# Thermodynamic Functions of 1,2-*trans*-Difluorodiazine

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THERMODYNAMIC functions, using the rigid-rotator-harmonic-oscillator approximation, have been calculated for *trans*-1,2-difluorodiazine, FN = NF. Heat capacities, enthalpies, free energies, and entropies are reported for the perfect gas state between 100 and 6000° K. The data used were as follows: ($r_{NF}$ = 1.44 ± .05A., $r_{NN}$ = 1.25 ± .04A. ∠FNN = 115 ± 5°, ∠FNF = 130°) (*3*): where $r_{NF}$ and $r_{NN}$ are the NF, and NN distances respectively, and ∠FNN, and ∠FNF are the angles between the atoms designated. The vibrational frequencies, and moments of inertia, following the nomenclature given by Herzberg (*6*) are: FN = NF; $\nu_1$ 1010; $\nu_2$ 1636; $\nu_3$ 592; $\nu_4$ 989; $\nu_5$ 421; and $\nu_6$ 360 cm.$^{-1}$ (*7*); $I_A = 107.45 \times 10^{-40}$; $I_B = 114.15 \times 10^{-40}$; $I_C = 221.60 \times 10^{-40}$ gram-cm.$^2$ The frequencies ($\nu_i$) are arranged in order of decreasing symmetry while the moments of inertia are in the following decreasing order $I_A < I_B < I_C$. Symmetry number, $\sigma = 2$. The physical constants used are those given by Cohen, Crowe, and Dumond (*4*).

The compound discussed here has been accepted as the trans-form of the difluorodiazines (*1, 2, 5*). The other form (active) which has been isolated is not as well characterized, and the evidence that it is the *cis*-1,2-difluorodiazine is not conclusive. At the time these calculations were done the thermodynamic functions for the 1,1-difluorodiazine were calculated assuming that the data for the active form applied to this isomer. This data will not be published unless more conclusive evidence is available about the structure of this isomer.

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Table I. Perfect Gas Thermodynamic Functions for *Trans*-1,2-difluoridiazine, FN = NF

| T. ° K. | $C_p^0/R^a$ | $(H^0 - E_0^0)/RT^a$ | $-(F^0 - E_0^0)/RT^a$ | $S^0/R^a$ |
|---|---|---|---|---|
| 100 | 4.044 | 4.005 | 25.80 | 22.11 |
| 200 | 4.853 | 4.189 | 28.79 | 24.93 |
| 300 | 6.029 | 4.608 | 30.99 | 26.70 |
| 400 | 6.995 | 5.090 | 32.86 | 28.09 |
| 500 | 7.702 | 5.546 | 34.50 | 29.28 |
| 600 | 8.212 | 5.950 | 35.95 | 30.33 |
| 700 | 8.581 | 6.301 | 37.25 | 31.27 |
| 800 | 8.854 | 6.604 | 38.41 | 32.13 |
| 900 | 9.059 | 6.866 | 39.47 | 32.93 |
| 1000 | 9.215 | 7.093 | 40.43 | 33.66 |
| 1100 | 9.337 | 7.292 | 41.32 | 34.35 |
| 1200 | 9.433 | 7.466 | 42.13 | 34.99 |
| 1300 | 9.510 | 7.621 | 42.89 | 35.59 |
| 1400 | 9.573 | 7.758 | 43.60 | 36.16 |
| 1500 | 9.625 | 7.881 | 44.26 | 36.70 |
| 1600 | 9.668 | 7.991 | 44.88 | 37.21 |
| 1700 | 9.704 | 8.091 | 45.47 | 37.70 |
| 1800 | 9.735 | 8.181 | 46.03 | 38.17 |
| 1900 | 9.761 | 8.264 | 46.55 | 38.61 |
| 2000 | 9.783 | 8.339 | 47.05 | 39.04 |
| 2100 | 9.803 | 8.409 | 47.53 | 39.45 |
| 2200 | 9.820 | 8.472 | 47.99 | 39.84 |
| 2300 | 9.835 | 8.531 | 48.42 | 40.22 |
| 2400 | 9.848 | 8.586 | 48.84 | 40.58 |
| 2500 | 9.860 | 8.637 | 49.25 | 40.93 |
| 2600 | 9.870 | 8.684 | 49.63 | 41.27 |
| 2700 | 9.880 | 8.728 | 50.01 | 41.60 |
| 2800 | 9.888 | 8.769 | 50.36 | 41.92 |
| 2900 | 9.895 | 8.808 | 50.71 | 42.23 |
| 3000 | 9.902 | 8.844 | 51.05 | 42.53 |
| 3100 | 9.908 | 8.879 | 51.37 | 42.82 |
| 3200 | 9.914 | 8.911 | 51.69 | 43.10 |
| 3300 | 9.919 | 8.941 | 51.99 | 43.37 |
| 3400 | 9.923 | 8.970 | 52.29 | 43.64 |
| 3500 | 9.928 | 8.997 | 52.58 | 43.90 |
| 3600 | 9.932 | 9.023 | 52.86 | 44.16 |
| 3700 | 9.935 | 9.048 | 53.13 | 44.40 |
| 3800 | 9.938 | 9.071 | 53.39 | 44.65 |
| 3900 | 9.942 | 9.093 | 53.65 | 44.88 |
| 4000 | 9.944 | 9.115 | 53.90 | 45.11 |
| 4100 | 9.947 | 9.135 | 54.15 | 45.34 |
| 4200 | 9.950 | 9.154 | 54.39 | 45.56 |
| 4300 | 9.952 | 9.173 | 54.62 | 45.77 |
| 4400 | 9.954 | 9.191 | 54.85 | 45.98 |
| 4500 | 9.956 | 9.208 | 55.17 | 46.19 |
| 4600 | 9.958 | 9.224 | 55.29 | 46.39 |
| 4700 | 9.960 | 9.239 | 55.51 | 46.59 |
| 4800 | 9.961 | 9.255 | 55.72 | 46.79 |
| 4900 | 9.963 | 9.269 | 55.92 | 46.98 |
| 5000 | 9.964 | 9.283 | 56.12 | 47.16 |
| 5100 | 9.966 | 9.296 | 56.32 | 47.35 |
| 5200 | 9.967 | 9.309 | 56.51 | 47.53 |
| 5300 | 9.968 | 9.322 | 56.70 | 47.71 |
| 5400 | 9.969 | 9.334 | 56.89 | 47.88 |
| 5500 | 9.970 | 9.345 | 57.07 | 48.05 |
| 5600 | 9.972 | 9.356 | 57.25 | 48.22 |
| 5700 | 9.973 | 9.367 | 57.43 | 48.39 |
| 5800 | 9.973 | 9.378 | 57.60 | 48.55 |
| 5900 | 9.974 | 9.388 | 57.77 | 48.71 |
| 6000 | 9.975 | 9.397 | 57.94 | 48.87 |

Table I. Perfect Gas Thermodynamic Functions for *Trans*-1,2-difluoridiazine, FN = NF (*Continued*)

[a] Dimensionsless

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