Supporting Information for

Coinage Metal-Ethylene Complexes Supported by Tris(pyrazolyl)borates: A Computational Study.

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Complete citation for reference 14.

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Table S-1. Optimized Geometries for Scorpionate Coinage Metal Ethylene Complexes. Coordinates are in Å, and individual files are in Sybyl MOL2 File Format. Atomic Symbols and Numbering are Indicated As Are Atom-Atom Connections.

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# Me-B(Pz)3Ag(C2H4)
# Created by GaussView 3.09
#
#

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Molecule Name
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SMALL
NO_CHARGES


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3 N3     -0.0831    -1.5398    -0.8751 N
4 N4      1.2510     1.2904    -0.7482 N
5 N5     -0.0838     1.5388    -0.8774 N
6 N6      1.3355    -0.0013     1.4780 N
7 N7      0.0124     0.0017     1.8087 N
8 C8     -0.2105    -2.7215    -1.5276 C
9 C9      1.0641    -3.2513    -1.8324 C
10 H10     1.2971    -4.1795    -2.3469 H
11 C11     1.9676    -2.3111    -1.3223 C
12 C12    -0.2114     2.7229    -1.5253 C
13 C13     1.0632     3.2575    -1.8220 C
14 H14     1.2959     4.1884    -2.3315 H
15 C15     1.9668     2.3177    -1.3114 C
16 C16    -0.0475    -0.0011     3.1617 C
17 C17     1.2540    -0.0061     3.7217 C
18 H18     1.5326    -0.0092     4.7723 H
19 C19     2.1103    -0.0062     2.6153 C
20 C20     3.4425     0.0005    -0.0901 C
21 H21     3.8738     0.8876     0.4104 H
22 H22     3.8090     0.0032    -1.1338 H
23 H23     3.8733    -0.8894     0.4057 H
24 C24    -3.6176    -0.6936     0.3372 C
25 H25    -3.5373    -1.2591     1.2737 H
26 C26    -3.6182     0.6925     0.3353 C
27 H27    -3.5383     1.2606     1.2703 H
28 B28     1.8275     0.0004    -0.0206 B
29 H29    -3.9607    -1.2573    -0.5393 H
30 H30    -3.9617     1.2536    -0.5427 H
31 H31     3.0532    -2.3067    -1.3288 H
32 H32    -1.1983    -3.1251    -1.7418 H
33 H33     3.0525     2.3162    -1.3130 H
34 H34    -1.0127     0.0005     3.6660 H
35 H35    -1.1992     3.1247    -1.7424 H
36 H36     3.1953    -0.0089     2.5659 H
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# Au(HB-(Pz)3)C2H4
# Created by GaussView 3.09
#

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NO_CHARGES


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5 N5     1.9282    -0.0042     1.2531 N
6 N6     0.7027    -0.0041     1.8494 N
7 C7    -0.2749    -2.6894    -1.3695 C
8 C8     0.9215    -3.2917    -1.8148 C
9 H9     1.0426    -4.2576    -2.2966 H
10 C10     1.9246    -2.3665    -1.4981 C
11 C11    -0.2777     2.6998    -1.3494 C
12 C12     0.9185     3.3082    -1.7868 C
13 H13     1.0388     4.2786    -2.2597 H
14 C14     1.9226     2.3821    -1.4763 C
15 C15     0.9314    -0.0119     3.1829 C
16 C16     2.3233    -0.0170     3.4602 C
17 H17     2.8147    -0.0234     4.4298 H
18 C18     2.9298    -0.0120     2.2005 C
19 C19     3.6298     0.0051    -0.7493 C
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20 H20     4.1678     0.8874    -0.3548 H
21 H21     3.7423     0.0141    -1.8495 H
22 H22     4.1666    -0.8843    -0.3694 H
23 C23    -3.1806    -0.7206     0.8635 C
24 H24    -2.9694    -1.2711     1.7897 H
25 C25    -3.1816     0.7111     0.8685 C
26 H26    -2.9712     1.2555     1.7985 H
27 B27     2.0761     0.0026    -0.3064 B
28 H28    -3.7994    -1.2637     0.1367 H
29 H29    -3.8013     1.2584     0.1454 H
30 H30     2.9975    -2.4138    -1.6563 H
31 H31    -1.2992    -3.0519    -1.4136 H
32 H32     2.9957     2.4326    -1.6320 H
33 H33     0.0937    -0.0132     3.8789 H
34 H34    -1.3026     3.0609    -1.3924 H
35 H35     3.9805    -0.0133     1.9236 H
36 Au36    -1.3918    -0.0005    -0.0040 Au
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# Cu(MeB-(Pz)3)C2H4
# Created by GaussView 3.09

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SMALL
NO_CHARGES


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4 N4    -0.3421     1.4843    -0.8071 N
5 N5     1.1147    -0.0395     1.4393 N
6 N6    -0.2193    -0.0460     1.7172 N
7 C7    -0.5349    -2.5996    -1.5577 C
8 C8     0.7062    -3.1789    -1.9077 C
9 H9     0.8807    -4.1070    -2.4447 H
10 C10     1.6680    -2.2900    -1.4094 C
11 C11    -0.5499     2.6845    -1.4046 C
12 C12     0.6881     3.2919    -1.7160 C
13 H13     0.8576     4.2514    -2.1964 H
14 C14     1.6547     2.3813    -1.2689 C
15 C15    -0.3338    -0.0921     3.0663 C
16 C16     0.9461    -0.1158     3.6738 C
17 H17     1.1833    -0.1527     4.7337 H
18 C18     1.8460    -0.0815     2.6018 C
19 C19     3.2319     0.0144    -0.1342 C
20 H20     3.6650     0.8886     0.3875 H
21 H21     3.5893     0.0478    -1.1807 H
22 H22     3.6701    -0.8880     0.3322 H
23 C23    -3.3458    -0.7150     0.2782 C
24 H24    -3.2706    -1.3087     1.1983 H
25 C25    -3.3501     0.6806     0.3185 C
26 H26    -3.2783     1.2207     1.2714 H
27 B27     1.6228     0.0070    -0.0513 B
28 H28    -3.7211    -1.2499    -0.6045 H
29 H29    -3.7287     1.2634    -0.5319 H
30 H30     2.7527    -2.3312    -1.4457 H
31 H31    -1.5453    -2.9544    -1.7500 H
32 H32     2.7392     2.4317    -1.3000 H
33 H33    -1.3174    -0.1060     3.5332 H
34 H34    -1.5622     3.0434    -1.5780 H
35 H35     2.9325    -0.0838     2.5907 H
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32 23 24 1
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# Me-B(3,5-CF3-Pz)3Ag(C2H4)
# Created by GaussView 3.09

#
#

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NO_CHARGES


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4 N4      0.6041     1.6333    -0.3024 N
5 N5     -0.2785     1.2173    -1.2397 N
6 N6      0.4096     0.0615     1.6948 N
7 N7     -0.8882     0.4246     1.6158 N
8 F8     -1.0628    -3.3744    -2.6304 F
9 F9      0.5922    -4.8398    -2.1638 F
10 F10    -3.1683     2.2990    -2.3127 F
11 F11    -1.7982     1.0209    -3.5721 F
12 F12    -3.7159    -0.9045     2.2842 F
13 F13    -3.2923     0.0519     4.2844 F
14 C14     0.8371    -2.6203    -1.3474 C
15 C15     2.0845    -2.3529    -1.9392 C
16 H16     2.6253    -2.9384    -2.6748 H
17 C17     2.4778    -1.1390    -1.3636 C
18 C18    -0.0909    -3.7343    -1.6520 C
19 C19    -0.8064     2.3270    -1.8121 C
20 C20    -0.2878     3.4932    -1.2207 C
21 H21    -0.5133     4.5289    -1.4509 H
22 C22     0.6007     3.0146    -0.2512 C
23 C23    -1.8564     2.2328    -2.8545 C
24 C24    -1.4932    -0.0612     2.7285 C
25 C25    -0.5899    -0.7891     3.5287 C
26 H26    -0.7726    -1.3018     4.4674 H
27 C27     0.6203    -0.6997     2.8318 C
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28 C28    -2.9487     0.1151     2.9307 C
29 C29     2.8223     0.9963     1.0861 C
30 H30     2.7085     1.6377     1.9735 H
31 H31     3.3962     1.5657     0.3414 H
32 H32     3.4432     0.1394     1.3871 H
33 C33    -3.4799    -1.9256    -0.7614 C
34 H34    -3.5933    -2.3197     0.2548 H
35 C35    -3.8429    -0.6341    -1.0669 C
36 H36    -4.2566     0.0356    -0.3034 H
37 B37     1.4047     0.5185     0.5290 B
38 H38    -3.2529    -2.6501    -1.5516 H
39 H39    -3.9206    -0.2980    -2.1072 H
40 F40    -3.4307     1.3270     2.4105 F
41 C41     1.8968    -1.3279     3.2539 C
42 F42     2.8310    -0.4267     3.7997 F
43 F43     2.5579    -1.9935     2.1934 F
44 F44     1.6493    -2.2891     4.2440 F
45 F45    -0.8253    -4.1593    -0.5280 F
46 C46     3.7214    -0.4033    -1.7147 C
47 F47     3.4856     0.9688    -1.9566 F
48 F48     4.2623    -0.9362    -2.8943 F
49 F49     4.7355    -0.4777    -0.7452 F
50 C50     1.3663     3.8832     0.6825 C
51 F51    -1.7615     3.2819    -3.7739 F
52 F52     1.2206     3.4928     2.0309 F
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15 10 23 1
16 11 23 1
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# Au(HB-(3,5-CF3-Pz)3)C2H4
# Created by GaussView 3.09

#
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NO_CHARGES


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4 N4    -0.6784     1.2143    -1.1171 N
5 N5     1.0925     0.4193     1.4689 N
6 N6    -0.1635     0.7550     1.8200 N
7 F7    -1.8706    -3.4049    -1.9672 F
8 F8    -0.2875    -5.0067    -1.7674 F
9 F9    -2.7866     3.3683    -3.1413 F
10 F10    -3.5436     2.5231    -1.1897 F
11 F11    -2.4243    -0.3925     3.6620 F
12 F12    -1.3782     0.8587     5.2257 F
13 C13     0.3312    -2.7959    -1.1810 C
14 C14     1.6006    -2.8690    -1.7873 C
15 H15     2.0227    -3.6837    -2.3650 H
16 C16     2.2010    -1.6460    -1.4721 C
17 C17    -0.7495    -3.8145    -1.2051 C
18 C18    -1.2013     2.3027    -1.7371 C
19 C19    -0.2652     3.3562    -1.7635 C
20 H20    -0.3819     4.3484    -2.1853 H
21 C21     0.8612     2.8251    -1.1289 C
22 C22    -2.6024     2.3263    -2.2280 C
23 C23    -0.2554     0.5333     3.1515 C
24 C24     0.9551     0.0289     3.6802 C
25 H25     1.1910    -0.2382     4.7050 H
26 C26     1.8014    -0.0286     2.5702 C
27 C27    -1.5499     0.7193     3.8447 C
28 C28    -3.4039    -1.5931     0.6814 C
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32 B32     1.5190     0.4992    -0.0337 B
33 H33    -3.6731    -2.4331     0.0300 H
34 H34    -4.4034    -0.0900    -0.5526 H
35 F35    -2.2649     1.8364     3.3790 F
36 C36     3.1976    -0.5183     2.5237 C
37 F37     4.1196     0.4368     2.0630 F
38 F38     3.3339    -1.6437     1.6692 F
39 F39     3.6175    -0.9211     3.7966 F
40 F40    -1.2435    -4.1138     0.0815 F
41 C41     3.5146    -1.1446    -1.9608 C
42 F42     3.3547     0.0122    -2.7554 F
43 F43     4.1181    -2.1208    -2.7652 F
44 F44     4.4273    -0.8158    -0.9528 F
45 C45     2.1572     3.5038    -0.8641 C
46 F46    -2.9728     1.1249    -2.8664 F
47 F47     2.5202     3.4394     0.4967 F
48 F48     2.0616     4.8579    -1.2087 F
49 F49     3.2302     2.9655    -1.5929 F
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51 H51     2.6611     0.8245    -0.1482 H
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# Au(MeB-(3,5-CF3-Pz)3)C2H4
# Created by GaussView 3.09

#
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SMALL
NO_CHARGES


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3 N3     0.0877     1.8165    -0.3205 N
4 N4    -0.6415     1.0423    -1.1599 N
5 N5     0.2440     0.3502     1.7541 N
6 N6    -1.0839     0.5830     1.7616 N
7 F7     0.4018    -3.4212    -2.5390 F
8 F8     2.4358    -4.2274    -1.9757 F
9 F9    -2.6055     2.3132    -3.9205 F
10 F10    -3.5938     0.9784    -2.3952 F
11 F11    -3.6699    -1.1777     2.3211 F
12 F12    -3.3372    -0.3865     4.4096 F
13 C13     1.8569    -2.0868    -1.1394 C
14 C14     3.0897    -1.4910    -1.4521 C
15 H15     3.9225    -1.9150    -2.0020 H
16 C16     3.0048    -0.2103    -0.8928 C
17 C17     1.3786    -3.4425    -1.5102 C
18 C18    -1.3937     1.8639    -1.9316 C
19 C19    -1.1821     3.2049    -1.5714 C
20 H20    -1.6350     4.0951    -1.9931 H
21 C21    -0.2407     3.1405    -0.5380 C
22 C22    -2.3431     1.3445    -2.9477 C
23 C23    -1.5808    -0.0843     2.8292 C
24 C24    -0.5700    -0.7831     3.5230 C
25 H25    -0.6571    -1.4046     4.4085 H
26 C26     0.5942    -0.4847     2.8074 C
27 C27    -3.0404    -0.1302     3.0654 C
28 C28     2.2166     2.0223     1.3569 C
29 H29     1.7316     2.6381     2.1314 H
30 H30     2.7436     2.7020     0.6744 H
31 H31     2.9788     1.4144     1.8689 H
32 C32    -2.3610    -2.8472    -0.4391 C
33 H33    -2.3757    -3.1311     0.6205 H
```

```
34 C34    -3.1619    -1.7725    -0.9017 C
35 H35    -3.7984    -1.2180    -0.2028 H
36 B36     1.1363     1.0841     0.6543 B
37 H37    -2.0270    -3.6275    -1.1336 H
38 H38    -3.4528    -1.7164    -1.9574 H
39 F39    -3.6967     1.0474     2.6885 F
40 C40     1.9601    -0.9121     3.1917 C
41 F41     2.6888     0.0811     3.8831 F
42 F42     2.7736    -1.2853     2.0932 F
43 F43     1.8970    -2.0216     4.0452 F
44 F44     0.7836    -4.1218    -0.4279 F
45 C45     4.0655     0.8262    -1.0195 C
46 F46     3.5505     2.0662    -1.4548 F
47 F47     5.0007     0.4159    -1.9815 F
48 F48     4.7898     1.0703     0.1573 F
49 C49     0.2587     4.3372     0.1956 C
50 F50    -1.8555     0.1959    -3.6064 F
51 F51     0.1055     4.2303     1.5902 F
52 F52    -0.4783     5.4622    -0.2056 F
53 F53     1.6087     4.6429    -0.0511 F
54 Au54    -1.1375    -1.1194    -0.6885 Au
@<TRIPOS>BOND
1 1 2 1
2 1 16 Ar
3 1 36 1
4 2 13 Ar
5 3 4 1
6 3 21 Ar
7 3 36 1
8 4 18 Ar
9 5 6 1
10 5 26 1
11 5 36 1
12 6 23 Ar
13 7 17 1
14 8 17 1
15 9 22 1
16 10 22 1
17 11 27 1
18 12 27 1
19 13 14 Ar
20 13 17 1
21 14 15 1
22 14 16 Ar
23 16 45 1
24 17 44 1
25 18 19 Ar
26 18 22 1
27 19 20 1
28 19 21 Ar
29 21 49 1
30 22 50 1
31 23 24 Ar
32 23 27 1
33 24 25 1
34 24 26 Ar
35 26 40 1
36 27 39 1
37 28 29 1
38 28 30 1
39 28 31 1
40 28 36 1
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41 32 33 1
42 32 34 Ar
43 32 37 1
44 32 54 1
45 34 35 1
46 34 38 1
47 34 54 1
48 40 41 1
49 40 42 1
50 40 43 1
51 45 46 1
52 45 47 1
53 45 48 1
54 49 51 1
55 49 52 1
56 49 53 1
# Cu(HB-(3,5-CF3-Pz)3)C2H4
# Created by GaussView 3.09

#
#

@<TRIPOS>MOLECULE
Molecule Name
51 52
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 N1     0.7560    -0.5092     1.3490 N
2 N2    -0.5490    -0.3528     1.6761 N
3 N3     0.5992    -1.0009    -1.1436 N
4 N4    -0.7360    -1.2255    -1.1185 N
5 N5     0.8412     1.4079    -0.3392 N
6 N6    -0.4605     1.6857    -0.5659 N
7 F7    -2.9678    -1.5893     3.0198 F
8 F8    -1.8628    -1.2415     4.9623 F
9 F9    -2.3544    -3.6700    -3.2750 F
10 F10    -3.1721    -1.5770    -3.0561 F
11 F11    -2.6133     3.8295     0.1391 F
12 F12    -1.6321     4.9889    -1.5313 F
13 C13    -0.6893    -0.7990     2.9520 C
14 C14     0.5403    -1.2651     3.4577 C
15 H15     0.7474    -1.6842     4.4359 H
16 C16     1.4399    -1.0674     2.4069 C
17 C17    -1.9971    -0.7763     3.6521 C
18 C18    -1.0060    -2.0985    -2.1235 C
19 C19     0.1682    -2.4250    -2.8316 C
20 H20     0.2760    -3.0873    -3.6833 H
21 C21     1.1724    -1.7067    -2.1785 C
22 C22    -2.3835    -2.5643    -2.4200 C
23 C23    -0.5340     3.0215    -0.7860 C
24 C24     0.7369     3.6274    -0.6818 C
25 H25     0.9974     4.6731    -0.8030 H
26 C26     1.5957     2.5639    -0.3975 C
27 C27    -1.8290     3.6979    -1.0350 C
28 C28    -3.6596     0.7131     0.7249 C
29 H29    -3.4823     1.7760     0.9237 H
30 C30    -3.7525     0.2248    -0.5680 C
31 H31    -3.6504     0.8845    -1.4370 H
32 B32     1.2756    -0.0716    -0.0699 B
```

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33 H33    -4.0171     0.1150     1.5694 H
34 H34    -4.1803    -0.7656    -0.7566 H
35 F35    -2.6379     3.0042    -1.9605 F
36 C36     3.0495     2.6468    -0.1094 C
37 F37     3.8425     1.8382    -0.9375 F
38 F38     3.3420     2.2717     1.2197 F
39 F39     3.4926     3.9666    -0.2721 F
40 F40    -2.5558     0.5180     3.7193 F
41 C41     2.8657    -1.4872     2.3674 C
42 F42     3.0860    -2.4857     1.3955 F
43 F43     3.2314    -2.0286     3.6074 F
44 F44     3.7615    -0.4472     2.0875 F
45 C45     2.6109    -1.6439    -2.5469 C
46 F46    -3.0911    -2.9425    -1.2592 F
47 F47     3.0176    -0.3299    -2.8537 F
48 F48     2.8407    -2.4271    -3.6862 F
49 F49     3.4729    -2.1103    -1.5432 F
50 Cu50    -1.8433    -0.0515     0.1357 Cu
51 H51     2.4606    -0.1802    -0.1198 H
@<TRIPOS>BOND
1 1 2 1
2 1 16 Ar
3 1 32 1
4 2 13 Ar
5 3 4 1
6 3 21 Ar
7 3 32 1
8 4 18 Ar
9 5 6 1
10 5 26 Ar
11 5 32 1
12 6 23 Ar
13 7 17 1
14 8 17 1
15 9 22 1
16 10 22 1
17 11 27 1
18 12 27 1
19 13 14 Ar
20 13 17 1
21 14 15 1
22 14 16 Ar
23 16 41 1
24 17 40 1
25 18 19 Ar
26 18 22 1
27 19 20 1
28 19 21 Ar
29 21 45 1
30 22 46 1
31 23 24 Ar
32 23 27 1
33 24 25 1
34 24 26 Ar
35 26 36 1
36 27 35 1
37 28 29 1
38 28 30 2
39 28 33 1
40 30 31 1
41 30 34 1
42 30 50 1
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43 32 51 1
44 36 37 1
45 36 38 1
46 36 39 1
47 41 42 1
48 41 43 1
49 41 44 1
50 45 47 1
51 45 48 1
52 45 49 1
# Cu(MeB-(3,5-CF3-Pz)3)C2H4
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
54 56
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 N1    -1.6582     0.3114    -0.0738 N
2 N2    -1.3883    -0.6642     0.8252 N
3 N3     0.5483     1.5674    -0.1408 N
4 N4     0.9052     0.9985     1.0378 N
5 N5     0.3180    -0.6023    -1.4524 N
6 N6     1.6549    -0.6255    -1.2586 N
7 F7    -1.5673    -1.6868     3.6092 F
8 F8    -3.7897    -1.9456     3.2439 F
9 F9     3.4639     0.7146     2.8996 F
10 F10     1.4090     0.8218     3.8287 F
11 F11     4.2038    -1.6793    -0.6298 F
12 F12     3.7567    -3.4839    -1.9328 F
13 C13    -2.5156    -0.8872     1.5450 C
14 C14    -3.5464    -0.0331     1.1190 C
15 H15    -4.5608     0.0376     1.4948 H
16 C16    -2.9657     0.7239     0.0946 C
17 C17    -2.5490    -1.9187     2.6093 C
18 C18     1.7183     1.8644     1.6870 C
19 C19     1.9302     3.0151     0.9096 C
20 H20     2.5310     3.8860     1.1455 H
21 C21     1.1770     2.7941    -0.2490 C
22 C22     2.3141     1.5303     3.0038 C
23 C23     2.0966    -1.7883    -1.7894 C
24 C24     1.0421    -2.5381    -2.3532 C
25 H25     1.0827    -3.5029    -2.8486 H
26 C26    -0.0920    -1.7522    -2.1188 C
27 C27     3.5456    -2.1007    -1.8075 C
28 C28    -0.9524     1.4623    -2.4108 C
29 H29    -0.1011     1.5650    -3.1036 H
30 H30    -1.3874     2.4598    -2.2648 H
31 H31    -1.7065     0.8431    -2.9220 H
32 C32     1.0224    -2.8552     1.7715 C
33 H33     0.9610    -3.3960     0.8168 H
34 C34     2.0894    -2.0089     2.0519 C
35 H35     2.9011    -1.8496     1.3327 H
36 B36    -0.4701     0.7431    -1.0764 B
37 H37     0.3651    -3.2194     2.5695 H
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38 H38     2.2830    -1.6832     3.0808 H
39 F39     4.2292    -1.4859    -2.8732 F
40 C40    -1.4504    -2.0672    -2.6257 C
41 F41    -1.7726    -1.3789    -3.8173 F
42 F42    -2.4962    -1.7685    -1.7211 F
43 F43    -1.5482    -3.4339    -2.9190 F
44 F44    -2.2929    -3.2174     2.1195 F
45 C45    -3.6706     1.8070    -0.6436 C
46 F46    -2.9654     3.0281    -0.6124 F
47 F47    -4.9151     2.0437    -0.0412 F
48 F48    -3.9294     1.5154    -1.9922 F
49 C49     1.1210     3.7540    -1.3875 C
50 F50     2.6995     2.6856     3.6866 F
51 F51     1.5374     3.1929    -2.6076 F
52 F52     1.9842     4.8286    -1.1246 F
53 F53    -0.1525     4.3121    -1.6012 F
54 Cu54     0.5085    -0.9423     1.3602 Cu
@<TRIPOS>BOND
1 1 2 1
2 1 16 Ar
3 1 36 1
4 2 13 Ar
5 3 4 1
6 3 21 1
7 3 36 1
8 4 18 Ar
9 5 6 1
10 5 26 1
11 5 36 1
12 6 23 Ar
13 7 17 1
14 8 17 1
15 9 22 1
16 10 22 1
17 11 27 1
18 12 27 1
19 13 14 Ar
20 13 17 1
21 14 15 1
22 14 16 Ar
23 16 45 1
24 17 44 1
25 18 19 Ar
26 18 22 1
27 19 20 1
28 19 21 Ar
29 21 49 1
30 22 50 1
31 23 24 Ar
32 23 27 1
33 24 25 1
34 24 26 Ar
35 26 40 1
36 27 39 1
37 28 29 1
38 28 30 1
39 28 31 1
40 28 36 1
41 32 33 1
42 32 34 Ar
43 32 37 1
44 32 54 1
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45 34 35 1
46 34 38 1
47 34 54 1
48 40 41 1
49 40 42 1
50 40 43 1
51 45 46 1
52 45 47 1
53 45 48 1
54 49 51 1
55 49 52 1
56 49 53 1
# H-B(3-CF3-Pz)3Ag(C2H4)
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
42 42
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 Ag1    -0.0480    -0.1612    -0.8259 Ag
2 N2    -1.4217    -0.3631     2.0453 N
3 N3    -1.7143    -0.5005     0.7314 N
4 N4     1.0635    -1.0026     2.0391 N
5 N5     1.2904    -1.2187     0.7227 N
6 N6     0.3762     1.4669     2.0539 N
7 F7    -2.9821    -1.8951    -1.4967 F
8 F8    -4.9821    -1.5198    -0.4958 F
9 C9    -3.0275    -0.8273     0.6661 C
10 C10    -3.5989    -0.8944     1.9596 C
11 H11    -4.6250    -1.1333     2.2196 H
12 C12    -2.5366    -0.5930     2.8163 C
13 C13    -3.6881    -1.0098    -0.6465 C
14 C14     2.2388    -2.1840     0.6533 C
15 C15     2.6393    -2.5960     1.9470 C
16 H16     3.3800    -3.3462     2.2042 H
17 C17     1.8609    -1.8170     2.8078 C
18 C18     1.0478     3.6015     1.9413 C
19 C19     0.8057     3.0540     0.6557 C
20 C20    -0.6315     0.3794    -2.9455 C
21 H21    -0.9398     1.4297    -2.8792 H
22 C22     0.7019     0.0285    -2.9524 C
23 H23     1.4886     0.7900    -2.8923 H
24 B24     0.0064     0.0362     2.5502 B
25 H25    -1.4106    -0.3439    -3.2137 H
26 H26     1.0195    -0.9847    -3.2254 H
27 F27    -3.8062     0.1983    -1.3784 F
28 H28    -2.4924    -0.5290     3.9001 H
29 H29     1.8169    -1.7823     3.8929 H
30 C30     2.7386    -2.6475    -0.6615 C
31 F31     3.4055    -1.6320    -1.3893 F
32 F32     3.6415    -3.7057    -0.5145 F
33 F33     1.7004    -3.0985    -1.5146 F
34 N34     0.4016     1.7655     0.7369 N
35 C35     0.7609     2.5494     2.8148 C
```

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36 H36     0.7980     2.4928     3.8996 H
37 C37     0.9593     3.6892    -0.6713 C
38 F38     1.3131     5.0373    -0.5572 F
39 F39    -0.2228     3.6310    -1.4514 F
40 F40     1.9563     3.0670    -1.4684 F
41 H41     1.3753     4.6071     2.1854 H
42 H42     0.0071     0.0220     3.7579 H
@<TRIPOS>BOND
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2 2 12 Ar
3 2 24 1
4 3 9 Ar
5 4 5 1
6 4 17 Ar
7 4 24 1
8 5 14 Ar
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10 6 34 1
11 6 35 Ar
12 7 13 1
13 8 13 1
14 9 10 Ar
15 9 13 1
16 10 11 1
17 10 12 Ar
18 12 28 1
19 13 27 1
20 14 15 Ar
21 14 30 1
22 15 16 1
23 15 17 Ar
24 17 29 1
25 18 19 Ar
26 18 35 Ar
27 18 41 1
28 19 34 Ar
29 19 37 1
30 20 21 1
31 20 22 2
32 20 25 1
33 22 23 1
34 22 26 1
35 24 42 1
36 30 31 1
37 30 32 1
38 30 33 1
39 35 36 1
40 37 38 1
41 37 39 1
42 37 40 1
# Me-B(3-CF3-Pz)3Ag(C2H4)
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
45 45
SMALL
NO_CHARGES
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@<TRIPOS>ATOM
1 Ag1    -0.0220    -0.1521    -0.9374 Ag
2 N2     -1.3670    -0.5308     1.9552 N
3 N3     -1.6083    -0.7129     0.6355 N
4 N4      1.1830    -0.8890     1.9427 N
5 N5      1.4311    -1.0235     0.6185 N
6 N6      0.2201     1.4941     1.9655 N
7 F7     -2.6346    -2.2545    -1.6210 F
8 F8     -4.6854    -2.1558    -0.6592 F
9 C9     -2.8686    -1.1997     0.5372 C
10 C10    -3.4635    -1.3271     1.8141 C
11 H11    -4.4591    -1.6883     2.0504 H
12 C12    -2.4705    -0.8930     2.6949 C
13 C13    -3.4710    -1.4724    -0.7873 C
14 C14     2.4849    -1.8676     0.5071 C
15 C15     2.9361    -2.2855     1.7807 C
16 H16     3.7599    -2.9546     2.0072 H
17 C17     2.0774    -1.6392     2.6727 C
18 C18     0.6185     3.6963     1.7938 C
19 C19     0.3978     3.0990     0.5279 C
20 C20     0.0190     0.0110     4.1230 C
21 H21     0.9825     0.3661     4.5338 H
22 H22    -0.1526    -1.0034     4.5286 H
23 H23    -0.7682     0.6663     4.5402 H
24 C24    -0.6860     0.2894    -3.0529 C
25 H25    -1.1489     1.2811    -2.9856 H
26 C26     0.6851     0.1427    -3.0646 C
27 H27     1.3485     1.0137    -3.0078 H
28 B28     0.0134     0.0263     2.5107 B
29 H29    -1.3471    -0.5432    -3.3196 H
30 H30     1.1503    -0.8108    -3.3404 H
31 F31    -3.7421    -0.2940    -1.5276 F
32 H32    -2.4779    -0.8243     3.7779 H
33 H33     2.0475    -1.6645     3.7573 H
34 C34     3.0274    -2.2219    -0.8243 C
35 F35     3.5358    -1.1047    -1.5311 F
36 F36     4.0721    -3.1457    -0.7139 F
37 F37     2.0539    -2.7954    -1.6815 F
38 N38     0.1606     1.7723     0.6448 N
39 C39     0.4955     2.6344     2.6921 C
40 H40     0.5811     2.6182     3.7742 H
41 C41     0.4263     3.7277    -0.8102 C
42 F42     0.5858     5.1143    -0.7219 F
43 F43    -0.7540     3.4896    -1.5589 F
44 F44     1.4834     3.2446    -1.6275 F
45 H45     0.8282     4.7386     2.0118 H
@<TRIPOS>BOND
1 2 3 1
2 2 12 Ar
3 2 28 1
4 3 9 Ar
5 4 5 1
6 4 17 Ar
7 4 28 1
8 5 14 Ar
9 6 28 1
10 6 38 1
11 6 39 Ar
12 7 13 1
13 8 13 1
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14 9 10 Ar
15 9 13 1
16 10 11 1
17 10 12 Ar
18 12 32 1
19 13 31 1
20 14 15 Ar
21 14 34 1
22 15 16 1
23 15 17 Ar
24 17 33 1
25 18 19 Ar
26 18 39 Ar
27 18 45 1
28 19 38 Ar
29 19 41 1
30 20 21 1
31 20 22 1
32 20 23 1
33 20 28 1
34 24 25 1
35 24 26 2
36 24 29 1
37 26 27 1
38 26 30 1
39 34 35 1
40 34 36 1
41 34 37 1
42 39 40 1
43 41 42 1
44 41 43 1
45 41 44 1
# Au(HB-(3-CF3-Pz)3)C2H4
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
42 44
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 N1    -0.2890     1.3048     2.1513 N
2 N2    -0.6622     1.5442     0.8715 N
3 N3    -0.4392    -1.2457     2.1641 N
4 N4    -0.8635    -1.4365     0.8922 N
5 N5     1.8517    -0.1010     1.9919 N
6 N6     2.0193    -0.1878     0.6561 N
7 F7    -2.6432     2.5744    -1.0858 F
8 F8    -2.3451     4.6133    -0.1479 F
9 F9     3.5449     0.8587    -1.7011 F
10 F10     5.2785    -0.3803    -0.9364 F
11 C11    -1.2160     2.7835     0.8529 C
12 C12    -1.1895     3.3594     2.1438 C
13 H13    -1.5583     4.3366     2.4372 H
14 C14    -0.5924     2.3823     2.9452 C
15 C15    -1.7121     3.3913    -0.4057 C
```

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16 C16    -1.5623    -2.5999     0.8857 C
17 C17    -1.5797    -3.1772     2.1764 C
18 H18    -2.0585    -4.1028     2.4782 H
19 C19    -0.8543    -2.2802     2.9652 C
20 C20     3.3553    -0.2121     0.4557 C
21 C21     4.0683    -0.1388     1.6818 C
22 H22     5.1439    -0.1417     1.8279 H
23 C23     3.0648    -0.0693     2.6505 C
24 C24     3.8819    -0.2801    -0.9252 C
25 C25    -0.0277     0.6942    -2.7283 C
26 H26     0.9497     1.1913    -2.7573 H
27 C27    -0.1107    -0.7243    -2.7153 C
28 H28     0.8031    -1.3311    -2.7279 H
29 B29     0.4279    -0.0168     2.6016 B
30 H30    -0.8716     1.2916    -3.0942 H
31 H31    -1.0169    -1.2270    -3.0743 H
32 F32     3.3778    -1.3847    -1.6542 F
33 F33    -0.6778     3.6526    -1.3353 F
34 H34    -0.3648     2.3741     4.0075 H
35 H35     3.1212    -0.0045     3.7342 H
36 H36    -0.6083    -2.3000     4.0232 H
37 C37    -2.1548    -3.1416    -0.3613 C
38 F38    -1.1819    -3.5602    -1.2998 F
39 F39    -2.9545    -4.2569    -0.0832 F
40 F40    -2.9657    -2.2042    -1.0399 F
41 Au41    -0.4130     0.0218    -0.7460 Au
42 H42     0.5087    -0.0123     3.8069 H
@<TRIPOS>BOND
1 1 2 1
2 1 14 Ar
3 1 29 1
4 2 11 Ar
5 3 4 1
6 3 19 Ar
7 3 29 1
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9 5 6 1
10 5 23 Ar
11 5 29 1
12 6 20 Ar
13 7 15 1
14 8 15 1
15 9 24 1
16 10 24 1
17 11 12 Ar
18 11 15 1
19 12 13 1
20 12 14 Ar
21 14 34 1
22 15 33 1
23 16 17 Ar
24 16 37 1
25 17 18 1
26 17 19 Ar
27 19 36 1
28 20 21 Ar
29 20 24 1
30 21 22 1
31 21 23 Ar
32 23 35 1
33 24 32 1
34 25 26 1
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35 25 27 Ar
36 25 30 1
37 25 41 1
38 27 28 1
39 27 31 1
40 27 41 1
41 29 42 1
42 37 38 1
43 37 39 1
44 37 40 1
# Au(MeB-(3-CF3-Pz)3)C2H4
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
45 47
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 N1     0.1443     1.3768     2.0558 N
2 N2    -0.0808     1.6781     0.7532 N
3 N3    -0.7184    -1.0387     2.1259 N
4 N4    -1.2544    -1.0423     0.8806 N
5 N5     1.7925    -0.5789     1.8509 N
6 N6     1.7743    -0.9314     0.5481 N
7 F7    -1.6866     3.2361    -1.2641 F
8 F8    -0.7182     5.0839    -0.3911 F
9 F9     3.3806    -0.4325    -2.0460 F
10 F10     4.6918    -2.0975    -1.2628 F
11 C11    -0.2714     3.0212     0.6874 C
12 C12    -0.1606     3.6020     1.9701 C
13 H13    -0.2597     4.6504     2.2313 H
14 C14     0.1034     2.5213     2.8147 C
15 C15    -0.5322     3.7115    -0.5993 C
16 C16    -2.2528    -1.9611     0.8857 C
17 C17    -2.3583    -2.5748     2.1540 C
18 H18    -3.0606    -3.3432     2.4599 H
19 C19    -1.3659    -1.9574     2.9173 C
20 C20     3.0571    -1.2059     0.2220 C
21 C21     3.9266    -1.0235     1.3288 C
22 H22     5.0009    -1.1761     1.3667 H
23 C23     3.0764    -0.6223     2.3603 C
24 C24     3.4030    -1.5557    -1.1722 C
25 C25     0.6533    -0.1093     4.1681 C
26 H26     0.9407    -1.1131     4.5324 H
27 H27    -0.2766     0.1815     4.6913 H
28 H28     1.4470     0.5833     4.5053 H
29 C29     0.1018     0.5914    -2.8424 C
30 H30     1.1888     0.7104    -2.9265 H
31 C31    -0.4730    -0.7062    -2.7785 C
32 H32     0.1673    -1.5962    -2.8091 H
33 B33     0.4802    -0.0965     2.5654 B
34 H34    -0.4952     1.4418    -3.1926 H
35 H35    -1.5150    -0.8636    -3.0816 H
36 F36     2.5096    -2.4873    -1.7470 F
37 F37     0.5291     3.5757    -1.5238 F
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38 H38     0.2631     2.4954     3.8876 H
39 H39     3.2942    -0.3793     3.3962 H
40 H40    -1.0875    -2.1068     3.9553 H
41 C41    -3.0386    -2.2696    -0.3332 C
42 F42    -2.2921    -2.9701    -1.3113 F
43 F43    -4.1406    -3.0751    -0.0177 F
44 F44    -3.5359    -1.1168    -0.9806 F
45 Au45    -0.3983     0.1334    -0.8246 Au
@<TRIPOS>BOND
1 1 2 1
2 1 14 Ar
3 1 33 1
4 2 11 Ar
5 3 4 1
6 3 19 Ar
7 3 33 1
8 4 16 Ar
9 5 6 1
10 5 23 1
11 5 33 1
12 6 20 Ar
13 7 15 1
14 8 15 1
15 9 24 1
16 10 24 1
17 11 12 Ar
18 11 15 1
19 12 13 1
20 12 14 Ar
21 14 38 1
22 15 37 1
23 16 17 Ar
24 16 41 1
25 17 18 1
26 17 19 Ar
27 19 40 1
28 20 21 Ar
29 20 24 1
30 21 22 1
31 21 23 Ar
32 23 39 1
33 24 36 1
34 25 26 1
35 25 27 1
36 25 28 1
37 25 33 1
38 29 30 1
39 29 31 Ar
40 29 34 1
41 29 45 1
42 31 32 1
43 31 35 1
44 31 45 1
45 41 42 1
46 41 43 1
47 41 44 1
# Cu(HB-(3-CF3-Pz)3)C2H4
# Created by GaussView 3.09
#

#
#
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@<TRIPOS>MOLECULE
Molecule Name
42 44
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 N1     1.0144    -1.0210     1.9562 N
2 N2     1.2776    -1.1455     0.6308 N
3 N3     0.2400     1.3979     1.9617 N
4 N4     0.3749     1.6571     0.6369 N
5 N5    -1.4745    -0.4831     1.9354 N
6 N6    -1.6966    -0.5585     0.6035 N
7 F7     3.2499    -1.3859    -1.5712 F
8 F8     3.9215    -3.3266    -0.6182 F
9 F9    -2.8874    -2.0440    -1.6833 F
10 F10    -4.9086    -1.6005    -0.7665 F
11 C11     2.2747    -2.0632     0.5302 C
12 C12     2.6504    -2.5419     1.8072 C
13 H13     3.4155    -3.2763     2.0361 H
14 C14     1.8218    -1.8491     2.6937 C
15 C15     2.8201    -2.4782    -0.7828 C
16 C16     0.6544     2.9835     0.5399 C
17 C17     0.6878     3.5865     1.8192 C
18 H18     0.8852     4.6278     2.0512 H
19 C19     0.4205     2.5379     2.7029 C
20 C20    -2.9861    -0.9567     0.4716 C
21 C21    -3.6034    -1.1370     1.7354 C
22 H22    -4.6230    -1.4499     1.9357 H
23 C23    -2.5982    -0.8238     2.6526 C
24 C24    -3.5947    -1.1295    -0.8659 C
25 C25     0.0829    -0.7006    -2.5168 C
26 H26    -0.6034    -1.5518    -2.4418 H
27 C27    -0.3836     0.6057    -2.4984 C
28 H28    -1.4531     0.8276    -2.4052 H
29 B29    -0.0859    -0.0410     2.4760 B
30 H30     1.0967    -0.9234    -2.8678 H
31 H31     0.2551     1.4297    -2.8347 H
32 F32    -3.6466     0.0762    -1.6102 F
33 F33     1.8794    -3.1783    -1.5750 F
34 H34     1.7502    -1.8823     3.7773 H
35 H35    -2.5980    -0.8187     3.7395 H
36 H36     0.3491     2.5188     3.7870 H
37 C37     0.8359     3.6474    -0.7717 C
38 F38    -0.3572     3.7024    -1.5312 F
39 F39     1.2700     4.9679    -0.6050 F
40 F40     1.7852     2.9973    -1.5940 F
41 Cu41     0.2292     0.0640    -0.6215 Cu
42 H42    -0.0926    -0.0453     3.6827 H
@<TRIPOS>BOND
1 1 2 1
2 1 14 Ar
3 1 29 1
4 2 11 Ar
5 3 4 1
6 3 19 Ar
7 3 29 1
8 4 16 Ar
9 5 6 1
10 5 23 Ar
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11 5 29 1
12 6 20 Ar
13 7 15 1
14 8 15 1
15 9 24 1
16 10 24 1
17 11 12 Ar
18 11 15 1
19 12 13 1
20 12 14 Ar
21 14 34 1
22 15 33 1
23 16 17 Ar
24 16 37 1
25 17 18 1
26 17 19 Ar
27 19 36 1
28 20 21 Ar
29 20 24 1
30 21 22 1
31 21 23 Ar
32 23 35 1
33 24 32 1
34 25 26 1
35 25 27 Ar
36 25 30 1
37 25 41 1
38 27 28 1
39 27 31 1
40 27 41 1
41 29 42 1
42 37 38 1
43 37 39 1
44 37 40 1
# Cu(MeB-(3-CF3-Pz)3)C2H4
# Created by GaussView 3.09
#

#

@<TRIPOS>MOLECULE
Molecule Name
45 47
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 N1     0.8518    -1.1648     1.8483 N
2 N2     1.0756    -1.3169     0.5177 N
3 N3     0.4484     1.3533     1.8547 N
4 N4     0.6139     1.5752     0.5254 N
5 N5    -1.5339    -0.2552     1.8193 N
6 N6    -1.7404    -0.2772     0.4820 N
7 F7     2.9697    -1.8266    -1.7193 F
8 F8     3.3685    -3.8443    -0.7758 F
9 F9    -3.1326    -1.6178    -1.8206 F
10 F10    -5.0541    -0.8050    -0.9476 F
11 C11     1.9304    -2.3658     0.3935 C
12 C12     2.2529    -2.9053     1.6597 C
13 H13     2.9082    -3.7436     1.8717 H
14 C14     1.5462    -2.1097     2.5634 C
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15 C15     2.3959    -2.8480    -0.9270 C
16 C16     1.0945     2.8409     0.4086 C
17 C17     1.2306     3.4472     1.6783 C
18 H18     1.5888     4.4479     1.8962 H
19 C19     0.8109     2.4643     2.5763 C
20 C20    -3.0695    -0.4921     0.3176 C
21 C21    -3.7309    -0.6072     1.5651 C
22 H22    -4.7877    -0.7793     1.7418 H
23 C23    -2.7119    -0.4506     2.5054 C
24 C24    -3.6757    -0.5759    -1.0292 C
25 C25    -0.1117    -0.0331     4.0220 C
26 H26    -0.7649     0.7618     4.4278 H
27 H27     0.8967     0.1253     4.4476 H
28 H28    -0.4883    -0.9920     4.4245 H
29 C29    -0.0314    -0.7011    -2.6356 C
30 H30    -0.8612    -1.4142    -2.5754 H
31 C31    -0.2530     0.6679    -2.6264 C
32 H32    -1.2650     1.0824    -2.5574 H
33 B33    -0.0932    -0.0262     2.4125 B
34 H34     0.9312    -1.1038    -2.9688 H
35 H35     0.5332     1.3578    -2.9510 H
36 F36    -3.5016     0.6059    -1.7919 F
37 F37     1.3585    -3.4078    -1.7102 F
38 H38     1.4958    -2.1532     3.6467 H
39 H39    -2.7473    -0.4660     3.5904 H
40 H40     0.7512     2.4827     3.6597 H
41 C41     1.3736     3.4599    -0.9076 C
42 F42     0.2039     3.6868    -1.6718 F
43 F43     1.9965     4.7042    -0.7474 F
44 F44     2.2219     2.6751    -1.7227 F
45 Cu45     0.2098     0.0290    -0.7334 Cu
@<TRIPOS>BOND
1 1 2 1
2 1 14 Ar
3 1 33 1
4 2 11 Ar
5 3 4 1
6 3 19 Ar
7 3 33 1
8 4 16 Ar
9 5 6 1
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11 5 33 1
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14 8 15 1
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21 14 38 1
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23 16 17 Ar
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25 17 18 1
26 17 19 Ar
27 19 40 1
28 20 21 Ar
29 20 24 1
30 21 22 1
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35 25 27 1
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40 29 34 1
41 29 45 1
42 31 32 1
43 31 35 1
44 31 45 1
45 41 42 1
46 41 43 1
47 41 44 1
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