2007, Volume 111A

Myrna H. Matus, Minh Tho Nguyen,* and David A. Dixon*: Heats of Formation of Diphosphene, Phosphinophosphinidene, Diphosphine and Their Methyl Derivatives, and Mechanism of the Borane-Assisted Hydrogen Release

Page 1726. Some of the heats of formation of the compounds containing nitrogen were incorrectly copied into Table 3 by us at the time of submission. None of the conclusions were changed.

TABLE 3: CCSD(T)/CBS Calculated and Experimental Heats of Formation (kcal/mol) at 0 and 298 K

molecule	ΔH_f (0 K)[a]	$\Delta H_f°$ (298 K)[a]	$\Delta H_f°$ (298 K) exptl
PH ($^3\Sigma^-$)	57.0	56.8	57.4 ± 0.6[b]
			$[60.6 \pm 8.0]$[c]
PH_2 ($^2B_1$)	32.7	31.8	33.1 ± 0.6[b]
			$[30.1 \pm 23.0]$[c]
PH_3 ($^1A_1$)	3.0	1.1	1.3 ± 0.4[d]
			1.1 ± 0.6[e]
P_2 ($^1\Sigma_g^+$)	35.2	34.7	34.3 ± 0.5[f]
P_2H ($^2A'$)	54.4	53.4	
trans-P_2H_2 (^1A_g)	30.6	28.7	
cis-P_2H_2 ($^1A_1$)	33.9	32.0	
H_2PP ($^1A_1$)	55.6	53.7	
H_2PP ($^3A''$)	58.3	56.5	
P_2H_3 (^2A)	34.8	32.3	
P_2H_4 (^1A)	9.1	5.7	5.0 ± 1.0[g]
CH_3PH_2 ($^1A'$)	−1.4	−5.0	
$BH_3PH_2PH_2$	12.9	7.5	
NH ($^3\Sigma^-$)	85.9[h]	85.9[i]	90 ± 4[f]
NH_2 ($^2B_1$)	45.3[h]	44.6[i]	44.50 ± 0.09[h]
NH_3 ($^1A_1$)	−9.1[j]	−10.7[j]	-10.98 ± 0.08[k]
			-10.97 ± 0.10[f]
			-10.891 ± 0.007[l]
N_2 ($^1\Sigma_g^+$)	0.6[m]	0.6[m]	0.0
N_2H ($^2A'$)	60.8[m]	60.1[m]	
trans-N_2H_2 (^1A_g)	49.9[m]	48.1[m]	$\geq 46.6 \pm 0.8$[n]
cis-N_2H_2 ($^1A_1$)	54.9[m]	53.2[m]	
H_2NN ($^1A_1$)	73.9	72.2	
H_2NN ($^3A''$)	89.5	87.8	
N_2H_3 (^2A)	56.2[m]	53.7[m]	
N_2H_4 (^1A)	26.6[m]	23.1[m]	22.8 ± 0.2[f]
CH_3NH_2 ($^1A'$)	−1.4[o]	−4.7[o]	-5.4 ± 0.2[p]

[a] Estimated error bar of ±1.0 kcal/mol. [b] Berkowitz, J. C. *J. Chem. Phys.* **1989**, *90*, 1. [c] Estimated values from: Chase, M. W., Jr. NIST-JANAF Tables, 4th ed. *J. Phys. Chem. Ref. Data* **1998**, *Monograph 9 (Suppl. 1)*. At 0 K, $\Delta H_{f,exptl}(PH) = 60.8 \pm 8.0$ and $\Delta H_{f,exptl}(PH_2) = 30.7 \pm 23.0$ kcal/mol. [d] Gunn, S. R.; Green, L. G. *J. Chem. Phys.* **1961**, *65*, 779. [e] (a) Gurvich, L. V.; Veyts, I. V.; Alcock, C. B. *Thermodynamic Properties of Individual Substances*, 4th ed.; : New York, **1989**. (b) Cox, J. D.; Wagman, D. D.; Medvedev, V. A. *CODATA Key Values for Thermodynamics*; : New York, **1989**. [f] Chase, M. W., Jr. NIST-JANAF Tables, 4th ed. *J. Phys. Chem. Ref. Data* **1998**, *Monograph 9 (Suppl. 1)*. At 0 K, $\Delta H_{f,exptl}(P_2) = 34.8 \pm 0.5$ kcal/mol. [g] (a) Berkowitz, J. C. *J. Chem. Phys.* **1989**, *90*, 1. (b). Wagman, D. D.; Evans, W. H.; Parker, V. B.; Schumm, R. H.; Halow, I.; Bailey, S. M.; Churney, K. L.; Nuttall, R. L. *J. Phys. Chem. Ref. Data* **1982**, *Monograph 11 (Suppl. 2)*. [h] Dixon, D. A.; Feller, D.; Peterson, K. A. *J. Chem. Phys.* **2001**, *115*, 2576. At 0 K, $\Delta H_{f,exptl}(NH) = 90.0 \pm 4$ kcal/mol (Chase, M. W., Jr. NIST-JANAF Tables, 4th ed. *J. Phys. Chem. Ref. Data* **1998**, *Monograph 9 (Suppl. 1)*) and $\Delta H_{f,exptl}(NH_2) = 45.17 \pm 0.09$ kcal/mol (Song, Y.; Qian, X-M.; Lau, K-C.; Ng, Y.; Liu, J.; Chen, W. *J. Chem. Phys.* **2001**, *115*, 2582). [i] Heats of formation at 298 K obtained with the values at 0 K and the CCSD(T)/aVTZ thermal corrections of NH and NH_2. [j] Grant, D. J.; Dixon, D. A. *J. Phys. Chem. A* **2006**, *110*, 12955. At 0 K, $\Delta H_{f,exptl}(NH_3) = -9.3 \pm 0.10$ kcal/mol (Chase, M. W., Jr. NIST-JANAF Tables, 4th ed. *J. Phys. Chem. Ref. Data* **1998**, *Monograph 9 (Suppl. 1)*). [k] Cox, J. D.; Wagman, D. D.; Medvedev, V. A. *CODATA Key Values for Thermodynamics*; : New York, **1989**. [l] Ruscic, B. Private communication of unpublished results 2005, obtained from Active Thermochemical Tables ver. 1.25 using the Core (Argonne) Thermochemical Network ver. 1.045. The Active Thermochemical Tables are described in detail in: Ruscic, B.; Pinzon, R. E.; Morton, M. L.; von Laszevski, G.; Bittner, S. J.; Nijsure, S. G.; Amin, K. A.; Minkoff, M.; Wagner, A. F. *J. Phys. Chem. A* **2004**, *108*, 9979. Ruscic, B. Active Thermochemical Tables. *2005 Yearbook of Science and Technology*; the yearly update of the McGraw-Hill Encyclopedia of Science and Technology; : New York, **2004**. [m] Matus, M. H.; Arduengo, A. J., III; Dixon, D. A. *J. Phys. Chem. A* **2006**, *110*, 10116. At 0 K, $\Delta H_{f,exptl}$(*trans*-N_2H_2) ≥ 48.8 ± 0.5 kcal/mol (Biehl, H.; Stuhl, F. *J. Chem. Phys.* **1994**, *100*, 141) and $\Delta H_{f,exptl}(N_2H_4) = 26.2$ kcal/mol (Chase, M. W., Jr. NIST-JANAF Tables, 4th ed. *J. Phys. Chem. Ref. Data* **1998**, *Monograph 9 (Suppl. 1)*). [n] Ruscic, B.; Berkowitz, J. C. *J. Chem. Phys.* **1991**, *95*, 4378. [o] Gutowski, K. E.; Rodgers, R. D.; Dixon, D. A. *J. Phys. Chem. A* **2006**, *110*, 11890. [p] (a) Pedley, J. B. *Thermodynamics of Organic Compounds in the Gas State*; : College Station, TX, **1994**; Vol. *II*. (b) Frenkel, M.; Kabo, G. J.; Marsh, K. N.; Roganov, G. N.; Wilhoit, R. C. *Thermodynamics of Organic Compounds in the Gas State*; : College Station, TX, **1994**; Vol. *II*. At 0 K, $\Delta H_{f,exptl}(CH_3NH_2) = -1.9 \pm 0.2$ kcal/mol.

10.1021/jp811432s
Published on Web 01/13/2009