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Thermophysical Properties Measurements and Models for Rocket Propellant RP-1: Phase I

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NIST
National Institute of Standards and Technology
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William A. Jeffrey, Director

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Accurate knowledge of thermophysical properties is a prerequisite to the design of efficient and cost-effective rocket engine systems that use the kerosene rocket propellant designated RP-1. A robust properties model that is based on reliable experimental measurements is the best means to provide this information to designers. Thus, a combined experimental and modeling study was carried out to elucidate the behavior of key properties over wide ranges of temperature and pressure. As a first step in this study, an RP-1 sample provided by the U.S. Air Force Research Lab (Wright-Patterson AFB, OH) was chemically characterized, which established that this sample had anomalously high concentrations of unsaturated compounds. Then, thermophysical properties were measured for this sample. Those experimental results were used to develop a mixture model based on a representative surrogate mixture. The results of this study were presented for review and comments during a December 11, 2003 workshop attended by representatives of NASA, U.S. Air Force, and their contractors.

Key words: chemical characterization; density; heat capacity; Helmholtz energy; hydrocarbons; mixture model; rocket propellant RP-1; surrogate mixture; thermal conductivity; viscosity

1. Introduction

1.1 Objective

Among the long-range objectives of research in thermophysical properties at the National Institute of Standards and Technology (NIST) is the development of accurate predictive methods for calculating the properties of gaseous and liquid mixtures of hydrocarbons. The underlying models may play a key role in design of equipment that is used in the transportation and energy sectors and for optimization of materials and energy usage. The ongoing development and testing of these models relies heavily on benchmark experimental measurements. The purpose of this report is to provide design engineers, data analysts, and experimentalists with a compilation of recent studies of the thermophysical properties for rocket propellant RP-1, a real fuel that is a complex hydrocarbon mixture. It is a well established fact that thermophysical properties of a complex mixture can vary considerably with composition. This report is denoted as Phase I since it covers thermophysical properties of the first sample of this real fuel that was furnished to NIST, with an expectation that studies of other samples would follow in Phases II, III, etc., until NIST had developed a robust compositionally variable model that was based on the measurements. The studies were carried out, during calendar year 2003, by the staff of the Experimental Properties of Fluids Group, the Theory and Modeling of Fluids Group, and the Properties for Process Separations Project, all of which are units of the Physical and Chemical Properties Division of the Chemical Science and Technology Laboratory (CSTL) of NIST. We begin with a report of the modeling effort because, while the model was the end product, its discussion provides a framework for the rest of the work. Following the models section, we present details of the underlying experimental measurements of chemical character, density, heat capacity, thermal conductivity and viscosity.

1.2 Scope

Knowledge of thermophysical properties is essential when a detailed analysis of the design and performance of a rocket propulsion system is needed. Both thermodynamic and transport properties are required. The present work stemmed from NASA's expressed need for accurate thermophysical properties that cover wide ranges of temperature and pressure. This property information is needed for a rational design of highly reliable reusable rocket engines for future launch vehicles in which the fuels are expected to encounter higher pressures and temperatures than in those previous designs. NASA's sensitivity study had concluded that property uncertainties accounted for 70 % of the uncertainty in a portion of the propulsion system design. NASA had also noted that, prior to this project, experimental data covered only limited ranges of conditions and, furthermore, the differences in RP-1 properties from different sources amounted to as much as 60 %.

To meet NASA's needs and expand knowledge in the field of kerosene-based fuels, a comprehensive program was planned and carried out. This program had both measurement and modeling components. Those results are the subject of this report.

1.3 Organization

This report is arranged in nine sections and begins with a discussion of property models. The modeling results are followed by those of measured thermophysical properties: chemical characterization, density, heat capacity, thermal conductivity, and viscosity. The experimental measurements are presented in tables and graphs. The report concludes with a discussion of a NIST workshop, some impacts of this research program, and recommendations for further studies. Section 10 following this report lists references, Appendix A details procedures for chemical analyses, and Appendix B reports computational results for the compounds in a surrogate fuel mixture.

2. Property Modeling

Since RP-1 is a complex mixture of several hundred components, modeling its properties using equations for the constituents of the mixture is not a practical solution. An alternative approach is to model the fuel as a surrogate mixture of between 10 and 20 components that can represent the thermodynamic and transport properties of the actual RP-1 fluid. Both thermodynamic properties (such as density, heat capacity, and normal boiling point) and transport properties (including thermal conductivity and viscosity) may be used in model development.

The first step in the modeling process was a chemical analysis (see Section 3) of a specific RP-1 fuel sample provided by the Fuels Branch of the Air Force Research Lab, Wright-Patterson AFB, OH. The analysis used a gas-chromatography mass/ spectrometry method and provided 37 constituent fluids. A detailed analysis shortened this list to 20 potential constituent fluids for a surrogate mixture. The lightest component identified was neohexane, and the heaviest was hexadecane. The list included linear and branched alkanes, mono and bicyclic paraffins, aromatics, and linear and branched olefins. For each of these fluids, we searched the open literature as well as databases such as TRC-SOURCE, DIPPR, Landolt-Bornstein, and NIST in-house databases for experimental physical property data. A bibliography of the results of these searches was constructed and is given in Table 1. In addition, we used predictive methods when data were not available.

In order to model the thermodynamic properties of these fluids, an equation of state of some form was required. Because of the very limited amount of data available, a generalized method was selected to describe the attributes of the fluids. A short form of a Helmholtz energy equation of state was used as a starting point. The equation is expressed with reducing variables, with the critical temperature and critical density of the fluid as the primary reducing properties.

The equation has 12 terms, and the coefficients of the equation are functions of the acentric factor. Experimental data for the normal alkanes from butane through hexatriacontane (C36) were fitted to determine the coefficients of the equation (48 in all, since each coefficient uses 4 parameters that are functions of the acentric factor). The experimental data included densities, vapor pressures, heat capacities, and sound speeds. Comparisons were made against data for both the normal alkanes as well as branched alkanes (which were not fitted) to determine that the final equation could successfully be applied to these hydrocarbons.

The generalized equation was then used to make equations for each of the 20 fluids in the surrogate. Only the critical temperature, critical density, and acentric factor are required to set up an equation for each component. The critical temperatures were taken from the literature or estimated from prediction schemes. The critical density and acentric factor were fitted using experimental vapor pressures at the boiling point and saturated liquid densities near atmospheric conditions. For fluids with additional data at other state points, the values of the critical density and acentric factor could be more closely tuned to achieve lower overall uncertainties. Viscosity and thermal conductivity surfaces for each of the constituent fluids were developed from experimental data, predictive methods, and an extended corresponding states model from sources summarized in Table 1.

The next step was to select a method for representing the properties of the RP-1 mixture. For the thermodynamic properties, we selected an excess Helmholtz energy mixture model used successfully at NIST for the representation of properties of natural gas and refrigerant mixtures [1,2]. The model uses the pure fluid equations of state with ideal mixing to account for most of the mixture properties. To account for the additional interaction between unlike molecules, an excess contribution can be used to account for the remainder of the mixture properties. However, experimental information for each binary system in the mixture is needed to determine the excess contribution. Since experimental data are not available, the excess part was set to zero. There are two additional parameters in the mixture model that can be adjusted to achieve better results. A general scheme had been developed in previous work at NIST to predict one of these parameters for systems where no data are available. This scheme was used here to improve the mixture calculations.

For transport properties, we use an extended corresponding states model [3,4]. In this approach, the properties of the mixture are represented in a two-step process that involves mapping onto a reference fluid. The reference fluid may be any well characterized fluid, but it is best to select a reference fluid that is chemically similar to the constituents of the mixture of interest. For this work, we chose n-dodecane as a reference fluid. Since it is important to have a very good representation of both the thermodynamic and transport properties of the reference fluid, as part of this project we developed a dedicated equation of state for n-dodecane and correlations for the viscosity and thermal conductivity. The results of this work are available as two publications in the journal Energy and Fuels [5,6]. The correlations for n-dodecane are valid over a wide range of fluid states, from the triple point to the onset of decomposition, and for pressures to 200 MPa. Uncertainties of properties calculated using the equation are 0.2 % in density at pressures up to 200 MPa, 0.5 % at higher pressures (up to 500 MPa), 1 % in heat capacities, 0.5 % in sound speeds, and 0.2 % in vapor pressures. The viscosity correlation has an estimated uncertainty of 0.5 % along the saturation boundary in the liquid phase, 3 % in the compressed liquid region, and 2 % in the vapor. The thermal conductivity has an estimated uncertainty of 3 % along the liquid saturation boundary and in the compressed liquid phase, and 5 % in the vapor region.

The final step in the modeling procedure was to determine the compositions of the constituent fluids that best represent the properties of the mixture. The properties that we selected for fitting were experimental densities, heat capacities, thermal conductivities, viscosities, and one boiling point that were measured as part of this work, described in separate sections of this report. Data at temperatures above 600 K were not used in the fitting process due to concerns about thermal decomposition during the measurements. A multi-property fitting routine was used to determine the compositions of the constituents of the surrogate mixture. The final mixture, summarized in Table 2, contains 14 constituent fluids, and represents the density to within 0.3 %, the heat capacity to within 7 %, the thermal conductivity to within 3 %, the viscosity to within 3 % at atmospheric pressures and 10 % at 60 MPa, and the boiling point at local atmospheric pressure to 0.5 %. It has an overall molar mass of 164.6, a hydrogen to carbon ratio (H/C) of 1.95, and an approximate chemical formula of $C_{11.8}\,H_{23.0}$. The overall composition is (by mole %) 27.4 % alkanes, 26.6 % alkenes, 18.5 % monocyclic paraffins, 22.4 % bicyclic paraffins, and 5.1 % aromatics. This mixture is a surrogate; it is not the actual mixture composition, but rather a mixture that approximates the behavior of the RP-1 sample that was investigated.

Table 1. Bibliography for property modeling.

Fuel Decomposition Studies

Author(s)	**Reference**	**Topic**
Andresen et al.	[7]	Solids formation jet fuels
Balster and Jones	[8]	Formation of insolubles in aviation fuels
Batti	[9]	Thermal stability jet fuels
Behar et al.	[10]	Thermal decomposition of dodecylbenzene
Chin et al.	[11]	Thermal stability of four kerosine-type fuels
Chin and Lefebvre	[12]	For characterizing the thermal oxidative tendencies of aviation fuels
Chin and Lefebvre	[13]	Thermal stability characteristics of kerosine-type fuels
Chin and Lefebvre	[14]	Thermal stability characteristics of hydrocarbon fuels
Edwards and Zabarnick	[15]	Surface deposition (fouling) of jet fuels
Giovanetti et al.	[16]	Thermal stability and heat-transfer characteristics of several hydrocarbon fuels
Goel and Boehman	[17]	Jet fuel degradation in flow reactors
Grinstead and Zabarnick	[18]	Oxidn. and deposition data for jet fuels
Han-Ying	[19]	Thermal stability of kerosene
Heneghan et al.	[20]	Jet fuel thermal stability
Heneghan and Harrison	[21]	development of an improved JP-8
Hines	[22]	Heat transfer to RP-1 kerosine
Kendall and Mills	[23]	Thermal stability of aviation kerosines
Lai and Song	[24]	Pyrolization of cyclohexane and seven n-alkylcyclohexanes
Liang et al.	[25]	Heat transfer characteristics of methane, propane, kerosene, aerokerosene and rocket kerosene
Ma	[26]	Thermal stability of kerosine
Marteney and Spadaccini	[27]	Thermal stability of jet fuels
Pande and Hardy	[28]	Soluble copper and stability
Roback et al.	[29]	Deposit formation in hydrocarbon fuels
Savage et al.	[30]	Review of fundamental studies and applications of reactions at supercritical conditions
Stekhun	[31]	Effect of hydrofining on thermal stability of jet fuels
Stewart et al.	[32]	Supercritical pyrolysis of decalin, tetralin, n-decane
Stiegemeier	[33]	Thermal Stability and Heat Transfer Investigation of Five Hydrocarbon Fuels
Wang	[34]	Thermophysics characterization of kerosene combustion
Watkinson and Wilson	[35]	Review of fouling of organic fluids
Wohlwend et al.	[36]	Thermal stability of RP-1, JP-10, and quadricyclane

Author(s)	Reference	Topic
Yu and Eser	[37]	Critical points of jet fuels
Yu and Eser	[38]	Thermal decomposition C10-C14 normal alkanes
Yu and Eser	[39]	Kinetics of thermal decomposition of C10-C14 normal alkanes
Yu and Eser	[40]	n-butylbenzene and n-butylcyclohexane
Yu and Eser	[41]	Thermal decomposition of decalin, tetralin
Yu and Eser	[42]	Thermal decomposition of binary mixtures of jet fuel model compounds
Volokhova and Zhorov	[43]	Pyrolysis of Russian kerosene

Surrogate Models

Author(s)	Reference	Topic
Edwards and Maurice	[44]	JP-4, JP-8, JP-5, RP-1 surrogates
Edwards	[45]	Surrogates, general petroleum distillate fuels
Farmer et al.	[46]	RP-1 surrogate
Patterson et al.	[47]	Kerosene surrogate
Violi et al.	[48]	JP-8 surrogate
Wang	[49]	Kerosene/RP-1 surrogate
Wood et al.	[50]	JP-4 surrogate

RP-1/kerosene Properties

Author(s)	Reference	Topic
Alexander et al.	[51]	Index of refraction
Blake and Sheard	[52]	Dielectric constant, kerosene
Chao	[53]	Isothermal compressibility
CPIA/M4	[54]	Properties of RP-1 including vapor pressure, density, viscosity, boiling point, fractional distillation curve, specific heat, thermal conductivity, composition
Dubovkin et al.	[55]	Vapor pressure, critical parameters Russian fuels
Kopylov	[56]	Viscosity, Russian T-1 kerosene
Kozyokov	[57]	Thermal conductivity, Russian T-1 kerosene
Liang et al.	[25]	Heat transfer characteristics of kerosene
Mehta et al.	[58]	Specific Gravity, viscosity, boiling point, chemical analysis of Russian kerosene
Piatibratov	[59]	Density, Russian T-1 kerosene
Sharma et al.	[60]	Correlation for flash point of kerosene
Sokolov and Tarlakov	[61]	Heat capacity, Russian T-1 kerosene
Sokolov and Tarlakov	[62]	Vapor pressure, Russian T-1 kerosene
Stiegemeier	[63]	RP-1, JP-7, JP-8, JP-8+100, JP-10 thermal stability

Author(s)	Reference	Topic
Vinogradov	[64]	Density, sound speed, viscosity of kerosene
Volyak	[65]	Surface tension, Russian T-1 kerosene
Wohlwend et al.	[36]	Thermal stability measurements RP-1, JP-10, quadricyclane
Wucherer and Wilson	[66]	Density, thermal conductivity
Zaytseva	[67]	Thermal conductivity, Russian T-1 kerosene

Estimation methods

Author(s)	Reference	Topic
American Petroleum Institute	[68]	viscosity, thermal conductivity
Baroncini et al.	[69]	Thermal conductivity
Chung et al.	[70]	Lennard-Jones parameters, viscosity, thermal conductivity
Constantinou and Gani	[71]	Critical point, boiling point
Deppmeier et al.	[72]	Dipole moment, radius of gyration
Ely and Hanley	[73,74]	Viscosity, thermal conductivity
Horvath	[75]	Critical point, boiling point, melting point, heat capacity, thermal conducitivty, viscosity
Joback	[76]	Critical point, boiling point, melting point
Marrero	[77]	Critical point, boiling point
Poling et al.	[78]	Critical point, boiling point, melting point, heat capacity, thermal conducitivy, viscosity
Quayle	[79]	Parachors
Rihani and Doraiswamy	[80]	Heat capacity
Stein and Brown	[81]	Heat capacity
Wilson and Jasperson	[82]	Critical point, boiling point
Yan et al.	[83]	Critical point

Potential Components in the Surrogate Model

Cyclododecane

Author(s)	Reference	Topic
Coops et al.	[84]	Melting point
Drotloff and Moller	[85]	Melting point
Fischer and Weiss	[86]	Viscosity, density, melting point, boiling point, self-diffusion coefficient
Gollis et al.	[87]	Viscosity
Ladygin et al	[88]	Viscosity
Matteoli et al.	[89]	Density

Author(s)	Reference	Topic
Meyer and Hotz	[90]	Density, vapor pressure
Mueller et al	[91]	Melting point
Ruzicka et al.	[92]	Density

Methylcyclododecane

Estimated properties

Cyclodecene

Author(s)	Reference	Topic
Allinger	[93]	Boiling point
Blomquist et al.	[94]	Density, boiling point
Cope et al.	[95]	Boiling point
Prelog et al.	[96]	Boiling point

2,10-dimethylundecane

Author(s)	Reference	Topic
Gibbons	[97]	boiling point

2,7,10-trimethyldodecane
Estimated values

3-methylundecane

Author(s)	Reference	Topic
Levene and Harris	[98]	Density, boiling point
Mann et al.	[99]	Density
Marsh et al.	[100]	Heat capacity
Petrov et al.	[101]	Melting point, density, boiling point
Prout et al.	[102]	Boiling point
Smith	[103]	Boiling point
Terres et al.	[104]	Melting point

2,9-dimethyldecane

Author(s)	Reference	Topic
Calingaert and Soroos	[105]	Density, boiling point

Author(s)	Reference	Topic
Calingaert and Soroos	[106]	Density
Dyke and Jones	[107]	Boiling point
Eykman	[108]	Density
Geist and Cannon	[109]	Density, viscosity
Mears et al.	[110]	Density, boiling point, melting point
Moore et al.	[111]	Density
Parks et al.	[112]	Triple point, melting point

2-methylnonane

Author(s)	Reference	Topic
Calingaert and Hladky	[113]	Density
Calingaert and Soroos	[105]	Boiling point, density
Eykman	[108]	Density
Geist and Cannon	[109]	Viscosity, density
Marsh et al.	[100]	Heat capacity
Mears et al.	[110]	Boiling point, freezing point
Moore et al	[111]	Density
Parks et al.	[112]	Triple point

3-methyldecane

Author(s)	Reference	Topic
Marsh et al.	[100]	Heat capacity

3-ethyl-4,4-dimethyl-2-pentene

Author(s)	Reference	Topic
Howard et al.	[114]	Density, boiling point

4-methyl-4-undecene
Estimated values

2-methylnaphthalene

Author(s)	Reference	Topic
Ambrose	[115]	Critical temperature
Briggs	[116]	Thermal conductivity
Byers and Williams	[117]	Viscosity

Author(s)	Reference	Topic
Camin and Rossini	[118]	Vapor pressure
Coulson	[119]	Boiling point
Cullinane and Chard	[120]	Freezing point
Cumper et al.	[121]	Freezing point
Evans	[122]	Viscosity, density
Glaser and Ruland	[123]	Vapor pressure
Grodde	[124]	Density
Grosse and Ipatieff	[125]	Boiling point
Hales and Townsend	[126]	Density
Huffman et al.	[127]	Triple point
Koelbel	[128]	Viscosity, boiling point
Larsen et al.	[129]	Freezing point
Luther and Wachter	[130]	Boiling point
Mair and Streiff	[131]	Density, boiling point, melting point
Marsh et al.	[100]	Heat capacity
Neuhaus	[132]	Density
Parks and Huffman	[133]	Freezing point
Rampolla and Smyth	[134]	Viscosity, density, freezing point
Salceanu	[135]	Density
Schiessler	[136]	Viscosity
Shreve and Lux	[137]	Density
Sirotenko, A.A.	[138]	Viscosity
Skvarchenko et al.	[139]	Boiling point, freezing point
Smyth	[140]	Viscosity
Streiff et al.	[141]	Freezing point
Szafranski	[142]	Freezing point
Von Auwers and Fruhling	[143]	Density
Wieczorek and Kobayashi	[144]	Vapor pressure
Yokoyama et al.	[145,146]	Viscosity

Decahydro-2-methylnaphthalene

Author(s)	Reference	Topic
Adkins and Davis	[147]	boiling point
Gollis et al.	[87]	viscosity, thermal conductivity
Gudzinowicz et al.	[148]	density, viscosity
Weissenberger et al.	[149]	boiling point, density

Heptylcyclohexane

Author(s)	Reference	Topic
Baylaucq et al.	[150]	viscosity, density
Luther	[151]	density
Marsh et al.	[100]	heat capacity
Mokbel et al.	[152]	vapor pressure
Schlenk	[153]	boiling point
Schmidt	[154]	freezing point
Schmidt and Grosser	[155]	boiling point, viscosity

Cis-decahydronaphthalene

Author(s)	Reference	Topic
Allinger and Coke	[156]	boiling point
Bird and Daly	[157]	viscosity
Boord et al.	[158]	freezing point, boiling point, density
Briggs	[116]	thermal conductivity
Camin and Rossini	[118]	density, vapor pressure, surface tension
Cheng et al.	[159]	boiling point, critical temperature
Chylinksi and Stryjek	[160]	density
Cooper et al.	[161]	boiling point
Daubin et al.	[162]	boiling point, density
Fenske et al.	[164]	density, vapor pressure
Fischer and Weiss	[86]	viscosity
Foehr and Fenske	[165]	boiling point, density
Frezzotti et al.	[166]	thermal conductivity
Glaser and Ruland	[123]	critical pressure, critical temperature
Gudzinowicz et al.	[167]	density, thermal conductivity
Guenthard et al.	[168]	density
Hibbit and Linstead	[169]	boiling point, density
Hogenboom et al.	[170]	viscosity, freezing point, density
Huckel	[171]	boiling point, freezing point, density
Huckel	[172]	density
Huckel et al	[173]	density
Ipatieff and Pines	[174]	boiling point
Jasper	[175]	surface tension
Korosi and Kovats	[176]	density, surface tension
Kuss	[177]	density
Lauer and King	[178]	density
Lozovoi et al.	[179]	density
Lyusternik and Zhdanov	[180]	viscosity
Marsh et al.	[100]	heat capacity

Author(s)	Reference	Topic
McCullough et al.	[181]	triple point
Nuzzi	[182]	viscosity
Pak and Kay	[183]	critical pressure, critical temperature
Parks and Hatton	[184]	freezing point
Parthasarathy	[185]	density
Petrov	[186]	freezing point
Polenske and Eisenlohr	[163]	boiling point, density
Prokopetz	[187]	boiling point, density
Rank et al.	[188]	boiling point
Ruzicka et al.	[189]	boiling point, density
Schiessler et al.	[190]	viscosity
Seyer and Barrow	[191]	freezing point, density
Seyer and Leslie	[192]	viscosity, freezing point
Seyer and Mann	[193]	freezing point, boiling point, vapor pressure
Seyer and Walker	[194]	density, surface tension
Shiohama et al	[195]	density
Shiohama et al	[196]	density
Sohda et al.	[197]	vapor pressure, surface tension
Stokkum	[198]	viscosity
Streiff et al.	[199]	freezing point
Timmermans	[200]	freezing point
Zeberg-Mikkelsen et al.	[201]	viscosity, density
Zelinskii	[202]	density

1- dodecene

Author(s)	Reference	Topic
Asinger	[203]	density, boiling point
Baumgarten	[204]	boiling point
Boord et al.	[205]	density, boiling point, freezing point
Engler and Hofer	[206]	density
Evans	[122]	density, viscosity, boiling point
Forziati et al.	[207]	density, vapor pressure, boiling point
Geldof and Wibaut	[208]	boiling point
Gude et al.	[209]	critical pressure, critical temperature
Hunig and Kiesel	[210]	boiling point
Jasper	[175]	surface tension
Jasper and Kerr	[211]	surface tension
Jasper and Kring	[212]	surface tension
Jeffery and Vogel	[213]	density, boiling point
Krafft	[214]	density, boiling point
Krassilchik	[215]	density
Labarre	[216]	density, boiling point

Author(s)	Reference	Topic
Lenneman et al.	[217]	boiling point
Luther	[151]	density
Lyusternik and Zhdanov	[180]	viscosity
Maman	[218]	density
Marsh et al.	[100]	heat capacity
McCullough et al.	[219]	triple point
Mukhamedzyanov and Usmanov	[220]	thermal conductivity
Petrov et al.	[221]	density, boiling point
Schiessler	[136]	viscosity
Schiessler et al.	[190]	viscosity
Schmidt	[154]	density, freezing point
Schmidt et al.	[222]	density, boiling point, freezing point, viscosity
Streiff et al.	[199]	freezing point
Tilicheev et al.	[223]	density, boiling point
Urry et al.	[224]	boiling point
Wibaut and Geldof	[225]	density
Zafiriadis and Mastagli	[226]	boiling point

1-tridecene

Author(s)	Reference	Topic
Camin and Rossini	[118]	density, vapor pressure
Jasper	[175]	surface tension
Kozacik and Reid	[227]	density
Lagemann et al.	[228]	density
Luther	[151]	density
Marsh et al.	[100]	heat capacity
Petrov et al.	[221]	density, boiling point
Pictet and Potok	[229]	density, boiling point
Scheissler	[230]	density
Schiessler	[136]	viscosity
Schiessler et al.	[190]	viscosity, density
Schmidt	[154]	density, freezing point
Schmidt et al.	[222]	density, freezing point, viscosity
Streiff et al.	[141]	freezing point
Tilicheev et al.	[223]	density, boiling point

2,2-dimethylbutane

Author(s)	Reference	Topic
Ambrose et al	[231]	critical temperature
Aucejo et al.	[232]	density, viscosity
Avery and Ellis	[233]	boiling point
Bazhulin et al.	[234]	density, boiling point
Bishop et al.	[235]	density, boiling point
Boord	[236]	boiling point
Brame and Hunter	[237]	density, boiling point
Brazier and Freeman	[238]	viscosity, density
Brewster et al.	[239]	boiling point
Brooks et al.	[240]	density, boiling point, freezing point
Chavanne and van Risseghem	[241]	density, boiling point, viscosity
Chavanne	[242]	density, boiling point
Chen and Zwolinski	[243]	density, vapor pressure
Compostizo et al.	[244]	density
Cramer and Mulligan	[245]	density, boiling point
Denyer et al.	[246]	density, boiling point, freezing point
Derfer et al.	[247]	density, boiling point
Desty and Whyman	[248]	boiling point
Dixon	[249]	density
Douslin and Huffman	[250]	triple point
Eicher and Zwolinski	[251]	viscosity
Felsing and Watson	[252]	density, boiling point
Fenske et al.	[253]	boiling point
Finke et al.	[254]	freezing point
Fischer	[255]	melting point
Foehr and Fenske	[165]	density, boiling point
Fomin and Sochanski	[256]	density
Forziati	[257]	density, boiling point, freezing point
Forziati et al.	[258]	density
Funk et al.	[259]	vapor pressure
Genco et al.	[260]	critical volume, critical temperature, critical pressure
Glasgow and Rossini	[261]	freezing point
Glasgow et al.	[262]	freezing point
Griskey and Canjar	[263]	vapor pressure
Griswold et al.	[264]	boiling point
Grummit et al.	[265]	density, boiling point
Haensel and Ipatieff	[266]	boiling point
Hickman	[267]	boiling point
Hicks-Brunn et al.	[268]	density, triple point, boiling point
Hoog et al.	[269]	density, boiling point
Howard et al.	[114]	density, boiling point, freezing point

Author(s)	Reference	Topic
Jasper	[175]	surface tension
Kay	[270]	vapor pressure, density, critical density, critical temperature, boiling point
Kay and Young	[271]	critical temperature, critical pressure
Kilpatrick and Pitzer	[272]	vapor pressure, triple point
Kimura and Benson	[273, 274, 275]	density
Kishner	[276]	density, boiling point
Kuss and Pollmann	[277]	viscosity
Lambert et al.	[278]	viscosity
Liberman et al.	[279]	density, boiling point
Lichtenfels et al.	[280]	boiling point
Maman	[281, 282]	density, boiling point
Mann et al.	[99]	density
Marker and Oakwood	[283]	density, boiling point
Markownikov	[284]	density, boiling point
Marsh et al.	[100]	heat capacity
McArdle and Robertson	[285]	density, boiling point
Moldavskii and Nizovkina	[286]	density
Nicolini and Laffitte	[287]	density, vapor pressure
Noller	[288]	density, boiling point
Oberfell and Frey	[289]	density, boiling point, freezing point
Paz Andrade	[290]	density
Pichler et al.	[291]	density, boiling point
Rank et al.	[188]	boiling point
Rodger et al.	[292]	density
Sakiadis and Coates	[293]	thermal conductivity
Sayegh and Ratcliff	[294]	vapor pressure
Schmerling et al.	[295]	density, boiling point
Serijan et al.	[296]	density
Seubold	[297]	boiling point
Shen and Williamson	[298]	density
Smittenberg at al.	[299]	triple point, boiling point
Smutny and Bondi	[300]	viscosity
Stull	[301]	vapor pressure, boiling point, freezing point
Timmermans	[302]	boiling point, freezing point
Tooke and Aston	[303]	freezing point
Treszczanowicz et al.	[304]	density
Van Risseghem	[305]	density, freezing point
Van Wijk and Versteeg	[306]	density, viscosity
Vilim	[307]	thermal conductivity
Waddington and Douslin	[308]	density
Westerdijk et al.	[309]	density, boiling point

Author(s)	Reference	Topic
Wibaut and Gitsels	[310]	boiling point
Wibaut et al.	[311]	density, boiling point, freezing point
Willingham et al.	[312]	vapor pressure, boiling point
Wojciechowski	[313]	boiling point, freezing point
Young	[314]	critical temperature, critical pressure
Zhang et al.	[315]	density

n-hexadecane

Author(s)	Reference	Topic
Ait-Kaci and Merlin	[316]	melting point
Ambrose	[115]	critical temperature
Aminabhavi and Gopalkrishma	[317]	density, viscosity
Anselme et al.	[318]	critical temperature, critical density
Aracil et al.	[319, 320]	density
Aralaguppi et al.	[321]	viscosity, density
Arenosa et al.	[322]	density
Asfour et al.	[323]	density
Assael et al.	[324]	thermal conductivity
Aucejo et al.	[232]	viscosity
Aucejo et al.	[325]	viscosity, density
Awwad et al.	[326]	viscosity
Awwad and Allos	[327]	density
Awwad and Pethwick	[328]	density
Awwad and Salman	[329, 330]	density
Awwad et al.	[331]	viscosity, density
Awwad et al.	[332, 333]	density
Banipal et al.	[334]	density
Banos et al.	[335]	density
Barber and English	[336]	boiling point, melting point, density
Behrends and Kaatze	[337]	viscosity
Benson and Handa	[338]	density
Berger	[339]	boiling point
Bhattacharyya et al.	[340]	density
Boelhouwer	[341]	density
Bogatov et al.	[342]	thermal conductivity
Boord et al.	[158]	boiling point, melting point, density
Bradley and Shellard	[343]	density
Bridgman	[344]	vapor pressure
Bronsted and Koefoed	[345]	density
Calingaert et al.	[346]	density
Camin et al	[347]	vapor pressure, density

Author(s)	**Reference**	**Topic**
Carey and Smith	[348]	melting point
Celda et al.	[349]	density
Chang et al.	[350]	density
Chawla et al.	[351]	density
Chevalier et al.	[352]	viscosity, density
Chylinski and Stryjek	[353]	viscosity
Chylinski and Stryjek	[160]	density
Cooper and Asfour	[354]	viscosity, density
Coursey and Heric	[355]	viscosity, density
Deanesly	[356]	density, melting point
DeLorenzi et al.	[357]	density, viscosity
Dernini et al.	[358]	density
Diaz Pena and Menduina	[359]	density
Diaz Pena and Nunez Delgado	[360]	density
Diaz-Pena and Tardajos	[361]	density
Dixon	[249]	density
Drahowzal	[362]	melting point
Ducooulombier et al.	[363]	viscosity
Dymond and Harris	[364]	density
Dymond and Young	[365]	viscosity, density
Dymond et al.	[366]	viscosity, density
Evans	[122]	viscosity, density
Evans	[367]	melting point
Fenby et al.	[368]	density
Ferhat-Hamida and Philippe	[369]	density
Fermeglia and Torriano	[370]	viscosity, density
Findenegg	[371]	density, melting point
Finke et al.	[372]	triple point
Foehr and Fenske	[165]	density, melting point
Fox et al.	[373]	surface tension
Francis and Wood	[374]	boiling point, vapor pressure
Gensler and Mahadevan	[375]	boiling point
Glaser et al.	[376]	density
Gollis et al.	[87]	thermal conductivity, melting point
Gouel	[377]	viscosity, density
Graaf et al.	[378]	density
Granovskaya	[379]	vapor pressure
Griot et al.	[380, 381]	density
Grolier et al.	[382]	density
Heric and Brewer	[383]	density, viscosity
Heric and Brewer	[384]	density
Heric and Coursey	[385]	density

Author(s)	**Reference**	**Topic**
Holmes et al.	[386]	thermal conductivity
Holzapfel et al.	[387, 388, 389]	density
Ivanov et al.	[390]	boiling point
Jasper	[175]	surface tension
Jasper et al.	[391]	surface tension
Kemula et al.	[392]	boiling point, melting point
Klofutar et al.	[393]	density
Korosi and Kovats	[176]	surface tension
Krafft	[394]	melting point, boiling point, density
Krafft	[395]	density, melting point
Krafft	[396]	density, vapor pressure, melting point
Lagerlof	[397]	boiling point
Lainez and Rodrigo	[398]	density
Lainez et al.	[399]	density
Lal et al.	[400]	density, viscosity
Langedijk and Smithuysen	[401]	density, melting point
Larkin et al.	[402]	melting point
Larsen et al.	[129]	boiling point, melting point
Lauer and King	[178]	density
Lee et al.	[403]	vapor pressure
Lenoir and Hipkin	[404]	density
Levene	[405]	boiling point
Levene et al.	[406]	boiling point, melting point
Lim and Williamson	[407]	density
Luther	[151]	density
Mabery	[408]	boiling point
Mabery	[409]	boiling point, density
Mansker et al.	[410]	density
Marsh et al.	[100]	heat capacity
Marsh and Organ	[411]	density
Matsui and Arakawa	[412]	boiling point, melting point, density
Matthews et al.	[413]	viscosity, density
McKinney	[414]	boiling point
McMakin and Van Winkle	[415]	density
Messow et al.	[416]	density
Mills and Fenton	[417]	vapor pressure
Mogollon et al.	[418]	critical temperature
Mukhamedzyanov et al.	[419]	thermal conductivity
Mumford and Phillips	[420]	density, melting point, boiling point, viscosity
Mustafaev	[421]	thermal conductivity
Myers	[422]	vapor pressure

Author(s)	Reference	Topic
Myers and Clever	[423]	surface tension, density
Myers and Fenske	[424]	vapor pressure
Nederbragt and Boelhouwer	[425]	viscosity
Nhaesi and Asfour	[426]	density, viscosity
Oddo	[427]	boiling point, melting point
Orwoll and Flory	[428]	melting point
Parks et al.	[429]	vapor pressure, triple point
Perez et al.	[430]	vapor pressure
Petrov	[186]	melting point
Petrov and Kaplan	[431]	boiling point, density
Philippe and Delmas	[432]	density
Pilcher	[433]	triple point
Plebanski et al.	[434]	density
Powell and Groot	[435]	thermal conductivity
Prophete	[436]	melting point
Queimada et al.	[437]	density, viscosity
Ralston et al.	[438]	melting point
Rasskazov et al.	[439]	viscosity
Rastorguev and Keramidi	[440]	viscosity
Ratkovics et al.	[441]	viscosity
Richardson and Parks	[442]	density
Rolo et al.	[443]	surface tension
Rosenthal and Teja	[444]	critical pressure, critical temperature
Sakiadis and Coates	[445]	thermal conductivity
Sanin and Melent'eva	[446]	viscosity
Schiessler	[136]	viscosity
Schiessler et al.	[190]	vapor pressure, density
Schiessler	[230]	melting point
Seyer et al.	[447]	density
Shen and Williamson	[298]	density
Smith	[448]	melting point
Smith et al.	[449, 450]	critical temperature
Snow et al.	[451]	melting point
Snyder and Winnick	[452]	density
Sondheimer and Amiel	[453]	boiling point, melting point
Sorabji	[454]	boiling point, melting point
Streiff et al.	[141]	melting point
Suehnel et al.	[455]	density
Tanaka et al.	[456]	viscosity, density
Tardajos et al.	[457, 458]	density
Tarzimanov and Mashirov	[459]	thermal conductivity
Teja and Rice	[460]	density

Author(s)	**Reference**	**Topic**
Teja et al.	[461]	critical temperature
Terhoff	[462]	density
Tilicheev and Kachmarchik	[463]	melting point, density
Tilicheev and Kachmarchik	[464]	density
Tilicheev et al.	[465]	boiling point, melting point, density
Trejo	[466]	density
Treszczanowicz et al.	[467]	density
Treszczanowicz et al.	[468]	density
Tuot and Guyard	[469]	boiling point, density
Ubbelohde	[470]	vapor pressure, melting point
Van Hook and Silver	[471]	density, melting point
Vavanellos et al.	[472]	viscosity
Vogel	[473]	boiling point, melting point, density
Wada et al.	[474]	thermal conductivity
Wakefield	[475]	viscosity, density
Wakefield and Marsh	[476]	viscosity, density
Wang et al.	[477]	density
Waterman et al.	[478]	boiling point, melting point, density
Whitmore et al.	[479]	viscosity
Wibaut et al.	[311]	density
Wilhelm et al.	[480, 481]	density
Witek et al.	[482]	density
Wu et al.	[483]	viscosity
Young	[484]	boiling point, vapor pressure
Zeinalov and Leikakh	[485]	density
Ziegler et al.	[486]	boiling point, melting point

n-dodecane

Author(s)	**Reference**	**Topic**
Aicart et al.	[487]	density
Allemand et al.	[488, 489]	vapor pressure
Ambrose and Townsend	[490]	critical pressure
Ambrose et al.	[231]	critical temperature
Aminabhavi and Banerjee	[491]	viscosity
Aminabhavi and Gopalkrishma	[317]	viscosity, density
Aminabhavi and Patil	[492]	viscosity, density
Anselme et al.	[318]	critical density, critical temperature
Aralaguppi et al.	[321 493]	viscosity, density
Arenosa et al.	[322]	density

Author(s)	Reference	Topic
Asfour et al.	[323]	density
Aucejo et al.	[494, 495]	density
Aucejo et al.	[496]	viscosity
Aucejo et al.	[232]	viscosity, density
Awwad and Salman	[329]	viscosity, density
Awwad et al.	[331]	viscosity
Awwad and Allos	[497]	viscosity, density
Awwad et al.	[331, 332]	density
Beale and Docksey	[498]	critical pressure, critical temperature, boiling point
Benson et al.	[499]	density
Berger	[339]	boiling point
Bessieres, D. et al.	[500]	
Bhattacharyya et al.	[340]	density
Bidlack and Anderson	[501]	viscosity
Bingham and Fornwalt	[502]	density, viscosity
Boelhouwer	[341]	density
Boord et al.	[158]	boiling point, density, freezing point
Bridgman	[344]	vapor pressure
Burgdorf et al.	[503]	viscosity, thermal conductivity, density
Campbell et al.	[504]	boiling point
Caudwell et al.	[505]	viscosity, density
Celda et al.	[349]	density
Celda et al.	[506]	viscosity
Chawla et al.	[351]	density
Chevalier et al.	[352]	viscosity, density
Cooper et al.	[161]	boiling point
Cooper and Asfour	[354]	viscosity, density
Crawford and Harbourn	[507]	freezing point
Cutler	[508]	density
Cutler et al.	[509]	density, viscosity
De Lorenzi et al.	[357]	viscosity, density
Deanesly and Carleton	[356]	density, freezing point
Dejoz et al.	[510]	density, boiling point, vapor pressure
DeLorenzi et al.	[357]	density
Dernini et al.	[358]	density
Diaz Pena and Menduina	[359]	density
Diaz Pena and Nunez Delgado	[360]	density
Diaz Pena and Tardajos	[361]	density
Dixon	[249]	density
Dornte and Smyth	[511]	density
Drabek and Cibulka	[512]	density
Ducoulombier et al.	[363]	viscosity
Dymond et al.	[366]	viscosity

Author(s)	Reference	Topic
Dymond et al.	[513]	viscosity, density
Dymond et al.	[514, 515]	density
Evans	[367]	viscosity, density, boiling point
Fenske et al.	[253]	boiling point
Ferhat-Hamida and Philippe	[369]	density
Findenegg	[371]	density
Finke et al.	[372]	triple point
Francis	[516]	critical temperature, density
Garcia et al.	[517]	viscosity
Gensler et al.	[518]	boiling point
Gierycz et al.	[519]	vapor pressure
Giller and Drickamer	[520]	viscosity, freezing point
Gollis et al.	[87]	thermal conductivity, freezing point
Gomez-Ibanez and Liu	[521]	boiling point, density
Gonzalez et al.	[522]	viscosity, density
Gouel	[377]	viscosity
Gouel	[523]	density
Grigg et al.	[524]	density
Griot et al.	[381]	density
Grolier and Benson	[525]	density
Grolier et al.	[382]	density
Guieu et al.	[526]	freezing point
Hamam et al.	[527]	density
Hansen and Hansen	[528]	boiling point
Hogenboom et al.	[529]	viscosity, freezing point
Horie and Morikawa	[530]	density, boiling point, freezing point
Houser and McLean	[531]	density, vapor pressure
Huffman et al.	[127]	triple point
Iwahashi et al.	[532]	viscosity
Jasper et al.	[391]	surface tension
Jessup and Stanley	[533]	boiling point, density, freezing point
Jobst	[534]	thermal conductivity
Kashiwagi and Makita	[535]	viscosity
Kashiwagi et al.	[536]	thermal conductivity
Keistler and Andrews	[537]	density, vapor pressure
Keramidi and Rastorguev	[538]	viscosity
Kharasch et al.	[539]	boiling point
Kincannon and Manning	[540]	boiling point, density
Knapstad et al.	[541]	viscosity
Knapstad et al.	[542]	viscosity, density
Korosi and Kovats	[176]	surface tension
Krafft	[396]	density, freezing point, vapor pressure
Kurtyka and Kurtyka	[543]	boiling point

Author(s)	Reference	Topic
Lainez et al.	[399]	density
Landau and Wuerflinger	[544]	density
Leslie and Heuer	[545]	freezing point
Luther	[151]	density
Lyusternik and Zhdanov	[180]	viscosity
Lyvers and Belyanina	[546]	density
Mair	[547]	freezing point
Mair and Streiff	[131]	density, boiling point, freezing point
Mallan et al.	[548]	thermal conductivity
Maman	[218]	boiling point, density
Mansker et al.	[410]	density
Marsh et al.	[100]	heat capacity
Mears et al.	[549]	boiling point, freezing point, density
Messow et al.	[416]	density
Mogollon et al.	[418]	critical temperature
Moreiras et al.	[550]	viscosity, density
Morse	[551]	boiling point
Mukhamedzyanov et al.	[552]	thermal conductivity
Mustafaev	[553]	thermal conductivity
Nayak et al.	[554]	viscosity, density
Neruchev et al.	[555]	density, boiling point
Ortega et al.	[556, 557, 558]	density
Ott and Goates	[559]	freezing point
Pak and Kay	[560]	critical pressure, critical temperature
Parks and Huffman	[133]	freezing point
Petrov and Kaplan	[431]	density, boiling point
Philippe and Delmas	[432]	density
Powell and Groot	[435]	thermal conductivity
Quayle et al.	[561]	density, boiling point
Ralston et al.	[438]	freezing point
Rosenthal and Teja	[444]	critical pressure, critical temperature
Sahgal and Hayduk	[562]	density
Sakiadis and Coates	[445]	thermal conductivity
Schiessler	[230]	freezing point, vapor pressure
Schiessler et al.	[190]	density
Schmidt et al.	[563]	density, surface tension
Seyer	[564]	freezing point
Shen and Williamson	[298]	density
Shen et al.	[565]	density
Shepard et al.	[566]	density, freezing point, viscosity, boiling point
Smith	[567]	thermal conductivity
Smith et al.	[450]	critical temperature
Snyder and Winnick	[452]	density

Author(s)	Reference	Topic
Sondheimer and Amiel	[453]	boiling point
Sondheimer et al.	[568]	freezing point
Streiff et al.	[141]	freezing point
Suri	[569]	density
Takagi and Teranishi	[570]	density
Tanaka	[456]	viscosity, density
Tanaka et al.	[571]	thermal conductivity
Tardajos et al.	[457, 458]	density
Teja et al.	[461]	critical temperature
Terhoff	[462]	density
Tilicheev et al.	[223]	boiling point, freezing point
Tilicheev et al.	[465]	density
Timmermans	[572]	freezing point
Trejo	[466]	density
Trenzado et al.	[573]	viscosity, density
Treszczanowicz and Lu	[574]	vapor pressure
Treszczanowicz et al.	[468, 575]	density
Tsimering and Kertes	[576]	density
Vogel	[473]	boiling point, density
Vogel and Schuberth	[577]	density
Wakefield and Marsh	[476]	viscosity
Wakefield	[475]	viscosity, density
Wang et al.	[477, 578]	density
Weissler and Del Grosso	[579]	density
Wilhelm et al.	[480, 481]	density
Willingham et al.	[312]	vapor pressure
Witek et al.	[482]	density
Wu et al.	[483]	viscosity
Yanes et al.	[580]	density
Young	[484]	vapor pressure, boiling point
Ziegler et al.	[486]	boiling point, freezing point
Zook and Goldey	[581]	boiling point

Table 2. Surrogate mixture formulation.

Fluid	CAS #	Formula	MW	Mole%
3-ethyl-4,4-dimethyl-2-pentene	53907-59-8	C_9H_{18}	126.24	9.98
Cyclodecene	3618-12-0	$C_{10}H_{18}$	138.25	2.11
2-methylnonane	871-83-0	$C_{10}H_{22}$	142.28	2.32
2-methylnaphthalene	91-57-6	$C_{11}H_{10}$	142.20	5.10
2-methyldecalin	2958-76-1	$C_{11}H_{20}$	152.28	22.35
3-methyldecane	13151-34-3	$C_{11}H_{24}$	156.31	10.84
1-dodecene	112-41-4	$C_{12}H_{24}$	168.32	2.64
Cyclododecane	294-62-2	$C_{12}H_{24}$	168.32	4.27
4-methyl-4-undecene	61142-40-3	$C_{12}H_{24}$	168.32	10.45
n-dodecane	112-40-3	$C_{12}H_{26}$	170.33	1.93
Heptylcyclohexane	5617-41-4	$C_{13}H_{26}$	182.35	14.22
1-tridecene	2437-56-1	$C_{13}H_{26}$	182.35	1.45
2,7,10-trimethyldodecane	74645-98-0	$C_{15}H_{32}$	212.41	10.38
n-hexadecane	544-76-3	$C_{16}H_{34}$	226.44	1.95

Σ = 99.99 %

3. Chemical Characterization

Rocket propellant RP-1 is a kerosene, a complex hydrocarbon mixture that may be thermally unstable at temperatures above 600 K. Thus, it was critical to the success of this project to characterize the components in RP-1, both before and after experimental properties studies. A discussion of the procedures, interpretation of results and identification of components are provided in Appendix B. Tables 3 to 7 provide the results of the chemical characterization of the RP-1 sample.

Table 3. Tier 1 - Identification of constituents of 2 % (mass/mass) or higher. These constituents represent 59 % of the total mass in the sample.

Peak	Retention time, min	Profile	Corr. coef.	Conf.	Name	CAS Reg. No.	RMM	%
1	4.480	S	50	M	2,2-dimethyl-butane	000075-83-2	86.11	2.375
2	4.619	A	64	H	3-methyl-decane	013151-34-3	156.19	3.985
3	5.117	A	43	M	3-ethyl-4,4-dimethyl-2-pentene	053907-59-8	126.14	2.726
4	5.486	A	47	M	2,9-dimethyl-decane	001002-17-1	170.2	6.280
5	5.808	S	94	H	2-methyl-cis-decalin	1000152-47-3	152.16	3.970
6	6.008	A	98	H	decahydro-2-methyl naphthalene	002958-76-1	152.16	2.574
7	6.307	S	50	M	cis-syn-1-methyl-decalin	1000158-89-1	152.16	4.652
8a†	6.468 6.537 6.653	S A S	46 43	M M	1-hexyl-3-methylcyclo pentane cyclo dodecane	061142-68-5 000294-62-2	168.19 168.19	5.099
9	7.443	S	43	M	1-dodecene	000112-41-4	168.19	5.995
10	7.789	S	78	H	2-methyl-undecane	007045-71-8	170.2	3.124
11	7.996	S	59	M	3-methyl-undecane	001002-43-3	170.2	2.839
12	8.150	A	56	M	2,2-dimethyl-decadi-3,5-ene	055638-50-1	166.17	2.735
13	8.464	S	NA	M	methylcyclo-dodecane	NA	182.22	3.580
14	9.194	S	90	H	dodecane	000112-40-3	170.20	5.327
15	9.746	S	50	M	2,7,10-trimethyl-dodecane	074645-98-0	212.25	3.765

† This peak consists of two coeluting solutes.

Table 4. Tier 2 - Identification of constituents of 1 % (mass/mass) or higher. These constituents represent 18.7 % of the total mass of the sample.

Peak	Retention time, min	Profile	Corr. coef.	Conf.	Name	CAS Reg. No.	RMM	%
a	3.144	A	50 38	M M	2,7-di-methyl octane or 2-methyl nonane	001072-16-8 000871-83-0	142.17 142.17	1.329
b	4.303	S	89	H	cyclodecene	003717-12-0	138.14	1.610
c	4.373	A	50	U	cis-deca-hydro naphthalene	108746-01-6	138.14	1.174
d	6.944	A	14	M	z-1,9-dodeca-diene	1000245-71-0	166.17	1.754
e	7.075	S	15	M	4-methyl-4-uncecene	061142-40-3	168.19	1.663
f	9.846	S	20	M	x-tridecene†	NA	182.2	1.115
g	10.230	A	30	M	1-tridecene	111270-56-1	182.2	1.241
h	10.514	S	72	H	heptylcyclo-hexane	005617-41-4	168.19	1.429
i	10.698	S	43	M	x-tridecene	NA	182.2	1.305
j	11.359	A	45	M	x-tridecene	NA	182.2	1.977
k	11.881	S	58	M	2,10-di-methyl undecane	017301-27-8	184.22	1.507
l	12.349	A	NA	M	x-methyl tridecane	NA	197.2	1.494
m	12.787	S	94	H	2-methyl naphthalene	000091-57-6	142.08	1.249
aa	13.623	S	97	H	tridecane	000629-50-5	184.22	1.080

† x signifies uncertainty in the location of the double bond or the methyl group.

Table 5. Light fraction-identification of constituents of lightest components. These components represent 1.7 % of the total mass of the sample.

Peak	Retention time, min	Profile	Corr. coef.	Conf.	Name	CAS Reg. No.	RMM	%
laa	0.795	A	2	M	methane	107902-82-8	16.03	trace
la	1.924	A	50	H	nonane	000111-84-2	128.16	0.179
lb	2.615	A	90	H	1,3,5-trimethyl-cyclohexane	001795-26-2	126.14	0.654
1d	3.551	A	52	H	2-methyldecane	006975-98-0	156.19	0.817

Table 6. Heavy fraction-identification of constituents of heaviest components. These constituents are not tabulated for mass percent.

Peak	Retention time, min	Profile	Corr. coef.	Conf.	Name	CAS Reg. No.	RMM	%
ha	21.776	S	30	M	5-methyl-2-undecene	056851-34-4	168.19	
hb	22.010	A	86	H	2,6,10-trimethyl-dodecene†	NA	210.25	
hc	22.433	A	59 47	U	3-methyl tridecane or tetradecane	006418-41-3 or 000629-59-4	198.24 198.24	
hd	24.083	A	43 22	U	hexadecane, or 1-tetradecene	000544-76-3 or 001120-36-1	226.27 196.22	

† The location of double bond is not clear.

Table 7. Thermal decomposition kinetics measurements on RP-1.

Temperature (ºC)	$k \pm 1\sigma$ (s^{-1})	$t_{1/2}$ (min)
375	$(6.92 \pm 0.75) \times 10^{-5}$	167
400	$(2.00 \pm 0.23) \times 10^{-4}$	58
425	$(3.85 \pm 0.53) \times 10^{-4}$	30
500	$(1.07 \pm 0.17) \times 10^{-3}$	11

4. Density

4.1 Density at Atmospheric Pressure

The density of RP-1 was measured with an Archimedes (buoyancy) technique over the temperature range 1 to 43 ˚C under a nitrogen blanket at the prevailing atmospheric pressure (approximately 83 kPa). These measurements provide a direct determination of the density. They were conducted to provide a consistency check on the wide-ranging measurements made at Azerbaijan State Oil Academy and to investigate the potential batch-to-batch variation in this property.

The core of the experimental apparatus consists of a cylindrical aluminum "sinker" (m = 11.54077 ± 0.00010 g; V = 4.2735 ± 0.0013 cm^3) that is housed in a test cell containing the fluid of interest. This sinker is suspended from a balance, and the experiment consists of weighing the (sinker + suspension device) and the suspension device alone (to give the "tare" weight). The density is given by

$$\rho = \frac{m_{\text{sinker}} - \left(W_{\text{sinker}} - W_{tare}\right)}{V_{\text{sinker}}},$$

where W_{sinker} and W_{tare} are the balance readings, and m_{sinker} and V_{sinker} are the mass and volume of the sinker. The volume of the sinker is adjusted for temperature from literature values for the thermal expansion of aluminum. Each density determination comprises multiple tare and sinker weighings, and the balance is calibrated before each determination by use of a small brass calibration mass placed on an auxiliary pan located above the test cell. The total uncertainty in the density is estimated to be ±0.10 % (k = 2).

Temperature is controlled by an external bath circulating a propylene gycol mixture through channels in a copper shield surrounding the test cell. The temperature of the fluid is measured with a standard platinum resistance thermometer located in a thermowell in the test cell; its resistance is read with a nanovolt-level multimeter. The uncertainty in the temperature is ±0.010 ˚C. The standard deviation in the temperature over the 20 minutes needed to complete a single density determination averaged 0.004 ˚C. The atmospheric pressure was read with a vibrating quartz crystal type pressure transducer with an uncertainty of ±0.07 kPa.

The results are presented in Table 8 and Figure 1(a) for the original sample of RP-1. Three repetitions were carried out at each temperature. The sample was held statically in the cell a total of 10 days, and repeats of the 25 ˚C point taken nine days apart exhibited variations less than 0.15 % in density. This provides an indication that the sample did not undergo any gross degradation or fractionation during the tests. These data have been correlated by a second-order polynomial (given in the figure) to facilitate comparisons.

Results for the ultra-low sulfur sample of RP-1 are given in Table 9. The percentage differences in density compared to the original RP-1 sample are shown in Figure 1(b) (where the baseline is the polynomial fit of the densities of the original sample). The differences between the two samples are seen to average 0.28 %, with the ultra-low sulfur sample having the higher densities.

Table 8. Experimental densities for RP-1 (original sample) under nitrogen.

Temperature, ˚C	Pressure, kPa	Density, kg/m^3
2.902	83.59	813.18
2.899	83.59	813.30
2.892	83.59	813.28
23.283	83.72	799.01
23.319	83.69	799.09
23.355	83.67	799.01
25.066	83.07	798.71
25.072	83.10	797.58
25.083	83.10	797.66
43.115	83.07	785.01
43.109	83.10	784.96
43.050	83.10	785.09

Table 9. Experimental densities for RP-1 (ultra-low sulfur) under nitrogen.

Temperature, ˚C	Pressure, kPa	Density, kg/m^3
1.081	82.13	816.71
1.091	82.12	816.70
1.106	82.10	816.60
23.941	82.61	800.88
23.911	82.61	800.91
23.878	82.63	801.15
39.693	82.25	790.01
39.705	82.23	789.79
39.720	82.25	789.68

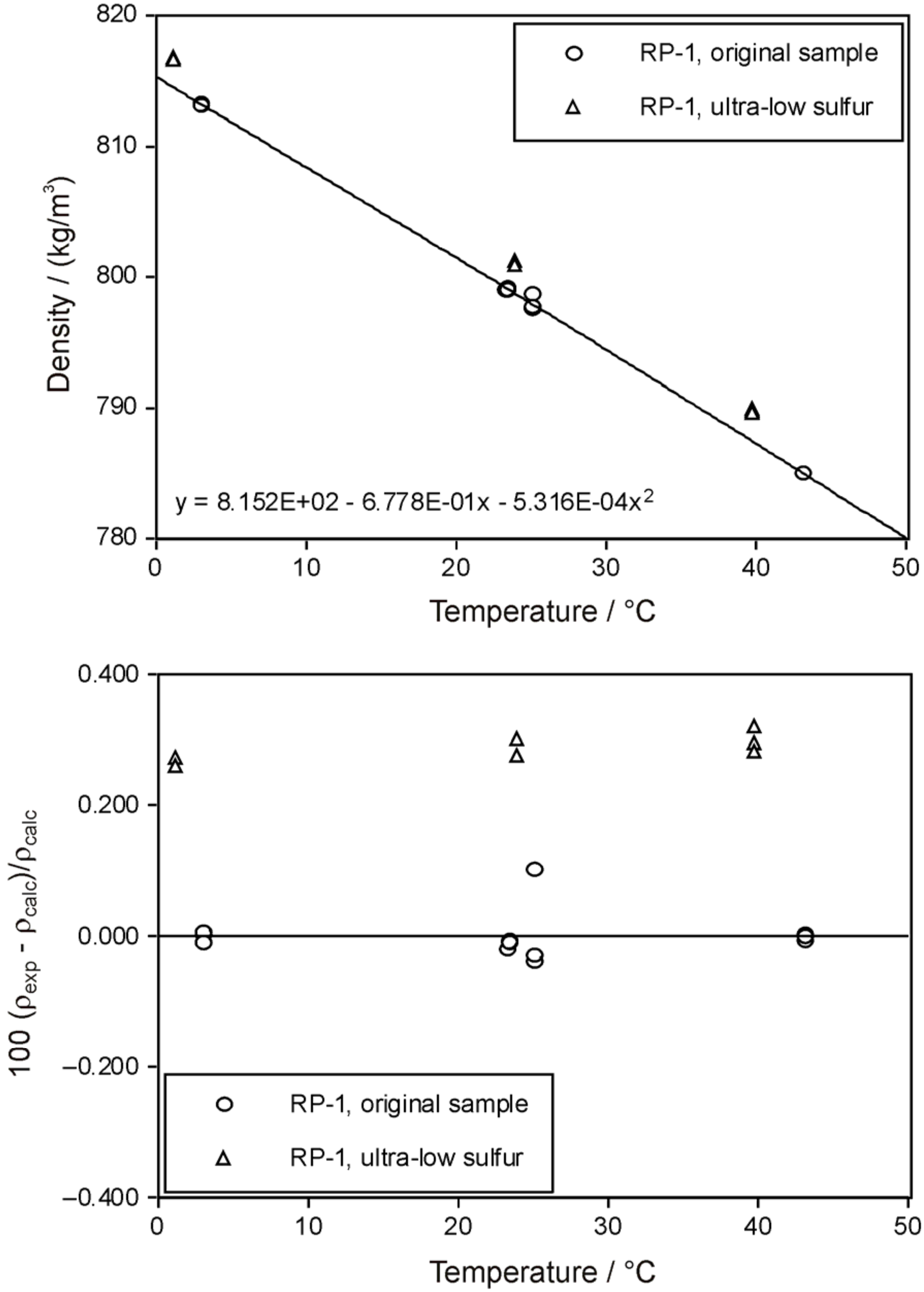

Figure 1. Density of RP-1 at atmospheric pressure; (a) measured densities; (b) deviations of density from the simple polynomial correlation.

4.2 Density at Elevated Pressures

Densities were measured with a constant-volume piezometer that operates at conditions up to 745 K and 60 MPa. This study was carried out under a contract to Prof. Ilmudin M. Abdulagatov (Russian Academy of Sciences, Makhachkala) who set up a collaborative project with Prof. Nazim D. Azizov (Azerbaijan State Oil Academy (ASOA), Baku). The uncertainty estimated by ASOA for the density measurements is 0.5 $kg \cdot m^{-3}$ (for $T<623$ K) and 0.1 % (for $T>623$ K). Those experimental data were privately communicated to NIST and were used, in addition to NIST measurements, to develop the models discussed in Section 2.

5. Heat Capacity

Heat capacities are fundamental to our knowledge of the thermal properties of any substance or mixture. They may be regarded as a measure of the rate of change of energy storage in molecular systems. Heat capacity is defined by the operational path taken during an exchange of energy with the surroundings; the path may be at a constant pressure, at constant density, or along a phase saturation curve. In practice, we may measure a change in enthalpy at constant pressure C_p or a change in internal energy at constant volume C_v. However, it is not possible to measure a heat capacity at a fixed pressure condition of vapor-liquid saturation. This is so because an addition of a small quantity of energy will evaporate a portion of the sample but will not raise its temperature, and thus an infinite heat capacity would be calculated. On the other hand, it is feasible to directly measure heat capacity in the vapor-liquid two-phase region, $C_v^{(2)}$, and then calculate the saturated liquid heat capacity from well-established thermodynamic relations.

Heat capacities at constant pressure were measured with a flow calorimeter that operates at conditions up to 671 K and 60 MPa. This study was carried out under a contract to Prof. Ilmudin M. Abdulagatov (Russian Academy of Sciences, Makhachkala) who set up a collaborative project with Prof. Nazim D. Azizov (Azerbaijan State Oil Academy (ASOA), Baku). The uncertainty estimated by ASOA for the heat capacity measurements is 2 % (for T<573 K) and 3 to 4 % (for T>573 K). Those experimental data were privately communicated to NIST and were used, in addition to NIST measurements, to develop the models discussed in Section 2.

6. Thermal Conductivity

Transient hot-wire measurements of the thermal conductivity of the RP-1 liquid sample were made along nine isotherms at temperatures from 300 to 700 K with pressures up to 70 MPa. Rapid decomposition was observed at 700 K. Only data up to 650 K (8 isotherms) are shown in Figure 2. The transient hot-wire instrument has been described in detail. The measurement cell is designed to closely approximate transient heating from a line source into an infinite fluid medium. The ideal (line source) temperature rise ΔT_{id} is given by,

$$\Delta T_{id} = \frac{q}{4\pi\lambda}\left[\ln(t) + \ln\left(\frac{4a}{r_0^{2} C}\right)\right] = \Delta T_w + \sum_{i=1}^{10} \delta T_i , \qquad (1)$$

where q is the power applied per unit length, λ is the thermal conductivity of the fluid, t is the elapsed time, $a = \lambda/\rho C_p$ is the thermal diffusivity of the fluid, ρ is the density of the fluid, C_p is the isobaric specific heat capacity of the fluid, r_0 is the radius of the hot wire, C = 1.781... is the exponential of Euler's constant, ΔT_w is the measured temperature rise of the wire, and δT_i are corrections to account for deviations from ideal line-source conduction. The significant corrections for the RP-1 measurements are for the finite wire diameter and thermal radiation from the IR absorbing fluid. A plot of ideal temperature rise versus logarithm of elapsed time should be linear, such that thermal conductivity can be found from the slope, and thermal diffusivity can be found from the intercept of a line fit to the data.

At time zero, a fixed voltage is applied to heat a small-diameter wire that is immersed in the fluid of interest. The wire is used as an electrical heat source, while its resistance increase allows determination of the transient temperature rise as a function of elapsed time. Two tungsten wires that have different lengths but the same 4 μm diameter are connected such that the response of the short wire is subtracted from the response of the long wire to eliminate the effects of axial heat conduction. Short experiment times (nominally 1 s) and small temperature rises (nominally 1 to 3 K) are selected to eliminate heat transfer by free convection. Experiments at several different heating powers (and temperature rises) allow verification that free convection is not significant. Heat transfer due to thermal radiation is more difficult to detect and correct when the fluid can absorb and re-emit infrared radiation such as RP-1. Thermal radiative heat transfer will increase roughly in proportion to the absolute temperature cubed and can be characterized from an increase in the apparent thermal conductivity as experiment time increases because radiative emission from the fluid increases as the thermal wave diffuses outward. Measurements of argon gas made prior to the RP-1 measurements verified that the apparatus was performing correctly.

The results of 465 transient hot-wire measurements are given in Table 10 for temperatures from 300 K to 650 K. Each experiment is characterized by the initial cell temperature T_0 and the mean experiment temperature T_e. There are generally five experiments at each initial cell temperature to verify that convection was not significant, since convection depends strongly on the temperature rise $(\Delta T = T_e - T_0)$. The conditions of the fluid during each measurement are given by the experimental temperature T_e, pressure P_e, and density ρ_e. Two values of measured thermal conductivity are reported. The thermal conductivity without correction for thermal radiation is given by λ_e, while the value corrected for thermal radiation is given by λ_c. The magnitude of the radiation correction can be found through comparison of these two values and varies from 0.1 % at 300 K to 3.5 % at 550 K, increasing to 6.6 % at 650 K. Both values of thermal conductivity are provided for comparison with literature data where the radiation correction has often not been considered. Details of the thermal radiation correction and validation of its use with liquid toluene have been presented elsewhere. Measured thermal conductivity data for RP-1, corrected for thermal radiation, are shown in Figure 3. Empirical values for the product of the mean absorption coefficient times the refractive index squared (Kn^2) are provided in Figure 4 as a function of fluid density (temperatures range from 300 K to 650 K). The solid line is given by a cubic polynomial fit in terms of density; the fit was used to correct the transient hot-wire data for thermal radiation.

Measurements were made at increasing temperatures on the original sample from 300 K to 600 K. The sample was collected for chemical analysis and the cell was charged with fresh RP-1 for measurements at 650 K. The 650 K sample was collected and the cell was charged again with fresh sample for the 700 K isotherm. Rapid decomposition of the RP-1 sample was observed at 700 K. Measured thermal conductivity at 700 K was significantly higher and inconsistent with values obtained at lower temperatures. The 700 K sample was collected and the three samples were analyzed for decomposition by gas chromatography-mass spectrometry-infrared detection (GC-MS-IR). There is clear evidence in the 650 K sample of sample reactions and discoloration with a significant increase in aromatics, including heavier aromatics such as naphthalenic compounds. The 700 K sample shows the predominance of these reactions with a further significant increase in aromatic and napthalenic components.

After significant reactions were observed at 700 K, a study of measured thermal conductivity as a function of residence time at 650 K was made. After filling and initial temperature equilibration at 650 K, there was a steady increase in cell pressure and decrease in cell temperature. While this would be characteristic of cracking reactions, which are endothermic and produce products of low molecular weight, chemical analysis suggests that other reactions are also responsible for the observed changes. The pressure increase was from 13.1 MPa to 14.8 MPa over a 9 h period. The thermal conductivity increased by 0.3 % over the same period, while the temperature decreased by 0.4 K. This thermal conductivity is 2.4 % smaller than expected based on the changes in temperature and pressure. Thus, the thermal conductivity changes by about 2 % due to changes in sample composition during this period at 650 K. This new isotherm agreed with the previous measurements at 650 K to within about 3 %. However, some of this disagreement is likely due to a solid coating that was present on the hot wires after exposure to the RP-1 sample at 700 K.

Figure 5 shows significant deposits of solid material that were found on the hot wires after measurements at 700 K. It appears that the material was molten but nonvolatile when the RP-1 sample was flashed and removed at 700 K. Small diameter cylindrical sections that are only slightly larger than the wire diameter are seen between the larger “beads”. The spherical-bead shape of the deposits was likely due to minimization of interfacial forces at the molten film-wire and film-gas boundaries. Measurements were made on liquid toluene near 300 K after the measurements at 700 K and excellent agreement (0.3 % difference) was found with reference data for the thermal conductivity of toluene even with the presence of the solid material on the wire. Thus, the thermal conductivity of the solid deposit is likely close to that of toluene, an aromatic material, but slightly different from` that of the original RP-1 sample. The deposit was not soluble in toluene at 300 K.

The uncertainty of the measured thermal conductivity data is less than 0.5 % for temperatures from 300 to 450 K where decomposition and thermal radiation were not significant. At higher temperatures, the uncertainty increases due to sample decomposition and increased thermal radiation heat transfer. This uncertainty is about 1.0 % at 550 K and increases significantly when the effects of decomposition are observable in the measured thermal conductivity as a function of sample residence time at 650 K. At 650 K the uncertainty is about 4 %, due largely to changes in sample composition.

Deviations between the measured thermal conductivity data, corrected for thermal radiation, and the corresponding states model developed in this project for the thermal conductivity of RP-1 are shown in Figure 6. The deviations are generally within 3 % for temperatures between 300 K and 400 K, but the model is systematically higher than the data as the density decreases along an isotherm and as temperature increases. The model is systematically 4 % to 12 % higher than the data along the 650 K isotherm. The data for each isotherm are consistent within the uncertainties given above, both within the isotherm and among the eight isotherms. There are some "discontinuities" of the order of 1 % in the deviation plot along the higher temperature isotherms. These "discontinuities" are not present in the measured thermal conductivity data, as shown in Figure 3. This is likely a convergence issue in the corresponding states model that would have a small impact on designs based on this model for the thermal conductivity of RP-1. The corresponding states model is based on thermal conductivity data for pure components that typically have not been corrected for thermal radiation. Thus it is expected that the corresponding states model will predict higher thermal conductivities, more like the uncorrected thermal conductivity values for RP-1 measured in this work. The correction for thermal radiation was as large as 6.6 % at the lowest densities along the 650 K isotherm. Thermal radiation accounts for about half of the systematic deviations shown in Figure 6. A thorough development of the corresponding states model would need to consider the contribution of thermal radiation on the pure components used in the model.

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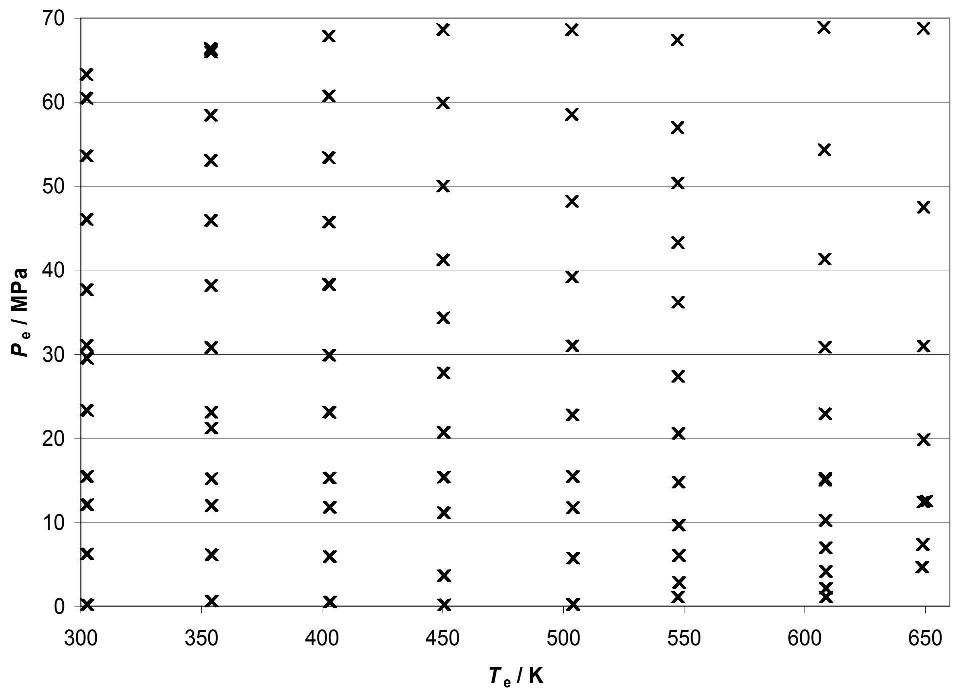

Figure 2. Range of thermal conductivity measurements on liquid RP-1.

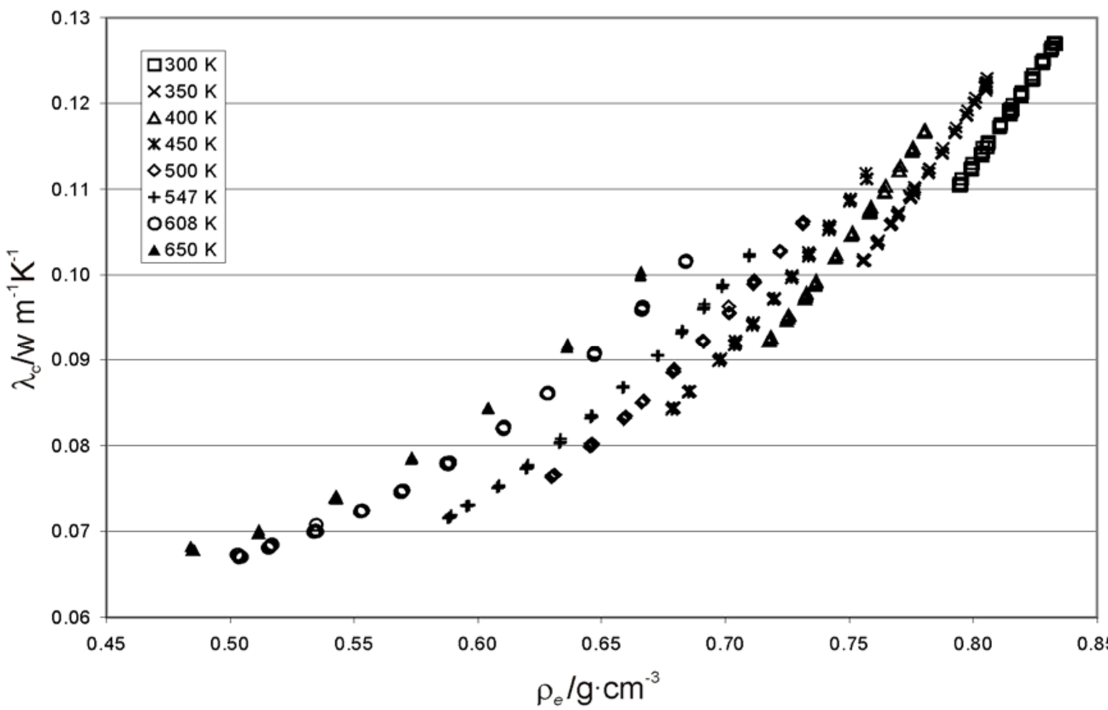

Figure 3. Measured thermal conductivity of RP-1 corrected for thermal radiation (pressure from 0.1 MPa to 70 MPa).

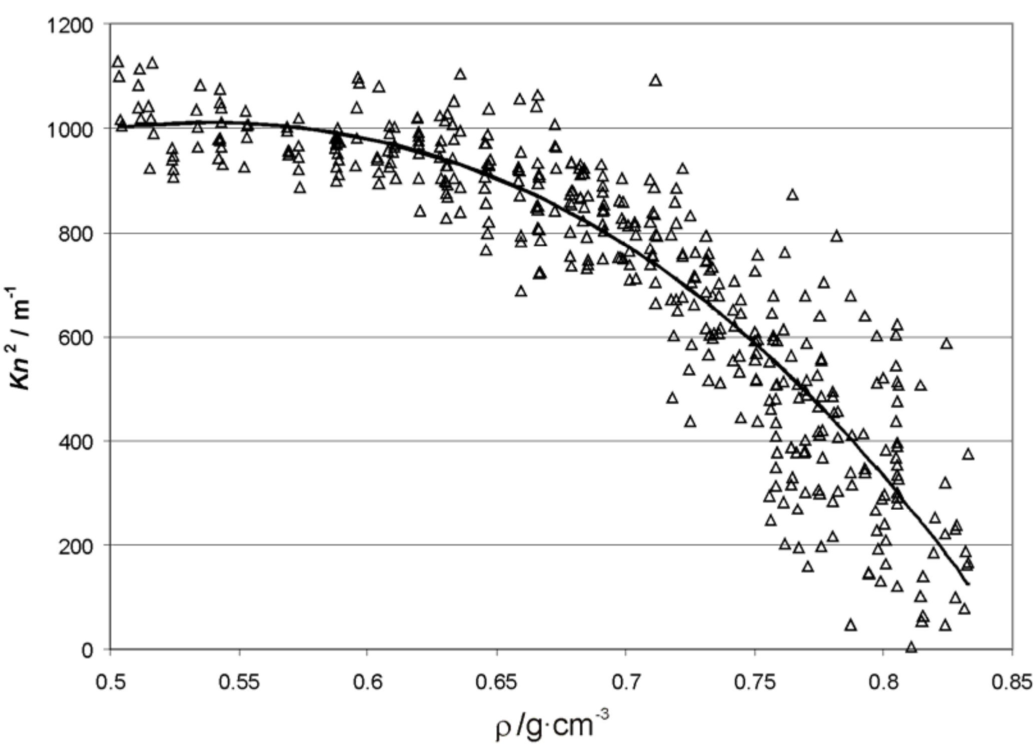

Figure 4. Empirical optical parameters for radiation correction of RP-1 data.

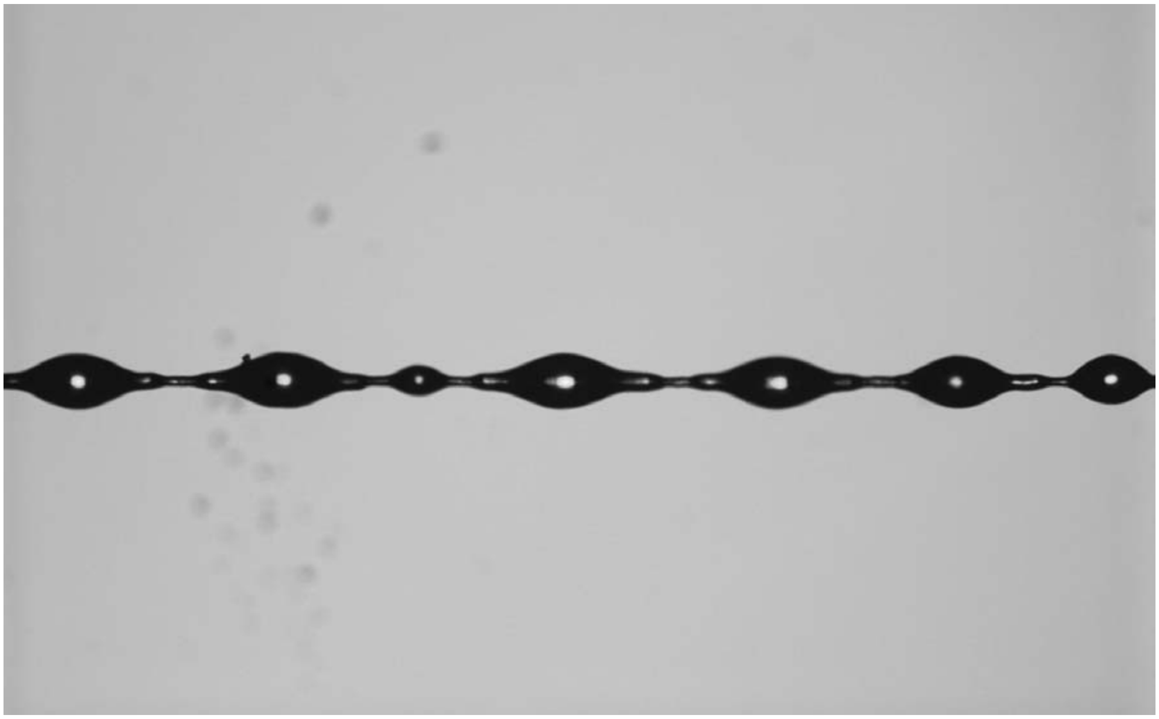

Figure 5. Solid deposits with diameters up to eight times that of the 4 μm hot wires were found after measurements on RP-1 at 650 K.

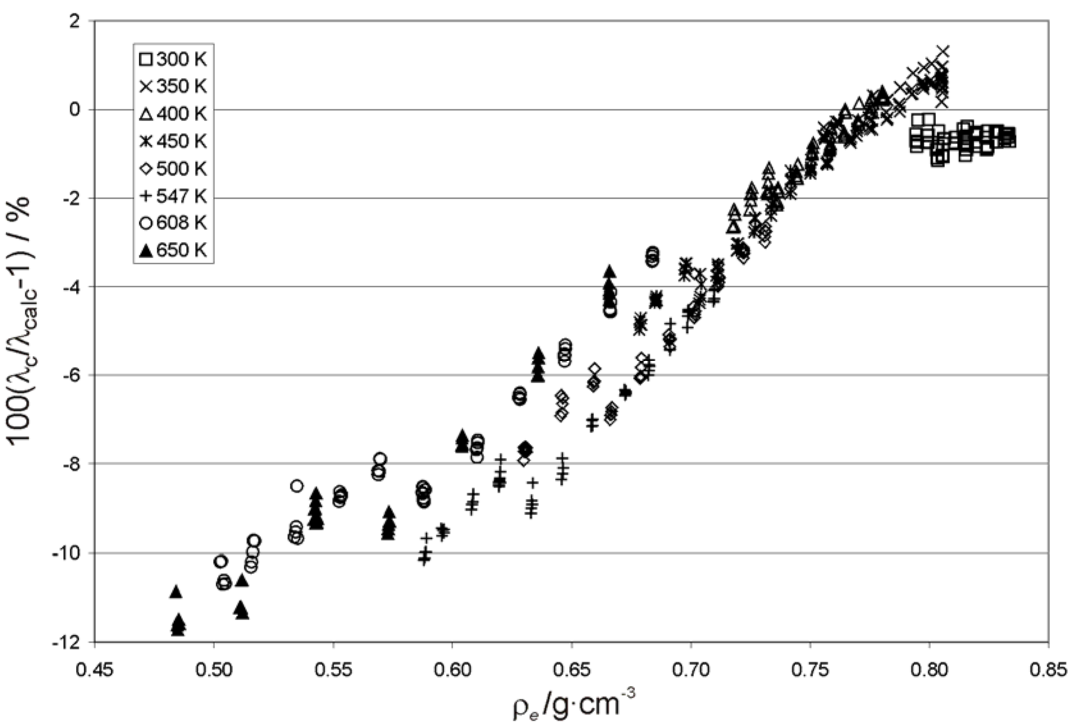

Figure 6. Deviations between the radiation corrected thermal conductivity data and the corresponding-states model for RP-1 developed in this work.

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e (g·cm^{-3})	λ_e (W·m^{-1}K^{-1})	λ_c (W·m^{-1}K^{-1})
2001	299.998	301.798	63.3444	0.83331	0.12705	0.12695
2002	299.998	302.036	63.3249	0.83316	0.12722	0.12712
2003	300.003	302.302	63.3083	0.83299	0.12710	0.12700
2004	300.004	302.559	63.2909	0.83283	0.12716	0.12706
2005	300.002	302.834	63.2699	0.83266	0.12712	0.12702
2006	299.985	301.802	60.5341	0.83192	0.12667	0.12656
2007	299.991	302.041	60.5107	0.83177	0.12659	0.12649
2008	300.002	302.302	60.4845	0.83160	0.12640	0.12633
2009	300.006	302.571	60.4609	0.83143	0.12631	0.12620
2010	300.003	302.844	60.4359	0.83125	0.12632	0.12621
2011	300.002	301.837	53.6465	0.82842	0.12523	0.12508
2012	300.018	302.092	53.6341	0.82825	0.12512	0.12499
2013	300.016	302.343	53.6227	0.82809	0.12479	0.12467
2014	300.025	302.616	53.6114	0.82792	0.12475	0.12462
2015	300.037	302.909	53.5993	0.82774	0.12495	0.12483
2016	300.021	301.875	46.0715	0.82440	0.12346	0.12332
2017	300.028	302.121	46.0630	0.82424	0.12295	0.12283
2018	300.030	302.383	46.0541	0.82408	0.12287	0.12274
2019	300.026	302.648	46.0468	0.82391	0.12280	0.12265
2020	300.036	302.946	46.0404	0.82372	0.12317	0.12295
2021	300.002	301.892	37.7058	0.81977	0.12145	0.12129
2022	300.000	302.132	37.7019	0.81961	0.12139	0.12122
2023	300.011	302.401	37.6976	0.81944	0.12100	0.12080
2024	300.008	302.674	37.6932	0.81926	0.12105	0.12088
2025	300.021	302.976	37.6688	0.81905	0.12118	0.12102
2026	299.999	301.908	31.0595	0.81591	0.11999	0.11981
2027	299.996	302.152	31.0539	0.81574	0.11942	0.11924
2028	300.011	302.427	31.0473	0.81556	0.11944	0.11926
2029	300.006	302.702	31.0387	0.81537	0.11922	0.11903
2030	300.016	303.006	31.0311	0.81517	0.11955	0.11936
2031	300.043	301.953	29.6071	0.81501	0.11886	0.11867
2032	300.056	302.217	29.5643	0.81481	0.11923	0.11905
2033	300.052	302.479	29.5309	0.81462	0.11907	0.11889
2034	300.062	302.767	29.5057	0.81441	0.11914	0.11895
2035	300.051	303.052	29.5016	0.81422	0.11936	0.11916
2036	300.011	301.954	23.3521	0.81119	0.11786	0.11759
2037	300.022	302.214	23.3541	0.81101	0.11777	0.11753
2038	300.028	302.486	23.3358	0.81081	0.11751	0.11731
2039	300.030	302.771	23.3001	0.81060	0.11744	0.11723
2040	300.039	303.078	23.2702	0.81037	0.11742	0.11721
2041	300.011	301.986	15.4211	0.80605	0.11570	0.11548
2042	300.012	302.240	15.4388	0.80588	0.11567	0.11544

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e (g·cm^{-3})	λ_e (W·m^{-1}K^{-1})	λ_c (W·m^{-1}K^{-1})
2043	300.027	302.526	15.4583	0.80569	0.11547	0.11525
2044	300.010	302.795	15.4736	0.80551	0.11511	0.11488
2045	300.025	303.113	15.4863	0.80530	0.11509	0.11486
2046	299.997	301.983	12.0832	0.80380	0.11504	0.11481
2047	300.016	302.262	12.0704	0.80359	0.11456	0.11432
2048	300.007	302.526	12.0827	0.80341	0.11420	0.11393
2049	300.022	302.828	12.1065	0.80321	0.11422	0.11395
2050	300.011	303.123	12.1261	0.80301	0.11434	0.11410
2051	299.987	302.001	6.2210	0.79967	0.11324	0.11299
2052	299.995	302.270	6.2334	0.79948	0.11278	0.11253
2053	300.013	302.565	6.2425	0.79927	0.11257	0.11232
2054	300.012	302.857	6.2477	0.79906	0.11251	0.11225
2055	300.015	303.168	6.2466	0.79883	0.11263	0.11238
2056	299.988	302.028	0.2179	0.79520	0.11148	0.11122
2057	299.999	302.308	0.1941	0.79497	0.11086	0.11060
2058	300.003	302.594	0.1755	0.79474	0.11070	0.11043
2059	300.003	302.892	0.1675	0.79450	0.11101	0.11067
2060	300.001	303.204	0.1792	0.79428	0.11072	0.11045
3001	351.854	353.436	66.4743	0.80567	0.12331	0.12296
3002	351.854	353.659	66.4227	0.80551	0.12212	0.12177
3003	351.870	353.904	66.3775	0.80535	0.12219	0.12184
3004	351.861	354.161	66.3535	0.80520	0.12179	0.12144
3005	351.865	354.379	66.3472	0.80508	0.12268	0.12236
3006	351.845	353.439	66.2878	0.80556	0.12285	0.12250
3007	351.847	353.706	66.2729	0.80540	0.12228	0.12189
3008	351.865	353.900	66.2542	0.80529	0.12236	0.12197
3009	351.846	354.127	66.2306	0.80515	0.12232	0.12196
3010	351.858	354.367	66.1862	0.80499	0.12238	0.12202
3011	351.847	353.444	65.9787	0.80538	0.12248	0.12212
3012	351.846	353.647	65.9703	0.80526	0.12250	0.12214
3013	351.849	353.872	65.9607	0.80513	0.12252	0.12216
3014	351.850	354.104	65.9512	0.80500	0.12246	0.12211
3015	351.856	354.356	65.9398	0.80486	0.12229	0.12193
3016	351.828	353.438	58.4753	0.80097	0.12102	0.12064
3017	351.825	353.652	58.4373	0.80083	0.12042	0.12004
3018	351.843	353.889	58.4229	0.80069	0.12051	0.12013
3019	351.839	354.120	58.4251	0.80056	0.12034	0.11995
3020	351.832	354.361	58.4319	0.80043	0.12045	0.12006
3021	351.823	353.454	53.0937	0.79767	0.11957	0.11917
3022	351.827	353.671	53.0800	0.79753	0.11895	0.11856
3023	351.836	353.904	53.0655	0.79739	0.11905	0.11865
3024	351.834	354.140	53.0528	0.79725	0.11897	0.11857
3025	351.839	354.396	53.0392	0.79709	0.11907	0.11866

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e (g·cm^{-3})	λ_e (W·m^{-1}K^{-1})	λ_c (W·m^{-1}K^{-1})
3026	351.829	353.484	45.9442	0.79308	0.11759	0.11716
3027	351.823	353.698	45.9346	0.79295	0.11702	0.11660
3028	351.833	353.936	45.9234	0.79280	0.11698	0.11655
3029	351.838	354.184	45.9124	0.79265	0.11707	0.11664
3030	351.823	354.424	45.9021	0.79250	0.11690	0.11647
3031	351.816	353.500	38.1685	0.78782	0.11518	0.11472
3032	351.816	353.724	38.1724	0.78769	0.11464	0.11419
3033	351.830	353.969	38.1784	0.78754	0.11448	0.11403
3034	351.829	354.213	38.1884	0.78740	0.11466	0.11421
3035	351.826	354.471	38.1983	0.78725	0.11463	0.11417
3036	351.808	353.523	30.8077	0.78253	0.11286	0.11238
3037	351.817	353.757	30.8057	0.78238	0.11233	0.11189
3038	351.833	354.008	30.8008	0.78222	0.11279	0.11231
3039	351.831	354.258	30.7953	0.78206	0.11226	0.11178
3040	351.837	354.528	30.7900	0.78189	0.11240	0.11192
3041	351.816	353.568	23.0974	0.77660	0.11061	0.11011
3042	351.825	353.808	23.0969	0.77645	0.11034	0.10983
3043	351.823	354.045	23.0942	0.77629	0.11074	0.11023
3044	351.835	354.313	23.0907	0.77611	0.10987	0.10936
3045	351.827	354.573	23.0858	0.77594	0.11005	0.10954
3046	351.849	353.609	21.2003	0.77506	0.10942	0.10891
3047	351.849	353.840	21.2056	0.77491	0.10962	0.10911
3048	351.868	354.104	21.2109	0.77474	0.10941	0.10890
3049	351.873	354.364	21.2156	0.77457	0.10962	0.10911
3050	351.864	354.629	21.2203	0.77440	0.10975	0.10923
3051	351.845	353.642	15.1613	0.77001	0.10788	0.10735
3052	351.848	353.875	15.1777	0.76986	0.10764	0.10711
3053	351.861	354.135	15.1951	0.76970	0.10754	0.10701
3054	351.853	354.390	15.2092	0.76954	0.10740	0.10687
3055	351.846	354.657	15.2224	0.76936	0.10738	0.10684
3056	351.832	353.645	11.9712	0.76722	0.10652	0.10598
3057	351.859	353.905	11.9842	0.76704	0.10635	0.10581
3058	351.868	354.163	11.9958	0.76687	0.10640	0.10585
3059	351.864	354.424	12.0053	0.76670	0.10635	0.10580
3060	351.862	354.700	12.0124	0.76651	0.10627	0.10573
3061	351.813	353.659	6.1880	0.76188	0.10450	0.10394
3062	351.828	353.909	6.1732	0.76168	0.10440	0.10383
3063	351.840	354.178	6.1425	0.76146	0.10404	0.10348
3064	351.840	354.448	6.1183	0.76124	0.10423	0.10367
3065	351.845	354.737	6.0987	0.76101	0.10430	0.10374
3066	351.818	353.696	0.6116	0.75633	0.10223	0.10165
3067	351.845	353.967	0.6214	0.75614	0.10225	0.10167
3068	351.847	354.228	0.6278	0.75594	0.10218	0.10159

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e (g·cm^{-3})	λ_e (W·m^{-1}K^{-1})	λ_c (W·m^{-1}K^{-1})
3069	351.851	354.505	0.6282	0.75573	0.10237	0.10179
3070	351.852	354.794	0.6056	0.75549	0.10213	0.10155
4001	400.446	402.270	67.8698	0.78064	0.11752	0.11682
4002	400.474	402.512	67.8711	0.78051	0.11731	0.11661
4003	400.464	402.724	67.8715	0.78041	0.11797	0.11668
4004	400.463	402.954	67.8743	0.78029	0.11748	0.11678
4005	400.466	403.201	67.8738	0.78016	0.11730	0.11659
4006	400.434	402.289	60.7558	0.77582	0.11560	0.11482
4007	400.435	402.506	60.7558	0.77570	0.11542	0.11474
4008	400.450	402.745	60.7602	0.77558	0.11528	0.11455
4009	400.453	402.986	60.7647	0.77545	0.11524	0.11450
4010	400.453	403.233	60.7700	0.77532	0.11508	0.11435
4011	400.424	402.304	53.4350	0.77058	0.11347	0.11270
4012	400.436	402.542	53.4325	0.77045	0.11291	0.11215
4013	400.446	402.778	53.4091	0.77030	0.11289	0.11212
4014	400.441	403.017	53.3763	0.77015	0.11292	0.11215
4015	400.447	403.274	53.3494	0.76999	0.11292	0.11215
4016	400.417	402.341	45.7511	0.76474	0.11113	0.11033
4017	400.428	402.573	45.7250	0.76459	0.11118	0.11038
4018	400.437	402.819	45.7046	0.76443	0.11054	0.10972
4019	400.449	403.074	45.7046	0.76429	0.11051	0.10976
4020	400.436	403.322	45.7239	0.76416	0.11041	0.10961
4021	400.410	402.368	38.3898	0.75877	0.10869	0.10787
4022	400.420	402.610	38.3544	0.75860	0.10823	0.10741
4023	400.440	402.868	38.3270	0.75842	0.10815	0.10732
4024	400.443	403.124	38.3062	0.75825	0.10806	0.10723
4025	400.440	403.385	38.2888	0.75809	0.10800	0.10717
4026	400.440	402.404	38.3049	0.75868	0.10862	0.10780
4027	400.444	402.635	38.2825	0.75852	0.10840	0.10757
4028	400.452	402.883	38.2644	0.75836	0.10810	0.10727
4029	400.455	403.138	38.2591	0.75821	0.10806	0.10724
4030	400.449	403.396	38.2724	0.75807	0.10833	0.10749
4031	400.420	402.438	29.9102	0.75132	0.10580	0.10494
4032	400.446	402.697	29.8883	0.75114	0.10567	0.10480
4033	400.437	402.929	29.8703	0.75098	0.10553	0.10467
4034	400.435	403.183	29.8701	0.75082	0.10546	0.10459
4035	400.441	403.461	29.8844	0.75066	0.10543	0.10456
4036	400.422	402.481	23.1390	0.74487	0.10323	0.10235
4037	400.439	402.738	23.1129	0.74468	0.10287	0.10199
4038	400.445	402.992	23.0911	0.74449	0.10291	0.10202
4039	400.448	403.263	23.0714	0.74430	0.10296	0.10207
4040	400.440	403.532	23.0644	0.74412	0.10279	0.10194
4041	400.421	402.543	15.2520	0.73665	0.10018	0.09926

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e (g·cm^{-3})	λ_e (W·m^{-1}K^{-1})	λ_c (W·m^{-1}K^{-1})
4042	400.409	402.774	15.2684	0.73651	0.10008	0.09916
4043	400.434	403.053	15.2832	0.73633	0.09982	0.09890
4044	400.432	403.324	15.2953	0.73616	0.09983	0.09891
4045	400.447	403.626	15.3055	0.73597	0.09970	0.09877
4046	400.428	402.578	11.7858	0.73274	0.09878	0.09785
4047	400.433	402.827	11.7687	0.73254	0.09862	0.09769
4048	400.443	403.097	11.7586	0.73234	0.09840	0.09746
4049	400.437	403.369	11.7652	0.73216	0.09811	0.09718
4050	400.441	403.661	11.7812	0.73197	0.09814	0.09721
4051	400.415	402.618	5.9253	0.72564	0.09625	0.09530
4052	400.417	402.870	5.9120	0.72544	0.09611	0.09516
4053	400.430	403.150	5.9089	0.72523	0.09592	0.09496
4054	400.423	403.423	5.9193	0.72504	0.09601	0.09506
4055	400.429	403.726	5.9348	0.72483	0.09570	0.09469
4056	400.407	402.659	0.5228	0.71842	0.09365	0.09268
4057	400.420	402.929	0.5313	0.71822	0.09371	0.09274
4058	400.419	403.200	0.5392	0.71802	0.09334	0.09237
4059	400.419	403.490	0.5450	0.71780	0.09328	0.09231
4060	400.435	403.808	0.5460	0.71755	0.09324	0.09227
5001	447.986	449.670	68.6898	0.75732	0.11230	0.11117
5002	447.991	449.870	68.6635	0.75721	0.11232	0.11118
5003	447.993	450.077	68.6272	0.75708	0.11238	0.11119
5004	447.983	450.283	68.5986	0.75695	0.11226	0.11112
5005	447.989	450.514	68.5747	0.75682	0.11300	0.11184
5006	447.928	449.652	59.8904	0.75048	0.11005	0.10887
5007	447.966	449.886	59.9032	0.75037	0.10986	0.10868
5008	447.944	450.075	59.9145	0.75029	0.10981	0.10863
5009	447.939	450.291	59.9247	0.75018	0.10975	0.10856
5010	447.935	450.518	59.9336	0.75008	0.10967	0.10848
5011	447.904	449.679	49.9987	0.74213	0.10681	0.10558
5012	447.905	449.882	50.0107	0.74203	0.10674	0.10551
5013	447.907	450.099	50.0219	0.74192	0.10654	0.10531
5014	447.911	450.330	50.0314	0.74180	0.10698	0.10574
5015	447.919	450.575	50.0394	0.74168	0.10641	0.10517
5016	447.906	449.729	41.2702	0.73404	0.10366	0.10239
5017	447.904	449.937	41.2462	0.73390	0.10364	0.10237
5018	447.911	450.166	41.2255	0.73375	0.10351	0.10223
5019	447.919	450.409	41.2089	0.73360	0.10334	0.10206
5020	447.907	450.637	41.2165	0.73348	0.10389	0.10260
5021	447.889	449.755	34.3025	0.72703	0.10121	0.09991
5022	447.895	449.974	34.3195	0.72691	0.10098	0.09968
5023	447.899	450.200	34.3354	0.72680	0.10122	0.09991
5024	447.923	450.468	34.3495	0.72665	0.10088	0.09957

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e (g·cm^{-3})	λ_e (W·m^{-1}K^{-1})	λ_c (W·m^{-1}K^{-1})
5025	447.917	450.714	34.3608	0.72652	0.10087	0.09956
5026	447.899	449.807	27.8189	0.71992	0.09862	0.09730
5027	447.903	450.031	27.7971	0.71975	0.09845	0.09712
5028	447.905	450.265	27.7795	0.71959	0.09856	0.09722
5029	447.913	450.520	27.7664	0.71942	0.09853	0.09720
5030	447.905	450.769	27.7621	0.71926	0.09835	0.09702
5031	447.893	449.857	20.7169	0.71137	0.09580	0.09445
5032	447.895	450.087	20.6985	0.71119	0.09573	0.09437
5033	447.905	450.333	20.6836	0.71101	0.09554	0.09418
5034	447.906	450.587	20.6850	0.71085	0.09550	0.09414
5035	447.905	450.851	20.6988	0.71069	0.09536	0.09400
5036	447.883	449.890	15.3503	0.70424	0.09352	0.09215
5037	447.889	450.128	15.3608	0.70409	0.09326	0.09188
5038	447.886	450.367	15.3694	0.70393	0.09370	0.09231
5039	447.898	450.640	15.3777	0.70376	0.09316	0.09178
5040	447.906	450.915	15.3851	0.70358	0.09306	0.09168
5041	447.888	449.937	11.1635	0.69816	0.09158	0.09019
5042	447.899	450.182	11.1639	0.69798	0.09154	0.09014
5043	447.919	450.449	11.1449	0.69776	0.09142	0.09002
5044	447.913	450.710	11.1238	0.69754	0.09136	0.08996
5045	447.910	450.983	11.1067	0.69731	0.09121	0.08981
5046	447.869	449.998	3.6297	0.68575	0.08778	0.08637
5047	447.889	450.267	3.6382	0.68555	0.08785	0.08643
5048	447.893	450.528	3.6454	0.68536	0.08783	0.08636
5049	447.889	450.798	3.6525	0.68515	0.08771	0.08629
5050	447.896	451.088	3.6577	0.68493	0.08764	0.08621
5051	447.882	450.059	0.1765	0.67919	0.08582	0.08440
5052	447.890	450.318	0.1697	0.67896	0.08591	0.08449
5053	447.908	450.599	0.1764	0.67873	0.08576	0.08434
5054	447.886	450.854	0.1878	0.67854	0.08579	0.08436
5055	447.902	451.159	0.1979	0.67830	0.08562	0.08419
6001	501.556	503.108	68.6557	0.73147	0.10791	0.10614
6002	501.565	503.294	68.6482	0.73138	0.10802	0.10624
6003	501.579	503.499	68.6109	0.73125	0.10790	0.10613
6004	501.561	503.682	68.5784	0.73113	0.10766	0.10583
6005	501.554	503.878	68.5536	0.73102	0.10773	0.10596
6006	501.492	503.091	58.5297	0.72228	0.10462	0.10279
6007	501.488	503.271	58.5390	0.72220	0.10456	0.10273
6008	501.503	503.479	58.5461	0.72211	0.10454	0.10271
6009	501.505	503.684	58.5529	0.72201	0.10442	0.10260
6010	501.506	503.900	58.5550	0.72191	0.10465	0.10282
6011	501.485	503.138	48.2361	0.71189	0.10097	0.09909
6012	501.491	503.336	48.2135	0.71177	0.10086	0.09898

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e (g·cm^{-3})	λ_e (W·m^{-1}K^{-1})	λ_c (W·m^{-1}K^{-1})
6013	501.500	503.542	48.1945	0.71164	0.10097	0.09909
6014	501.493	503.749	48.1807	0.71151	0.10122	0.09933
6015	501.487	503.966	48.1838	0.71140	0.10068	0.09885
6016	501.454	503.160	39.1892	0.70169	0.09746	0.09555
6017	501.471	503.375	39.1977	0.70158	0.09740	0.09548
6018	501.486	503.596	39.2047	0.70146	0.09732	0.09540
6019	501.497	503.826	39.2083	0.70134	0.09824	0.09629
6020	501.480	504.039	39.2048	0.70121	0.09753	0.09560
6021	501.469	503.232	30.9930	0.69126	0.09424	0.09228
6022	501.475	503.441	30.9816	0.69112	0.09405	0.09209
6023	501.475	503.657	30.9862	0.69099	0.09419	0.09222
6024	501.488	503.893	31.0013	0.69087	0.09454	0.09221
6025	501.501	504.142	31.0161	0.69074	0.09428	0.09231
6026	501.470	503.297	22.7998	0.67936	0.09099	0.08900
6027	501.487	503.526	22.8038	0.67921	0.09060	0.08861
6028	501.493	503.753	22.8028	0.67906	0.09078	0.08879
6029	501.506	504.000	22.7819	0.67887	0.09059	0.08859
6030	501.516	504.254	22.7625	0.67868	0.09053	0.08853
6031	501.487	503.385	15.4641	0.66692	0.08729	0.08528
6032	501.492	503.609	15.4503	0.66673	0.08721	0.08520
6033	501.506	503.854	15.4406	0.66654	0.08713	0.08511
6034	501.506	504.098	15.4385	0.66636	0.08710	0.08508
6035	501.507	504.354	15.4490	0.66620	0.08701	0.08499
6036	501.489	503.429	11.7229	0.65968	0.08549	0.08347
6037	501.498	503.660	11.7341	0.65953	0.08525	0.08323
6038	501.497	503.893	11.7437	0.65937	0.08523	0.08321
6039	501.488	504.135	11.7521	0.65921	0.08519	0.08317
6040	501.506	504.407	11.7591	0.65902	0.08511	0.08309
6041	501.473	503.483	5.7558	0.64636	0.08228	0.08025
6042	501.484	503.723	5.7489	0.64614	0.08216	0.08013
6043	501.475	503.961	5.7334	0.64590	0.08198	0.07995
6044	501.501	504.244	5.7211	0.64563	0.08196	0.08021
6045	501.499	504.508	5.7106	0.64538	0.08188	0.07984
6046	501.489	503.584	0.2293	0.63093	0.07857	0.07654
6047	501.497	503.834	0.2292	0.63069	0.07857	0.07654
6048	501.482	504.069	0.2293	0.63046	0.07858	0.07655
6049	501.500	504.352	0.2300	0.63019	0.07857	0.07653
6050	501.482	504.618	0.2307	0.62993	0.07834	0.07630
6051	501.361	503.455	0.2316	0.63107	0.07865	0.07663
6052	501.373	503.707	0.2319	0.63082	0.07862	0.07659
6053	501.380	503.969	0.2321	0.63057	0.07857	0.07654
6054	501.361	504.216	0.2322	0.63033	0.07861	0.07657
6055	501.365	504.503	0.2324	0.63005	0.07850	0.07646

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e ($g \cdot cm^{-3}$)	λ_e ($W \cdot m^{-1}K^{-1}$)	λ_c ($W \cdot m^{-1}K^{-1}$)
7001	545.383	546.851	67.4191	0.70986	0.10481	0.10239
7002	545.381	547.018	67.4082	0.70977	0.10458	0.10217
7003	545.381	547.197	67.4029	0.70968	0.10478	0.10236
7004	545.388	547.394	67.3987	0.70959	0.10451	0.10209
7005	545.383	547.581	67.3945	0.70950	0.10451	0.10209
7006	545.396	546.916	56.9830	0.69905	0.10122	0.09880
7007	545.399	547.094	56.9839	0.69896	0.10133	0.09884
7008	545.415	547.292	56.9840	0.69886	0.10130	0.09882
7009	545.421	547.490	56.9823	0.69876	0.10119	0.09870
7010	545.424	547.695	56.9813	0.69866	0.10093	0.09845
7011	545.430	546.986	50.3613	0.69148	0.09904	0.09652
7012	545.456	547.191	50.3670	0.69138	0.09868	0.09617
7013	545.449	547.372	50.3813	0.69131	0.09868	0.09617
7014	545.452	547.570	50.3948	0.69122	0.09849	0.09597
7015	545.465	547.792	50.4064	0.69112	0.09848	0.09596
7016	545.436	547.031	43.2920	0.68268	0.09594	0.09340
7017	545.441	547.220	43.2966	0.68258	0.09597	0.09342
7018	545.459	547.431	43.2993	0.68247	0.09606	0.09351
7019	545.453	547.630	43.2938	0.68236	0.09583	0.09328
7020	545.467	547.860	43.2682	0.68220	0.09572	0.09316
7021	545.442	547.089	36.1910	0.67288	0.09311	0.09053
7022	545.438	547.270	36.1943	0.67278	0.09306	0.09048
7023	545.459	547.493	36.1931	0.67265	0.09311	0.09053
7024	545.476	547.716	36.1896	0.67252	0.09302	0.09043
7025	545.475	547.936	36.1673	0.67236	0.09310	0.09051
7026	545.426	547.138	27.3687	0.65893	0.08951	0.08689
7027	545.457	547.363	27.3756	0.65880	0.08939	0.08677
7028	545.461	547.573	27.3780	0.65867	0.08948	0.08685
7029	545.461	547.790	27.3805	0.65854	0.08949	0.08686
7030	545.451	548.008	27.3644	0.65838	0.08935	0.08672
7031	545.426	547.197	20.5868	0.64631	0.08607	0.08344
7032	545.435	547.411	20.5896	0.64617	0.08596	0.08333
7033	545.445	547.635	20.5911	0.64602	0.08623	0.08359
7034	545.458	547.874	20.5770	0.64583	0.08622	0.08357
7035	545.464	548.116	20.5600	0.64563	0.08582	0.08318
7036	545.430	547.256	14.7485	0.63351	0.08344	0.08078
7037	545.419	547.460	14.7549	0.63337	0.08307	0.08042
7038	545.421	547.681	14.7604	0.63322	0.08312	0.08047
7039	545.443	547.939	14.7656	0.63304	0.08298	0.08033
7040	545.454	548.197	14.7698	0.63286	0.08289	0.08024
7041	545.420	547.317	9.6654	0.62017	0.08041	0.07776
7042	545.436	547.555	9.6709	0.61999	0.08001	0.07736
7043	545.429	547.775	9.6760	0.61982	0.08008	0.07743

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 **(K)**	T_e **(K)**	P_e **(MPa)**	ρ_e **(g·cm^{-3})**	λ_e **(W·m^{-1}K^{-1})**	λ_c **(W·m^{-1}K^{-1})**
7044	545.443	548.028	9.6803	0.61962	0.08002	0.07737
7045	545.431	548.272	9.6840	0.61943	0.07993	0.07728
7046	545.426	547.321	9.6400	0.62009	0.08019	0.07754
7047	545.444	547.557	9.6388	0.61989	0.08005	0.07741
7048	545.450	547.789	9.6465	0.61972	0.08001	0.07736
7049	545.441	548.021	9.6550	0.61955	0.07992	0.07727
7050	545.443	548.279	9.6619	0.61936	0.07996	0.07731
7051	545.412	547.356	6.0392	0.60874	0.07802	0.07537
7052	545.410	547.578	6.0433	0.60855	0.07787	0.07523
7053	545.435	547.836	6.0470	0.60832	0.07782	0.07518
7054	545.447	548.093	6.0494	0.60810	0.07781	0.07516
7055	545.437	548.348	6.0515	0.60787	0.07772	0.07507
7056	545.420	547.422	2.8458	0.59656	0.07562	0.07300
7057	545.406	547.635	2.8430	0.59633	0.07567	0.07304
7058	545.436	547.907	2.8335	0.59601	0.07563	0.07300
7059	545.426	548.151	2.8249	0.59572	0.07552	0.07289
7060	545.435	548.429	2.8180	0.59541	0.07561	0.07297
7061	544.931	546.966	1.0907	0.58916	0.07449	0.07188
7062	544.952	547.222	1.0966	0.58891	0.07427	0.07167
7063	544.962	547.477	1.1018	0.58864	0.07425	0.07164
7064	544.946	547.716	1.1060	0.58840	0.07416	0.07155
7065	544.966	548.006	1.1101	0.58809	0.07411	0.07150
8001	605.887	608.009	15.0088	0.58786	0.08163	0.07782
8002	605.896	608.232	15.0091	0.58769	0.08181	0.07800
8003	605.889	608.454	15.0098	0.58751	0.08170	0.07789
8004	605.885	608.687	15.0109	0.58733	0.08183	0.07800
8005	605.901	608.954	15.0124	0.58713	0.08171	0.07788
8006	605.901	607.571	68.9229	0.68401	0.10529	0.10169
8007	605.902	607.754	68.9080	0.68391	0.10525	0.10165
8008	605.908	607.937	68.9000	0.68382	0.10510	0.10151
8009	605.907	608.117	68.9029	0.68375	0.10520	0.10160
8010	605.919	608.329	68.9171	0.68367	0.10508	0.10147
8011	605.970	607.725	54.3640	0.66635	0.10000	0.09631
8012	605.986	607.920	54.3665	0.66626	0.09978	0.09610
8013	605.988	608.114	54.3508	0.66614	0.09956	0.09588
8014	606.003	608.325	54.3318	0.66602	0.09998	0.09592
8015	606.015	608.541	54.3142	0.66589	0.09958	0.09588
8016	605.989	607.838	41.3265	0.64724	0.09465	0.09090
8017	605.993	608.034	41.3139	0.64711	0.09458	0.09082
8018	606.000	608.237	41.3159	0.64701	0.09446	0.09071
8019	606.011	608.454	41.3281	0.64691	0.09431	0.09056
8020	606.012	608.674	41.3388	0.64681	0.09443	0.09067
8021	605.989	607.926	30.8369	0.62830	0.08999	0.08619

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e (g·cm^{-3})	λ_e (W·m^{-1}K^{-1})	λ_c (W·m^{-1}K^{-1})
8022	605.992	608.130	30.8407	0.62819	0.08988	0.08609
8023	605.990	608.336	30.8421	0.62807	0.08997	0.08617
8024	606.013	608.574	30.8294	0.62790	0.08990	0.08609
8025	606.003	608.792	30.8140	0.62774	0.08990	0.08609
8026	605.958	607.983	22.9257	0.61062	0.08607	0.08226
8027	605.969	608.201	22.9273	0.61048	0.08601	0.08220
8028	605.985	608.430	22.9169	0.61030	0.08592	0.08211
8029	606.005	608.681	22.9027	0.61010	0.08573	0.08192
8030	606.010	608.922	22.8928	0.60991	0.08586	0.08204
8031	605.986	608.109	15.2320	0.58853	0.08187	0.07806
8032	605.986	608.326	15.2214	0.58832	0.08187	0.07805
8033	605.996	608.564	15.2123	0.58811	0.08167	0.07785
8034	606.009	608.814	15.2060	0.58789	0.08165	0.07783
8035	606.007	609.062	15.2004	0.58768	0.08166	0.07783
8036	605.901	608.103	10.2436	0.56965	0.07862	0.07483
8037	605.927	608.356	10.2371	0.56939	0.07862	0.07482
8038	605.918	608.579	10.2284	0.56915	0.07841	0.07462
8039	605.931	608.846	10.2215	0.56888	0.07834	0.07455
8040	605.961	609.137	10.2159	0.56859	0.07840	0.07459
8041	605.890	608.158	6.9713	0.55351	0.07621	0.07245
8042	605.923	608.426	6.9734	0.55324	0.07619	0.07242
8043	605.937	608.680	6.9744	0.55298	0.07616	0.07239
8044	605.936	608.936	6.9695	0.55269	0.07625	0.07247
8045	605.944	609.210	6.9636	0.55237	0.07608	0.07230
8046	605.898	608.242	4.1257	0.53490	0.07371	0.07000
8047	605.903	608.483	4.1296	0.53463	0.07451	0.07076
8048	605.907	608.736	4.1333	0.53434	0.07388	0.07016
8049	605.881	608.974	4.1364	0.53406	0.07380	0.07007
8050	605.915	609.279	4.1394	0.53370	0.07371	0.06998
8051	605.854	608.251	2.1312	0.51694	0.07215	0.06849
8052	605.878	608.520	2.1330	0.51655	0.07215	0.06849
8053	605.885	608.783	2.1344	0.51616	0.07198	0.06832
8054	605.881	609.047	2.1350	0.51575	0.07183	0.06817
8055	605.889	609.336	2.1321	0.51527	0.07174	0.06809
8056	605.824	608.259	1.1099	0.50456	0.07062	0.06705
8057	605.825	608.509	1.1098	0.50411	0.07066	0.06708
8058	605.858	608.804	1.1085	0.50355	0.07060	0.06701
8059	605.832	609.047	1.1080	0.50310	0.07092	0.06731
8060	605.839	609.340	1.1078	0.50256	0.07090	0.06729
9006	647.900	649.976	12.5113	0.54280	0.07897	0.07423
9007	647.882	650.176	12.5159	0.54265	0.07885	0.07411
9008	647.875	650.394	12.5162	0.54246	0.07873	0.07400
9009	647.888	650.643	12.5153	0.54223	0.07871	0.07398

Table 10. Thermal conductivity of liquid RP-1.

Point ID	T_0 (K)	T_e (K)	P_e (MPa)	ρ_e ($g \cdot cm^{-3}$)	λ_e ($W \cdot m^{-1} K^{-1}$)	λ_c ($W \cdot m^{-1} K^{-1}$)
9010	647.862	650.862	12.5150	0.54204	0.07855	0.07381
9011	647.288	648.869	68.7755	0.66590	0.10489	0.10039
9012	647.299	649.038	68.7679	0.66582	0.10444	0.09990
9013	647.277	649.189	68.7776	0.66577	0.10447	0.09998
9014	647.275	649.365	68.7887	0.66570	0.10432	0.09977
9015	647.279	649.550	68.7983	0.66564	0.10469	0.10013
9016	647.084	648.793	47.5140	0.63622	0.09659	0.09192
9017	647.119	649.006	47.5050	0.63610	0.09648	0.09180
9018	647.120	649.193	47.4964	0.63599	0.09610	0.09144
9019	647.125	649.390	47.4906	0.63588	0.09630	0.09162
9020	647.138	649.601	47.4928	0.63578	0.09612	0.09145
9021	646.936	648.790	30.9474	0.60426	0.08905	0.08433
9022	646.946	648.983	30.9604	0.60417	0.08922	0.08448
9023	646.931	649.165	30.9726	0.60410	0.08918	0.08444
9024	646.923	649.366	30.9838	0.60400	0.08903	0.08429
9025	646.936	649.599	30.9946	0.60389	0.08906	0.08431
9026	646.823	648.804	19.8446	0.57356	0.08326	0.07853
9027	646.825	649.005	19.8431	0.57341	0.08343	0.07869
9028	646.832	649.225	19.8429	0.57326	0.08322	0.07848
9029	646.832	649.447	19.8457	0.57311	0.08314	0.07841
9030	646.839	649.688	19.8528	0.57296	0.08307	0.07834
9031	646.565	648.662	12.4149	0.54348	0.07850	0.07382
9032	646.581	648.893	12.4166	0.54328	0.07853	0.07385
9033	646.586	649.124	12.4191	0.54309	0.07844	0.07375
9034	646.575	649.349	12.4242	0.54292	0.07845	0.07376
9035	646.551	649.569	12.4331	0.54277	0.07843	0.07374
9036	646.212	648.432	7.3542	0.51194	0.07428	0.06971
9037	646.207	648.654	7.3563	0.51170	0.07453	0.07018
9038	646.206	648.890	7.3593	0.51145	0.07435	0.06978
9039	646.211	649.144	7.3632	0.51119	0.07437	0.06978
9040	646.201	649.394	7.3687	0.51095	0.07437	0.06978
9041	645.805	648.101	4.6461	0.48546	0.07235	0.06785
9042	645.818	648.348	4.6503	0.48514	0.07242	0.06791
9043	645.846	648.627	4.6544	0.48477	0.07227	0.06777
9044	645.856	648.894	4.6581	0.48442	0.07234	0.06783
9045	645.875	649.180	4.6613	0.48403	0.07284	0.06828

7. Viscosity

7.1 Viscosity at Atmospheric Pressure

The kinematic viscosities (ν) of the RP-1 samples were measured at atmospheric pressure (approximately 83 kPa) by open gravitational capillary viscometry. With this technique, the time (t) required for a given volume of the liquid to flow through a calibrated capillary under the influence of gravity was measured. The flow time is proportional to the kinematic viscosity:

$$\nu = C \cdot t,$$

where the proportionality constant, C, is determined by calibrating the capillary with standard reference liquids. The absolute viscosity (η) can be determined from the kinematic viscosity if the density (ρ) of the liquid is known:

$$\eta = \nu \cdot \rho.$$

For these measurements we used the procedure outlined in ASTM method D 445 – 03; however, instead of averaging two determinations of the kinematic viscosity, at least eight determinations were averaged for each entry in Table 11. Commercially obtained Ubbelohde capillary viscometers were used for all the measurements. The capillary viscometers were calibrated at NIST using commercially obtained standard reference liquids. The calibration constant, C, for each capillary was found to be within the stated uncertainty of the manufacturer's calibration constant. During a measurement, the viscometers were immersed in an insulated, continuously stirred bath (ethylene glycol + water) whose temperature was maintained with a refrigerated circulator, an electric heater, and a precision temperature controller. The bath temperature was measured with an ITS-90 calibrated platinum resistance thermometer accurate to ±0.01 K. Flow times were measured automatically.

With this apparatus, the expanded uncertainty in the kinematic viscosity is estimated to be 1 % (k = 2). The primary contribution to the uncertainty is the 0.5 % standard uncertainty in *C*, which results in a 0.5 % standard uncertainty in the kinematic viscosity. Including fluctuations and temperature gradients, the uncertainty in the temperature is estimated to be 0.02 K, which leads to a negligible standard uncertainty in the kinematic viscosity of ≤0.074 %. The Hagenbach (kinetic energy) correction was ≤0.13 %, so it was also neglected. The uncertainty in the flow time measurement also leads to a negligible standard uncertainty of about 0.01 % in the kinematic viscosity. Since the RP-1 samples are hydrocarbon-based, no correction was necessary to account for the difference in surface tension between the hydrocarbon-based calibration liquids and the test samples.

Kinematic viscosities were measured as a function of temperature for four RP-1 samples. The first sample was the original sample of RP-1 (acquired May 2003, designated by batch number P000016660,) which has anomalously high olefin (unsaturated hydrocarbon) content. Viscosities were measured from 243.29 K to 333.15 K (approximately –30 ºC to 60 ºC). The kinematic viscosities of the other three samples—a second sample of normal grade RP-1 (acquired November 2004, designated 11/03), an ultra-low sulfur RP-1 (batch number not provided), and a TS-5 RP-1 (batch number not provided)—were measured only at 298.15 K (25 ºC) and 313.15 K (40 ºC). All of these data are collected in Table 11. At some temperatures the kinematic viscosity of the original sample of RP-1 was determined multiple times using different aliquots of that sample. Such independent determinations are listed separately in Table 11.

Figure 7(a) shows a graph of the kinematic viscosity as a function of temperature for the original sample of RP-1. Figure 7(b) shows an Arrhenius plot of the same data with a correlation to a modified Arrhenius equation of the form,

$$\ln(\nu) = A + B(1/T) + C(1/T)^2 + D(1/T)^3, \quad (1)$$

where A, B, C, and D are constants and T is the temperature in kelvins. A regression analysis gave the following values for the coefficients: A = −7.812, B = 5.530 × 10^3, C = −1.503 × 10^6, and D = 1.801 × 10^8. Figure 7(c) shows the percent deviation of the measured kinematic viscosities from the correlation given in Eq. (1). All of the data points are within 1.1 % of Eq. (1).

Figure 8 shows the percent deviation of the kinematic viscosities of the three other rocket propellant samples compared to the correlation of the data for the original sample of RP-1, Eq. (1). The error bars in Figure 8 correspond to the repeatability of the measurements at the 2-sigma level, not to the total uncertainty in the measurement. Figure 8 shows that the viscosities for the second RP-1 sample, the TS-5 sample and the ultra-low sulfur sample are all about 7 to 10 % higher than the correlation at 298.15 K and 313.15 K. Hence, capillary viscosity measurements easily distinguish all three of these samples from the original sample of RP-1. The second RP-1 sample is also distinguishable from the TS-5 and the ultra-low sulfur samples. However, the viscosities of the TS-5 and the ultra-low sulfur samples cannot be distinguished with this apparatus.

These measurements show that the anomalous composition of the original sample of RP-1 results in a significant change in the viscosity behavior of that sample compared to a "normal" RP-1 sample whose composition is on specification. Consequently, these data provide strong motivation for additional measurements on a "normal" RP-1 sample. These measurements also show that the two low-sulfur versions of RP-1 are significantly different from normal grade RP-1. Hence, accurate models of such low-sulfur rocket propellants will require separate viscosity measurements.

Table 11. Experimental kinematic viscosities (ν) for four RP-1 samples.

	Temperature / K	ν / (mm^2·s^{-1})	**Capillary used**
Original sample of RP-1 (acquired 05/03, P000016660)	243.29	7.667	I
	243.93	7.431	I*
	248.15	6.530	I
	248.16	6.368	I*
	253.15	5.369	I
	258.15	4.601	I
	263.15	4.027	I
	263.15	3.990	I
	268.15	3.496	I
	273.15	3.093	I
	278.15	2.758	I
	283.15	2.479	I
	288.15	2.242	I
	288.15	2.255	0b
	293.15	2.053	0b
	293.15	2.040	I
	298.15	1.867	I
	298.15	1.870	I
	298.15	1.867	I
	298.15	1.875	0b
	298.15	1.878	0b
	298.15	1.880	0b
	298.15	1.865	I*
	303.15	1.723	0b
	308.15	1.591	0b
	313.15	1.475	0b
	323.15	1.282	0b
	333.15	1.126	0b
Second sample of RP-1 (acquired 11/03)	298.15	2.0214	0b
	313.15	1.5768	0b
Ultra-low sulfur RP-1	298.15	2.0491	0b
	313.15	1.5968	0b
TS-5 RP-1	298.15	2.0581	0b
	313.15	1.6021	0b

* These values were determined with a second capillary viscometer of size I.

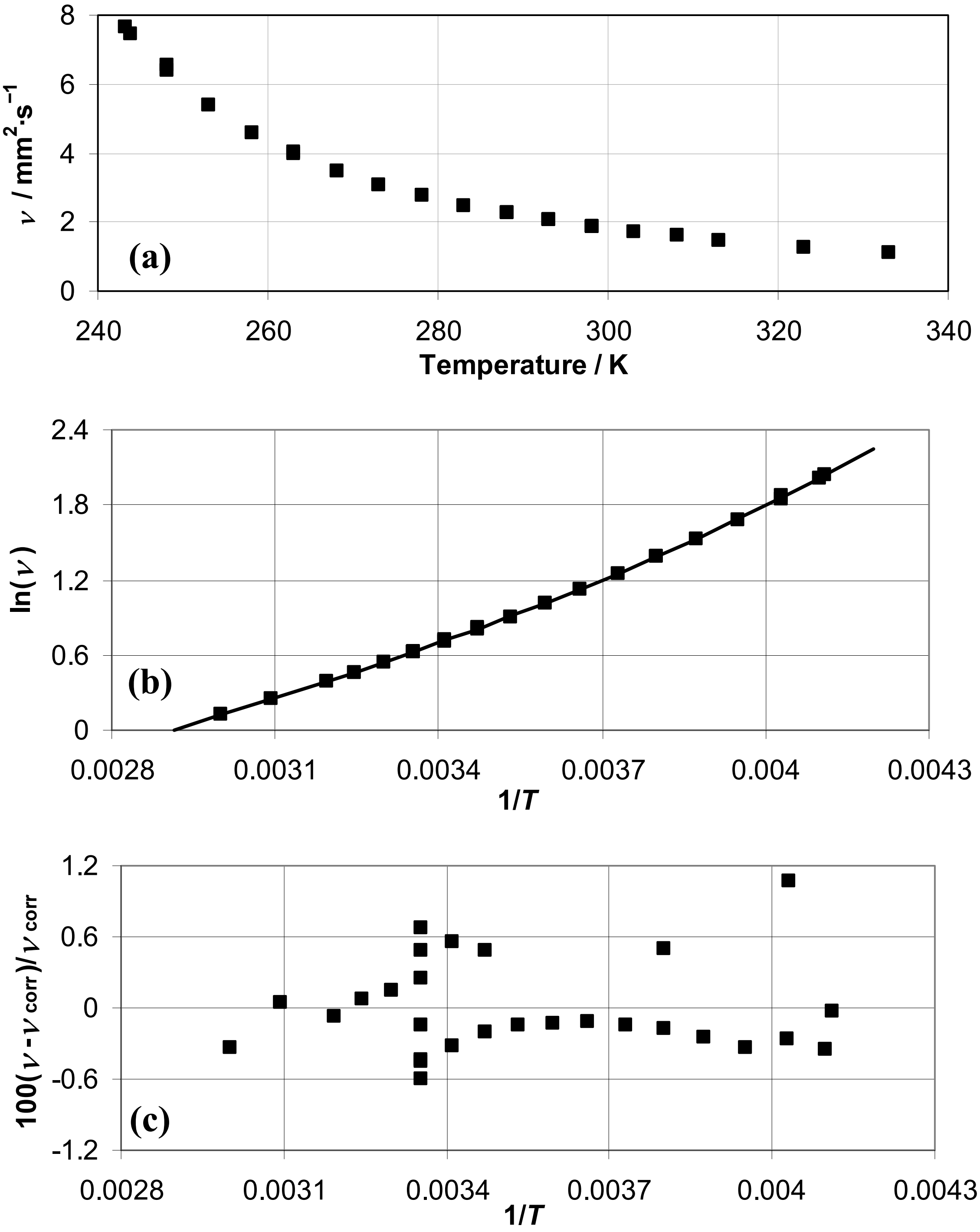

Figure 7. (a) Kinematic viscosity of the original sample of RP-1 as a function of temperature; (b) Arrhenius plot of the same data; solid curve is correlation; (c) deviations of kinematic viscosity from the correlation.

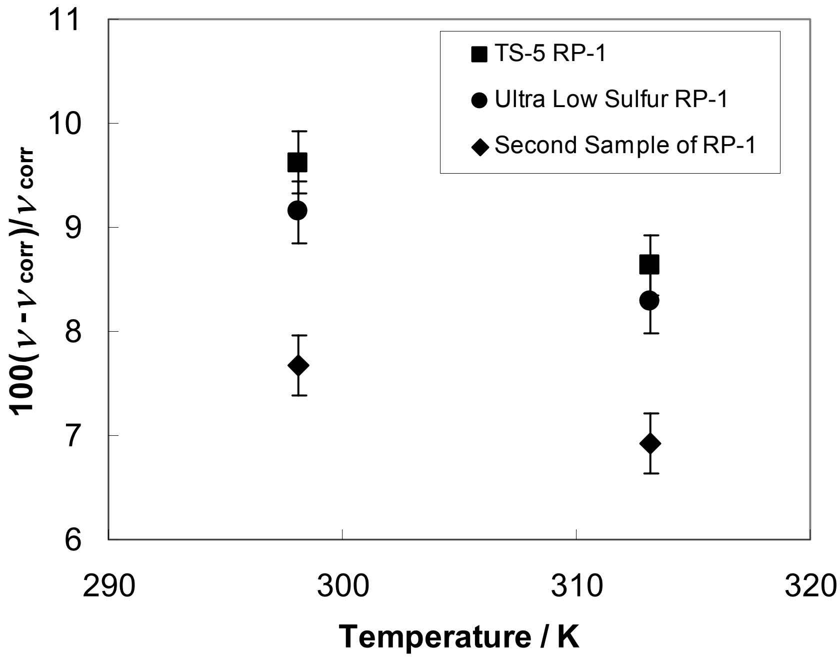

Figure 8. Percent deviations of the kinematic viscosities of three rocket propellant samples compared to the correlation of the kinematic viscosities for the original sample of RP-1.

7.2 Viscosity at Elevated Pressures

The viscosity of RP-1 kerosene was measured at elevated pressures up to 65.7 MPa with a torsional crystal viscometer by mechanical spectroscopy in the frequency domain. Three isotherms were measured, two of which were near room temperature to validate the repeatability of the instrument, and one was at 400 K. Table 12 presents the results of the measurements numerically, while the pressure dependence is shown in Figure 9.

Before introducing the sample fluid with a pressure generator, the viscometer was evacuated for three days. The internal damping of the torsional crystal transducer was measured in vacuo at room temperature prior to the RP-1 measurements. The transducer performance was consistent with the long-term results measured during the last decade. The pressure generator was cleaned with toluene and evacuated for 24 h before it was filled with RP-1.

After charging the cell with RP-1, the quartz crystal viscosity transducer indicated no increase of the measured conductance. The susceptance rose by about 6 microsiemens (μS) over its vacuum level. This is a typical increase for dense hydrocarbons. It is much lower than values observed with hydrofluorocarbons. These observations indicate the presence of no polar impurities in the sample fluid that might have caused electroviscous contributions in the measured viscosity data.

Each line in Table 12 represents an average of four measurements, except the line at 5.5 MPa, which is based on only three measurements. The columns with the experimental data are followed by columns with their absolute and relative standard deviations. Included are columns with the averaged resonance frequencies f^* and bandwidths Δf, which are the original experimental information. The product (viscosity × density) rather than the absolute viscosity is shown because measurements with this viscometer yield this product and the density needs to be supplied either from other measurements or from correlations or equations of state to obtain the viscosity. The pressure dependence of the measured (viscosity × density) results is illustrated in Figure 9.

The uncertainty of the pressure transducer is estimated at 0.01 MPa, while the uncertainty of the measured temperatures is estimated to be 0.05 K. The typical uncertainty of the (viscosity × density) results measured with this instrument is 2 %. However, the RP-1 measurements were conducted at the resolution limit of the impedance analyzer, so that higher uncertainties were incurred. These will be discussed below. The internal damping of the vibrating crystal was not accounted for in the data analysis at room temperature because the bandwidth in vacuo (0.08 Hz) is at most only 0.01 % of the bandwidths of the resonances in the kerosene sample. The internal damping was included in the analysis of the data at 400 K.

Figure 10 compares the viscosities derived from Table 12 with viscosities calculated with the model that was developed in this project. The figure displays percent deviations of the experimental viscosities relative to those calculated with the model as a function of pressure. The deviations range between −3.5 % at 400 K and 0.1 MPa and −11.7 % at 295 K and 41.5 MPa. Consequently, the model predicts higher viscosities than those measured. Given the complexity of the surrogate mixture, the agreement between the model and the measured data can be considered satisfactory. This is supported by a consideration of the uncertainties of the experimental data. They were assessed by calculating the change in the viscosity due to a change in the measured bandwidth Δf resulting from the resolution of the impedance analyzer of ±0.01 Hz. The uncertainties are indicated in Figure 10 by horizontal bars above and below the data points at the highest and at the lowest pressure. The highest uncertainties of the viscosity data occur at the highest pressures due to the flatness of the resonance curves at high external damping of the torsionally vibrating crystal. While the measurement at the highest pressure of Series 2 at 296 K is 9.2 % lower than the viscosity predicted by the model, the uncertainty of the measurement due to the impedance analyzer resolution of ±0.1 Hz results in a deviation interval from –15 % to –0.3 %. This puts the deviations between the experimental and the calculated model data in perspective.

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Table 12. Results of viscosity measurements at elevated pressures.

$\boldsymbol{P}_{exp}$ MPa	$\boldsymbol{T}_{exp}$ K	$\boldsymbol{f}$* Hz	s_f* Hz	$\Delta \boldsymbol{f}$ Hz	$s_{\Delta f}$ Hz	$\eta \times \rho$ $kg^2 \cdot m^{-4} \cdot s$	$s_{\eta \cdot \rho}$ Hz	s_η / η %
65.7032	295.23	39479.7920	1.5476	91.0156	0.8436	2.5287	0.047	1.85
63.6221	295.37	39480.1843	1.8560	90.1313	2.0625	2.4804	0.115	4.62
51.1380	295.57	39481.1876	1.0860	84.1500	0.7194	2.1606	0.037	1.71
41.5231	295.68	39486.1139	1.2056	78.2529	0.6358	1.8676	0.030	1.63
31.5127	295.78	39486.6795	0.6816	74.3371	1.1402	1.6851	0.052	3.07
21.5319	295.91	39489.3690	1.0328	70.5069	0.2671	1.5151	0.011	0.76
11.3880	297.23	39491.8394	0.6729	64.9280	0.0320	1.2843	0.001	0.10
5.54529	297.22	39491.4181	0.9675	62.9383	0.3212	1.2066	0.012	1.02
1.16686	297.30	39493.5601	0.3737	61.0921	0.8900	1.1368	0.033	2.91
0.1190	297.31	39491.6728	0.6652	60.6646	0.4787	1.1209	0.018	1.58
67.3416	296.12	39479.8022	2.7331	90.4688	0.8398	2.4985	0.046	1.86
60.7903	296.22	39481.3354	2.1428	87.7083	0.4166	2.3477	0.022	0.95
49.5042	296.27	39483.3182	0.8905	82.9125	1.1698	2.0974	0.059	2.83
40.0488	297.12	39485.5269	1.4492	77.4432	0.6889	1.8290	0.032	1.77
29.8420	297.14	39489.1896	1.5698	72.6040	0.2903	1.6069	0.013	0.80
20.1337	297.25	39490.8163	0.9642	68.7578	0.9207	1.4408	0.039	2.69
10.1259	297.29	39490.7615	1.5726	64.4845	0.7253	1.2669	0.029	2.25
5.0746	297.36	39490.9510	1.3958	62.7792	0.2912	1.2005	0.011	0.93
1.2191	297.38	39493.5878	1.4182	61.1579	0.5500	1.1392	0.020	1.79
0.1984	297.42	39493.9507	1.3361	60.6076	0.3710	1.1187	0.014	1.23
68.1731	400.08	39508.6993	1.1045	45.1800	0.2298	0.6202	0.006	1.01
60.0641	400.06	39510.1366	0.6027	43.8570	0.3088	0.5842	0.008	1.41
50.2712	400.07	39509.5068	0.6400	42.1027	0.1064	0.5383	0.003	0.50
39.8690	400.04	39510.9737	0.5615	39.9416	0.2524	0.4843	0.006	1.26
29.4055	400.06	39511.1211	0.2013	37.7958	0.1313	0.4335	0.003	0.69
19.4202	400.06	39511.9547	0.2073	35.9434	0.2801	0.3919	0.006	1.56
10.1350	400.06	39512.9821	0.0000	33.6950	0.0272	0.3443	0.001	0.16
5.0553	400.04	39513.4951	0.0008	32.6561	0.0621	0.3234	0.001	0.38
1.0233	400.06	39512.7072	1.0937	31.8197	0.1076	0.3070	0.002	0.68
0.1008	399.07	39512.7240	1.0627	31.7850	0.1672	0.3063	0.003	1.05

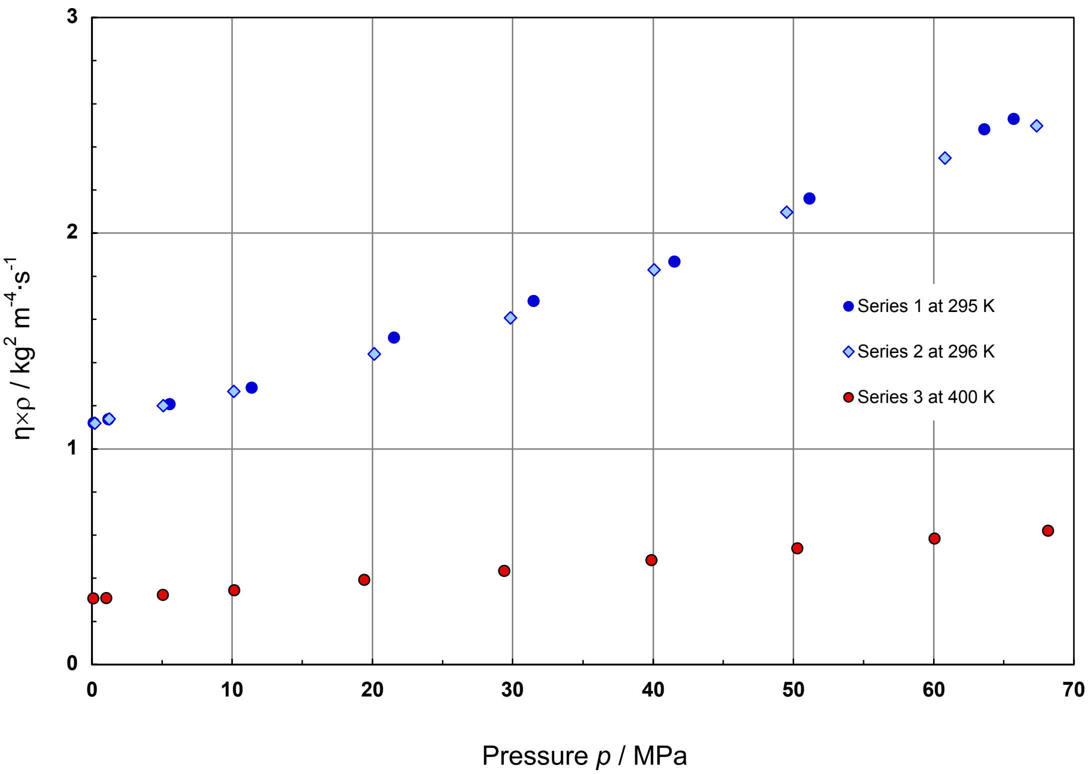

Figure 9. (Viscosity × density) product of RP-1 at elevated pressures measured in the torsional crystal viscometer at room temperature and at 400 K.

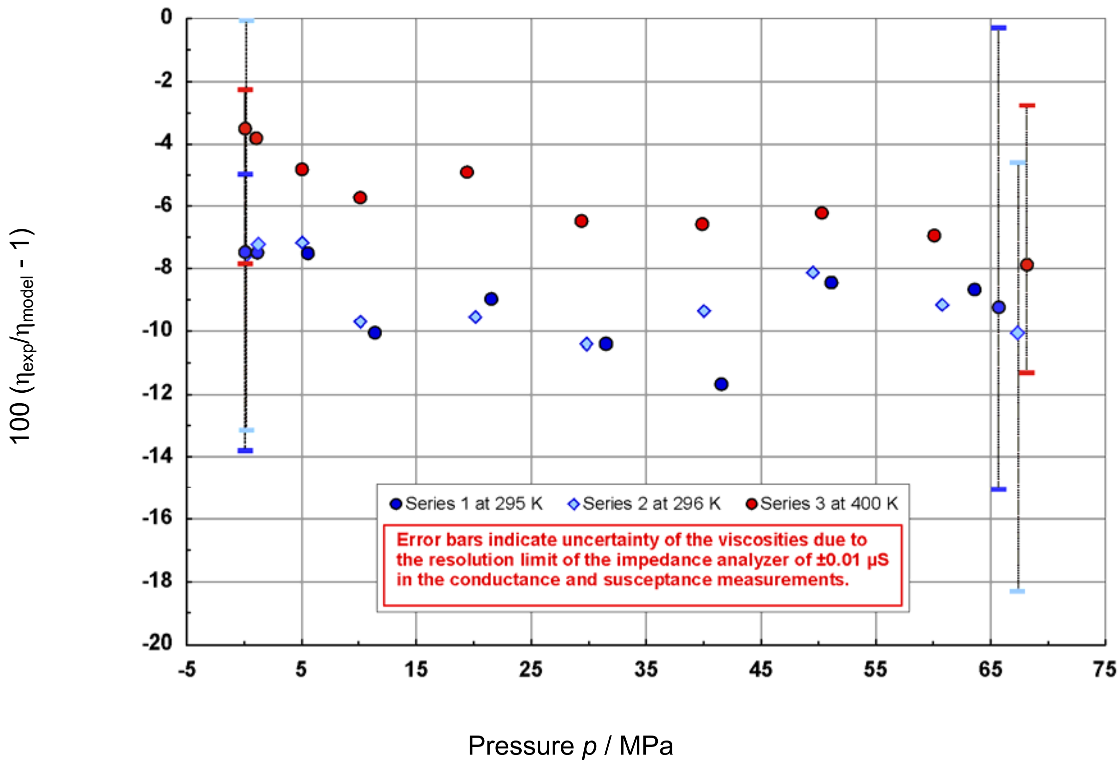

Figure 10. Percent deviations of the measured viscosities of RP-1 at elevated pressures from the model for the surrogate mixture.

8. Project Workshop at NIST Boulder on December 11, 2003

On December 11, 2003, the Physical and Chemical Properties Division of CSTL hosted a project workshop at the Boulder campus of NIST on the thermophysical properties of the rocket propellant designated RP-1. Specialists in rocket fuels (from NASA, the U.S. Air Force, commercial rocket engine manufacturers, and academia) convened with NIST researchers to hear about recent NIST work conducted to help better define the properties of this fuel and to plan future activities required to achieve consensus standards for the properties of fuels over the broad ranges of conditions encountered in their use.

NIST researchers reported new, high sensitivity compositional characterizations of RP-1 fuels and new metrological quality property results for density, viscosity, heat capacity, and thermal conductivity with temperatures extending beyond a decomposition limit (near 600 K) and pressures to about 70 MPa. These data were used to establish accurate preliminary property surfaces for this complex fluid. A software implementation of the preliminary models was delivered to NASA engineers and their contractors for testing and to assist in the resolution of current engine design problems. Participants in the workshop, listed in Table 13, were eager to use the current results, and were very interested in continued NIST efforts to explore the effects of sample-to-sample variation and refined processing methods on fuel properties, to help establish new protocols for fuel characterization, and to expand the range of conditions and properties.

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9. Summary and Recommendations

A combined experimental and modeling study was carried out to elucidate the behavior of key properties over wide ranges of temperature and pressure. An RP-1 sample provided by the Air Force Research Lab (Wright-Patterson AFB, OH) was chemically characterized. Thermophysical properties were then measured for this sample. The experimental results were used to develop a mixture model based on a representative surrogate mixture. The results of this study were presented for review and comments in the December 11, 2003 workshop attended by representatives of NASA, the U.S. Air Force and their contractors.

The anticipated impact of the knowledge of thermophysical properties developed in this study will be more efficient and cost-effective rocket engine systems that use the kerosene rocket propellant designated RP-1. For future work, it is recommend that the variation of RP-1 properties be systematically explored based on studies of RP-1 samples from different lots. This will help design engineers to better understand the effects of batch-to-batch variability on the thermophysical properties of RP-1, and thus to lead to a more flexible engine design that performs equally well with RP-1 from various distillation batches or vendors. In the longer term, it is recommended that the mixture property model developed here, and the approach used to obtain the model from accurate experimental measurements, be applied to other kerosene-type fuels that are widely used in jet aviation. This information is expected to enhance the design and performance characterization of jet engines, especially those that will see applications in supersonic flight where fuels encounter both high temperatures and pressures.

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Appendix A. Discussion of Chemical Characterization

A.1. Procedures

A sample of RP-1 kerosene-based rocket propellant was presented for analysis. The sample was drawn with a disposable pipette from a 5-gallon steel pail supplied by the Air Force Research Lab (designated P000016660). The liquid sample had a pale-red cast provided by a dying agent, and appeared to have the viscosity of a typical kerosene. The liquid had the characteristic kerosene odor.

The sample was analyzed with a gas chromatography/mass spectrometry method. A 30 m capillary column with a 0.1 μm coating of 5 % phenyl polydimethyl siloxane was chosen as the stationary phase. This phase provides separations based upon boiling temperature and also the polarity of the solute. In this context, polarity also includes points of unsaturation or aromaticity on the solute molecule. The sample was injected via a syringe into a split/splitless injector set with a 100 to 1 split ratio. The injector was operated at 350 °C and a constant head pressure of 69 kPa (10 psig). The sample residence time in the injector was very short, thus the effect of sample exposure to this high temperature is expected to be minimal. The column was temperature programmed to provide complete and rapid elution with minimal loss of peak shape. Initially, the temperature was maintained isothermally at 60 °C for 2 min, followed by a 2 °C /min ramp to 90 °C, followed by a 10 °C /min ramp to 250 °C. Although the analysis was allowed to run for 40 min, all peaks were eluted after approximately 27 min. Mass spectra were collected for each peak from 15 to 550 RMM (relative molecular mass) units. The areas under each peak were integrated with a commercial algorithm optimized to identify peaks that were at least an order of magnitude larger than the noise level.

A.2. Results

Approximately 250 peaks can be discerned on the total ion chromatogram. Not all of these were chosen for integration, however. The integration protocol mentioned above selected only 70 peaks as exceeding the threshold peak width and intensity established for recognition. Of these, a subset was chosen for examination. These were divided into four groups:

First tier: Peaks representing 2 % (mass/mass) or higher

Second tier: Peaks representing 1 % or higher

Lights: Peaks that elute very early

Heavies: Peaks that elute very late

A few comments about the above categories are in order. First, the mass percents referred to are based on the assumption that all peaks have identical response factors. Thus, the mass percents obtained from the total ion chromatogram were recorded without calibration. To apply a calibration to the mass, one would have to make standard mixtures of each of the components of RP-1. Since we do not have all of the pure components to make up calibration mixtures, or the time and resources to do so, the only practical alternative was the assumption of equal response. What is the consequence of this assumption?

In general, the total ion current, and therefore the intensity of the peaks on a total ion chromatogram, depends upon the number and intensity of the fragments produced by the constituents. A greater ion current will be produced by species that produce more fragments. Thus larger heavier species that produce a richer fragmentation pattern will tend to be over-represented in intensity on the total ion chromatogram. On the other hand, smaller, lighter species, which will produce a less rich fragmentation pattern, will be more efficiently carried into the source. The larger heavier ones will be more likely to adsorb on surfaces along the way, despite efforts to prevent that. These two effects will cancel to some extent. In the case of RP-1, even the smaller molecules are reasonably rich in fragments. Therefore, the assumption of equal response factor is unlikely to be a major source of uncertainty.

The terms heavy and light need some explanation. In this context, they refer only to the time that is required for the components producing the peaks to emerge from the column. Note however that the column is not a pure boiling point column. Thus, the last component out is not necessarily the heaviest in terms of RMM. Unsaturation will play a role in this as well. Thus, if components of lighter RMM emerge after components of heavier RMM, this is not a concern. Rather, this is expected.

The constituents in the heavy category were not integrated for mass percent. This is because as the chromatogram proceeds, the peaks broaden and are less amenable to integration. Thus, to integrate these peaks, one needs a protocol different from that used with the earlier peaks. While this could have been done, there was no reason to do so for the purpose of this study.

The components that have been identified represent 70 % of the total constituents of the RP-1 sample. Note that the dye is not among those materials identified.

A.3. Identification of Components

The ability to view the mass spectrum of each peak provides a great deal of insight into the identity of the constituent that produced it. It must be understood that it is not necessarily unequivocal, however. Not all peaks on a mass spectrum are created equally. Some are very instructive, some are ubiquitous, and some are distractions. The automated search routines that are available seek to match mass spectra with library file spectra. In all of these routines, match quality is determined by the intensity of a peak and also the m/e, or RMM value, of the fragment that the peak represents. Once a database routine finds a "match," it provides a quality factor based upon the match up of these two parameters: intensity and m/e. A higher quality factor results from the match of a heavier and more intense m/e peak. An unfortunate consequence of the procedure is that very often, the highest quality factor matches are nonsense, and that the slate of matches that is produced is of matches unrelated chemically. For this reason, it is very rare for one to be able to have "the computer" find the matches for you. Rather, each mass spectrum will have to be interpreted individually, by hand.

It is critical to correctly identify the parent ion packet on the mass spectrum, and make sure that the computer has done so properly. If the computer has failed to do so, it is time to ignore the computer and to start analyzing the mass spectrum. In 80 % of the spectra analyzed here, the software failed to properly identify the parent ion packet. In the tables shown in the text of this report, the quality factor is normalized to 100 and is referred to as the correlation coefficient. Sometimes a high number is obtained for this, sometimes not. Occasionally, the software will "identify" a compound and assign it a correlation coefficient of 90 (very high). Then, upon looking at the spectrum, it is apparent that the match is 200 m/e units heavier than the compound being matched. The parent ion packed was misidentified by the computer, leading the operator "down the garden path." It is always possible to calculate the correlation coefficient, however, even if it is meaningless. In these instances, one must scroll through the spectrum until the correct pattern is recognized. Thus, even when a relatively low quality factor is obtained, the identification may be very certain. It becomes a matter of ignoring the m/e peaks that the computer weighted too heavily.

In the tables of results, the correlation coefficient is given, as well as a confidence indication. These range from U,S (uncertain and/or speculative) to M (confident) to H (highly confident). The purpose of the foregoing discussion on mass spectral interpretation, while by no means complete, was to give proper context for interpretation of the correlation coefficient and confidence columns in the tables of results.

In all cases, the chromatographic peaks were examined for mass spectral purity. What is meant by this is that each peak was examined to determine whether the beginning, centroid, and end of the peak represented the mass spectrum of the same compound. When two peaks closely elute, there is inevitably some chemical impurity of the overlapping tails of the peak. Examining the peak for mass spectral purity ensures that the most reliable region will be chosen for the identification.

The peaks are listed in the tables by retention time on the total ion chromatogram. This is determined at the peak apex. Usually, well shaped Gaussian-like peaks were obtained, consistent with high efficiency and high selectivity. Nearly all resolved peaks were resolved to baseline. In some cases, the mass spectra were determined from the spectrum taken at the peak apex, while in other cases, an average over just part or all of the chromatographic peak was used. This is denoted in the profile column in each table as a S(ingle) or A(verage). We conclude that the RP-1 sample used in this work is unusual because it has a surprising number of unsaturated compounds present.

A.4. Thermal Decomposition

The global decomposition kinetics of RP-1 was investigated at elevated temperatures and a function of time. From these experiments, a global pseudo-first-order rate constant was derived that describes the overall decomposition of the RP-1 sample. Those results are presented in Table 7.

Bibliography for Chemical Characterization

Bruno, T. J.; Svoronos, P. D. N. CRC handbook of basic tables for chemical analysis, CRC Press: Boca Raton, 1989.

Bruno, T. J.; Svoronos, P. D. N. CRC handbook of basic tables for chemical analysis, 2nd. ed., CRC Press: Boca Raton, 2004.

Andersen, P. C.; Bruno, T. J. Thermal decomposition kinetics of RP-1 rocket propellant. Ind. Eng. Chem. Res. 44: 1670-1676 (2005).

Appendix B. Computational Characterization of Surrogate Mixture Compounds

The following four steps were taken to computationally characterize the compounds that were selected for the surrogate fuel mixture:

(a) Obtain equilibrium geometries from ab initio molecular orbital calculations.
Use Hartree-Fock approximation as theory level with 6-31G* basis sets (low level approximation, sufficient for visualization purposes).

(b) Calculate isosurfaces for two electron density values:

- Isosurface of electron density 0.002 e-/au3 contains approx. 98% of a molecule. Rendered as a mesh;
- Isosurface of electron density 0.08 e-/au3 rendered as a solid surface to illustrate the core of the molecule;
- 1 au (atomic unit) = 5.292 nm.

(c) Color-map the electrostatic potential onto the electron density isosurfaces.
The electrostatic potential is defined as the energy of interaction of a point positive charge with the nuclei and electrons of a molecule. The color-mapping indicates electron-rich regions in red and electron-poor regions in blue.

(d) Combining this information leads to molecular representations that comprise four dimensions:

- three dimensions conveying structure, and;
- one dimension conveying intramolecular charge distribution as a function of location.

The still images illustrated below were created with PC Spartan for Windows, version '02.*

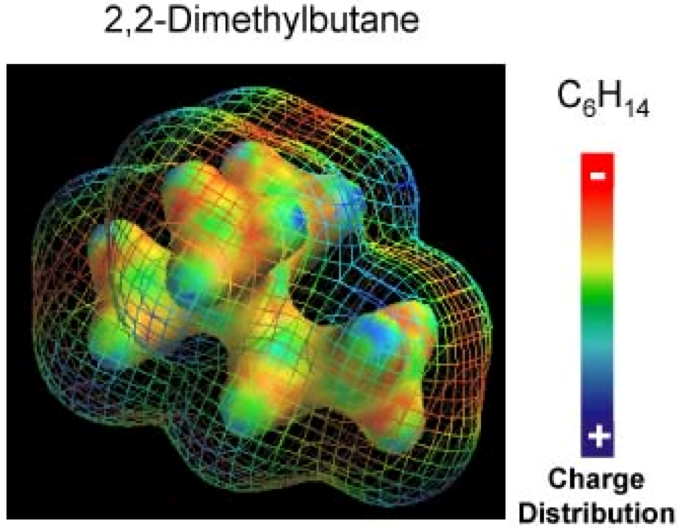
Bibliography for Computational Characterization

Shusterman, G. P.; Shusterman, A. J. Teaching chemistry with electron density models. J. Chem. Educ. 74: 771-776 (1997).

Gillespie, R. J. Electron densities, atomic charges, and ionic, covalent, and polar bonds. J. Chem. Educ. 78: 1688-1690 (2001).

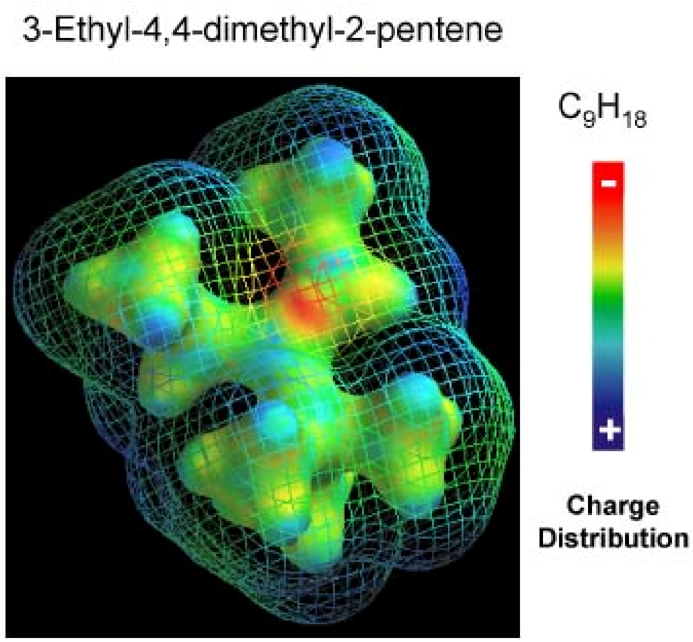
Gillespie, R. J.; Popelier, P. L. A. Chemical bonding and molecular geometry: from Lewis to electron densities, Oxford University Press: New York, 2001.

*Certain commercial entities, equipment, or materials may be identified in this document in order to describe an experimental procedure or concept adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the entities, materials, or equipment are necessarily the best available for the purpose.



Surface Area of Molecule / $Å^2$	146.66
Volume of Molecule / $Å^3$	123.59
Dipol moment / d	0.04

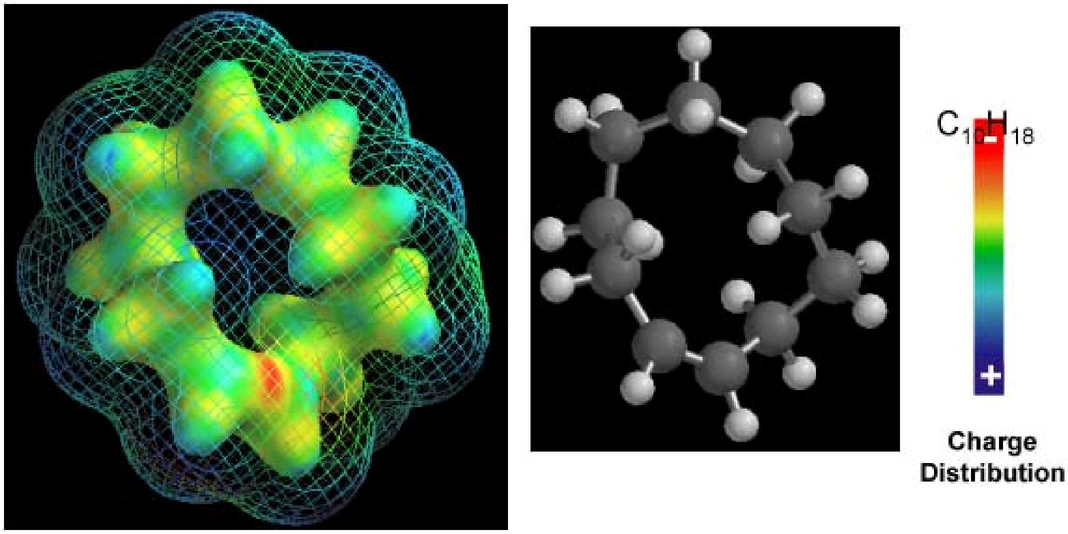
Figure 11. Molecular representation of 2,2-dimethylbutane.



Surface Area of Molecule / $Å^2$	191.18
Volume of Molecule / $Å^3$	173.28
Dipol moment / d	0.11

Figure 12. Molecular representation of 3-ethyl-4,4-dimethyl-2-pentene.

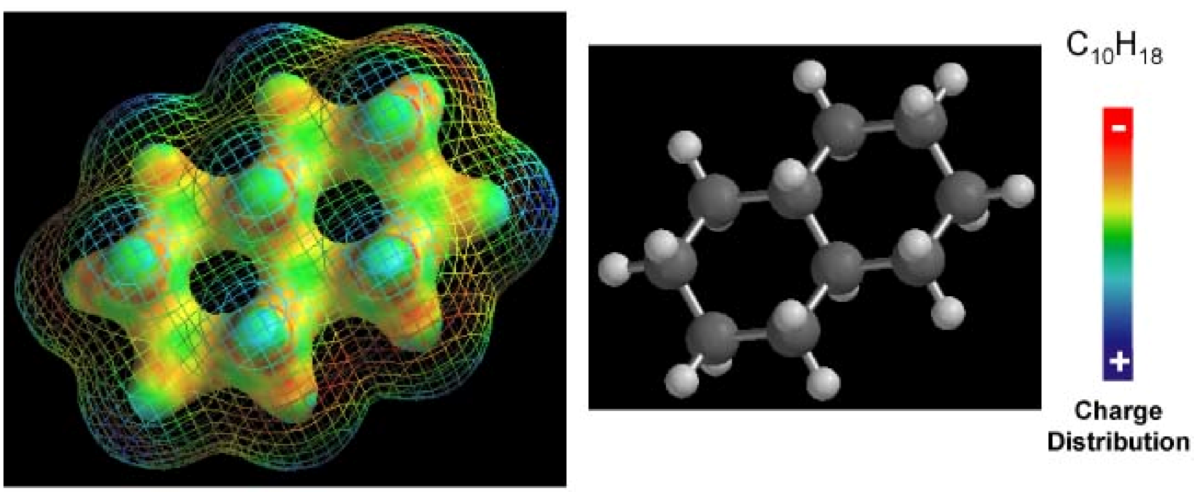
Cyclodecene



Surface Area of Molecule / Å^2	186.26
Volume of Molecule / Å^3	178.71
Dipol moment / d	0.25

Figure 13. Molecular representation of cyclodecene.

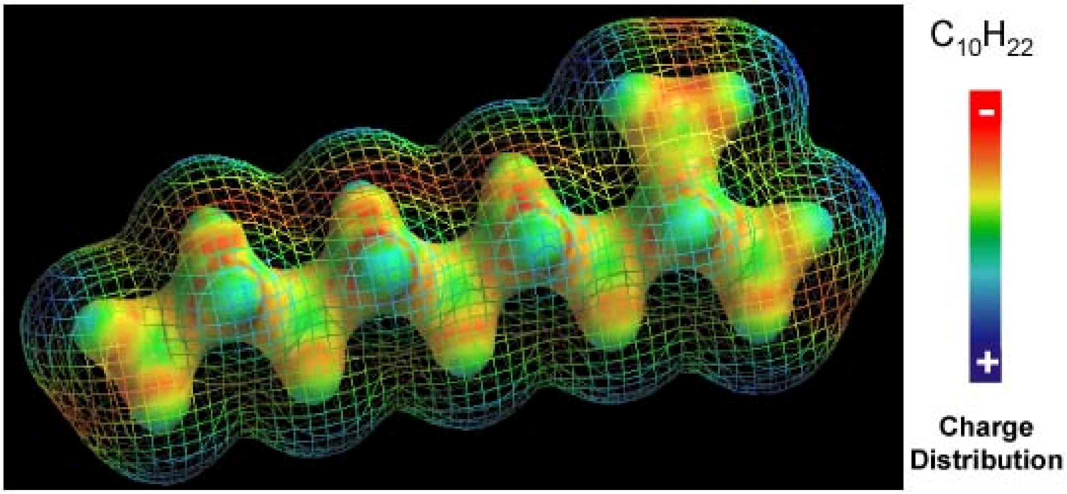
Cis-decaline



Surface Area of Molecule / Å^2	184.50
Volume of Molecule / Å^3	170.89
Dipol moment / d	0

Figure 14. Molecular representation of cis-decaline.

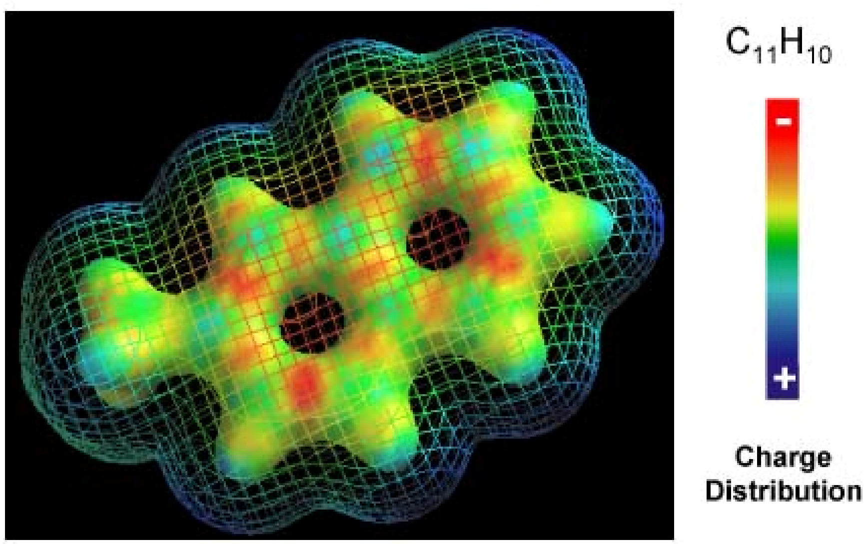
2-Methylnonane



Surface Area of Molecule / Å^2	230.60
Volume of Molecule / Å^3	197.63
Dipol moment / d	0.1

Figure 15. Molecular representation of 2-methylnonane.

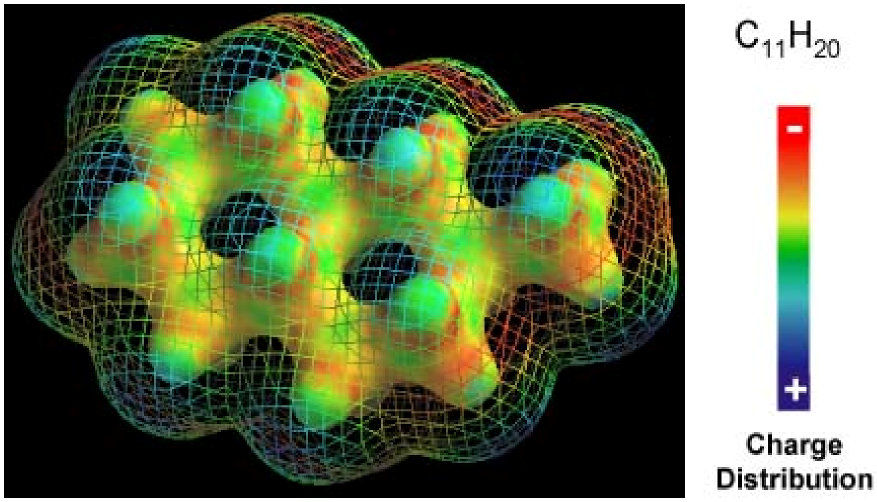
2-Methylnaphthalene



Surface Area of Molecule / Å^2	180.57
Volume of Molecule / Å^3	167.61
Dipol moment / d	0.34

Figure 16. Molecular representation of 2-methylnaphthalene.

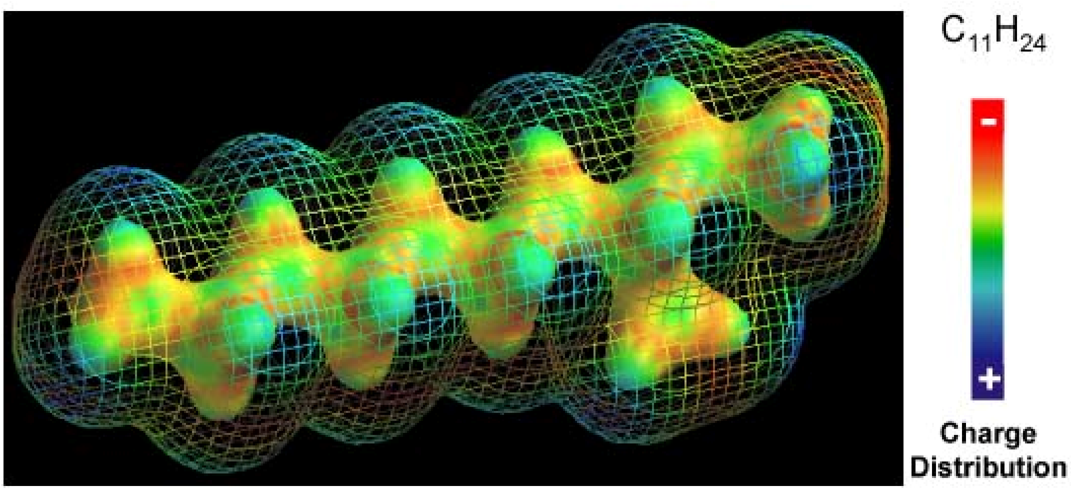
Decahydro-2-methylnaphthalene



Surface Area of Molecule / Å^2	203.58
Volume of Molecule / Å^3	188.94
Dipol moment / d	0.09

Figure 17. Molecular representation of decahydro-2-methylnaphthalene.

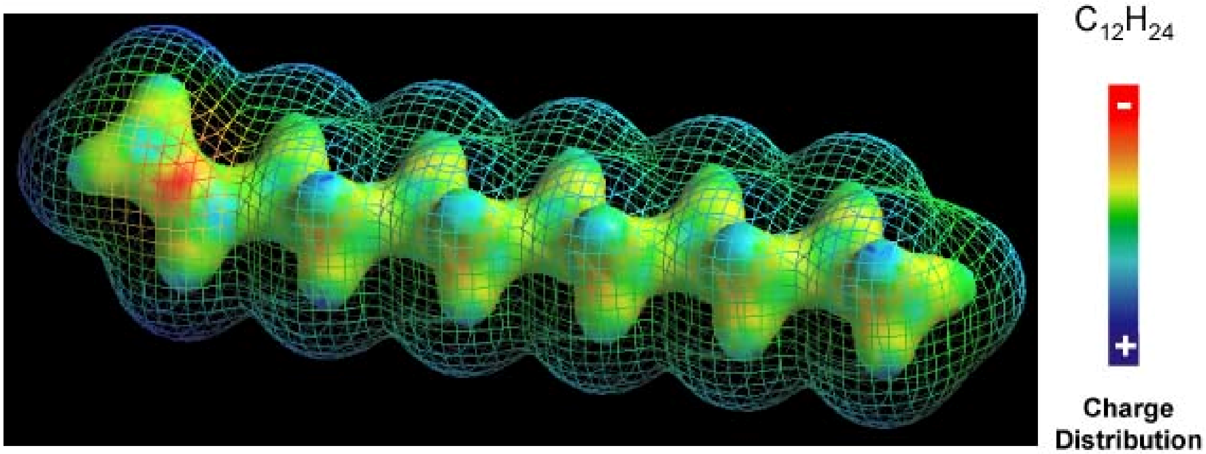
3-Methyldecane



Surface Area of Molecule / Å^2	249.55
Volume of Molecule / Å^3	215.88
Dipol moment / d	0.06

Figure 18. Molecular representation of 3-methyldecane.

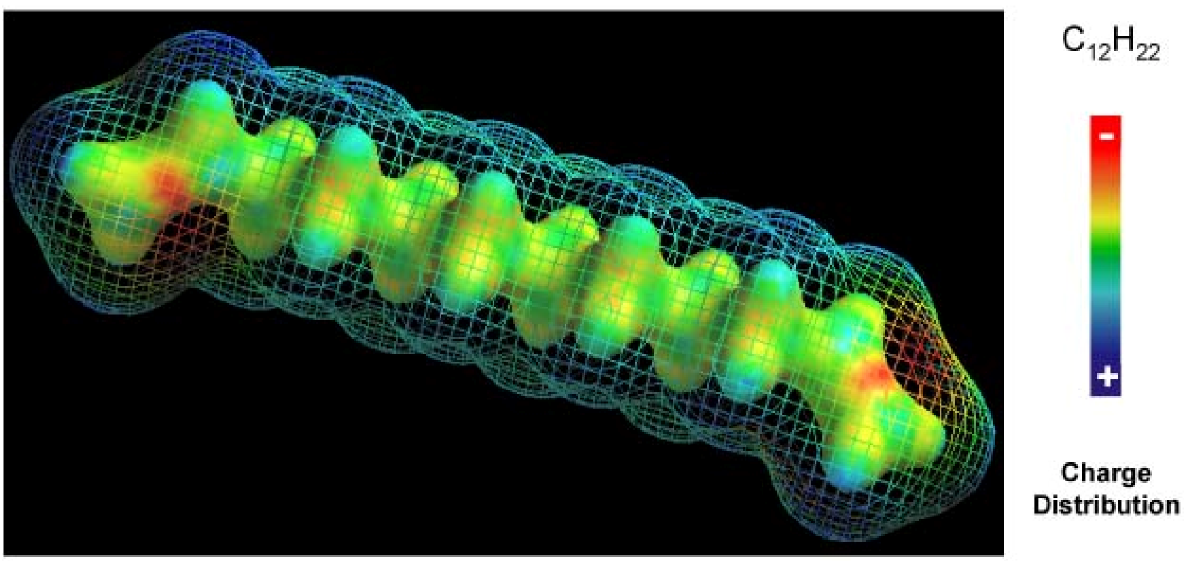
1-Dodecene



Surface Area of Molecule / Å^2	268.02
Volume of Molecule / Å^3	230.62
Dipol moment / d	0.35

Figure 19. Molecular representation of 1-dodecene.

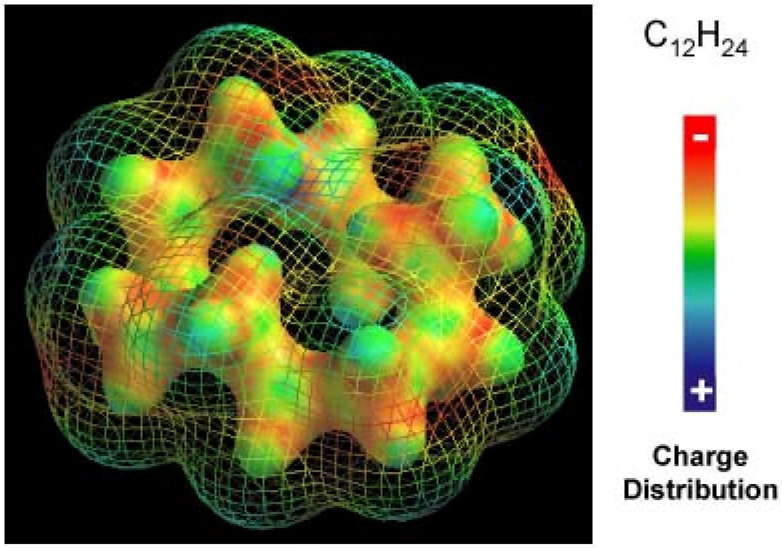
1,11-Dodecadiene



Surface Area of Molecule / Å^2	263.10
Volume of Molecule / Å^3	226.61
Dipol moment / d	0.26

Figure 20. Molecular representation of 1,11-dodecadiene.

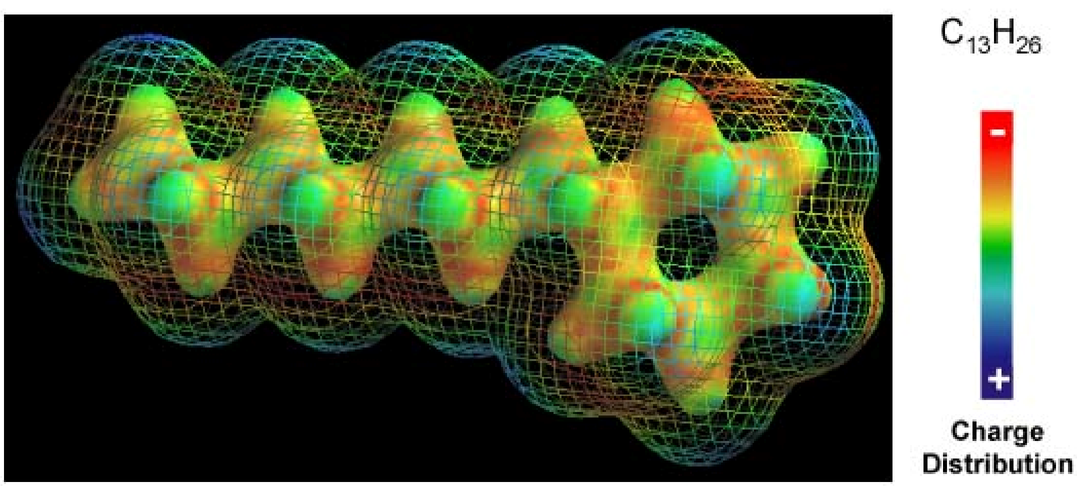
Cyclododecane



Surface Area of Molecule / Å^2	232.77
Volume of Molecule / Å^3	220.67
Dipol moment / d	0.01

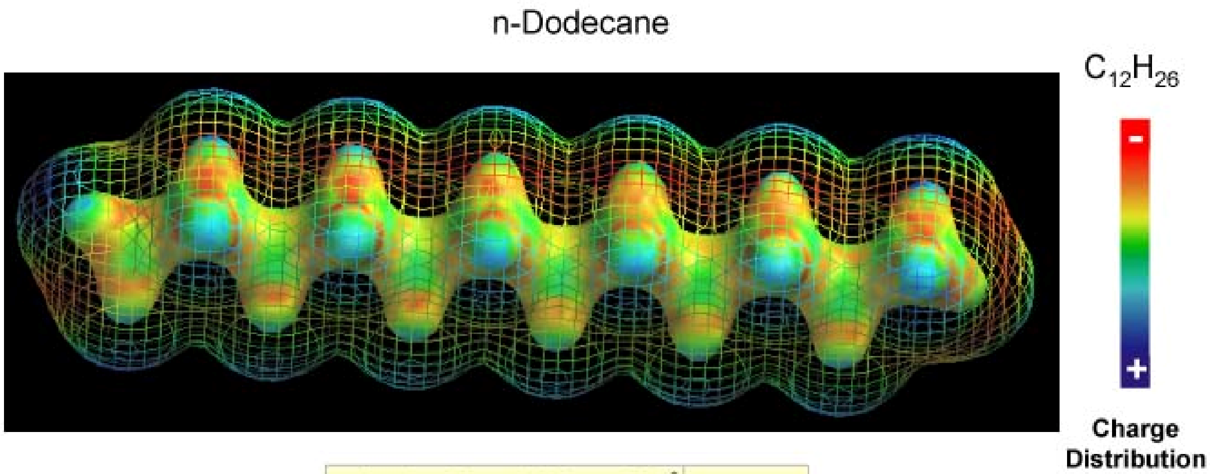
Figure 21. Molecular representation of cyclododecane.

Heptylcyclohexane



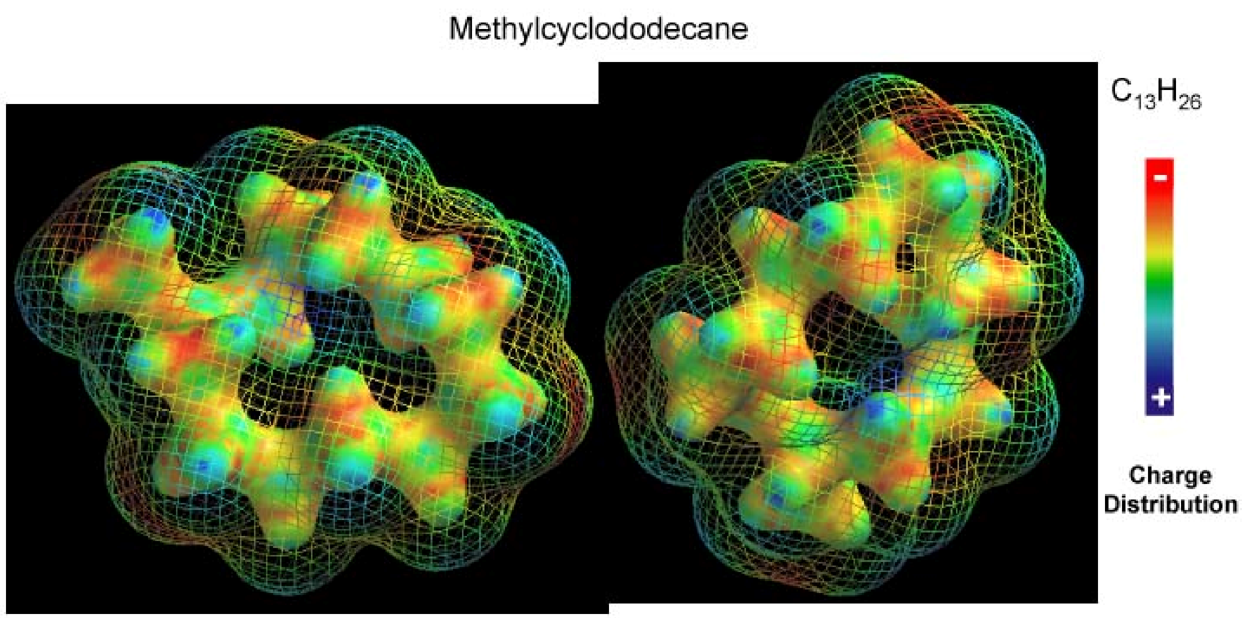
Surface Area of Molecule / Å^2	266.87
Volume of Molecule / Å^3	239.37
Dipol moment / d	0.06

Figure 22. Molecular representation of heptylcyclohexane.



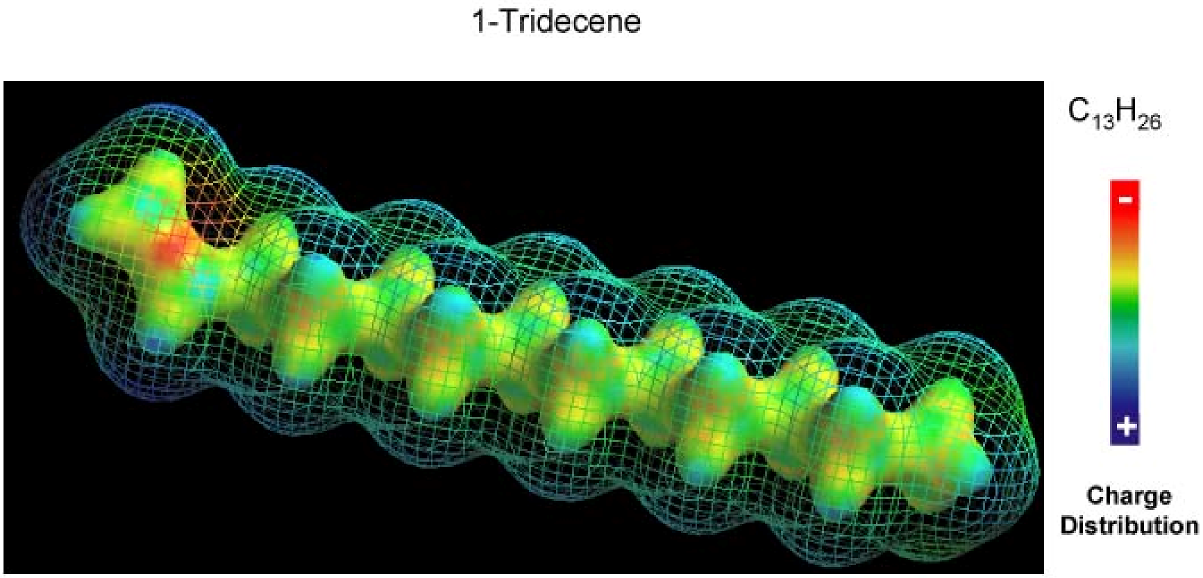
Surface Area of Molecule / Å^2	272.94
Volume of Molecule / Å^3	234.62
Dipol moment / d	0

Figure 23. Molecular representation of n-dodecane.



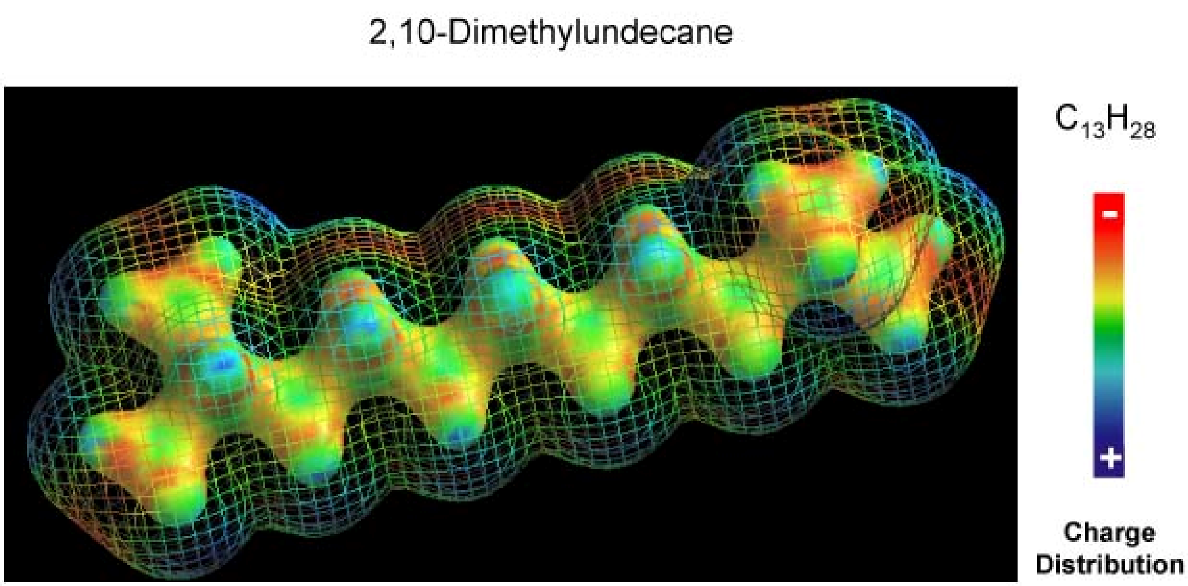
Surface Area of Molecule / Å^2	246.77
Volume of Molecule / Å^3	237.57
Dipol moment / d	0.04

Figure 24. Molecular representation of methylcyclododecane.



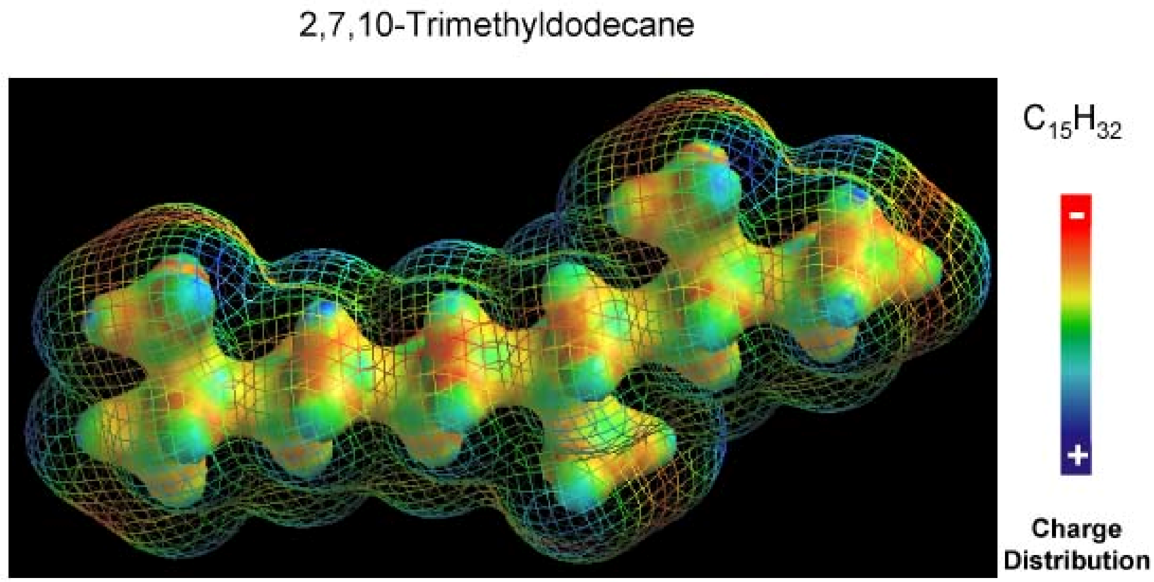
Surface Area of Molecule / Å^2	288.12
Volume of Molecule / Å^3	248.93
Dipol moment / d	0.34

Figure 25. Molecular representation of 1-tridecene.



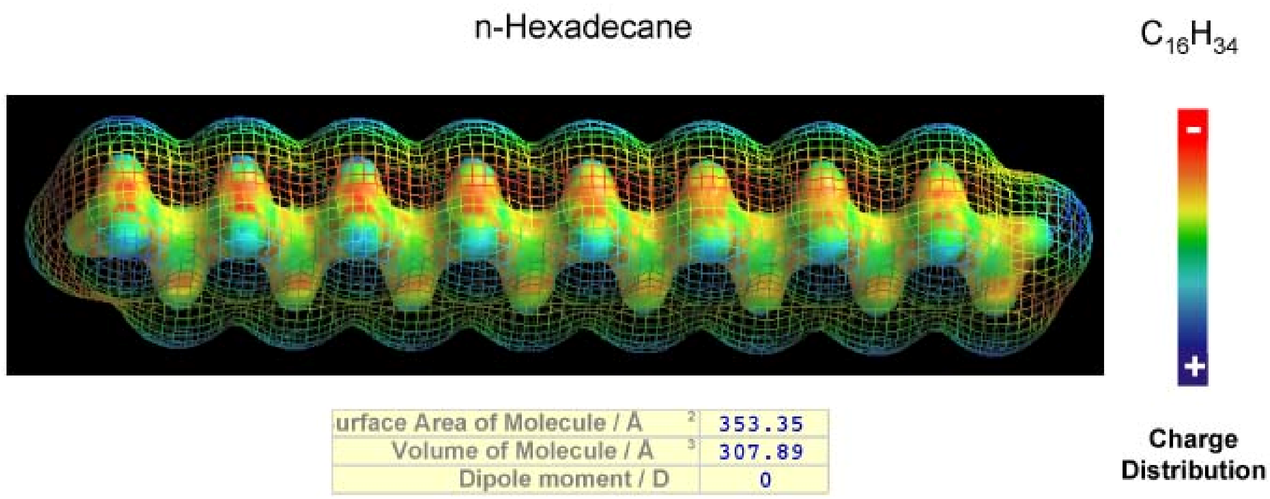
Surface Area of Molecule / Å^2	288.76
Volume of Molecule / Å^3	252.2
Dipol moment / d	0.08

Figure 26. Molecular representation of 2,10-dimethylundecane.



Surface Area of Molecule / Å^2	324.25
Volume of Molecule / Å^3	288.36
Dipol moment / d	0.07

Figure 27. Molecular representation of 2,7,10-trimethyldodecane.



urface Area of Molecule / Å^2	353.35
Volume of Molecule / Å^3	307.89
Dipole moment / D	0

Figure 28. Molecular representation of n-hexadecane.