ADDITIONS AND CORRECTIONS

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David M. Golden,* John R. Barker,* and Lawrence L. Lohr*: Master Equation Models for the Pressure- and Temperature-Dependent Reactions $HO + NO_2 \rightarrow HONO_2$ and $HO + NO_2 \rightarrow HOONO$

Page 11057. A bug, since corrected, in the Multiwell suite (ref 53) caused a small error in the calculated entropy and deduced enthalpy of the HOONO species. Changes in the last few sentences of the Appendix and Table 10 are in bold font.

Appendix: Thermochemistry of $HO + NO_2 = HOONO$

.... From this, we compute, as shown in Table 10, a third law value of the heat of formation of the cis−cis isomer to be **−9.28** kJ mol^{-1}. Using this value, we compute the value of the equilibrium constant for cis−cis formation and then for trans−perp formation using the same ratios as above. (Calculations of the individual equilibrium constant for the trans−perp isomer, with heats of formation adjusted from the QCISD(T)/cc-pVDZ value relative to the value for the cis−cis isomer yield the same result, as they should.) These values are shown in Table 10. Figure 11 shows a van't Hoff plot of the Hippler et al.[4] data and the third law function deduced above. **(Changes are too small to be discerned.)** The equilibrium constants used in obtaining the recombination rate constants from the dissociation rate constants for the individual isomers are presented in Table 8. **(These will change slightly but are largely offset by the concomitant change in the barriers for the dissociation.)**

TABLE 10: Third Law Heat of Formation for *cis*−*cis*-HOONO

T (K)	K_{equil} (bar^{-1})	factor	$K_{cis-cis}$ (bar^{-1})	ΔG(expt) (kJ mol^{-1})	ΔS(rxn) (J mol^{-1} K^{-1})	$\Delta H = \Delta G + T\Delta S$ (kJ mol^{-1})	$\Delta[H(T) - H(0)]$ (kJ mol^{-1})	ΔH(0K) (kJ mol^{-1})
430	670	1.03	653	−23.17	**−147.2**	**−86.47**	**−6.18**	**−80.29**
435	650	1.03	632	−23.33	**−147.3**	**−87.40**	**−6.22**	**−81.18**
440	520	1.03	505	−22.77	**−147.4**	**−87.63**	**−6.27**	**−81.36**
443	510	1.03	495	−22.85	**−147.4**	**−88.15**	**−6.30**	**−81.85**
445	450	1.03	437	−22.49	**−147.5**	**−88.13**	**−6.31**	**−81.82**
448	510	1.03	494	−23.10	**−147.5**	**−89.18**	**−6.34**	**−82.84**
450	340	1.03	329	−21.69	**−147.6**	**−88.11**	**−6.36**	**−81.75**
455	280	1.03	271	−21.19	**−147.7**	**−88.39**	**−6.41**	**−81.98**
460	240	1.04	232	−20.83	**−147.8**	**−88.81**	**−6.45**	**−82.36**
465	220	1.04	212	−20.71	**−147.9**	**−89.48**	**−6.49**	**−82.99**
470	190	1.04	183	−20.35	**−148.0**	**−89.91**	**−6.54**	**−83.37**
475	140	1.04	134	−19.36	**−148.1**	**−89.70**	**−6.59**	**−83.11**
							av =	**−82.08**
							ΔH_f(HOONO)	**−9.28**

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