*Supplementary Materials*

Длины связей, валентные и невалентные углы в гетеролигандных комплексах M(IV) [M**L**(O)] с порфиразином и оксо-анионом

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Параметр | Ti | V | Cr | Mn | Fe | Co | Ni | Cu |
| Длины связей M–N, *пм* | | | | | | | | |
| (M1N1) | 207.5 | 199.1 | 196.4 | 194.6 | 192.5 | 190.4 | 189.9 | 195.5 |
| (M1N2) | 207.5 | 198.8 | 196.4 | 194.6 | 192.5 | 190.4 | 189.9 | 196.4 |
| (M1N3) | 207.5 | 199.1 | 196.4 | 194.6 | 192.5 | 190.4 | 189.9 | 195.5 |
| (M1N4) | 207.5 | 198.8 | 196.4 | 194.6 | 192.5 | 190.4 | 189.9 | 196.4 |
| Длины связей M–O, *пм* | | | | | | | | |
| (M1O1) | 161.9 | 157.5 | 158.0 | 164.0 | 161.8 | 170.1 | 197.8 | 193.1 |
| Длины связей C–N, *пм* | | | | | | | | |
| (N1C3) | 137.0 | 138.8 | 138.3 | 137.3 | 137.2 | 137.4 | 137.1 | 136.7 |
| (N1C4) | 137.0 | 138.8 | 138.3 | 137.3 | 137.2 | 137.4 | 137.1 | 136.7 |
| (N2C1) | 137.0 | 138.9 | 138.3 | 137.3 | 137.2 | 137.2 | 137.0 | 136.5 |
| (N2C2) | 137.0 | 138.9 | 138.3 | 137.3 | 137.2 | 137.2 | 137.0 | 136.5 |
| (N3C7) | 137.0 | 138.8 | 138.3 | 137.3 | 137.2 | 137.4 | 137.1 | 136.7 |
| (N3C8) | 137.0 | 138.8 | 138.3 | 137.3 | 137.2 | 137.4 | 137.1 | 136.7 |
| (N4C5) | 137.0 | 138.9 | 138.3 | 137.3 | 137.2 | 137.2 | 137.0 | 136.5 |
| (N4C6) | 137.0 | 138.9 | 138.3 | 137.3 | 137.2 | 137.2 | 137.0 | 136.5 |
| (N5C2) | 133.0 | 133.7 | 132.5 | 132.4 | 132.3 | 132.0 | 132.1 | 132.8 |
| (N5C3) | 133.0 | 130.6 | 132.5 | 132.4 | 132.3 | 132.2 | 132.1 | 132.8 |
| (N6C6) | 133.0 | 133.7 | 132.5 | 132.4 | 132.3 | 132.0 | 132.1 | 132.8 |
| (N6C7) | 133.0 | 130.6 | 132.5 | 132.4 | 132.3 | 132.2 | 132.1 | 132.8 |
| (N7C4) | 133.0 | 130.6 | 132.5 | 132.4 | 132.3 | 132.2 | 132.1 | 132.8 |
| (N7C5) | 133.0 | 133.7 | 132.5 | 132.4 | 132.3 | 132.0 | 132.1 | 132.8 |
| (N8C1) | 133.0 | 133.7 | 132.5 | 132.4 | 132.3 | 132.0 | 132.1 | 132.8 |
| (N8C8) | 133.0 | 130.6 | 132.5 | 132.4 | 132.3 | 132.2 | 132.1 | 132.8 |

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Длины связей C–C, *пм* | | | | | | | | |
| (C7C14) | 145.3 | 145.3 | 145.0 | 144.9 | 144.8 | 144.8 | 144.5 | 145.3 |
| (C14C13) | 136.0 | 135.3 | 135.7 | 135.8 | 135.7 | 135.8 | 135.6 | 135.9 |
| (C13C8) | 145.3 | 145.3 | 145.0 | 144.9 | 144.8 | 144.8 | 144.5 | 145.3 |
| (C1C11) | 145.3 | 142.4 | 145.0 | 144.9 | 144.8 | 144.9 | 144.5 | 145.4 |
| (C11C12) | 136.0 | 137.5 | 135.7 | 135.8 | 135.7 | 135.5 | 135.5 | 135.9 |
| (C12C2) | 145.3 | 142.4 | 145.0 | 144.9 | 144.8 | 144.9 | 144.5 | 145.4 |
| (C3C10) | 145.3 | 145.3 | 145.0 | 144.9 | 144.8 | 144.8 | 144.5 | 145.3 |
| (C10C9) | 136.0 | 135.3 | 135.7 | 135.8 | 135.7 | 135.8 | 135.6 | 135.9 |
| (C9C4) | 145.3 | 145.3 | 145.0 | 144.9 | 144.8 | 144.8 | 144.5 | 145.3 |
| (C5C15) | 145.3 | 142.4 | 145.0 | 144.9 | 144.8 | 144.9 | 144.5 | 145.4 |
| (C15C16) | 136.0 | 137.5 | 135.7 | 135.8 | 135.7 | 135.5 | 135.5 | 135.9 |
| (C16C6) | 145.3 | 142.4 | 145.0 | 144.9 | 144.8 | 144.9 | 144.5 | 145.4 |
| Длины связей C–H, *пм* | | | | | | | | |
| (C10H1) | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.5 |
| (C9H2) | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.5 |
| (C12H3) | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.5 |
| (C11H4) | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.5 |
| (C13H5) | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.5 |
| (C14H6) | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.5 |
| (C16H7) | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.5 |
| (C15H8) | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.4 | 108.5 |
| Валентные углы в хелатном узле MN4, град | | | | | | | | |
| (N1M1N2) | 83.5 | 86.1 | 87.1 | 88.6 | 88.8 | 89.4 | 89.7 | 88.9 |
| (N2M1N3) | 83.5 | 86.1 | 87.1 | 88.6 | 88.8 | 89.4 | 89.7 | 88.9 |
| (N3M1N4) | 83.5 | 86.1 | 87.1 | 88.6 | 88.8 | 89.4 | 89.7 | 88.9 |
| (N4M1N1) | 83.5 | 86.1 | 87.1 | 88.6 | 88.8 | 89.4 | 89.7 | 88.9 |
| *Сумма углов*  (***VAS***) | **334.0** | **344.4** | **348.4** | **354.4** | **355.2** | **357.6** | **358.8** | **355.6** |

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Невалентные углы в хелатном узле MN4, град | | | | | | | | |
| (N1N2N3) | 90.0 | 90.8 | 90.0 | 90.0 | 90.0 | 89.9 | 90.0 | 89.9 |
| (N2N3N4) | 90.0 | 89.1 | 90.0 | 90.0 | 90.0 | 90.1 | 90.0 | 90.1 |
| (N3N4N1) | 90.0 | 90.8 | 90.0 | 90.0 | 90.0 | 89.9 | 90.0 | 89.9 |
| (N4N1N2) | 90.0 | 89.1 | 90.0 | 90.0 | 90.0 | 90.1 | 90.0 | 90.1 |
| *Сумма углов*  (NVAS) | 360.0 | 359.8 | 360.0 | 360.0 | 360.0 | 360.0 | 360.0 | 360.0 |
| Валентные углы в 6-членном хелатном цикле (N1C4N7C5N4M1), град | | | | | | | | |
| (M1N1C4) | 125.5 | 126.9 | 126.5 | 126.2 | 126.5 | 126.6 | 126.8 | 125.8 |
| (N1C4N7) | 127.5 | 126.9 | 127.8 | 127.5 | 127.7 | 127.8 | 128.0 | 127.8 |
| (C4N7C5) | 122.9 | 122.5 | 121.0 | 121.9 | 121.0 | 120.5 | 120.3 | 122.2 |
| (N7C5N4) | 127.5 | 126.0 | 127.8 | 127.5 | 127.7 | 127.7 | 128.0 | 127.7 |
| (C5N4M1) | 125.5 | 124.0 | 126.5 | 126.2 | 126.5 | 126.8 | 126.7 | 125.6 |
| (N4M1N1) | 83.5 | 86.1 | 87.1 | 88.6 | 88.8 | 89.4 | 89.7 | 88.9 |
| *Сумма углов*  (VAS61) | **712.4** | **712.4** | **716.7** | **717.9** | **718.2** | **718.8** | **719.5** | **718.0** |
| Валентные углы в 6-членном хелатном цикле (N1C3N5C2N2M1), град | | | | | | | | |
| (M1N2C2) | 125.5 | 124.0 | 126.5 | 126.2 | 126.5 | 126.8 | 126.7 | 125.8 |
| (N2C2N5) | 127.5 | 126.0 | 127.8 | 127.5 | 127.7 | 127.7 | 128.0 | 127.8 |
| (C2N5C3) | 122.9 | 120.5 | 121.0 | 121.9 | 121.0 | 120.5 | 120.3 | 122.2 |
| (N5C3N1) | 127.5 | 126.9 | 127.8 | 127.5 | 127.7 | 127.8 | 128.0 | 127.7 |
| (C3N1M1) | 125.5 | 126.9 | 126.5 | 126.2 | 126.5 | 126.6 | 126.8 | 125.6 |
| (N1M1N2) | 83.5 | 86.1 | 87.1 | 88.6 | 88.8 | 89.4 | 89.7 | 88.9 |
| *Сумма углов*  (VAS62) | **712.4** | **712.4** | **716.7** | **717.9** | **718.2** | **718.8** | **719.5** | **718.0** |
| Валентные углы в 6-членном хелатном цикле (N2C1N8C8N3M1), град | | | | | | | | |
| (M1N3C8) | 125.5 | 126.9 | 126.5 | 126.2 | 126.5 | 126.6 | 126.8 | 125.8 |
| (N3C8N8) | 127.5 | 126.9 | 127.8 | 127.5 | 127.7 | 127.8 | 128.0 | 127.8 |
| (C8N8C1) | 122.9 | 122.5 | 121.0 | 121.9 | 121.0 | 120.5 | 120.3 | 122.2 |

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| (N8C1N2) | 127.5 | 126.0 | 127.8 | 127.5 | 127.7 | 127.7 | 128.0 | 127.7 |
| (C1N2M1) | 125.5 | 124.0 | 126.5 | 126.2 | 126.5 | 126.8 | 126.7 | 125.6 |
| (N2M1N3) | 83.5 | 86.1 | 87.1 | 88.6 | 88.8 | 89.4 | 89.7 | 88.9 |
| *Сумма углов*  (VAS63) | **712.4** | **712.4** | **716.7** | **717.9** | **718.2** | **718.8** | **719.5** | **718.0** |
| Валентные углы в 6-членном хелатном цикле (N3C7N6C6N4M1), град | | | | | | | | |
| (M1N4C6) | 125.5 | 124.0 | 126.5 | 126.2 | 126.5 | 126.8 | 126.7 | 125.8 |
| (N4C6N6) | 127.5 | 126.0 | 127.8 | 127.5 | 127.7 | 127.7 | 128.0 | 127.8 |
| (C6N6C7) | 122.9 | 120.5 | 121.0 | 121.9 | 121.0 | 120.5 | 120.3 | 122.2 |
| (N6C7N3) | 127.5 | 126.9 | 127.8 | 127.5 | 127.7 | 127.8 | 128.0 | 127.7 |
| (C7N3M1) | 125.5 | 126.9 | 126.5 | 126.2 | 126.5 | 126.6 | 126.8 | 125.6 |
| (N3M1N4) | 83.5 | 86.1 | 87.1 | 88.6 | 88.8 | 89.4 | 89.7 | 88.9 |
| *Сумма углов*  (VAS64) | **712.4** | **712.4** | **716.7** | **717.9** | **718.2** | **718.8** | **719.5** | **718.0** |
| Валентные углы в 5-членном нехелатном цикле (C3N1C4C9C10), град | | | | | | | | |
| (C3N1C4) | 107.4 | 106.2 | 106.4 | 106.9 | 106.3 | 106.0 | 106.3 | 107.7 |
| (N1C4C9) | 109.3 | 109.6 | 109.6 | 109.5 | 110.0 | 110.1 | 110.1 | 109.2 |
| (C4C9C10) | 107.0 | 107.3 | 107.2 | 107.0 | 106.8 | 106.9 | 106.8 | 107.0 |
| (C9C10C3) | 107.0 | 107.3 | 107.2 | 107.0 | 106.8 | 106.9 | 106.8 | 106.9 |
| (C10C3N1) | 109.3 | 109.6 | 109.6 | 109.5 | 110.0 | 110.1 | 110.1 | 109.2 |
| *Сумма углов*  (VAS5) | **540.0** | **540.0** | **540.0** | **540.0** | **539.9** | **540.0** | **540.0** | **540.0** |
| Валентные углы (OMN), град | | | | | | | | |
| (O1M1N1) | 109.6 | 103.8 | 103.0 | 98.9 | 98.5 | 96.5 | 94.3 | 97.6 |
| (O1M1N2) | 109.6 | 106.7 | 103.0 | 98.9 | 98.5 | 95.3 | 94.3 | 98.5 |
| (O1M1N3) | 109.6 | 103.8 | 103.0 | 98.9 | 98.5 | 96.5 | 94.3 | 97.6 |
| (O1M1N4) | 109.6 | 106.7 | 103.0 | 98.9 | 98.5 | 95.3 | 94.3 | 98.5 |

Координаты атомов в гетеролигандных комплексах M(IV) [M**L**(O)] с порфиразином и оксо-анионом (M= Ti, V, Cr, Mn, Fe, Co, Ni, Cu)

[Ti**L**(O)]

|  |  |  |  |
| --- | --- | --- | --- |
| Атом | *x* | *y* | *z* |
| Ti1 | -0.000014 | 0.000001 | 0.658648 |
| N1 | -0.000024 | -1.954448 | -0.037703 |
| N2 | 1.954485 | -0.000025 | -0.037629 |
| N3 | 0.000026 | 1.954448 | -0.037708 |
| N4 | -1.954483 | 0.000025 | -0.037713 |
| C1 | 2.756889 | 1.104331 | -0.154987 |
| C2 | 2.756860 | -1.104403 | -0.154984 |
| C3 | 1.104338 | -2.756897 | -0.155049 |
| C4 | -1.104402 | -2.756868 | -0.155100 |
| C5 | -2.756882 | -1.104331 | -0.155104 |
| C6 | -2.756853 | 1.104402 | -0.155106 |
| C7 | -1.104331 | 2.756896 | -0.155107 |
| C8 | 1.104409 | 2.756868 | -0.155056 |
| N5 | 2.379176 | -2.379202 | -0.187825 |
| N6 | -2.379168 | 2.379201 | -0.187935 |
| N7 | -2.379230 | -2.379140 | -0.187929 |
| N8 | 2.379238 | 2.379140 | -0.187831 |
| C9 | -0.680018 | -4.136094 | -0.320581 |
| C10 | 0.679924 | -4.136110 | -0.320567 |
| C11 | 4.136183 | 0.679892 | -0.320473 |
| C12 | 4.136165 | -0.680000 | -0.320471 |
| C13 | 0.680031 | 4.136092 | -0.320578 |
| C14 | -0.679910 | 4.136111 | -0.320592 |
| C15 | -4.136169 | -0.679893 | -0.320649 |
| C16 | -4.136152 | 0.679999 | -0.320651 |
| H1 | -1.362849 | -4.969272 | -0.445588 |
| H2 | 1.362739 | -4.969305 | -0.445557 |
| H3 | 4.969255 | -1.362948 | -0.445447 |
| H4 | 4.969291 | 1.362818 | -0.445450 |
| H5 | 1.362868 | 4.969268 | -0.445570 |
| H6 | -1.362720 | 4.969307 | -0.445600 |
| H7 | -4.969236 | 1.362947 | -0.445664 |
| H8 | -4.969272 | -1.362819 | -0.445661 |
| O1 | -0.000049 | 0.000003 | 2.277565 |

[V**L**(O)]

|  |  |  |  |
| --- | --- | --- | --- |
| Атом | *x* | *y* | *z* |
| V1 | -0.000001 | -0.000009 | 0.443017 |
| N1 | 1.933109 | 0.000051 | -0.031812 |
| N2 | -0.000052 | 1.903881 | -0.128625 |
| N3 | -1.933109 | -0.000050 | -0.031817 |
| N4 | 0.000052 | -1.903876 | -0.128705 |
| C1 | -1.107703 | 2.738416 | -0.047792 |
| C2 | 1.107556 | 2.738476 | -0.047791 |
| C3 | 2.744041 | 1.109486 | -0.226782 |
| C4 | 2.744103 | -1.109330 | -0.226824 |
| C5 | 1.107703 | -2.738414 | -0.047905 |
| C6 | -1.107556 | -2.738474 | -0.047910 |
| C7 | -2.744041 | -1.109477 | -0.226835 |
| C8 | -2.744102 | 1.109339 | -0.226784 |
| N5 | 2.384403 | 2.363365 | -0.172033 |
| N6 | -2.384403 | -2.363358 | -0.172139 |
| N7 | 2.384532 | -2.363231 | -0.172130 |
| N8 | -2.384531 | 2.363238 | -0.172036 |
| C9 | 4.098640 | -0.676336 | -0.523557 |
| C10 | 4.098607 | 0.676579 | -0.523510 |
| C11 | -0.687365 | 4.092218 | 0.089589 |
| C12 | 0.687145 | 4.092255 | 0.089593 |
| C13 | -4.098639 | 0.676358 | -0.523538 |
| C14 | -4.098606 | -0.676557 | -0.523549 |
| C15 | 0.687365 | -4.092222 | 0.089417 |
| C16 | -0.687145 | -4.092259 | 0.089418 |
| H1 | 4.917309 | -1.364371 | -0.702411 |
| H2 | 4.917241 | 1.364666 | -0.702321 |
| H3 | 1.367670 | 4.934579 | 0.137719 |
| H4 | -1.367936 | 4.934506 | 0.137713 |
| H5 | -4.917308 | 1.364401 | -0.702365 |
| H6 | -4.917240 | -1.364637 | -0.702391 |
| H7 | -1.367670 | -4.934585 | 0.137507 |
| H8 | 1.367936 | -4.934511 | 0.137507 |
| O1 | -0.000003 | -0.000042 | 2.017912 |

[Cr**L**(O)]

|  |  |  |  |
| --- | --- | --- | --- |
| Атом | *x* | *y* | *z* |
| Cr1 | 0.000001 | -0.000008 | 0.402436 |
| N1 | 1.913324 | 0.010787 | -0.039671 |
| N2 | -0.010786 | 1.913371 | -0.039466 |
| N3 | -1.913324 | -0.010785 | -0.039664 |
| N4 | 0.010786 | -1.913370 | -0.039543 |
| C1 | -1.122608 | 2.731968 | -0.123473 |
| C2 | 1.091736 | 2.744452 | -0.123475 |
| C3 | 2.731955 | 1.122611 | -0.123330 |
| C4 | 2.744438 | -1.091734 | -0.123376 |
| C5 | 1.122608 | -2.731963 | -0.123586 |
| C6 | -1.091736 | -2.744446 | -0.123582 |
| C7 | -2.731955 | -1.122606 | -0.123364 |
| C8 | -2.744438 | 1.091739 | -0.123320 |
| N5 | 2.371030 | 2.397910 | -0.129340 |
| N6 | -2.371031 | -2.397905 | -0.129426 |
| N7 | 2.397916 | -2.371020 | -0.129434 |
| N8 | -2.397916 | 2.371025 | -0.129328 |
| C9 | 4.121353 | -0.655389 | -0.251483 |
| C10 | 4.113702 | 0.701816 | -0.251466 |
| C11 | -0.701812 | 4.113667 | -0.252078 |
| C12 | 0.655395 | 4.121315 | -0.252108 |
| C13 | -4.121354 | 0.655399 | -0.251435 |
| C14 | -4.113703 | -0.701806 | -0.251473 |
| C15 | 0.701811 | -4.113656 | -0.252256 |
| C16 | -0.655396 | -4.121305 | -0.252262 |
| H1 | 4.941595 | 1.395292 | -0.346297 |
| H2 | 4.957011 | -1.339487 | -0.346332 |
| H3 | 1.339484 | 4.956945 | -0.347279 |
| H4 | -1.395276 | 4.941536 | -0.347223 |
| H5 | -4.957013 | 1.339501 | -0.346251 |
| H6 | -4.941597 | -1.395278 | -0.346327 |
| H7 | -1.339485 | -4.956932 | -0.347456 |
| H8 | 1.395274 | -4.941520 | -0.347446 |
| O1 | 0.000004 | -0.000040 | 1.982454 |

[Mn**L**(O)]

|  |  |  |  |
| --- | --- | --- | --- |
| Атом | *x* | *y* | *z* |
| Mn1 | 0.000000 | -0.000004 | 0.220507 |
| N1 | 1.922949 | -0.000613 | -0.079690 |
| N2 | 0.000614 | 1.922952 | -0.079622 |
| N3 | -1.922950 | 0.000616 | -0.079681 |
| N4 | -0.000614 | -1.922949 | -0.079699 |
| C1 | -1.102346 | 2.740671 | -0.107815 |
| C2 | 1.104102 | 2.739959 | -0.107821 |
| C3 | 2.740674 | 1.102348 | -0.107738 |
| C4 | 2.739962 | -1.104100 | -0.107783 |
| C5 | 1.102346 | -2.740667 | -0.107931 |
| C6 | -1.104102 | -2.739955 | -0.107925 |
| C7 | -2.740675 | -1.102344 | -0.107769 |
| C8 | -2.739963 | 1.104104 | -0.107725 |
| N5 | 2.376917 | 2.375398 | -0.111322 |
| N6 | -2.376918 | -2.375393 | -0.111406 |
| N7 | 2.375396 | -2.376914 | -0.111418 |
| N8 | -2.375397 | 2.376919 | -0.111310 |
| C9 | 4.123891 | -0.680527 | -0.169175 |
| C10 | 4.124332 | 0.677864 | -0.169147 |
| C11 | -0.677860 | 4.124322 | -0.169419 |
| C12 | 0.680529 | 4.123881 | -0.169422 |
| C13 | -4.123892 | 0.680533 | -0.169127 |
| C14 | -4.124333 | -0.677857 | -0.169155 |
| C15 | 0.677859 | -4.124316 | -0.169588 |
| C16 | -0.680530 | -4.123874 | -0.169586 |
| H1 | 4.961717 | 1.364931 | -0.217474 |
| H2 | 4.960823 | -1.368146 | -0.217528 |
| H3 | 1.368151 | 4.960806 | -0.217870 |
| H4 | -1.364928 | 4.961700 | -0.217865 |
| H5 | -4.960824 | 1.368155 | -0.217449 |
| H6 | -4.961718 | -1.364923 | -0.217505 |
| H7 | -1.368152 | -4.960797 | -0.218066 |
| H8 | 1.364928 | -4.961691 | -0.218070 |
| O1 | 0.000004 | -0.000037 | 1.860116 |

[Fe**L**(O)]

|  |  |  |  |
| --- | --- | --- | --- |
| Атом | *x* | *y* | *z* |
| Fe1 | -0.000004 | -0.000003 | 0.189344 |
| N1 | -0.000425 | -1.903785 | -0.094268 |
| N2 | 1.903849 | -0.000425 | -0.094058 |
| N3 | 0.000429 | 1.903786 | -0.094259 |
| N4 | -1.903845 | 0.000429 | -0.094135 |
| C1 | 2.726855 | 1.097368 | -0.106643 |
| C2 | 2.726362 | -1.098587 | -0.106649 |
| C3 | 1.097379 | -2.726833 | -0.106781 |
| C4 | -1.098597 | -2.726341 | -0.106825 |
| C5 | -2.726850 | -1.097365 | -0.106758 |
| C6 | -2.726359 | 1.098590 | -0.106753 |
| C7 | -1.097374 | 2.726834 | -0.106813 |
| C8 | 1.098601 | 2.726342 | -0.106769 |
| N5 | 2.372832 | -2.373897 | -0.105581 |
| N6 | -2.372828 | 2.373900 | -0.105665 |
| N7 | -2.373892 | -2.372834 | -0.105677 |
| N8 | 2.373896 | 2.372836 | -0.105569 |
| C9 | -0.679603 | -4.112016 | -0.149826 |
| C10 | 0.677767 | -4.112320 | -0.149800 |
| C11 | 4.112353 | 0.677768 | -0.149605 |
| C12 | 4.112048 | -0.679609 | -0.149609 |
| C13 | 0.679609 | 4.112018 | -0.149780 |
| C14 | -0.677761 | 4.112322 | -0.149808 |
| C15 | -4.112346 | -0.677767 | -0.149775 |
| C16 | -4.112043 | 0.679610 | -0.149771 |
| H1 | 1.367845 | -4.947979 | -0.184865 |
| H2 | -1.370053 | -4.947367 | -0.184919 |
| H3 | 4.947388 | -1.370077 | -0.184555 |
| H4 | 4.948001 | 1.367862 | -0.184547 |
| H5 | 1.370061 | 4.947368 | -0.184841 |
| H6 | -1.367838 | 4.947980 | -0.184898 |
| H7 | -4.947381 | 1.370078 | -0.184747 |
| H8 | -4.947993 | -1.367862 | -0.184754 |
| O1 | -0.000036 | -0.000008 | 1.807683 |

[Co**L**(O)]

|  |  |  |  |
| --- | --- | --- | --- |
| Атом | *x* | *y* | *z* |
| Co1 | -0.000003 | 0.000002 | 0.090261 |
| N1 | 0.000002 | -1.891256 | -0.126522 |
| N2 | 1.895425 | -0.000001 | -0.085880 |
| N3 | 0.000003 | 1.891256 | -0.126511 |
| N4 | -1.895421 | 0.000000 | -0.085952 |
| C1 | 2.721218 | 1.095672 | -0.078292 |
| C2 | 2.721218 | -1.095675 | -0.078298 |
| C3 | 1.097939 | -2.717231 | -0.113179 |
| C4 | -1.097937 | -2.717230 | -0.113223 |
| C5 | -2.721215 | -1.095673 | -0.078405 |
| C6 | -2.721214 | 1.095674 | -0.078400 |
| C7 | -1.097935 | 2.717231 | -0.113209 |
| C8 | 1.097941 | 2.717230 | -0.113165 |
| N5 | 2.373176 | -2.369320 | -0.086879 |
| N6 | -2.373173 | 2.369320 | -0.086963 |
| N7 | -2.373174 | -2.369318 | -0.086974 |
| N8 | 2.373178 | 2.369318 | -0.086868 |
| C9 | -0.678893 | -4.099571 | -0.142272 |
| C10 | 0.678895 | -4.099572 | -0.142245 |
| C11 | 4.108554 | 0.677554 | -0.093629 |
| C12 | 4.108554 | -0.677557 | -0.093633 |
| C13 | 0.678899 | 4.099571 | -0.142225 |
| C14 | -0.678890 | 4.099572 | -0.142253 |
| C15 | -4.108550 | -0.677554 | -0.093798 |
| C16 | -4.108549 | 0.677557 | -0.093795 |
| H1 | 1.371370 | -4.933533 | -0.162179 |
| H2 | -1.371367 | -4.933532 | -0.162234 |
| H3 | 4.941823 | -1.370967 | -0.113167 |
| H4 | 4.941824 | 1.370963 | -0.113160 |
| H5 | 1.371373 | 4.933532 | -0.162156 |
| H6 | -1.371362 | 4.933534 | -0.162212 |
| H7 | -4.941818 | 1.370966 | -0.113361 |
| H8 | -4.941819 | -1.370963 | -0.113367 |
| O1 | -0.000035 | -0.000003 | 1.791594 |

[Ni**L**(O)]

|  |  |  |  |
| --- | --- | --- | --- |
| Атом | *x* | *y* | *z* |
| Ni1 | 0.000001 | -0.000002 | 0.034307 |
| N1 | 0.000603 | -1.893916 | -0.107181 |
| N2 | 1.893925 | 0.000610 | -0.107048 |
| N3 | -0.000611 | 1.893926 | -0.107001 |
| N4 | -1.893937 | -0.000601 | -0.106858 |
| C1 | 2.715887 | 1.096274 | -0.091980 |
| C2 | 2.716600 | -1.094520 | -0.092091 |
| C3 | 1.097404 | -2.716022 | -0.109405 |
| C4 | -1.095667 | -2.716733 | -0.109285 |
| C5 | -2.715896 | -1.096265 | -0.091810 |
| C6 | -2.716609 | 1.094528 | -0.091709 |
| C7 | -1.097414 | 2.716030 | -0.109033 |
| C8 | 1.095657 | 2.716745 | -0.109136 |
| N5 | 2.372259 | -2.369988 | -0.097391 |
| N6 | -2.372268 | 2.369997 | -0.096922 |
| N7 | -2.370741 | -2.371512 | -0.097134 |
| N8 | 2.370732 | 2.371522 | -0.097147 |
| C9 | -0.676570 | -4.102091 | -0.138545 |
| C10 | 0.679202 | -4.101649 | -0.138639 |
| C11 | 4.102893 | 0.678930 | -0.091059 |
| C12 | 4.103336 | -0.676273 | -0.091206 |
| C13 | 0.676556 | 4.102105 | -0.138218 |
| C14 | -0.679216 | 4.101661 | -0.138176 |
| C15 | -4.102903 | -0.678920 | -0.090705 |
| C16 | -4.103346 | 0.676282 | -0.090722 |
| H1 | -1.370649 | -4.934691 | -0.158283 |
| H2 | 1.373824 | -4.933793 | -0.158472 |
| H3 | 4.935530 | -1.371121 | -0.094847 |
| H4 | 4.934629 | 1.374325 | -0.094561 |
| H5 | 1.370631 | 4.934708 | -0.157946 |
| H6 | -1.373841 | 4.933806 | -0.157858 |
| H7 | -4.935540 | 1.371131 | -0.094211 |
| H8 | -4.934639 | -1.374316 | -0.094188 |
| O1 | 0.000101 | -0.000095 | 2.012106 |

[Cu**L**(O)]

|  |  |  |  |
| --- | --- | --- | --- |
| Атом | *x* | *y* | *z* |
| Cu1 | 0.000019 | -0.000051 | 0.146124 |
| N1 | 0.006540 | 1.938250 | -0.112394 |
| N2 | -1.942365 | 0.006490 | -0.143745 |
| N3 | -0.006504 | -1.938153 | -0.113576 |
| N4 | 1.942407 | -0.006432 | -0.143652 |
| C1 | -2.752326 | -1.092411 | -0.123891 |
| C2 | -2.744857 | 1.110839 | -0.123558 |
| C3 | -1.094321 | 2.748114 | -0.119469 |
| C4 | 1.112791 | 2.740697 | -0.119612 |
| C5 | 2.752350 | 1.092463 | -0.123614 |
| C6 | 2.744911 | -1.110787 | -0.123704 |
| C7 | 1.094364 | -2.748045 | -0.119838 |
| C8 | -1.112754 | -2.740640 | -0.120007 |
| N5 | -2.371723 | 2.385347 | -0.118729 |
| N6 | 2.371766 | -2.385288 | -0.118960 |
| N7 | 2.387750 | 2.369447 | -0.118899 |
| N8 | -2.387714 | -2.369385 | -0.119214 |
| C9 | 0.693599 | 4.131126 | -0.155722 |
| C10 | -0.665783 | 4.135712 | -0.155694 |
| C11 | -4.141850 | -0.665528 | -0.127931 |
| C12 | -4.137229 | 0.693408 | -0.127796 |
| C13 | -0.693563 | -4.131069 | -0.155258 |
| C14 | 0.665833 | -4.135648 | -0.155208 |
| C15 | 4.141886 | 0.665594 | -0.127767 |
| C16 | 4.137278 | -0.693340 | -0.127856 |
| H1 | 1.381994 | 4.968577 | -0.186571 |
| H2 | -1.348489 | 4.977810 | -0.186437 |
| H3 | -4.975040 | 1.382032 | -0.135635 |
| H4 | -4.984351 | -1.348414 | -0.136019 |
| H5 | -1.381944 | -4.968551 | -0.185568 |
| H6 | 1.348529 | -4.977775 | -0.185386 |
| H7 | 4.975093 | -1.381958 | -0.135845 |
| H8 | 4.984381 | 1.348491 | -0.135720 |
| O1 | -0.000474 | -0.000447 | 2.076916 |

**Summary of Natural Population Analysis:**

[Ti**L**(O)]

**Atom No Charge Core Valence Rydberg Total**

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

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Ti** | **1** | **0.88958** | **17.96779** | **3.09461** | **0.04802** | **21.11042** |
| **N** | **2** | **-0.47268** | **1.99929** | **5.45174** | **0.02166** | **7.47268** |
| **N** | **3** | **-0.47268** | **1.99929** | **5.45173** | **0.02166** | **7.47268** |
| **N** | **4** | **-0.47269** | **1.99929** | **5.45174** | **0.02166** | **7.47269** |
| **N** | **5** | **-0.47268** | **1.99929** | **5.45173** | **0.02166** | **7.47268** |
| **C** | **6** | **0.33760** | **1.99928** | **3.64265** | **0.02047** | **5.66240** |
| **C** | **7** | **0.33760** | **1.99928** | **3.64265** | **0.02047** | **5.66240** |
| **C** | **8** | **0.33757** | **1.99927** | **3.64268** | **0.02047** | **5.66243** |
| **C** | **9** | **0.33757** | **1.99927** | **3.64268** | **0.02047** | **5.66243** |
| **C** | **10** | **0.33760** | **1.99928** | **3.64265** | **0.02047** | **5.66240** |
| **C** | **11** | **0.33760** | **1.99928** | **3.64265** | **0.02047** | **5.66240** |
| **C** | **12** | **0.33757** | **1.99927** | **3.64268** | **0.02047** | **5.66243** |
| **C** | **13** | **0.33757** | **1.99927** | **3.64268** | **0.02047** | **5.66243** |
| **N** | **14** | **-0.36245** | **1.99936** | **5.34853** | **0.01457** | **7.36245** |
| **N** | **15** | **-0.36245** | **1.99936** | **5.34853** | **0.01457** | **7.36245** |
| **N** | **16** | **-0.36245** | **1.99936** | **5.34853** | **0.01457** | **7.36245** |
| **N** | **17** | **-0.36245** | **1.99936** | **5.34853** | **0.01457** | **7.36245** |
| **C** | **18** | **-0.21903** | **1.99912** | **4.20812** | **0.01179** | **6.21903** |
| **C** | **19** | **-0.21903** | **1.99912** | **4.20812** | **0.01179** | **6.21903** |
| **C** | **20** | **-0.21903** | **1.99912** | **4.20811** | **0.01179** | **6.21903** |
| **C** | **21** | **-0.21903** | **1.99912** | **4.20811** | **0.01179** | **6.21903** |
| **C** | **22** | **-0.21903** | **1.99912** | **4.20812** | **0.01179** | **6.21903** |
| **C** | **23** | **-0.21903** | **1.99912** | **4.20812** | **0.01179** | **6.21903** |
| **C** | **24** | **-0.21903** | **1.99912** | **4.20811** | **0.01179** | **6.21903** |
| **C** | **25** | **-0.21903** | **1.99912** | **4.20811** | **0.01179** | **6.21903** |
| **H** | **26** | **0.24370** | **0.00000** | **0.75477** | **0.00153** | **0.75630** |
| **H** | **27** | **0.24370** | **0.00000** | **0.75477** | **0.00153** | **0.75630** |
| **H** | **28** | **0.24370** | **0.00000** | **0.75477** | **0.00153** | **0.75630** |
| **H** | **29** | **0.24370** | **0.00000** | **0.75477** | **0.00153** | **0.75630** |
| **H** | **30** | **0.24370** | **0.00000** | **0.75477** | **0.00153** | **0.75630** |
| **H** | **31** | **0.24370** | **0.00000** | **0.75477** | **0.00153** | **0.75630** |
| **H** | **32** | **0.24370** | **0.00000** | **0.75477** | **0.00153** | **0.75630** |
| **H** | **33** | **0.24370** | **0.00000** | **0.75477** | **0.00153** | **0.75630** |
| **O** | **34** | **-0.44709** | **1.99985** | **6.44255** | **0.00469** | **8.44709** |

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

**\* Total \* -0.00000 67.94941 121.58264 0.46795 190.00000**

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

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **1** | **Ti** | **1** | **S** | **Cor(** | **1S)** | **2.00000** |
| **2** | **Ti** | **1** | **S** | **Cor(** | **2S)** | **1.99999** |
| **3** | **Ti** | **1** | **S** | **Cor(** | **3S)** | **1.99219** |
| **4** | **Ti** | **1** | **S** | **Val(** | **4S)** | **0.20210** |
| **5** | **Ti** | **1** | **S** | **Ryd(** | **5S)** | **0.00168** |
| **6** | **Ti** | **1** | **S** | **Ryd(** | **6S)** | **0.00040** |
| **7** | **Ti** | **1** | **px** | **Cor(** | **2p)** | **2.00000** |
| **8** | **Ti** | **1** | **px** | **Cor(** | **3p)** | **1.99663** |
| **9** | **Ti** | **1** | **px** | **Val(** | **4p)** | **0.16051** |
| **10** | **Ti** | **1** | **px** | **Ryd(** | **5p)** | **0.00039** |
| **11** | **Ti** | **1** | **py** | **Cor(** | **2p)** | **2.00000** |
| **12** | **Ti** | **1** | **py** | **Cor(** | **3p)** | **1.99663** |
| **13** | **Ti** | **1** | **py** | **Val(** | **4p)** | **0.16051** |
| **14** | **Ti** | **1** | **py** | **Ryd(** | **5p)** | **0.00039** |
| **15** | **Ti** | **1** | **pz** | **Cor(** | **2p)** | **1.99999** |
| **16** | **Ti** | **1** | **pz** | **Cor(** | **3p)** | **1.98235** |
| **17** | **Ti** | **1** | **pz** | **Val(** | **4p)** | **0.14542** |
| **18** | **Ti** | **1** | **pz** | **Ryd(** | **5p)** | **0.00048** |
| **19** | **Ti** | **1** | **dxy** | **Val(** | **3d)** | **0.06646** |
| **20** | **Ti** | **1** | **dxy** | **Ryd(** | **4d)** | **0.00173** |
| **21** | **Ti** | **1** | **dxy** | **Ryd(** | **5d)** | **0.00008** |
| **22** | **Ti** | **1** | **dxz** | **Val(** | **3d)** | **0.59549** |
| **23** | **Ti** | **1** | **dxz** | **Ryd(** | **4d)** | **0.00271** |
| **24** | **Ti** | **1** | **dxz** | **Ryd(** | **5d)** | **0.00014** |
| **25** | **Ti** | **1** | **dyz** | **Val(** | **3d)** | **0.59550** |
| **26** | **Ti** | **1** | **dyz** | **Ryd(** | **4d)** | **0.00271** |
| **27** | **Ti** | **1** | **dyz** | **Ryd(** | **5d)** | **0.00014** |
| **28** | **Ti** | **1** | **dx2y2** | **Val(** | **3d)** | **0.57389** |
| **29** | **Ti** | **1** | **dx2y2** | **Ryd(** | **4d)** | **0.00758** |
| **30** | **Ti** | **1** | **dx2y2** | **Ryd(** | **5d)** | **0.00005** |
| **31** | **Ti** | **1** | **dz2** | **Val(** | **3d)** | **0.59473** |
| **32** | **Ti** | **1** | **dz2** | **Ryd(** | **4d)** | **0.02932** |
| **33** | **Ti** | **1** | **dz2** | **Ryd(** | **5d)** | **0.00021** |

[V**L**(O)]

**Atom No Charge Core Valence Rydberg Total**

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

**V 1 0.53441 17.97034 4.45886 0.03639 22.46559**

**N 2 -0.42610 1.99932 5.40249 0.02428 7.42610**

**N 3 -0.40439 1.99932 5.38162 0.02346 7.40439**

**N 4 -0.42610 1.99932 5.40249 0.02428 7.42610**

**N 5 -0.40439 1.99932 5.38162 0.02346 7.40439**

**C 6 0.30306 1.99922 3.67768 0.02005 5.69694**

**C 7 0.30305 1.99922 3.67768 0.02005 5.69695**

**C 8 0.33921 1.99928 3.64094 0.02057 5.66079**

**C 9 0.33921 1.99928 3.64094 0.02057 5.66079**

**C 10 0.30306 1.99922 3.67768 0.02005 5.69694**

**C 11 0.30305 1.99922 3.67768 0.02005 5.69695**

**C 12 0.33921 1.99928 3.64094 0.02057 5.66079**

**C 13 0.33921 1.99928 3.64094 0.02057 5.66079**

**N 14 -0.35163 1.99930 5.33761 0.01472 7.35163**

**N 15 -0.35163 1.99930 5.33761 0.01472 7.35163**

**N 16 -0.35163 1.99930 5.33761 0.01472 7.35163**

**N 17 -0.35163 1.99930 5.33761 0.01472 7.35163**

**C 18 -0.21717 1.99910 4.20625 0.01183 6.21717**

**C 19 -0.21717 1.99910 4.20625 0.01183 6.21717**

**C 20 -0.23752 1.99911 4.22653 0.01188 6.23752**

**C 21 -0.23752 1.99911 4.22653 0.01188 6.23752**

**C 22 -0.21717 1.99910 4.20625 0.01183 6.21717**

**C 23 -0.21717 1.99910 4.20625 0.01183 6.21717**

**C 24 -0.23752 1.99911 4.22653 0.01188 6.23752**

**C 25 -0.23752 1.99911 4.22653 0.01188 6.23752**

**H 26 0.24537 0.00000 0.75312 0.00151 0.75463**

**H 27 0.24537 0.00000 0.75312 0.00151 0.75463**

**H 28 0.24273 0.00000 0.75572 0.00154 0.75727**

**H 29 0.24274 0.00000 0.75572 0.00154 0.75726**

**H 30 0.24537 0.00000 0.75312 0.00151 0.75463**

**H 31 0.24537 0.00000 0.75312 0.00151 0.75463**

**H 32 0.24273 0.00000 0.75572 0.00154 0.75727**

**H 33 0.24273 0.00000 0.75572 0.00154 0.75727**

**O 34 -0.16963 1.99987 6.16340 0.00635 8.16963**

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

**\* Total \* -0.00000 67.95149 122.58191 0.46659 191.00000**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **1** | **V** | **1** | **S** | **Cor(** | **1S)** | **2.00000** |
| **2** | **V** | **1** | **S** | **Cor(** | **2S)** | **1.99999** |
| **3** | **V** | **1** | **S** | **Cor(** | **3S)** | **1.99388** |
| **4** | **V** | **1** | **S** | **Val(** | **4S)** | **0.23837** |
| **5** | **V** | **1** | **S** | **Ryd(** | **5S)** | **0.00159** |
| **6** | **V** | **1** | **S** | **Ryd(** | **6S)** | **0.00043** |
| **7** | **V** | **1** | **px** | **Cor(** | **2p)** | **2.00000** |
| **8** | **V** | **1** | **px** | **Cor(** | **3p)** | **1.99697** |
| **9** | **V** | **1** | **px** | **Val(** | **4p)** | **0.19180** |
| **10** | **V** | **1** | **px** | **Ryd(** | **5p)** | **0.00060** |
| **11** | **V** | **1** | **py** | **Cor(** | **2p)** | **2.00000** |
| **12** | **V** | **1** | **py** | **Cor(** | **3p)** | **1.99643** |
| **13** | **V** | **1** | **py** | **Val(** | **4p)** | **0.18942** |
| **14** | **V** | **1** | **py** | **Ryd(** | **5p)** | **0.00066** |
| **15** | **V** | **1** | **pz** | **Cor(** | **2p)** | **2.00000** |
| **16** | **V** | **1** | **pz** | **Cor(** | **3p)** | **1.98308** |
| **17** | **V** | **1** | **pz** | **Val(** | **4p)** | **0.16389** |
| **18** | **V** | **1** | **pz** | **Ryd(** | **5p)** | **0.00055** |
| **19** | **V** | **1** | **dxy** | **Val(** | **3d)** | **0.45907** |
| **20** | **V** | **1** | **dxy** | **Ryd(** | **4d)** | **0.00362** |
| **21** | **V** | **1** | **dxy** | **Ryd(** | **5d)** | **0.00012** |
| **22** | **V** | **1** | **dxz** | **Val(** | **3d)** | **0.79296** |
| **23** | **V** | **1** | **dxz** | **Ryd(** | **4d)** | **0.00154** |
| **24** | **V** | **1** | **dxz** | **Ryd(** | **5d)** | **0.00009** |
| **25** | **V** | **1** | **dyz** | **Val(** | **3d)** | **0.76995** |
| **26** | **V** | **1** | **dyz** | **Ryd(** | **4d)** | **0.00247** |
| **27** | **V** | **1** | **dyz** | **Ryd(** | **5d)** | **0.00012** |
| **28** | **V** | **1** | **dx2y2** | **Val(** | **3d)** | **0.86531** |
| **29** | **V** | **1** | **dx2y2** | **Ryd(** | **4d)** | **0.00818** |
| **30** | **V** | **1** | **dx2y2** | **Ryd(** | **5d)** | **0.00011** |
| **31** | **V** | **1** | **dz2** | **Val(** | **3d)** | **0.78810** |
| **32** | **V** | **1** | **dz2** | **Ryd(** | **4d)** | **0.01606** |
| **33** | **V** | **1** | **dz2** | **Ryd(** | **5d)** | **0.00023** |

[Cr**L**(O)]

**Atom No Charge Core Valence Rydberg Total**

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

**Cr 1 0.38213 17.97795 5.60390 0.03601 23.61787**

**N 2 -0.41420 1.99930 5.38285 0.03205 7.41420**

**N 3 -0.41418 1.99930 5.38282 0.03205 7.41418**

**N 4 -0.41420 1.99930 5.38285 0.03205 7.41420**

**N 5 -0.41418 1.99930 5.38282 0.03205 7.41418**

**C 6 0.36734 1.99927 3.61265 0.02074 5.63266**

**C 7 0.36734 1.99927 3.61265 0.02074 5.63266**

**C 8 0.36735 1.99927 3.61264 0.02074 5.63265**

**C 9 0.36735 1.99927 3.61264 0.02074 5.63265**

**C 10 0.36734 1.99927 3.61265 0.02074 5.63266**

**C 11 0.36734 1.99927 3.61265 0.02074 5.63266**

**C 12 0.36735 1.99927 3.61264 0.02074 5.63265**

**C 13 0.36735 1.99927 3.61264 0.02074 5.63265**

**N 14 -0.40448 1.99936 5.38983 0.01529 7.40448**

**N 15 -0.40448 1.99936 5.38983 0.01529 7.40448**

**N 16 -0.40448 1.99936 5.38983 0.01529 7.40448**

**N 17 -0.40448 1.99936 5.38983 0.01529 7.40448**

**C 18 -0.22999 1.99911 4.21868 0.01220 6.22999**

**C 19 -0.22999 1.99911 4.21868 0.01220 6.22999**

**C 20 -0.23000 1.99911 4.21870 0.01220 6.23000**

**C 21 -0.23001 1.99911 4.21870 0.01220 6.23001**

**C 22 -0.22999 1.99911 4.21868 0.01220 6.22999**

**C 23 -0.22999 1.99911 4.21868 0.01220 6.22999**

**C 24 -0.23000 1.99911 4.21870 0.01220 6.23000**

**C 25 -0.23000 1.99911 4.21870 0.01220 6.23000**

**H 26 0.24382 0.00000 0.75463 0.00155 0.75618**

**H 27 0.24382 0.00000 0.75463 0.00155 0.75618**

**H 28 0.24382 0.00000 0.75463 0.00155 0.75618**

**H 29 0.24382 0.00000 0.75463 0.00155 0.75618**

**H 30 0.24382 0.00000 0.75463 0.00155 0.75618**

**H 31 0.24382 0.00000 0.75463 0.00155 0.75618**

**H 32 0.24382 0.00000 0.75463 0.00155 0.75618**

**H 33 0.24382 0.00000 0.75463 0.00155 0.75618**

**O 34 -0.15683 1.99990 6.14555 0.01138 8.15683**

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

**\* Total \* 0.00000 67.95945 123.52788 0.51267 192.00000**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **1** | **Cr** | **1** | **S** | **Cor(** | **1S)** | **2.00000** |
| **2** | **Cr** | **1** | **S** | **Cor(** | **2S)** | **1.99999** |
| **3** | **Cr** | **1** | **S** | **Cor(** | **3S)** | **1.99520** |
| **4** | **Cr** | **1** | **S** | **Val(** | **4S)** | **0.24817** |
| **5** | **Cr** | **1** | **S** | **Ryd(** | **5S)** | **0.00164** |
| **6** | **Cr** | **1** | **S** | **Ryd(** | **6S)** | **0.00047** |
| **7** | **Cr** | **1** | **px** | **Cor(** | **2p)** | **2.00000** |
| **8** | **Cr** | **1** | **px** | **Cor(** | **3p)** | **1.99759** |
| **9** | **Cr** | **1** | **px** | **Val(** | **4p)** | **0.20771** |
| **10** | **Cr** | **1** | **px** | **Ryd(** | **5p)** | **0.00058** |
| **11** | **Cr** | **1** | **py** | **Cor(** | **2p)** | **2.00000** |
| **12** | **Cr** | **1** | **py** | **Cor(** | **3p)** | **1.99759** |
| **13** | **Cr** | **1** | **py** | **Val(** | **4p)** | **0.20771** |
| **14** | **Cr** | **1** | **py** | **Ryd(** | **5p)** | **0.00058** |
| **15** | **Cr** | **1** | **pz** | **Cor(** | **2p)** | **2.00000** |
| **16** | **Cr** | **1** | **pz** | **Cor(** | **3p)** | **1.98759** |
| **17** | **Cr** | **1** | **pz** | **Val(** | **4p)** | **0.17014** |
| **18** | **Cr** | **1** | **pz** | **Ryd(** | **5p)** | **0.00040** |
| **19** | **Cr** | **1** | **dxy** | **Val(** | **3d)** | **1.05141** |
| **20** | **Cr** | **1** | **dxy** | **Ryd(** | **4d)** | **0.00372** |
| **21** | **Cr** | **1** | **dxy** | **Ryd(** | **5d)** | **0.00041** |
| **22** | **Cr** | **1** | **dxz** | **Val(** | **3d)** | **0.99132** |
| **23** | **Cr** | **1** | **dxz** | **Ryd(** | **4d)** | **0.00382** |
| **24** | **Cr** | **1** | **dxz** | **Ryd(** | **5d)** | **0.00017** |
| **25** | **Cr** | **1** | **dyz** | **Val(** | **3d)** | **0.99150** |
| **26** | **Cr** | **1** | **dyz** | **Ryd(** | **4d)** | **0.00383** |
| **27** | **Cr** | **1** | **dyz** | **Ryd(** | **5d)** | **0.00017** |
| **28** | **Cr** | **1** | **dx2y2** | **Val(** | **3d)** | **0.89288** |
| **29** | **Cr** | **1** | **dx2y2** | **Ryd(** | **4d)** | **0.00969** |
| **30** | **Cr** | **1** | **dx2y2** | **Ryd(** | **5d)** | **0.00005** |
| **31** | **Cr** | **1** | **dz2** | **Val(** | **3d)** | **0.84307** |
| **32** | **Cr** | **1** | **dz2** | **Ryd(** | **4d)** | **0.01031** |
| **33** | **Cr** | **1** | **dz2** | **Ryd(** | **5d)** | **0.00018** |

[Mn**L**(O)]

**Atom No Charge Core Valence Rydberg Total**

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

**Mn 1 0.43123 17.98270 6.55837 0.02769 24.56877**

**N 2 -0.38905 1.99925 5.36412 0.02567 7.38905**

**N 3 -0.38904 1.99925 5.36411 0.02567 7.38904**

**N 4 -0.38905 1.99925 5.36412 0.02567 7.38905**

**N 5 -0.38904 1.99925 5.36411 0.02567 7.38904**

**C 6 0.32804 1.99927 3.65211 0.02058 5.67196**

**C 7 0.32803 1.99927 3.65211 0.02058 5.67197**

**C 8 0.32804 1.99927 3.65211 0.02058 5.67196**

**C 9 0.32803 1.99927 3.65211 0.02058 5.67197**

**C 10 0.32804 1.99927 3.65211 0.02058 5.67196**

**C 11 0.32803 1.99927 3.65211 0.02058 5.67197**

**C 12 0.32804 1.99927 3.65211 0.02058 5.67196**

**C 13 0.32803 1.99927 3.65211 0.02058 5.67197**

**N 14 -0.35611 1.99936 5.34208 0.01467 7.35611**

**N 15 -0.35611 1.99936 5.34208 0.01467 7.35611**

**N 16 -0.35611 1.99936 5.34208 0.01467 7.35611**

**N 17 -0.35611 1.99936 5.34208 0.01467 7.35611**

**C 18 -0.22128 1.99911 4.21039 0.01178 6.22128**

**C 19 -0.22127 1.99911 4.21039 0.01178 6.22127**

**C 20 -0.22128 1.99911 4.21039 0.01178 6.22128**

**C 21 -0.22128 1.99911 4.21039 0.01178 6.22128**

**C 22 -0.22128 1.99911 4.21039 0.01178 6.22128**

**C 23 -0.22127 1.99911 4.21039 0.01178 6.22127**

**C 24 -0.22128 1.99911 4.21039 0.01178 6.22128**

**C 25 -0.22128 1.99911 4.21039 0.01178 6.22128**

**H 26 0.24388 0.00000 0.75457 0.00154 0.75612**

**H 27 0.24389 0.00000 0.75457 0.00154 0.75611**

**H 28 0.24389 0.00000 0.75457 0.00154 0.75611**

**H 29 0.24388 0.00000 0.75457 0.00154 0.75612**

**H 30 0.24389 0.00000 0.75457 0.00154 0.75611**

**H 31 0.24388 0.00000 0.75457 0.00154 0.75612**

**H 32 0.24389 0.00000 0.75457 0.00154 0.75611**

**H 33 0.24388 0.00000 0.75457 0.00154 0.75612**

**O 34 -0.25575 1.99994 6.24953 0.00629 8.25575**

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

**\* Total \* 0.00000 67.96411 124.56929 0.46660 193.00000**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **1** | **Mn** | **1** | **S** | **Cor(** | **1S)** | **2.00000** |
| **2** | **Mn** | **1** | **S** | **Cor(** | **2S)** | **2.00000** |
| **3** | **Mn** | **1** | **S** | **Cor(** | **3S)** | **1.99578** |
| **4** | **Mn** | **1** | **S** | **Val(** | **4S)** | **0.26344** |
| **5** | **Mn** | **1** | **S** | **Ryd(** | **5S)** | **0.00163** |
| **6** | **Mn** | **1** | **S** | **Ryd(** | **6S)** | **0.00046** |
| **7** | **Mn** | **1** | **px** | **Cor(** | **2p)** | **2.00000** |
| **8** | **Mn** | **1** | **px** | **Cor(** | **3p)** | **1.99810** |
| **9** | **Mn** | **1** | **px** | **Val(** | **4p)** | **0.21852** |
| **10** | **Mn** | **1** | **px** | **Ryd(** | **5p)** | **0.00069** |
| **11** | **Mn** | **1** | **py** | **Cor(** | **2p)** | **2.00000** |
| **12** | **Mn** | **1** | **py** | **Cor(** | **3p)** | **1.99810** |
| **13** | **Mn** | **1** | **py** | **Val(** | **4p)** | **0.21852** |
| **14** | **Mn** | **1** | **py** | **Ryd(** | **5p)** | **0.00069** |
| **15** | **Mn** | **1** | **pz** | **Cor(** | **2p)** | **2.00000** |
| **16** | **Mn** | **1** | **pz** | **Cor(** | **3p)** | **1.99073** |
| **17** | **Mn** | **1** | **pz** | **Val(** | **4p)** | **0.16319** |
| **18** | **Mn** | **1** | **pz** | **Ryd(** | **5p)** | **0.00067** |
| **19** | **Mn** | **1** | **dxy** | **Val(** | **3d)** | **1.05819** |
| **20** | **Mn** | **1** | **dxy** | **Ryd(** | **4d)** | **0.00319** |
| **21** | **Mn** | **1** | **dxy** | **Ryd(** | **5d)** | **0.00041** |
| **22** | **Mn** | **1** | **dxz** | **Val(** | **3d)** | **1.35703** |
| **23** | **Mn** | **1** | **dxz** | **Ryd(** | **4d)** | **0.00553** |
| **24** | **Mn** | **1** | **dxz** | **Ryd(** | **5d)** | **0.00013** |
| **25** | **Mn** | **1** | **dyz** | **Val(** | **3d)** | **1.35702** |
| **26** | **Mn** | **1** | **dyz** | **Ryd(** | **4d)** | **0.00553** |
| **27** | **Mn** | **1** | **dyz** | **Ryd(** | **5d)** | **0.00013** |
| **28** | **Mn** | **1** | **dx2y2** | **Val(** | **3d)** | **0.94879** |
| **29** | **Mn** | **1** | **dx2y2** | **Ryd(** | **4d)** | **0.00511** |
| **30** | **Mn** | **1** | **dx2y2** | **Ryd(** | **5d)** | **0.00003** |
| **31** | **Mn** | **1** | **dz2** | **Val(** | **3d)** | **0.97368** |
| **32** | **Mn** | **1** | **dz2** | **Ryd(** | **4d)** | **0.00346** |
| **33** | **Mn** | **1** | **dz2** | **Ryd(** | **5d)** | **0.00003** |

[Fe**L**(O)]

**Atom No Charge Core Valence Rydberg Total**

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

**Fe 1 0.24195 17.98564 7.75178 0.02063 25.75805**

**N 2 -0.36223 1.99922 5.33783 0.02518 7.36223**

**N 3 -0.36222 1.99922 5.33782 0.02518 7.36222**

**N 4 -0.36223 1.99922 5.33783 0.02518 7.36223**

**N 5 -0.36222 1.99922 5.33782 0.02518 7.36222**

**C 6 0.32801 1.99927 3.65181 0.02091 5.67199**

**C 7 0.32801 1.99927 3.65181 0.02091 5.67199**

**C 8 0.32801 1.99927 3.65181 0.02091 5.67199**

**C 9 0.32801 1.99927 3.65181 0.02091 5.67199**

**C 10 0.32801 1.99927 3.65181 0.02091 5.67199**

**C 11 0.32801 1.99927 3.65181 0.02091 5.67199**

**C 12 0.32801 1.99927 3.65181 0.02091 5.67199**

**C 13 0.32801 1.99927 3.65181 0.02091 5.67199**

**N 14 -0.35948 1.99937 5.34510 0.01501 7.35948**

**N 15 -0.35948 1.99937 5.34510 0.01501 7.35948**

**N 16 -0.35948 1.99937 5.34510 0.01501 7.35948**

**N 17 -0.35948 1.99937 5.34510 0.01501 7.35948**

**C 18 -0.22055 1.99910 4.20960 0.01185 6.22055**

**C 19 -0.22055 1.99910 4.20960 0.01185 6.22055**

**C 20 -0.22056 1.99910 4.20961 0.01185 6.22056**

**C 21 -0.22056 1.99910 4.20961 0.01185 6.22056**

**C 22 -0.22055 1.99910 4.20960 0.01185 6.22055**

**C 23 -0.22055 1.99910 4.20960 0.01185 6.22055**

**C 24 -0.22056 1.99910 4.20961 0.01185 6.22056**

**C 25 -0.22056 1.99910 4.20961 0.01185 6.22056**

**H 26 0.24320 0.00000 0.75524 0.00156 0.75680**

**H 27 0.24320 0.00000 0.75524 0.00156 0.75680**

**H 28 0.24320 0.00000 0.75524 0.00156 0.75680**

**H 29 0.24320 0.00000 0.75524 0.00156 0.75680**

**H 30 0.24320 0.00000 0.75524 0.00156 0.75680**

**H 31 0.24320 0.00000 0.75524 0.00156 0.75680**

**H 32 0.24320 0.00000 0.75524 0.00156 0.75680**

**H 33 0.24320 0.00000 0.75524 0.00156 0.75680**

**O 34 -0.16035 1.99994 6.15421 0.00620 8.16035**

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

**\* Total \* -0.00000 67.96694 125.57089 0.46217 194.00000**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **1** | **Fe** | **1** | **S** | **Cor(** | **1S)** | **2.00000** |
| **2** | **Fe** | **1** | **S** | **Cor(** | **2S)** | **2.00000** |
| **3** | **Fe** | **1** | **S** | **Cor(** | **3S)** | **1.99625** |
| **4** | **Fe** | **1** | **S** | **Val(** | **4S)** | **0.27065** |
| **5** | **Fe** | **1** | **S** | **Ryd(** | **5S)** | **0.00144** |
| **6** | **Fe** | **1** | **S** | **Ryd(** | **6S)** | **0.00048** |
| **7** | **Fe** | **1** | **px** | **Cor(** | **2p)** | **2.00000** |
| **8** | **Fe** | **1** | **px** | **Cor(** | **3p)** | **1.99836** |
| **9** | **Fe** | **1** | **px** | **Val(** | **4p)** | **0.22928** |
| **10** | **Fe** | **1** | **px** | **Ryd(** | **5p)** | **0.00067** |
| **11** | **Fe** | **1** | **py** | **Cor(** | **2p)** | **2.00000** |
| **12** | **Fe** | **1** | **py** | **Cor(** | **3p)** | **1.99836** |
| **13** | **Fe** | **1** | **py** | **Val(** | **4p)** | **0.22929** |
| **14** | **Fe** | **1** | **py** | **Ryd(** | **5p)** | **0.00067** |
| **15** | **Fe** | **1** | **pz** | **Cor(** | **2p)** | **2.00000** |
| **16** | **Fe** | **1** | **pz** | **Cor(** | **3p)** | **1.99267** |
| **17** | **Fe** | **1** | **pz** | **Val(** | **4p)** | **0.16906** |
| **18** | **Fe** | **1** | **pz** | **Ryd(** | **5p)** | **0.00077** |
| **19** | **Fe** | **1** | **dxy** | **Val(** | **3d)** | **1.97782** |
| **20** | **Fe** | **1** | **dxy** | **Ryd(** | **4d)** | **0.00306** |
| **21** | **Fe** | **1** | **dxy** | **Ryd(** | **5d)** | **0.00037** |
| **22** | **Fe** | **1** | **dxz** | **Val(** | **3d)** | **1.44668** |
| **23** | **Fe** | **1** | **dxz** | **Ryd(** | **4d)** | **0.00417** |
| **24** | **Fe** | **1** | **dxz** | **Ryd(** | **5d)** | **0.00016** |
| **25** | **Fe** | **1** | **dyz** | **Val(** | **3d)** | **1.44667** |
| **26** | **Fe** | **1** | **dyz** | **Ryd(** | **4d)** | **0.00417** |
| **27** | **Fe** | **1** | **dyz** | **Ryd(** | **5d)** | **0.00016** |
| **28** | **Fe** | **1** | **dx2y2** | **Val(** | **3d)** | **0.95643** |
| **29** | **Fe** | **1** | **dx2y2** | **Ryd(** | **4d)** | **0.00253** |
| **30** | **Fe** | **1** | **dx2y2** | **Ryd(** | **5d)** | **0.00003** |
| **31** | **Fe** | **1** | **dz2** | **Val(** | **3d)** | **1.02589** |
| **32** | **Fe** | **1** | **dz2** | **Ryd(** | **4d)** | **0.00193** |
| **33** | **Fe** | **1** | **dz2** | **Ryd(** | **5d)** | **0.00002** |

[Co**L**(O)]

**Atom No Charge Core Valence Rydberg Total**

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

**Co 1 0.33092 17.98922 8.66489 0.01497 26.66908**

**N 2 -0.35967 1.99917 5.33616 0.02434 7.35967**

**N 3 -0.35318 1.99917 5.32942 0.02459 7.35318**

**N 4 -0.35967 1.99917 5.33616 0.02434 7.35967**

**N 5 -0.35318 1.99917 5.32942 0.02459 7.35318**

**C 6 0.32475 1.99927 3.65478 0.02120 5.67525**

**C 7 0.32475 1.99927 3.65478 0.02120 5.67525**

**C 8 0.31985 1.99927 3.65968 0.02119 5.68015**

**C 9 0.31985 1.99927 3.65968 0.02119 5.68015**

**C 10 0.32475 1.99927 3.65478 0.02120 5.67525**

**C 11 0.32475 1.99927 3.65478 0.02120 5.67525**

**C 12 0.31985 1.99927 3.65968 0.02119 5.68015**

**C 13 0.31985 1.99927 3.65968 0.02119 5.68015**

**N 14 -0.35637 1.99937 5.34192 0.01509 7.35637**

**N 15 -0.35637 1.99937 5.34192 0.01509 7.35637**

**N 16 -0.35637 1.99937 5.34192 0.01509 7.35637**

**N 17 -0.35637 1.99937 5.34192 0.01509 7.35637**

**C 18 -0.22106 1.99910 4.21012 0.01185 6.22106**

**C 19 -0.22106 1.99910 4.21012 0.01185 6.22106**

**C 20 -0.22018 1.99910 4.20923 0.01185 6.22018**

**C 21 -0.22018 1.99910 4.20923 0.01185 6.22018**

**C 22 -0.22106 1.99910 4.21012 0.01185 6.22106**

**C 23 -0.22106 1.99910 4.21012 0.01185 6.22106**

**C 24 -0.22018 1.99910 4.20923 0.01185 6.22018**

**C 25 -0.22018 1.99910 4.20923 0.01185 6.22018**

**H 26 0.24399 0.00000 0.75445 0.00156 0.75601**

**H 27 0.24399 0.00000 0.75445 0.00156 0.75601**

**H 28 0.24360 0.00000 0.75484 0.00156 0.75640**

**H 29 0.24360 0.00000 0.75484 0.00156 0.75640**

**H 30 0.24399 0.00000 0.75445 0.00156 0.75601**

**H 31 0.24399 0.00000 0.75445 0.00156 0.75601**

**H 32 0.24360 0.00000 0.75484 0.00156 0.75640**

**H 33 0.24360 0.00000 0.75484 0.00156 0.75640**

**O 34 -0.24351 1.99995 6.23799 0.00556 8.24351**

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

**\* Total \* -0.00000 67.97027 126.57412 0.45561 195.00000**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **1** | **Co** | **1** | **S** | **Cor(** | **1S)** | **2.00000** |
| **2** | **Co** | **1** | **S** | **Cor(** | **2S)** | **2.00000** |
| **3** | **Co** | **1** | **S** | **Cor(** | **3S)** | **1.99649** |
| **4** | **Co** | **1** | **S** | **Val(** | **4S)** | **0.28248** |
| **5** | **Co** | **1** | **S** | **Ryd(** | **5S)** | **0.00140** |
| **6** | **Co** | **1** | **S** | **Ryd(** | **6S)** | **0.00055** |
| **7** | **Co** | **1** | **px** | **Cor(** | **2p)** | **2.00000** |
| **8** | **Co** | **1** | **px** | **Cor(** | **3p)** | **1.99857** |
| **9** | **Co** | **1** | **px** | **Val(** | **4p)** | **0.23827** |
| **10** | **Co** | **1** | **px** | **Ryd(** | **5p)** | **0.00069** |
| **11** | **Co** | **1** | **py** | **Cor(** | **2p)** | **2.00000** |
| **12** | **Co** | **1** | **py** | **Cor(** | **3p)** | **1.99860** |
| **13** | **Co** | **1** | **py** | **Val(** | **4p)** | **0.23290** |
| **14** | **Co** | **1** | **py** | **Ryd(** | **5p)** | **0.00071** |
| **15** | **Co** | **1** | **pz** | **Cor(** | **2p)** | **2.00000** |
| **16** | **Co** | **1** | **pz** | **Cor(** | **3p)** | **1.99557** |
| **17** | **Co** | **1** | **pz** | **Val(** | **4p)** | **0.16519** |
| **18** | **Co** | **1** | **pz** | **Ryd(** | **5p)** | **0.00086** |
| **19** | **Co** | **1** | **dxy** | **Val(** | **3d)** | **1.98126** |
| **20** | **Co** | **1** | **dxy** | **Ryd(** | **4d)** | **0.00231** |
| **21** | **Co** | **1** | **dxy** | **Ryd(** | **5d)** | **0.00032** |
| **22** | **Co** | **1** | **dxz** | **Val(** | **3d)** | **1.89913** |
| **23** | **Co** | **1** | **dxz** | **Ryd(** | **4d)** | **0.00316** |
| **24** | **Co** | **1** | **dxz** | **Ryd(** | **5d)** | **0.00014** |
| **25** | **Co** | **1** | **dyz** | **Val(** | **3d)** | **1.69176** |
| **26** | **Co** | **1** | **dyz** | **Ryd(** | **4d)** | **0.00192** |
| **27** | **Co** | **1** | **dyz** | **Ryd(** | **5d)** | **0.00015** |
| **28** | **Co** | **1** | **dx2y2** | **Val(** | **3d)** | **1.03878** |
| **29** | **Co** | **1** | **dx2y2** | **Ryd(** | **4d)** | **0.00133** |
| **30** | **Co** | **1** | **dx2y2** | **Ryd(** | **5d)** | **0.00005** |
| **31** | **Co** | **1** | **dz2** | **Val(** | **3d)** | **1.13513** |
| **32** | **Co** | **1** | **dz2** | **Ryd(** | **4d)** | **0.00132** |
| **33** | **Co** | **1** | **dz2** | **Ryd(** | **5d)** | **0.00005** |

[Ni**L**(O)]

**Atom No Charge Core Valence Rydberg Total**

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

**Ni 1 0.56277 17.99276 9.43418 0.01028 27.43723**

**N 2 -0.34440 1.99913 5.32090 0.02436 7.34440**

**N 3 -0.38879 1.99912 5.36534 0.02433 7.38879**

**N 4 -0.34440 1.99913 5.32090 0.02436 7.34440**

**N 5 -0.38879 1.99912 5.36534 0.02433 7.38879**

**C 6 0.30825 1.99927 3.67078 0.02170 5.69175**

**C 7 0.30824 1.99927 3.67079 0.02170 5.69176**

**C 8 0.27909 1.99927 3.69975 0.02188 5.72091**

**C 9 0.27911 1.99927 3.69974 0.02188 5.72089**

**C 10 0.30825 1.99927 3.67078 0.02170 5.69175**

**C 11 0.30824 1.99927 3.67079 0.02170 5.69176**

**C 12 0.27909 1.99927 3.69975 0.02188 5.72091**

**C 13 0.27911 1.99927 3.69974 0.02188 5.72089**

**N 14 -0.35489 1.99937 5.34045 0.01507 7.35489**

**N 15 -0.35489 1.99937 5.34045 0.01507 7.35489**

**N 16 -0.35490 1.99937 5.34045 0.01507 7.35490**

**N 17 -0.35490 1.99937 5.34045 0.01507 7.35490**

**C 18 -0.23830 1.99909 4.22703 0.01218 6.23830**

**C 19 -0.23830 1.99909 4.22702 0.01218 6.23830**

**C 20 -0.21840 1.99909 4.20735 0.01195 6.21840**

**C 21 -0.21840 1.99909 4.20735 0.01195 6.21840**

**C 22 -0.23830 1.99909 4.22703 0.01218 6.23830**

**C 23 -0.23830 1.99909 4.22702 0.01218 6.23830**

**C 24 -0.21840 1.99909 4.20735 0.01195 6.21840**

**C 25 -0.21840 1.99909 4.20735 0.01195 6.21840**

**H 26 0.24192 0.00000 0.75652 0.00157 0.75808**

**H 27 0.24192 0.00000 0.75652 0.00157 0.75808**

**H 28 0.24618 0.00000 0.75228 0.00153 0.75382**

**H 29 0.24618 0.00000 0.75228 0.00153 0.75382**

**H 30 0.24192 0.00000 0.75652 0.00157 0.75808**

**H 31 0.24192 0.00000 0.75652 0.00157 0.75808**

**H 32 0.24618 0.00000 0.75228 0.00153 0.75382**

**H 33 0.24618 0.00000 0.75228 0.00153 0.75382**

**O 34 -0.15185 1.99997 6.14827 0.00360 8.15185**

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

**\* Total \* -0.00000 67.97361 127.57157 0.45482 196.00000**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **1** | **Ni** | **1** | **S** | **Cor(** | **1S)** | **2.00000** |
| **2** | **Ni** | **1** | **S** | **Cor(** | **2S)** | **2.00000** |
| **3** | **Ni** | **1** | **S** | **Cor(** | **3S)** | **1.99625** |
| **4** | **Ni** | **1** | **S** | **Val(** | **4S)** | **0.30271** |
| **5** | **Ni** | **1** | **S** | **Ryd(** | **5S)** | **0.00160** |
| **6** | **Ni** | **1** | **S** | **Ryd(** | **6S)** | **0.00064** |
| **7** | **Ni** | **1** | **px** | **Cor(** | **2p)** | **2.00000** |
| **8** | **Ni** | **1** | **px** | **Cor(** | **3p)** | **1.99883** |
| **9** | **Ni** | **1** | **px** | **Val(** | **4p)** | **0.22940** |
| **10** | **Ni** | **1** | **px** | **Ryd(** | **5p)** | **0.00078** |
| **11** | **Ni** | **1** | **py** | **Cor(** | **2p)** | **2.00000** |
| **12** | **Ni** | **1** | **py** | **Cor(** | **3p)** | **1.99885** |
| **13** | **Ni** | **1** | **py** | **Val(** | **4p)** | **0.23306** |
| **14** | **Ni** | **1** | **py** | **Ryd(** | **5p)** | **0.00076** |
| **15** | **Ni** | **1** | **pz** | **Cor(** | **2p)** | **2.00000** |
| **16** | **Ni** | **1** | **pz** | **Cor(** | **3p)** | **1.99884** |
| **17** | **Ni** | **1** | **pz** | **Val(** | **4p)** | **0.17074** |
| **18** | **Ni** | **1** | **pz** | **Ryd(** | **5p)** | **0.00060** |
| **19** | **Ni** | **1** | **dxy** | **Val(** | **3d)** | **1.98579** |
| **20** | **Ni** | **1** | **dxy** | **Ryd(** | **4d)** | **0.00112** |
| **21** | **Ni** | **1** | **dxy** | **Ryd(** | **5d)** | **0.00026** |
| **22** | **Ni** | **1** | **dxz** | **Val(** | **3d)** | **1.93604** |
| **23** | **Ni** | **1** | **dxz** | **Ryd(** | **4d)** | **0.00080** |
| **24** | **Ni** | **1** | **dxz** | **Ryd(** | **5d)** | **0.00013** |
| **25** | **Ni** | **1** | **dyz** | **Val(** | **3d)** | **1.97662** |
| **26** | **Ni** | **1** | **dyz** | **Ryd(** | **4d)** | **0.00139** |
| **27** | **Ni** | **1** | **dyz** | **Ryd(** | **5d)** | **0.00013** |
| **28** | **Ni** | **1** | **dx2y2** | **Val(** | **3d)** | **1.21698** |
| **29** | **Ni** | **1** | **dx2y2** | **Ryd(** | **4d)** | **0.00087** |
| **30** | **Ni** | **1** | **dx2y2** | **Ryd(** | **5d)** | **0.00008** |
| **31** | **Ni** | **1** | **dz2** | **Val(** | **3d)** | **1.38284** |
| **32** | **Ni** | **1** | **dz2** | **Ryd(** | **4d)** | **0.00102** |
| **33** | **Ni** | **1** | **dz2** | **Ryd(** | **5d)** | **0.00010** |

[Cu**L**(O)]

**Atom No Charge Core Valence Rydberg Total**

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

**Cu 1 0.81729 17.99460 10.17719 0.01091 28.18271**

**N 2 -0.35150 1.99914 5.32535 0.02701 7.35150**

**N 3 -0.38348 1.99913 5.35789 0.02646 7.38348**

**N 4 -0.35150 1.99914 5.32537 0.02699 7.35150**

**N 5 -0.38350 1.99913 5.35791 0.02646 7.38350**

**C 6 0.31204 1.99926 3.66692 0.02178 5.68796**

**C 7 0.31205 1.99926 3.66691 0.02178 5.68795**

**C 8 0.28233 1.99926 3.69640 0.02200 5.71767**

**C 9 0.28230 1.99926 3.69643 0.02200 5.71770**

**C 10 0.31203 1.99926 3.66693 0.02178 5.68797**

**C 11 0.31207 1.99926 3.66689 0.02178 5.68793**

**C 12 0.28232 1.99926 3.69641 0.02200 5.71768**

**C 13 0.28228 1.99926 3.69645 0.02200 5.71772**

**N 14 -0.35614 1.99937 5.34205 0.01473 7.35614**

**N 15 -0.35616 1.99937 5.34206 0.01473 7.35616**

**N 16 -0.35611 1.99937 5.34201 0.01473 7.35611**

**N 17 -0.35611 1.99937 5.34201 0.01473 7.35611**

**C 18 -0.22934 1.99910 4.21819 0.01205 6.22934**

**C 19 -0.22935 1.99910 4.21820 0.01205 6.22935**

**C 20 -0.21125 1.99910 4.20035 0.01180 6.21125**

**C 21 -0.21124 1.99910 4.20034 0.01180 6.21124**

**C 22 -0.22926 1.99910 4.21811 0.01205 6.22926**

**C 23 -0.22929 1.99910 4.21814 0.01205 6.22929**

**C 24 -0.21124 1.99910 4.20035 0.01180 6.21124**

**C 25 -0.21127 1.99910 4.20037 0.01180 6.21127**

**H 26 0.24456 0.00000 0.75388 0.00156 0.75544**

**H 27 0.24456 0.00000 0.75388 0.00156 0.75544**

**H 28 0.24820 0.00000 0.75027 0.00153 0.75180**

**H 29 0.24820 0.00000 0.75027 0.00153 0.75180**

**H 30 0.24456 0.00000 0.75389 0.00156 0.75544**

**H 31 0.24455 0.00000 0.75389 0.00156 0.75545**

**H 32 0.24820 0.00000 0.75027 0.00153 0.75180**

**H 33 0.24820 0.00000 0.75027 0.00153 0.75180**

**O 34 -0.50900 1.99997 6.50594 0.00309 8.50900**

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

**\* Total \* 0.00000 67.97549 128.56179 0.46272 197.00000**

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

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

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

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **1** | **Cu** | **1** | **S** | **Cor(** | **1S)** | **2.00000** |
| **2** | **Cu** | **1** | **S** | **Cor(** | **2S)** | **2.00000** |
| **3** | **Cu** | **1** | **S** | **Cor(** | **3S)** | **1.99766** |
| **4** | **Cu** | **1** | **S** | **Val(** | **4S)** | **0.32424** |
| **5** | **Cu** | **1** | **S** | **Ryd(** | **5S)** | **0.00171** |
| **6** | **Cu** | **1** | **S** | **Ryd(** | **6S)** | **0.00058** |
| **7** | **Cu** | **1** | **px** | **Cor(** | **2p)** | **2.00000** |
| **8** | **Cu** | **1** | **px** | **Cor(** | **3p)** | **1.99925** |
| **9** | **Cu** | **1** | **px** | **Val(** | **4p)** | **0.22856** |
| **10** | **Cu** | **1** | **px** | **Ryd(** | **5p)** | **0.00066** |
| **11** | **Cu** | **1** | **py** | **Cor(** | **2p)** | **2.00000** |
| **12** | **Cu** | **1** | **py** | **Cor(** | **3p)** | **1.99923** |
| **13** | **Cu** | **1** | **py** | **Val(** | **4p)** | **0.22871** |
| **14** | **Cu** | **1** | **py** | **Ryd(** | **5p)** | **0.00065** |
| **15** | **Cu** | **1** | **pz** | **Cor(** | **2p)** | **2.00000** |
| **16** | **Cu** | **1** | **pz** | **Cor(** | **3p)** | **1.99848** |
| **17** | **Cu** | **1** | **pz** | **Val(** | **4p)** | **0.16257** |
| **18** | **Cu** | **1** | **pz** | **Ryd(** | **5p)** | **0.00050** |
| **19** | **Cu** | **1** | **dxy** | **Val(** | **3d)** | **1.99177** |
| **20** | **Cu** | **1** | **dxy** | **Ryd(** | **4d)** | **0.00067** |
| **21** | **Cu** | **1** | **dxy** | **Ryd(** | **5d)** | **0.00031** |
| **22** | **Cu** | **1** | **dxz** | **Val(** | **3d)** | **1.99318** |
| **23** | **Cu** | **1** | **dxz** | **Ryd(** | **4d)** | **0.00180** |
| **24** | **Cu** | **1** | **dxz** | **Ryd(** | **5d)** | **0.00023** |
| **25** | **Cu** | **1** | **dyz** | **Val(** | **3d)** | **1.99203** |
| **26** | **Cu** | **1** | **dyz** | **Ryd(** | **4d)** | **0.00173** |
| **27** | **Cu** | **1** | **dyz** | **Ryd(** | **5d)** | **0.00021** |
| **28** | **Cu** | **1** | **dx2y2** | **Val(** | **3d)** | **1.49265** |
| **29** | **Cu** | **1** | **dx2y2** | **Ryd(** | **4d)** | **0.00089** |
| **30** | **Cu** | **1** | **dx2y2** | **Ryd(** | **5d)** | **0.00013** |
| **31** | **Cu** | **1** | **dz2** | **Val(** | **3d)** | **1.76348** |
| **32** | **Cu** | **1** | **dz2** | **Ryd(** | **4d)** | **0.00064** |
| **33** | **Cu** | **1** | **dz2** | **Ryd(** | **5d)** | **0.00020** |