 119.8 |
| C(334)-C(333)-C(332) | 120.3 |
| C(334)-C(333)-H(333) | 119.8 |
| C(333)-C(334)-C(335) | 120.2 |
| C(333)-C(334)-C(337) | 121.9 |
| C(335)-C(334)-C(337) | 117.3 |
| C(334)-C(335)-H(335) | 120.7 |
| C(334)-C(335)-C(336) | 118.7 |
| C(336)-C(335)-H(335) | 120.7 |
| C(331)-C(336)-C(335) | 119.4 |
| C(331)-C(336)-H(336) | 120.3 |
| C(335)-C(336)-H(336) | 120.3 |
| C(334)-C(337)-C(338) | 109.8 |
| C(334)-C(337)-C(339) | 109.2 |
| C(334)-C(337)-C(340) | 111.2 |
| C(338)-C(337)-C(339) | 104.0 |
| C(338)-C(337)-C(340) | 112.5 |
| C(340)-C(337)-C(339) | 110.0 |
| C(337)-C(338)-H(33D) | 109.5 |
| C(337)-C(338)-H(33E) | 109.5 |
| C(337)-C(338)-H(33F) | 109.5 |
| H(33D)-C(338)-H(33E) | 109.5 |

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| H(33D)-C(338)-H(33F) | 109.5 |
| H(33E)-C(338)-H(33F) | 109.5 |
| C(337)-C(339)-H(33G) | 109.5 |
| C(337)-C(339)-H(33H) | 109.5 |
| C(337)-C(339)-H(33I) | 109.5 |
| H(33G)-C(339)-H(33H) | 109.5 |
| H(33G)-C(339)-H(33I) | 109.5 |
| H(33H)-C(339)-H(33I) | 109.5 |
| C(337)-C(340)-H(34A) | 109.5 |
| C(337)-C(340)-H(34B) | 109.5 |
| C(337)-C(340)-H(34C) | 109.5 |
| H(34A)-C(340)-H(34B) | 109.5 |
| H(34A)-C(340)-H(34C) | 109.5 |
| H(34B)-C(340)-H(34C) | 109.5 |
| C(342)-C(341)-S(35)  | 120.9 |
| C(346)-C(341)-S(35)  | 124.6 |
| C(346)-C(341)-C(342) | 114.6 |
| C(341)-C(342)-H(342) | 119.0 |
| C(343)-C(342)-C(341) | 122.0 |
| C(343)-C(342)-H(342) | 119.0 |
| C(342)-C(343)-H(343) | 120.5 |
| C(342)-C(343)-C(344) | 119.0 |
| C(344)-C(343)-H(343) | 120.5 |
| C(343)-C(344)-C(345) | 121.4 |
| C(343)-C(344)-C(347) | 119.0 |
| C(345)-C(344)-C(347) | 119.5 |
| C(344)-C(345)-H(345) | 121.2 |
| C(346)-C(345)-C(344) | 117.6 |
| C(346)-C(345)-H(345) | 121.2 |
| C(341)-C(346)-H(346) | 117.4 |
| C(345)-C(346)-C(341) | 125.1 |
| C(345)-C(346)-H(346) | 117.4 |
| C(344)-C(347)-C(349) | 108.5 |
| C(348)-C(347)-C(344) | 110.6 |
| C(348)-C(347)-C(349) | 108.2 |
| C(350)-C(347)-C(344) | 110.6 |
| C(350)-C(347)-C(348) | 125.5 |

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|----------------------|-------|
| C(350)-C(347)-C(349) | 90.8  |
| C(347)-C(348)-H(34D) | 109.5 |
| C(347)-C(348)-H(34E) | 109.5 |
| C(347)-C(348)-H(34F) | 109.5 |
| H(34D)-C(348)-H(34E) | 109.5 |
| H(34D)-C(348)-H(34F) | 109.5 |
| H(34E)-C(348)-H(34F) | 109.5 |
| C(347)-C(349)-H(34G) | 109.5 |
| C(347)-C(349)-H(34H) | 109.5 |
| C(347)-C(349)-H(34I) | 109.5 |
| H(34G)-C(349)-H(34H) | 109.5 |
| H(34G)-C(349)-H(34I) | 109.5 |
| H(34H)-C(349)-H(34I) | 109.5 |
| C(347)-C(350)-H(35A) | 109.5 |
| C(347)-C(350)-H(35B) | 109.5 |
| C(347)-C(350)-H(35C) | 109.5 |
| H(35A)-C(350)-H(35B) | 109.5 |
| H(35A)-C(350)-H(35C) | 109.5 |
| H(35B)-C(350)-H(35C) | 109.5 |
| C(352)-C(351)-S(36)  | 124.9 |
| C(352)-C(351)-C(356) | 117.8 |
| C(356)-C(351)-S(36)  | 117.1 |
| C(351)-C(352)-H(352) | 118.9 |
| C(351)-C(352)-C(353) | 122.3 |
| C(353)-C(352)-H(352) | 118.9 |
| C(352)-C(353)-H(353) | 119.8 |
| C(354)-C(353)-C(352) | 120.4 |
| C(354)-C(353)-H(353) | 119.8 |
| C(353)-C(354)-C(355) | 117.5 |
| C(353)-C(354)-C(357) | 125.0 |
| C(355)-C(354)-C(357) | 116.9 |
| C(354)-C(355)-H(355) | 119.2 |
| C(356)-C(355)-C(354) | 121.6 |
| C(356)-C(355)-H(355) | 119.2 |
| C(351)-C(356)-H(356) | 120.3 |
| C(355)-C(356)-C(351) | 119.4 |
| C(355)-C(356)-H(356) | 120.3 |

|                      |       |
|----------------------|-------|
| C(354)-C(357)-C(358) | 113.4 |
| C(354)-C(357)-C(359) | 113.3 |
| C(358)-C(357)-C(359) | 109.4 |
| C(360)-C(357)-C(354) | 110.0 |
| C(360)-C(357)-C(358) | 103.5 |
| C(360)-C(357)-C(359) | 106.6 |
| C(357)-C(358)-H(35D) | 109.5 |
| C(357)-C(358)-H(35E) | 109.5 |
| C(357)-C(358)-H(35F) | 109.5 |
| H(35D)-C(358)-H(35E) | 109.5 |
| H(35D)-C(358)-H(35F) | 109.5 |
| H(35E)-C(358)-H(35F) | 109.5 |
| C(357)-C(359)-H(35G) | 109.5 |
| C(357)-C(359)-H(35H) | 109.5 |
| C(357)-C(359)-H(35I) | 109.5 |
| H(35G)-C(359)-H(35H) | 109.5 |
| H(35G)-C(359)-H(35I) | 109.5 |
| H(35H)-C(359)-H(35I) | 109.5 |
| C(357)-C(360)-H(36A) | 109.5 |
| C(357)-C(360)-H(36B) | 109.5 |
| C(357)-C(360)-H(36C) | 109.5 |
| H(36A)-C(360)-H(36B) | 109.5 |
| H(36A)-C(360)-H(36C) | 109.5 |
| H(36B)-C(360)-H(36C) | 109.5 |