A Matrix Isolation ESR and Theoretical Study of ZnN

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**Table S1.** Observed and Simulated Line Positions in Gauss for the $xy_1$, oa and $xy_3$ Lines of $Zn^{15}N$ and the $xy_1$ lines of $^{67}ZnN$.

| $Zn^{15}N$ | | | |
|---|---|---|---|
| frequency (MHz) | $M_I$[a] | Obs.[b] | Calc.[c] |
| 9714.181 | 1/2 | 1887.6(3) | 1887.53 |
| | -1/2 | 1896.6(3) | 1896.51 |
| 9714.483 | 1/2 | 5035.5(3) | 5035.45 |
| | -1/2 | 5040.3(3) | 5040.30 |
| 9714.379 | 1/2 | 5888.8(3) | 5888.80 |
| | -1/2 | 5897.6(3) | 5897.76 |
| | | | |
| $^{67}ZnN$[d] | | | |
| $M_I$[e] | $M_I$[a] | Obs.[b] | Calc.[c] |
| 5/2 | 1 | | 1737.83 |
| | 0 | | 1744.22 |
| | -1 | 1750.7(3) | 1750.59 |
| 3/2 | 1 | 1791.7(3) | 1791.45 |
| | 0 | 1797.9(3) | 1797.83 |
| | -1 | 1804.1(3) | 1804.23 |
| 1/2 | 1 | 1846.1(3) | 1846.25 |
| | 0 | 1852.8(3) | 1852.64 |

| | | | |
|---|---|---|---|
| | -1 | 1859.1(3) | 1859.02 |
| -1/2 | 1 | 1902.1(3) | 1902.23 |
| | 0 | 1908.8(3) | 1908.61 |
| | -1 | 1915.2(3) | 1914.99 |
| -3/2 | 1 | 1958.9(3) | 1959.40 |
| | 0 | 1965.3(3) | 1965.78 |
| | -1 | 1971.9(3) | 1972.16 |
| -5/2 | 1 | 2017.9(3) | 2017.71 |
| | 0 | 2024.2(3) | 2024.09 |
| | -1 | 2030.4(3) | 2030.47 |

[a]The magnetic quantum number for the N (I=1/2) nucleus or the $^{15}$N (I=1) nucleus.

[b]Peak positions as measured at the apex. The radical was trapped in a neon matrix at 4.3 K. Uncertainty in position is ± 0.3 G.

[c]Peak positions of a simulated spectra generated by direct diagonalisation of the spin Hamiltonian using the magnetic parameters found in Table 2.

[d]Microwave frequency of 9683.086 MHz

[e]The magnetic quantum number for the Zn-67 (I=5/2) nucleus.

**Table S2.** Comparison of Potential Energy Surface dissociation energy levels to experimentally determined energy level combinations for atomic Zn and N in Hartree.

| **Zn** | **N** | $S_z$ | Experiment[a] | PES[b] |
|---|---|---|---|---|
| **$^1$S** | **$^4$S$^0$** | 1.5 | 0[c] | 0[c] |
| **$^1$S** | **$^2$D$^0$** | 0.5 | 0.0876 | 0.100 |
| **$^1$S** | **$^2$P$^0$** | 0.5 | 0.1314 | 0.110 |
| **$^3$P$^0$** | **$^4$S$^0$** | 2.5 | 0.1484 | 0.144 |
| **$^1$P$^0$** | **$^4$S$^0$** | 1.5 | 0.2130 | 0.1687 |
| **$^3$P$^0$** | **$^2$D$^0$** | 1.5 | 0.23481 | 0.244 |

[a]Experimental values from Ref. 55 and 56

[b]Potential energy values are taken from the PES shown in Figure 5 at a bond length of 6.0 Å

[c]Set to 0