*Supplementary Materials*

*Таблица 1*

Длины связей, валентные и невалентные углы в гетеролигандных комплексах M(III) с фталоцианином и фторид-анионом

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Sc | Ti | V | Cr | Mn | Fe | Co | Ni | Cu |
| Длины связей M–N, *пм* | | | | | | | | | |
| (M1N1) | 215.6 | 204.0 | 202.7 | 198.8 | 195.8 | 196.1 | 192.1 | 192.6 | 194.5 |
| (M1N2) | 215.6 | 203.0 | 200.3 | 198.8 | 195.1 | 196.1 | 192.1 | 192,6 | 194.5 |
| (M1N3) | 215.6 | 204.0 | 202.7 | 198.8 | 195.8 | 196.1 | 192.1 | 192.6 | 194.5 |
| (M1N4) | 215.6 | 203.0 | 200.3 | 198.8 | 196.9 | 196.1 | 192.1 | 192,6 | 194.5 |
| Длины связей M–F, *пм* | | | | | | | | | |
| (M1F1) | 185.7 | 177.9 | 175.9 | 178.1 | 174.1 | 183.2 | 178.5 | 192.7 | 200.5 |
| Длины связей C–N, *пм* | | | | | | | | | |
| (N1C3) | 137.3 | 139.2 | 137.8 | 137.5 | 137.8 | 137.3 | 137.6 | 137.3 | 136.9 |
| (N1C4) | 137.3 | 139.2 | 137.8 | 137.5 | 137.6 | 137.3 | 137.6 | 137.3 | 136.9 |
| (N2C1) | 137.3 | 138.9 | 138.5 | 137.5 | 137.6 | 137.3 | 137.6 | 137.3 | 136.9 |
| (N2C2) | 137.3 | 138.9 | 138.5 | 137.5 | 137.6 | 137.3 | 137.6 | 137.3 | 136.9 |
| (N3C7) | 137.3 | 139.2 | 137.8 | 137.5 | 137.6 | 137.3 | 137.6 | 137.3 | 136.9 |
| (N3C8) | 137.3 | 139.2 | 137.8 | 137.5 | 137.8 | 137.3 | 137.6 | 137.3 | 136.9 |
| (N4C5) | 137.3 | 138.9 | 138.5 | 137.5 | 137.7 | 137.3 | 137.6 | 137.3 | 136.9 |
| (N4C6) | 137.3 | 138.9 | 138.5 | 137.5 | 137.7 | 137.3 | 137.6 | 137.3 | 136.9 |
| (N5C2) | 132.8 | 133.0 | 132.4 | 132.3 | 132.1 | 132.0 | 131.6 | 131.6 | 131.6 |
| (N5C3) | 132.8 | 130.9 | 131.8 | 132.3 | 132.0 | 132.0 | 131.6 | 131.6 | 131.6 |
| (N6C6) | 132.8 | 133.0 | 132.4 | 132.3 | 132.1 | 132.0 | 131.6 | 131.6 | 131.6 |
| (N6C7) | 132.8 | 130.9 | 131.8 | 132.3 | 131.9 | 132.0 | 131.6 | 131.6 | 131.6 |
| (N7C4) | 132.8 | 130.9 | 131.8 | 132.3 | 131.9 | 132.0 | 131.6 | 131.6 | 131.6 |
| (N7C5) | 132.8 | 133.0 | 132.4 | 132.3 | 132.1 | 132.0 | 131.6 | 131.6 | 131.6 |
| (N8C1) | 132.8 | 133.0 | 132.4 | 132.3 | 132.1 | 132.0 | 131.6 | 131.6 | 131.6 |
| (N8C8) | 132.8 | 130.9 | 131.8 | 132.3 | 132.0 | 132.0 | 131.6 | 131.6 | 131.6 |
| Длины связей C–C, *пм* | | | | | | | | | |
| (C7C14) | 145.7 | 145.5 | 145.6 | 145.4 | 145.2 | 145.2 | 145.1 | 145.2 | 145.3 |
| (C14C13) | 140.9 | 140.4 | 140.5 | 140.7 | 140.5 | 140.4 | 140.1 | 140.0 | 140.2 |
| (C13C8) | 145.7 | 145.5 | 145.6 | 145.4 | 145.3 | 145.2 | 145.1 | 145.2 | 145.3 |
| (C1C11) | 145.7 | 143.9 | 144.6 | 145.4 | 145.1 | 145.2 | 145.1 | 145.2 | 145.3 |
| (C11C12) | 140.9 | 141.2 | 140.8 | 140.7 | 140.6 | 140.4 | 140.1 | 140.0 | 140.2 |
| (C12C2) | 145.7 | 143.9 | 144.6 | 145.4 | 145.1 | 145.2 | 145.1 | 145.2 | 145.3 |
| (C3C10) | 145.7 | 145.5 | 145.6 | 145.4 | 145.3 | 145.2 | 145.1 | 145.2 | 145.3 |
| (C10C9) | 140.9 | 140.4 | 140.5 | 140.7 | 140.5 | 140.4 | 140.1 | 140.0 | 140.2 |
| (C9C4) | 145.7 | 145.5 | 145.6 | 145.4 | 145.2 | 145.2 | 145.1 | 145.2 | 145.3 |
| (C5C15) | 145.7 | 143.9 | 144.6 | 145.4 | 145.1 | 145.2 | 145.1 | 145.2 | 145.3 |
| (C15C16) | 140.9 | 141.2 | 140.8 | 140.7 | 140.6 | 140.4 | 140.1 | 140.0 | 140.2 |
| (C16C6) | 145.7 | 143.9 | 144.6 | 145.4 | 145.1 | 145.2 | 145.1 | 145.2 | 145.3 |
| Длины связей C–H, *пм* | | | | | | | | | |
| (C17H1) | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 |
| (C18H2) | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 |
| (C19H3) | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 |
| (C20H4) | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 | 108.8 |
| (C25H9) | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 |
| (C26H10) | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 |
| (C27H11) | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 |
| (C28H12) | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 | 109.0 |
| Валентные углы ∠NMN в хелатном узле, *град* | | | | | | | | | |
| (N1M1N2) | 81.6 | 86.0 | 86.9 | 88.8 | 89.4 | 88.6 | 89.7 | 89.7 | 89.5 |
| (N2M1N3) | 81.6 | 86.0 | 86.9 | 88.8 | 89.4 | 88.6 | 89.7 | 89.7 | 89.5 |
| (N3M1N4) | 81.6 | 86.0 | 86.9 | 88.8 | 88.3 | 88.6 | 89.7 | 89.7 | 89.5 |
| (N4M1N1) | 81.6 | 86.0 | 86.9 | 88.8 | 88.3 | 88.6 | 89.7 | 89.7 | 89.5 |
| *Сумма углов*  ***VAS*** | **326.4** | **344.0** | **349.6** | **355.2** | **355.4** | **354.4** | **358.8** | **358.8** | **358.0** |
| Невалентные углы ∠NNN в группировке атомов N4 хелатного узла, *град* | | | | | | | | | |
| (N1N2N3) | 90.0 | 91.1 | 91.5 | 90.0 | 89.7 | 90.0 | 90.0 | 90.0 | 90.0 |
| (N2N3N4) | 90.0 | 88.7 | 88.2 | 90.0 | 90.0 | 90.0 | 90.0 | 90.0 | 90.0 |
| (N3N4N1) | 90.0 | 91.1 | 91.5 | 90.0 | 90.3 | 90.0 | 90.0 | 90.0 | 90.0 |
| (N4N1N2) | 90.0 | 88.7 | 88.2 | 90.0 | 90.0 | 90.0 | 90.0 | 90.0 | 90.0 |
| *Сумма углов*  (NVAS) | 360.0 | 359.6 | 359.4 | 360.0 | 360.0 | 360.0 | 360.0 | 360.0 | 360.0 |
| Валентные углы в 6-членном хелатном цикле (N1C4N7C5N4M1), *град* | | | | | | | | | |
| (M1N1C4) | 124.4 | 126.1 | 126.0 | 125.4 | 126.5 | 125.6 | 126.2 | 126.0 | 125.3 |
| (N1C4N7) | 127.6 | 127.0 | 127.1 | 127.6 | 127.5 | 128.0 | 127.9 | 128.2 | 128.8 |
| (C4N7C5) | 124.3 | 123.5 | 123.2 | 123.6 | 122.3 | 122.0 | 121.5 | 121.2 | 121.2 |
| (N7C5N4) | 127.6 | 127.0 | 127.1 | 127.6 | 127.5 | 128.0 | 127.9 | 128.2 | 128.8 |
| (C5N4M1) | 124.4 | 126.1 | 126.0 | 125.4 | 126.5 | 125.6 | 126.2 | 126.0 | 125.3 |
| (N4M1N1) | 81.6 | 86.0 | 86.9 | 88.8 | 88.3 | 88.6 | 89.7 | 89.7 | 89.5 |
| *Сумма углов*  (VAS6) | **709.9** | **712.8** | **715.6** | **718.4** | **718.0** | **717.8** | **718.4** | **719.3** | **718.9** |
| Валентные углы в 6-членном хелатном цикле (M1N2C2N5C3N1), *град* | | | | | | | | | |
| (M1N2C2) | 124.4 | 126.1 | 126.0 | 125.4 | 125.8 | 125.6 | 126.2 | 126.0 | 125.3 |
| (N2C2N5) | 127.6 | 127.0 | 127.1 | 127.6 | 127.6 | 128.0 | 127.9 | 128.2 | 128.8 |
| (C2N5C3) | 124.3 | 123.5 | 123.2 | 123.6 | 122.6 | 122.0 | 121.5 | 121.2 | 121.2 |
| (N5C3N1) | 127.6 | 127.0 | 127.1 | 127.6 | 127.9 | 128.0 | 127.9 | 128.2 | 128.8 |
| (C3N1M1) | 124.4 | 126.1 | 126.0 | 125.4 | 125.1 | 125.6 | 126.2 | 126.0 | 125.3 |
| (N1M1N2) | 81.6 | 86.0 | 86.9 | 88.8 | 89.4 | 88.6 | 89.7 | 89.7 | 89.5 |
| *Сумма углов*  (VAS6) | **709.9** | **712.8** | **715.6** | **718.4** | **718.4** | **717.8** | **718.4** | **719.3** | **718.9** |
| Валентные углы (FMN), *deg* | | | | | | | | | |
| (F1M1N1) | 112.5 | 103.8 | 101.5 | 98.3 | 98.0 | 99.0 | 94.1 | 94.2 | 95.5 |
| (F1M1N2) | 112.5 | 107.1 | 105.6 | 98.3 | 97.0 | 99.0 | 94.1 | 94.2 | 95.5 |
| (F1M1N3) | 112.5 | 103.8 | 101.5 | 98.3 | 98.0 | 99.0 | 94.1 | 94.2 | 95.5 |
| (F1M1N4) | 112.5 | 107.1 | 105.6 | 98.3 | 99.2 | 99.0 | 94.1 | 94.2 | 95.5 |
| Валентные углы в 5-членном нехелатном цикле (C3N1C4C9C10), *град* | | | | | | | | | |
| (C3N1C4) | 109.0 | 107.8 | 108.0 | 108.8 | 107.8 | 108.0 | 107.2 | 107.7 | 108.6 |
| (N1C4C9) | 109.0 | 109.3 | 109.5 | 109.0 | 109.7 | 109.6 | 110.1 | 109.8 | 109.2 |
| (C4C9C10) | 106.5 | 106.8 | 106.5 | 106.6 | 106.4 | 106.4 | 106.3 | 106.3 | 106.5 |
| (C9C10C3) | 106.5 | 106.8 | 106.5 | 106.6 | 106.5 | 106.4 | 106.3 | 106.3 | 106.5 |
| (C10C3N1) | 109.0 | 109.3 | 109.5 | 109.0 | 109.6 | 109.6 | 110.1 | 109.8 | 109.2 |
| *Сумма углов*  (VAS5) | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 |
| Валентные углы в 5-членном нехелатном цикле (C2N2C1C11C12), *град* | | | | | | | | | |
| (C2N2C1) | 109.0 | 108.1 | 108.2 | 108.8 | 108.0 | 108.0 | 107.2 | 107.7 | 108.6 |
| (N2C1C11) | 109.0 | 109.0 | 109.1 | 109.0 | 109.5 | 109.6 | 110.1 | 109.8 | 109.2 |
| (C1C11C12) | 106.5 | 106.9 | 106.8 | 106.6 | 106.5 | 106.4 | 106.3 | 106.3 | 106.5 |
| (C11C12C2) | 106.5 | 106.9 | 106.8 | 106.6 | 106.5 | 106.4 | 106.3 | 106.3 | 106.5 |
| (C12C2N2) | 109.0 | 109.1 | 109.1 | 109.0 | 109.5 | 109.6 | 110.1 | 109.8 | 109.2 |
| *Сумма углов*  (VAS5) | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 | 540.0 |
| Валентные углы в 6-членном нехелатном цикле (C9C10C18C26C25C17), *град* | | | | | | | | | |
| (C9C10C18) | 121.0 | 121.1 | 121.1 | 121.1 | 121.2 | 121.2 | 121.3 | 121.3 | 121.4 |
| (C10C18C26) | 117.8 | 117.7 | 121.1 | 117.7 | 117.6 | 117.5 | 117.5 | 117.4 | 117.3 |
| (C18C26C25) | 121.2 | 121.2 | 117.7 | 121.2 | 121.2 | 121.3 | 121.2 | 121.3 | 121.3 |
| (C26C25C17) | 121.2 | 121.2 | 121.2 | 121.2 | 121.2 | 121.3 | 121.2 | 121.3 | 121.3 |
| (C25C17C9) | 117.8 | 117.7 | 121.2 | 117.7 | 117.6 | 117.5 | 117.5 | 117.4 | 117.3 |
| (C17C9C10) | 121.0 | 121.1 | 117.7 | 121.1 | 121.2 | 121.2 | 121.3 | 121.3 | 121.4 |
| *Сумма углов*  (VAS6) | 720.0 | 720.0 | 720.0 | 720.0 | 720.0 | 720.0 | 720.0 | 720.0 | 720.0 |

*Таблица 2*

Стандартные термодинамические параметры образования комплексов M(III) с фталоцианином и фторид-анионом в газовой фазе

|  |  |  |  |
| --- | --- | --- | --- |
| M(III) | Термодинамические параметры | | |
| *H*0f, 298, кДж/моль | *S*0f, 298, Дж/моль∙К | *G*0f, 298, кДж/моль |
| Sc | –305.6 | 1122.3 | –62.0 |
| Ti | –598.6 | 1119.4 | –355.3 |
| V | –228.0 | 1121.0 | 12.7 |
| Cr | –120.5 | 1113.3 | 364.5 |
| Mn | –35.7 | 1120.0 | 207.9 |
| Fe | 63.0 | 1130.4 | 302.1 |
| Co | 173.6 | 1118.5 | 417.1 |
| Ni | 252.2 | 1141.9 | 488.5 |
| Cu | 483.6 | 1130.1 | 724.5 |

**NBO Analysis Data**

**Sc(III) Complex**

**<S^2> = 0.0000**

**Summary of Natural Population Analysis:**

**Natural Population**

**Natural -----------------------------------------------**

**Atom No Charge Core Valence Rydberg Total**

**-----------------------------------------------------------------------**

**Sc 1 1.42605 17.97955 1.54587 0.04852 19.57395**

**N 2 -0.53943 1.99925 5.52363 0.01656 7.53943**

**N 3 -0.53943 1.99925 5.52363 0.01656 7.53943**

**N 4 -0.53943 1.99925 5.52363 0.01656 7.53943**

**N 5 -0.53943 1.99925 5.52363 0.01656 7.53943**

**C 6 0.36132 1.99921 3.61987 0.01959 5.63868**

**C 7 0.36133 1.99921 3.61987 0.01959 5.63867**

**C 8 0.36132 1.99921 3.61987 0.01959 5.63868**

**C 9 0.36133 1.99921 3.61987 0.01959 5.63867**

**C 10 0.36132 1.99921 3.61987 0.01959 5.63868**

**C 11 0.36133 1.99921 3.61987 0.01959 5.63867**

**C 12 0.36132 1.99921 3.61987 0.01959 5.63868**

**C 13 0.36133 1.99921 3.61987 0.01959 5.63867**

**N 14 -0.39442 1.99935 5.38125 0.01382 7.39442**

**N 15 -0.39442 1.99935 5.38125 0.01382 7.39442**

**N 16 -0.39442 1.99935 5.38125 0.01382 7.39442**

**N 17 -0.39442 1.99935 5.38125 0.01382 7.39442**

**C 18 -0.08225 1.99907 4.06731 0.01587 6.08225**

**C 19 -0.08225 1.99907 4.06731 0.01587 6.08225**

**C 20 -0.08225 1.99907 4.06731 0.01587 6.08225**

**C 21 -0.08225 1.99907 4.06731 0.01587 6.08225**

**C 22 -0.08225 1.99907 4.06731 0.01587 6.08225**

**C 23 -0.08225 1.99907 4.06731 0.01587 6.08225**

**C 24 -0.08225 1.99907 4.06731 0.01587 6.08225**

**C 25 -0.08225 1.99907 4.06731 0.01587 6.08225**

**C 26 -0.17394 1.99913 4.16296 0.01185 6.17394**

**C 27 -0.17394 1.99913 4.16296 0.01185 6.17394**

**C 28 -0.17394 1.99913 4.16296 0.01185 6.17394**

**C 29 -0.17394 1.99913 4.16296 0.01185 6.17394**

**C 30 -0.17394 1.99913 4.16296 0.01185 6.17394**

**C 31 -0.17394 1.99913 4.16296 0.01185 6.17394**

**C 32 -0.17394 1.99913 4.16296 0.01185 6.17394**

**C 33 -0.17394 1.99913 4.16296 0.01185 6.17394**

**C 34 -0.20802 1.99926 4.19692 0.01184 6.20802**

**H 35 0.23594 0.00000 0.76219 0.00187 0.76406**

**C 36 -0.20802 1.99926 4.19692 0.01184 6.20802**

**H 37 0.23594 0.00000 0.76219 0.00187 0.76406**

**C 38 -0.20802 1.99926 4.19692 0.01184 6.20802**

**H 39 0.23594 0.00000 0.76219 0.00187 0.76406**

**C 40 -0.20802 1.99926 4.19692 0.01184 6.20802**

**H 41 0.23594 0.00000 0.76219 0.00187 0.76406**

**C 42 -0.20802 1.99926 4.19692 0.01184 6.20802**

**H 43 0.23594 0.00000 0.76219 0.00187 0.76406**

**C 44 -0.20802 1.99926 4.19692 0.01184 6.20802**

**H 45 0.23594 0.00000 0.76219 0.00187 0.76406**

**C 46 -0.20802 1.99926 4.19692 0.01184 6.20802**

**H 47 0.23594 0.00000 0.76219 0.00187 0.76406**

**C 48 -0.20802 1.99926 4.19692 0.01184 6.20802**

**H 49 0.23594 0.00000 0.76219 0.00187 0.76406**

**H 50 0.22311 0.00000 0.77564 0.00125 0.77689**

**H 51 0.22311 0.00000 0.77564 0.00125 0.77689**

**H 52 0.22311 0.00000 0.77564 0.00125 0.77689**

**H 53 0.22311 0.00000 0.77564 0.00125 0.77689**

**H 54 0.22311 0.00000 0.77564 0.00125 0.77689**

**H 55 0.22311 0.00000 0.77564 0.00125 0.77689**

**H 56 0.22311 0.00000 0.77564 0.00125 0.77689**

**H 57 0.22311 0.00000 0.77564 0.00125 0.77689**

**F 58 -0.53997 1.99996 7.53693 0.00308 9.53997**

**=======================================================================**

**\* Total \* -0.00000 99.94730 193.38145 0.67125 294.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

**NAO Atom No lang Type(AO) Occupancy Energy**

**----------------------------------------------------------**

**1 Sc 1 S Cor( 1S) 2.00000 -157.69887**

**2 Sc 1 S Cor( 2S) 1.99999 -19.37071**

**3 Sc 1 S Cor( 3S) 1.99472 -2.62157**

**4 Sc 1 S Val( 4S) 0.15705 0.20222**

**5 Sc 1 S Ryd( 6S) 0.00056 1.08689**

**6 Sc 1 S Ryd( 5S) 0.00021 0.85430**

**7 Sc 1 px Cor( 2p) 2.00000 -14.21120**

**8 Sc 1 px Cor( 3p) 1.99476 -1.20918**

**9 Sc 1 px Val( 4p) 0.10543 0.24450**

**10 Sc 1 px Ryd( 5p) 0.00032 1.44827**

**11 Sc 1 py Cor( 2p) 2.00000 -14.21120**

**12 Sc 1 py Cor( 3p) 1.99476 -1.20918**

**13 Sc 1 py Val( 4p) 0.10543 0.24450**

**14 Sc 1 py Ryd( 5p) 0.00032 1.44827**

**15 Sc 1 pz Cor( 2p) 2.00000 -14.21001**

**16 Sc 1 pz Cor( 3p) 1.99532 -1.20290**

**17 Sc 1 pz Val( 4p) 0.08934 0.19427**

**18 Sc 1 pz Ryd( 5p) 0.00030 1.44252**

**19 Sc 1 dxy Val( 3d) 0.02854 -0.02916**

**20 Sc 1 dxy Ryd( 4d) 0.00147 0.45675**

**21 Sc 1 dxy Ryd( 5d) 0.00008 1.70706**

**22 Sc 1 dxz Val( 3d) 0.24342 -0.00594**

**23 Sc 1 dxz Ryd( 4d) 0.00403 0.52314**

**24 Sc 1 dxz Ryd( 5d) 0.00022 1.37221**

**25 Sc 1 dyz Val( 3d) 0.24342 -0.00594**

**26 Sc 1 dyz Ryd( 4d) 0.00403 0.52314**

**27 Sc 1 dyz Ryd( 5d) 0.00022 1.37221**

**28 Sc 1 dx2y2 Val( 3d) 0.34461 -0.00227**

**29 Sc 1 dx2y2 Ryd( 4d) 0.00847 0.45177**

**30 Sc 1 dx2y2 Ryd( 5d) 0.00008 1.59698**

**31 Sc 1 dz2 Val( 3d) 0.22863 0.00786**

**32 Sc 1 dz2 Ryd( 4d) 0.02812 0.47705**

**33 Sc 1 dz2 Ryd( 5d) 0.00007 1.63282**

**Ti(III) Complex**

**<S^2>= 0.7532**

**Summary of Natural Population Analysis:**

**Natural Population**

**Natural -----------------------------------------------**

**Atom No Charge Core Valence Rydberg Total**

**-----------------------------------------------------------------------**

**Ti 1 1.07001 17.97701 2.90839 0.04458 20.92999**

**N 2 -0.48401 1.99930 5.46576 0.01896 7.48401**

**N 3 -0.46098 1.99926 5.44398 0.01775 7.46098**

**N 4 -0.48401 1.99930 5.46576 0.01896 7.48401**

**N 5 -0.46098 1.99926 5.44398 0.01775 7.46098**

**C 6 0.33352 1.99917 3.64811 0.01920 5.66648**

**C 7 0.33352 1.99917 3.64811 0.01920 5.66648**

**C 8 0.36260 1.99922 3.61841 0.01978 5.63740**

**C 9 0.36260 1.99922 3.61841 0.01978 5.63740**

**C 10 0.33352 1.99917 3.64811 0.01920 5.66648**

**C 11 0.33352 1.99917 3.64811 0.01920 5.66648**

**C 12 0.36260 1.99922 3.61841 0.01978 5.63740**

**C 13 0.36260 1.99922 3.61841 0.01978 5.63740**

**N 14 -0.38305 1.99931 5.36958 0.01416 7.38305**

**N 15 -0.38305 1.99931 5.36958 0.01416 7.38305**

**N 16 -0.38305 1.99931 5.36958 0.01416 7.38305**

**N 17 -0.38305 1.99931 5.36958 0.01416 7.38305**

**C 18 -0.08014 1.99905 4.06532 0.01577 6.08014**

**C 19 -0.08014 1.99905 4.06532 0.01577 6.08014**

**C 20 -0.08506 1.99907 4.07022 0.01577 6.08506**

**C 21 -0.08506 1.99907 4.07022 0.01577 6.08506**

**C 22 -0.08014 1.99905 4.06532 0.01577 6.08014**

**C 23 -0.08014 1.99905 4.06532 0.01577 6.08014**

**C 24 -0.08506 1.99907 4.07022 0.01577 6.08506**

**C 25 -0.08506 1.99907 4.07022 0.01577 6.08506**

**C 26 -0.17508 1.99913 4.16409 0.01185 6.17508**

**C 27 -0.17508 1.99913 4.16409 0.01185 6.17508**

**C 28 -0.17519 1.99914 4.16420 0.01186 6.17519**

**C 29 -0.17519 1.99914 4.16420 0.01186 6.17519**

**C 30 -0.17508 1.99913 4.16409 0.01185 6.17508**

**C 31 -0.17508 1.99913 4.16409 0.01185 6.17508**

**C 32 -0.17519 1.99914 4.16420 0.01186 6.17519**

**C 33 -0.17519 1.99914 4.16420 0.01186 6.17519**

**C 34 -0.20788 1.99926 4.19678 0.01184 6.20788**

**H 35 0.23629 0.00000 0.76185 0.00186 0.76371**

**C 36 -0.20788 1.99926 4.19678 0.01184 6.20788**

**H 37 0.23629 0.00000 0.76185 0.00186 0.76371**

**C 38 -0.21164 1.99926 4.20039 0.01199 6.21164**

**H 39 0.23474 0.00000 0.76340 0.00187 0.76526**

**C 40 -0.21164 1.99926 4.20039 0.01199 6.21164**

**H 41 0.23474 0.00000 0.76340 0.00187 0.76526**

**C 42 -0.20788 1.99926 4.19678 0.01184 6.20788**

**H 43 0.23629 0.00000 0.76185 0.00186 0.76371**

**C 44 -0.20788 1.99926 4.19678 0.01184 6.20788**

**H 45 0.23629 0.00000 0.76185 0.00186 0.76371**

**C 46 -0.21163 1.99926 4.20039 0.01199 6.21163**

**H 47 0.23474 0.00000 0.76340 0.00187 0.76526**

**C 48 -0.21164 1.99926 4.20039 0.01199 6.21164**

**H 49 0.23474 0.00000 0.76340 0.00187 0.76526**

**H 50 0.22343 0.00000 0.77533 0.00124 0.77657**

**H 51 0.22343 0.00000 0.77533 0.00124 0.77657**

**H 52 0.22231 0.00000 0.77644 0.00125 0.77769**

**H 53 0.22231 0.00000 0.77644 0.00125 0.77769**

**H 54 0.22343 0.00000 0.77533 0.00124 0.77657**

**H 55 0.22343 0.00000 0.77533 0.00124 0.77657**

**H 56 0.22231 0.00000 0.77644 0.00125 0.77769**

**H 57 0.22231 0.00000 0.77644 0.00125 0.77769**

**F 58 -0.35935 1.99995 7.35504 0.00436 9.35935**

**=======================================================================**

**\* Total \* 0.00000 99.94447 194.37943 0.67610 295.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

**NAO Atom No lang Type(AO) Occupancy**

**--------------------------------------------**

**1 Ti 1 S Cor( 1S) 2.00000**

**2 Ti 1 S Cor( 2S) 1.99999**

**3 Ti 1 S Cor( 3S) 1.99349**

**4 Ti 1 S Val( 4S) 0.19900**

**5 Ti 1 S Ryd( 5S) 0.00093**

**6 Ti 1 S Ryd( 6S) 0.00040**

**7 Ti 1 px Cor( 2p) 2.00000**

**8 Ti 1 px Cor( 3p) 1.99410**

**9 Ti 1 px Val( 4p) 0.14150**

**10 Ti 1 px Ryd( 5p) 0.00047**

**11 Ti 1 py Cor( 2p) 2.00000**

**12 Ti 1 py Cor( 3p) 1.99547**

**13 Ti 1 py Val( 4p) 0.14925**

**14 Ti 1 py Ryd( 5p) 0.00043**

**15 Ti 1 pz Cor( 2p) 2.00000**

**16 Ti 1 pz Cor( 3p) 1.99397**

**17 Ti 1 pz Val( 4p) 0.11294**

**18 Ti 1 pz Ryd( 5p) 0.00049**

**19 Ti 1 dxy Val( 3d) 0.21541**

**20 Ti 1 dxy Ryd( 4d) 0.00283**

**21 Ti 1 dxy Ryd( 5d) 0.00011**

**22 Ti 1 dxz Val( 3d) 0.41189**

**23 Ti 1 dxz Ryd( 4d) 0.00361**

**24 Ti 1 dxz Ryd( 5d) 0.00018**

**25 Ti 1 dyz Val( 3d) 0.56958**

**26 Ti 1 dyz Ryd( 4d) 0.00682**

**27 Ti 1 dyz Ryd( 5d) 0.00012**

**28 Ti 1 dx2y2 Val( 3d) 0.67027**

**29 Ti 1 dx2y2 Ryd( 4d) 0.00968**

**30 Ti 1 dx2y2 Ryd( 5d) 0.00016**

**31 Ti 1 dz2 Val( 3d) 0.43855**

**32 Ti 1 dz2 Ryd( 4d) 0.01826**

**33 Ti 1 dz2 Ryd( 5d) 0.00009**

**V(III) Complex**

**<S^2>= 2.0261**

**Summary of Natural Population Analysis:**

**Natural Population**

**Natural -----------------------------------------------**

**Atom No Charge Core Valence Rydberg Total**

**-----------------------------------------------------------------------**

**V 1 0.72854 17.98072 4.25145 0.03929 22.27146**

**N 2 -0.42284 1.99936 5.39916 0.02431 7.42284**

**N 3 -0.41113 1.99932 5.39166 0.02015 7.41113**

**N 4 -0.42284 1.99936 5.39916 0.02431 7.42284**

**N 5 -0.41113 1.99932 5.39166 0.02015 7.41113**

**C 6 0.35175 1.99918 3.62950 0.01957 5.64825**

**C 7 0.35175 1.99918 3.62950 0.01957 5.64825**

**C 8 0.36335 1.99921 3.61761 0.01983 5.63665**

**C 9 0.36335 1.99921 3.61761 0.01983 5.63665**

**C 10 0.35175 1.99918 3.62950 0.01957 5.64825**

**C 11 0.35175 1.99918 3.62950 0.01957 5.64825**

**C 12 0.36335 1.99921 3.61761 0.01983 5.63665**

**C 13 0.36335 1.99921 3.61761 0.01983 5.63665**

**N 14 -0.38960 1.99934 5.37593 0.01433 7.38960**

**N 15 -0.38960 1.99934 5.37593 0.01433 7.38960**

**N 16 -0.38960 1.99934 5.37593 0.01433 7.38960**

**N 17 -0.38960 1.99934 5.37593 0.01433 7.38960**

**C 18 -0.08137 1.99906 4.06666 0.01566 6.08137**

**C 19 -0.08137 1.99906 4.06666 0.01566 6.08137**

**C 20 -0.08049 1.99906 4.06556 0.01586 6.08049**

**C 21 -0.08049 1.99906 4.06556 0.01586 6.08049**

**C 22 -0.08137 1.99906 4.06666 0.01566 6.08137**

**C 23 -0.08137 1.99906 4.06666 0.01566 6.08137**

**C 24 -0.08049 1.99906 4.06556 0.01586 6.08049**

**C 25 -0.08049 1.99906 4.06556 0.01586 6.08049**

**C 26 -0.17542 1.99913 4.16440 0.01189 6.17542**

**C 27 -0.17542 1.99913 4.16440 0.01189 6.17542**

**C 28 -0.17453 1.99913 4.16352 0.01188 6.17453**

**C 29 -0.17453 1.99913 4.16352 0.01188 6.17453**

**C 30 -0.17542 1.99913 4.16440 0.01189 6.17542**

**C 31 -0.17542 1.99913 4.16440 0.01189 6.17542**

**C 32 -0.17453 1.99913 4.16352 0.01188 6.17453**

**C 33 -0.17453 1.99913 4.16352 0.01188 6.17453**

**C 34 -0.20893 1.99926 4.19780 0.01187 6.20893**

**H 35 0.23551 0.00000 0.76262 0.00187 0.76449**

**C 36 -0.20893 1.99926 4.19780 0.01187 6.20893**

**H 37 0.23551 0.00000 0.76262 0.00187 0.76449**

**C 38 -0.20833 1.99926 4.19718 0.01189 6.20833**

**H 39 0.23628 0.00000 0.76185 0.00187 0.76372**

**C 40 -0.20833 1.99926 4.19718 0.01189 6.20833**

**H 41 0.23628 0.00000 0.76185 0.00187 0.76372**

**C 42 -0.20893 1.99926 4.19780 0.01187 6.20893**

**H 43 0.23551 0.00000 0.76262 0.00187 0.76449**

**C 44 -0.20893 1.99926 4.19780 0.01187 6.20893**

**H 45 0.23551 0.00000 0.76262 0.00187 0.76449**

**C 46 -0.20833 1.99926 4.19718 0.01189 6.20833**

**H 47 0.23628 0.00000 0.76185 0.00187 0.76372**

**C 48 -0.20833 1.99926 4.19718 0.01189 6.20833**

**H 49 0.23628 0.00000 0.76185 0.00187 0.76372**

**H 50 0.22283 0.00000 0.77592 0.00125 0.77717**

**H 51 0.22283 0.00000 0.77592 0.00125 0.77717**

**H 52 0.22295 0.00000 0.77581 0.00125 0.77705**

**H 53 0.22295 0.00000 0.77581 0.00125 0.77705**

**H 54 0.22283 0.00000 0.77592 0.00125 0.77717**

**H 55 0.22283 0.00000 0.77592 0.00125 0.77717**

**H 56 0.22295 0.00000 0.77581 0.00125 0.77705**

**H 57 0.22295 0.00000 0.77581 0.00125 0.77705**

**F 58 -0.31662 1.99996 7.31193 0.00472 9.31662**

**=======================================================================**

**\* Total \* -0.00000 99.94857 195.36242 0.68901 296.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

**NAO Atom No lang Type(AO) Occupancy**

**--------------------------------------------**

**1 V 1 S Cor( 1S) 2.00000**

**2 V 1 S Cor( 2S) 1.99999**

**3 V 1 S Cor( 3S) 1.99381**

**4 V 1 S Val( 4S) 0.21551**

**5 V 1 S Ryd( 5S) 0.00107**

**6 V 1 S Ryd( 6S) 0.00043**

**7 V 1 px Cor( 2p) 2.00000**

**8 V 1 px Cor( 3p) 1.99680**

**9 V 1 px Val( 4p) 0.16389**

**10 V 1 px Ryd( 5p) 0.00044**

**11 V 1 py Cor( 2p) 2.00000**

**12 V 1 py Cor( 3p) 1.99545**

**13 V 1 py Val( 4p) 0.15887**

**14 V 1 py Ryd( 5p) 0.00045**

**15 V 1 pz Cor( 2p) 2.00000**

**16 V 1 pz Cor( 3p) 1.99467**

**17 V 1 pz Val( 4p) 0.11923**

**18 V 1 pz Ryd( 5p) 0.00054**

**19 V 1 dxy Val( 3d) 1.01639**

**20 V 1 dxy Ryd( 4d) 0.00438**

**21 V 1 dxy Ryd( 5d) 0.00024**

**22 V 1 dxz Val( 3d) 0.89249**

**23 V 1 dxz Ryd( 4d) 0.00934**

**24 V 1 dxz Ryd( 5d) 0.00009**

**25 V 1 dyz Val( 3d) 0.44507**

**26 V 1 dyz Ryd( 4d) 0.00257**

**27 V 1 dyz Ryd( 5d) 0.00011**

**28 V 1 dx2y2 Val( 3d) 0.72743**

**29 V 1 dx2y2 Ryd( 4d) 0.01064**

**30 V 1 dx2y2 Ryd( 5d) 0.00008**

**31 V 1 dz2 Val( 3d) 0.51258**

**32 V 1 dz2 Ryd( 4d) 0.00885**

**33 V 1 dz2 Ryd( 5d) 0.00006**

**Cr(III) Complex**

**<S^2>= 3.7965**

**Summary of Natural Population Analysis:**

**Natural Population**

**Natural -----------------------------------------------**

**Atom No Charge Core Valence Rydberg Total**

**-----------------------------------------------------------------------**

**Cr 1 0.71836 17.98564 5.24764 0.04835 23.28164**

**N 2 -0.41777 1.99933 5.38661 0.03182 7.41777**

**N 3 -0.41777 1.99933 5.38661 0.03182 7.41777**

**N 4 -0.41777 1.99933 5.38661 0.03182 7.41777**

**N 5 -0.41777 1.99933 5.38662 0.03182 7.41777**

**C 6 0.36388 1.99920 3.61711 0.01981 5.63612**

**C 7 0.36389 1.99920 3.61711 0.01981 5.63611**

**C 8 0.36388 1.99920 3.61711 0.01981 5.63612**

**C 9 0.36388 1.99920 3.61711 0.01981 5.63612**

**C 10 0.36388 1.99920 3.61711 0.01981 5.63612**

**C 11 0.36388 1.99920 3.61711 0.01981 5.63612**

**C 12 0.36388 1.99920 3.61711 0.01981 5.63612**

**C 13 0.36388 1.99920 3.61711 0.01981 5.63612**

**N 14 -0.38825 1.99934 5.37479 0.01413 7.38825**

**N 15 -0.38825 1.99934 5.37479 0.01413 7.38825**

**N 16 -0.38825 1.99934 5.37479 0.01413 7.38825**

**N 17 -0.38825 1.99934 5.37479 0.01413 7.38825**

**C 18 -0.08017 1.99906 4.06538 0.01573 6.08017**

**C 19 -0.08017 1.99906 4.06537 0.01573 6.08017**

**C 20 -0.08017 1.99906 4.06537 0.01573 6.08017**

**C 21 -0.08017 1.99906 4.06538 0.01573 6.08017**

**C 22 -0.08017 1.99906 4.06538 0.01573 6.08017**

**C 23 -0.08017 1.99906 4.06537 0.01573 6.08017**

**C 24 -0.08017 1.99906 4.06537 0.01573 6.08017**

**C 25 -0.08017 1.99906 4.06538 0.01573 6.08017**

**C 26 -0.17475 1.99913 4.16375 0.01187 6.17475**

**C 27 -0.17475 1.99913 4.16375 0.01187 6.17475**

**C 28 -0.17475 1.99913 4.16375 0.01187 6.17475**

**C 29 -0.17475 1.99913 4.16375 0.01187 6.17475**

**C 30 -0.17475 1.99913 4.16375 0.01187 6.17475**

**C 31 -0.17475 1.99913 4.16375 0.01187 6.17475**

**C 32 -0.17475 1.99913 4.16375 0.01187 6.17475**

**C 33 -0.17475 1.99913 4.16375 0.01187 6.17475**

**C 34 -0.20830 1.99926 4.19717 0.01186 6.20830**

**H 35 0.23598 0.00000 0.76215 0.00187 0.76402**

**C 36 -0.20830 1.99926 4.19718 0.01186 6.20830**

**H 37 0.23598 0.00000 0.76215 0.00187 0.76402**

**C 38 -0.20830 1.99926 4.19718 0.01186 6.20830**

**H 39 0.23598 0.00000 0.76215 0.00187 0.76402**

**C 40 -0.20830 1.99926 4.19717 0.01186 6.20830**

**H 41 0.23598 0.00000 0.76215 0.00187 0.76402**

**C 42 -0.20830 1.99926 4.19717 0.01186 6.20830**

**H 43 0.23598 0.00000 0.76215 0.00187 0.76402**

**C 44 -0.20830 1.99926 4.19718 0.01186 6.20830**

**H 45 0.23598 0.00000 0.76215 0.00187 0.76402**

**C 46 -0.20830 1.99926 4.19718 0.01186 6.20830**

**H 47 0.23598 0.00000 0.76215 0.00187 0.76402**

**C 48 -0.20830 1.99926 4.19717 0.01186 6.20830**

**H 49 0.23598 0.00000 0.76215 0.00187 0.76402**

**H 50 0.22306 0.00000 0.77569 0.00125 0.77694**

**H 51 0.22306 0.00000 0.77569 0.00125 0.77694**

**H 52 0.22306 0.00000 0.77569 0.00125 0.77694**

**H 53 0.22306 0.00000 0.77569 0.00125 0.77694**

**H 54 0.22306 0.00000 0.77569 0.00125 0.77694**

**H 55 0.22306 0.00000 0.77569 0.00125 0.77694**

**H 56 0.22306 0.00000 0.77569 0.00125 0.77694**

**H 57 0.22306 0.00000 0.77569 0.00125 0.77694**

**F 58 -0.37188 1.99997 7.36357 0.00834 9.37188**

**=======================================================================**

**\* Total \* 0.00000 99.95348 196.30688 0.73964 297.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

**NAO Atom No lang Type(AO) Occupancy**

**--------------------------------------------**

**1 Cr 1 S Cor( 1S) 2.00000**

**2 Cr 1 S Cor( 2S) 1.99999**

**3 Cr 1 S Cor( 3S) 1.99452**

**4 Cr 1 S Val( 4S) 0.22947**

**5 Cr 1 S Ryd( 5S) 0.00133**

**6 Cr 1 S Ryd( 6S) 0.00040**

**7 Cr 1 px Cor( 2p) 2.00000**

**8 Cr 1 px Cor( 3p) 1.99760**

**9 Cr 1 px Val( 4p) 0.17965**

**10 Cr 1 px Ryd( 5p) 0.00040**

**11 Cr 1 py Cor( 2p) 2.00000**

**12 Cr 1 py Cor( 3p) 1.99760**

**13 Cr 1 py Val( 4p) 0.17965**

**14 Cr 1 py Ryd( 5p) 0.00040**

**15 Cr 1 pz Cor( 2p) 2.00000**

**16 Cr 1 pz Cor( 3p) 1.99594**

**17 Cr 1 pz Val( 4p) 0.12074**

**18 Cr 1 pz Ryd( 5p) 0.00060**

**19 Cr 1 dxy Val( 3d) 1.01799**

**20 Cr 1 dxy Ryd( 4d) 0.00454**

**21 Cr 1 dxy Ryd( 5d) 0.00045**

**22 Cr 1 dxz Val( 3d) 1.07371**

**23 Cr 1 dxz Ryd( 4d) 0.00929**

**24 Cr 1 dxz Ryd( 5d) 0.00016**

**25 Cr 1 dyz Val( 3d) 1.07370**

**26 Cr 1 dyz Ryd( 4d) 0.00929**

**27 Cr 1 dyz Ryd( 5d) 0.00016**

**28 Cr 1 dx2y2 Val( 3d) 0.80430**

**29 Cr 1 dx2y2 Ryd( 4d) 0.01400**

**30 Cr 1 dx2y2 Ryd( 5d) 0.00009**

**31 Cr 1 dz2 Val( 3d) 0.56843**

**32 Cr 1 dz2 Ryd( 4d) 0.00719**

**33 Cr 1 dz2 Ryd( 5d) 0.00005**

**Mn(III) Complex**

**<S^2>= 2.0561**

**Summary of Natural Population Analysis:**

**Natural Population**

**Natural -----------------------------------------------**

**Atom No Charge Core Valence Rydberg Total**

**-----------------------------------------------------------------------**

**Mn 1 0.52793 17.98621 6.46092 0.02493 24.47207**

**N 2 -0.38031 1.99930 5.35689 0.02412 7.38031**

**N 3 -0.37575 1.99930 5.35232 0.02412 7.37575**

**N 4 -0.38028 1.99930 5.35686 0.02412 7.38028**

**N 5 -0.38463 1.99931 5.36128 0.02404 7.38463**

**C 6 0.35891 1.99920 3.62192 0.01996 5.64109**

**C 7 0.35889 1.99920 3.62195 0.01996 5.64111**

**C 8 0.36071 1.99921 3.62016 0.01992 5.63929**

**C 9 0.36189 1.99921 3.61883 0.02008 5.63811**

**C 10 0.35991 1.99920 3.62088 0.02001 5.64009**

**C 11 0.35986 1.99920 3.62092 0.02001 5.64014**

**C 12 0.36184 1.99921 3.61888 0.02008 5.63816**

**C 13 0.36074 1.99921 3.62013 0.01992 5.63926**

**N 14 -0.38809 1.99934 5.37417 0.01457 7.38809**

**N 15 -0.38882 1.99934 5.37483 0.01465 7.38882**

**N 16 -0.38885 1.99934 5.37485 0.01465 7.38885**

**N 17 -0.38811 1.99934 5.37419 0.01457 7.38811**

**C 18 -0.08114 1.99905 4.06649 0.01560 6.08114**

**C 19 -0.08020 1.99905 4.06552 0.01563 6.08020**

**C 20 -0.08080 1.99906 4.06617 0.01557 6.08080**

**C 21 -0.08079 1.99906 4.06616 0.01557 6.08079**

**C 22 -0.08021 1.99905 4.06553 0.01563 6.08021**

**C 23 -0.08112 1.99905 4.06647 0.01560 6.08112**

**C 24 -0.08098 1.99905 4.06628 0.01565 6.08098**

**C 25 -0.08096 1.99905 4.06626 0.01565 6.08096**

**C 26 -0.17460 1.99913 4.16355 0.01191 6.17460**

**C 27 -0.17467 1.99913 4.16361 0.01192 6.17467**

**C 28 -0.17480 1.99913 4.16376 0.01191 6.17480**

**C 29 -0.17481 1.99913 4.16377 0.01191 6.17481**

**C 30 -0.17466 1.99913 4.16361 0.01192 6.17466**

**C 31 -0.17460 1.99913 4.16356 0.01191 6.17460**

**C 32 -0.17449 1.99913 4.16344 0.01192 6.17449**

**C 33 -0.17451 1.99913 4.16345 0.01192 6.17451**

**C 34 -0.20816 1.99926 4.19704 0.01186 6.20816**

**H 35 0.23601 0.00000 0.76212 0.00187 0.76399**

**C 36 -0.20800 1.99926 4.19688 0.01186 6.20800**

**H 37 0.23609 0.00000 0.76204 0.00187 0.76391**

**C 38 -0.20836 1.99926 4.19723 0.01188 6.20836**

**H 39 0.23592 0.00000 0.76220 0.00187 0.76408**

**C 40 -0.20835 1.99926 4.19721 0.01188 6.20835**

**H 41 0.23592 0.00000 0.76220 0.00187 0.76408**

**C 42 -0.20801 1.99926 4.19689 0.01186 6.20801**

**H 43 0.23609 0.00000 0.76204 0.00187 0.76391**

**C 44 -0.20816 1.99926 4.19704 0.01186 6.20816**

**H 45 0.23600 0.00000 0.76212 0.00187 0.76400**

**C 46 -0.20819 1.99926 4.19707 0.01187 6.20819**

**H 47 0.23605 0.00000 0.76208 0.00187 0.76395**

**C 48 -0.20817 1.99926 4.19704 0.01187 6.20817**

**H 49 0.23605 0.00000 0.76208 0.00187 0.76395**

**H 50 0.22292 0.00000 0.77583 0.00125 0.77708**

**H 51 0.22292 0.00000 0.77583 0.00125 0.77708**

**H 52 0.22289 0.00000 0.77587 0.00125 0.77711**

**H 53 0.22288 0.00000 0.77587 0.00125 0.77712**

**H 54 0.22292 0.00000 0.77583 0.00125 0.77708**

**H 55 0.22293 0.00000 0.77583 0.00125 0.77707**

**H 56 0.22286 0.00000 0.77590 0.00125 0.77714**

**H 57 0.22285 0.00000 0.77590 0.00125 0.77715**

**F 58 -0.29839 1.99998 7.29509 0.00332 9.29839**

**=======================================================================**

**\* Total \* -0.00000 99.95397 197.36283 0.68320 298.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

**NAO Atom No lang Type(AO) Occupancy**

**--------------------------------------------**

**1 Mn 1 S Cor( 1S) 2.00000**

**2 Mn 1 S Cor( 2S) 1.99999**

**3 Mn 1 S Cor( 3S) 1.99412**

**4 Mn 1 S Val( 4S) 0.24215**

**5 Mn 1 S Ryd( 5S) 0.00106**

**6 Mn 1 S Ryd( 6S) 0.00052**

**7 Mn 1 px Cor( 2p) 2.00000**

**8 Mn 1 px Cor( 3p) 1.99787**

**9 Mn 1 px Val( 4p) 0.19443**

**10 Mn 1 px Ryd( 5p) 0.00046**

**11 Mn 1 py Cor( 2p) 2.00000**

**12 Mn 1 py Cor( 3p) 1.99787**

**13 Mn 1 py Val( 4p) 0.19418**

**14 Mn 1 py Ryd( 5p) 0.00046**

**15 Mn 1 pz Cor( 2p) 2.00000**

**16 Mn 1 pz Cor( 3p) 1.99637**

**17 Mn 1 pz Val( 4p) 0.13040**

**18 Mn 1 pz Ryd( 5p) 0.00103**

**19 Mn 1 dxy Val( 3d) 1.89000**

**20 Mn 1 dxy Ryd( 4d) 0.00401**

**21 Mn 1 dxy Ryd( 5d) 0.00038**

**22 Mn 1 dxz Val( 3d) 1.15253**

**23 Mn 1 dxz Ryd( 4d) 0.00502**

**24 Mn 1 dxz Ryd( 5d) 0.00013**

**25 Mn 1 dyz Val( 3d) 1.12733**

**26 Mn 1 dyz Ryd( 4d) 0.00510**

**27 Mn 1 dyz Ryd( 5d) 0.00013**

**28 Mn 1 dx2y2 Val( 3d) 0.84596**

**29 Mn 1 dx2y2 Ryd( 4d) 0.00402**

**30 Mn 1 dx2y2 Ryd( 5d) 0.00004**

**31 Mn 1 dz2 Val( 3d) 0.68394**

**32 Mn 1 dz2 Ryd( 4d) 0.00252**

**33 Mn 1 dz2 Ryd( 5d) 0.00005**

**Fe(III) Complex**

**<S^2>= 3.7899**

**Summary of Natural Population Analysis:**

**Natural Population**

**Natural -----------------------------------------------**

**Atom No Charge Core Valence Rydberg Total**

**-----------------------------------------------------------------------**

**Fe 1 0.69070 17.99132 7.29960 0.01838 25.30930**

**N 2 -0.39789 1.99926 5.37275 0.02588 7.39789**

**N 3 -0.39789 1.99926 5.37275 0.02588 7.39789**

**N 4 -0.39789 1.99926 5.37275 0.02588 7.39789**

**N 5 -0.39789 1.99926 5.37275 0.02588 7.39789**

**C 6 0.36332 1.99920 3.61708 0.02040 5.63668**

**C 7 0.36333 1.99920 3.61707 0.02040 5.63667**

**C 8 0.36332 1.99920 3.61708 0.02040 5.63668**

**C 9 0.36333 1.99920 3.61707 0.02040 5.63667**

**C 10 0.36332 1.99920 3.61708 0.02040 5.63668**

**C 11 0.36333 1.99920 3.61707 0.02040 5.63667**

**C 12 0.36332 1.99920 3.61708 0.02040 5.63668**

**C 13 0.36333 1.99920 3.61707 0.02040 5.63667**

**N 14 -0.39145 1.99935 5.37732 0.01479 7.39145**

**N 15 -0.39145 1.99935 5.37732 0.01479 7.39145**

**N 16 -0.39145 1.99935 5.37732 0.01479 7.39145**

**N 17 -0.39145 1.99935 5.37732 0.01479 7.39145**

**C 18 -0.07952 1.99905 4.06481 0.01566 6.07952**

**C 19 -0.07951 1.99905 4.06480 0.01566 6.07951**

**C 20 -0.07951 1.99905 4.06480 0.01566 6.07951**

**C 21 -0.07952 1.99905 4.06481 0.01566 6.07952**

**C 22 -0.07952 1.99905 4.06481 0.01566 6.07952**

**C 23 -0.07951 1.99905 4.06480 0.01566 6.07951**

**C 24 -0.07951 1.99905 4.06480 0.01566 6.07951**

**C 25 -0.07952 1.99905 4.06481 0.01566 6.07952**

**C 26 -0.17357 1.99913 4.16251 0.01193 6.17357**

**C 27 -0.17357 1.99913 4.16251 0.01193 6.17357**

**C 28 -0.17358 1.99913 4.16251 0.01193 6.17358**

**C 29 -0.17357 1.99913 4.16251 0.01193 6.17357**

**C 30 -0.17357 1.99913 4.16251 0.01193 6.17357**

**C 31 -0.17357 1.99913 4.16251 0.01193 6.17357**

**C 32 -0.17357 1.99913 4.16251 0.01193 6.17357**

**C 33 -0.17357 1.99913 4.16251 0.01193 6.17357**

**C 34 -0.20706 1.99926 4.19596 0.01184 6.20706**

**H 35 0.23671 0.00000 0.76143 0.00186 0.76329**

**C 36 -0.20706 1.99926 4.19596 0.01184 6.20706**

**H 37 0.23671 0.00000 0.76142 0.00186 0.76329**

**C 38 -0.20706 1.99926 4.19596 0.01184 6.20706**

**H 39 0.23671 0.00000 0.76142 0.00186 0.76329**

**C 40 -0.20706 1.99926 4.19596 0.01184 6.20706**

**H 41 0.23671 0.00000 0.76143 0.00186 0.76329**

**C 42 -0.20706 1.99926 4.19596 0.01184 6.20706**

**H 43 0.23671 0.00000 0.76143 0.00186 0.76329**

**C 44 -0.20706 1.99926 4.19596 0.01184 6.20706**

**H 45 0.23671 0.00000 0.76142 0.00186 0.76329**

**C 46 -0.20706 1.99926 4.19596 0.01184 6.20706**

**H 47 0.23671 0.00000 0.76142 0.00186 0.76329**

**C 48 -0.20706 1.99926 4.19596 0.01184 6.20706**

**H 49 0.23671 0.00000 0.76143 0.00186 0.76329**

**H 50 0.22339 0.00000 0.77537 0.00124 0.77661**

**H 51 0.22338 0.00000 0.77538 0.00124 0.77662**

**H 52 0.22338 0.00000 0.77538 0.00124 0.77662**

**H 53 0.22339 0.00000 0.77537 0.00124 0.77661**

**H 54 0.22338 0.00000 0.77537 0.00124 0.77662**

**H 55 0.22338 0.00000 0.77538 0.00124 0.77662**

**H 56 0.22338 0.00000 0.77538 0.00124 0.77662**

**H 57 0.22339 0.00000 0.77537 0.00124 0.77661**

**F 58 -0.43951 1.99998 7.43722 0.00231 9.43951**

**=======================================================================**

**\* Total \* -0.00000 99.95887 198.35435 0.68678 299.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

**NAO Atom No lang Type(AO) Occupancy**

**--------------------------------------------**

**1 Fe 1 S Cor( 1S) 2.00000**

**2 Fe 1 S Cor( 2S) 2.00000**

**3 Fe 1 S Cor( 3S) 1.99622**

**4 Fe 1 S Val( 4S) 0.26192**

**5 Fe 1 S Ryd( 5S) 0.00162**

**6 Fe 1 S Ryd( 6S) 0.00071**

**7 Fe 1 px Cor( 2p) 2.00000**

**8 Fe 1 px Cor( 3p) 1.99837**

**9 Fe 1 px Val( 4p) 0.20015**

**10 Fe 1 px Ryd( 5p) 0.00047**

**11 Fe 1 py Cor( 2p) 2.00000**

**12 Fe 1 py Cor( 3p) 1.99837**

**13 Fe 1 py Val( 4p) 0.20015**

**14 Fe 1 py Ryd( 5p) 0.00047**

**15 Fe 1 pz Cor( 2p) 2.00000**

**16 Fe 1 pz Cor( 3p) 1.99836**

**17 Fe 1 pz Val( 4p) 0.15058**

**18 Fe 1 pz Ryd( 5p) 0.00100**

**19 Fe 1 dxy Val( 3d) 1.10208**

**20 Fe 1 dxy Ryd( 4d) 0.00199**

**21 Fe 1 dxy Ryd( 5d) 0.00015**

**22 Fe 1 dxz Val( 3d) 1.16224**

**23 Fe 1 dxz Ryd( 4d) 0.00325**

**24 Fe 1 dxz Ryd( 5d) 0.00017**

**25 Fe 1 dyz Val( 3d) 1.16224**

**26 Fe 1 dyz Ryd( 4d) 0.00325**

**27 Fe 1 dyz Ryd( 5d) 0.00017**

**28 Fe 1 dx2y2 Val( 3d) 1.79733**

**29 Fe 1 dx2y2 Ryd( 4d) 0.00301**

**30 Fe 1 dx2y2 Ryd( 5d) 0.00038**

**31 Fe 1 dz2 Val( 3d) 1.26292**

**32 Fe 1 dz2 Ryd( 4d) 0.00153**

**33 Fe 1 dz2 Ryd( 5d) 0.00022**

**Co(III) Complex**

**<S^2> = 0.0000**

**Summary of Natural Population Analysis:**

**Natural Population**

**Natural -----------------------------------------------**

**Atom No Charge Core Valence Rydberg Total**

**-----------------------------------------------------------------------**

**Co 1 0.50665 17.99042 8.49076 0.01216 26.49335**

**N 2 -0.35072 1.99922 5.32761 0.02388 7.35072**

**N 3 -0.35072 1.99922 5.32761 0.02388 7.35072**

**N 4 -0.35072 1.99922 5.32761 0.02388 7.35072**

**N 5 -0.35072 1.99922 5.32761 0.02388 7.35072**

**C 6 0.35103 1.99920 3.62933 0.02044 5.64897**

**C 7 0.35102 1.99920 3.62934 0.02044 5.64898**

**C 8 0.35103 1.99920 3.62933 0.02044 5.64897**

**C 9 0.35102 1.99920 3.62934 0.02044 5.64898**

**C 10 0.35103 1.99920 3.62933 0.02044 5.64897**

**C 11 0.35102 1.99920 3.62934 0.02044 5.64898**

**C 12 0.35103 1.99920 3.62933 0.02044 5.64897**

**C 13 0.35102 1.99920 3.62934 0.02044 5.64898**

**N 14 -0.38080 1.99934 5.36665 0.01480 7.38080**

**N 15 -0.38080 1.99934 5.36665 0.01480 7.38080**

**N 16 -0.38080 1.99934 5.36665 0.01480 7.38080**

**N 17 -0.38080 1.99934 5.36665 0.01480 7.38080**

**C 18 -0.08028 1.99904 4.06565 0.01558 6.08028**

**C 19 -0.08027 1.99904 4.06565 0.01558 6.08027**

**C 20 -0.08027 1.99904 4.06565 0.01558 6.08027**

**C 21 -0.08028 1.99904 4.06565 0.01558 6.08028**

**C 22 -0.08028 1.99904 4.06565 0.01558 6.08028**

**C 23 -0.08027 1.99904 4.06565 0.01558 6.08027**

**C 24 -0.08027 1.99904 4.06565 0.01558 6.08027**

**C 25 -0.08028 1.99904 4.06565 0.01558 6.08028**

**C 26 -0.17499 1.99913 4.16393 0.01193 6.17499**

**C 27 -0.17499 1.99913 4.16393 0.01193 6.17499**

**C 28 -0.17499 1.99913 4.16393 0.01193 6.17499**

**C 29 -0.17499 1.99913 4.16393 0.01193 6.17499**

**C 30 -0.17499 1.99913 4.16393 0.01193 6.17499**

**C 31 -0.17499 1.99913 4.16393 0.01193 6.17499**

**C 32 -0.17499 1.99913 4.16393 0.01193 6.17499**

**C 33 -0.17499 1.99913 4.16393 0.01193 6.17499**

**C 34 -0.20865 1.99926 4.19752 0.01186 6.20865**

**H 35 0.23618 0.00000 0.76196 0.00186 0.76382**

**C 36 -0.20865 1.99926 4.19753 0.01186 6.20865**

**H 37 0.23617 0.00000 0.76196 0.00186 0.76383**

**C 38 -0.20865 1.99926 4.19753 0.01186 6.20865**

**H 39 0.23617 0.00000 0.76196 0.00186 0.76383**

**C 40 -0.20865 1.99926 4.19752 0.01186 6.20865**

**H 41 0.23618 0.00000 0.76196 0.00186 0.76382**

**C 42 -0.20865 1.99926 4.19752 0.01186 6.20865**

**H 43 0.23618 0.00000 0.76196 0.00186 0.76382**

**C 44 -0.20865 1.99926 4.19753 0.01186 6.20865**

**H 45 0.23617 0.00000 0.76196 0.00186 0.76383**

**C 46 -0.20865 1.99926 4.19753 0.01186 6.20865**

**H 47 0.23617 0.00000 0.76196 0.00186 0.76383**

**C 48 -0.20865 1.99926 4.19752 0.01186 6.20865**

**H 49 0.23618 0.00000 0.76196 0.00186 0.76382**

**H 50 0.22301 0.00000 0.77575 0.00124 0.77699**

**H 51 0.22301 0.00000 0.77575 0.00124 0.77699**

**H 52 0.22301 0.00000 0.77575 0.00124 0.77699**

**H 53 0.22301 0.00000 0.77575 0.00124 0.77699**

**H 54 0.22301 0.00000 0.77575 0.00124 0.77699**

**H 55 0.22301 0.00000 0.77575 0.00124 0.77699**

**H 56 0.22301 0.00000 0.77575 0.00124 0.77699**

**H 57 0.22301 0.00000 0.77575 0.00124 0.77699**

**F 58 -0.35099 1.99998 7.34882 0.00219 9.35099**

**=======================================================================**

**\* Total \* 0.00000 99.95773 199.36983 0.67244 300.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

**NAO Atom No lang Type(AO) Occupancy Energy**

**----------------------------------------------------------**

**1 Co 1 S Cor( 1S) 2.00000 -269.85362**

**2 Co 1 S Cor( 2S) 2.00000 -37.19486**

**3 Co 1 S Cor( 3S) 1.99544 -4.96984**

**4 Co 1 S Val( 4S) 0.25717 0.33362**

**5 Co 1 S Ryd( 5S) 0.00097 0.52892**

**6 Co 1 S Ryd( 6S) 0.00073 1.32046**

**7 Co 1 px Cor( 2p) 2.00000 -28.07896**

**8 Co 1 px Cor( 3p) 1.99858 -2.37305**

**9 Co 1 px Val( 4p) 0.21221 0.44522**

**10 Co 1 px Ryd( 5p) 0.00045 1.72225**

**11 Co 1 py Cor( 2p) 2.00000 -28.07896**

**12 Co 1 py Cor( 3p) 1.99858 -2.37305**

**13 Co 1 py Val( 4p) 0.21221 0.44522**

**14 Co 1 py Ryd( 5p) 0.00045 1.72225**

**15 Co 1 pz Cor( 2p) 2.00000 -28.08078**

**16 Co 1 pz Cor( 3p) 1.99782 -2.38722**

**17 Co 1 pz Val( 4p) 0.13169 0.20660**

**18 Co 1 pz Ryd( 5p) 0.00052 1.82788**

**19 Co 1 dxy Val( 3d) 1.17058 -0.24194**

**20 Co 1 dxy Ryd( 4d) 0.00139 2.11507**

**21 Co 1 dxy Ryd( 5d) 0.00013 3.07688**

**22 Co 1 dxz Val( 3d) 1.92957 -0.23631**

**23 Co 1 dxz Ryd( 4d) 0.00173 1.06827**

**24 Co 1 dxz Ryd( 5d) 0.00014 3.46326**

**25 Co 1 dyz Val( 3d) 1.92957 -0.23631**

**26 Co 1 dyz Ryd( 4d) 0.00173 1.06827**

**27 Co 1 dyz Ryd( 5d) 0.00014 3.46326**

**28 Co 1 dx2y2 Val( 3d) 1.80312 -0.23524**

**29 Co 1 dx2y2 Ryd( 4d) 0.00227 1.63849**

**30 Co 1 dx2y2 Ryd( 5d) 0.00025 3.27978**

**31 Co 1 dz2 Val( 3d) 0.84463 -0.25378**

**32 Co 1 dz2 Ryd( 4d) 0.00118 1.80505**

**33 Co 1 dz2 Ryd( 5d) 0.00006 3.36703**

**Ni(III) Complex**

**<S^2>= 0.7563**

**Summary of Natural Population Analysis:**

**Natural Population**

**Natural -----------------------------------------------**

**Atom No Charge Core Valence Rydberg Total**

**-----------------------------------------------------------------------**

**Ni 1 0.67672 17.99352 9.32091 0.00885 27.32328**

**N 2 -0.37444 1.99917 5.35084 0.02444 7.37444**

**N 3 -0.37443 1.99917 5.35082 0.02444 7.37443**

**N 4 -0.37444 1.99917 5.35084 0.02444 7.37444**

**N 5 -0.37443 1.99917 5.35082 0.02444 7.37443**

**C 6 0.35539 1.99920 3.62482 0.02059 5.64461**

**C 7 0.35539 1.99920 3.62482 0.02059 5.64461**

**C 8 0.35539 1.99920 3.62482 0.02059 5.64461**

**C 9 0.35539 1.99920 3.62482 0.02059 5.64461**

**C 10 0.35539 1.99920 3.62482 0.02059 5.64461**

**C 11 0.35539 1.99920 3.62482 0.02059 5.64461**

**C 12 0.35539 1.99920 3.62482 0.02059 5.64461**

**C 13 0.35539 1.99920 3.62482 0.02059 5.64461**

**N 14 -0.38381 1.99934 5.36949 0.01497 7.38381**

**N 15 -0.38381 1.99934 5.36949 0.01497 7.38381**

**N 16 -0.38381 1.99934 5.36949 0.01497 7.38381**

**N 17 -0.38381 1.99934 5.36949 0.01497 7.38381**

**C 18 -0.07901 1.99904 4.06417 0.01580 6.07901**

**C 19 -0.07901 1.99904 4.06417 0.01580 6.07901**

**C 20 -0.07901 1.99904 4.06417 0.01580 6.07901**

**C 21 -0.07901 1.99904 4.06417 0.01580 6.07901**

**C 22 -0.07901 1.99904 4.06417 0.01580 6.07901**

**C 23 -0.07901 1.99904 4.06417 0.01580 6.07901**

**C 24 -0.07901 1.99904 4.06417 0.01580 6.07901**

**C 25 -0.07901 1.99904 4.06417 0.01580 6.07901**

**C 26 -0.17375 1.99913 4.16268 0.01193 6.17375**

**C 27 -0.17375 1.99913 4.16268 0.01193 6.17375**

**C 28 -0.17375 1.99913 4.16268 0.01193 6.17375**

**C 29 -0.17375 1.99913 4.16268 0.01193 6.17375**

**C 30 -0.17375 1.99913 4.16268 0.01193 6.17375**

**C 31 -0.17375 1.99913 4.16268 0.01193 6.17375**

**C 32 -0.17375 1.99913 4.16268 0.01193 6.17375**

**C 33 -0.17375 1.99913 4.16268 0.01193 6.17375**

**C 34 -0.20761 1.99926 4.19650 0.01184 6.20761**

**H 35 0.23689 0.00000 0.76125 0.00186 0.76311**

**C 36 -0.20761 1.99926 4.19650 0.01184 6.20761**

**H 37 0.23689 0.00000 0.76125 0.00186 0.76311**

**C 38 -0.20761 1.99926 4.19650 0.01184 6.20761**

**H 39 0.23689 0.00000 0.76125 0.00186 0.76311**

**C 40 -0.20761 1.99926 4.19650 0.01184 6.20761**

**H 41 0.23689 0.00000 0.76125 0.00186 0.76311**

**C 42 -0.20761 1.99926 4.19650 0.01184 6.20761**

**H 43 0.23689 0.00000 0.76125 0.00186 0.76311**

**C 44 -0.20761 1.99926 4.19650 0.01184 6.20761**

**H 45 0.23689 0.00000 0.76125 0.00186 0.76311**

**C 46 -0.20761 1.99926 4.19650 0.01184 6.20761**

**H 47 0.23689 0.00000 0.76125 0.00186 0.76311**

**C 48 -0.20761 1.99926 4.19650 0.01184 6.20761**

**H 49 0.23689 0.00000 0.76125 0.00186 0.76311**

**H 50 0.22355 0.00000 0.77521 0.00124 0.77645**

**H 51 0.22355 0.00000 0.77521 0.00124 0.77645**

**H 52 0.22355 0.00000 0.77521 0.00124 0.77645**

**H 53 0.22355 0.00000 0.77521 0.00124 0.77645**

**H 54 0.22355 0.00000 0.77521 0.00124 0.77645**

**H 55 0.22355 0.00000 0.77521 0.00124 0.77645**

**H 56 0.22355 0.00000 0.77521 0.00124 0.77645**

**H 57 0.22355 0.00000 0.77521 0.00124 0.77645**

**F 58 -0.48745 1.99999 7.48597 0.00149 9.48745**

**=======================================================================**

**\* Total \* 0.00000 99.96055 200.36537 0.67408 301.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

**NAO Atom No lang Type(AO) Occupancy**

**--------------------------------------------**

**1 Ni 1 S Cor( 1S) 2.00000**

**2 Ni 1 S Cor( 2S) 2.00000**

**3 Ni 1 S Cor( 3S) 1.99696**

**4 Ni 1 S Val( 4S) 0.28302**

**5 Ni 1 S Ryd( 5S) 0.00163**

**6 Ni 1 S Ryd( 6S) 0.00076**

**7 Ni 1 px Cor( 2p) 2.00000**

**8 Ni 1 px Cor( 3p) 1.99888**

**9 Ni 1 px Val( 4p) 0.20942**

**10 Ni 1 px Ryd( 5p) 0.00045**

**11 Ni 1 py Cor( 2p) 2.00000**

**12 Ni 1 py Cor( 3p) 1.99888**

**13 Ni 1 py Val( 4p) 0.20942**

**14 Ni 1 py Ryd( 5p) 0.00045**

**15 Ni 1 pz Cor( 2p) 2.00000**

**16 Ni 1 pz Cor( 3p) 1.99881**

**17 Ni 1 pz Val( 4p) 0.13789**

**18 Ni 1 pz Ryd( 5p) 0.00056**

**19 Ni 1 dxy Val( 3d) 1.98402**

**20 Ni 1 dxy Ryd( 4d) 0.00103**

**21 Ni 1 dxy Ryd( 5d) 0.00024**

**22 Ni 1 dxz Val( 3d) 1.95892**

**23 Ni 1 dxz Ryd( 4d) 0.00091**

**24 Ni 1 dxz Ryd( 5d) 0.00012**

**25 Ni 1 dyz Val( 3d) 1.95891**

**26 Ni 1 dyz Ryd( 4d) 0.00091**

**27 Ni 1 dyz Ryd( 5d) 0.00012**

**28 Ni 1 dx2y2 Val( 3d) 1.11430**

**29 Ni 1 dx2y2 Ryd( 4d) 0.00053**

**30 Ni 1 dx2y2 Ryd( 5d) 0.00013**

**31 Ni 1 dz2 Val( 3d) 1.46500**

**32 Ni 1 dz2 Ryd( 4d) 0.00081**

**33 Ni 1 dz2 Ryd( 5d) 0.00021**

**Cu(III) Complex**

**<S^2> = 0.0000**

**Summary of Natural Population Analysis:**

**Natural Population**

**Natural -----------------------------------------------**

**Atom No Charge Core Valence Rydberg Total**

**-----------------------------------------------------------------------**

**Cu 1 0.80982 17.99555 10.18462 0.01001 28.19018**

**N 2 -0.37123 1.99918 5.34526 0.02680 7.37123**

**N 3 -0.37123 1.99918 5.34526 0.02680 7.37123**

**N 4 -0.37123 1.99918 5.34525 0.02680 7.37123**

**N 5 -0.37123 1.99918 5.34526 0.02680 7.37123**

**C 6 0.35874 1.99919 3.62122 0.02086 5.64126**

**C 7 0.35872 1.99919 3.62124 0.02086 5.64128**

**C 8 0.35874 1.99919 3.62122 0.02086 5.64126**

**C 9 0.35872 1.99919 3.62124 0.02086 5.64128**

**C 10 0.35874 1.99919 3.62122 0.02086 5.64126**

**C 11 0.35872 1.99919 3.62124 0.02086 5.64128**

**C 12 0.35874 1.99919 3.62122 0.02086 5.64126**

**C 13 0.35872 1.99919 3.62124 0.02086 5.64128**

**N 14 -0.38471 1.99934 5.37039 0.01498 7.38471**

**N 15 -0.38471 1.99934 5.37039 0.01498 7.38471**

**N 16 -0.38471 1.99934 5.37039 0.01498 7.38471**

**N 17 -0.38471 1.99934 5.37039 0.01498 7.38471**

**C 18 -0.07488 1.99904 4.05997 0.01588 6.07488**

**C 19 -0.07488 1.99904 4.05997 0.01588 6.07488**

**C 20 -0.07488 1.99904 4.05996 0.01588 6.07488**

**C 21 -0.07488 1.99904 4.05997 0.01588 6.07488**

**C 22 -0.07489 1.99904 4.05997 0.01588 6.07489**

**C 23 -0.07488 1.99904 4.05997 0.01588 6.07488**

**C 24 -0.07488 1.99904 4.05997 0.01588 6.07488**

**C 25 -0.07488 1.99904 4.05997 0.01588 6.07488**

**C 26 -0.17321 1.99913 4.16215 0.01193 6.17321**

**C 27 -0.17321 1.99913 4.16215 0.01193 6.17321**

**C 28 -0.17321 1.99913 4.16215 0.01193 6.17321**

**C 29 -0.17321 1.99913 4.16215 0.01193 6.17321**

**C 30 -0.17321 1.99913 4.16215 0.01193 6.17321**

**C 31 -0.17321 1.99913 4.16215 0.01193 6.17321**

**C 32 -0.17321 1.99913 4.16215 0.01193 6.17321**

**C 33 -0.17321 1.99913 4.16215 0.01193 6.17321**

**C 34 -0.20550 1.99926 4.19442 0.01182 6.20550**

**H 35 0.23807 0.00000 0.76009 0.00184 0.76193**

**C 36 -0.20550 1.99926 4.19442 0.01182 6.20550**

**H 37 0.23806 0.00000 0.76010 0.00184 0.76194**

**C 38 -0.20550 1.99926 4.19442 0.01182 6.20550**

**H 39 0.23806 0.00000 0.76010 0.00184 0.76194**

**C 40 -0.20550 1.99926 4.19442 0.01182 6.20550**

**H 41 0.23807 0.00000 0.76009 0.00184 0.76193**

**C 42 -0.20550 1.99926 4.19442 0.01182 6.20550**

**H 43 0.23807 0.00000 0.76009 0.00184 0.76193**

**C 44 -0.20550 1.99926 4.19442 0.01182 6.20550**

**H 45 0.23806 0.00000 0.76010 0.00184 0.76194**

**C 46 -0.20550 1.99926 4.19442 0.01182 6.20550**

**H 47 0.23806 0.00000 0.76010 0.00184 0.76194**

**C 48 -0.20550 1.99926 4.19442 0.01182 6.20550**

**H 49 0.23807 0.00000 0.76009 0.00184 0.76193**

**H 50 0.22445 0.00000 0.77431 0.00124 0.77555**

**H 51 0.22445 0.00000 0.77431 0.00124 0.77555**

**H 52 0.22445 0.00000 0.77431 0.00124 0.77555**

**H 53 0.22445 0.00000 0.77431 0.00124 0.77555**

**H 54 0.22445 0.00000 0.77431 0.00124 0.77555**

**H 55 0.22445 0.00000 0.77431 0.00124 0.77555**

**H 56 0.22445 0.00000 0.77431 0.00124 0.77555**

**H 57 0.22445 0.00000 0.77431 0.00124 0.77555**

**F 58 -0.72728 1.99999 7.72571 0.00158 9.72728**

**=======================================================================**

**\* Total \* 0.00000 99.96255 201.35026 0.68719 302.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

**NAO Atom No lang Type(AO) Occupancy Energy**

**----------------------------------------------------------**

**1 Cu 1 S Cor( 1S) 2.00000 -315.13723**

**2 Cu 1 S Cor( 2S) 2.00000 -42.99396**

**3 Cu 1 S Cor( 3S) 1.99765 -5.99792**

**4 Cu 1 S Val( 4S) 0.30356 0.18445**

**5 Cu 1 S Ryd( 5S) 0.00263 0.46115**

**6 Cu 1 S Ryd( 6S) 0.00080 1.36193**

**7 Cu 1 px Cor( 2p) 2.00000 -33.66775**

**8 Cu 1 px Cor( 3p) 1.99918 -2.84677**

**9 Cu 1 px Val( 4p) 0.21116 0.45834**

**10 Cu 1 px Ryd( 5p) 0.00046 1.49566**

**11 Cu 1 py Cor( 2p) 2.00000 -33.66775**

**12 Cu 1 py Cor( 3p) 1.99918 -2.84677**

**13 Cu 1 py Val( 4p) 0.21116 0.45834**

**14 Cu 1 py Ryd( 5p) 0.00046 1.49563**

**15 Cu 1 pz Cor( 2p) 2.00000 -33.63803**

**16 Cu 1 pz Cor( 3p) 1.99955 -2.79971**

**17 Cu 1 pz Val( 4p) 0.17181 0.19772**

**18 Cu 1 pz Ryd( 5p) 0.00058 2.02783**

**19 Cu 1 dxy Val( 3d) 1.93547 -0.33648**

**20 Cu 1 dxy Ryd( 4d) 0.00072 1.82988**

**21 Cu 1 dxy Ryd( 5d) 0.00025 3.06362**

**22 Cu 1 dxz Val( 3d) 1.98401 -0.30473**

**23 Cu 1 dxz Ryd( 4d) 0.00101 1.15594**

**24 Cu 1 dxz Ryd( 5d) 0.00019 3.28036**

**25 Cu 1 dyz Val( 3d) 1.98401 -0.30473**

**26 Cu 1 dyz Ryd( 4d) 0.00101 1.15596**

**27 Cu 1 dyz Ryd( 5d) 0.00019 3.28036**

**28 Cu 1 dx2y2 Val( 3d) 1.40636 -0.34535**

**29 Cu 1 dx2y2 Ryd( 4d) 0.00061 2.40044**

**30 Cu 1 dx2y2 Ryd( 5d) 0.00021 2.77840**

**31 Cu 1 dz2 Val( 3d) 1.97707 -0.29519**

**32 Cu 1 dz2 Ryd( 4d) 0.00061 2.07163**

**33 Cu 1 dz2 Ryd( 5d) 0.00030 3.19220**