Thermodynamic Properties of Ideal Gas Nitro and Nitrate Compounds

Cite as: Journal of Physical and Chemical Reference Data **28**, 63 (1999); https://doi.org/10.1063/1.556033
Submitted: 06 July 1998 . Published Online: 25 March 1999

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Received July 6, 1998; final manuscript received December 4, 1998

The ideal gas thermodynamic properties of 27 organic nitro and nitrate organic compounds and two of their radicals are presented. Most of these compounds are high explosives (TNT, RDX, HMX, PETN, NPN, and NG), while others serve as propellants or specialty fuels (such as nitromethane). The thermodynamic properties were calculated using fundamental molecular data. The molecular data were gathered from the literature or calculated for this purpose. The enthalpy of formation of gaseous 1-nitropentane was estimated to be $-164.431\,\mathrm{kJ\,mol^{-1}}$ ($-39.3\pm0.5\,\mathrm{kcal\,mol^{-1}}$); that of 1-nitrohexane to be $-185.351\,\mathrm{kJ\,mol^{-1}}$ ($-44.3\pm0.7\,\mathrm{kcal\,mol^{-1}}$) for the ideal gas and $-241.835\,\mathrm{kJ\,mol^{-1}}$ ($-57.8\pm0.7\,\mathrm{kcal\,mol^{-1}}$) for the liquid. All values refer to 298.15 K. © *1999 American Institute of Physics and American Chemical Society.* [S0047-2689(99)00301-3]

Key words: explosives; nitro-compounds; nitrate compounds; thermodynamics.

Contents

List of Figures

List of Tables

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1. Introduction

This is an attempt to publish the detailed thermodynamics of a list of organic nitro and nitrate compounds, some of which are known as explosives, and others as propellants or specialty fuels. The detailed thermodynamics of most propellants and explosive compounds are not known or are unpublished in the open literature. The thermodynamic and thermochemical properties are involved in most computational aspects of these compounds including the enthalpy of reaction, the adiabatic flame temperature obtained during combustion, the temperature and pressure obtained during [gaseous] detonation, safety aspects, etc.

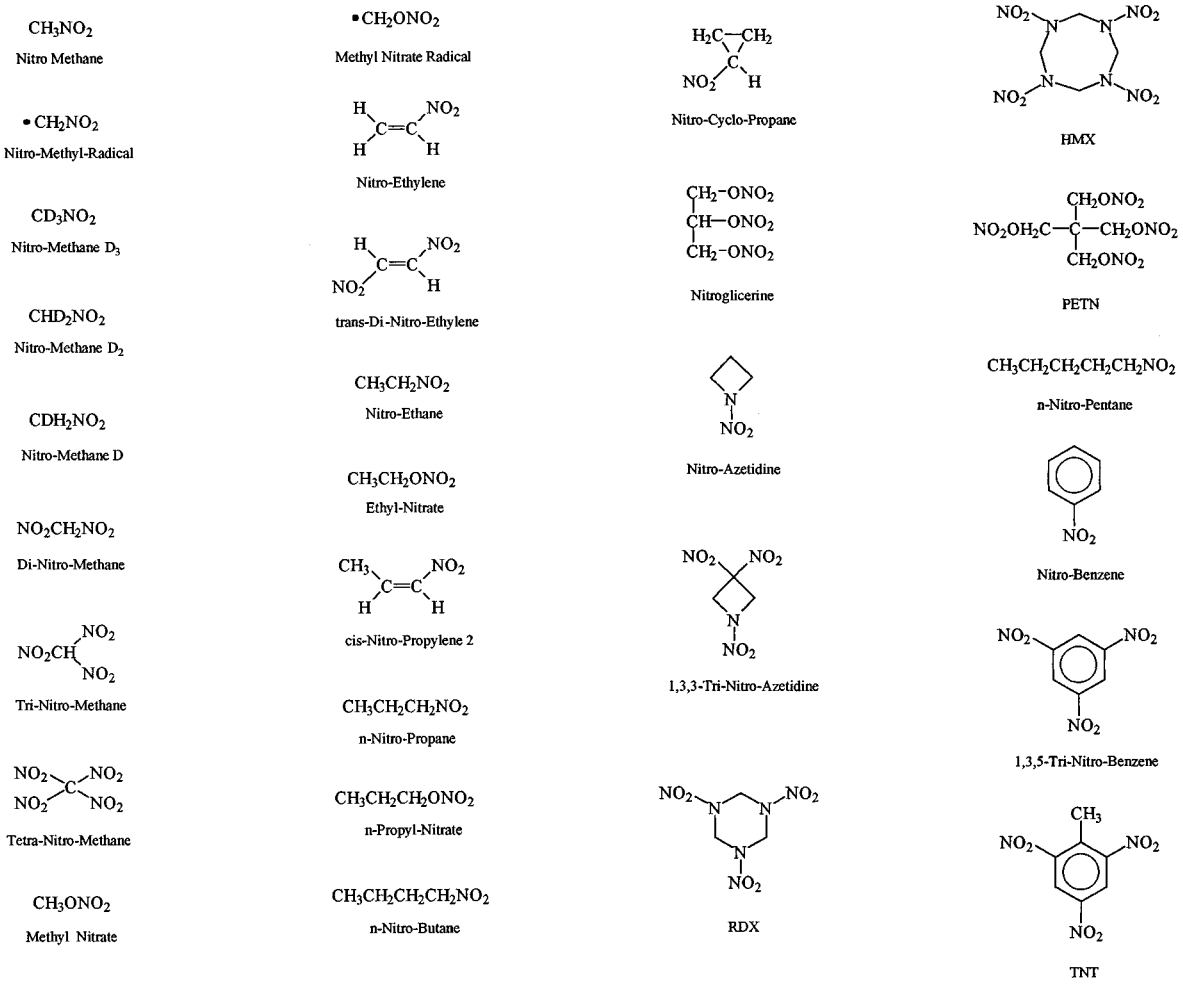
The fundamental molecular data such as molecular vibrations, moments of inertia, internal rotation barriers and enthalpies of formation were taken from existing sources (The NIST Webbook[1] for the experimental infrared (IR) spectrum and the experimental enthalpies of formation, Melius' BAC/MP4/MP2 collections,[35] and the open literature) or were calculated using GAUSSIAN 94[18] and mostly, semiempirical methods such as MOPAC.[54] In all cases the calculated data were supplemented where possible with experimental data. Checking with group additivity methods was done where possible using the NIST 94 thermodynamic program and database,[51] and Bozzelli's Therm program.[48]

It is known that the *ab initio* methods are by far more accurate than semiempirical ones, but lately the difference has been narrowed, and the semiempirical methods of today are almost as good as the *ab initio* ones regarding the optimization of a molecule's structure and the estimation of its molecular vibrations. However, the estimation of the enthalpies of formation are still unacceptable by semiempirical methods.

The list of compounds that will be covered in this work are:
Nitromethane CH_3NO_2,
Nitromethane-d_3 CD_3NO_2,
Nitromethane-d_2 CHD_2NO_2,
Nitromethane-d CH_2DNO_2,
Nitromethyl radical $\cdot CH_2NO_2$,
Dinitromethane $CH_2(NO_2)_2$,
Trinitromethane $CH(NO_2)_3$ (TNF),
Tetranitomethane $C(NO_2)_4$,
Methynitrate CH_3ONO_2
Methynitrate radical $\cdot CH_2ONO_2$,
Nitroethylene $CH_2{=}CHNO_2$,
Trans-dinitroethylene $O_2NHC{=}CHNO_2$,
Nitroethane $C_2H_5NO_2$,
Ethylnitrate $C_2H_5ONO_2$,
Nitropropene-2 $CH_3CH{=}CHNO_2$,
Nitrocyclo-propane $C_3H_5NO_2$,
Nitroglycerin $C_3H_5O_3(NO_2)_3$,
Nitroazetidine Cy $(CH_2)_3N\text{-}NO_2$,
1,3,3-Trinitroazetidine $C_3H_4N(NO_2)_3$,
Hexogen 1,3,5-trinitrotriazine $C_3H_6N_6O_6$ (RDX),
N-nitropropane $C_3H_7NO_2$,
N-propylnitrate $C_3H_7ONO_2$ (NPN),
Octogen Cyclotetramethylene Tetranitramine $C_4H_8N_8O_8$ (HMX),
N-nitrobutane $C_4H_9NO_2$,
Penta-trithrytoltetranitrate $C_5H_8(ONO_2)_4$ (PETN),
N-nitropentane $C_5H_{11}NO_2$,
Nitrolbenzene $C_6H_5NO_2$,
N-nitrohexane $C_6H_{13}NO_2$,
1,3,5-Trinitrobenzene $C_6H_3(NO_2)_3$,
1,3,5-Trinitrotolluene $CH_3C_6H_2(NO_2)_3$ (TNT).

There are 30 compounds covered in this work. Their structures are given in Table 1. The fundamental vibrational frequencies, the bond lengths, and the moments of inertia were calculated using MOPAC 6 semiempirical methods;[54] PM3, PM3/UHF, AM1, and AM1/UHF as well as GAUSSIAN 94 *ab initio* calculations. For simple molecules, the Brinkman and Burcat program[7] was used to calculate moments of inertia and internal moments of rotation. The results have been compared to existing experimental or *ab initio* calculations. The enthalpies of formation were treated in each case separately as reported in the following sections. In Table 2, all

TABLE 1. Configuration formulas of the nitro and nitrate compounds.



known values for the enthalpy of formation found in the literature are listed. Finally, recommendations were made and thermodynamic tables were calculated accordingly.

2. Thermodynamic Calculations

The thermodynamic calculations were made with the McBride and Gordon thermodynamic program,[31] version PAC97 at a standard pressure of 1 bar. The fundamental constants were taken from Cohen and Taylor,[11] and the atomic weights from DeLaeter and Heumann.[14] Where needed, the calculated fundamental frequencies were supplemented with internal rotation information taken from other nitro compounds as shown in Table 3.

3. The Individual Substances

3.1. Nitromethane CH_3NO_2

Nitromethane is the simplest organic nitro compound, and has been investigated both experimentally[33] and by calculations.[5] All MOPAC calculations resulted in transition states as seen from the vibrational results of PM3 (one imaginary vibration). Therefore the calculated enthalpies of formation are not mentioned. The IR spectrum[1] was adopted for the thermodynamic calculations, although McKean[33] published an assigned experimental spectrum. The actual difference in the calculated thermodynamic data (C_p, S, etc) was less than 0.3 calories when using the McKean[33] and the IR spectra.[1] Thus the IR spectra was preferred for the sake of compatibility with nitromethyl radical, the deuterated nitromethanes, nitroethane, nitropropane, nitrobutane and nitrobenzene. The molecular data available are listed in Table 4 and the thermodynamic calculations are listed in Table 5.

3.2. Nitromethyl Radical: $\cdot CH_2NO_2$

The experimental and calculated vibrational spectrum of this radical was published by McKee,[32] and calculated by Melius in 1997.[35] The PM3/UHF calculation resulted in a transition state. The experimental values were adopted and the two missing vibrations were taken from the GAUSSIAN 6-31G* calculation of McKee.[29] The PM3 moments of inertia were chosen and the reduced moments of inertia were calculated with the Brinkmann and Burcat[7] program. The molecular data available are listed in Table 6 and the thermodynamic calculations are listed in Table 7.

3.3. Nitromethane-d_3 CD_3NO_2

The vibrational spectrum was calculated by Bock *et al.*[3] using *ab initio* methods at HF/631G* levels. MOPAC calculations for PM3 and PM3/UHF have resulted in transition state species only, as can be seen from the enclosed vibrations. The experimental spectral results[5] were adopted. The moments of inertia were calculated using the Brinkmann and Burcat[7] program. The enthalpy of formation was calculated from the value of the nondeuterated molecule according to the equations:

$$\Delta_f H_0(\text{deuterated comp}) = \Delta_f H_0(\text{Parent compound}) - \Delta E_{\text{comp}} + \Delta E_{\text{elements}}$$

where

$$\Delta E_{\text{comp}} = \left(\sum \nu_I(\text{parent compound}) - \sum \nu_I(\text{deuterated comp}) \right) \times \frac{2.859\,121}{2} \text{ calories/mole}$$

$$\Delta E_{\text{elements}} = n\left(\sum \nu_{i\text{H}_2} - \sum \nu_{i\text{D}_2} \right) = n \times 1.8 \text{ kcal/mol},$$

where n is the number of hydrogen molecules H_2, that were deuterated. The molecular data available are listed in Table 8 and the thermodynamic calculations are listed in Table 9.

3.4. Nitromethane-d_2 CHD_2NO_2

The experimental spectrum was published by McKean and Watt.[33] As with all the deuterated and nondeuterated methane molecules the MOPAC PM3 and PM3/UHF calculations showed transition states. The enthalpy of formation was calculated from the CH_3NO_2 value, using the equations described for the previous species. For the thermodynamic calculations, the experimental values were adopted together with the moments of inertia calculated using the Brinkmann and Burcat[7] program. The molecular data available are listed in Table 10 and the thermodynamic calculations are listed in Table 11.

3.5. Nitromethane-d_1 CH_2DNO_2

The experimental vibrational spectrum was measured by Engelke *et al.*[17] As with all the deuterated and nondeuterated methane molecules the MOPAC PM3 and PM3/UHF calculations showed a transition state. The enthalpy of formation was calculated as described in the former deuterated species. For the thermodynamic calculations, the experimental values were adopted[19] together with the moments of inertia calculated using the Brinkmann and Burcat[7] program. The molecular data available are listed in Table 12 and the thermodynamic calculations are listed in Table 13.

3.6. Dinitromethane (TNF): $CH_2(NO_2)_2$

Dinitromethane is rarely mentioned in the literature. Melius calculates only transition states for this molecule. For the thermodynamic compilation, the PM3 calculations were chosen. The vibrations were not scaled since comparison of PM3 values of nitromethane showed no need to scale, if the vibrations are compared with the experimental (IR) values.[1] For the internal moments of inertia as well as energy barriers the Melius's values[35] from nitroethane were taken. The experimental enthalpy of formation recommended by NIST 97[40] was taken. The molecular data available are listed in Table 14 and the thermodynamic calculations are listed in Table 15.

3.7. Trinitromethane: $CH(NO_2)_3$

This propellant is mentioned in the literature where measured enthalpies of formation in the liquid and solid form are presented.[2] Benson[3] gives an estimate of its gaseous enthalpy of formation. The MOPAC calculations for AM1 and AM1/UHF have failed, resulting in transition states. The PM3 and PM3/UHF were successful with enthalpies of formation very far from Benson's estimate. The other values are very close together. For the thermodynamic calculations the PM3 vibrations were chosen since this species caused Stewart[52] to calibrate the PM3 system. The heat of formation found experimentally by Carpenter[9] was chosen. The internal rotation values were taken from Melius[35] or estimated. The molecular data available are listed in Table 16 and the thermodynamic calculations are listed in Table 17.

3.8. Tetranitromethane: $C(NO_2)_4$

Tetranitromethane served as one of 28 nitro compounds used by Stewart[52] to calibrate the PM3 method for the enthalpy of formation of nitro compounds. Our calculations with AM1 and AM1/UHF resulted in transition states only. The values of the calculated enthalpies of formation for PM1 are very far apart from those of Stewart. The NIST 97 experimental value was adopted. The molecular data available are listed in Table 18 and the thermodynamic calculations are listed in Table 19.

3.9. Methyl Nitrate: CH_3ONO_2

Experimental values are given by Brand and Cawthon,[6] and also by Czuchajowsky and Kucharski,[13] who calculated part of the vibrations. Additional BAC/MP4 calculations were made by Melius.[35] The vibrations of Brand and Cawthon[6] were adopted, and the Melius moments of inertia were preferred since this configuration is tighter than that of Dixon and Wilson.[16] The NIST 97[40] recommended that enthalpy of formation[50] be used. The molecular data available are listed in Table 20 and the thermodynamic calculations are listed in Table 21.

TABLE 2. Listed values of the enthalpy of formation at 298 K for nitro and nitrate species in kcal/mol.

Name	PM3	PM3 /UHF	AMI	AM1 /UHF	Melius	Pedley	NIST 94[b]	Experimental, (NIST 97)
Nitromethane	−15.9[a]		−9.9[a]		−16.85±2.1	−7.9	(−15.1)	−19.3±0.3
CH_3NO_2								
$*CH_2NO_2$	21.83				36.44			
CD_3NO_2								−18.008
CD_2HNO_2								−16.971
CDH_2NO_2								−15.686
Dinitromethane	−11.91	−11.91	74.41	2.91	−11.87±4.2			−14.7±0.3
$CH_2(NO_2)_2$			2.9[a]					
Trinitromethane	165.75	165.65	-	-	-		−0.2	−3.2[a]
$CH(NO_2)_3$	−4.7[a]		25.0[a]					
Tetranitromethane	189.57	189.57	224.39	224.39				(19.69)
$C(NO_2)_4$	6.4[a]							
Methylnitrate	−32.4[a]		−31.3[a]		−26.12±3.55	−29.±1.0	−29.6	−29.16±0.3
CH_3ONO_2								
$^aCH_2ONO_2$					23.65			
Nitroethylene	7.17	7.17	15.95	15.95	7.94		13.4	
$H_2C{=}CHNO_2$								
Dinitroethylene	−26.42	−26.42	−19.42	−19.50	85.12±5.22		14.2	
$C_2H_2(NO_2)_2$								
Nitroethane	−20.9[a]		−16.9[a]		−24.8±1.2	−24.4	−24.6	−23.5[a]
$C_2H_5NO_2$								
Ethylnitrate	−38.03	−38.03	−38.11	−38.11	−34.50			−37.04±
$C_2H_5ONO_2$								0.7
Nitropropene					2.39±2.12		5.5	
$CH_3CH{=}CHNO_2$								
Nitrocypropane							4.2	
$C_3H_5NO_2$							(6.42)	
Nitroglycerin	17.96	17.96	18.92	18.92			−81.5	−66.70±0.65
	−76.6[a]		−71.2[a]					−92.5[a]
Nitroazetidine					27.28±5.1			
$C_3H_6N\text{-}NO_2$								
Trinitroazetidine								30.7
RDX Hexogen	141.65		198.31					45.89
Nitropropane	−26.21	−26.21	−23.8[a]	−23.58		−29.7	−29.5	−30.0[a]
Propylnitrate	−42.68	−42.68	−44.38	−44.38		−41.60	−42.60	
HMX Octogen	93.37		174.98	174.45			24.1	
Nitrobutane	−32.1	-	−30.4	−29.6		−34.4	−34.4	−34.4[a]
PETN	−98.2[a]		−95.3[a]		−89.89			−92.5[a]
n-Nitropentane	−36.9	−36.9	−35.5	−35.5			−39.3	−39.3±0.5
Nitrobenzene	14.5[a]		25.3[a]		14.18±2.6			16.38±0.16
Trinitrobenzene	189.65	94.64		136.84		14.9		
$C_6H_{13}NO_2$							−44.3	−44.3±0.7
Trinitrotoluene	3.3[a]	89.73	41.3[a]					5.76±1.0
								12.9[a]

[a]Data reported by Stewart[52] as part of the optimization of the MOPAC AM1 and PM3 methods.
[b]Values in parenthesis were evaluated with the program THERM.[48]

3.10. Methyl Nitrate Radical: $\cdot CH_2ONO_2$

This radical was calculated by Melius[35] with the BAC/MP4 method at the HF/6-31G/* level. These data are used for the thermodynamic calculation. The molecular data are listed in Table 22 and the thermodynamic calculations are listed in Table 23.

3.11. Nitroethylene: $CH_2{=}CHNO_2$

The only source for this species is that of Melius BAC/MP4/6-31G** calculations. The MOPAC calculations are in very good agreement with those of Melius.[35] Thus all the Melius values including the enthalpy of formation were adopted. The molecular data available are listed in Table 24 and the thermodynamic calculations are listed in Table 25.

3.12. Trans-dinitroethylene: $O_2NHC{=}CHNO_2$

There are three possible isomers for dinitroethylene, the *cis*-form, the *trans*-form and the 1,1-form ($CH_2{=}C(NO_2)_2$). No calculations were found for this species. Melius[35] using MP4/G2 calculated transition states only. It was decided to

TABLE 3. Internal rotation values for different nitro and nitrate compounds.

Compound	$I_r(CH_3)$ ($\times 10^{40}$ g cm^2)	$I_r(NO_2)$ ($\times 10^{40}$ g cm^2)	V(2)NO_2[a] (kcal/mol)	V(3)CH_3[a] (kcal/mol)	V(2)NO_2[b] (kcal/mol)	$I_r(CX_3)$ ($\times 10^{40}$ g cm^2)	$I_r(NO_2)$[c] ($\times 10^{40}$ g cm^2)
CH_3NO_2	5.1666	59.60		9.1	0.0	5.187	59.316
[a]CH_2NO_2						3.46	59.32
CD3NO2						10.36	
CHD_2NO_2						8.64	
CDH_2NO_2						6.91	
$C_2H_3NO_2$	-	59.710	5.04	-	4.8		
$C_2H_5NO_2$	5.1666	59.548	0.08	3.50			
$CH_3CH{=}CHNO_2$	5.1536	59.606	1.50	8.8			
N-nitroazetidine					4.6		
$C_6H_5NO_2$	-	59.350	3.11	-	2.8-3.3		
CH_3ONO_2	5.280	17.4	2.32	9.1			
$(CH_3)_2NNO_2$					>9		

[a]Values taken from Melius.[35]
[b]Values taken from Habibullahzadeh[20]
[c]Values calculated using Brinkmann and Burcat's program.[7]

calculate the most abundant of the isomers, the *trans*-form, although the differences between the isomers should be minimal. The PM3 calculations were adopted. The NIST 94[41] estimation was used for the enthalpy of formation. The molecular data available are listed in Table 26 and the thermodynamic calculations are listed in Table 27.

3.13. Nitroethane: $C_2H_5NO_2$

The thermodynamic properties of Nitroethane were published by Stull *et al.*[55] BAC/MP4 calculations were done by Melius and the enthalpy of formation was recalculated with the MP4/G2 method in 1997.[35] The IR vibrational spectrum[1] was adopted and supplemented with the missing vibrations from Melius' calculations. The enthalpy of formation of Melius (1997)[35] was adopted. The molecular data available are listed in Table 28 and the thermodynamic calculations are listed in Table 29.

3.14. Ethyl Nitrate: $C_2H_5ONO_2$

Ethylnitrate was estimated by Stull *et al.*[55] and calculated by Melius. The MOPAC calculations gave results very close to those of Melius. The Melius values were adopted for the thermodynamic calculations, and for the enthalpy of formation, the NIST 97[40] recommendations were included. The molecular data available are listed in Table 30 and the thermodynamic calculations are listed in Table 31.

3.15. Nitropropene-2: $CH_3CH{=}CHNO_2$

This compound was calculated by Melius.[35] His values were adopted for the thermodynamic calculations. The molecular data available are listed in Table 32 and the thermodynamic calculations are listed in Table 33.

3.16. Nitrocyclopropane: $C_3H_5NO_2$

Holtzclaw, Harris and Bush[22] have published the vibrations and internal rotation barrier for nitrocyclopropane. Mochel, Britt and Boggs[39] published the moments of inertia externally and internally. The enthalpy of formation was estimated using NIST 94.[41] The molecular data available are listed in Table 34 and the thermodynamic calculations are listed in Table 35.

3.17. Nitroglycerin: $C_3H_5O_3(NO_2)_3$

No information was found in the literature for nitroglycerin, except for the heat of formation. In our case, the MOPAC, restricted Hartree–Fock (RHF) and UHF calculations gave the same results, as predicted by the theory, and the differences between PM3 and AM1 calculations are minimal. The PM3 results were chosen for the thermodynamic calculations, and the enthalpy of formation recommended by NIST 97.[40] The molecular data available are listed in Table 36 and the thermodynamic calculations are listed in Table 37.

3.18. N-Nitroazetidine (Cyclotrimethylene Nitramine): $(CH_2)_3N{-}NO_2$

This compound was calculated by Melius.[35] No other source is available. The molecular data available are listed in Table 38 and the thermodynamic calculations are listed in Table 39.

3.19. 1,3,3-Trinitroazetidine: $C_3H_4N(NO_2)_3$

This compound was investigated, measured and calculated by Yu, Zang and Bauer.[60] Their assignment and calculation is adopted, except for an internal rotation of the NO_2 group connected to the N ring atom. They seem not to have included internal rotations of the nitro groups. The two nitro groups on carbon atom 3 were not considered to be rotors and the vibration assignment of Bauer *et al.*[60] was adopted. The enthalpy of formation is the one proposed by Politzer.[47] The molecular data available are listed in Table 40 and the thermodynamic calculations are listed in Table 41.

TABLE 4. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for Nitromethane CH_3NO_2 (molecular wt.=61.040360)[a]

PM3 (transition state)												
	i-42.3	476	607	621	949	1016	1025	1361	1373	1385	1610	1905
	3048	3063	3153									
Melius[b]												
	18.7	470.5	627	657	938	1100	1134	1402	1436	1446	1507	1679
	2922	3005	3039									
Bock *et al.*[c]												
	34	465	592	639	885	1093	1146	1366	1430	1436	1458	1503
	2916	3010	3043									
Experimental[d]												
		483	607	661	922	1102	1119	1376	1410	1428	1438	1562
	2966	3044	3078									
IR spectrum[e]												
		598	**639**	**666**	**928**	**1083**	**1157**	**1380**	**1400**	**1440**	**1481**	**1561**
	2484	**2767**	**2962**									

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia=65.300 430 Ib=84.208 414 Ic=144.302 455
Melius Ia=65.029 Ib=77.264 Ic=137.079
Brinkman Ia=**64.5024** Ib=**82.4944** Ic=**141.8103**
Brinkman Ir(NO_2)=59.31583 Ir(CH_3)=5.186 56 I(reduced)=**4.769 52** V(2)=**0.0** kcal/mol[f] ROSYM=**2**
PM3 heat of formation=−15.9 kcal/mol (transition state)
PM3[g] $\Delta H_f(298) = -15.9$ kcal/mol
AM1[g] $\Delta H_f(298) = -9.9$ kcal/mol
Melius[b] $\Delta H_f(0) = -13.43$ $\Delta H_f(300) = -16.85$ kcal/mol spin=1 $S^2 = 0.3050$
Melius MP4/G2 1997[b] $\Delta H_f(298) = -18.76 \pm 1.02$ kcal/mol
NIST 1997 $\Delta H_f(298) = -$**19.3±0.3** kcal/mol[h]
Pedley and Rylance[i] $\Delta H_f(298) = -17.9 \pm 0.2$ kcal/mol
Stull *et al.*[j] $\Delta H_f(298) = -17.86$ kcal/mol
TRC ΔH_f solid(298) $= -27.03$ kcal/mol
PM3 zero point energy 30.76 kcal/mol (transition state)
R(CN)=1.4787[b]
R(CH)=1.0754–1.0789
R(NO)=1.1908–1.1923

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 35.
[c]See Ref. 5.
[d]See Ref. 33.
[e]See Ref. 1.
[f]See Ref. 20.
[g]See Ref. 52.
[h]See Ref. 23.
[i]See Ref. 44.
[j]See Ref. 55.

3.20. 1,3,5-Trinitrotriazine (RDX, hexogen): $C_3H_6N_6O_6$

This compound known as high explosive[21] was calculated by Wu *et al.*[58] The MOPAC-PM3/UHF and AM1/UHF calculations failed. For the thermodynamic calculations the GAUSSIAN 94 values of Wu[58] were adopted including the moments of inertia. The vibrations were scaled by a factor of 0.9. The internal moments of inertia for NO_2 were taken from Melius and the rotation barrier from Habibollahzadeh's[20] calculations for Nitropiperidine. The enthalpy of formation is the experimental value chosen by NIST 1997, and based on the publication of Pepekin *et al.*[46] The molecular data available are listed in Table 42 and the thermodynamic calculations are listed in Table 43.

3.21. N-Nitropropane: $C_3H_7NO_2$

Stull *et al.*[55] have calculated the thermodynamics of N-nitropropane. The IR of this species is presented in the NIST WebBook.[1] The MOPAC RHF and UHF calculations of the PM3 method gave almost exact values as predicted by the theory. The AM1 calculations failed, but AM1/UHF was successful. For the thermodynamic calculations the IR spectrum was adopted and supplemented with the missing vibrations from PM3. The enthalpy of formation of Pedley and Rylance[44] was accepted. The molecular data available are listed in Table 44 and the thermodynamic calculations are listed in Table 45.

3.22. N-Propyl Nitrate (NPN): $C_3H_7ONO_2$

N-propyl nitrate is a known explosive.[21] The thermodynamic data of this species were estimated by Stull *et al.*[55] For this calculation the PM3 vibrations were adopted and the moments of inertia were taken from AM1 because it showed a tighter molecular configuration. Stull's[55] estimate for the

TABLE 5. Ideal gas thermodynamic properties for nitromethane CH_3NO_2

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−12.610	-------	-------	−93.361	−66.590	-------
100	37.655	−8.866	235.722	324.380	−89.617	−71.758	28.6270
200	43.933	−4.859	263.252	287.545	−85.610	−76.486	9.4024
298.15	55.528	0.000	282.863	282.863	−80.751	−80.751	2.6636
300	55.767	0.103	283.207	282.864	−80.648	−80.826	2.5764
400	68.766	6.331	301.036	285.207	−74.420	−84.408	−1.0155
500	80.800	13.822	317.701	290.057	−66.929	−87.157	−3.2549
600	91.177	22.435	333.376	295.984	−58.316	−89.166	−4.7898
700	99.913	32.003	348.107	302.389	−48.748	−90.555	−5.9074
800	107.224	42.371	361.940	308.977	−38.381	−91.431	−6.7563
900	113.342	53.408	374.933	315.591	−27.343	−91.883	−7.4215
1000	118.475	65.006	387.149	322.142	−15.745	−91.998	−7.9552
1100	122.793	77.076	398.649	328.580	−3.676	−91.841	−8.3917
1200	126.440	89.542	409.494	334.875	8.791	−91.466	−8.7545
1300	129.533	102.345	419.740	341.013	21.594	−90.925	−9.0600
1400	132.170	115.434	429.438	346.986	34.683	−90.255	−9.3199
1500	134.427	128.766	438.636	352.792	48.015	−89.484	−9.5436
1600	136.371	142.309	447.376	358.433	61.558	−88.642	−9.7375
1700	138.051	156.032	455.695	363.911	75.281	−87.747	−9.9069
1800	139.512	169.912	463.628	369.232	89.161	−86.818	−10.0558
1900	140.788	183.928	471.206	374.401	103.177	−85.866	−10.1878
2000	141.907	198.064	478.456	379.424	117.313	−84.905	−10.3051
2100	142.894	212.305	485.404	384.307	131.554	−83.942	−10.4101
2200	143.767	226.639	492.072	389.055	145.888	−82.986	−10.5045
2300	144.542	241.055	498.480	393.674	160.304	−82.041	−10.5896
2400	145.234	255.545	504.647	398.170	174.793	−81.113	−10.6669
2500	145.853	270.100	510.588	402.549	189.348	−80.209	−10.7371
2600	146.409	284.713	516.320	406.815	203.962	−79.326	−10.8012
2700	146.910	299.380	521.855	410.974	218.628	−78.474	−10.8599
2800	147.363	314.094	527.206	415.030	233.342	−77.649	−10.9139
2900	147.774	328.851	532.385	418.988	248.100	−76.857	−10.9635
3000	148.148	343.647	537.401	422.852	262.896	−76.099	−11.0093
3100	148.488	358.479	542.264	426.626	277.728	−75.371	−11.0521
3200	148.800	373.344	546.983	430.313	292.593	−74.682	−11.0915
3300	149.085	388.238	551.567	433.919	307.487	−74.030	−11.1282
3400	149.347	403.160	556.021	437.445	322.409	−73.412	−11.1626
3500	149.588	418.107	560.354	440.895	337.356	−72.833	−11.1947
3600	149.810	433.077	564.571	444.272	352.326	−72.292	−11.2247
3700	150.016	448.068	568.679	447.579	367.317	−71.790	−11.2530
3800	150.206	463.080	572.682	450.819	382.328	−71.327	−11.2796
3900	150.383	478.109	576.586	453.994	397.358	−70.901	−11.3047
4000	150.547	493.156	580.395	457.106	412.405	−70.519	−11.3283
4100	150.699	508.218	584.115	460.159	427.467	−70.173	−11.3508
4200	150.842	523.295	587.748	463.154	442.544	−69.868	−11.3720
4300	150.975	538.386	591.299	466.093	457.635	−69.605	−11.3921
4400	151.099	553.490	594.771	468.978	472.739	−69.385	−11.4113
4500	151.215	568.606	598.168	471.811	487.854	−69.201	−11.4296
4600	151.324	583.733	601.493	474.594	502.982	−69.059	−11.4470
4700	151.427	598.870	604.748	477.329	518.119	−68.954	−11.4637
4800	151.523	614.018	607.937	480.017	533.267	−68.889	−11.4796
4900	151.614	629.175	611.063	482.659	548.424	−68.863	−11.4950
5000	151.699	644.340	614.126	485.258	563.589	−68.883	−11.5096
5100	151.780	659.514	617.131	487.815	578.763	−68.933	−11.5238
5200	151.856	674.696	620.079	490.330	593.945	−69.025	−11.5374
5300	151.928	689.885	622.973	492.805	609.134	−69.153	−11.5505
5400	151.996	705.082	625.813	495.242	624.331	−69.319	−11.5631
5500	152.060	720.285	628.603	497.642	639.533	−69.519	−11.5753
5600	152.122	735.494	631.343	500.005	654.742	−69.754	−11.5871
5700	152.180	750.709	634.036	502.333	669.958	−70.022	−11.5986
5800	152.235	765.930	636.683	504.626	685.178	−70.322	−11.6097
5900	152.287	781.156	639.286	506.887	700.404	−70.652	−11.6204
6000	152.337	796.387	641.846	509.115	715.636	−71.011	−11.6309

TABLE 6. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for nitromethyl radical $\bullet CH_2(NO_2)$ (molecular wt. = 60.032420)[a]

PM3											
150	440	593	612	713	986	1037	1283	1614	1891	3105	3158
Melius BAC/MP4[b]											
262	409	496	676	705	988	1066	1381	1416	1647	3027	3173
McKee 6-31G*[c]											
291	**457**	**555**	756	789	1106	1194	1546	1586	1845	3391	3554
Experimental[c]											
			693	**719**	**986**	**1095**	**1297**	**1419**	**1461**	**3055**	**3200**

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia = 63.203120 Ib = 78.014956 Ic = 135.435 809
Melius Ia = **63.450869** Ib = **67.566103** Ic = **131.016 97** spin = 2 $S^2 = 0.773$
Brinkmann Ia = 62.478 Ib = 75.9714 Ic = 136.1148 Ir(NO_2) = 59.315 83 Ir(CH_2) = 3.457 11 I(reduced) = **3.26725** V(2) = **0.08** est. ROSYM = **2**
PM3 heat of formation = 21.8 kcal/mol
Melius $\Delta H_f(0) = 38.68$ kcal/mol $\Delta H_f(298) =$ **36.44** kcal/mol
PM3 Zero point energy 22.32 kcal/mol
STATWT = **2**

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 35.
[c]See Ref. 32.

enthalpy of formation was adopted. The molecular data available are listed in Table 46 and the thermodynamic calculations are listed in Table 47.

3.23. Cyclotetramethylene Tetranitramine (HMX): $C_4H_8N_8O_8$

Octogen is considered the most powerful explosive material available today. It is roughly 50% stronger than TNT.[21] No thermodynamic data were found in the literature. This is the first attempt to calculate its molecular properties. The MOPAC calculations result in distorted molecular configurations; therefore the confidence in these results is very low. The PM3/UHF calculation has failed to give any nontransitional state, while the others give values quite different from each other. The AM1/UHF calculation is preferred because it has the lowest distortion. The enthalpy of formation was estimated using the difference between the solid and the gaseous enthalpy of formation of RDX and other explosives. The value estimated at 44.6 ± 6 kcal/mol is in itself very doubtful. This species has the lowest reliability of all the groups. The molecular data available are listed in Table 48 and the thermodynamic calculations are listed in Table 49.

3.24. N-Nitrobutane: $C_4H_9NO_2$

Except for Stull *et al.*[55] the species was mentioned in the literature by Stewart[52] and by Cox and Pilcher.[12] The MOPAC PM3 and PM3/UHF have failed by giving transition states. However, the values found for the RHF and UHF transition states were identical. For the thermodynamic calculation the IR vibrations[1] were adopted and supplemented with the missing vibrations from the AM1 calculation. The enthalpy of formation recommended by Stull *et al.*,[55] Pedley and Nylor[45] and NIST 94[51] was included. The molecular data available are listed in Table 50 and the thermodynamic calculations are listed in Table 51.

3.25. Penta-Erythritoltetranitrate (PETN): $C_5H_8(O-NO_2)_4$

No experimental value is known for this explosive material. It was calculated by Melius.[35] The moments of internal rotation and the rotation barrier were taken from Melius's methyl nitrate. The enthalpy of formation was taken from Cox and Pilcher.[12] The molecular data available are listed in Table 52 and the thermodynamic calculations are listed in Table 53.

3.26. N-Nitropentane: $C_5H_{11}NO_2$

This species is not mentioned in the literature. It is calculated here for the first time using the MOPAC program.[54] For the thermodynamic calculations the PM3 results were chosen. The enthalpy of formation was estimated graphically. See Sec. 4. The molecular data available are listed in Table 54 and the thermodynamic calculations are listed in Table 55.

3.27. Nitrobenzene: $C_6H_5NO_2$

Nitrobenzene was calculated by Stull *et al.*,[55] by Stewart[52] and by Melius.[35] For the thermodynamic calculations the IR spectrum[1] was used and supplemented with Melius's values. The enthalpy of formation was taken from Pedley, Naylor and Kirby.[45] The molecular data available are listed in Table 56 and the thermodynamic calculations are listed in Table 57.

TABLE 7. Ideal gas thermodynamic properties for nitromethane radical ● CH_2NO_2

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−13.143	-------	-------	139.322	161.858	-------
100	38.259	−9.389	238.511	332.402	143.076	158.200	−88.7115
200	46.980	−5.192	267.253	293.215	147.272	155.009	−47.7287
298.15	58.862	0.000	288.218	288.218	152.465	152.465	−34.5012
300	59.083	0.109	288.583	288.219	152.574	152.423	−34.3364
400	70.213	6.589	307.147	290.675	159.054	150.545	−27.7413
500	79.347	14.084	323.834	295.666	166.549	149.261	−23.8263
600	86.596	22.395	338.967	301.642	174.860	148.414	−21.2348
700	92.387	31.355	352.766	307.974	183.820	147.887	−19.3925
800	97.103	40.837	365.421	314.375	193.302	147.602	−18.0145
900	101.014	50.748	377.091	320.704	203.213	147.511	−16.9442
1000	104.303	61.019	387.909	326.890	213.484	147.571	−16.0880
1100	107.095	71.592	397.984	332.900	224.057	147.751	−15.3868
1200	109.481	82.424	407.408	338.721	234.889	148.030	−14.8017
1300	111.531	93.477	416.254	344.348	245.942	148.382	−14.3055
1400	113.300	104.721	424.585	349.785	257.186	148.790	−13.8790
1500	114.834	116.130	432.456	355.036	268.595	149.240	−13.5085
1600	116.168	127.681	439.911	360.110	280.146	149.717	−13.1832
1700	117.334	139.358	446.989	365.014	291.823	150.212	−12.8952
1800	118.356	151.143	453.725	369.757	303.608	150.714	−12.6384
1900	119.256	163.025	460.149	374.347	315.490	151.216	−12.4078
2000	120.051	174.991	466.287	378.791	327.456	151.713	−12.1996
2100	120.756	187.032	472.161	383.099	339.497	152.198	−12.0106
2200	121.384	199.139	477.794	387.276	351.604	152.667	−11.8383
2300	121.945	211.306	483.202	391.330	363.771	153.118	−11.6804
2400	122.447	223.526	488.403	395.267	375.991	153.547	−11.5354
2500	122.898	235.794	493.411	399.093	388.259	153.949	−11.4015
2600	123.306	248.105	498.239	402.814	400.570	154.327	−11.2777
2700	123.674	260.454	502.899	406.435	412.919	154.674	−11.1627
2800	124.008	272.838	507.403	409.961	425.303	154.994	−11.0558
2900	124.311	285.254	511.760	413.397	437.719	155.282	−10.9559
3000	124.588	297.700	515.979	416.746	450.165	155.536	−10.8625
3100	124.841	310.171	520.069	420.014	462.636	155.763	−10.7753
3200	125.073	322.667	524.036	423.203	475.132	155.953	−10.6931
3300	125.285	335.185	527.888	426.317	487.650	156.111	−10.6159
3400	125.481	347.724	531.631	429.359	500.189	156.236	−10.5432
3500	125.661	360.281	535.271	432.334	512.746	156.327	−10.4747
3600	125.828	372.855	538.813	435.243	525.320	156.384	−10.4098
3700	125.982	385.446	542.263	438.089	537.911	156.407	−10.3485
3800	126.125	398.051	545.625	440.874	550.516	156.395	−10.2904
3900	126.258	410.671	548.903	443.603	563.136	156.350	−10.2353
4000	126.382	423.303	552.101	446.275	575.768	156.268	−10.1829
4100	126.497	435.947	555.223	448.895	588.412	156.154	−10.1332
4200	126.604	448.602	558.273	451.463	601.067	156.005	−10.0859
4300	126.705	461.267	561.253	453.981	613.732	155.820	−10.0407
4400	126.799	473.943	564.167	456.453	626.408	155.598	−9.9977
4500	126.887	486.627	567.017	458.878	639.092	155.344	−9.9567
4600	126.969	499.320	569.807	461.259	651.785	155.056	−9.9175
4700	127.047	512.021	572.539	463.598	664.486	154.735	−9.8801
4800	127.120	524.729	575.214	465.896	677.194	154.382	−9.8443
4900	127.189	537.444	577.836	468.153	689.909	153.994	−9.8101
5000	127.254	550.167	580.406	470.373	702.632	153.566	−9.7773
5100	127.315	562.895	582.927	472.555	715.360	153.115	−9.7460
5200	127.373	575.629	585.399	474.701	728.094	152.626	−9.7158
5300	127.427	588.370	587.826	476.813	740.835	152.107	−9.6870
5400	127.479	601.115	590.209	478.891	753.580	151.555	−9.6592
5500	127.528	613.865	592.548	480.936	766.330	150.973	−9.6327
5600	127.575	626.621	594.846	482.950	779.085	150.361	−9.6071
5700	127.619	639.380	597.105	484.933	791.845	149.720	−9.5826
5800	127.661	652.144	599.325	486.886	804.609	149.051	−9.5589
5900	127.701	664.912	601.507	488.810	817.377	148.355	−9.5362
6000	127.739	677.684	603.654	490.707	830.149	147.634	−9.5144

TABLE 8. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for deuterated nitromethane $CD_3(NO_2)$ (molecular wt. = 64.058846)[a]

PM3 (transition state)											
	i-16.3	432	538	600	801	842	863	1011	1020	1128	1608	1900
	2261	2264	2271									
PM3 UHF(transition state)											
	i-16.5	432	538	600	801	842	863	1011	1020	1128	1608	1900
	2261	2264	2271									
Book *et al.*[b]											
	25	419	535	610	866	877	948	1049	1051	1088	1376	1466
	2090	2231	2263									
Experimental[b]											
		435	**542**	**631**	**885**	**898**	**942**	**1038**	**1046**	**1075**	**1404**	**1548**
	2147	**2283**	**2317**									

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia = 70.506612 Ib = 102.650 884 Ic = 162.783 371
PM3 UHF Ia = 70.506620 Ib = 102.650 905 Ic = 162.783 392 spin = 0 $S^2 = 0$
Brinkmann Ia = **69.6802** Ib = **100.1365** Ic = **159.4523** Ir = 59.6 ROSYM = **2** V(2) = **0.16** kcal/mol [estimated]; V(2) = 0.063 kcal/mol[c]
Brinkmann Ir(NO_2) = 59.31583 Ir(CD_3) = 10.36439 I(reduced) = **8.82277**
$\Delta H_f(0) = \mathbf{-18.008}$ kcal/mol [calculated from CH_3NO_2 $\Delta H_f(0) = -15.915$ kcal/mol].

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 5.
[c]See Ref. 17.

3.28. 1,3,5-Trinitrobenzene: $C_6H_3(NO_2)_3$

The fundamental properties of this species were not mentioned in the literature. The MOPAC/AM1 calculation failed since it optimized a transition state. The calculations of PM3, PM3/UHF, and AM1/UHF disagree with each other although the S^2 values found in both PM3/UHF and AM1/UHF are very small. For the thermodynamic calculations the PM3 values were taken and the enthalpy of formation was taken from Pedley, Naylor and Kirby.[45] The molecular data available are listed in Table 58 and the thermodynamic calculations are listed in Table 59.

3.29. N-Nitrohexane: $C_6H_{13}NO_2$

This species is not found in the literature. The MOPAC calculations of PM3 and AM1 resulted in ''intersection points'' (two imaginary vibrations). The enthalpies of formation of the gaseous and the liquid state could be estimated including the uncertainties from the straight line extrapolation of the first four nitro-homologues. The enthalpy of formation found is $\Delta H_f(298) = -44.3 \pm 0.7$ kcal/mol for the gaseous state and -57.8 ± 0.7 kcal/mol for the liquid state. The NIST 94[51] program that uses Benson's group additivity method gave exactly the same result for the gaseous enthalpy of formation. See Table 60.

3.30. 2,4,6-Trinitrotoluene (TNT): $C_7H_5(NO_2)_3$

There are no experimental thermodynamic or other data of this basic explosive in the literature. The MOPAC calculations of AM1 and AM1/UHF have failed, and the PM3 calculation showed a transition state. Since there are no reported IR spectra of TNT, the IR spectra of toluene, 2-nitrotoluene, 4-nitrotoluene and 2,4-dinitrotoluene[1] were analyzed and combined and the missing vibrations were added using the calculated MOPAC PM3/UHF. The internal moments of inertia for NO_2 and CH_3 were taken from Melius, and the V(2) value for the rotation barrier of NO_2 in the para position from Nitrobenzene. The V(2) values for the two NO_2 groups adjacent to CH_3 have been estimated to be approximately twice the free (para) NO_2 value. The enthalpy of formation was taken from the NIST 97[1] recommendation.[28] The molecular data available are listed in Table 61 and the thermodynamic calculations are listed in Table 62.

4. Discussion

4.1. Fundamental Vibrations

Melius[36] explains that the BAC/MP4 method scales all the *ab initio* calculated vibrations automatically by 12%. But since not all the vibrations differ from the experimental by the same percentage it has been found[4] that Melius' calculated vibrations are 1%–3% lower if less than 1000 cm^{-1}, 1%–3% higher between 1000 and 1500 cm^{-1} and 1% lower around 3000 cm^{-1}, while the average difference is less than 1%. Judging from the compound vibrations we can agree with this statement while, our GAUSSIAN 94 calculations[18] show an error roughly 10% higher. The MOPAC calculations and specifically the PM3 show very good correlation with the IR spectrum as well as with the Melius BAC/MP4 data. Since the thermodynamic data are not very sensitive to the exact value of the vibrations, the MOPAC and BAC/MP4 values of the vibrations were used as is, and only the Gaussian data were scaled by 10%.

TABLE 9. Ideal gas thermodynamic properties for nitromethane-d_3 CD_3NO_2

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−13.556	-------	-------	−75.345	−48.423	-------
100	38.853	−9.736	240.387	337.743	−71.525	−53.141	18.2015
200	48.348	−5.458	269.664	296.953	−67.247	−57.988	3.8178
298.15	63.166	0.000	291.669	291.669	−61.789	−61.789	−1.3171
300	63.453	0.117	292.061	291.670	−61.672	−61.851	−1.3838
400	78.223	7.216	312.382	294.341	−54.573	−64.588	−4.1337
500	90.757	15.685	331.228	299.857	−46.104	−66.368	−5.8440
600	101.029	25.292	348.715	306.561	−36.497	−67.414	−7.0089
700	109.382	35.827	364.938	313.756	−25.962	−67.898	−7.8507
800	116.167	47.116	380.003	321.107	−14.673	−67.960	−8.4846
900	121.688	59.019	394.015	328.439	−2.771	−67.705	−8.9768
1000	126.197	71.420	407.077	335.657	9.631	−67.211	−9.3686
1100	129.899	84.231	419.285	342.711	22.442	−66.544	−9.6862
1200	132.957	97.379	430.723	349.574	35.589	−65.747	−9.9480
1300	135.500	110.805	441.468	356.233	49.016	−64.855	−10.1668
1400	137.630	124.465	451.590	362.686	62.676	−63.898	−10.3515
1500	139.427	138.320	461.149	368.935	76.531	−62.891	−10.5093
1600	140.953	152.341	470.197	374.984	90.552	−61.857	−10.6452
1700	142.258	166.504	478.782	380.839	104.714	−60.811	−10.7629
1800	143.381	180.787	486.946	386.509	118.998	−59.754	−10.8659
1900	144.352	195.175	494.725	392.002	133.385	−58.705	−10.9563
2000	145.198	209.653	502.151	397.325	147.864	−57.660	−11.0362
2100	145.938	224.211	509.254	402.487	162.421	−56.631	−11.1074
2200	146.589	238.838	516.058	407.496	177.049	−55.624	−11.1708
2300	147.165	253.526	522.587	412.359	191.737	−54.640	−11.2277
2400	147.675	268.269	528.862	417.083	206.479	−53.681	−11.2790
2500	148.130	283.059	534.899	421.676	221.270	−52.749	−11.3253
2600	148.537	297.893	540.717	426.143	236.104	−51.851	−11.3673
2700	148.903	312.765	546.330	430.491	250.976	−50.982	−11.4056
2800	149.232	327.673	551.751	434.726	265.883	−50.154	−11.4406
2900	149.530	342.611	556.993	438.852	280.821	−49.356	−11.4725
3000	149.800	357.578	562.067	442.875	295.788	−48.594	−11.5019
3100	150.046	372.570	566.983	446.800	310.781	−47.866	−11.5291
3200	150.270	387.586	571.751	450.630	325.797	−47.177	−11.5541
3300	150.475	402.623	576.378	454.371	340.834	−46.530	−11.5772
3400	150.663	417.680	580.873	458.026	355.891	−45.918	−11.5987
3500	150.835	432.755	585.243	461.598	370.966	−45.342	−11.6188
3600	150.994	447.847	589.494	465.092	386.058	−44.813	−11.6375
3700	151.140	462.954	593.633	468.511	401.164	−44.319	−11.6550
3800	151.275	478.075	597.666	471.857	416.285	−43.862	−11.6713
3900	151.401	493.209	601.597	475.133	431.419	−43.446	−11.6867
4000	151.517	508.355	605.431	478.343	446.565	−43.074	−11.7012
4100	151.625	523.512	609.174	481.488	461.722	−42.735	−11.7149
4200	151.725	538.679	612.829	484.572	476.890	−42.444	−11.7278
4300	151.818	553.856	616.400	487.597	492.067	−42.187	−11.7400
4400	151.906	569.043	619.892	490.564	507.253	−41.977	−11.7515
4500	151.987	584.237	623.306	493.476	522.448	−41.804	−11.7626
4600	152.063	599.440	626.648	496.335	537.651	−41.667	−11.7732
4700	152.134	614.650	629.919	499.142	552.860	−41.572	−11.7832
4800	152.200	629.866	633.122	501.900	568.077	−41.520	−11.7929
4900	152.262	645.090	636.261	504.610	583.300	−41.506	−11.8021
5000	152.320	660.319	639.338	507.274	598.529	−41.532	−11.8109
5100	152.374	675.553	642.355	509.893	613.764	−41.598	−11.8195
5200	152.425	690.793	645.314	512.469	629.004	−41.697	−11.8276
5300	152.473	706.038	648.218	515.003	644.249	−41.834	−11.8356
5400	152.518	721.288	651.069	517.497	659.499	−41.997	−11.8433
5500	152.560	736.542	653.868	519.951	674.752	−42.216	−11.8507
5600	152.599	751.800	656.617	522.367	690.010	−42.457	−11.8579
5700	152.635	767.062	659.318	524.746	705.272	−42.728	−11.8648
5800	152.670	782.327	661.973	527.089	720.537	−43.037	−11.8716
5900	152.702	797.595	664.583	529.397	735.806	−43.375	−11.8782
6000	152.731	812.867	667.150	531.672	751.078	−43.731	−11.8846

TABLE 10. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for dideuterated nitromethane $CHD_2(NO_2)$ (molecular wt.=63.052684)[a]

PM3 (transition state)											
i-34.3	444	553	612	824	849	968	1037	1238	1251	1610	1903
2261	2271	3091									
PM3 UHF (transition state)											
i-38.5	444	553	612	824	849	968	1037	1238	1251	1610	1903
2261	2271	3091									
Experimental[b]											
	443	**577**	**643**	**896**	**923**	**977**	**1060**	**1285**	**1285**	**1405**	**1554**
2187	**2313**	**3000**									

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia=68.533 928 Ib=96.721 700 Ic=156.931 323
PM3 UHF Ia=68.533 928 Ib=96.721 700 Ic=156.931 323
Brinkmann Ia=**67.6188** Ib=**95.5869** Ic=**152.8413**
Brinkmann Ir(NO_2)=59.31583 Ir(CHD_2)=8.63845 I(reduced)=**7.54032**
estimated V(2)=**0.125** kcal/mol ROSYM=**2**
PM3 heat of formation=−15.9 kcal/mol (transition state)
PM3 UHF heat of formation=−15.9 kcal/mol (transition state)
$\Delta H_f(0)$=**−16.971** kcal/mol [calculated from CH_3NO_2 $\Delta H_f(0)$=−15.915 kcal/mol].
PM3 zero point energy 26.94 kcal/mol (transition state)
PM3 UHF zero point energy 26.92 kcal/mol (transition state)

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 33

TABLE 11. Ideal gas thermodynamic properties for nitromethane-d_2 CD_2HNO_2

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−13.290	-------	-------	−71.007	−44.135	-------
100	38.525	−9.499	239.079	334.071	−67.215	−49.007	16.2886
200	47.226	−5.285	267.943	294.370	−63.002	−53.787	2.9938
298.15	60.806	0.000	289.264	289.264	−57.716	−57.716	−1.7834
300	61.074	0.113	289.641	289.265	−57.604	−57.782	−1.8456
400	75.107	6.932	309.162	291.832	−50.784	−60.790	−4.4236
500	87.369	15.073	327.278	297.131	−42.643	−62.895	−6.0385
600	97.565	24.337	344.138	303.578	−33.380	−64.274	−7.1457
700	105.939	34.526	359.828	310.506	−23.191	−65.083	−7.9503
800	112.810	45.474	374.438	317.595	−12.242	−65.450	−8.5594
900	118.467	57.047	388.062	324.677	−0.669	−65.472	−9.0344
1000	123.145	69.135	400.794	331.659	11.419	−65.227	−9.4139
1100	127.034	81.650	412.719	338.492	23.934	−64.779	−9.7226
1200	130.286	94.521	423.916	345.149	36.804	−64.172	−9.9778
1300	133.021	107.690	434.455	351.617	49.974	−63.447	−10.1916
1400	135.336	121.111	444.400	357.893	63.395	−62.634	−10.3724
1500	137.306	134.746	453.807	363.976	77.029	−61.752	−10.5273
1600	138.993	148.563	462.723	369.872	90.846	−60.826	−10.6608
1700	140.447	162.536	471.194	375.585	104.820	−59.873	−10.7766
1800	141.705	176.645	479.259	381.122	118.929	−58.898	−10.8780
1900	142.801	190.872	486.950	386.491	133.156	−57.919	−10.9672
2000	143.759	205.201	494.300	391.699	147.485	−56.937	−11.0461
2100	144.602	219.620	501.335	396.754	161.904	−55.964	−11.1164
2200	145.346	234.118	508.079	401.662	176.402	−55.004	−11.1791
2300	146.006	248.686	514.555	406.430	190.970	−54.063	−11.2354
2400	146.594	263.317	520.782	411.066	205.601	−53.142	−11.2861
2500	147.119	278.003	526.777	415.575	220.287	−52.245	−11.3320
2600	147.591	292.739	532.556	419.964	235.023	−51.377	−11.3736
2700	148.015	307.520	538.134	424.238	249.803	−50.536	−11.4116
2800	148.398	322.341	543.524	428.403	264.624	−49.731	−11.4462
2900	148.745	337.198	548.738	432.463	279.482	−48.956	−11.4779
3000	149.060	352.089	553.786	436.423	294.372	−48.214	−11.5070
3100	149.348	367.009	558.678	440.288	309.293	−47.505	−11.5340
3200	149.610	381.957	563.424	444.063	324.241	−46.833	−11.5588
3300	149.851	396.931	568.032	447.750	339.214	−46.201	−11.5818
3400	150.071	411.927	572.509	451.354	354.210	−45.603	−11.6032
3500	150.274	426.944	576.862	454.878	369.228	−45.040	−11.6231
3600	150.461	441.981	581.098	458.325	384.265	−44.522	−11.6416
3700	150.634	457.036	585.223	461.699	399.320	−44.038	−11.6590
3800	150.794	472.107	589.242	465.003	414.391	−43.592	−11.6753
3900	150.942	487.194	593.161	468.239	429.478	−43.185	−11.6906
4000	151.080	502.295	596.984	471.410	444.579	−42.822	−11.7050
4100	151.208	517.410	600.716	474.519	459.693	−42.491	−11.7186
4200	151.327	532.537	604.361	477.567	474.820	−42.206	−11.7314
4300	151.438	547.675	607.923	480.557	489.959	−41.957	−11.7436
4400	151.542	562.824	611.406	483.492	505.108	−41.754	−11.7551
4500	151.640	577.983	614.813	486.372	520.267	−41.586	−11.7661
4600	151.731	593.152	618.147	489.201	535.435	−41.456	−11.7766
4700	151.816	608.329	621.411	491.979	550.613	−41.367	−11.7866
4800	151.896	623.515	624.608	494.709	565.798	−41.318	−11.7962
4900	151.972	638.708	627.741	497.392	580.992	−41.307	−11.8054
5000	152.043	653.909	630.812	500.030	596.193	−41.339	−11.8141
5100	152.109	669.117	633.823	502.624	611.400	−41.406	−11.8227
5200	152.172	684.331	636.777	505.175	626.614	−41.509	−11.8308
5300	152.232	699.551	639.677	507.686	641.835	−41.650	−11.8387
5400	152.287	714.777	642.523	510.157	657.061	−41.820	−11.8463
5500	152.340	730.008	645.317	512.589	672.292	−42.038	−11.8537
5600	152.390	745.245	648.063	514.983	687.528	−42.282	−11.8609
5700	152.437	760.486	650.761	517.342	702.770	−42.557	−11.8678
5800	152.481	775.732	653.412	519.665	718.016	−42.867	−11.8746
5900	152.523	790.982	656.019	521.954	733.266	−43.207	−11.8811
6000	152.563	806.237	658.583	524.210	748.520	−43.568	−11.8875

TABLE 12. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for monodeuterated nitromethane $CH_2D(NO_2)$ (molecular wt.=62.046522)[a]

PM3 (transition state)											
	i-38	454	600	614	833	952	1001	1180	1285	1372	1610	1903
	2271	3048	3125									
PM3 UHF (transition state)											
	i-42.8	454	600	614	833	952	1001	1180	1285	1372	1610	1903
	2271	3048	3125									
Experimental (calculated in parenthesis)[b]												
		463	**579**	**651**	**893**	**957**	(**1099**	**1254**	**1304**)	**1338**	(**1480**)	**1557**
	2221	**2997**	(**3082**)									

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia=66.617 938 Ib=90.189 686 Ic=151.462 017
PM3 UHF Ia=66.617 938 Ib=90.189 686 Ic=151.462 017
Brinkmann Ia=**66.0202** Ib=**89.0396** Ic=**147.5046**
Brinkmann Ir(NO_2)=59.31583 Ir(CDH_2)=6.91251 I(reduced)=**6.19102**
estimated V(2)=**0.104** kcal/mol ROSYM=**2**
PM3 heat of formation=−15.9 kcal/mol
PM3 UHF heat of formation=−15.9 kcal/mol
$\Delta H_f(0) = -$**15.686** kcal/mol [calculated from CH_3NO_2 $\Delta H_f(0) = -15.915$ kcal/mol].
PM3 zero point energy 28.84 kcal/mol
PM3 UHF zero point energy 28.82 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 17.

TABLE 13. Ideal gas thermodynamic properties for nitromethane-*d* CH_2DNO_2

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−13.098	-------	-------	−65.630	−38.809	-------
100	38.302	−9.327	237.550	330.817	−61.859	−43.825	13.8170
200	46.440	−5.157	266.129	291.915	−57.689	−48.520	1.8861
298.15	58.983	0.000	286.942	286.942	−52.532	−52.532	−2.4401
300	59.233	0.109	287.308	286.943	−52.423	−52.600	−2.4967
400	72.553	6.705	306.190	289.428	−45.827	−55.824	−4.8531
500	84.468	14.571	323.694	294.551	−37.961	−58.201	−6.3415
600	94.493	23.535	340.009	300.784	−28.997	−59.870	−7.3693
700	102.795	33.412	355.218	307.486	−19.119	−60.969	−8.1209
800	109.673	44.046	369.408	314.350	−8.485	−61.614	−8.6928
900	115.401	55.309	382.666	321.212	2.777	−61.894	−9.1410
1000	120.197	67.096	395.081	327.985	14.564	−61.886	−9.5003
1100	124.236	79.323	406.731	334.620	26.791	−61.648	−9.7936
1200	127.653	91.922	417.692	341.090	39.390	−61.227	−10.0368
1300	130.559	104.836	428.028	347.384	52.305	−60.665	−10.2410
1400	133.043	118.020	437.796	353.496	65.488	−59.995	−10.4141
1500	135.176	131.433	447.050	359.428	78.901	−59.239	−10.5625
1600	137.017	145.045	455.834	365.181	92.513	−58.423	−10.6906
1700	138.613	158.828	464.190	370.761	106.297	−57.564	−10.8020
1800	140.004	172.761	472.153	376.175	120.229	−56.674	−10.8995
1900	141.221	186.823	479.756	381.428	134.292	−55.767	−10.9854
2000	142.291	201.000	487.027	386.527	148.468	−54.852	−11.0614
2100	143.236	215.277	493.993	391.480	162.746	−53.936	−11.1291
2200	144.073	229.644	500.676	396.292	177.112	−53.028	−11.1895
2300	144.818	244.089	507.097	400.971	191.557	−52.132	−11.2438
2400	145.483	258.605	513.275	405.523	206.073	−51.252	−11.2927
2500	146.080	273.183	519.226	409.953	220.651	−50.393	−11.3370
2600	146.616	287.819	524.966	414.267	235.287	−49.557	−11.3771
2700	147.100	302.505	530.508	418.470	249.973	−48.748	−11.4137
2800	147.537	317.237	535.866	422.567	264.705	−47.968	−11.4472
2900	147.935	332.011	541.051	426.564	279.479	−47.218	−11.4777
3000	148.296	346.823	546.072	430.464	294.291	−46.500	−11.5058
3100	148.626	361.669	550.940	434.273	309.137	−45.811	−11.5319
3200	148.928	376.547	555.664	437.993	324.015	−45.160	−11.5557
3300	149.204	391.454	560.251	441.628	338.922	−44.544	−11.5779
3400	149.459	406.387	564.709	445.183	353.855	−43.962	−11.5985
3500	149.693	421.345	569.044	448.660	368.813	−43.416	−11.6177
3600	149.909	436.325	573.264	452.063	383.793	−42.909	−11.6356
3700	150.108	451.326	577.375	455.395	398.794	−42.438	−11.6524
3800	150.293	466.346	581.380	458.658	413.814	−42.005	−11.6680
3900	150.465	481.384	585.286	461.855	428.852	−41.609	−11.6828
4000	150.624	496.439	589.098	464.988	443.907	−41.255	−11.6966
4100	150.773	511.509	592.819	468.061	458.977	−40.936	−11.7098
4200	150.911	526.593	596.454	471.075	474.061	−40.658	−11.7221
4300	151.041	541.691	600.007	474.032	489.159	−40.419	−11.7338
4400	151.162	556.801	603.480	476.935	504.269	−40.223	−11.7449
4500	151.275	571.923	606.879	479.785	519.391	−40.064	−11.7555
4600	151.381	587.056	610.205	482.584	534.524	−39.942	−11.7656
4700	151.481	602.199	613.461	485.334	549.667	−39.859	−11.7752
4800	151.575	617.352	616.652	488.037	564.820	−39.816	−11.7845
4900	151.663	632.514	619.778	490.693	579.982	−39.811	−11.7934
5000	151.746	647.684	622.843	493.306	595.152	−39.850	−11.8018
5100	151.825	662.863	625.848	495.875	610.331	−39.921	11.8100
5200	151.899	678.049	628.797	498.403	625.517	−40.030	−11.8179
5300	151.969	693.242	631.691	500.891	640.711	−40.175	−11.8255
5400	152.035	708.443	634.533	503.340	655.911	−40.354	−11.8328
5500	152.098	723.649	637.323	505.750	671.118	−40.574	−11.8400
5600	152.157	738.862	640.064	508.124	686.330	−40.823	−11.8469
5700	152.214	754.081	642.758	510.463	701.549	−41.105	−11.8536
5800	152.267	769.305	645.405	512.767	716.773	−41.419	−11.8601
5900	152.318	784.534	648.009	515.037	732.002	−41.763	−11.8664
6000	152.366	799.768	650.569	517.274	747.236	−42.131	−11.8726

TABLE 14. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for dinitromethane $CH_2(NO_2)_2$ (molecular wt. = 106.037960)[a]

PM3												
	28.5	66.4	194	412	430	568	585	638	746	895	915	971
	1063	1275	1358	1555	1602	1951	1959	2875	2962			
PM3 UHF												
	25.9	66.1	**194**	**412**	**430**	**568**	**585**	**638**	**746**	**895**	**915**	**971**
	1063	**1275**	**1358**	**1555**	**1602**	**1951**	**1959**	**2875**	**2962**			
AM1												
	33.5	69	168	352	393	442	485	586	629	760	888	952
	977	1026	1166	1292	1346	1588	1935	2906	2969			
AM1 UHF												
	43	49	216	449	460	586	613	754	828	1039	1051	1097
	1134	1317	1335	1746	1783	2094	2106	2956	2996			

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia = 134.973 668 Ib = 499.300 239 Ic = 507.077 699 σ(external) = **2**
PM3 UHF Ia = **134.973 668** Ib = **499.300 239** Ic = **507.077 699**
AM1 Ia = 160.087 397 Ib = 426.750 031 Ic = 459.397 104
AM1 UHF Ia = 132.737 881 Ib = 488.868 410 Ic = 497.142 751 (Ir(NO_2) = **59.6** ROSYM = **2** V(2) = **0.08** kcal/mol) × **2**[Melius nitroethane]
PM3 heat of formation = −11.9 kcal/mol
PM3 UHF heat of formation = −11.9 kcal/mol
PM3[b] $\Delta H_f(298) = -11.9$ kcal/mol
AM1 heat of formation = 74.4 kcal/mol
AM1 UHF heat of formation = 2.9 kcal/mol spin = 0.0 $S^2 = 0.0$
AM1[b] $\Delta H_f(298) = 2.9$ kcal/mol
NIST 1997 $\Delta H_f(298) = -$ **14.7 ± 1.02** kcal/mol[c]
Melius MP4/G2 1997 $\Delta H_f(298) = -7.63 \pm 3.1$ kcal/mol (transition state)
PM3 zero point energy 33.00 kcal/mol
PM3 UHF zero point energy 32.99 kcal/mol
AM1 zero point energy 30.03 kcal/mol
AM1 UHF zero point energy 35.31 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 52.
[c]See Ref. 23.

TABLE 15. Ideal gas thermodynamic properties for dinitromethane $CH_2(NO_2)_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−17.721	-------	-------	−79.226	−43.674	-------
100	48.236	−13.167	289.300	420.972	−74.672	−50.885	9.9272
200	66.314	−7.503	327.843	365.356	−69.008	−56.974	−4.0080
298.15	86.352	0.000	358.098	358.098	−61.505	−61.505	−9.0854
300	86.712	0.160	358.633	358.099	−61.345	−61.578	−9.1516
400	104.677	9.755	386.111	361.724	−51.750	−64.770	−11.8996
500	119.603	20.993	411.127	369.141	−40.511	−66.840	−13.6184
600	131.814	33.585	434.051	378.076	−27.920	−68.058	−14.7931
700	141.781	47.281	455.144	387.599	−14.223	−68.625	−15.6434
800	149.933	61.881	474.626	397.276	0.376	−68.685	−16.2841
900	156.620	77.219	492.685	406.886	15.714	−68.343	−16.7815
1000	162.119	93.165	509.481	416.315	31.660	−67.691	−17.1765
1100	166.654	109.611	525.152	425.505	48.106	−66.799	−17.4958
1200	170.404	126.470	539.818	434.427	64.965	−65.717	−17.7582
1300	173.513	143.670	553.585	443.069	82.166	−64.499	−17.9763
1400	176.100	161.155	566.541	451.430	99.650	−63.183	−18.1595
1500	178.260	178.876	578.766	459.516	117.371	−61.797	−18.3151
1600	180.069	196.795	590.331	467.333	135.290	−60.372	−18.4481
1700	181.590	214.880	601.294	474.894	153.376	−58.925	−18.5627
1800	182.874	233.105	611.711	482.208	171.601	−57.477	−18.6620
1900	183.961	251.449	621.628	489.287	189.944	−56.041	−18.7488
2000	184.886	269.892	631.088	496.142	208.387	−54.628	−18.8247
2100	185.676	288.421	640.129	502.785	226.917	−53.247	−18.8918
2200	186.352	307.024	648.782	509.226	245.519	−51.906	−18.9513
2300	186.934	325.689	657.079	515.475	264.184	−50.609	−19.0042
2400	187.435	344.408	665.046	521.543	282.903	−49.362	−19.0515
2500	187.870	363.173	672.706	527.437	301.669	−48.172	−19.0940
2600	188.247	381.980	680.082	533.167	320.475	−47.034	−19.1323
2700	188.575	400.821	687.193	538.741	339.316	−45.959	−19.1668
2800	188.863	419.693	694.056	544.166	358.189	−44.941	−19.1983
2900	189.114	438.592	700.688	549.449	377.088	−43.984	−19.2268
3000	189.335	457.515	707.103	554.598	396.010	−43.090	−19.2529
3100	189.530	476.459	713.315	559.618	414.954	−42.252	−19.2771
3200	189.703	495.421	719.335	564.516	433.916	−41.480	−19.2990
3300	189.855	514.399	725.175	569.296	452.894	−40.769	−19.3193
3400	189.991	533.391	730.845	573.965	471.886	−40.117	−19.3381
3500	190.111	552.396	736.354	578.526	490.891	−39.525	−19.3556
3600	190.219	571.413	741.711	582.985	509.908	−38.993	−19.3718
3700	190.315	590.439	746.924	587.346	528.935	−38.520	−19.3871
3800	190.401	609.475	752.000	591.612	547.971	−38.105	−19.4013
3900	190.478	628.519	756.947	595.788	567.015	−37.747	−19.4147
4000	190.547	647.571	761.771	599.878	586.066	−37.450	−19.4272
4100	190.610	666.629	766.477	603.884	605.124	−37.206	−19.4392
4200	190.666	685.692	771.070	607.810	624.188	−37.020	−19.4505
4300	190.717	704.762	775.558	611.659	643.257	−36.889	−19.4611
4400	190.763	723.836	779.943	615.434	662.331	−36.816	−19.4712
4500	190.805	742.914	784.230	619.138	681.409	−36.795	−19.4810
4600	190.843	761.997	788.424	622.773	700.492	−36.827	−19.4902
4700	190.877	781.083	792.529	626.341	719.578	−36.910	−19.4992
4800	190.909	800.172	796.548	629.845	738.667	−37.045	−19.5077
4900	190.937	819.264	800.484	633.288	757.759	−37.232	−19.5160
5000	190.963	838.359	804.342	636.670	776.854	−37.476	−19.5239
5100	190.987	857.457	808.124	639.995	795.952	−37.762	−19.5317
5200	191.009	876.557	811.833	643.264	815.052	−38.101	−19.5391
5300	191.029	895.658	815.471	646.479	834.154	−38.487	−19.5464
5400	191.047	914.762	819.042	649.642	853.257	−38.921	−19.5535
5500	191.064	933.868	822.548	652.754	872.363	−39.401	−19.5604
5600	191.079	952.975	825.991	655.817	891.470	−39.925	−19.5672
5700	191.093	972.084	829.373	658.832	910.579	−40.495	−19.5737
5800	191.106	991.194	832.697	661.801	929.689	−41.104	−19.5801
5900	191.118	1010.305	835.963	664.725	948.800	−41.755	−19.5864
6000	191.129	1029.417	839.176	667.606	967.912	−42.445	−19.5927

TABLE 16. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for trinitromethane (TNF) $CH(NO_2)_3$ (molecular wt. = 151.035560)[a]

PM3												
	19.4	35.7	52.3	**157**	**170**	**210**	**335**	**347**	**368**	**421**	**449**	**490**
	563	**619**	**670**	**708**	**724**	**884**	**993**	**1064**	**1135**	**1167**	**1232**	**1261**
	1572	**1962**	**2749**									
PM3 UHF												
	13	32.8	55.7	159	171	209	336	347	370	421	447	491
	571	619	674	709	724	885	995	1053	1140	1168	1234	1263
	1572	1962	2745									

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia = **508.309 479** Ib = **684.055 572** Ic = **992.098 743** σ(external) = **3**
PM3 UHF Ia = 513.554 691 Ib = 683.471 748 Ic = 987.177484 (Ir(NO_2) = **59.6** ROSYM = **2** V(2) = **0.1** kcal/mol(estimated).) × **3**
PM3 heat of formation = 165.75 kcal/mol
PM3 UHF heat of formation = 165.65 kcal/mol spin = 0.0 S^2 = 0.0
PM3[b] $\Delta H_f(298) = -4.7$ kcal/mol
AM1[b] $\Delta H_f(298) = 25.0$ kcal/mol
Carpenter *et al.*[c] $\Delta H_f(298) = \mathbf{-3.2}$ kcal/mol
Benson[d] $\Delta H_f(298) = -0.2$ kcal/mol
Carpenter *et al.*[c] $\Delta H_{f\ \mathrm{liquid}}(298) = -16.25 \pm 0.75$ kcal/mol
Mirishnichenko[e] $\Delta H_{f\ \mathrm{solid}}(298) = -11.5 \pm 0.5$ kcal/mol
PM3 ionization potential = 11.966 eV
PM3 UHF ionization potential = 11.990 eV
PM3 zero point energy 29.14 kcal/mol
PM3 UHF zero point energy 29.12 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 52.
[c]See Ref. 9.
[d]See Ref. 3.
[e]See Ref. 37.

TABLE 17. Ideal gas thermodynamic properties for trinitromethane $CH(NO_2)_3$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−25.968	-------	-------	−39.357	4.976	-------
100	67.454	−20.333	330.117	533.452	−33.722	−4.006	−23.0224
200	103.994	−11.743	388.198	446.912	−25.132	−10.189	−24.7626
298.15	134.090	0.000	435.569	435.569	−13.389	−13.389	−25.7752
300	134.589	0.249	436.400	435.571	−13.140	−13.429	−25.7893
400	158.086	14.937	478.494	441.151	1.548	−14.505	−26.4017
500	175.701	31.669	515.758	452.419	18.281	−14.148	−26.7787
600	188.895	49.930	549.015	465.798	36.542	−12.883	−27.0156
700	198.886	69.342	578.918	479.858	55.953	−11.043	−27.1654
800	206.553	89.630	605.998	493.960	76.242	−8.830	−27.2588
900	212.505	110.596	630.685	507.801	97.207	−6.368	−27.3145
1000	217.166	132.089	653.326	521.237	118.700	−3.751	−27.3443
1100	220.840	153.996	674.203	534.207	140.607	−1.037	−27.3557
1200	223.750	176.231	693.548	546.689	162.842	1.736	−27.3546
1300	226.062	198.726	711.553	558.686	185.337	4.526	−27.3442
1400	227.903	221.428	728.376	570.213	208.039	7.310	−27.3272
1500	229.372	244.294	744.151	581.288	230.906	10.068	−27.3059
1600	230.545	267.293	758.994	591.936	253.904	12.778	−27.2810
1700	231.481	290.396	772.999	602.178	277.007	15.433	−27.2541
1800	232.228	313.582	786.252	612.040	300.194	18.016	−27.2255
1900	232.824	336.836	798.825	621.543	323.447	20.521	−27.1961
2000	233.297	360.143	810.780	630.708	346.754	22.942	−27.1661
2100	233.672	383.492	822.172	639.556	370.103	25.273	−27.1361
2200	233.967	406.875	833.049	648.106	393.486	27.511	−27.1063
2300	234.197	430.283	843.455	656.375	416.895	29.654	−27.0768
2400	234.376	453.713	853.426	664.379	440.324	31.700	−27.0478
2500	234.512	477.157	862.997	672.134	463.768	33.644	−27.0194
2600	234.613	500.614	872.196	679.653	487.225	35.495	−26.9917
2700	234.687	524.079	881.052	686.949	510.690	37.242	−26.9645
2800	234.738	547.550	889.588	694.035	534.162	38.894	−26.9384
2900	234.771	571.026	897.826	700.921	557.637	40.450	−26.9127
3000	234.788	594.504	905.786	707.618	581.115	41.910	−26.8879
3100	234.794	617.983	913.484	714.135	604.594	43.281	−26.8643
3200	234.789	641.462	920.939	720.482	628.074	44.558	−26.8410
3300	234.777	664.941	928.163	726.666	651.552	45.744	−26.8185
3400	234.759	688.418	935.172	732.696	675.029	46.844	−26.7971
3500	234.736	711.892	941.977	738.579	698.504	47.861	−26.7763
3600	234.708	735.365	948.589	744.321	721.976	48.792	−26.7562
3700	234.678	758.834	955.019	749.929	745.445	49.643	−26.7370
3800	234.646	782.300	961.277	755.409	768.911	50.415	−26.7184
3900	234.612	805.763	967.372	760.766	792.374	51.110	−26.7005
4000	234.576	829.223	973.311	766.006	815.834	51.726	−26.6832
4100	234.540	852.678	979.103	771.133	839.290	52.269	−26.6668
4200	234.504	876.131	984.755	776.152	862.742	52.740	−26.6508
4300	234.467	899.579	990.272	781.068	886.190	53.139	−26.6355
4400	234.430	923.024	995.662	785.884	909.635	53.465	−26.6207
4500	234.394	946.465	1000.930	790.604	933.076	53.725	−26.6066
4600	234.357	969.903	1006.081	795.233	956.514	53.916	−26.5930
4700	234.322	993.337	1011.121	799.773	979.948	54.045	−26.5800
4800	234.287	1016.767	1016.054	804.228	1003.378	54.109	−26.5674
4900	234.252	1040.194	1020.885	808.600	1026.805	54.108	−26.5554
5000	234.218	1063.618	1025.617	812.893	1050.229	54.040	−26.5438
5100	234.185	1087.038	1030.255	817.110	1073.649	53.917	−26.5329
5200	234.153	1110.455	1034.802	821.253	1097.066	53.729	−26.5222
5300	234.121	1133.868	1039.262	825.324	1120.479	53.486	−26.5121
5400	234.090	1157.279	1043.637	829.327	1143.890	53.181	−26.5024
5500	234.060	1180.686	1047.933	833.262	1167.297	52.821	−26.4931
5600	234.031	1204.091	1052.150	837.133	1190.702	52.408	−26.4842
5700	234.002	1227.493	1056.292	840.942	1214.104	51.937	−26.4756
5800	233.975	1250.891	1060.361	844.690	1237.503	51.416	−26.4674
5900	233.948	1274.287	1064.361	848.380	1260.899	50.845	−26.4596
6000	233.922	1297.681	1068.292	852.012	1284.292	50.224	−26.4522

TABLE 18. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for tetranitromethane $C(NO_2)_4$ (molecular wt. = 196.033160)[a]

PM3

36	49	70.5	71.9	**138**	**146**	**183**	**191**	**206**	**333**	**344**	**355**
357	**378**	**408**	**482**	**491**	**563**	**594**	**640**	**646**	**672**	**687**	**702**
791	**1015**	**1129**	**1147**	**1193**	**1193**	**1213**	**1565**	**1985**			

PM3 UHF

36.9	49.1	71.5	73.4	138	146	183	191	206	333	344	354
357	378	407	481	490	562	594	640	646	672	687	701
791	1015	1128	1146	1192	1192	1213	1565	1985			

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia = 811.789 190 Ib = 1090.935 512 Ic = 1199.663 730 σ(external) = **4**
PM3 UHF Ia = 811.565 714 Ib = 1090.954 078 Ic = 1199.964 043 spin = 0 S^2 = 0 (Ir(NO_2) = **59.6** ROSYM = **2** V(2) = **0.2** kcal/mol (estimated)) × 4
PM3 heat of formation = 259.02 kcal/mol
PM3 UHF heat of formation = 259.03 kcal/mol
PM3[b] ΔH_f(298) = 6.4 kcal/mol
NIST 97 ΔH_f(298) = **19.69** ± **0.5** kcal/mol[c]
PM3 ionization potential = 11.920 eV
PM3 UHF ionization potential = 11.922 eV
PM3 zero point energy 28.57 kcal/mol
PM3 UHF zero point energy 28.58 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 52.
[c]See Ref. 25.

TABLE 19. Ideal gas thermodynamic properties for tetranitromethane $C(NO_2)_4$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−33.993	-------	-------	48.389	101.504	-------
100	88.370	−26.842	364.554	632.976	55.541	91.185	−81.5409
200	137.754	−15.503	441.166	518.681	66.880	84.731	−58.4745
298.15	176.119	0.000	503.723	503.723	82.383	82.383	−51.3006
300	176.729	0.326	504.814	503.726	82.709	82.366	−51.2111
400	204.622	19.473	559.703	511.021	101.856	82.770	−47.6260
500	224.516	40.985	607.623	525.653	123.368	84.840	−45.4421
600	238.833	64.191	649.893	542.908	146.574	87.862	−43.9411
700	249.276	88.623	687.535	560.930	171.006	91.415	−42.8278
800	257.000	113.956	721.350	578.906	196.339	95.257	−41.9583
900	262.781	139.959	751.970	596.461	222.342	99.249	−41.2534
1000	267.145	166.465	779.894	613.429	248.848	103.299	−40.6663
1100	270.456	193.353	805.518	629.743	275.735	107.352	−40.1661
1200	272.976	220.530	829.164	645.389	302.913	111.382	−39.7338
1300	274.891	247.928	851.092	660.379	330.311	115.354	−39.3543
1400	276.343	275.493	871.520	674.739	357.876	119.250	−39.0176
1500	277.435	303.184	890.624	688.502	385.567	123.061	−38.7166
1600	278.249	330.970	908.557	701.700	413.353	126.765	−38.4447
1700	278.846	358.827	925.445	714.370	441.210	130.363	−38.1980
1800	279.273	386.734	941.396	726.544	469.117	133.840	−37.9725
1900	279.569	414.677	956.504	738.253	497.060	137.191	−37.7656
2000	279.761	442.644	970.849	749.527	525.027	140.417	−37.5745
2100	279.874	470.627	984.502	760.394	553.009	143.512	−37.3980
2200	279.924	498.617	997.523	770.879	581.000	146.475	−37.2342
2300	279.925	526.610	1009.966	781.005	608.993	149.304	−37.0815
2400	279.890	554.601	1021.879	790.795	636.984	152.002	−36.9390
2500	279.827	582.587	1033.303	800.269	664.970	154.562	−36.8056
2600	279.742	610.565	1044.277	809.444	692.948	156.997	−36.6805
2700	279.642	638.535	1054.833	818.338	720.918	159.296	−36.5627
2800	279.530	666.493	1065.000	826.967	748.876	161.470	−36.4520
2900	279.410	694.441	1074.807	835.345	776.823	163.520	−36.3473
3000	279.285	722.375	1084.278	843.486	804.758	165.449	−36.2486
3100	279.157	750.297	1093.433	851.402	832.680	167.261	−36.1554
3200	279.028	778.207	1102.294	859.105	860.590	168.954	−36.0667
3300	278.898	806.103	1110.878	866.605	888.486	170.532	−35.9826
3400	278.770	833.986	1119.202	873.912	916.369	172.003	−35.9030
3500	278.643	861.857	1127.281	881.037	944.240	173.370	−35.8272
3600	278.518	889.715	1135.129	887.986	972.098	174.631	−35.7550
3700	278.396	917.561	1142.759	894.769	999.944	175.794	−35.6864
3800	278.276	945.394	1150.182	901.394	1027.777	176.861	−35.6208
3900	278.161	973.216	1157.408	907.866	1055.599	177.832	−35.5583
4000	278.048	1001.026	1164.449	914.193	1083.409	178.709	−35.4986
4100	277.939	1028.826	1171.314	920.381	1111.209	179.498	−35.4417
4200	277.833	1056.614	1178.010	926.435	1138.997	180.200	−35.3871
4300	277.731	1084.393	1184.546	932.362	1166.776	180.818	−35.3349
4400	277.633	1112.161	1190.930	938.166	1194.544	181.350	−35.2849
4500	277.537	1139.919	1197.168	943.853	1222.302	181.802	−35.2369
4600	277.446	1167.668	1203.267	949.426	1250.051	182.175	−35.1910
4700	277.357	1195.408	1209.233	954.891	1277.791	182.473	−35.1470
4800	277.272	1223.140	1215.072	960.251	1305.523	182.696	−35.1047
4900	277.189	1250.863	1220.788	965.510	1333.246	182.843	−35.0641
5000	277.110	1278.578	1226.387	970.671	1360.961	182.914	−35.0250
5100	277.034	1306.285	1231.874	975.739	1388.668	182.918	−34.9877
5200	276.960	1333.985	1237.253	980.717	1416.368	182.848	−34.9516
5300	276.889	1361.677	1242.527	985.607	1444.060	182.714	−34.9170
5400	276.821	1389.363	1247.702	990.413	1471.746	182.507	−34.8837
5500	276.755	1417.041	1252.781	995.137	1499.424	182.236	−34.8517
5600	276.692	1444.714	1257.767	999.783	1527.097	181.903	−34.8209
5700	276.630	1472.380	1262.664	1004.352	1554.763	181.502	−34.7909
5800	276.571	1500.040	1267.475	1008.847	1582.423	181.043	−34.7623
5900	276.514	1527.694	1272.202	1013.271	1610.077	180.524	−34.7347
6000	276.460	1555.343	1276.849	1017.625	1637.726	179.947	−34.7082

TABLE 20. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for CH_3ONO_2HCON Trans (molecular wt.=77.039760)[a]

Brand and Cawthon[b]

		340	**578**	**657**	**759**	**854**	**1017**	**1136**	**1176**	**1287**	**1434**
1435	**1468**	**1672**	**2907**	**2940**	**3008**						

Czuchajowski and Kucharski[c]

	262	540	630	760	863	993	1089	1104	1177	1283	1431
1438	1458	1635	2905	2991	2992						

Melius[d]

130	217	342	598	707	815	943	1083	1152	1190	1392	1458
1464	1473	1708	2922	3010	3016						

Principal moments of inertia in units of 10^{-40} g cm^2

Melius[c] Ia=**66.7244** Ib=**172.0275** Ic=**233.4975**
Dixon and Wilson[e] Ia=71.17 Ib=178.32 Ic=244.149 Ir(CH3)=**5.3436** ROSYM=**3** V(3)=**2.32** kcal/mol Ir(NO2)=**59.6** ROSYM=**2**
V(2)=**9.1** kcal/mol
Melius BAC-MP4 $\Delta H_f(0) = -22.31$ $\Delta H_f(300) = -26.14$ kcal/mol spin=0 $S^2=0.000$
NIST 97 $\Delta H_f(298) = -29.16 \pm 0.3$ kcal/mol[f]
NIST 94 $\Delta H_f(298) = -29.6$ kcal/mol[g]
Pedley and Rylance[b] $\Delta H_f(298) = -$**29.0**$\pm$**1** kcal/mol IP=11.53$\pm$0.01 eV
Stull *et al.*[i] $\Delta H_f(298) = -28.8$ kcal/mol
R(CO)=1.4277[d]
R(CH)=1.07741–1.0781
R(NO)=1.17721–1.3305

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 6.
[c]See Ref. 13.
[d]See Ref. 35.
[e]See Ref. 16.
[f]See Ref. 50.
[g]See Ref. 51.
[h]See Ref. 44.
[i]See Ref. 55.

TABLE 21. Ideal gas thermodynamic properties for methyl nitrate CH_3ONO_2

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−16.234	-------	-------	−138.239	−107.128	-------
100	47.710	−12.241	241.119	363.528	−134.246	−113.498	46.1849
200	61.695	−6.784	278.395	312.312	−128.789	−118.231	16.0425
298.15	76.597	0.000	305.793	305.793	−122.005	−122.005	5.7308
300	76.878	0.142	306.267	305.794	−121.863	−122.068	5.5992
400	91.538	8.574	330.423	308.988	−113.431	−124.932	0.2257
500	104.421	18.389	352.272	315.493	−103.616	−126.887	−3.0626
600	115.251	29.389	372.297	323.315	−92.616	−128.089	−5.2826
700	124.238	41.378	390.760	331.649	−80.628	−128.684	−6.8796
800	131.678	54.185	407.851	340.119	−67.820	−128.789	−8.0807
900	137.834	67.671	423.727	348.538	−54.335	−128.497	−9.0143
1000	142.925	81.717	438.521	356.805	−40.289	−127.895	−9.7585
1100	147.135	96.226	452.347	364.869	−25.779	−127.054	−10.3638
1200	150.618	111.119	465.304	372.704	−10.886	−126.028	−10.8647
1300	153.504	126.330	477.477	380.300	4.325	−124.871	−11.2849
1400	155.902	141.804	488.944	387.655	19.799	−123.623	−11.6414
1500	157.900	157.497	499.770	394.772	35.492	−122.314	−11.9475
1600	159.570	173.373	510.016	401.657	51.368	−120.973	−12.2123
1700	160.974	189.402	519.733	408.320	67.397	−119.619	−12.4433
1800	162.157	205.560	528.968	414.768	83.555	−118.271	−12.6463
1900	163.159	221.828	537.763	421.012	99.822	−116.940	−12.8260
2000	164.012	238.187	546.154	427.061	116.182	−115.638	−12.9858
2100	164.741	254.626	554.175	432.924	132.620	−114.373	−13.1288
2200	165.367	271.132	561.853	438.611	149.127	−113.151	−13.2575
2300	165.907	287.697	569.216	444.131	165.691	−111.975	−13.3736
2400	166.374	304.311	576.287	449.491	182.306	−110.851	−13.4791
2500	166.781	320.969	583.088	454.700	198.964	−109.785	−13.5751
2600	167.135	337.666	589.636	459.765	215.660	−108.771	−13.6630
2700	167.446	354.395	595.950	464.692	232.389	−107.819	−13.7435
2800	167.719	371.153	602.044	469.489	249.148	−106.923	−13.8178
2900	167.960	387.938	607.934	474.162	265.932	−106.088	−13.8862
3000	168.174	404.745	613.632	478.717	282.739	−105.314	−13.9496
3100	168.363	421.572	619.149	483.158	299.566	−104.595	−14.0087
3200	168.533	438.417	624.497	487.492	316.411	−103.940	−14.0635
3300	168.684	455.278	629.686	491.723	333.272	−103.344	−14.1147
3400	168.819	472.153	634.723	495.855	350.147	−102.805	−14.1628
3500	168.941	489.041	639.619	499.893	367.035	−102.326	−14.2078
3600	169.051	505.941	644.380	503.841	383.935	−101.906	−14.2501
3700	169.150	522.851	649.013	507.702	400.845	−101.542	−14.2900
3800	169.239	539.770	653.525	511.480	417.765	−101.237	−14.3277
3900	169.321	556.698	657.922	515.179	434.693	−100.987	−14.3633
4000	169.395	573.634	662.210	518.801	451.629	−100.797	−14.3970
4100	169.463	590.577	666.394	522.350	468.572	−100.660	−14.4292
4200	169.525	607.527	670.478	525.829	485.521	−100.579	−14.4597
4300	169.581	624.482	674.468	529.239	502.476	−100.554	−14.4888
4400	169.633	641.443	678.367	532.584	519.437	−100.586	−14.5165
4500	169.681	658.408	682.180	535.867	536.403	−100.669	−14.5431
4600	169.725	675.379	685.909	539.088	553.373	−100.807	−14.5685
4700	169.765	692.353	689.560	542.251	570.348	−100.994	−14.5929
4800	169.803	709.332	693.135	545.357	587.326	−101.233	−14.6163
4900	169.837	726.314	696.636	548.409	604.308	−101.523	−14.6388
5000	169.870	743.299	700.068	551.408	621.294	−101.871	−14.6604
5100	169.899	760.288	703.432	554.356	638.282	−102.259	−14.6815
5200	169.927	777.279	706.731	557.255	655.273	−102.699	−14.7016
5300	169.953	794.273	709.968	560.105	672.267	−103.186	−14.7211
5400	169.977	811.269	713.145	562.910	689.264	−103.720	−14.7400
5500	169.999	828.268	716.264	565.670	706.263	−104.298	−14.7583
5600	170.020	845.269	719.328	568.387	723.264	−104.919	−14.7760
5700	170.040	862.272	722.337	571.061	740.267	−105.583	−14.7933
5800	170.058	879.277	725.295	573.695	757.272	−106.285	−14.8100
5900	170.075	896.284	728.202	576.289	774.278	−107.026	−14.8262
6000	170.091	913.292	731.060	578.845	791.287	−107.803	−14.8421

TABLE 22. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for $\cdot CH_2ONO_2$ (molecular wt.=76.031820)[a]

Melius BAC/MP4[b]

132.6	211	**364**	**608**	**683**	**718**	**766**	**921**	**1120**	**1165**	**1306**	**1412**
1727	**3009**	**3142**									

Principal moments of inertia in units of 10^{-40} g cm^2

Melius 1997 Ia=**65.230 882** Ib=**162.460 15** Ic=**226.9382** spin=2 S^2=0.857
Brinkmann Ir(CH_2)=**3.45711** ROSYM=**2** V(2)=**2.3** kcal/mol (methyl nitrate) Ir(NO2)=**59.6** ROSYM=**2** V(2)=**9.1** kcal/mol (methyl nitrate)
Melius MP4 $\Delta H_f(0)$=26.39 kcal/mol $\Delta H_f(298)$=**23.65** kcal/mol
STATWT=**2**
R(OC)=1.3809[b]
R(ON)=1.1798–1.3422
R(CH)=1.0685–1.0697

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 35.

TABLE 23. Ideal gas thermodynamic properties for methyl nitrate radical $\cdot CH_2ONO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	-(G-H_{298})/T (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−16.347	-------	-------	82.605	109.481	-------
100	48.261	−12.303	247.158	370.186	86.649	104.663	−64.8216
200	62.003	−6.819	284.626	318.721	92.133	101.303	−37.8483
298.15	76.780	0.000	312.169	312.169	98.952	98.952	−29.2329
300	77.045	0.142	312.645	312.171	99.094	98.916	−29.1258
400	90.066	8.519	336.654	315.356	107.471	97.449	−24.8523
500	100.552	18.070	357.923	321.783	117.022	96.692	−22.3178
600	108.889	28.558	377.022	329.425	127.510	96.442	−20.6368
700	115.562	39.793	394.327	337.480	138.744	96.562	−19.4370
800	120.951	51.628	410.122	345.588	150.579	96.961	−18.5348
900	125.326	63.949	424.630	353.575	162.901	97.577	−17.8294
1000	128.888	76.666	438.025	361.359	175.618	98.351	−17.2610
1100	131.791	89.705	450.450	368.900	188.656	99.241	−16.7919
1200	134.159	103.006	462.023	376.184	201.958	100.214	−16.3974
1300	136.093	116.522	472.840	383.207	215.474	101.237	−16.0602
1400	137.676	130.213	482.985	389.976	229.165	102.284	−15.7681
1500	138.973	144.048	492.530	396.498	242.999	103.339	−15.5126
1600	140.041	158.000	501.534	402.784	256.952	104.382	−15.2865
1700	140.921	172.050	510.051	408.845	271.001	105.403	−15.0851
1800	141.650	186.179	518.127	414.694	285.131	106.389	−14.9043
1900	142.256	200.376	525.803	420.342	299.327	107.335	−14.7412
2000	142.760	214.627	533.113	425.799	313.579	108.234	−14.5929
2100	143.182	228.925	540.088	431.077	327.877	109.081	−14.4578
2200	143.537	243.261	546.758	436.184	342.213	109.872	−14.3341
2300	143.836	257.631	553.145	441.132	356.582	110.608	−14.2202
2400	144.088	272.027	559.272	445.927	370.979	111.284	−14.1153
2500	144.302	286.447	565.158	450.580	385.398	111.897	−14.0181
2600	144.484	300.886	570.822	455.096	399.838	112.453	−13.9280
2700	144.639	315.343	576.278	459.484	414.294	112.944	−13.8441
2800	144.771	329.813	581.540	463.750	428.765	113.376	−13.7660
2900	144.885	344.296	586.622	467.900	443.248	113.747	−13.6929
3000	144.983	358.790	591.536	471.939	457.741	114.056	−13.6244
3100	145.067	373.292	596.291	475.874	472.244	114.309	−13.5605
3200	145.139	387.803	600.898	479.710	486.754	114.500	−13.5001
3300	145.202	402.320	605.365	483.450	501.272	114.633	−13.4434
3400	145.257	416.843	609.701	487.100	515.795	114.711	−13.3901
3500	145.304	431.371	613.912	490.663	530.323	114.731	−13.3397
3600	145.345	445.904	618.006	494.144	544.855	114.696	−13.2921
3700	145.380	460.440	621.989	497.546	559.391	114.606	−13.2472
3800	145.411	474.979	625.866	500.872	573.931	114.463	−13.2046
3900	145.438	489.522	629.644	504.125	588.473	114.267	−13.1643
4000	145.461	504.067	633.326	507.310	603.018	114.016	−13.1261
4100	145.482	518.614	636.918	510.427	617.566	113.717	−13.0899
4200	145.500	533.163	640.424	513.481	632.115	113.365	−13.0554
4300	145.515	547.714	643.848	516.473	646.665	112.963	−13.0227
4400	145.529	562.266	647.194	519.406	661.218	112.508	−12.9915
4500	145.540	576.820	650.464	522.282	675.771	112.007	−12.9619
4600	145.551	591.374	653.663	525.104	690.326	111.457	−12.9337
4700	145.560	605.930	656.794	527.872	704.881	110.862	−12.9069
4800	145.567	620.486	659.858	530.590	719.438	110.222	−12.8813
4900	145.574	635.043	662.860	533.259	733.995	109.534	−12.8569
5000	145.580	649.601	665.801	535.881	748.552	108.795	−12.8335
5100	145.585	664.159	668.684	538.456	763.111	108.020	−12.8115
5200	145.589	678.718	671.511	540.988	777.669	107.198	−12.7902
5300	145.592	693.277	674.284	543.477	792.228	106.335	−12.7700
5400	145.595	707.836	677.005	545.925	806.788	105.428	−12.7507
5500	145.598	722.396	679.677	548.332	821.347	104.482	−12.7323
5600	145.600	736.956	682.300	550.701	835.907	103.497	−12.7146
5700	145.602	751.516	684.878	553.033	850.467	102.473	−12.6977
5800	145.603	766.076	687.410	555.328	865.027	101.413	−12.6816
5900	145.604	780.636	689.899	557.588	879.588	100.319	−12.6662
6000	145.605	795.197	692.346	559.813	894.148	99.190	−12.6515

TABLE 24. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for nitroethylene $H_2C{=}CHNO_2$ $C_2H_3NO_2$ (molecular wt. = 73.051360)[a]

PM3												
	79.0	311	503	553	641	772	901	950	1073	1082	1214	1325
	1605	1819	1904	2997	3104	3131						
PM3 UHF												
	77.5	311	502	553	641	772	901	950	1073	1082	1214	1325
	1605	1819	1904	2997	3104	3131						
AM1												
	91.2	310	503	607	730	770	951	990	1081	1180	1272	1392
	1781	1825	2060	3137	3162	3191						
AM1 UHF												
	91.6	310	503	607	730	770	951	990	1080	1180	1272	1392
	1781	1824	2060	3137	3162	3191						
Melius MP4/6-31G**//RHF/6-31G**[b]												
	104	**323**	**536**	**544**	**654**	**828**	**904**	**966**	**1026**	**1066**	**1264**	**1378**
	1479	**1628**	**1699**	**3013**	**3094**	**3103**						

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia = 68.632 659 Ib = 189.023 663 Ic = 257.466 854
PM3 UHF Ia = 68.632 659 Ib = 189.023 663 Ic = 257.466 854
AM1 Ia = 67.617 782 Ib = 186.082 234 Ic = 253.700 017
AM1 UHF Ia = 67.617 949 Ib = 186.083 365 Ic = 253.701 307
Melius Ia = **67.7795** Ib = **174.725** Ic = **242.505** σ = **1** Ir = **59.71** ROSYM = **2** V(3) = **5.04** kcal/mol[c] V(2)(Experimental) = 4.8 kcal/mol
PM3 heat of formation = 7.17 kcal/mol
PM3 UHF heat of formation = 7.17 kcal/mol
AM1 heat of formation = 15.95 kcal/mol
AM1 UHF heat of formation = 15.95 kcal/mol spin = 0 $S^2 = 0$
Melius $\Delta H_f(0) = 11.1$ $\Delta H_f(298) = \mathbf{7.95 \pm 2.06}$ kcal/mol spin = 1 $S^2 = 0.3850$
Luo and Holmes[d] (Benson's estimation) $\Delta H_f(298) = 9.0$ kcal/mol
AM1 ionization potential = 11.891 eV
AM1 UHF ionization potential = 11.891 eV
PM3 zero point energy 34.347 kcal/mol
PM3 UHF zero point energy 34.340 kcal/mol
AM1 zero point energy 35.857 kcal/mol
AM1 UHF zero point energy 35.860 kcal/mol
Melius zero-point vibrational energy 33.750 kcal/mol
R(CC) = 1.3120[b]
R(CH) = 1.0689–1.0732
R(CN) = 1.4525
R(NO) = 1.1932–1.1938

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 35.
[c]See Ref. 43.
[d]See Ref. 30.

TABLE 25. Ideal gas thermodynamic properties for nitroethylene $CH_2=CHNO_2$

T (deg K)	C_P (J/mol K)	$H-H_{298}$ (kJ/mol)	S (J/mol K)	$-(G-H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−15.108	-------	-------	18.176	46.001	-------
100	43.027	−11.309	241.157	354.246	21.975	40.826	−29.9445
200	56.591	−6.383	274.763	306.679	26.900	36.690	−19.7146
298.15	73.680	0.000	300.503	300.503	33.284	33.284	−16.6924
300	74.007	0.137	300.960	300.505	33.420	33.227	−16.6564
400	90.791	8.394	324.599	303.614	41.678	30.651	−15.2642
500	104.910	18.204	346.431	310.023	51.488	28.894	−14.4866
600	116.200	29.281	366.596	317.794	62.565	27.771	−13.9934
700	125.182	41.367	385.208	326.113	74.651	27.128	−13.6522
800	132.420	54.260	402.413	334.589	87.543	26.857	−13.4007
900	138.340	67.807	418.363	343.022	101.091	26.880	−13.2060
1000	143.242	81.894	433.200	351.307	115.178	27.129	−13.0493
1100	147.339	96.429	447.051	359.388	129.713	27.558	−12.9195
1200	150.784	111.340	460.023	367.240	144.624	28.126	−12.8094
1300	153.698	126.568	472.210	374.850	159.852	28.794	−12.7143
1400	156.173	142.065	483.694	382.219	175.349	29.533	−12.6305
1500	158.284	157.790	494.542	389.349	191.074	30.323	−12.5563
1600	160.092	173.712	504.817	396.247	206.995	31.140	−12.4894
1700	161.647	189.801	514.570	402.923	223.084	31.969	−12.4288
1800	162.990	206.034	523.849	409.385	239.318	32.796	−12.3735
1900	164.154	222.393	532.693	415.644	255.676	33.610	−12.3229
2000	165.166	238.860	541.139	421.710	272.143	34.404	−12.2760
2100	166.051	255.422	549.220	427.590	288.705	35.170	−12.2328
2200	166.827	272.066	556.963	433.296	305.350	35.899	−12.1926
2300	167.510	288.784	564.394	438.836	322.068	36.593	−12.1552
2400	168.113	305.566	571.536	444.217	338.849	37.244	−12.1203
2500	168.647	322.404	578.410	449.448	355.688	37.846	−12.0876
2600	169.123	339.293	585.034	454.536	372.577	38.405	−12.0570
2700	169.547	356.227	591.425	459.489	389.511	38.911	−12.0282
2800	169.927	373.201	597.598	464.311	406.485	39.368	−12.0013
2900	170.268	390.211	603.567	469.011	423.495	39.772	−11.9757
3000	170.574	407.253	609.344	473.593	440.537	40.119	−11.9516
3100	170.852	424.325	614.942	478.063	457.609	40.421	−11.9292
3200	171.103	441.423	620.370	482.426	474.707	40.663	−11.9077
3300	171.330	458.545	625.639	486.686	491.828	40.851	−11.8875
3400	171.537	475.688	630.757	490.848	508.972	40.987	−11.8685
3500	171.727	492.852	635.732	494.917	526.135	41.065	−11.8506
3600	171.899	510.033	640.572	498.896	543.317	41.090	−11.8334
3700	172.058	527.231	645.284	502.789	560.515	41.059	−11.8174
3800	172.203	544.444	649.875	506.600	577.728	40.973	−11.8021
3900	172.337	561.671	654.349	510.331	594.955	40.834	−11.7878
4000	172.460	578.911	658.714	513.986	612.195	40.634	−11.7740
4100	172.574	596.163	662.974	517.568	629.446	40.386	−11.7613
4200	172.679	613.425	667.134	521.080	646.709	40.080	−11.7490
4300	172.776	630.698	671.198	524.524	663.982	39.718	−11.7374
4400	172.867	647.980	675.171	527.903	681.264	39.294	−11.7264
4500	172.951	665.271	679.057	531.219	698.555	38.823	−11.7161
4600	173.029	682.570	682.859	534.474	715.854	38.297	−11.7064
4700	173.102	699.877	686.581	537.671	733.161	37.721	−11.6972
4800	173.171	717.191	690.226	540.812	750.475	37.093	−11.6886
4900	173.235	734.511	693.798	543.897	767.795	36.412	−11.6805
5000	173.294	751.838	697.298	546.931	785.121	35.662	−11.6727
5100	173.350	769.170	700.730	549.913	802.454	34.882	−11.6657
5200	173.403	786.508	704.097	552.846	819.791	34.041	−11.6588
5300	173.452	803.850	707.400	555.731	837.134	33.151	−11.6525
5400	173.499	821.198	710.643	558.569	854.482	32.210	−11.6465
5500	173.543	838.550	713.827	561.363	871.834	31.221	−11.6409
5600	173.584	855.906	716.954	564.114	889.190	30.185	−11.6357
5700	173.623	873.267	720.027	566.822	906.550	29.103	−11.6309
5800	173.660	890.631	723.047	569.490	923.915	27.976	−11.6264
5900	173.695	907.999	726.016	572.118	941.282	26.806	−11.6221
6000	173.728	925.370	728.936	574.707	958.653	25.595	−11.6183

TABLE 26. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for *trans*-dinitroethylene $NO_2HC{=}CHNO_2$ $C_2H_2(NO_2)_2$ (molecular wt.=118.048960)[a]

PM3												
	94.1	108	**140**	**291**	**353**	**418**	**474**	**512**	**630**	**676**	**698**	**771**
	944	**996**	**1081**	**1168**	**1439**	**1527**	**1620**	**1794**	**1906**	**2035**	**3033**	**3618**
PM3 UHF												
	90.3	107	140	291	353	418	474	512	629	674	698	771
	943	996	1081	1167	1439	1527	1620	1794	1906	2035	3033	3618
AM1												
	72.2	75.6	170	218	338	395	421	492	571	673	779	826
	899	1061	1191	1249	1471	1581	1759	1847	2051	2186	3143	3329
AM1 UHF												
	67.8	75.3	180	207	333	385	427	496	571	673	776	824
	901	1064	1192	1252	1475	1583	1760	1848	2051	2187	3139	3333

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia=**150.866 142** Ib=**703.065 060** Ic=**832.326 544** σ(external)=**2**
PM3 UHF Ia=150.866 142 Ib=703.065 060 Ic=832.326 544
AM1 Ia=138.327 798 Ib=728.543 236 Ic=859.306 753
AM1 UHF Ia=136.390 804 Ib=729.945 159 Ic=861.717 112 (Ir(NO_2)=**59.6** ROSYM=**2** V(3)=**5.04** kcal/mol)×2
PM3 Heat of formation=−26.42 kcal/mol
PM3 UHF heat of formation=−26.42 kcal/mol
AM1 heat of formation=−19.42 kcal/mol
AM1 UHF heat of formation=−19.51 kcal/mol spin=0.0 S^2=0.0
Melius 97 $\Delta H_f(298)$=85.12±5.22 kcal/mol (transition state)
NIST 94 $\Delta H_f(298)$=**14.2** kcal/mol
AM1 ionization potential=11.120 eV
AM1 UHF ionization potential=11.146 eV
PM3 zero point energy 37.667 kcal/mol
PM3 UHF zero point energy 37.651 kcal/mol
AM1 zero point energy 38.352 kcal/mol
AM1 UHF zero point energy 38.305 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.

TABLE 27. Ideal gas thermodynamic properties for dinitroethylene $NO_2CH{=}CHNO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-----	−21.514	-----	-----	37.898	74.504	-----
100	59.546	−16.968	270.697	440.378	42.445	67.224	−52.7858
200	86.262	−9.686	320.104	368.535	49.727	62.425	−35.7559
298.15	110.488	0.000	359.186	359.186	59.413	59.413	−30.5117
300	110.907	0.205	359.871	359.189	59.618	59.369	−30.4473
400	131.436	12.357	394.688	363.797	71.770	57.710	−27.9003
500	147.927	26.357	425.861	373.147	85.770	57.076	−26.4028
600	160.888	41.824	454.025	384.318	101.237	57.156	−25.4090
700	171.023	58.440	479.619	396.132	117.853	57.736	−24.6952
800	179.002	75.957	502.997	408.051	135.370	58.672	−24.1528
900	185.350	94.187	524.461	419.809	153.599	59.870	−23.7232
1000	190.457	112.986	544.263	431.278	172.399	61.252	−23.3719
1100	194.602	132.246	562.617	442.393	191.659	62.765	−23.0775
1200	197.993	151.881	579.700	453.132	211.294	64.372	−22.8262
1300	200.784	171.825	595.662	463.489	231.237	66.034	−22.6080
1400	203.094	192.022	610.628	473.470	251.435	67.723	−22.4159
1500	205.015	212.430	624.708	483.088	271.843	69.423	−22.2457
1600	206.619	233.014	637.992	492.358	292.427	71.109	−22.0928
1700	207.964	253.746	650.560	501.298	313.158	72.770	−21.9547
1800	209.097	274.600	662.480	509.924	334.013	74.392	−21.8291
1900	210.055	295.559	673.811	518.254	354.972	75.964	−21.7143
2000	210.868	316.606	684.607	526.304	376.019	77.482	−21.6087
2100	211.560	337.729	694.913	534.089	397.142	78.939	−21.5115
2200	212.151	358.915	704.768	541.625	418.328	80.327	−21.4214
2300	212.658	380.156	714.210	548.925	439.569	81.647	−21.3378
2400	213.094	401.444	723.270	556.002	460.857	82.894	−21.2600
2500	213.470	422.773	731.977	562.868	482.186	84.060	−21.1874
2600	213.796	444.137	740.356	569.534	503.549	85.157	−21.1194
2700	214.079	465.531	748.430	576.011	524.944	86.171	−21.0556
2800	214.325	486.951	756.220	582.309	546.364	87.109	−20.9959
2900	214.540	508.395	763.745	588.437	567.808	87.969	−20.9394
3000	214.728	529.858	771.022	594.402	589.271	88.749	−20.8863
3100	214.893	551.340	778.065	600.214	610.752	89.458	−20.8365
3200	215.039	572.836	784.890	605.879	632.249	90.085	−20.7891
3300	215.166	594.347	791.509	611.404	653.760	90.636	−20.7443
3400	215.280	615.869	797.934	616.796	675.282	91.115	−20.7020
3500	215.380	637.402	804.176	622.061	696.815	91.518	−20.6620
3600	215.468	658.945	810.245	627.205	718.358	91.848	−20.6239
3700	215.547	680.496	816.150	632.232	739.908	92.105	−20.5879
3800	215.617	702.054	821.899	637.148	761.467	92.292	−20.5536
3900	215.680	723.619	827.500	641.957	783.032	92.408	−20.5211
4000	215.736	745.190	832.962	646.664	804.602	92.450	−20.4901
4100	215.786	766.766	838.289	651.273	826.179	92.428	−20.4608
4200	215.831	788.347	843.490	655.788	847.760	92.336	−20.4327
4300	215.871	809.932	848.569	660.213	869.345	92.175	−20.4060
4400	215.907	831.521	853.532	664.550	890.934	91.940	−20.3805
4500	215.940	853.113	858.385	668.804	912.526	91.646	−20.3563
4600	215.969	874.709	863.131	672.977	934.121	91.286	−20.3332
4700	215.995	896.307	867.776	677.072	955.720	90.865	−20.3112
4800	216.019	917.908	872.324	681.093	977.320	90.381	−20.2902
4900	216.041	939.511	876.778	685.041	998.923	89.835	−20.2703
5000	216.060	961.116	881.143	688.920	1020.528	89.211	−20.2511
5100	216.077	982.722	885.422	692.731	1042.135	88.546	−20.2331
5200	216.093	1004.331	889.618	696.477	1063.744	87.811	−20.2156
5300	216.108	1025.941	893.734	700.160	1085.354	87.018	−20.1991
5400	216.121	1047.553	897.773	703.782	1106.965	86.164	−20.1833
5500	216.133	1069.165	901.739	707.346	1128.578	85.253	−20.1683
5600	216.143	1090.779	905.634	710.852	1150.192	84.288	−20.1539
5700	216.153	1112.394	909.459	714.303	1171.807	83.265	−20.1401
5800	216.162	1134.010	913.219	717.700	1193.422	82.191	−20.1271
5900	216.170	1155.626	916.914	721.045	1215.039	81.064	−20.1146
6000	216.177	1177.244	920.547	724.340	1236.656	79.888	−20.1027

TABLE 28. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for nitroethane $C_2H_5NO_2$ HCCN *trans* (molecular wt. = 75.067240)[a]

Melius MP4/6-31G**//rhf/6-31g* ump4(sdq)/6-31g**//hf/6-31g*[b]

10.7	233	**286**	**501**	**591**	**639**	797	881	984	1089	**1141**	1274
1348	1405	**1447**	1457	**1465**	1503	1672	2884	**2929**	2947	**2961**	2982

IR spectrum[c]

					774	**881**	**996**	**1117**		**1252**
1386	**1400**		**1460**		**1561**	**1582**	**2754**		**2956**		**3003**

Principal moments of inertia in units of 10^{-40} g cm^2

Melius Ia = **74.804** Ib = **198.289** Ic = **262.826** σ = **1**
Ir(CH_3) = **5.1666** ROSYM = **3** V(3) = **3.5** kcal/mol
Ir(NO_2) = 59.548 ROSYM = **2** V(2) = **0.08** kcal/mol
Table 3 Ir(NO_2) = **59.7**
Melius $\Delta H_f(0) = -19.8$ $\Delta H_f(298) = -$ **24.81** $\pm$ **1.23** kcal/mol spin = 1 $S^2 = 0.2840$
Melius MP4/G2(1997) $\Delta H_f(298) = -26.80 \pm 1.01$ kcal/mol
NIST 94 $\Delta H_f(298) = -24.6$ kcal/mol[d]
Pedley and Rylance[e] $\Delta H_f(298) = -24.6 \pm 0.1$ kcal/mol IP = 10.9 ± 0.05 eV
Stull *et al.*[f] $\Delta H_f(298) = -24.2$ kcal/mol
NIST 97 ΔH_f liquid (298) = -34.41 kcal/mol C_p liquid (298) = 32.08 kcal/mol[g]
zero point vibrational energy = 47.78243 kcal/mol[b]
R(CC) = 1.5150[b]
R(CN) = 1.4927
R(NO) = 1.1904–1.1931
R(CH) = 1.0805–1.0848

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 35.
[c]See Ref. 1.
[d]See Ref. 51.
[e]See Ref. 44.
[f]See Ref. 55.
[g]See Ref. 27.

TABLE 29. Ideal gas thermodynamic properties for nitroethane $CH_3CH_2NO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-----	−16.015	-----	-----	−119.799	−83.506	-----
100	44.130	−12.016	257.654	377.812	−115.800	−91.480	34.7636
200	60.324	−6.824	292.999	327.120	−110.608	−98.044	10.1886
298.15	79.018	0.000	320.512	320.512	−103.784	−103.784	1.5399
300	79.382	0.147	321.002	320.514	−103.638	−103.884	1.4278
400	98.662	9.059	346.509	323.861	−94.725	−108.710	−3.1933
500	115.884	19.808	370.423	330.807	−83.976	−112.451	−6.0799
600	130.471	32.147	392.880	339.301	−71.637	−115.241	−8.0618
700	142.706	45.824	413.938	348.475	−57.960	−117.231	−9.5074
800	153.008	60.624	433.686	357.906	−43.160	−118.548	−10.6073
900	161.724	76.373	452.225	367.366	−27.411	−119.298	−11.4703
1000	169.125	92.925	469.658	376.733	−10.859	−119.587	−12.1636
1100	175.421	110.161	486.080	385.934	6.377	−119.496	−12.7313
1200	180.788	127.978	501.580	394.932	24.194	−119.100	−13.2035
1300	185.373	146.292	516.237	403.704	42.508	−118.467	−13.6014
1400	189.300	165.031	530.122	412.243	61.247	−117.650	−13.9401
1500	192.673	184.134	543.300	420.544	80.350	−116.690	−14.2318
1600	195.579	203.550	555.830	428.611	99.766	−115.629	−14.4847
1700	198.092	223.237	567.764	436.449	119.453	−114.496	−14.7057
1800	200.274	243.158	579.150	444.063	139.373	−113.316	−14.9001
1900	202.175	263.282	590.030	451.461	159.498	−112.107	−15.0723
2000	203.837	283.585	600.444	458.652	179.800	−110.889	−15.2255
2100	205.297	304.043	610.425	465.643	200.259	−109.672	−15.3627
2200	206.583	324.638	620.006	472.443	220.854	−108.470	−15.4860
2300	207.721	345.354	629.214	479.060	241.570	−107.288	−15.5973
2400	208.731	366.178	638.077	485.503	262.394	−106.136	−15.6984
2500	209.630	387.097	646.616	491.777	283.313	−105.024	−15.7902
2600	210.434	408.101	654.854	497.892	304.317	−103.947	−15.8742
2700	211.154	429.181	662.810	503.854	325.397	−102.919	−15.9512
2800	211.803	450.329	670.501	509.669	346.545	−101.936	−16.0221
2900	212.387	471.539	677.943	515.344	367.755	−101.004	−16.0873
3000	212.916	492.805	685.153	520.884	389.021	−100.131	−16.1474
3100	213.395	514.121	692.142	526.297	410.337	−99.303	−16.2037
3200	213.831	535.483	698.924	531.586	431.698	−98.538	−16.2557
3300	214.229	556.886	705.510	536.757	453.102	−97.831	−16.3042
3400	214.592	578.327	711.911	541.815	474.543	−97.180	−16.3496
3500	214.925	599.803	718.137	546.764	496.019	−96.592	−16.3923
3600	215.230	621.311	724.195	551.609	517.527	−96.063	−16.4320
3700	215.511	642.848	730.096	556.354	539.064	−95.596	−16.4697
3800	215.770	664.413	735.847	561.002	560.629	−95.193	−16.5051
3900	216.009	686.002	741.455	565.557	582.218	−94.850	−16.5387
4000	216.230	707.614	746.927	570.023	603.830	−94.578	−16.5702
4100	216.435	729.247	752.269	574.403	625.463	−94.362	−16.6005
4200	216.626	750.901	757.487	578.701	647.116	−94.213	−16.6291
4300	216.803	772.572	762.586	582.918	668.788	−94.131	−16.6562
4400	216.968	794.261	767.572	587.058	690.477	−94.120	−16.6821
4500	217.121	815.965	772.450	591.124	712.181	−94.167	−16.7070
4600	217.265	837.685	777.223	595.118	733.901	−94.279	−16.7308
4700	217.399	859.418	781.897	599.042	755.634	−94.452	−16.7536
4800	217.525	881.164	786.476	602.900	777.380	−94.688	−16.7755
4900	217.643	902.923	790.962	606.692	799.139	−94.986	−16.7966
5000	217.754	924.693	795.360	610.422	820.909	−95.365	−16.8167
5100	217.859	946.473	799.673	614.090	842.689	−95.784	−16.8366
5200	217.957	968.264	803.905	617.700	864.480	−96.273	−16.8554
5300	218.049	990.065	808.057	621.253	886.280	−96.822	−16.8737
5400	218.137	1011.874	812.134	624.750	908.090	−97.430	−16.8915
5500	218.219	1033.692	816.137	628.193	929.908	−98.096	−16.9087
5600	218.297	1055.518	820.070	631.585	951.733	−98.816	−16.9253
5700	218.371	1077.351	823.934	634.925	973.567	−99.590	−16.9416
5800	218.440	1099.191	827.733	638.217	995.407	−100.415	−16.9574
5900	218.506	1121.039	831.468	641.461	1017.255	−101.291	−16.9727
6000	218.569	1142.893	835.141	644.658	1039.109	−102.212	−16.9878

TABLE 30. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for ethylnitrate $C_2H_5ONO_2$ (molecular wt.=91.066640)[a]

PM3												
	58.8	104	161	265	317	413	535	609	644	847	957	1096
	1112	1119	1149	1316	1355	1403	1405	1411	1530	2090	2950	3026
	3085	3089	3185									
PM3 UHF												
	58.5	104	158	264	317	413	535	609	644	847	958	1096
	1112	1119	1148	1316	1355	1403	1405	1411	1530	2090	2950	3026
	3085	3089	3185									
AM1												
	74.9	109	164	325	440	652	683	729	860	1010	1130	1176
	1211	1263	1309	1374	1380	1388	1423	1433	1733	2149	3040	3065
	3069	3096	3157									
AM1 UHF												
	74.9	109	164	325	440	652	683	729	860	1010	1130	1176
	1211	1263	1309	1374	1380	1388	1423	1433	1733	2149	3040	3065
	3069	3096	3157									
Melius BAC-MP4												
	86.8	125	**207**	**342**	**396**	**589**	**692**	**790**	**815**	**878**	**968**	**1066**
	1086	**1172**	**1296**	**1355**	**1403**	**1427**	**1455**	**1468**	**1481**	**1703**	**2877**	**2933**
	2946	**2959**	**3003**									

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia=108.848 086 Ib=347.796 885 Ic=394.385 230
PM3 UHF Ia=108.848 086 Ib=347.796 885 Ic=394.385 230
AM1 Ia=101.367 498 Ib=328.292 964 Ic=370.178 298
AM1 UHF Ia=101.367 077 Ib=328.294 744 Ic=370.179 691 spin=0 $S^2=0$
Melius Ia=**99.190 168** Ib=**323.569 95** Ic=**364.527** spin=0 $S^2=0$
Ir(NO_2)=**59.6** ROSYM=**2** V(2)=**9.1** kcal/mol[b]
Ir(CH_3)=**5.166** ROSYM=**3** V(3)=**3.5** kcal/mol[b]
PM3 heat of formation=−38.03 kcal/mol
PM3 UHF heat of formation=−38.03 kcal/mol
AM1 heat of formation=−38.11 kcal/mol
AM1 UHF heat of formation=−38.11 kcal/mol
Melius BAC-MP4 $\Delta H_f(0)=-29.13$ $\Delta H_f(298)=-34.50$ kcal/mol
Stull[c] $\Delta H_f(298)=-36.80$ kcal/mol
NIST 97[d] $\Delta H_f(298)=-$**37.04**$\pm$**0.7** kcal/mol
ΔH_f liquid (298)=−45.5$\pm$0.25 kcal/mol S liquid (298)=59.08 cal/mole K
C_p liquid (298)=40.70 cal/mole
AM1 ionization potential=12.305 eV
AM1 UHF ionization potential=12.305 eV
PM3 zero point energy 50.413 kcal/mol
PM3 UHF zero point energy 50.403 kcal/mol
AM1 zero point energy 53.566 kcal/mol
AM1 UHF zero point energy 53.566 kcal/mol
R(OC)=1.4412[e]
R(CC)=1.5153
R(ON)=1.1774–1.3292
R(CH)=1.0772–1.0852

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 20.
[c]See Ref. 55.
[d]See Ref. 1.
[e]See Ref. 35.

TABLE 31. Ideal gas thermodynamic properties for ethyl nitrate $CH_3CH_2ONO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-----	−18.480	-----	-----	−173.455	−132.823	-----
100	51.268	−14.411	253.641	397.746	−169.386	−142.176	56.5082
200	72.585	−8.215	295.741	336.818	−163.191	−149.192	18.6368
298.15	95.103	0.000	328.863	328.863	−154.975	−154.975	5.5865
300	95.537	0.176	329.452	328.865	−154.799	−155.073	5.4192
400	118.284	10.884	360.099	332.889	−144.091	−159.590	−1.4251
500	138.169	23.735	388.693	341.223	−131.240	−162.758	−5.6341
600	154.716	38.406	415.395	351.385	−116.570	−164.796	−8.4859
700	168.377	54.582	440.304	362.329	−100.393	−165.914	−10.5428
800	179.700	72.003	463.550	373.546	−82.972	−166.279	−12.0926
900	189.125	90.459	485.276	384.767	−64.517	−166.025	−13.2984
1000	196.992	109.776	505.622	395.846	−45.199	−165.280	−14.2600
1100	203.572	129.814	524.715	406.702	−25.161	−164.143	−15.0423
1200	209.087	150.455	542.672	417.292	−4.520	−162.699	−15.6891
1300	213.720	171.602	559.596	427.594	16.627	−161.025	−16.2313
1400	217.626	193.175	575.581	437.599	38.200	−159.182	−16.6907
1500	220.929	215.107	590.712	447.307	60.132	−157.214	−17.0845
1600	223.735	237.344	605.062	456.722	82.369	−155.167	−17.4246
1700	226.128	259.840	618.700	465.852	104.865	−153.071	−17.7205
1800	228.178	282.558	631.684	474.707	127.583	−150.954	−17.9800
1900	229.942	305.466	644.070	483.298	150.491	−148.833	−18.2091
2000	231.467	328.539	655.904	491.634	173.563	−146.728	−18.4120
2100	232.791	351.753	667.230	499.728	196.778	−144.649	−18.5933
2200	233.946	375.091	678.087	507.591	220.116	−142.612	−18.7557
2300	234.958	398.538	688.509	515.232	243.562	−140.617	−18.9019
2400	235.847	422.079	698.528	522.662	267.103	−138.677	−19.0341
2500	236.633	445.704	708.172	529.890	290.728	−136.800	−19.1539
2600	237.329	469.402	717.466	536.927	314.427	−134.980	−19.2632
2700	237.949	493.167	726.435	543.781	338.192	−133.230	−19.3630
2800	238.501	516.990	735.099	550.460	362.015	−131.546	−19.4546
2900	238.997	540.865	743.477	556.972	385.890	−129.933	−19.5386
3000	239.442	564.788	751.587	563.325	409.812	−128.397	−19.6159
3100	239.843	588.752	759.445	569.525	433.777	−126.925	−19.6879
3200	240.205	612.755	767.065	575.580	457.779	−125.533	−19.7542
3300	240.534	636.792	774.462	581.495	481.817	−124.215	−19.8160
3400	240.833	660.861	781.647	587.277	505.885	−122.969	−19.8735
3500	241.105	684.958	788.632	592.930	529.982	−121.801	−19.9273
3600	241.353	709.081	795.428	598.461	554.105	−120.707	−19.9774
3700	241.581	733.228	802.044	603.874	578.252	−119.689	−20.0247
3800	241.790	757.396	808.489	609.175	602.421	−118.748	−20.0689
3900	241.982	781.585	814.773	614.366	626.610	−117.879	−20.1107
4000	242.159	805.792	820.901	619.453	650.817	−117.093	−20.1499
4100	242.322	830.016	826.883	624.440	675.041	−116.375	−20.1873
4200	242.474	854.256	832.724	629.330	699.281	−115.736	−20.2224
4300	242.614	878.511	838.431	634.126	723.535	−115.174	−20.2557
4400	242.744	902.779	844.010	638.833	747.803	−114.693	−20.2873
4500	242.865	927.059	849.467	643.454	772.084	−114.281	−20.3176
4600	242.977	951.351	854.806	647.990	796.376	−113.944	−20.3464
4700	243.082	975.654	860.033	652.447	820.679	−113.675	−20.3739
4800	243.180	999.967	865.151	656.825	844.992	−113.479	−20.4002
4900	243.272	1024.290	870.167	661.128	869.315	−113.355	−20.4255
5000	243.358	1048.622	875.082	665.358	893.646	−113.318	−20.4495
5100	243.439	1072.962	879.902	669.517	917.986	−113.332	−20.4729
5200	243.514	1097.309	884.630	673.609	942.334	−113.422	−20.4952
5300	243.585	1121.664	889.269	677.634	966.689	−113.579	−20.5167
5400	243.652	1146.026	893.823	681.596	991.051	−113.804	−20.5375
5500	243.715	1170.395	898.294	685.495	1015.419	−114.092	−20.5576
5600	243.775	1194.769	902.686	689.335	1039.794	−114.442	−20.5769
5700	243.831	1219.149	907.001	693.116	1064.174	−114.852	−20.5957
5800	243.884	1243.535	911.243	696.840	1088.560	−115.319	−20.6139
5900	243.935	1267.926	915.412	700.509	1112.951	−115.842	−20.6314
6000	243.982	1292.322	919.512	704.125	1137.347	−116.416	−20.6486

TABLE 32. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for CH3–C=C–NO_2 *cis*-1-methyl-2-nitroethylene (molecular wt.=87.078240)[a]

Melius MP4/6-31G**//RHF/6-31G*

37.4	128	**223**	**362**	**382**	**575**	**655**	**762**	**831**	**887**	**955**	**972**
1072	**1081**	**1228**	**1354**	**1400**	**1448**	**1457**	**1477**	**1629**	**1696**	**2888**	**2954**
2954	**3001**	**3091**									

Principal moments of inertia in units of 10^{-40} g cm^2

Melius Ia=**95.524** Ib=**309.429** Ic=**399.889**

Ir(NO_2)=**59.606** ROSYM=**2** V(2)=**1.5** kcal/mol

Ir(CH_3)=**5.1536** ROSYM=**3** V(3)=**8.8** kcal/mol

Melius $\Delta H_f(0)$=6.8 $\Delta H_f(298)$=**2.39**±**2.12** kcal/mol spin=1 S^2=0.3460

zero point vibrational energy 50.745 kcal/mol[b]

R(CC)=1.3208–1.5040[b]

R(CN)=1.4439

R(NO)=1.1941–1.1965

R(CH)=1.0688–1.0822

[a]The properties marked with bold characters were chosen for thermodynamic calculations.

[b]See Ref. 35.

TABLE 33. Ideal gas thermodynamic properties for nitropropylene $CH_3CH{=}CHNO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-----	−18.288	-----	-----	−8.300	29.046	-----
100	49.706	−14.159	256.209	397.803	−4.172	21.140	−24.1861
200	71.560	−8.098	297.352	337.843	1.889	15.119	−19.2989
298.15	93.590	0.000	330.004	330.004	9.987	9.987	−18.1956
300	94.009	0.174	330.584	330.006	10.161	9.899	−18.1847
400	116.051	10.691	360.688	333.961	20.678	5.653	−17.8415
500	135.596	23.298	388.740	342.143	33.286	2.445	−17.7348
600	152.096	37.708	414.966	352.120	47.695	0.148	−17.7121
700	165.856	53.626	439.477	362.868	63.613	−1.373	−17.7199
800	177.332	70.803	462.396	373.893	80.790	−2.235	−17.7371
900	186.922	89.030	483.853	384.931	99.017	−2.541	−17.7547
1000	194.951	108.135	503.975	395.840	118.122	−2.401	−17.7692
1100	201.682	127.977	522.881	406.539	137.964	−1.899	−17.7795
1200	207.338	148.436	540.679	416.983	158.423	−1.112	−17.7856
1300	212.102	169.415	557.469	427.150	179.402	−0.112	−17.7879
1400	216.126	190.832	573.339	437.030	200.819	1.043	−17.7864
1500	219.539	212.619	588.369	446.623	222.607	2.315	−17.7826
1600	222.445	234.723	602.633	455.932	244.710	3.659	−17.7762
1700	224.930	257.095	616.196	464.964	267.082	5.046	−17.7678
1800	227.064	279.697	629.114	473.727	289.684	6.451	−17.7580
1900	228.906	302.498	641.441	482.232	312.485	7.857	−17.7472
2000	230.502	325.470	653.224	490.489	335.457	9.246	−17.7352
2100	231.891	348.591	664.505	498.509	358.578	10.608	−17.7230
2200	233.105	371.842	675.321	506.302	381.829	11.928	−17.7102
2300	234.171	395.207	685.707	513.878	405.194	13.207	−17.6972
2400	235.111	418.672	695.694	521.247	428.659	14.431	−17.6843
2500	235.942	442.226	705.308	528.418	452.213	15.592	−17.6711
2600	236.681	465.858	714.577	535.401	475.845	16.698	−17.6581
2700	237.339	489.559	723.522	542.204	499.546	17.733	−17.6454
2800	237.928	513.323	732.164	548.835	523.310	18.704	−17.6329
2900	238.456	537.143	740.523	555.301	547.130	19.604	−17.6205
3000	238.931	561.012	748.615	561.611	571.000	20.425	−17.6082
3100	239.360	584.927	756.457	567.770	594.915	21.186	−17.5968
3200	239.749	608.883	764.062	573.786	618.870	21.865	−17.5854
3300	240.102	632.876	771.445	579.665	642.863	22.470	−17.5744
3400	240.423	656.903	778.618	585.411	666.890	23.003	−17.5638
3500	240.716	680.960	785.591	591.031	690.947	23.455	−17.5537
3600	240.984	705.045	792.376	596.531	715.032	23.834	−17.5438
3700	241.230	729.156	798.982	601.913	739.143	24.134	−17.5345
3800	241.456	753.290	805.419	607.184	763.277	24.356	−17.5254
3900	241.663	777.446	811.693	612.348	787.434	24.504	−17.5168
4000	241.855	801.622	817.814	617.409	811.610	24.565	−17.5085
4100	242.032	825.817	823.788	622.370	835.804	24.559	−17.5009
4200	242.196	850.028	829.623	627.235	860.016	24.469	−17.4934
4300	242.349	874.256	835.324	632.008	884.243	24.300	−17.4862
4400	242.490	898.498	840.897	636.693	908.485	24.042	−17.4794
4500	242.622	922.753	846.348	641.291	932.741	23.716	−17.4732
4600	242.744	947.022	851.682	645.807	957.009	23.312	−17.4672
4700	242.859	971.302	856.903	650.243	981.289	22.837	−17.4616
4800	242.966	995.593	862.017	654.602	1005.580	22.286	−17.4565
4900	243.066	1019.895	867.028	658.886	1029.882	21.661	−17.4517
5000	243.160	1044.206	871.940	663.099	1054.193	20.934	−17.4469
5100	243.248	1068.527	876.756	667.241	1078.514	20.166	−17.4431
5200	243.331	1092.856	881.480	671.316	1102.843	19.310	−17.4391
5300	243.409	1117.193	886.116	675.325	1127.180	18.381	−17.4355
5400	243.482	1141.537	890.666	679.271	1151.524	17.381	−17.4323
5500	243.551	1165.889	895.135	683.155	1175.876	16.313	−17.4293
5600	243.616	1190.247	899.524	686.980	1200.234	15.177	−17.4266
5700	243.678	1214.612	903.836	690.746	1224.599	13.974	−17.4243
5800	243.736	1238.983	908.075	694.457	1248.970	12.709	−17.4222
5900	243.792	1263.359	912.242	698.113	1273.346	11.382	−17.4203
6000	243.844	1287.741	916.340	701.716	1297.728	9.996	−17.4187

TABLE 34. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for nitrocyclopropane $C_3H_5NO_2$ (molecular wt. = 87.078240)[a]

Holtzclaw Harris and Bush[b]

70	**289**	**309**	**483**	**645**	**730**	**770**	**828**	**854**	**(880)**	**921**	**936**
1042	**1075**	**1110**	**1118**	**1202**	**1325**	**1373**	**1407**	**1443**	**1571**	**2934**	**3019**
3019	**3095**	**3103**									

Principal moments of inertia in units of 10^{-40} g cm^2

Mochel Britt and Boggs[c] Ia = **105.515** Ib = **285.698** Ic = **324.822** σ(external) = **2**
Ir = 26.1 V(2) = 3.3 ± 1.5 kcal/mol
Holtzclaw *et al.*[b] Ir = **59.6** [Melius] ROSYM = **2** V(2) = **4.7** ± **0.15** kcal/mol
Estimated $\Delta H_f(298) = 6.42$ kcal/mol
NIST 94[d] $\Delta H_f(298) =$ **4.2** kcal/mol $S(298) = 76.6$ cal/mole K

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 22.
[c]See Ref. 39.
[d]See Ref. 51.

TABLE 35. Ideal gas thermodynamic properties for nitrocyclopropane $C_3H_5NO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-----	−16.913	-----	-----	0.659	38.005	-----
100	45.662	−13.041	249.488	379.900	4.532	29.844	−29.0834
200	64.686	−7.596	286.488	324.468	9.977	23.206	−21.9787
298.15	90.787	0.000	317.042	317.042	17.573	17.573	−20.2016
300	91.302	0.168	317.605	317.043	17.741	17.479	−20.1825
400	117.888	10.656	347.593	320.952	28.229	13.205	−19.5115
500	139.918	23.589	376.360	329.182	41.162	10.321	−19.2043
600	157.205	38.481	403.463	339.328	56.054	8.506	−19.0406
700	170.825	54.908	428.759	350.319	72.481	7.495	−18.9414
800	181.785	72.558	452.310	361.613	90.130	7.105	−18.8738
900	190.783	91.200	474.257	372.924	108.773	7.215	−18.8222
1000	198.281	110.664	494.758	384.094	128.237	7.714	−18.7790
1100	204.591	130.817	513.961	395.036	148.390	8.527	−18.7405
1200	209.938	151.551	531.998	405.706	169.123	9.588	−18.7048
1300	214.492	172.778	548.987	416.081	190.351	10.837	−18.6709
1400	218.387	194.427	565.029	426.152	212.000	12.224	−18.6376
1500	221.733	216.437	580.213	435.921	234.010	13.718	−18.6057
1600	224.617	238.758	594.617	445.393	256.331	15.280	−18.5743
1700	227.114	261.348	608.311	454.577	278.920	16.884	−18.5434
1800	229.283	284.170	621.356	463.483	301.743	18.510	−18.5131
1900	231.176	307.195	633.804	472.123	324.768	20.140	−18.4837
2000	232.833	330.397	645.705	480.506	347.970	21.759	−18.4548
2100	234.289	353.755	657.101	488.646	371.328	23.358	−18.4269
2200	235.574	377.249	668.030	496.553	394.822	24.921	−18.3995
2300	236.712	400.865	678.528	504.239	418.438	26.450	−18.3730
2400	237.722	424.587	688.624	511.712	442.160	27.932	−18.3474
2500	238.624	448.406	698.347	518.984	465.978	29.357	−18.3223
2600	239.430	472.309	707.722	526.064	489.882	30.735	−18.2982
2700	240.153	496.289	716.772	532.961	513.862	32.048	−18.2749
2800	240.804	520.337	725.517	539.683	537.910	33.303	−18.2525
2900	241.391	544.447	733.978	546.237	562.020	34.494	−18.2305
3000	241.923	568.614	742.171	552.633	586.186	35.612	−18.2092
3100	242.405	592.830	750.111	558.876	610.403	36.674	−18.1893
3200	242.845	617.093	757.814	564.973	634.666	37.661	−18.1696
3300	243.245	641.398	765.293	570.930	658.971	38.578	−18.1507
3400	243.611	665.741	772.560	576.754	683.314	39.427	−18.1325
3500	243.947	690.119	779.627	582.450	707.692	40.200	−18.1152
3600	244.255	714.530	786.503	588.023	732.102	40.904	−18.0982
3700	244.539	738.969	793.200	593.478	756.542	41.533	−18.0821
3800	244.800	763.437	799.725	598.820	781.009	42.088	−18.0665
3900	245.042	787.929	806.087	604.054	805.502	42.572	−18.0517
4000	245.265	812.444	812.293	609.182	830.017	42.973	−18.0372
4100	245.473	836.981	818.352	614.210	854.554	43.309	−18.0237
4200	245.665	861.538	824.270	619.142	879.111	43.565	−18.0105
4300	245.844	886.114	830.053	623.980	903.687	43.743	−17.9977
4400	246.011	910.707	835.706	628.728	928.280	43.837	−17.9855
4500	246.167	935.316	841.237	633.389	952.889	43.864	−17.9740
4600	246.312	959.940	846.649	637.966	977.513	43.816	−17.9629
4700	246.449	984.578	851.948	642.463	1002.151	43.699	−17.9523
4800	246.576	1009.229	857.137	646.881	1026.802	43.508	−17.9423
4900	246.696	1033.893	862.223	651.224	1051.466	43.245	−17.9328
5000	246.808	1058.568	867.208	655.494	1076.141	42.881	−17.9234
5100	246.914	1083.254	872.097	659.694	1100.827	42.479	−17.9150
5200	247.014	1107.951	876.892	663.825	1125.524	41.990	−17.9065
5300	247.108	1132.657	881.598	667.889	1150.230	41.431	−17.8987
5400	247.196	1157.372	886.218	671.890	1174.945	40.802	−17.8912
5500	247.280	1182.096	890.755	675.828	1199.669	40.105	−17.8841
5600	247.359	1206.828	895.211	679.706	1224.401	39.343	−17.8773
5700	247.434	1231.568	899.590	683.525	1249.140	38.515	−17.8710
5800	247.505	1256.315	903.894	687.288	1273.887	37.627	−17.8650
5900	247.572	1281.068	908.125	690.995	1298.641	36.677	−17.8592
6000	247.636	1305.829	912.287	694.649	1323.402	35.670	−17.8539

TABLE 36. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for Nitroglycerin $C_3H_5(ONO_2)_3$ $CH_2(ONO_2)CH(ONO_2)CH_2ONO_2$ (molecular wt.=227.087520)[a]

PM3

22.9 33.4 35.1 43.6 54.1 60 62 97.7 173 188 232 264
276 312 318 348 379 409 463 470 478 582 622 627
639 654 676 701 798 915 928 971 1083 1093 1117 1144
1150 1159 1211 1230 1302 1317 1329 1358 1363 1522 1538 2132
2142 2833 2942 2954 3015 3023

PM3 UHF

23.9 33.8 34.2 **44.4** **53.9** **59.8** **61.8** **97** **173** **188** **232** **264**
276 **311** **316** **348** **378** **409** **463** **471** **478** **582** **621** **627**
638 **654** **675** **701** **798** **915** **928** **971** **1085** **1093** **1118** **1145**
1151 **1160** **1209** **1231** **1303** **1318** **1329** **1359** **1363** **1522** **1537** **2132**
2142 **2831** **2941** **2953** **3014** **3024**

AM1

15.9 29 40.2 54.1 59.2 73 78.3 123 201 203 273 307
358 403 477 556 578 626 669 678 684 717 764 781
954 976 1013 1059 1076 1102 1176 1191 1242 1261 1273 1304
1311 1323 1348 1357 1371 1375 1424 1462 1717 1723 1779 2162
2168 3030 3039 3045 3085 3092

AM1 UHF

15.9 28.9 39.4 53.9 58.9 73 78 123 201 203 273 307
358 403 477 556 578 626 669 678 684 717 764 781
954 976 1013 1059 1076 1102 1176 1192 1241 1261 1273 1304
1311 1323 1348 1357 1371 1375 1424 1462 1717 1723 1779 2162
2168 3030 3039 3045 3085 3092

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia=**1130.230 874** Ib=**2164.117 177** Ic=**2600.035 548** σ(external)=**2**
PM3 UHF Ia=1131.482 395 Ib=2165.539 807 Ic=2602.579 955
AM1 Ia=970.193 760 Ib=2126.474 567 Ic=2424.746 670
AM1 UHF Ia=970.349 036 Ib=2126.249 488 Ic=2424.619 088
(Ir(NO_2)=**59.6** ROSYM=**2** V(2)=**9.1** kcal/mol [methyl nitrate])×**3**
PM3 heat of formation=17.97 kcal/mol
PM3 UHF heat of formation=17.96 kcal/mol spin=0 $S^2=0$
PM3[b] $\Delta H_f(298)=-76.6$ kcal/mol
AM1 heat of formation=18.22 kcal/mol
AM1 UHF heat of formation=18.22 kcal/mol spin=0 $S^2=0$
AM1[b] $\Delta H_f(298)=-71.4$ kcal/mol
NIST 94 $\Delta H_f(298)=-87.5$ kcal/mol[c]
Cox and Pilcher[d] $\Delta H_f(298)=-88.6$ kcal/mol
NIST 1997 $\Delta H_f(298)=-$**66.70**$\pm$**0.65** kcal/mol[e]
ΔH_f liquid $(298)=-88.43$ kcal/mol[f,e]
PM3 ionization potential=11.834 eV
PM3 UHF ionization potential=11.833 eV
AM1 ionization potential=12.517 eV
AM1 UHF ionization potential=12.518 eV
PM3 zero point energy 72.615 kcal/mol
PM3 UHF zero point energy 72.618 kcal/mol
AM1 zero point energy 83.207 kcal/mol
AM1 UHF zero point energy 83.203 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 52.
[c]See Ref. 51.
[d]See Ref. 12.
[e]See Ref. 38.
[f]See Ref. 1.

TABLE 37. Ideal gas thermodynamic properties for nitroglycerin $C_3H_5O_3(ONO_2)_3$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−43.458	-------	-------	−322.531	−246.135	-------
100	119.652	−35.832	359.569	717.890	−314.905	−263.598	89.9099
200	183.226	−20.557	462.915	565.700	−299.630	−273.505	19.9539
298.15	234.240	0.000	545.865	545.865	−279.073	−279.073	−3.7928
300	235.121	0.434	547.317	545.870	−278.639	−279.147	−4.0938
400	278.317	26.180	621.084	555.635	−252.893	−281.480	−16.3013
500	312.944	55.810	687.058	575.438	−223.263	−281.313	−23.6554
600	340.321	88.526	746.632	599.088	−190.546	−279.346	−28.5392
700	362.096	123.688	800.790	624.093	−155.385	−276.059	−31.9950
800	379.571	160.803	850.324	649.321	−118.270	−271.775	−34.5516
900	393.676	199.490	895.875	674.219	−79.583	−266.718	−36.5061
1000	405.097	239.449	937.965	698.516	−39.624	−261.085	−38.0386
1100	414.358	280.438	977.025	722.081	1.365	−255.022	−39.2643
1200	421.879	322.262	1013.412	744.860	43.190	−248.643	−40.2614
1300	427.997	364.767	1047.430	766.841	85.694	−242.059	−41.0833
1400	432.985	407.824	1079.337	788.034	128.751	−235.350	−41.7684
1500	437.063	451.333	1109.354	808.465	172.261	−228.576	−42.3460
1600	440.407	495.212	1137.672	828.164	216.140	−221.800	−42.8362
1700	443.159	539.395	1164.456	847.165	260.322	−215.057	−43.2559
1800	445.432	583.828	1189.853	865.504	304.755	−208.386	−43.6172
1900	447.316	628.469	1213.988	883.215	349.396	−201.812	−43.9307
2000	448.884	673.281	1236.974	900.333	394.208	−195.352	−44.2033
2100	450.193	718.237	1258.908	916.890	439.164	−189.026	−44.4425
2200	451.290	763.313	1279.877	932.916	484.240	−182.846	−44.6528
2300	452.213	808.489	1299.958	948.441	529.416	−176.815	−44.8384
2400	452.991	853.750	1319.221	963.492	574.677	−170.944	−45.0031
2500	453.650	899.083	1337.727	978.093	620.010	−165.247	−45.1494
2600	454.210	944.477	1355.530	992.270	665.404	−159.706	−45.2800
2700	454.686	989.922	1372.682	1006.044	710.850	−154.344	−45.3968
2800	455.093	1035.412	1389.225	1019.435	756.339	−149.146	−45.5019
2900	455.442	1080.939	1405.201	1032.463	801.866	−144.119	−45.5960
3000	455.740	1126.499	1420.646	1045.147	847.426	−139.265	−45.6809
3100	455.997	1172.086	1435.594	1057.502	893.013	−134.566	−45.7583
3200	456.219	1217.697	1450.075	1069.545	938.624	−130.042	−45.8276
3300	456.410	1263.329	1464.117	1081.290	984.256	−125.682	−45.8908
3400	456.575	1308.978	1477.745	1092.751	1029.905	−121.478	−45.9484
3500	456.718	1354.643	1490.982	1103.941	1075.570	−117.435	−46.0009
3600	456.842	1400.321	1503.850	1114.872	1121.248	−113.548	−46.0486
3700	456.950	1446.011	1516.368	1125.554	1166.938	−109.814	−46.0926
3800	457.044	1491.711	1528.556	1136.000	1212.638	−106.232	−46.1327
3900	457.125	1537.419	1540.428	1146.218	1258.346	−102.799	−46.1695
4000	457.195	1583.135	1552.003	1156.219	1304.062	−99.521	−46.2033
4100	457.257	1628.858	1563.293	1166.011	1349.785	−96.379	−46.2348
4200	457.310	1674.586	1574.312	1175.601	1395.514	−93.385	−46.2634
4300	457.357	1720.320	1585.074	1184.999	1441.247	−90.534	−46.2900
4400	457.397	1766.058	1595.589	1194.212	1486.985	−87.832	−46.3144
4500	457.432	1811.799	1605.868	1203.246	1532.726	−85.259	−46.3373
4600	457.463	1857.544	1615.922	1212.108	1578.471	−82.824	−46.3585
4700	457.489	1903.292	1625.761	1220.805	1624.219	−80.515	−46.3783
4800	457.512	1949.042	1635.393	1229.342	1669.969	−78.336	−46.3967
4900	457.531	1994.794	1644.826	1237.726	1715.721	−76.289	−46.4140
5000	457.548	2040.548	1654.070	1245.960	1761.475	−74.390	−46.4297
5100	457.562	2086.303	1663.131	1254.052	1807.230	−72.589	−46.4452
5200	457.575	2132.060	1672.016	1262.004	1852.988	−70.923	−46.4592
5300	457.585	2177.818	1680.732	1269.823	1898.745	−69.375	−46.4725
5400	457.593	2223.577	1689.285	1277.512	1944.504	−67.951	−46.4851
5500	457.601	2269.337	1697.682	1285.075	1990.264	−66.638	−46.4970
5600	457.606	2315.097	1705.927	1292.517	2036.024	−65.435	−46.5082
5700	457.611	2360.858	1714.027	1299.841	2081.785	−64.344	−46.5187
5800	457.615	2406.619	1721.985	1307.051	2127.546	−63.354	−46.5288
5900	457.617	2452.381	1729.808	1314.150	2173.308	−62.465	−46.5384
6000	457.619	2498.143	1737.499	1321.142	2219.070	−61.673	−46.5476

TABLE 38. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for N-nitroazetidine (cyclotrimethylene Nitramine) (molecular wt.=102.092920)[a]

Melius hf/6-31g*[b]

128	**137**	**242**	**247**	**475**	**593**	**722**	**806**	**823**	**827**	**900**	**902**
946	**1113**	**1131**	**1148**	**1182**	**1188**	**1213**	**1263**	**1284**	**1318**	**1431**	**1464**
1481	**1507**	**1641**	**2911**	**2914**	**2925**	**2964**	**2973**	**2982**			

Principal moments of inertia in units of 10^{-40} g cm^2

Melius Ia=**177.086** Ib=**361.404** Ic=**475.02** σ (external)=**2.0**
Ir=**59.6** [nitropropene] ROSYM=**2** V(2)=1.23 kcal/mol
Habibollahzadeh *et al.*[c] V(2)=**12.5**–15.2 kcal/mol
Melius $\Delta H_f(0)$=33.9 $\Delta H_f(298)$=**27.28**±**5.10** kcal/mol spin=0.0 S^2=0.0
Melius zero-point vibration energy 62.58515 kcal/mol
R(CN)=1.4642[b]
R(CC)=1.5447
R(NN)=1.3433
R(NO)=1.1948
R(CH)=1.0793–1.0827

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 35.
[c]See Ref. 20.

TABLE 39. Ideal gas thermodynamic properties for N-nitroazetidine $(CH_2)_3N–NO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−18.840	-------	-------	95.283	141.198	-------
100	52.614	−14.789	251.963	399.854	99.334	130.264	−88.2116
200	73.600	−8.502	294.725	337.236	105.621	121.666	−55.0821
298.15	100.656	0.000	328.954	328.954	114.123	114.123	−44.9113
300	101.211	0.187	329.578	328.955	114.310	113.994	−44.7879
400	130.969	11.808	362.805	333.285	125.931	107.942	−39.9520
500	157.440	26.266	394.956	342.425	140.389	103.651	−37.1884
600	179.426	43.145	425.670	353.762	157.268	100.869	−35.4083
700	197.484	62.020	454.730	366.130	176.143	99.314	−34.1640
800	212.409	82.538	482.105	378.933	196.660	98.762	−33.2410
900	224.842	104.419	507.863	391.842	218.542	99.035	−32.5241
1000	235.256	127.439	532.108	404.669	241.562	99.968	−31.9469
1100	244.009	151.415	554.953	417.303	265.537	101.435	−31.4689
1200	251.384	176.195	576.509	429.680	290.318	103.330	−31.0640
1300	257.610	201.653	596.884	441.766	315.776	105.553	−30.7146
1400	262.878	227.685	616.173	453.541	341.808	108.023	−30.4080
1500	267.347	254.202	634.466	464.998	368.325	110.686	−30.1365
1600	271.148	281.132	651.845	476.137	395.255	113.482	−29.8927
1700	274.391	308.413	668.383	486.963	422.536	116.369	−29.6720
1800	277.169	335.995	684.147	497.484	450.117	119.312	−29.4709
1900	279.556	363.834	699.199	507.707	477.957	122.285	−29.2865
2000	281.614	391.895	713.592	517.644	506.018	125.264	−29.1162
2100	283.397	420.148	727.376	527.306	534.270	128.232	−28.9587
2200	284.946	448.566	740.596	536.702	562.689	131.171	−28.8121
2300	286.298	477.130	753.293	545.845	591.253	134.077	−28.6752
2400	287.482	505.820	765.503	554.745	619.943	136.933	−28.5470
2500	288.523	534.622	777.260	563.412	648.745	139.728	−28.4265
2600	289.441	563.521	788.595	571.856	677.644	142.470	−28.3132
2700	290.254	592.507	799.534	580.087	706.629	145.139	−28.2063
2800	290.976	621.569	810.103	588.114	735.692	147.742	−28.1052
2900	291.620	650.699	820.325	595.946	764.822	150.270	−28.0092
3000	292.196	679.890	830.221	603.591	794.013	152.715	−27.9180
3100	292.712	709.136	839.811	611.057	823.259	155.095	−27.8319
3200	293.177	738.431	849.112	618.352	852.554	157.387	−27.7495
3300	293.596	767.770	858.140	625.482	881.893	159.597	−27.6711
3400	293.976	797.149	866.910	632.455	911.272	161.729	−27.5963
3500	294.320	826.564	875.437	639.276	940.687	163.773	−27.5250
3600	294.633	856.012	883.733	645.951	970.135	165.735	−27.4565
3700	294.918	885.490	891.809	652.488	999.613	167.612	−27.3913
3800	295.179	914.995	899.678	658.890	1029.118	169.402	−27.3286
3900	295.418	944.525	907.348	665.162	1058.648	171.110	−27.2687
4000	295.638	974.078	914.830	671.311	1088.201	172.721	−27.2110
4100	295.839	1003.652	922.133	677.340	1117.775	174.257	−27.1560
4200	296.025	1033.245	929.264	683.253	1147.368	175.701	−27.1028
4300	296.197	1062.857	936.232	689.056	1176.979	177.056	−27.0517
4400	296.356	1092.484	943.043	694.751	1206.607	178.314	−27.0024
4500	296.503	1122.127	949.705	700.343	1236.250	179.495	−26.9553
4600	296.640	1151.785	956.223	705.835	1265.908	180.589	−26.9099
4700	296.767	1181.455	962.604	711.231	1295.578	181.602	−26.8662
4800	296.886	1211.138	968.853	716.533	1325.261	182.530	−26.8240
4900	296.996	1240.832	974.976	721.745	1354.955	183.376	−26.7836
5000	297.100	1270.537	980.977	726.870	1384.660	184.111	−26.7441
5100	297.196	1300.252	986.862	731.910	1414.375	184.796	−26.7067
5200	297.287	1329.976	992.633	736.869	1444.099	185.385	−26.6701
5300	297.371	1359.709	998.297	741.748	1473.832	185.892	−26.6350
5400	297.451	1389.450	1003.856	746.551	1503.573	186.321	−26.6010
5500	297.526	1419.199	1009.315	751.279	1533.322	186.673	−26.5683
5600	297.597	1448.955	1014.677	755.935	1563.078	186.949	−26.5365
5700	297.663	1478.718	1019.944	760.520	1592.841	187.152	−26.5060
5800	297.726	1508.488	1025.122	765.038	1622.611	187.285	−26.4764
5900	297.785	1538.263	1030.212	769.489	1652.386	187.348	−26.4477
6000	297.841	1568.045	1035.217	773.877	1682.168	187.347	−26.4201

TABLE 40. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for 1,3,3-trinitroazetidine $C_3H_4N(NO_2)_3$ (molecular wt. = 192.088120)[a]

Yu, Zhang and Bauer[b]

80	**162**	**4801**	**480**	**564**	**564**	**564**	**601**	**626**	**626**	**626**	**662**
662	**712**	**760**	**760**	**816**	**843**	**843**	**865**	**865**	**906**	**1057**	**1057**
1085	**1113**	**1172**	**1183**	**1200**	**1216**	**1280**	**1325**	**1340**	**1365**	**1380**	**1403**
1428	**1510**	**1538**	**1589**	**1589**	**2900**	**2973**	**3021**	**3036**			

Principal moments of inertia in units of 10^{-40} g cm^2

Bauer *et al.* Ia = **605.9091** Ib = **1473.316** Ic = **1696.545**
Ir(NO_2) = **59.6** ROSYM = **2** V(2) = **12.5** (nitroazetidine)
Politzer[c] $\Delta H_f(298)$ = **30.7** kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 60.
[c]See Ref. 47.

TABLE 41. Ideal gas thermodynamic properties for 1,3,3-trinitroazetidine $C_3H_4N(NO_2)_3$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−20.706	-------	-------	107.743	171.220	-------
100	46.685	−16.876	272.994	441.752	111.573	154.361	−120.8904
200	82.869	−10.664	314.626	367.947	117.785	139.648	−82.1159
298.15	134.987	0.000	357.315	357.315	128.449	128.449	−70.5535
300	135.974	0.251	358.153	357.317	128.699	128.273	−70.4144
400	185.832	16.406	404.285	363.269	144.855	120.801	−64.9918
500	226.630	37.109	450.312	376.094	165.558	116.621	−61.8937
600	258.545	61.435	494.575	392.184	189.884	114.910	−59.8800
700	283.384	88.582	536.374	409.828	217.031	115.013	−58.4519
800	302.908	117.935	575.540	428.121	246.384	116.464	−57.3737
900	318.455	149.032	612.149	446.558	277.481	118.939	−56.5208
1000	330.981	181.526	646.373	464.847	309.974	122.183	−55.8218
1100	341.174	215.150	678.413	482.822	343.599	126.019	−55.2327
1200	349.533	249.699	708.469	500.387	378.148	130.312	−54.7261
1300	356.437	285.009	736.728	517.491	413.457	134.942	−54.2824
1400	362.172	320.948	763.359	534.111	449.397	139.820	−53.8880
1500	366.963	357.412	788.515	550.240	485.860	144.884	−53.5345
1600	370.986	394.315	812.330	565.883	522.764	150.065	−53.2137
1700	374.381	431.588	834.926	581.051	560.037	155.323	−52.9206
1800	377.261	469.174	856.409	595.756	597.623	160.618	−52.6510
1900	379.715	507.026	876.874	610.018	635.475	165.920	−52.4018
2000	381.817	545.105	896.405	623.853	673.554	171.206	−52.1698
2100	383.624	583.380	915.079	637.279	711.828	176.456	−51.9538
2200	385.186	621.822	932.962	650.316	750.271	181.652	−51.7514
2300	386.542	660.410	950.115	662.980	788.859	186.787	−51.5613
2400	387.723	699.125	966.592	675.290	827.573	191.846	−51.3822
2500	388.757	737.950	982.441	687.261	866.398	196.815	−51.2131
2600	389.665	776.872	997.706	698.909	905.321	201.704	−51.0530
2700	390.466	815.879	1012.427	710.250	944.328	206.492	−50.9011
2800	391.175	854.962	1026.641	721.297	983.411	211.185	−50.7570
2900	391.805	894.112	1040.379	732.065	1022.560	215.777	−50.6195
3000	392.367	933.321	1053.671	742.564	1061.770	220.262	−50.4884
3100	392.869	972.583	1066.545	752.809	1101.032	224.654	−50.3639
3200	393.320	1011.893	1079.026	762.809	1140.342	228.933	−50.2443
3300	393.725	1051.245	1091.135	772.576	1179.694	233.107	−50.1299
3400	394.091	1090.636	1102.894	782.119	1219.085	237.179	−50.0205
3500	394.422	1130.062	1114.323	791.448	1258.511	241.143	−49.9156
3600	394.722	1169.520	1125.439	800.572	1297.969	245.003	−49.8147
3700	394.996	1209.006	1136.257	809.499	1337.455	248.759	−49.7181
3800	395.245	1248.518	1146.794	818.237	1376.967	252.410	−49.6249
3900	395.473	1288.054	1157.064	826.794	1416.503	255.960	−49.5354
4000	395.681	1327.612	1167.079	835.176	1456.061	259.397	−49.4489
4100	395.873	1367.190	1176.852	843.391	1495.639	262.741	−49.3660
4200	396.049	1406.786	1186.394	851.445	1535.235	265.979	−49.2858
4300	396.212	1446.399	1195.715	859.343	1574.848	269.113	−49.2083
4400	396.362	1486.028	1204.825	867.092	1614.477	272.137	−49.1335
4500	396.501	1525.671	1213.734	874.696	1654.120	275.069	−49.0613
4600	396.630	1565.328	1222.451	882.162	1693.777	277.901	−48.9915
4700	396.749	1604.997	1230.982	889.493	1733.446	280.640	−48.9241
4800	396.860	1644.678	1239.336	896.695	1773.126	283.282	−48.8588
4900	396.964	1684.369	1247.520	903.771	1812.818	285.828	−48.7958
5000	397.061	1724.070	1255.541	910.727	1852.519	288.254	−48.7343
5100	397.151	1763.781	1263.404	917.565	1892.230	290.616	−48.6754
5200	397.236	1803.500	1271.117	924.290	1931.949	292.868	−48.6178
5300	397.315	1843.228	1278.685	930.906	1971.676	295.031	−48.5622
5400	397.389	1882.963	1286.112	937.415	2011.412	297.100	−48.5081
5500	397.459	1922.705	1293.404	943.822	2051.154	299.081	−48.4558
5600	397.524	1962.455	1300.567	950.128	2090.903	300.977	−48.4049
5700	397.586	2002.210	1307.603	956.338	2130.659	302.782	−48.3554
5800	397.644	2041.972	1314.518	962.454	2170.420	304.509	−48.3074
5900	397.699	2081.739	1321.316	968.479	2210.188	306.152	−48.2608
6000	397.751	2121.511	1328.001	974.416	2249.960	307.718	−48.2156

TABLE 42. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for RDX $C_3H_6(N-NO_2)_3$ 1,3,5-trinitrotriazine (molecular wt.=222.117480)[a]

PM3												
	25.7	34	47.7	49.5	62	81	105	132	173	193	202	234
	235	289	315	326	363	391	453	464	491	542	581	622
	661	663	677	702	752	855	888	929	954	973	998	1048
	1108	1139	1160	1191	1233	1235	1347	1362	1372	1382	1506	1528
	1809	2011	2022	2900	2940	2950	3032	3045	3118			
AM1												
	25.2	44.3	65.1	66.7	73.9	92.3	213	235	260	335	373	381
	401	474	498	572	629	646	675	708	726	737	816	907
	988	996	1007	1032	1044	1056	1095	1122	1150	1178	1253	1269
	1314	1345	1350	1354	1373	1379	1383	1391	1426	1431	1710	1719
	1725	2073	2076	2910	2911	2921	2974	2978	2991			
GAUSSIAN 94[b]												
	9.8	16.1	27.9	**79.0**	**90.2**	**91.3**	**152**	**154**	**266**	**266**	**273**	**302**
	303	**307**	**320**	**501**	**501**	**528**	**554**	**554**	**581**	**583**	**590**	**638**
	702	**702**	**762**	**806**	**807**	**818**	**907**	**907**	**1012**	**1012**	**1027**	**1042**
	1081	**1097**	**1104**	**1104**	**1180**	**1181**	**1207**	**1218**	**1218**	**1280**	**1295**	**1295**
	1332	**1332**	**1337**	**2684**	**2684**	**2688**	**2767**	**2767**	**2770**			

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia=890.467 328 Ib=2289.066 106 Ic=2706.848 559 σ (ext)=**6**
AM1 Ia=894.849 465 Ib=1629.167 934 Ic=2207.576 954
GAUSSIAN 94 Ia=**1378.906** Ib=**1378.906** Ic=**2455.315**
3×(Ir=**59.6** ROSYM=**2** V(2)=**16.7** kcal/mol[c])
PM3 heat of formation=141.66 kcal/mol
AM1 heat of formation=198.31 kcal/mol
Rosen and Dickinson[d] $\Delta H_f(298)$=45.76 kcal/mol
NIST 1997 $\Delta H_f(298)$=**45.89** kcal/mol[e]
ΔH_f solid (298)=18.90 kcal/mol C_p solid (298)=59.49 cal/mol[c]
PM3 ionization potential=10.997 eV
AM1 ionization potential=11.623 eV
PM3 zero point energy 79.967 kcal/mol
AM1 zero point energy 91.360 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]Calculated by Wu and Fried 1997, private communication[58] scaled by 0.9
[c]See Ref. 20.
[d]See Ref. 49.
[e]See Ref. 46.

TABLE 43. Ideal gas thermodynamic properties for hexogen (RDX) $C_3H_6(N-NO_2)_3$ 1,3,5-trinitrotriazine

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−39.331	-------	-------	152.669	233.285	-------
100	101.186	−33.222	311.893	644.111	158.778	212.803	−162.9938
200	169.009	−19.637	403.371	501.555	172.363	199.859	−108.8440
298.15	230.174	0.000	482.441	482.441	192.000	192.000	−91.9856
300	231.261	0.427	483.868	482.446	192.427	191.893	−91.7779
400	284.446	26.308	557.955	492.186	218.308	188.324	−83.5103
500	326.076	56.926	626.105	512.254	248.926	188.196	−78.5998
600	357.937	91.197	688.500	536.506	283.197	190.519	−75.3068
700	382.601	128.274	745.606	562.358	320.274	194.571	−72.9149
800	402.076	167.545	798.016	588.585	359.545	199.877	−71.0774
900	417.724	208.562	846.310	614.574	400.562	206.123	−69.6063
1000	430.466	250.993	891.003	640.010	442.993	213.060	−68.3909
1100	440.935	294.580	932.538	664.738	486.580	220.521	−67.3619
1200	449.588	339.119	971.287	688.687	531.119	228.379	−66.4745
1300	456.765	384.448	1007.566	711.836	576.448	236.513	−65.6966
1400	462.728	430.432	1041.641	734.189	622.432	244.838	−65.0059
1500	467.683	476.960	1073.740	755.766	668.960	253.290	−64.3871
1600	471.799	523.941	1104.059	776.596	715.941	261.798	−63.8268
1700	475.212	571.297	1132.767	796.710	763.297	270.321	−63.3161
1800	478.036	618.964	1160.012	816.143	810.964	278.814	−62.8475
1900	480.367	666.888	1185.922	834.929	858.888	287.245	−62.4154
2000	482.283	715.023	1210.612	853.101	907.023	295.589	−62.0146
2100	483.851	763.332	1234.182	870.691	955.332	303.824	−61.6421
2200	485.128	811.784	1256.722	887.729	1003.784	311.930	−61.2941
2300	486.160	860.350	1278.310	904.245	1052.350	319.900	−60.9680
2400	486.989	909.009	1299.019	920.265	1101.009	327.717	−60.6616
2500	487.647	957.742	1318.913	935.816	1149.742	335.367	−60.3730
2600	488.162	1006.533	1338.049	950.921	1198.533	342.864	−60.1006
2700	488.558	1055.370	1356.480	965.602	1247.370	350.180	−59.8428
2800	488.856	1104.242	1374.254	979.881	1296.242	357.330	−59.5986
2900	489.071	1153.139	1391.412	993.778	1345.139	364.305	−59.3662
3000	489.218	1202.054	1407.995	1007.310	1394.054	371.099	−59.1452
3100	489.308	1250.980	1424.038	1020.496	1442.980	377.731	−58.9355
3200	489.352	1299.914	1439.574	1033.351	1491.914	384.181	−58.7346
3300	489.358	1348.850	1454.632	1045.890	1540.850	390.457	−58.5429
3400	489.333	1397.784	1469.240	1058.127	1589.784	396.566	−58.3598
3500	489.282	1446.715	1483.424	1070.077	1638.715	402.504	−58.1846
3600	489.211	1495.640	1497.207	1081.751	1687.640	408.273	−58.0163
3700	489.123	1544.557	1510.610	1093.162	1736.557	413.878	−57.8554
3800	489.022	1593.464	1523.652	1104.320	1785.464	419.318	−57.7005
3900	488.911	1642.361	1536.354	1115.235	1834.361	424.601	−57.5518
4000	488.793	1691.246	1548.730	1125.919	1883.246	429.713	−57.4087
4100	488.668	1740.119	1560.798	1136.379	1932.119	434.677	−57.2713
4200	488.539	1788.980	1572.572	1146.625	1980.980	439.482	−57.1386
4300	488.408	1837.827	1584.066	1156.665	2029.827	444.133	−57.0108
4400	488.275	1886.661	1595.293	1166.507	2078.661	448.621	−56.8873
4500	488.141	1935.482	1606.265	1176.158	2127.482	452.969	−56.7685
4600	488.008	1984.290	1616.992	1185.625	2176.290	457.169	−56.6537
4700	487.875	2033.084	1627.486	1194.915	2225.084	461.230	−56.5428
4800	487.743	2081.865	1637.756	1204.034	2273.865	465.148	−56.4355
4900	487.613	2130.632	1647.811	1212.988	2322.632	468.928	−56.3319
5000	487.485	2179.387	1657.661	1221.784	2371.387	472.544	−56.2313
5100	487.360	2228.130	1667.313	1230.425	2420.130	476.055	−56.1346
5200	487.237	2276.860	1676.776	1238.918	2468.860	479.417	−56.0403
5300	487.116	2325.577	1686.056	1247.268	2517.577	482.651	−55.9492
5400	486.998	2374.283	1695.160	1255.478	2566.283	485.754	−55.8608
5500	486.883	2422.977	1704.095	1263.554	2614.977	488.732	−55.7752
5600	486.771	2471.660	1712.867	1271.499	2663.660	491.591	−55.6921
5700	486.662	2520.331	1721.481	1279.318	2712.331	494.326	−55.6114
5800	486.556	2568.992	1729.944	1287.015	2760.992	496.951	−55.5330
5900	486.452	2617.643	1738.261	1294.593	2809.643	499.460	−55.4569
6000	486.352	2666.283	1746.436	1302.055	2858.283	501.864	−55.3831

TABLE 44. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for N-nitropropane $CH_3CH_2CH_2NO_2$ (molecular wt. = 89.094120)[a]

PM3												
	24.8	93.4	176	**268**	**417**	**474**	597	691	818	906	919	962
	1052	**1068**	**1134**	**1140**	**1155**	1278	1330	1377	**1392**	**1403**	**1415**	1426
	1612	**1907**	2916	2956	2992	**3031**	**3080**	**3088**	**3187**			
PM3 UHF												
	25.1	88.4	167.8	268	417	473	597	691	817	906	919	962
	1052	1068	1135	1141	1155	1278	1330	1377	1392	1403	1415	1426
	1612	1908	2916	2956	2992	3031	3080	3088	3187			
AM1 UHF												
	24.7	79.4	166.8	264	420	498	656	732	855	954	1003	1047
	1139	1148	1203	1225	1256	1352	1371	1389	1393	1394	1407	1441
	1801	2069	3002	3016	3056	3059	3064	3088	3157			
IR spectrum[b]												
							569	**601**	**619**	**727**	**796**	**885**
						1225	**1232**	**1377**				**1447**
	1567		**2280**	**2905**	**2981**							

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia = 132.818 245 Ib = 359.744 519 Ic = 380.242 873
PM3 UHF Ia = 132.818 245 Ib = 359.744 519 Ic = 380.242 873
AM1 UHF Ia = **130.940 160** Ib = **354.575 741** Ic = **373.826 884**
Table 3 Ir(NO_2) = **59.6** ROSYM = **2** V(2) = **0.08** kcal/mol [nitroethane]
Ir(CH_3) = **5.166** ROSYM = **3** V(3) = **3.5** kcal/mol [nitroethane]
Ir(C_2H_5) = **21.04** ROSYM = **2** $V(2)$ = **9.0** kcal/mol[c]
PM3 heat of formation = −26.21 kcal/mol
PM3 UHF heat of formation = −26.21 kcal/mol
AM1 UHF heat of formation = −23.58 kcal/mol spin = 0 $S^2 = 0$
NIST 94[d] $\Delta H_f(298) = -29.5$ kcal/mol
Pedley and Rylance[e] $\Delta H_f(298) = -$ **29.7** $\pm$ **0.1** kcal/mol IP = 10.81 $\pm$ 0.03 eV
Stull *et al.*[f] $\Delta H_f(298) = -29.8$ kcal/mol
NIST 97[b] ΔH_f liquid $(298) = -39.91$ kcal/mol
PM3 zero point energy 66.153 kcal/mol
PM3 UHF zero point energy 66.118 kcal/mol
AM1 UHF zero point energy 68.291 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 1.
[c]See Ref. 10.
[d]See Ref. 51.
[e]See Ref. 44.
[f]See Ref. 55.

TABLE 45. Ideal gas thermodynamic properties for nitropropane $C_3H_7NO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−19.344	-------	-------	−143.609	−97.795	-------
100	50.150	−15.140	271.840	423.238	−139.405	−108.623	39.1488
200	76.293	−8.846	314.430	358.659	−133.111	−117.106	9.8885
298.15	104.085	0.000	350.046	350.046	−124.265	−124.265	−0.4548
300	104.610	0.193	350.692	350.048	−124.072	−124.387	−0.5890
400	131.802	12.037	384.578	354.485	−112.227	−130.210	−6.1238
500	155.356	26.429	416.595	363.736	−97.835	−134.558	−9.5800
600	174.995	42.977	446.711	375.082	−81.287	−137.645	−11.9496
700	191.332	61.318	474.951	387.354	−62.947	−139.681	−13.6743
800	205.012	81.155	501.420	399.976	−43.109	−140.836	−14.9830
900	216.528	102.249	526.251	412.641	−22.016	−141.249	−16.0067
1000	226.253	124.401	549.582	425.181	0.137	−141.066	−16.8261
1100	234.480	147.449	571.543	437.498	23.185	−140.396	−17.4945
1200	241.451	171.255	592.253	449.540	46.991	−139.341	−18.0481
1300	247.372	195.705	611.819	461.277	71.440	−137.991	−18.5127
1400	252.413	220.701	630.341	472.698	96.436	−136.421	−18.9063
1500	256.720	246.163	647.906	483.798	121.898	−134.683	−19.2439
1600	260.411	272.024	664.595	494.580	147.759	−132.832	−19.5351
1700	263.588	298.228	680.481	505.052	173.963	−130.907	−19.7883
1800	266.333	324.727	695.626	515.222	200.463	−128.938	−20.0101
1900	268.713	351.482	710.092	525.101	227.218	−126.950	−20.2057
2000	270.787	378.460	723.929	534.699	254.195	−124.965	−20.3786
2100	272.599	405.631	737.185	544.028	281.366	−122.998	−20.5330
2200	274.189	432.972	749.904	553.099	308.707	−121.067	−20.6709
2300	275.590	460.463	762.124	561.923	336.198	−119.174	−20.7949
2400	276.827	488.085	773.879	570.511	363.820	−117.333	−20.9069
2500	277.924	515.823	785.203	578.873	391.559	−115.558	−21.0081
2600	278.899	543.665	796.123	587.020	419.401	−113.838	−21.1003
2700	279.768	571.600	806.665	594.961	447.335	−112.194	−21.1845
2800	280.545	599.616	816.854	602.705	475.351	−110.619	−21.2616
2900	281.240	627.706	826.711	610.260	503.441	−109.122	−21.3321
3000	281.865	655.862	836.256	617.635	531.597	−107.712	−21.3969
3100	282.426	684.077	845.508	624.838	559.812	−106.369	−21.4574
3200	282.932	712.345	854.482	631.874	588.080	−105.118	−21.5129
3300	283.389	740.662	863.196	638.753	616.397	−103.951	−21.5646
3400	283.801	769.021	871.662	645.479	644.757	−102.868	−21.6128
3500	284.175	797.421	879.894	652.060	673.156	−101.877	−21.6579
3600	284.513	825.855	887.904	658.500	701.590	−100.971	−21.6997
3700	284.820	854.322	895.704	664.806	730.057	−100.157	−21.7393
3800	285.099	882.818	903.303	670.983	758.554	−99.435	−21.7762
3900	285.352	911.341	910.712	677.035	787.076	−98.801	−21.8113
4000	285.582	939.888	917.940	682.968	815.623	−98.269	−21.8441
4100	285.792	968.457	924.994	688.785	844.192	−97.818	−21.8756
4200	285.982	997.046	931.883	694.492	872.781	−97.466	−21.9051
4300	286.156	1025.653	938.615	700.091	901.388	−97.210	−21.9331
4400	286.314	1054.276	945.195	705.587	930.012	−97.058	−21.9598
4500	286.458	1082.915	951.631	710.983	958.650	−96.990	−21.9855
4600	286.590	1111.568	957.929	716.284	987.303	−97.016	−22.0100
4700	286.710	1140.233	964.093	721.491	1015.968	−97.130	−22.0334
4800	286.819	1168.909	970.131	726.608	1044.644	−97.336	−22.0560
4900	286.918	1197.596	976.046	731.638	1073.331	−97.632	−22.0778
5000	287.009	1226.293	981.843	736.585	1102.028	−98.046	−22.0984
5100	287.092	1254.998	987.528	741.450	1130.733	−98.517	−22.1188
5200	287.167	1283.711	993.103	746.236	1159.446	−99.090	−22.1382
5300	287.235	1312.431	998.574	750.945	1188.166	−99.752	−22.1570
5400	287.298	1341.158	1003.943	755.581	1216.893	−100.498	−22.1754
5500	287.354	1369.890	1009.216	760.145	1245.625	−101.328	−22.1931
5600	287.405	1398.628	1014.394	764.639	1274.363	−102.239	−22.2103
5700	287.452	1427.371	1019.481	769.065	1303.106	−103.228	−22.2272
5800	287.494	1456.118	1024.481	773.426	1331.854	−104.292	−22.2436
5900	287.532	1484.870	1029.396	777.723	1360.605	−105.429	−22.2595
6000	287.566	1513.625	1034.229	781.958	1389.360	−106.634	−22.2752

TABLE 46. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for N-propylnitrate $C_3H_7ONO_2$ (molecular wt. = 105.093520)[a]

PM3												
	47	58.7	116	184	243	301	359	461	541	609	641	816
	917	941	1025	1106	1109	1129	1155	1161	1300	1341	1359	1401
	1403	1415	1430	1537	2099	2948	2955	3027	3048	3077	3088	3182
PM3 UHF												
	46.1	58.3	114	**179**	**244**	**301**	**359**	**461**	**541**	**609**	**641**	**815**
	917	**941**	**1025**	**1105**	**1108**	**1129**	**1155**	**1161**	**1300**	**1341**	**1359**	**1401**
	1403	**1415**	**1430**	**1537**	**2099**	**2948**	**2955**	**3027**	**3049**	**3077**	**3088**	**3182**
AM1												
	51.2	70.8	122	163	275	383	487	651	682	733	841	946
	1020	1069	1133	1191	1216	1237	1267	1318	1368	1389	1393	1401
	1412	1426	1438	1733	2148	3018	3045	3063	3064	3090	3096	3157
AM1 UHF												
	51.2	70.8	122	163	275	383	487	651	682	733	841	946
	1020	1069	1133	1191	1216	1237	1267	1318	1368	1389	1393	1401
	1412	1426	1438	1733	2148	3018	3045	3063	3064	3090	3096	3157

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia = 158.717 321 Ib = 549.581 214 Ic = 588.811 793
PM3 UHF Ia = 158.717 321 Ib = 549.581 214 Ic = 588.811 793
AM1 Ia = 152.364 460 Ib = 516.552 959 Ic = 551.178 261
AM1 UHF Ia = **152.364 435** Ib = 516.552 716 Ic = **551.180 418** spin = 0 $S^2 = 0$
Melius Ir(NO_2) = **59.6** ROSYM = **2** V(2) = **9.1** kcal/mol
Ir(CH_3) = **5.1666** ROSYM = **3** V(3) = **3.5** kcal/mol
Chao[b] Ir(C_2H_5) = **30.27** ROSYM = **2** V(2) = **9** kcal/mol
PM3 heat of formation = −42.68 kcal/mol
PM3 UHF heat of formation = −42.68 kcal/mol
AM1 heat of formation = −44.38 kcal/mol
AM1 UHF heat of formation = −44.38 kcal/mol
Stull *et al.*[c] $\Delta H_f(298) = -$ **41.60** kcal/mol
NIST 94[d] $\Delta H_f(298) = -42.60$ kcal/mol
Pedley and Rylance[e] $\Delta H_f(298) = -$ **41.60** ± **0.3** kcal/mol
Pedley, Naylor and Kirby[f] ΔH_f solid (298) = −51.27 kcal/mol
AM1 ionization potential = 12.12 eV
AM1 UHF ionization potential = 12.12 eV
PM3 zero point energy 67.987 kcal/mol
PM3 UHF zero point energy 67.982 kcal/mol
AM1 zero point energy 71.662 kcal/mol
AM1 UHF zero point energy 71.662 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 10.
[c]See Ref. 55.
[d]See Ref. 51.
[e]See Ref. 44.
[f]See Ref. 45.

TABLE 47. Ideal gas thermodynamic properties for propyl nitrate $C_3H_7ONO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−23.008	-------	-------	−197.063	−146.909	-------
100	62.454	−18.554	266.166	451.708	−192.609	−158.938	60.6071
200	94.145	−10.663	319.608	372.924	−184.718	−167.279	18.2092
298.15	123.239	0.000	362.601	362.601	−174.054	−174.054	3.5658
300	123.789	0.229	363.365	362.603	−173.826	−174.168	3.3779
400	152.484	14.065	402.971	367.809	−159.990	−179.485	−4.3142
500	177.462	30.598	439.760	378.564	−143.456	−183.221	−9.0502
600	198.260	49.417	474.014	391.652	−124.638	−185.618	−12.2615
700	215.512	70.132	505.912	405.723	−103.923	−186.907	−14.5785
800	229.911	92.424	535.658	420.127	−81.630	−187.275	−16.3242
900	241.984	116.037	563.455	434.526	−58.018	−186.873	−17.6819
1000	252.128	140.757	589.491	448.734	−33.297	−185.853	−18.7638
1100	260.659	166.409	613.933	462.653	−7.646	−184.336	−19.6429
1200	267.840	192.844	636.930	476.227	18.789	−182.426	−20.3688
1300	273.894	219.939	658.615	489.431	45.885	−180.223	−20.9762
1400	279.009	247.591	679.105	502.254	73.537	−177.804	−21.4898
1500	283.343	275.715	698.507	514.697	101.660	−175.227	−21.9293
1600	287.027	304.238	716.914	526.765	130.184	−172.548	−22.3079
1700	290.170	333.102	734.412	538.469	159.048	−169.810	−22.6367
1800	292.861	362.257	751.076	549.822	188.203	−167.045	−22.9241
1900	295.174	391.662	766.973	560.835	217.608	−164.279	−23.1773
2000	297.169	421.281	782.166	571.525	247.227	−161.535	−23.4011
2100	298.896	451.087	796.707	581.904	277.032	−158.829	−23.6004
2200	300.396	481.053	810.647	591.987	306.999	−156.179	−23.7784
2300	301.703	511.159	824.030	601.787	337.105	−153.588	−23.9383
2400	302.846	541.388	836.895	611.317	367.334	−151.070	−24.0826
2500	303.849	571.724	849.279	620.589	397.670	−148.638	−24.2129
2600	304.730	602.154	861.213	629.616	428.099	−146.283	−24.3314
2700	305.507	632.667	872.729	638.408	458.612	−144.023	−24.4395
2800	306.193	663.252	883.852	646.976	489.198	−141.852	−24.5384
2900	306.802	693.903	894.608	655.331	519.848	−139.779	−24.6289
3000	307.342	724.610	905.018	663.481	550.556	−137.810	−24.7119
3100	307.822	755.369	915.104	671.436	581.315	−135.928	−24.7892
3200	308.250	786.173	924.883	679.204	612.118	−134.156	−24.8601
3300	308.632	817.017	934.375	686.794	642.963	−132.484	−24.9260
3400	308.974	847.898	943.593	694.212	673.844	−130.912	−24.9873
3500	309.280	878.811	952.554	701.466	704.756	−129.449	−25.0446
3600	309.554	909.753	961.271	708.562	735.698	−128.086	−25.0978
3700	309.801	940.721	969.756	715.507	766.666	−126.829	−25.1479
3800	310.023	971.712	978.021	722.307	797.658	−125.678	−25.1947
3900	310.222	1002.725	986.076	728.967	828.670	−124.628	−25.2389
4000	310.403	1033.756	993.933	735.494	859.702	−123.693	−25.2803
4100	310.565	1064.805	1001.599	741.891	890.750	−122.851	−25.3199
4200	310.712	1095.868	1009.085	748.164	921.814	−122.120	−25.3570
4300	310.845	1126.946	1016.398	754.317	952.892	−121.496	−25.3920
4400	310.965	1158.037	1023.545	760.355	983.983	−120.987	−25.4254
4500	311.074	1189.139	1030.535	766.282	1015.085	−120.572	−25.4573
4600	311.172	1220.251	1037.373	772.101	1046.197	−120.262	−25.4877
4700	311.262	1251.373	1044.066	777.817	1077.319	−120.048	−25.5167
4800	311.343	1282.503	1050.620	783.432	1108.449	−119.935	−25.5445
4900	311.416	1313.641	1057.041	788.951	1139.587	−119.921	−25.5713
5000	311.483	1344.787	1063.333	794.376	1170.732	−120.033	−25.5966
5100	311.544	1375.938	1069.502	799.710	1201.883	−120.211	−25.6216
5200	311.599	1407.095	1075.552	804.957	1233.041	−120.498	−25.6452
5300	311.649	1438.258	1081.488	810.118	1264.203	−120.880	−25.6681
5400	311.695	1469.425	1087.313	815.198	1295.370	−121.355	−25.6902
5500	311.737	1500.596	1093.033	820.197	1326.542	−121.920	−25.7116
5600	311.774	1531.772	1098.651	825.120	1357.718	−122.571	−25.7323
5700	311.808	1562.951	1104.169	829.967	1388.897	−123.307	−25.7525
5800	311.840	1594.133	1109.592	834.742	1420.079	−124.122	−25.7720
5900	311.868	1625.319	1114.923	839.445	1451.265	−125.017	−25.7910
6000	311.893	1656.507	1120.165	844.081	1482.453	−125.984	−25.8095

TABLE 48. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for Cyclotetramethylene Tetranitramine (HMX) $C_4H_8(N-NO_2)_4$ (molecular wt.=296.156640)[a]

PM3

16.5 20.9 28.5 33.2 48.5 52.1 57 60.6 75 88.9 96.4 104
149 173 205 240 272 286 296 309 324 353 377 384
405 466 476 476 496 540 601 614 643 675 684 707
725 728 745 752 835 885 905 939 986 1031 1033 1044
1055 1063 1093 1113 1125 1164 1206 1242 1254 1257 1320 1328
1338 1463 1519 1534 1542 1829 1961 1968 1994 2019 2892 2900
2900 2939 2941 2972 3025 3087

AM1

11.7 20.6 34.6 42.3 46.8 64.2 71 78.6 92.8 108 119 135
140 212 253 315 335 348 360 394 429 449 492 545
613 617 626 649 665 691 699 729 741 781 809 819
955 987 1001 1007 1016 1037 1074 1105 1130 1141 1168 1185
1217 1260 1271 1313 1328 1355 1368 1370 1382 1388 1398 1405
1418 1496 1711 1728 1748 1891 2000 2050 2063 2077 2912 2916
2979 2980 2986 3032 3075 3111

AM1 UHF

20.6 24.9 32.1 34.4 **55.5** **64.6** **74.6** **80.3** **97.1** **108** **122** **130**
143 **218** **256** **312** **338** **348** **358** **393** **434** **471** **494** **544**
608 **624** **625** **638** **662** **676** **696** **714** **736** **758** **776** **819**
963 **990** **1004** **1005** **1021** **1046** **1071** **1109** **1127** **1141** **1167** **1179**
1224 **1258** **1271** **1312** **1338** **1356** **1366** **1367** **1382** **1385** **1397** **1406**
1412 **1464** **1706** **1726** **1747** **1892** **1968** **2051** **2062** **2076** **2912** **2914**
2977 **2979** **2992** **3034** **3076** **3110**

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia=1860.412 216 Ib=3728.904 799 Ic=4090.327 649 σ (total)=**128**
AM1 Ia=1623.802 091 Ib=3459.396 376 Ic=3637.911 304
AM1 UHF Ia=**1667.115 446** Ib=**3336.503 086** Ic=**3551.744 536**
4×(Ir(NO_2)=**59.6** ROSYM=2 V(2)=**16.7** kcal/mol)[b]
PM3 heat of formation=93.37 kcal/mol
AM1 heat of formation=174.98 kcal/mol
AM1 UHF heat of formation=174.45 kcal/mol spin=0 S^2=0.339 05
Ornellas[c] ΔH_f solid (298)=17.9 kcal/mol
NIST 94[d] ΔH_f(298)=24.1 kcal/mol (*erroneous)
Estimate ΔH_f(298)=**44.9**±**6.0** kcal/mol
PM3 ionization potential=11.119 eV
AM1 ionization potential=11.337 eV
AM1 UHF ionization potential=11.321 eV
PM3 zero point energy 108.241 kcal/mol
AM1 zero point energy 120.931 kcal/mol
AM1 zero point energy 120.804 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 20.
[c]See Ref. 42.
[d]See Ref. 51.

TABLE 49. Ideal gas thermodynamic properties for octogen (HMX) $C_4H_8(N-NO_2)_4$

T (deg K)	C_P (J/mol K)	$H-H_{298}$ (kJ/mol)	S (J/mol K)	$-(G-H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−50.045	-------	-------	137.817	245.304	-------
100	140.462	−41.391	353.785	767.691	146.471	218.504	−186.4938
200	209.769	−23.830	472.763	591.913	164.032	200.692	−131.3427
298.15	275.455	0.000	568.833	568.833	187.862	187.862	−114.5976
300	276.664	0.511	570.541	568.838	188.372	187.661	−114.3942
400	338.582	31.336	658.791	580.452	219.197	179.220	−106.4085
500	391.744	67.931	740.230	604.368	255.792	174.820	−101.7890
600	435.762	109.378	815.675	633.379	297.240	173.669	−98.7584
700	471.916	154.821	885.654	664.481	342.683	175.078	−96.5925
800	501.709	203.550	950.678	696.241	391.411	178.521	−94.9457
900	526.406	254.993	1011.242	727.916	442.855	183.602	−93.6340
1000	546.991	308.694	1067.802	759.108	496.556	189.979	−92.5511
1100	564.219	364.280	1120.768	789.604	552.141	197.396	−91.6320
1200	578.678	421.446	1170.499	819.295	609.307	205.653	−90.8355
1300	590.837	479.939	1217.312	848.129	667.801	214.554	−90.1326
1400	601.071	539.549	1261.484	876.091	727.411	223.952	−89.5034
1500	609.691	600.099	1303.256	903.189	787.961	233.733	−88.9351
1600	616.950	661.442	1342.843	929.441	849.303	243.779	−88.4158
1700	623.064	723.451	1380.434	954.874	911.313	254.012	−87.9380
1800	628.210	786.022	1416.197	979.518	973.884	264.351	−87.4957
1900	632.540	849.066	1450.282	1003.405	1036.928	274.738	−87.0844
2000	636.181	912.508	1482.822	1026.569	1100.369	285.123	−86.6992
2100	639.239	976.283	1513.938	1049.041	1164.145	295.466	−86.3385
2200	641.805	1040.339	1543.736	1070.855	1228.200	305.729	−85.9987
2300	643.956	1104.630	1572.314	1092.040	1292.492	315.892	−85.6779
2400	645.757	1169.118	1599.760	1112.627	1356.980	325.924	−85.3743
2500	647.261	1233.772	1626.153	1132.644	1421.633	335.801	−85.0863
2600	648.515	1298.562	1651.564	1152.117	1486.424	345.531	−84.8127
2700	649.557	1363.468	1676.059	1171.071	1551.329	355.075	−84.5520
2800	650.420	1428.468	1699.698	1189.531	1616.329	364.447	−84.3038
2900	651.133	1493.547	1722.535	1207.519	1681.408	373.629	−84.0661
3000	651.717	1558.690	1744.620	1225.056	1746.552	382.612	−83.8387
3100	652.194	1623.886	1765.997	1242.163	1811.748	391.416	−83.6221
3200	652.579	1689.126	1786.710	1258.858	1876.987	400.011	−83.4134
3300	652.887	1754.400	1806.796	1275.160	1942.261	408.404	−83.2133
3400	653.130	1819.701	1826.290	1291.084	2007.563	416.605	−83.0214
3500	653.317	1885.024	1845.226	1306.647	2072.885	424.603	−82.8369
3600	653.459	1950.363	1863.632	1321.865	2138.225	432.402	−82.6590
3700	653.560	2015.714	1881.538	1336.750	2203.576	440.004	−82.4883
3800	653.629	2081.074	1898.968	1351.317	2268.936	447.408	−82.3233
3900	653.670	2146.439	1915.947	1365.578	2334.301	454.620	−82.1645
4000	653.688	2211.807	1932.497	1379.545	2399.669	461.624	−82.0108
4100	653.686	2277.176	1948.638	1393.229	2465.038	468.448	−81.8632
4200	653.667	2342.544	1964.390	1406.642	2530.406	475.075	−81.7199
4300	653.635	2407.909	1979.771	1419.792	2595.771	481.512	−81.5815
4400	653.592	2473.270	1994.797	1432.690	2661.132	487.745	−81.4474
4500	653.540	2538.627	2009.485	1445.345	2726.489	493.805	−81.3181
4600	653.480	2603.978	2023.848	1457.766	2791.840	499.679	−81.1927
4700	653.414	2669.323	2037.901	1469.960	2857.185	505.380	−81.0714
4800	653.343	2734.661	2051.657	1481.936	2922.522	510.901	−80.9537
4900	653.269	2799.992	2065.128	1493.701	2987.853	516.247	−80.8398
5000	653.191	2865.314	2078.325	1505.262	3053.176	521.385	−80.7288
5100	653.112	2930.630	2091.259	1516.626	3118.491	526.391	−80.6221
5200	653.030	2995.937	2103.941	1527.799	3183.799	531.208	−80.5176
5300	652.948	3061.236	2116.379	1538.787	3249.097	535.862	−80.4167
5400	652.866	3126.526	2128.583	1549.597	3314.388	540.350	−80.3184
5500	652.783	3191.809	2140.562	1560.233	3379.671	544.678	−80.2232
5600	652.700	3257.083	2152.323	1570.701	3444.945	548.853	−80.1305
5700	652.618	3322.349	2163.875	1581.007	3510.210	552.870	−80.0402
5800	652.537	3387.607	2175.224	1591.154	3575.468	556.746	−79.9525
5900	652.456	3452.856	2186.378	1601.149	3640.718	560.475	−79.8671
6000	652.377	3518.098	2197.344	1610.994	3705.960	564.068	−79.7843

TABLE 50. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for nitrobutane $C_4H_9NO_2$ (molecular wt.=103.121000)[a]

AM1

19.3	32.9	100	197	**243**	**368**	**446**	**535**	631	728	818	918
947	**1033**	**1054**	**1088**	1148	**1160**	**1191**	1223	**1241**	**1278**	**1346**	**1374**
1390	**1394**	**1400**	**1405**	**1408**	**1425**	1442	1800	2067	2997	3010	3018
3056	**3060**	**3062**	**3083**	**3092**	**3157**						

AM1 UHF

21.4	39.9	104	194	247	361	441	564	595	722	822	915
945	1033	1050	1089	1154	1158	1190	1227	1246	1279	1338	1376
1390	1394	1399	1405	1410	1426	1443	1799	2066	2996	3011	3019
3056	3060	3063	3084	3093	3157						

IR spectrum[b]

								611	**712**	**752**	**860**
900				**1123**			**1211**				
1379						**1440**	**1568**	**2276**	**2760**	**2889**	**2970**

Principal moments of inertia in units of 10^{-40} g cm^2

AM1 Ia=179.144 716 Ib=528.009 756 Ic=574.685 911
AM1 UHF Ia=168.338 441 Ib=557.318 842 Ic=584.065 216
Table 3 Ir(NO_2)=**59.6** ROSYM=**2** V(2)=**0.08** kcal/mol
Ir(CH_3)=**5.1666** ROSYM=**3** V(3)=**3.5** kcal/mol
Ir(C_2H_5)=**21.04**[c] ROSYM=**2** V(3)=**9** kcal/mol
Ir(C_3H_7)=**22.2**[c] ROSYM=**2** V(3)=**13.64** kcal/mol[c]
AM1 heat of formation=−29.68 kcal/mol
AM1 UHF heat of formation=−29.62 kcal/mol spin=0.0 S^2=0.0
PM3[d] $\Delta H_f(298)=-32.1$ kcal/mol
AM1[d] $\Delta H_f(298)=-30.4$ kcal/mol
NIST 94[e] $\Delta H_f(298)=-$**34.4** kcal/mol
Stull *et al.*[f] $\Delta H_f(298)=-$**34.4** kcal/mol
Pedley and Nylor[g] $\Delta H_f(298)=-$**34.4** kcal/mol
ΔH_f liquid (298)=−46.00±0.3 kcal/mol
AM1 ionization potential=11.618 eV
AM1 UHF ionization potential=11.609 eV
AM1 zero point energy 86.384 kcal/mol
AM1 UHF zero point energy 86.369 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 1.
[c]See Ref. 10.
[d]See Ref. 52.
[e]See Ref. 51.
[f]See Ref. 55.
[g]See Ref. 45.

TABLE 51. Ideal gas thermodynamic properties for nitrobutane $C_4H_9NO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−21.040	-------	-------	−164.969	−109.634	-------
100	54.863	−16.697	283.584	450.551	−160.626	−123.384	42.1618
200	84.015	−9.737	330.675	379.360	−153.667	−134.222	8.8092
298.15	115.119	0.000	369.874	369.874	−143.930	−143.930	−3.0995
300	115.741	0.214	370.588	369.876	−143.716	−144.100	−3.2549
400	149.218	13.472	408.498	374.819	−130.458	−152.438	−9.6983
500	179.601	29.949	445.140	385.242	−113.981	−158.950	−13.7621
600	205.466	49.239	480.239	398.173	−94.690	−163.801	−16.5713
700	227.248	70.906	513.595	412.300	−73.024	−167.222	−18.6298
800	245.669	94.577	545.176	426.954	−49.352	−169.417	−20.2004
900	261.321	119.948	575.040	441.765	−23.982	−170.562	−21.4341
1000	274.647	146.764	603.281	456.517	2.834	−170.843	−22.4250
1100	285.999	174.811	630.005	471.085	30.882	−170.407	−23.2354
1200	295.669	203.908	655.316	485.393	59.978	−169.390	−23.9079
1300	303.908	233.898	679.316	499.395	89.968	−167.919	−24.4730
1400	310.936	264.649	702.102	513.067	120.719	−166.097	−24.9521
1500	316.937	296.051	723.765	526.398	152.121	−164.001	−25.3632
1600	322.074	328.008	744.387	539.383	184.078	−161.709	−25.7178
1700	326.480	360.441	764.049	552.025	216.511	−159.279	−26.0260
1800	330.271	393.283	782.820	564.329	249.354	−156.758	−26.2957
1900	333.541	426.478	800.766	576.304	282.548	−154.182	−26.5333
2000	336.372	459.977	817.948	587.960	316.047	−151.584	−26.7433
2100	338.829	493.740	834.421	599.307	349.810	−148.989	−26.9304
2200	340.968	527.732	850.234	610.356	383.802	−146.423	−27.0973
2300	342.836	561.924	865.433	621.118	417.995	−143.890	−27.2471
2400	344.472	596.292	880.059	631.604	452.362	−141.414	−27.3823
2500	345.908	630.812	894.151	641.826	486.883	−139.013	−27.5041
2600	347.172	665.467	907.743	651.794	521.538	−136.677	−27.6149
2700	348.287	700.242	920.866	661.518	556.312	−134.431	−27.7159
2800	349.272	735.121	933.551	671.008	591.191	−132.269	−27.8082
2900	350.143	770.092	945.823	680.274	626.163	−130.204	−27.8925
3000	350.916	805.146	957.707	689.325	661.216	−128.249	−27.9697
3100	351.602	840.272	969.224	698.169	696.343	−126.378	−28.0417
3200	352.212	875.464	980.397	706.815	731.534	−124.626	−28.1075
3300	352.754	910.713	991.244	715.270	766.783	−122.981	−28.1688
3400	353.236	946.012	1001.782	723.543	802.083	−121.443	−28.2256
3500	353.665	981.358	1012.027	731.639	837.428	−120.026	−28.2789
3600	354.047	1016.744	1021.996	739.567	872.814	−118.719	−28.3281
3700	354.388	1052.166	1031.701	747.332	908.236	−117.532	−28.3746
3800	354.690	1087.620	1041.156	754.940	943.691	−116.465	−28.4179
3900	354.959	1123.103	1050.373	762.398	979.173	−115.513	−28.4589
4000	355.198	1158.611	1059.363	769.710	1014.681	−114.694	−28.4972
4100	355.410	1194.142	1068.136	776.882	1050.212	−113.983	−28.5340
4200	355.598	1229.692	1076.703	783.919	1085.763	−113.401	−28.5684
4300	355.764	1265.261	1085.073	790.826	1121.331	−112.946	−28.6009
4400	355.911	1300.845	1093.253	797.607	1156.915	−112.628	−28.6318
4500	356.040	1336.442	1101.253	804.266	1192.513	−112.420	−28.6617
4600	356.152	1372.052	1109.080	810.807	1228.122	−112.336	−28.6900
4700	356.251	1407.672	1116.740	817.235	1263.743	−112.368	−28.7172
4800	356.336	1443.302	1124.241	823.553	1299.372	−112.521	−28.7432
4900	356.410	1478.939	1131.590	829.765	1335.009	−112.792	−28.7685
5000	356.473	1514.583	1138.791	835.874	1370.654	−113.220	−28.7922
5100	356.526	1550.233	1145.850	841.883	1406.304	−113.723	−28.8159
5200	356.571	1585.888	1152.774	847.795	1441.959	−114.361	−28.8382
5300	356.608	1621.547	1159.566	853.614	1477.618	−115.116	−28.8600
5400	356.638	1657.210	1166.232	859.342	1513.280	−115.982	−28.8811
5500	356.661	1692.875	1172.776	864.981	1548.945	−116.959	−28.9016
5600	356.679	1728.542	1179.203	870.535	1584.612	−118.043	−28.9215
5700	356.691	1764.210	1185.516	876.006	1620.281	−119.231	−28.9410
5800	356.699	1799.880	1191.720	881.396	1655.950	−120.517	−28.9599
5900	356.702	1835.550	1197.817	886.707	1691.620	−121.902	−28.9783
6000	356.701	1871.220	1203.813	891.943	1727.291	−123.377	−28.9965

TABLE 52. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for PETN penta-erythritoltetranitrate $C_5H_8N_4O_{12}$ ($C(CH_2ONO_2)_4$) (molecular wt.=316.138280)[a]

Melius[d]

29.9	37.8	45.6	55.4	**57.0**	**60.0**	**65.1**	**67.8**	**75.4**	**113**	**114**	**139**
166	**184**	**199**	**218**	**222**	**249**	**274**	**284**	**372**	**408**	**409**	**462**
541	**590**	**645**	**663**	**667**	**694**	**696**	**724**	**764**	**773**	**807**	**807**
810	**811**	**865**	**918**	**923**	**962**	**969**	**974**	**988**	**1022**	**1055**	**1072**
1079	**1098**	**1130**	**1198**	**1199**	**1256**	**1288**	**1326**	**1334**	**1362**	**1363**	**1380**
1390	**1417**	**1424**	**1435**	**1445**	**1469**	**1473**	**1485**	**1494**	**1710**	**1711**	**1730**
1735	**2929**	**2936**	**2971**	**2972**	**2999**	**3006**	**3028**	**3029**			

Principal moments of inertia in units of 10^{-40} g cm^2

Melius Ia=**1724.17** Ib=**4611.38** Ic=**4626.187**[d]
4×(Ir(NO_2)=**59.6** ROSYM=**2** V(2)=**9.1** kcal/mol) [from methylnitrate]
Melius $\Delta H_f(0) = -76.87$ $\Delta H_f(300) = -89.89$ kcal/mol spin=0.0 $S^2=0.0$
Cox and Pilcher[b] $\Delta H_f(298) = -$**92.5** kcal/mol
PM3[c] $\Delta H_f(298) = -98.2$ kcal/mol
AM1[c] $\Delta H_f(298) = -95.3$ kcal/mol
R(CC)=1.5404[d]
R(CH)=1.0760–1.0805
R(CO)=1.4261–1.4290
R(NO)=1.3373
R(NO)=1.1707–1.3421

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 12.
[c]See Ref. 52.
[d]See Ref. 35.

TABLE 53. Ideal gas thermodynamic properties for PETN penta-erythritoltetranitrate $C_5H_8(ONO_2)_4$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−53.542	-------	-------	−440.562	−332.001	-------
100	152.429	−44.455	383.299	827.846	−431.475	−358.427	114.9395
200	224.749	−25.481	511.979	639.382	−412.501	−375.153	19.5261
298.15	294.758	0.000	614.706	614.706	−387.020	−387.020	−13.2011
300	296.077	0.547	616.534	614.712	−386.473	−387.202	−13.6186
400	364.039	33.618	711.206	627.160	−353.402	−394.529	−30.6340
500	422.024	73.015	798.876	652.846	−314.005	−397.692	−40.9844
600	469.130	117.658	880.140	684.043	−269.362	−397.578	−47.9114
700	506.880	166.529	955.399	717.501	−220.491	−394.938	−52.8425
800	537.110	218.784	1025.131	751.652	−168.236	−390.347	−56.5073
900	561.377	273.752	1089.847	785.678	−113.268	−384.236	−59.3187
1000	580.915	330.902	1150.042	819.140	−56.118	−376.981	−61.5290
1100	596.691	389.810	1206.175	851.803	2.790	−368.861	−63.3003
1200	609.472	450.140	1258.662	883.545	63.120	−360.094	−64.7434
1300	619.862	511.625	1307.870	914.312	124.605	−350.882	−65.9343
1400	628.344	574.049	1354.128	944.092	187.029	−341.372	−66.9277
1500	635.297	637.243	1397.724	972.895	250.223	−331.670	−67.7657
1600	641.023	701.068	1438.914	1000.746	314.048	−321.888	−68.4771
1700	645.761	765.414	1477.922	1027.678	378.394	−312.088	−69.0861
1800	649.700	830.194	1514.948	1053.729	443.174	−302.337	−69.6105
1900	652.990	895.333	1550.166	1078.938	508.313	−292.679	−70.0652
2000	655.751	960.774	1583.732	1103.345	573.754	−283.148	−70.4605
2100	658.078	1026.469	1615.784	1126.990	639.449	−273.774	−70.8071
2200	660.049	1092.378	1646.445	1149.909	705.358	−264.582	−71.1115
2300	661.726	1158.469	1675.823	1172.141	771.449	−255.579	−71.3800
2400	663.158	1224.715	1704.017	1193.719	837.695	−246.782	−71.6178
2500	664.386	1291.093	1731.114	1214.677	904.073	−238.218	−71.8289
2600	665.443	1357.586	1757.193	1235.044	970.566	−229.859	−72.0170
2700	666.357	1424.177	1782.324	1254.851	1037.157	−221.742	−72.1850
2800	667.149	1490.854	1806.573	1274.125	1103.834	−213.848	−72.3359
2900	667.839	1557.604	1829.996	1292.892	1170.584	−206.188	−72.4706
3000	668.441	1624.418	1852.647	1311.175	1237.398	−198.768	−72.5918
3100	668.968	1691.289	1874.574	1328.997	1304.269	−191.559	−72.7022
3200	669.431	1758.210	1895.821	1346.380	1371.190	−184.595	−72.8008
3300	669.839	1825.174	1916.426	1363.343	1438.154	−177.860	−72.8903
3400	670.200	1892.176	1936.429	1379.906	1505.156	−171.344	−72.9717
3500	670.519	1959.212	1955.861	1396.086	1572.192	−165.056	−73.0457
3600	670.803	2026.279	1974.754	1411.899	1639.259	−158.987	−73.1126
3700	671.055	2093.372	1993.137	1427.361	1706.352	−153.136	−73.1741
3800	671.280	2160.489	2011.036	1442.486	1773.469	−147.503	−73.2298
3900	671.481	2227.627	2028.475	1457.289	1840.607	−142.079	−73.2809
4000	671.662	2294.784	2045.478	1471.782	1907.764	−136.882	−73.3274
4100	671.824	2361.959	2062.065	1485.977	1974.939	−131.877	−73.3706
4200	671.970	2429.149	2078.256	1499.887	2042.129	−127.086	−73.4098
4300	672.101	2496.352	2094.069	1513.522	2109.332	−122.503	−73.4457
4400	672.220	2563.569	2109.522	1526.893	2176.549	−118.138	−73.4787
4500	672.327	2630.796	2124.630	1540.009	2243.776	−113.959	−73.5094
4600	672.424	2698.034	2139.408	1552.879	2311.014	−109.978	−73.5376
4700	672.512	2765.280	2153.870	1565.513	2378.260	−106.181	−73.5638
4800	672.592	2832.535	2168.030	1577.918	2445.515	−102.575	−73.5880
4900	672.665	2899.799	2181.899	1590.103	2512.779	−99.159	−73.6106
5000	672.732	2967.069	2195.489	1602.076	2580.049	−95.967	−73.6309
5100	672.792	3034.345	2208.812	1613.842	2647.325	−92.910	−73.6509
5200	672.848	3101.627	2221.877	1625.410	2714.607	−90.057	−73.6687
5300	672.898	3168.914	2234.694	1636.785	2781.894	−87.376	−73.6856
5400	672.945	3236.206	2247.272	1647.975	2849.186	−84.875	−73.7013
5500	672.988	3303.503	2259.620	1658.984	2916.483	−82.540	−73.7162
5600	673.027	3370.804	2271.747	1669.818	2983.784	−80.366	−73.7300
5700	673.063	3438.108	2283.660	1680.483	3051.088	−78.358	−73.7429
5800	673.096	3505.416	2295.366	1690.983	3118.396	−76.499	−73.7551
5900	673.126	3572.727	2306.872	1701.325	3185.707	−74.789	−73.7666
6000	673.154	3640.041	2318.186	1711.512	3253.021	−73.222	−73.7776

TABLE 54. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for $C_5H_{11}NO_2$ N-nitropentane (molecular wt. = 117.147880)[a]

PM3												
	11.9	54.3	73.5	138	**214**	**295**	**315**	**394**	**470**	**480**	**615**	**691**
	805	**830**	**866**	**926**	**965**	**990**	**1020**	**1039**	**1081**	**1121**	**1129**	**1146**
	1153	**1167**	**1173**	**1253**	**1300**	**1341**	**1367**	**1386**	**1398**	**1402**	**1403**	**1410**
	1421	**1474**	**1611**	**1901**	**2893**	**2947**	**2949**	**2955**	**2992**	**3024**	**3027**	**3034**
	3069	**3088**	**3183**									
PM3 UHF												
	19.4	51.5	69.3	135	215	295	314	394	470	480	615	691
	804	829	866	926	965	989	1020	1039	1081	1121	1129	1147
	1153	1167	1173	1253	1300	1341	1367	1386	1398	1402	1404	1410
	1421	1474	1611	1901	2894	2947	2949	2955	2992	3024	3027	3034
	3069	3088	3183									
AM1												
	23.7	50.7	81.5	88.0	203	210	327	360	478	503	638	777
	800	848	915	984	1045	1088	1097	1122	1155	1192	1199	1235
	1245	1260	1284	1328	1369	1388	1394	1398	1403	1405	1416	1420
	1429	1441	1800	2068	2992	3009	3018	3023	3050	3059	3062	3083
	3090	3096	3156									
AM1 UHF												
	23.7	50.7	81.5	88.0	203	210	327	360	478	503	638	777
	800	848	915	984	1045	1088	1097	1122	1155	1192	1199	1235
	1245	1260	1284	1328	1369	1388	1394	1398	1403	1405	1416	1420
	1429	1441	1800	2068	2992	3009	3018	3023	3050	3059	3062	3083
	3090	3096	3156									

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia = **212.647 702** Ib = **858.897 159** Ic = **1004.047 696** σ = **1**
PM3 UHF Ia = 212.647 702 Ib = 858.897 159 Ic = 1004.047 696
AM1 Ia = 198.265 314 Ib = 879.381 235 Ic = 1009.141 087
AM1 UHF Ia = 198.265 314 Ib = 879.381 235 Ic = 1009.141 087
Table 3 Ir(NO_2) = **59.6** ROSYM = **2** V(2) = **0.08** kcal/mol Ir(CH_3) = **5.1666** ROSYM = **3** V(3) = **3.5** kcal/mol
Chao[b] Ir(C_2H_5) = **21.04** ROSYM = **2** V(2) = **9** kcal/mol
Chao[b] Ir(C_3H_7) = **22.2** ROSYM = **2** V(2) = **13.64** kcal/mol
PM3 heat of formation = −36.87 kcal/mol
PM3 UHF heat of formation = −36.87 kcal/mol
AM1 heat of formation = −35.5 kcal/mol
AM1 UHF heat of formation = −35.5 kcal/mol
NIST 97 ΔH_f (liquid) (298) = −51.4 kcal/mol[c]
NIST 94 $\Delta H_f(298) = -$ **39.3** kcal/mol $S(298) = 103.5$ cal/mole[d]
Estimated $\Delta H_f(298) = -$ **39.3** ± **0.5** kcal/mol (see Sec. IV).
AM1 ionization potential = 11.592 eV
AM1 UHF ionization potential = 11.592 eV
PM3 zero point energy 101.546 kcal/mol
PM3 UHF zero point energy 101.553 kcal/mol
AM1 zero point energy 104.537 kcal/mol
AM1 UHF zero point energy 104.537 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 10.
[c]See Ref. 27.
[d]See Ref. 51.

TABLE 55. Ideal gas thermodynamic properties for N-nitropentane $C_5H_{11}NO_2$

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G$-$H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−23.792	-------	-------	−188.223	−123.366	-------
100	59.466	−19.329	291.760	485.052	−183.760	−140.057	45.9873
200	97.288	−11.460	344.813	402.113	−175.891	−153.006	8.0556
298.15	137.100	0.000	390.905	390.905	−164.431	−164.431	−5.5346
300	137.890	0.254	391.756	390.908	−164.177	−164.629	−5.7122
400	179.964	16.168	437.246	396.826	−148.263	−174.241	−13.0762
500	217.350	36.084	481.532	409.364	−128.347	−181.563	−17.7201
600	248.673	59.434	524.017	424.960	−104.997	−186.862	−20.9271
700	274.765	85.644	564.369	442.020	−78.787	−190.449	−23.2736
800	296.686	114.248	602.531	459.721	−50.183	−192.585	−25.0607
900	315.245	144.870	638.577	477.611	−19.561	−193.488	−26.4618
1000	331.022	177.204	672.630	495.426	12.773	−193.379	−27.5847
1100	344.460	210.996	704.827	513.013	46.565	−192.431	−28.5010
1200	355.917	246.030	735.304	530.278	81.599	−190.806	−29.2595
1300	365.696	282.124	764.189	547.170	117.693	−188.650	−29.8952
1400	374.052	319.122	791.604	563.659	154.691	−186.086	−30.4327
1500	381.208	356.894	817.661	579.731	192.463	−183.200	−30.8927
1600	387.348	395.330	842.464	595.383	230.899	−180.085	−31.2882
1700	392.632	434.335	866.110	610.618	269.904	−176.807	−31.6309
1800	397.193	473.832	888.684	625.444	309.401	−173.421	−31.9297
1900	401.141	513.754	910.268	639.871	349.322	−169.969	−32.1922
2000	404.570	554.043	930.933	653.911	389.612	−166.491	−32.4232
2100	407.559	594.653	950.746	667.578	430.222	−163.011	−32.6284
2200	410.171	635.542	969.767	680.884	471.111	−159.564	−32.8106
2300	412.461	676.676	988.052	693.844	512.245	−156.153	−32.9736
2400	414.475	718.025	1005.649	706.472	553.594	−152.806	−33.1199
2500	416.251	759.563	1022.606	718.780	595.132	−149.543	−33.2513
2600	417.821	801.269	1038.962	730.782	636.837	−146.352	−33.3702
2700	419.212	843.122	1054.758	742.491	678.690	−143.266	−33.4782
2800	420.448	885.106	1070.026	753.917	720.675	−140.275	−33.5763
2900	421.548	927.207	1084.800	765.073	762.775	−137.395	−33.6654
3000	422.529	969.411	1099.108	775.971	804.980	−134.641	−33.7466
3100	423.405	1011.709	1112.977	786.619	847.278	−131.984	−33.8220
3200	424.189	1054.089	1126.432	797.029	889.658	−129.464	−33.8907
3300	424.891	1096.544	1139.496	807.210	932.113	−127.067	−33.9541
3400	425.520	1139.065	1152.190	817.171	974.634	−124.794	−34.0127
3500	426.085	1181.646	1164.533	826.920	1017.215	−122.662	−34.0673
3600	426.592	1224.280	1176.543	836.466	1059.849	−120.657	−34.1174
3700	427.048	1266.962	1188.238	845.816	1102.531	−118.791	−34.1645
3800	427.458	1309.688	1199.632	854.977	1145.257	−117.066	−34.2082
3900	427.827	1352.453	1210.740	863.958	1188.021	−115.474	−34.2493
4000	428.159	1395.252	1221.576	872.763	1230.821	−114.039	−34.2875
4100	428.457	1438.083	1232.152	881.400	1273.652	−112.728	−34.3240
4200	428.726	1480.943	1242.480	889.875	1316.511	−111.570	−34.3579
4300	428.967	1523.828	1252.571	898.193	1359.396	−110.560	−34.3898
4400	429.184	1566.735	1262.436	906.360	1402.304	−109.712	−34.4199
4500	429.379	1609.664	1272.083	914.380	1445.232	−108.993	−34.4489
4600	429.554	1652.610	1281.522	922.259	1488.179	−108.419	−34.4764
4700	429.711	1695.574	1290.762	930.002	1531.143	−107.980	−34.5025
4800	429.851	1738.552	1299.810	937.612	1574.121	−107.684	−34.5275
4900	429.976	1781.544	1308.675	945.095	1617.112	−107.528	−34.5517
5000	430.088	1824.547	1317.363	952.453	1660.116	−107.559	−34.5742
5100	430.187	1867.561	1325.881	959.692	1703.129	−107.674	−34.5968
5200	430.276	1910.584	1334.235	966.815	1746.153	−107.950	−34.6179
5300	430.353	1953.615	1342.432	973.825	1789.184	−108.364	−34.6384
5400	430.422	1996.654	1350.476	980.726	1832.223	−108.910	−34.6583
5500	430.482	2039.700	1358.375	987.520	1875.268	−109.586	−34.6775
5600	430.535	2082.751	1366.132	994.212	1918.319	−110.389	−34.6960
5700	430.580	2125.806	1373.753	1000.804	1961.375	−111.314	−34.7143
5800	430.619	2168.866	1381.242	1007.299	2004.435	−112.355	−34.7320
5900	430.653	2211.930	1388.603	1013.700	2047.499	−113.512	−34.7491
6000	430.681	2254.997	1395.841	1020.009	2090.566	−114.776	−34.7660

TABLE 56. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for $C_6H_5NO_2$ nitrobenzene (molecular wt.=123.111240)[a]

Melius rhf/6-31g*[b]

49.6	**171**	**254**	**388**	**409**	**436**	**510**	**599**	**665**	**674**	723	807
855	**860**	968	**977**	**999**	**1004**	**1019**	1057	1102	1108	1159	1211
1308	1449	1464	1484	1594	1602	1667	3011	3025	3034	3071	3071

IR spectrum[c]

										692	**787**
854		**928**					**1020**	**1070**	**1103**	**1171**	**1245**
1312	**1353**	**1481**	**1541**	**1609**	**1797**	**1912**	**1966**	**2700**	**2888**	**2935**	**3084**

Principal moments of inertia in units of 10^{-40} g cm^2

Melius Ia=**206.002** Ib=**639.627** Ic=**845.628** σ (external)=**2**
Ir=**59.350** ROSYM=**2** V(2)=3.11 kcal/mol
V(2)(experimental)=**2.8**–3.3 kcal/mol[d]
PM3[e] $\Delta H_f(298)$=14.5 kcal/mol
AM1[e] $\Delta H_f(298)$=25.3 kcal/mol
Melius $\Delta H_f(0)$=19.0 $\Delta H_f(298)$=14.18±1.66 kcal/mol spin=1 S^2=0.4230
Pedley, Nylor and Kirby[f] $\Delta H_f(298)$=**16.38**±**0.16** kcal/mol
Stull *et al.*[g] $\Delta H_f(298)$=15.4 kcal/mol
Zero-point vibrational energy 62.594 kcal/mol[b]
R(CC)=1.3832–1.3867[b]
R(CH)=1.0709–1.0750
R(CN)=1.4588
R(NO)=1.1938
R(CN)=1.465[h]

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 35.
[c]See Ref. 1.
[d]See Ref. 18.
[e]See Ref. 52.
[f]See Ref. 45.
[g]See Ref. 55.
[h]Politzer *et al.*, J. Phys. Chem. A **102**, 6697 (1998).

TABLE 57. Ideal gas thermodynamic properties for nitrobenzene $C_6H_5NO_2$.

T (deg K)	C_P (J/mol K)	H-H_{298} (kJ/mol)	S (J/mol K)	$-(G-H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−20.903	-------	-------	47.631	88.137	-------
100	52.534	−16.735	263.198	430.544	51.799	80.088	−54.7587
200	83.769	−10.013	308.553	358.618	58.521	73.746	−34.5072
298.15	120.380	0.000	348.800	348.800	68.534	68.534	−28.3692
300	121.062	0.223	349.546	348.802	68.757	68.448	−28.2952
400	155.443	14.094	389.212	353.977	82.628	64.485	−25.3986
500	183.861	31.110	427.064	364.844	99.644	61.705	−23.7504
600	206.678	50.679	462.679	378.215	119.213	59.836	−22.6922
700	224.998	72.296	495.965	392.686	140.829	58.696	−21.9555
800	239.829	95.562	527.012	407.559	164.096	58.161	−21.4110
900	251.941	120.171	555.983	422.459	188.705	58.133	−20.9894
1000	261.910	145.879	583.060	437.180	214.413	58.504	−20.6511
1100	270.171	172.496	608.422	451.607	241.030	59.199	−20.3718
1200	277.060	199.868	632.234	465.678	268.402	60.146	−20.1358
1300	282.838	227.871	654.646	479.360	296.405	61.276	−19.9328
1400	287.712	256.406	675.790	492.643	324.939	62.528	−19.7549
1500	291.845	285.389	695.785	505.525	353.923	63.877	−19.5982
1600	295.370	314.754	714.735	518.014	383.288	65.271	−19.4578
1700	298.392	344.446	732.735	530.120	412.980	66.681	−19.3310
1800	300.996	374.419	749.866	541.856	442.953	68.089	−19.2160
1900	303.251	404.634	766.202	553.237	473.168	69.472	−19.1110
2000	305.212	435.059	781.808	564.278	503.593	70.818	−19.0143
2100	306.926	465.668	796.742	574.995	534.202	72.114	−18.9257
2200	308.432	496.438	811.055	585.402	564.971	73.341	−18.8433
2300	309.758	527.348	824.795	595.514	595.882	74.506	−18.7671
2400	310.933	558.384	838.004	605.344	626.918	75.594	−18.6962
2500	311.976	589.531	850.718	614.906	658.064	76.590	−18.6298
2600	312.907	620.776	862.973	624.213	689.310	77.512	−18.5678
2700	313.739	652.109	874.798	633.276	720.643	78.337	−18.5100
2800	314.487	683.521	886.222	642.107	752.055	79.072	−18.4558
2900	315.161	715.004	897.269	650.716	783.538	79.712	−18.4045
3000	315.769	746.551	907.964	659.114	815.085	80.243	−18.3561
3100	316.320	778.156	918.327	667.309	846.689	80.695	−18.3114
3200	316.821	809.813	928.378	675.312	878.347	81.036	−18.2687
3300	317.277	841.518	938.134	683.129	910.052	81.278	−18.2285
3400	317.694	873.267	947.612	690.769	941.801	81.420	−18.1905
3500	318.075	905.056	956.827	698.240	973.590	81.453	−18.1550
3600	318.425	936.881	965.793	705.548	1005.415	81.391	−18.1210
3700	318.747	968.740	974.521	712.700	1037.274	81.219	−18.0893
3800	319.043	1000.630	983.026	719.702	1069.163	80.944	−18.0590
3900	319.316	1032.548	991.317	726.561	1101.082	80.567	−18.0307
4000	319.569	1064.492	999.404	733.281	1133.026	80.072	−18.0036
4100	319.804	1096.461	1007.298	739.869	1164.995	79.488	−17.9785
4200	320.021	1128.452	1015.007	746.328	1196.986	78.791	−17.9545
4300	320.224	1160.465	1022.540	752.665	1228.999	77.982	−17.9315
4400	320.412	1192.497	1029.904	758.882	1261.031	77.048	−17.9099
4500	320.588	1224.547	1037.107	764.985	1293.081	76.026	−17.8897
4600	320.752	1256.614	1044.155	770.978	1325.148	74.902	−17.8707
4700	320.906	1288.697	1051.054	776.864	1357.231	73.679	−17.8527
4800	321.049	1320.795	1057.812	782.647	1389.329	72.355	−17.8360
4900	321.184	1352.906	1064.433	788.330	1421.440	70.930	−17.8203
5000	321.311	1385.031	1070.923	793.917	1453.565	69.346	−17.8049
5100	321.430	1417.168	1077.287	799.411	1485.702	67.730	−17.7915
5200	321.542	1449.317	1083.530	804.815	1517.851	65.977	−17.7782
5300	321.648	1481.477	1089.656	810.132	1550.010	64.123	−17.7659
5400	321.748	1513.646	1095.669	815.364	1582.180	62.169	−17.7544
5500	321.842	1545.826	1101.574	820.514	1614.360	60.116	−17.7436
5600	321.931	1578.015	1107.374	825.585	1646.549	57.965	−17.7336
5700	322.015	1610.212	1113.073	830.579	1678.746	55.718	−17.7243
5800	322.095	1642.418	1118.674	835.498	1710.951	53.376	−17.7157
5900	322.171	1674.631	1124.180	840.345	1743.165	50.943	−17.7077
6000	322.243	1706.852	1129.596	845.120	1775.386	48.420	−17.7004

TABLE 58. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for 2,4,6-trinitrobenzene $C_6H_3(NO_2)_3$ (Molecular wt. = 213.106440)[a]

PM3

23.5	29.5	38.3	**66.8**	**87.5**	**129**	**147**	**251**	**256**	**294**	**323**	**335**
350	**393**	**448**	**504**	**522**	**568**	**591**	**644**	**680**	**688**	**748**	**751**
778	**843**	**939**	**952**	**970**	**1000**	**1018**	**1113**	**1121**	**1183**	**1209**	**1321**
1368	**1431**	**1580**	**1594**	**1671**	**1720**	**1742**	**1913**	**1923**	**2993**	**3038**	**3071**

PM3 UHF

29.4	39.3	43.6	104	144	153	162	166	296	304	337	363
397	442	460	516	535	583	635	658	678	684	743	762
780	967	970	973	1013	1033	1063	1160	1194	1203	1274	1355
1417	1560	1579	1587	1598	1776	1781	1912	1924	2978	2997	3000

AM1 UHF

30.8	44	46	111	153	165	175	179	302	350	401	405
470	481	559	565	615	692	734	772	779	783	871	982
984	990	1026	1051	1102	1117	1171	1251	1264	1313	1410	1493
1585	1616	1736	1757	1781	1783	1788	2072	2077	3113	3124	3129

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 Ia=1114.285 965 Ib=**1721.862 748** Ic=**2528.621 471** σ(external)=**6**
PM3-UHF Ia=1441.571 867 Ib=1592.043 009 Ic=2990.684 436
AM1-UHF Ia=1368.532 505 Ib=1601.686 761 Ic=2929.695 958
3×(Ir=**59.35** ROSYM=**2** V(2)=**3.11** kcal/mol) [from nitrobenzene]
PM3 heat of formation=189.36 kcal/mol
PM3 UHF heat of formation=94.64 kcal/mol spin=0.0 S^2=0.000 003
AM1 UHF heat of formation=136.84 kcal/mol spin=0.0 S^2=0.000 181
NIST 97 ΔH_f solid(298)=−8.9±0.3 kcal/mol[b]
Pedley Naylor and Kirby[c] ΔH_f(298)=**14.9** kcal/mol
PM3 UHF ionization potential=11.21 eV
AM1 UHF ionization potential=11.734 eV
PM3 zero point energy 64.870 kcal/mol
PM3 UHF zero point energy 66.283 kcal/mol
AM1 UHF zero point energy 72.094 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 26.
[c]See Ref. 45.

TABLE 59. Ideal gas thermodynamic properties for trinitrobenzene $C_6H_3(NO_2)_3$

T (deg K)	C_P (J/mol K)	$H-H_{298}$ (kJ/mol)	S (J/mol K)	$-(G-H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−37.794	-------	-------	24.548	82.617	-------
100	101.282	−30.823	325.756	633.989	31.518	71.664	−68.2820
200	157.154	−17.881	413.239	502.643	44.461	65.504	−50.2635
298.15	205.633	0.000	485.335	485.335	62.342	62.342	−44.7665
300	206.453	0.381	486.609	485.338	62.723	62.302	−44.6989
400	245.654	23.068	551.604	493.935	85.409	61.202	−42.0148
500	276.134	49.221	609.837	511.395	111.563	61.424	−40.4161
600	299.926	78.072	662.373	532.253	140.414	62.462	−39.3388
700	318.688	109.039	710.071	554.301	171.381	64.058	−38.5530
800	333.646	141.683	753.639	576.535	204.025	66.068	−37.9470
900	345.692	175.672	793.658	598.467	238.013	68.405	−37.4598
1000	355.471	210.746	830.604	619.857	273.088	70.981	−37.0557
1100	363.465	246.706	864.871	640.593	309.048	73.738	−36.7123
1200	370.038	283.392	896.788	660.628	345.734	76.629	−36.4150
1300	375.472	320.676	926.628	679.954	383.018	79.597	−36.1538
1400	379.985	358.456	954.624	698.584	420.797	82.594	−35.9208
1500	383.751	396.648	980.972	716.540	458.990	85.605	−35.7122
1600	386.909	435.186	1005.843	733.852	497.527	88.584	−35.5228
1700	389.569	474.013	1029.381	750.550	536.355	91.510	−35.3499
1800	391.819	513.086	1051.714	766.666	575.428	94.365	−35.1913
1900	393.731	552.366	1072.951	782.232	614.708	97.129	−35.0451
2000	395.363	591.823	1093.189	797.278	654.165	99.795	−34.9094
2100	396.761	631.431	1112.514	811.833	693.772	102.350	−34.7838
2200	397.963	671.169	1131.000	825.923	733.510	104.779	−34.6668
2300	399.002	711.018	1148.713	839.575	773.360	107.088	−34.5574
2400	399.902	750.964	1165.714	852.812	813.306	109.265	−34.4552
2500	400.685	790.995	1182.055	865.657	853.336	111.294	−34.3591
2600	401.369	831.098	1197.784	878.131	893.440	113.200	−34.2689
2700	401.968	871.266	1212.943	890.252	933.607	114.955	−34.1840
2800	402.495	911.489	1227.572	902.040	973.831	116.572	−34.1043
2900	402.959	951.762	1241.704	913.510	1014.104	118.047	−34.0285
3000	403.370	992.079	1255.372	924.679	1054.421	119.370	−33.9570
3100	403.734	1032.435	1268.604	935.561	1094.777	120.569	−33.8901
3200	404.058	1072.825	1281.428	946.170	1135.166	121.615	−33.8262
3300	404.347	1113.245	1293.866	956.519	1175.587	122.521	−33.7656
3400	404.605	1153.693	1305.941	966.619	1216.035	123.290	−33.7084
3500	404.836	1194.165	1317.673	976.482	1256.507	123.916	−33.6543
3600	405.044	1234.660	1329.080	986.119	1297.001	124.411	−33.6027
3700	405.232	1275.174	1340.180	995.539	1337.515	124.765	−33.5540
3800	405.401	1315.705	1350.990	1004.751	1378.047	124.986	−33.5074
3900	405.553	1356.253	1361.522	1013.765	1418.595	125.075	−33.4635
4000	405.692	1396.816	1371.792	1022.588	1459.157	125.019	−33.4214
4100	405.818	1437.391	1381.811	1031.227	1499.733	124.845	−33.3819
4200	405.932	1477.979	1391.591	1039.692	1540.320	124.535	−33.3441
4300	406.036	1518.577	1401.144	1047.987	1580.919	124.090	−33.3080
4400	406.132	1559.186	1410.480	1056.120	1621.527	123.498	−33.2735
4500	406.219	1599.803	1419.608	1064.096	1662.145	122.795	−33.2411
4600	406.298	1640.429	1428.537	1071.922	1702.771	121.968	−33.2101
4700	406.372	1681.063	1437.276	1079.603	1743.404	121.023	−33.1808
4800	406.439	1721.703	1445.832	1087.144	1784.045	119.957	−33.1531
4900	406.501	1762.350	1454.213	1094.550	1824.692	118.770	−33.1267
5000	406.558	1803.003	1462.426	1101.825	1865.345	117.409	−33.1012
5100	406.610	1843.662	1470.478	1108.975	1906.003	115.996	−33.0778
5200	406.659	1884.325	1478.374	1116.003	1946.667	114.426	−33.0550
5300	406.704	1924.993	1486.120	1122.914	1987.335	112.742	−33.0335
5400	406.746	1965.666	1493.723	1129.711	2028.007	110.936	−33.0131
5500	406.784	2006.342	1501.187	1136.397	2068.684	109.016	−32.9939
5600	406.820	2047.022	1508.516	1142.977	2109.364	106.982	−32.9756
5700	406.854	2087.706	1515.717	1149.453	2150.048	104.832	−32.9581
5800	406.885	2128.393	1522.794	1155.829	2190.735	102.574	−32.9417
5900	406.914	2169.083	1529.749	1162.108	2231.425	100.205	−32.9262
6000	406.941	2209.776	1536.589	1168.293	2272.118	97.731	−32.9117

TABLE 60. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for 1-nitrohexane $C_6H_{13}NO_2$

Estimate	$\Delta H_f(298) = -44.3 \pm 0.7$ kcal/mol
NIST 94	$\Delta H_f(298) = -44.3$ kcal/mol $S(298) = 112.9$ cal/mole K[a]
Estimate	ΔH_fliquid$(298) = -57.8 \pm 0.7$ kcal/mol (see Sec. 4)

[a]See Ref. 4.

TABLE 61. Fundamental vibrations, moments of inertia, bond lengths, and enthalpies of formation for 2,4,6-tri nitrotoluene TNT $C_7H_5(NO_2)_3$ (molecular wt.$=227.133320$)[a]

PM3 UHF											
24.7	30.6	38.3	69.3	**70.6**	**106**	**144**	**150**	**159**	**264**	**274**	**301**
320	**346**	**360**	**371**	460	**497**	510	**543**	599	**651**	672	685
737	748	767	795	860	961	979	989	1010	1024	1060	1150
1200	1259	1283	1351	1370	1373	1429	1447	1564	1587	1602	1615
1766	1788	1915	1919	2989	2993	3061	3067	3170			
IR spectra of toluene[b]											
457	524	591	686	726	888				1023	1070	
1218		1380	1440	1494		1602	1723	1784	1858	1945	2747
2875	2935	3030	3070								
IR spectra of 2 nitrotoluene[b]											
470			666	726	780	854	901	942	1036	1090	1151
1204	1305	1353	1386	1427	1481	1534	1609	1804	1918	1966	2828
2882	2942	3036	3077								
IR Spectra of 4 nitrotoluene[b]											
490		612	679	733	780	827	854	948	1023	1049	1103
1177	1204	1238	1346	1413	1467	1534	1602	1656	1790	1918	2450
2700	2747	2875	2942	3010	3050	3084					
IR spectra of 2,4-dinitrotoluene[b]											
		625	666	733	780	834		908	1029	1063	1151
1198		1265	1346	1393		1555	1609	1716	1797	1817	1925
2693	2740	2888	2942	2989	3050	3090					
Combined spectrum											
				457		**524**		**600**		**666**	**733**
780	**827**	**854**	**908**	**942**	**1023**	**1063**	**1103**	**1151**	**1204**	**1265**	**1345**
1393	**1430**	**1490**	**1554**	**1609**	**1656**	**1716**	**1790**	**1817**	**1858**	**1915**	**1945**
2450	**2700**	**2747**	**2828**	**2875**	**2942**	**2989**	**3050**	**3080**			

Principal moments of inertia in units of 10^{-40} g cm^2

PM3 UHF Ia$=$**1585.062 915** Ib$=$**1716.536 176** Ic$=$**3149.299 127** σ(external)$=$**2**
Table 3 **3**$\times$(Ir(NO_2)$=$**59.6** ROSYM$=$**2**) (V(2)$=$**3.11** kcal/mol)$\times$**1**
(V(2)$=$**7.0** kcal/mol)$\times$**2** (estimated)
Ir(CH_3)$=$**5.17** ROSYM$=$**3** V(3)$=$**3.5** kcal/mol [nitroethane]
PM3 UHF heat of formation$=$89.74 kcal/mol spin$=0$ $S^2=0$
PM3[c] $\Delta H_f(298) = 3.3$ kcal/mol
Cox and Pilcher[d] $\Delta H_f(298) = 12.9$ kcal/mol
NIST 97 $\Delta H_f(298) = \mathbf{5.76 \pm 1.0}$ kcal/mol[e]
NIST 97 ΔH_fsolid$(298) = -15.1 \pm 1.2$ kcal/mol[b]
ΔH_fsolid$(298) = -19.25 \pm 0.74$ kcal/mol.[e]
PM3 UHF zero point energy 83.610 kcal/mol

[a]The properties marked with bold characters were chosen for thermodynamic calculations.
[b]See Ref. 1.
[c]See Ref. 48.
[d]See Ref. 12.
[e]See Ref. 28.

TABLE 62. Ideal gas thermodynamic properties for trinitrotoluene CH_3–$C_6H_2(NO_2)_3$

T (deg K)	C_P (J/mol K)	$H-H_{298}$ (kJ/mol)	S (J/mol K)	$-(G-H_{298})/T$ (J/mol K)	H (kJ/mol)	ΔH (kJ/mol)	Log K
0	-------	−39.554	-------	-------	−15.454	52.136	-------
100	107.329	−32.660	331.800	658.401	−8.560	38.046	−55.7173
200	167.244	−18.804	425.455	519.475	5.296	29.779	−46.6932
298.15	214.425	0.000	501.324	501.324	24.100	24.100	−44.3571
300	215.233	0.397	502.653	501.328	24.497	24.008	−44.3308
400	255.226	23.978	570.215	510.270	48.078	19.873	−43.3724
500	288.947	51.234	630.895	528.427	75.334	16.948	−42.8912
600	317.404	81.592	686.166	550.178	105.692	14.987	−42.6130
700	341.368	114.565	736.947	573.282	138.665	13.879	−42.4340
800	361.496	149.738	783.883	596.711	173.838	13.543	−42.3068
900	378.366	186.756	827.465	619.958	210.856	13.901	−42.2078
1000	392.487	225.320	868.082	642.763	249.420	14.838	−42.1247
1100	404.310	265.177	906.062	664.991	289.277	16.259	−42.0510
1200	414.221	306.118	941.679	686.580	330.218	18.076	−41.9833
1300	422.546	347.968	975.172	707.504	372.068	20.192	−41.9197
1400	429.560	390.584	1006.750	727.762	414.683	22.520	−41.8581
1500	435.492	433.844	1036.595	747.365	457.944	25.019	−41.7996
1600	440.526	477.652	1064.866	766.333	501.752	27.612	−41.7426
1700	444.817	521.925	1091.705	784.690	546.025	30.259	−41.6870
1800	448.490	566.595	1117.237	802.462	590.695	32.921	−41.6331
1900	451.648	611.606	1141.572	819.674	635.706	35.565	−41.5809
2000	454.374	656.910	1164.809	836.354	681.010	38.169	−41.5298
2100	456.737	702.469	1187.037	852.528	726.568	40.711	−41.4810
2200	458.795	748.248	1208.333	868.220	772.347	43.166	−41.4335
2300	460.594	794.219	1228.768	883.455	818.319	45.534	−41.3878
2400	462.172	840.359	1248.404	898.255	864.459	47.795	−41.3438
2500	463.562	886.647	1267.300	912.641	910.747	49.926	−41.3011
2600	464.791	933.066	1285.506	926.634	957.166	51.951	−41.2601
2700	465.881	979.601	1303.068	940.253	1003.700	53.835	−41.2209
2800	466.852	1026.238	1320.029	953.515	1050.338	55.589	−41.1833
2900	467.719	1072.968	1336.427	966.438	1097.067	57.207	−41.1467
3000	468.495	1119.779	1352.296	979.037	1143.879	58.671	−41.1116
3100	469.193	1166.664	1367.670	991.327	1190.764	60.016	−41.0788
3200	469.822	1213.615	1382.576	1003.321	1237.715	61.202	−41.0467
3300	470.390	1260.626	1397.042	1015.034	1284.726	62.244	−41.0160
3400	470.904	1307.691	1411.093	1026.477	1331.791	63.145	−40.9869
3500	471.372	1354.806	1424.750	1037.662	1378.905	63.893	−40.9592
3600	471.797	1401.964	1438.035	1048.600	1426.064	64.502	−40.9323
3700	472.185	1449.164	1450.967	1059.301	1473.264	64.960	−40.9072
3800	472.540	1496.400	1463.564	1069.774	1520.500	65.272	−40.8827
3900	472.866	1543.671	1475.843	1080.030	1567.771	65.442	−40.8599
4000	473.165	1590.973	1487.819	1090.075	1615.072	65.450	−40.8377
4100	473.440	1638.303	1499.506	1099.920	1662.403	65.330	−40.8173
4200	473.693	1685.660	1510.917	1109.570	1709.760	65.057	−40.7975
4300	473.927	1733.041	1522.066	1119.034	1757.141	64.633	−40.7785
4400	474.144	1780.445	1532.964	1128.318	1804.545	64.042	−40.7604
4500	474.345	1827.869	1543.622	1137.429	1851.969	63.327	−40.7436
4600	474.531	1875.313	1554.050	1146.373	1899.413	62.471	−40.7277
4700	474.705	1922.775	1564.257	1155.156	1946.875	61.481	−40.7128
4800	474.866	1970.254	1574.253	1163.783	1994.354	60.353	−40.6989
4900	475.016	2017.748	1584.046	1172.260	2041.848	59.088	−40.6858
5000	475.157	2065.257	1593.644	1180.592	2089.357	57.620	−40.6729
5100	475.288	2112.779	1603.054	1188.784	2136.879	56.095	−40.6619
5200	475.411	2160.314	1612.285	1196.840	2184.414	54.390	−40.6509
5300	475.526	2207.861	1621.342	1204.764	2231.961	52.553	−40.6408
5400	475.635	2255.419	1630.231	1212.561	2279.519	50.577	−40.6314
5500	475.736	2302.988	1638.960	1220.235	2327.088	48.470	−40.6228
5600	475.832	2350.566	1647.533	1227.789	2374.666	46.231	−40.6147
5700	475.922	2398.154	1655.955	1235.227	2422.254	43.861	−40.6073
5800	476.007	2445.750	1664.233	1242.552	2469.850	41.367	−40.6006
5900	476.087	2493.355	1672.371	1249.768	2517.455	38.747	−40.5944
6000	476.162	2540.968	1680.373	1256.879	2565.068	36.007	−40.5889

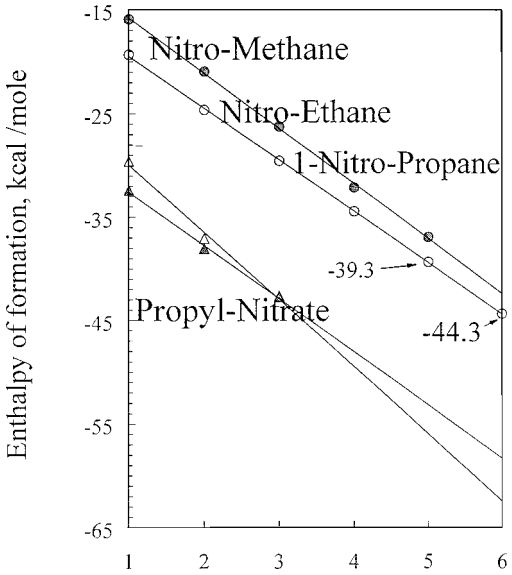


FIG. 1. The enthalpy of formation of the first four N-nitro−carbons and the first three N-nitrate-homologues as a function of the number of carbon atoms in the molecule. The open symbols are experimental enthalpies of formation and the filled symbols are the PM3 calculations. The 1-nitropentane and 1-nitrohexane value can be estimated from this graph.

4.2. IR spectrum

It is known that the IR spectra are a good indicator of the fundamental vibrations, but not necessarily a correct one. Looking at the assignment of vibrations in the literature it is possible to see that some of the bands are not pure, but the sum of two or more vibrations. Therefore the use of the IR spectrum as is can only approximate the real vibrational spectrum of the molecule. Nevertheless, it can be seen for nitromethane that the IR spectra are very similar to the assigned spectrum and to the MOPAC or BAC/MP4 calculated vibrations. Therefore, wherever available, the IR spectra[1] were used and supplemented with the missing vibrations from the calculations.

4.3. Internal Rotations

In the rigid-rotor-harmonic-oscillator (RRHO) approximation of a polyatomic molecule, it is generally expected that the C_p increases gradually and it approaches asymptotically to $C_p(\infty)$. However it is observed that in many cases, specifically when the number of internal rotors is greater than two, the C_p value arrives at a maximum and then decreases. It has been observed with trinitromethane, tetranitromethane, trinitroazetidine, RDX, and HMX. The explanation for this

TABLE 63. Comparison of the thermodynamic data with the literature (cal/mol K units)

		Stull *et al.*		Melius[a]		This study	
Compound	T (K)	C_p	S	C_p	S	C_p	S
CH_3NO_2	300	13.76	65.82			13.329	67.688
	1000	28.17	90.87			28.316	92.531
CH_3ONO_2	300	18.34	72.27			18.374	73.200
	1000	34.19	103.87			34.160	104.809
$CH_2{=}CHNO_2$	300		70.6[b]	17.648	70.581	17.688	71.931
	1000			34.272	102.179	34.236	103.537
$C_2H_5NO_2$	300	18.78	75.51	18.948	77.742	18.973	76.721
	1000	40.67	111.24	40.407	114.425	40.422	112.251
$C_2H_5ONO_2$	300	23.36	83.40			22.834	78.741
	1000	46.69	125.68			47.082	120.847
$CH_3CH{=}CHNO_2$	300		79.3[b]	22.868	80.373	22.469	79.012
	1000			46.688	122.310	46.594	120.453
$C_3H_6N{-}NO_2$	300			23.890	79.392	24.190	78.771
	1000			55.042	127.357	56.227	127.177
$C_3H_4N{-}(NO_3)_3$	300			32.498[c]	85.787[c]	32.498	85.601
	1000			78.835[c]	154.299[d]	79.106	154.487
$C_3H_7NO_2$	300	24.52	85.16			25.002	83.817
	1000	53.06	131.64			54.076	131.353
$C_3H_7ONO_2$	300	29.10	92.28			29.586	86.746
	1000	59.08	145.32			60.260	140.892
$C_4H_8N_8O_8$	300	69.57[d]				66.124	
$C_4H_9NO_2$	300	29.99	94.47			27.663	88.573
	1000	65.39	151.57			65.642	144.188
$C_5H_{11}NO_2$	300		103.5[b]				93.632
$C_6H_5NO_2$	300			28.771	82.940	28.935	83.544
	1000			62.110	138.514	62.598	139.355
$C_7H_5(NO_2)_3$	300	58.90[d]				51.442	

[a]Data unavailable to the public. Received as private communication.
[b]Estimate from NIST 94.[51]
[c]Results from Yu, Zhang and Bauer.[60]
[d]Experimental measurements averaged by Yin *et al.*[59]

phenomenon is the transition from a hindered rotation of the internal rotor to a free rotation at a higher temperature. The hindered rotation has a C_p value which is higher than the equivalent free rotation. Thus after a certain temperature the C_p decreases.

4.4. Enthalpies of Formation

It has been found in practice that while MOPAC and other *ab initio* programs give results regarding the fundamental vibrations of the molecules in close relation to each other, the predictions of the enthalpy of formation can differ up to a factor of 2. The mean absolute error of the AM1 method was reported to be 12 kcal/mol.[15,53] For 26 nitro-organic compounds and three organic nitrates the optimized error was found to be 5.2 kcal/mol for the PM3 and 15.7 kcal/mol for the AM1 method.[53] Some authors[56,57] have tried methods to improve these results. Melius[35] explains the way the BAC/MP4 method calculates and corrects the enthalpies of formation, but from Table 2 it can be seen that his results are on the average 3 kcal/mol lower than the experimental values, although mostly within the assigned error value. It is found that Benson's group additivity method is far more reliable than any other estimate. But even this method does not give a uniform answer since there are disputes among different groups of researchers regarding specific values of some of the groups. In this research, the NIST 94[51] program was used to evaluate all the species that were possible, since none of them were incorporated in the program's database.

The enthalpy of formation of the first four homologous mononitrocarbons and the first three nitrate compounds, were plotted in Fig. 1 as a function of the number of carbon atoms in the molecule. In both cases a perfect straight line is obtained which raises the question of whether these values were not evaluated this way. In any case if these values are correct then the value of the gaseous enthalpy of formation of 1-nitropentane can be estimated. The value found is -39.3 ± 0.5 kcal/mol as compared to the value of the liquid enthalpy of formation of 51.5 ± 0.4 kcal/mol.[45] The estimate of butylnitrate cannot be done the same way, since the three points scatter from the straight line which causes the error of the estimate to be bigger than ~5 kcal/mol.

4.5. Accuracy of Calculations

For most of the nitro compounds, the thermodynamic properties have not been measured experimentally except for the very simple nitromethane and methyl nitrate. In Table 63, the present results are compared with other calculations of simple nitro and nitrate compounds previously made by Stull *et al.*,[55] by Melius (private communication) and others.

Most of our species meet the general standard of RRHO thermodynamic calculations[8] with the exception of (1) trinitrobenzene which shows that the MOPAC calculations differ very much between themselves, (2) TNT, since it's vibration spectrum is a combination of vibrations from other toluene nitro compounds, and (3) HMX, due to the fact that the molecular data were obtained for distorted molecules, and there is also a very big uncertainty regarding its gaseous enthalpy of formation.

5. Acknowledgments

The author thanks Bonnie McBride and Dr. Martin Rabinowitz from NASA-Lewis Research Center, for the very careful checking of the results, for their suggestions to the manuscript content, and for pointing out the internal rotation contributions to the C_p maximum.

6. References

[1] H. Y. Afeefy, J. F. Liebman, and S. E. Stein, ''Neutral Thermochemical Data'' in *NIST Standard Reference Database Number 69*, edited by W. G. Mallard and P. J. Linstrom (National Institute of Standards and Technology, Gaithersburg MD, 1997); ⟨http://webbook.nist.gov⟩.
[2] E. Baroody, Naval Surface Weapons Center Report HITR 368 (October 1972).
[3] S. Benson, *Thermochemical Kinetics* (Wiley, New York, 1976).
[4] J. Berry, D. R. F. Burgess, Jr., M. R. Nyden, M. R. Zachariah, C. F. Melius, and M. Schwarz, J. Phys. Chem. **100**, 7405 (1996).
[5] C. W. Bock, S. V. Krasnoshchiokov, L. V. Kristenko, Yu. N. Panchenko, and Yu. A. Pentin, J. Mol. Struct.: THEOCHEM **149**, 201 (1987).
[6] J. C. D. Brand and T. M. Cawthon, J. Am. Chem. Soc. **77**, 319 (1955).
[7] U. Brinkmann and A. Burcat, ''A program for calculating moments of inertia of a molecule'' Technion Aerospace Reports TAE 382 (October 1979).
[8] A. Burcat and B. McBride, ''1997 Ideal gas Thermodynamic Data for Combustion and Air-Pollution Use'' Technion Aerospace Report TAE 804 (June 1997). Available at ⟨ftp://ftp.technion.ac.il/pub/supported/aetdd/thermodynamics⟩.
[9] G. A. Carpenter, M. F. Zimmer, E. E. Baroody, and R. A. Robb, J. Chem. Eng. Data **15**, 553 (1970).
[10] J. Chao, K. R. Hall, K. N. Marsh, and R. C. Wilhoit, J. Phys. Chem. Ref. Data **15**, 1369 (1986).
[11] E. R. Cohen and B. N. Taylor, J. Res. Natl. Bur. Stand. **92**, 1239 (1987).
[12] J. O. Cox and G. Pilcher, *Thermochemistry of Organic and Organometalic Compounds* (Academic, New York, 1970).
[13] L. Czuchajowski and S. A. Kucharski, Bull. Acad. Polon. Sci. Ser. Chim. Sci. **20**, 789 (1972).
[14] J. R. DeLaeter and K. G. Heumann, J. Phys. Chem. Ref. Data **20**, 1313 (1991).
[15] M. J. S. Dewar, E. G. Zobisch, F. Healy, and J. J. P Stewart, J. Am. Chem. Soc. **107**, 3902 (1985).
[16] W. B. Dixon and E. B. Wilson, Jr., J. Chem. Phys. **35**, 191 (1961).
[17] R. Engelke, D. Schiferl, C. B. Storm, and W. L. Earl, J. Phys. Chem. **92**, 6815 (1998).
[18] M. J. Frisch *et al.*, Gaussian 94, Gaussian Inc., Pittsburgh PA, 1995.
[19] D. Gorse, D. Cavagnat, M. Pesquer, and C. Lapouge, J. Phys. Chem. **97**, 4262 (1993).
[20] D. Habibollahzadeh, J. S. Murray, M. E. Grice, and P. Politzer, Int. J. Quantum. Chem. **45**, 15 (1993).
[21] G. R. Handrick, ''Report of the study of pure explosive compounds. Part IV. Calculation of heat of combustion of organic compounds from structural features and calculation of power of high explosives,'' Rpt. C-58247, Office of the Chief of Ordnance, Contract DA-19-020-ORD-47 (Arthur D. Little, Inc., Cambridge, MA, 1956), pp. 467–573.
[22] J. R. Holtzclaw, W. C. Harris, and S. F. Bush, J. Raman Spectrosc. **9**, 257 (1980).
[23] Y. K. Knobel, E. A. Miroshnichenko, and Y. A. Lebedev, Bull. Acad. Sci. USSR Div. Chem. Sci. 425 (1971).
[24] G. Krien, H. H. Licht, and J. Zierath, Thermochim. Acta **6**, 465 (1973).
[25] V. P. Lebedev, Russ. J. Phys. Chem. **49**, 1133 (1975).
[26] N. D. Lebedeva, V. L. Ryadnenko, and I. N. Kuznetsova, Russ. J. Phys. Chem. **45**, 549 (1971).

[27] N. D. Lebedeva and V. L. R. Ryadenko, Russ. J. Phys. Chem. **47**, 1382 (1973).
[28] C. Lenchitz, R. W. Velicky, G. Silvestro, and L. P. Schlosberg, J. Chem. Thermodyn. **3**, 689 (1971).
[29] J. F. Liebmann, J. Phys. Chem. Ref. Data **17**, Suppl. 1 (1988).
[30] Y. R. Luo and J. L. Holmes, J. Phys. Chem. **96**, 9568 (1992).
[31] B. J. McBride and S. Gordon, ''Computer Program for Calculating and Fitting Thermodynamic Functions,'' Report NASA-RP-1271 (November 1992).
[32] M. L. McKee, J. Am. Chem. Soc. **107**, 1900 (1985).
[33] C. McKean and R. A. Watt, J. Mol. Struct. **61**, 164 (1976).
[34] D. F. McMillan and D. M. Golden, Annu. Rev. Phys. Chem. **33**, 493 (1982).
[35] C. Melius, A database for 4000 specie calculated using the BAC/MP4, BAC/MP2 (1988) and MP4/G2 (1997) methods at Sandia Nat. Labs. and partially available at: ⟨http://herzberg.ca.sandia.gov/~melius/index.html⟩
[36] C. F. Melius, ''Thermochemical modeling application to decomposition of energetic materials,'' in *Chemistry and Physics of Energetic Materials*, edited by S. N. Bulusu (Kluwer Academic, Dordrecht, 1990), pp. 21–49.
[37] E. A. Mirishnichenko, Yu. A. Lebedev, S. A. Shevelev, V. I. Gulevskaya, A. A. Fainzil'berg, and A. Ya. Apin, Zh. Fiz. Khim. **41**, 1477 (1967).
[38] E. A. Miroshnichenko, L. I. Korchatova, V. P. Shelaputina, S. A. Zyuz'kevich, and Yu. A. Lebedev, Bull. Acad. Sci. USSR, Chem. Sci., 1778 (1988).
[39] P. R. Mochel, C. O. Britt, and J. E. Boggs, J. Chem. Phys. **58**, 3221 (1973).
[40] Afeefy *et al.*, National Institute of Standards and Technology (NIST) WebBook (1997). ⟨http://webbook.nist.gov/chemistry⟩.
[41] NIST 94, S. E. Stein (1994).
[42] D. L. Ornellas, Combust. Flame **23**, 37 (1974).
[43] P. W. Payne and L. C. Allen, *Modern Theoretical Chemistry*, edited by H. F. Schaefer III (Plenum, New York, 1977), Vol. 4.
[44] J. B. Pedley and J. Rylance, *Thermochemical Data of Organic Compounds* (University of Sussex Press, Sussex, 1977).
[45] J. B. Pedley, R. D Naylor, and S. P. Kirby, *Thermochemical Data of Organic Compounds*, 2nd ed. (Chapman and Hall, London, 1986).
[46] V. I. Pepekin, Yu. N. Matyushin, and Yu. A. Lebedev, Bull. Acad. Sci. USSR, Div. Chem. Sci., 1707 (1974).
[47] P. Politzer, P. Lane, M. E. Grice, M. C. Concha, and P. C. Redfem, J. Mol. Struct.: THEOCHEM **338**, 249 (1995).
[48] E. R. Ritter and J. W. Bozzelli, Int. J. Chem. Kinet **23**, 767 (1991).
[49] J. M. Rosen and C. Dikinson, J. Chem. Eng. Data **14**, 120 (1969).
[50] J. D. Roy and R. A. Ogg, Jr., J. Phys. Chem. **63**, 1522 (1959).
[51] S. E. Stein, NIST ''Structures and Properties and Estimation Program,'' Version 2.0 Computerized Database 25 (NIST 1994).
[52] J. J. P. Stewart, J. Comput. Chem. **10**, 209 (1989); **10**, 221 (1989).
[53] J. J. P. Stewart *Reviews of Computational Chemistry*, edited by K. B. Lipkowitz and D. B. Boyd (VCH, New York, 1990), p. 45.
[54] J. J. P. Stewart, *MOPAC 7 Manual* (1993); USAF Academy, Colorado Springs, CO 80840-6528.
[55] D. R. Stull, E. F. Westroom, and G. C. Sinke, *The Chemical Thermodynamics of Organic Compounds* (Wiley, New York, 1969).
[56] H. Wang and M. Frenklach, J. Phys. Chem. **97**, 3867 (1993).
[57] H. Wang and M. Frenklach, J. Phys. Chem. **98**, 11465 (1994).
[58] C. J. Wu and L. E. Fried, J. Phys. Chem. **101**, 8675 (1997).
[59] C. Yin *et al.*, ''Determination of heat capacity of explosives and related materials by DSC,'' Proceedings of the 17th International Pyrotechnical Seminar (1991), Vol. 1, p. 515.
[60] C. L. Yu, Y. X. Zhang, and S. H. Bauer, J. Mol. Struct. THEOCHEM **432**, 63 (1998).